

Supplementary Material

Hydrolysis Mechanisms for A-Series (Novichok) Nerve Agents at Different pH V and Computational Simulant Screening

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Supplementary Tables

- **Geometrical parameters:** Cartesian coordinates of the Boltzmann weighted average conformers used for pKa calculation were optimized at the G4mp2-xp level.

Cartesian coordinates of transition states (TS) for studied NAs and simulants were optimized at the PCM(H₂O)/B3LYP-D3(BJ)/def2-SVP level .

Table S1. Dissociation constants of different protonation sites in NAs.

$G_i^\circ(\text{A}, \text{aq})$		$G_i^\circ(-\text{N}_1\text{H}^+, \text{aq})$		$G_i^\circ(-\text{N}_2\text{H}^+, \text{aq})$		$G^\circ(-\text{OH}^+, \text{aq})$	
$G_i^\circ(\text{A}, \text{aq})$ (Hartree)	Boltzmann distribution	$G_i^\circ(-\text{N}_1\text{H}^+, \text{aq})$ (Hartree)	Boltzmann distribution	$G_i^\circ(-\text{N}_2\text{H}^+, \text{aq})$ (Hartree)	Boltzmann distribution	$G^\circ(-\text{OH}^+, \text{aq})$ (Hartree)	Boltzmann distribution
A230							
-901.2877493	29.79%	-901.725990	44.55%	-901.7034195	1.48%	-901.7097472	5.68%
-901.2863426	6.72%	-901.724558	9.78%	-901.7060597	24.29%	-901.7096252	4.99%
-901.2863654	6.88%	-901.724408	8.34%	-901.7060634	24.37%	-901.7095820	4.77%

-901.2863526	6.79%	-901.724343	7.79%	-901.7036355	1.86%	-901.7106508	14.79%
-901.2861346	5.39%	-901.724122	6.16%	-901.7061344	26.28%	-901.7103127	10.34%
-901.2851447	1.89%	-901.723994	5.38%	-901.7045033	4.67%	-901.7098258	6.17%
-901.2879522	36.93%	-901.724632	10.58%	-901.7043996	4.19%	-901.7111138	24.15%
-901.2851240	1.85%	-901.722947	1.78%	-901.7044175	4.27%	-901.7089803	2.51%
-901.2850537	1.71%	-901.723015	1.91%	-901.7044196	4.28%	-901.7107800	16.96%
-901.2852222	2.05%	-901.723648	3.73%	-901.7044266	4.31%	-901.7102469	9.64%
$\sum_i = -901.2872569$		$\sum_i = -901.7250249$		$\sum_i = -901.7056431$		$\sum_i = -901.7104643$	
<i>pKa</i>		3.23531949		-5.679627891		-3.462055343	
A232							
-976.462999	29.94%	-976.896021	6.06%	-976.878079	19.62%	-976.881172	5.79%
-976.461586	6.70%	-976.894664	1.44%	-976.876478	3.60%	-976.881339	6.91%
-976.461641	7.11%	-976.896846	14.50%	-976.878079	19.60%	-976.882321	19.56%
-976.462422	16.26%	-976.895957	5.65%	-976.878073	19.50%	-976.882276	18.64%

-976.461960	9.96%	-976.897140	19.80%	-976.878073	19.49%	-976.881704	10.17%
-976.462053	10.99%	-976.896889	15.18%	-976.876479	3.60%	-976.881181	5.84%
-976.461657	7.23%	-976.896524	10.32%	-976.876476	3.59%	-976.879931	1.55%
-976.460577	2.30%	-976.897107	19.12%	-976.876481	3.61%	-976.881426	7.58%
-976.461633	7.05%	-976.895981	5.80%	-976.876508	3.71%	-976.881304	6.66%
-976.460638	2.46%	-976.895034	2.13%	-976.876498	3.68%	-976.882205	17.30%
$\sum_i = -976.4621991$		$\sum_i = -976.896707$		$\sum_i = -976.8777299$		$\sum_i = -976.8818561$	
<i>pKa</i>		1.7357942		-6.993045756		-5.095137136	
A234							
-1015.711012	52.25%	-1016.144621	7.98%	-1016.126227	14.45%	-1016.129353	18.03%
-1015.708892	5.53%	-1016.144311	5.75%	-1016.126233	14.55%	-1016.129879	31.47%
-1015.708938	5.81%	-1016.145127	13.64%	-1016.126248	14.78%	-1016.128305	5.94%
-1015.709427	9.75%	-1016.145253	15.58%	-1016.126230	14.50%	-1016.128533	7.56%
-1015.708156	2.54%	-1016.144852	10.19%	-1016.126228	14.47%	-1016.128493	7.25%

-1015.709072	6.69%	-1016.144441	6.59%	-1016.124914	3.60%	-1016.128611	8.21%
-1015.708879	5.46%	-1016.144883	10.53%	-1016.126229	14.49%	-1016.127707	3.16%
-1015.707797	1.73%	-1016.144288	5.62%	-1016.125085	4.31%	-1016.128599	8.11%
-1015.709190	7.59%	-1016.145094	13.17%	-1016.124586	2.54%	-1016.127709	3.16%
-1015.708197	2.65%	-1016.144920	10.95%	-1016.124495	2.31%	-1016.128475	7.11%
$\sum_i = -1015.710033$		$\sum_i = -1016.144886$		$\sum_i = -1016.126054$		$\sum_i = -1016.129044$	
pKa		1.894788601		-6.767517528		-5.392284272	

Table S2. Dissociation constants of simulants protonated at the S₂ (N₁-H⁺) site.

AMP				AMOP			
$G^\circ (A, aq)$		$G^\circ (-N_1H^+, aq)$		$G^\circ (A, aq)$		$G^\circ (-N_1H^+, aq)$	
$G_i^\circ (A, aq)$	Boltzmann distribution	$G_i^\circ (-N_1H^+, aq)$	Boltzmann distribution	$G_i^\circ (A, aq)$	Boltzmann distribution	$G_i^\circ (-N_1H^+, aq)$	Boltzmann distribution
- 1107.930005	1.11%	-1108.374947	23.29%	- 1183.110501	4.98%	-1183.548245	12.97%
- 1107.930836	2.68%	-1108.374323	12.03%	- 1183.112922	64.70%	-1183.548767	22.55%
- 1107.933925	70.66%	-1108.374964	23.70%	-1183.1105	4.98%	-1183.548283	13.50%
- 1107.932208	11.47%	-1108.374305	11.80%	- 1183.110374	4.35%	-1183.548201	12.38%
-	12.83%	-1108.367974	0.01%	-	12.96%	-1183.547459	5.64%

1107.932314				1183.111404			
- 1107.928771	0.30%	-1108.374951	23.39%	- 1183.109692	2.11%	-1183.548253	13.08%
- 1107.928789	0.31%	-1108.367986	0.01%	- 1183.110271	3.90%	-1183.547369	5.13%
- 1107.928914	0.35%	-1108.372972	2.88%	- 1183.109645	2.02%	-1183.547726	7.49%
- 1107.928768	0.29%	-1108.372976	2.89%			-1183.547308	4.81%
- 1107.930005	1.11%	-1108.374947	23.29%			-1183.54667	2.45%
$\sum_i = -1107.933331$		$\sum_i = -1108.374686$		$\sum_i = -1183.112135$		$\sum_i = -1183.548152$	
pKa		4.885246638		pKa		2.429634548	
AEOP				ADDP			

$G^\circ (A, aq)$		$G^\circ (-N_1H^+, aq)$		$G^\circ (A, aq)$		$G^\circ (-N_1H^+, aq)$	
$G_i^\circ (A, aq)$	Boltzmann distribution	$G_i^\circ (-N_1H^+, aq)$	Boltzmann distribution	$G_i^\circ (A, aq)$	Boltzmann distribution	$G_i^\circ (-N_1H^+, aq)$	Boltzmann distribution
- 1222.356392	1.72%	-1222.796605	13.55%	-1217.61391	6.84%	-1218.050664	10.75%
- 1222.358889	24.37%	-1222.796486	11.95%	- 1217.613887	6.67%	-1218.050716	11.36%
- 1222.358011	9.62%	-1222.796505	12.19%	- 1217.614679	15.44%	-1218.050352	7.72%
- 1222.356876	2.89%	-1222.79672	15.31%	- 1217.615638	42.63%	-1218.050369	7.86%
- 1222.357068	3.54%	-1222.796677	14.63%	- 1217.614898	19.47%	-1218.050699	11.15%
-	37.46%	-1222.796658	14.33%	-	4.43%	-1218.0507	11.17%

1222.359295				1217.613498			
- 1222.358721	20.40%	-1222.795673	5.05%	-1217.61352	4.52%	-1218.050392	8.06%
		-1222.796565	12.99%			-1218.050398	8.11%
						-1218.050754	11.82%
						-1218.050768	12.00%
$\sum_i = -1222.358757$		$\sum_i = -1222.796562$		$\sum_i = -1217.61492$		$\sum_i = -1218.05061$	
<i>pKa</i>		3.252443107		<i>pKa</i>		2.279518154	
ANMP				ANMOP			
$G^\circ (A,aq)$		$G^\circ (-N_1H^+,aq)$		$G^\circ (A,aq)$		$G^\circ (-N_1H^+,aq)$	
$G_i^\circ (A,aq)$	Boltzmann distribution	$G_i^\circ (-N_1H^+,aq)$	Boltzmann distribution	$G_i^\circ (A,aq)$	Boltzmann distribution	$G_i^\circ (-N_1H^+,aq)$	Boltzmann distribution
- 1312.264077	96.10%	-1312.705707	28.01%	- 1387.439238	8.14%	-1387.877757	32.57%

- 1312.259809	1.05%	-1312.704308	6.37%	- 1387.439363	9.29%	-1387.876524	8.82%
- 1312.259848	1.09%	-1312.704394	6.97%	- 1387.440361	26.73%	-1387.876521	8.80%
- 1312.259892	1.14%	-1312.704411	7.10%	- 1387.439216	7.94%	-1387.876701	10.64%
- 1312.259316	0.62%	-1312.704861	11.43%	- 1387.439462	10.32%	-1387.877189	17.85%
		-1312.705051	13.98%	- 1387.440138	21.11%	-1387.876414	7.85%
		-1312.704784	10.54%	- 1387.439228	8.05%	-1387.875611	3.36%
		-1312.704502	7.82%	-1387.43927	8.42%	-1387.875578	3.25%
		-1312.704482	7.65%			-1387.875621	3.39%

		-1312.70056	0.13%			-1387.875644	3.47%
$\sum_i = -1312.263909$		$\sum_i = -1312.704954$		$\sum_i = -1387.439763$		$\sum_i = -1387.876932$	
pKa		4.74277384		pKa		2.959688151	
ANEOP							
$G^\circ (A,aq)$		$G^\circ (- N_1H^+,aq)$					
$G_i^\circ (A,aq)$	Boltzmann distribution	$G_i^\circ (- N_1H^+,aq)$	Boltzmann distribution				
- 1426.688226	20.95%	-1427.125565	12.83%				
- 1426.687951	15.66%	-1427.125562	12.79%				
- 1426.686628	3.86%	-1427.124817	5.81%				
-	4.21%	-1427.125563	12.80%				

1426.686712							
- 1426.687968	15.94%	-1427.124821	5.83%				
- 1426.686649	3.94%	-1427.125566	12.84%				
- 1426.686917	5.24%	-1427.125662	14.22%				
-1426.68666	3.99%	-1427.125658	14.16%				
-1426.68614	2.30%	-1427.124906	6.38%				
- 1426.688351	23.91%	-1427.123956	2.34%				
$\sum_i = -1426.687805$		$\sum_i = -1427.125425$					
pKa		3.167284857					

Table S3. Gibbs free energy barriers (kcal/mol) for water assisted hydrogen atom transfer in different reaction paths.

	A230	A232	A234	A230-H ₂ O	A232-H ₂ O	A234-H ₂ O
Path1	56.58	53.34	51.48	52.46	56.20	56.08
Path2	84.63	53.52	53.38	91.73	47.79	45.35
Path3	37.94	41.94	42.26	33.57	37.03	37.33
Path4	38.04	42.12	40.08	36.80	37.03	36.82
Path6	52.31	49.70	47.59	40.35	40.73	42.68
Path7	79.49	47.16	42.68	74.39	34.06	35.65
Path8	54.30	54.10	55.26	38.49	42.61	43.95
Path9	39.12	41.00	40.65	29.00	26.20	27.15

Supplementary Figures

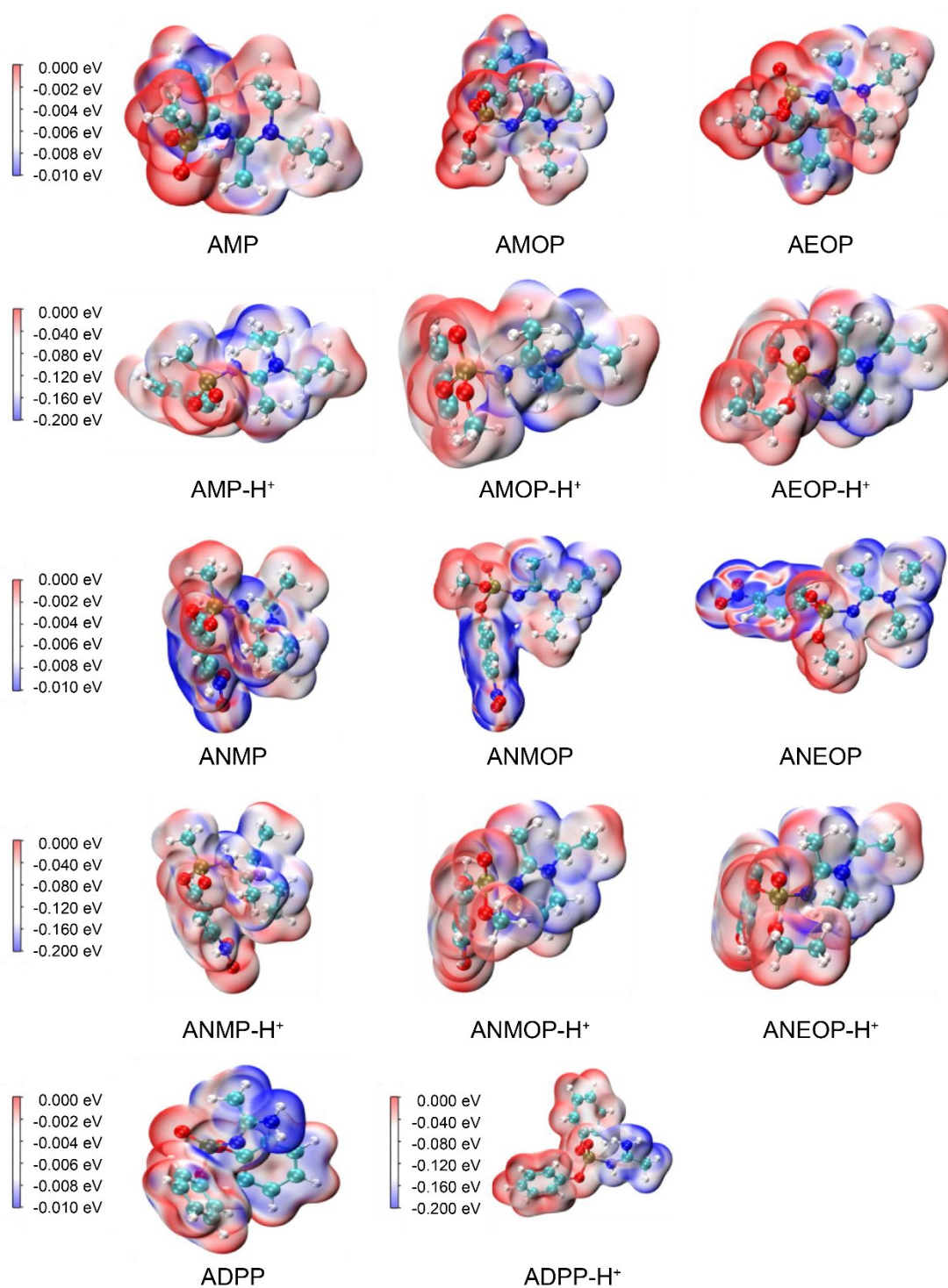


Fig. S1: Local electron attachment energy (LEAE) of the simulants.

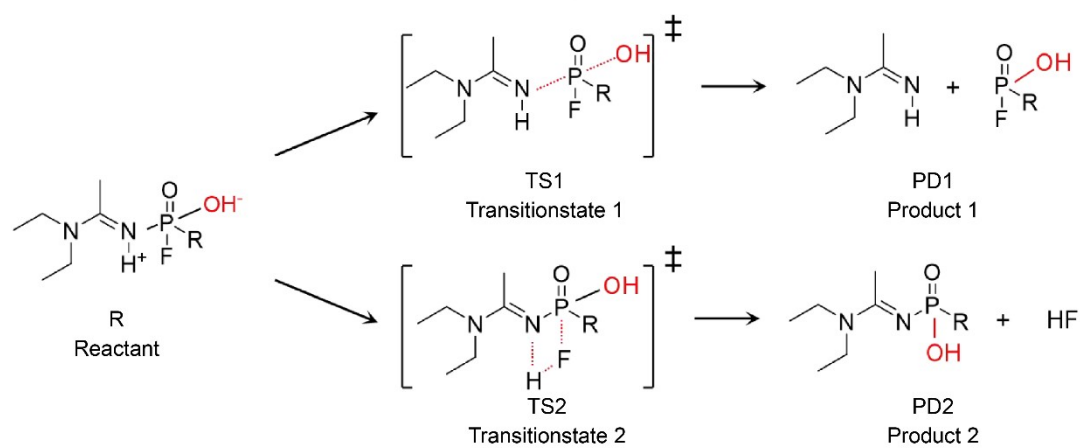
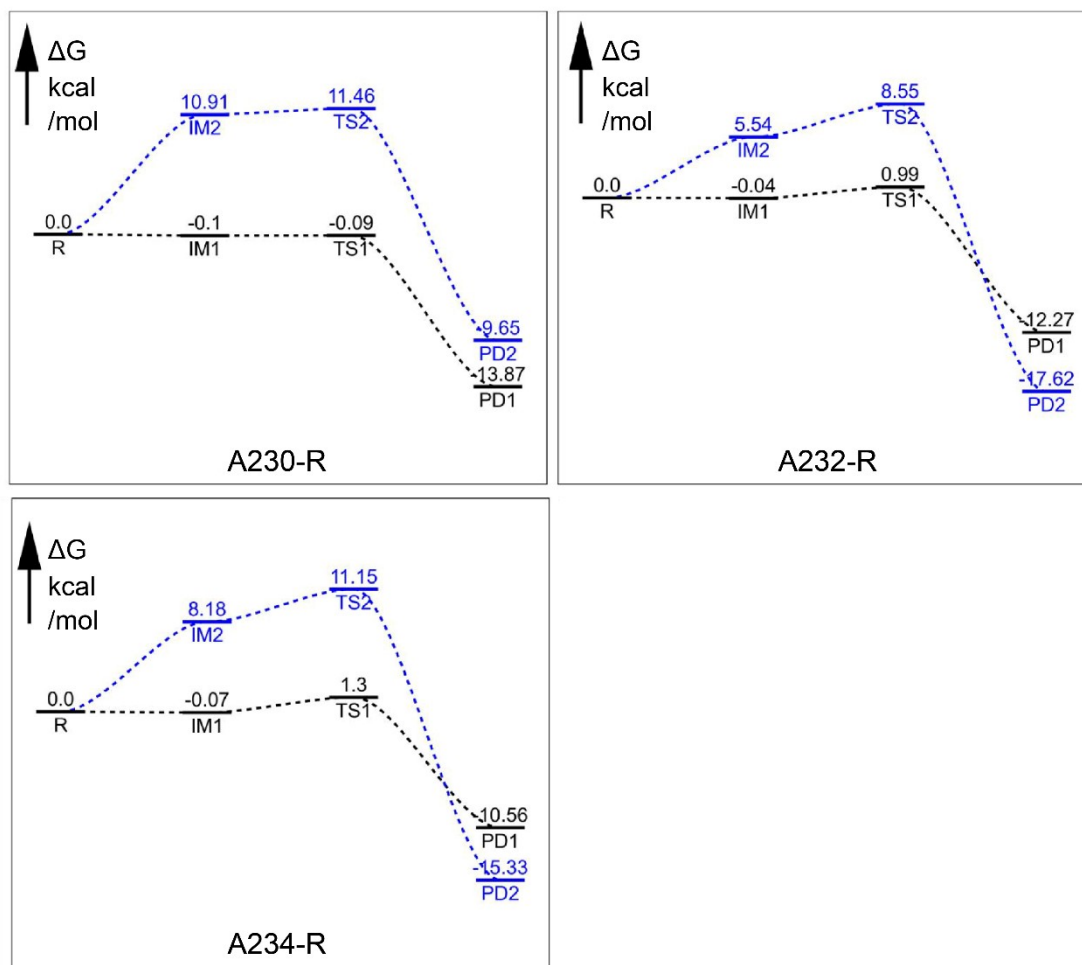


Fig. S2: Reaction path of intermediate in protonation of NAs, R=Me,OMe,OEt.

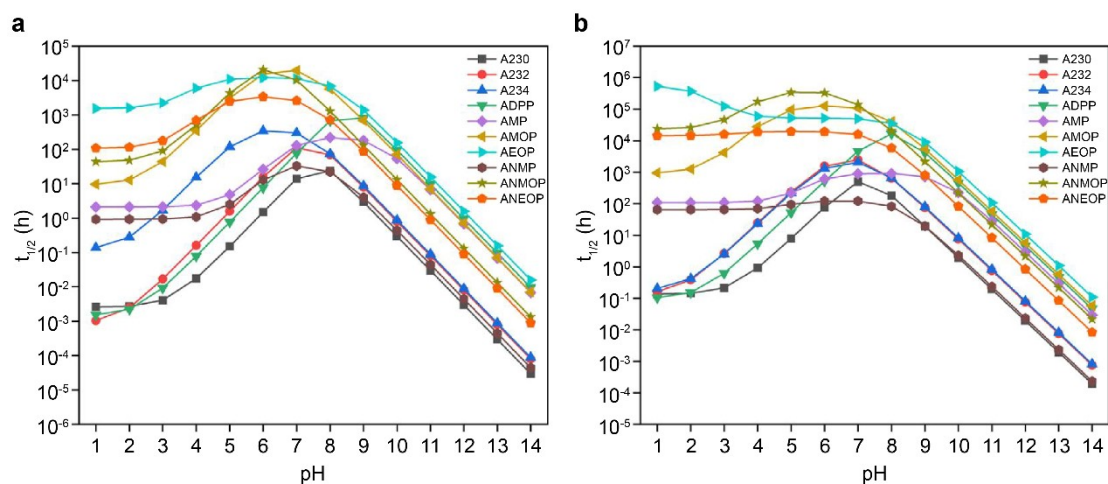


Fig. S3: Predicted half-lives ($t_{1/2}$) via two computational methods. a: ω B97M-V/def2-TZVPP; b: DLPNO-

CCSD(T)/def2-TZVPP.

Cartesian coordinates of the Boltzmann weighted average conformers used for pKa calculation were optimized at the G4mp2-xp level.

A230

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Energy =	-901.28795220 a.u.	#Cluster:	1
P	-5.12974800	-4.98279000	-2.20294100
O	-4.08491300	-3.91890800	-2.10500200
C	-5.92113600	-5.12430500	-3.81850200
H	-6.74474000	-5.85262000	-3.78141700
H	-6.30717900	-4.13951100	-4.12142600
H	-5.17139300	-5.46044100	-4.54993600
C	-5.26944500	-7.50916500	-1.25159600
F	-6.41530500	-4.54215400	-1.28727100
N	-4.64086000	-6.45124200	-1.70245900
C	-6.73985300	-7.54191200	-0.89653100
H	-7.24979000	-8.37187300	-1.40568700
H	-6.86427800	-7.69020400	0.18780800
H	-7.22417700	-6.60067400	-1.16736300
C	-5.13158500	-9.87913000	-0.52723500
H	-5.95854100	-9.63544600	0.15058900
H	-4.35250600	-10.34538200	0.09547500
C	-5.59261300	-10.85529700	-1.60804300

H	-6.40210400	-10.42245900	-2.21630600
H	-4.76316900	-11.12312700	-2.28153900
H	-5.96752300	-11.78120400	-1.14407700
C	-3.13620900	-8.68019400	-1.41279000
H	-2.98076500	-8.06115900	-2.30564400
H	-2.88922700	-9.71915500	-1.67680600
C	-2.24955500	-8.19299400	-0.26938300
H	-2.40705000	-8.79552800	0.63967600
H	-1.18774500	-8.27216100	-0.55208000
H	-2.46795100	-7.14047500	-0.03449800
N	-4.56289100	-8.64314000	-1.07289700

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Energy = -901.28774930 a.u. #Cluster: 2

P	-5.93068900	-5.31216400	-2.32499700
O	-6.99144400	-4.85576700	-1.37002900
C	-4.73577600	-4.05774600	-2.80494100
H	-5.27243700	-3.17097500	-3.17251700
H	-4.13730900	-3.78031600	-1.92469900
H	-4.07057900	-4.44597900	-3.58940500
C	-5.53189800	-7.82110000	-1.63373400
F	-6.62546300	-5.62369500	-3.77558600
N	-5.04887400	-6.64297600	-1.96471500

C	-7.00715200	-8.15103600	-1.69436500
H	-7.47569300	-7.89699600	-0.72963300
H	-7.48503400	-7.54335800	-2.47146900
H	-7.20414000	-9.20717800	-1.90990000
C	-5.09205300	-10.09249500	-0.73196800
H	-6.09896800	-10.03077500	-0.30066200
H	-4.42210700	-10.35911600	0.09983600
C	-5.02977100	-11.16270900	-1.81893700
H	-5.29656900	-12.14469600	-1.39744300
H	-5.72883300	-10.93721700	-2.63975500
H	-4.01597000	-11.23697600	-2.24309200
C	-3.23976600	-8.47851600	-1.13968100
H	-2.98413400	-7.83163900	-1.98868800
H	-2.70883000	-9.43304300	-1.27103800
C	-2.83174700	-7.81441800	0.17273500
H	-3.33322000	-6.84153100	0.28453700
H	-3.09368300	-8.44552500	1.03716900
H	-1.74294500	-7.64753800	0.18961000
N	-4.67716600	-8.76716700	-1.20451500

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Energy = -901.28636540 a.u. #Cluster: 3

P	-5.59840300	-5.33735300	-2.74482600
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O	-6.80276000	-5.41958800	-3.63843300
C	-5.63270500	-3.96389400	-1.58239500
H	-4.67222900	-3.88499700	-1.05411200
H	-5.83923200	-3.03282100	-2.13050200
H	-6.43710400	-4.13879500	-0.85219000
C	-5.29571000	-7.90204300	-2.05054600
F	-4.30210100	-4.93099100	-3.64355500
N	-5.04391500	-6.62146700	-1.90189500
C	-6.24419200	-8.46297200	-3.08595400
H	-6.78423800	-7.64197400	-3.56800800
H	-5.67570500	-9.01418000	-3.85235700
H	-6.96244700	-9.16283700	-2.63624700
C	-4.83674500	-10.22352400	-1.30780300
H	-3.85514400	-10.67617700	-1.09841500
H	-5.09426100	-10.51364400	-2.33373700
C	-5.87840600	-10.74962000	-0.32241200
H	-5.93743800	-11.84765800	-0.38610600
H	-5.61602400	-10.48168700	0.71328600
H	-6.87575600	-10.33677100	-0.54099200
C	-3.72167100	-8.27396700	-0.22719100
H	-3.69056800	-9.01584600	0.58431900
H	-4.12250000	-7.33959700	0.18723000

C	-2.32381500	-8.04324000	-0.79646800
H	-1.91402100	-8.96966500	-1.23020800
H	-2.35152200	-7.27135700	-1.58015400
H	-1.64009600	-7.70619500	-0.00105200
N	-4.66354100	-8.76979100	-1.23715800

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Energy = -901.28635260 a.u. #Cluster: 4

P	-5.72094900	-5.36880600	-2.73577300
O	-7.04220600	-5.46231700	-3.44337200
C	-5.55561800	-3.93334600	-1.66423400
H	-6.25390000	-4.04118100	-0.82070400
H	-4.52880400	-3.85901100	-1.27962300
H	-5.81248900	-3.02729600	-2.23242200
C	-5.30994100	-7.91082300	-2.04228200
F	-4.55500100	-5.05849000	-3.83149400
N	-5.10079500	-6.62229300	-1.88919200
C	-6.21280400	-8.49831100	-3.10352600
H	-5.60090500	-8.96939900	-3.89016300
H	-6.87946600	-9.26827500	-2.69188100
H	-6.81352500	-7.70045900	-3.55200200
C	-4.77750700	-10.21921000	-1.30807700
H	-3.78375200	-10.63163800	-1.07436900

H	-4.99158400	-10.50808000	-2.34441700
C	-5.82292300	-10.80050300	-0.35844700
H	-5.60199400	-10.53144700	0.68659200
H	-6.83096900	-10.42972800	-0.60201100
H	-5.83144500	-11.89937500	-0.43350900
C	-3.77455400	-8.23892100	-0.17711300
H	-3.75567600	-8.97711300	0.63831000
H	-4.21193500	-7.31296700	0.21847000
C	-2.36287300	-7.97743900	-0.69646600
H	-2.38003800	-7.21016200	-1.48495700
H	-1.71720700	-7.62042100	0.12170400
H	-1.91488700	-8.89553300	-1.10965200
N	-4.66850300	-8.76010600	-1.21727200

28

Energy = -901.28634260 a.u. #Cluster: 5

P	-6.01559400	-5.38811300	-2.47895300
O	-7.48864300	-5.47557500	-2.75401700
C	-5.49273100	-3.88282900	-1.64760100
H	-5.87789700	-3.01349800	-2.20016800
H	-5.90803100	-3.87770500	-0.62896700
H	-4.39571900	-3.83883400	-1.59351400
C	-5.31430600	-7.88660600	-1.99996500

F	-5.22230100	-5.24342300	-3.89868200
N	-5.24615900	-6.60705000	-1.70176600
C	-6.06425000	-8.41344000	-3.20318000
H	-6.52537000	-9.39194000	-3.02346900
H	-6.85056000	-7.70033400	-3.47730000
H	-5.36830400	-8.51225900	-4.05277300
C	-4.57259800	-10.20003100	-1.50094400
H	-3.56832400	-10.52850900	-1.19216700
H	-4.62540900	-10.36460700	-2.58453500
C	-5.63812600	-11.01707300	-0.77360500
H	-6.65052500	-10.73215100	-1.10052100
H	-5.49739100	-12.08974000	-0.98031700
H	-5.57594200	-10.86828800	0.31605100
C	-3.92793400	-8.28904700	-0.03722000
H	-3.92556700	-9.10979000	0.69552800
H	-4.49049400	-7.45250500	0.39671600
C	-2.50046300	-7.85564500	-0.36122900
H	-1.98393300	-7.53655000	0.55800400
H	-1.92383200	-8.68224600	-0.80669000
H	-2.50501500	-7.01183700	-1.06735700
N	-4.65683000	-8.76302400	-1.21924100

Energy = -901.28613460 a.u. #Cluster: 6

P	-5.62584000	-5.48459200	-3.03269600
O	-7.08309900	-5.42967000	-3.39084300
C	-4.99954700	-3.99507200	-2.23800700
H	-5.26773000	-3.11959400	-2.84776200
H	-5.46734200	-3.90122900	-1.24637000
H	-3.90833400	-4.05346900	-2.12190500
C	-5.50566600	-7.85633400	-1.79147000
F	-4.74646800	-5.47659000	-4.40097800
N	-4.96471800	-6.74397200	-2.23029700
C	-6.97863000	-8.18155700	-1.89708800
H	-7.13580700	-9.17181900	-2.34758600
H	-7.43243100	-8.19669400	-0.89307600
H	-7.47932500	-7.41906100	-2.50124600
C	-5.18549500	-10.02284500	-0.62709500
H	-6.22364000	-9.90550100	-0.29348400
H	-4.59264400	-10.21928200	0.27967200
C	-5.06244700	-11.19554100	-1.59841800
H	-5.68079300	-11.03449600	-2.49528800
H	-4.01879400	-11.33483200	-1.92188700
H	-5.39603400	-12.12556200	-1.11159000
C	-3.26546600	-8.49908400	-1.06944400

H	-2.93793200	-7.96238600	-1.96911600
H	-2.75672800	-9.47445300	-1.05484300
C	-2.91794200	-7.69612400	0.18141800
H	-3.25014100	-8.21690400	1.09393500
H	-1.82786100	-7.55147200	0.24872800
H	-3.39712600	-6.70601600	0.14991400
N	-4.70427000	-8.75849700	-1.19105700

28

Energy = -901.28522220 a.u. #Cluster: 7

P	-5.25166600	-4.91027800	-1.75951800
O	-4.40758900	-3.75945900	-1.31613000
C	-5.43592400	-5.07772100	-3.54659600
H	-5.79149400	-4.12471900	-3.96596400
H	-4.45438500	-5.32095300	-3.97972100
H	-6.14868700	-5.88004600	-3.78768500
C	-5.44215000	-7.48451100	-0.96047200
F	-6.80760500	-4.61150000	-1.33642500
N	-4.81969500	-6.34373500	-1.12606500
C	-6.93155000	-7.67477200	-1.14473600
H	-7.13542300	-8.46947700	-1.87735600
H	-7.40274600	-7.96928800	-0.19427800
H	-7.39881700	-6.74616800	-1.48206700

C	-5.29108500	-9.88321900	-0.35521600
H	-6.34115000	-9.77397500	-0.06038200
H	-4.77009900	-10.31937700	0.51123200
C	-5.17760100	-10.82065100	-1.55697600
H	-4.12670700	-11.02557900	-1.81096200
H	-5.66445000	-11.78136700	-1.32596500
H	-5.66870000	-10.38892900	-2.44335300
C	-3.25737500	-8.41816400	-0.44069300
H	-2.91835800	-9.25012000	0.19311300
H	-3.05942600	-7.48004000	0.09753100
C	-2.49936400	-8.41871800	-1.76755600
H	-2.65520100	-9.35612900	-2.32203800
H	-2.82216300	-7.57883000	-2.39964600
H	-1.41959400	-8.30964600	-1.57695100
N	-4.71324400	-8.55527700	-0.58300400

28

Energy = -901.28514470 a.u. #Cluster: 8

P	-5.91161900	-5.32623000	-2.45275600
O	-7.26642300	-5.11807200	-1.83992100
C	-4.77093100	-3.95497000	-2.22790700
H	-4.52882200	-3.86700400	-1.15826900
H	-3.84728400	-4.13145000	-2.79689300

H	-5.25158300	-3.02598400	-2.56774200
C	-5.48217300	-7.90794200	-2.01671000
F	-6.05906200	-5.32913600	-4.07712700
N	-5.04160500	-6.67443500	-2.13003500
C	-6.92675500	-8.30099600	-2.23332100
H	-7.04137200	-8.76744000	-3.22559400
H	-7.27499300	-9.01988000	-1.47992800
H	-7.55697500	-7.40634600	-2.18567300
C	-4.95339900	-10.29453000	-1.62381900
H	-4.12206400	-10.86817700	-2.06162000
H	-5.82663800	-10.48766600	-2.25829200
C	-5.21773200	-10.76708900	-0.19541200
H	-6.03930000	-10.19556100	0.26482600
H	-5.49806900	-11.83232000	-0.20083200
H	-4.32398600	-10.65322200	0.43647600
C	-3.19162500	-8.51534100	-1.46327100
H	-2.87885500	-7.80006500	-2.23746400
H	-2.59652600	-9.43097300	-1.58906300
C	-2.95413300	-7.91253000	-0.07960200
H	-1.88652600	-7.66784900	0.04023200
H	-3.53473900	-6.98714300	0.04307000
H	-3.23613500	-8.61418700	0.71984300

N	-4.59292500	-8.87611000	-1.72107700
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28

Energy = -901.28512400 a.u. #Cluster: 9

P	-5.71482700	-5.35602100	-2.75187800
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O	-7.21137600	-5.30706500	-2.86644200
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C	-4.99728900	-3.97252700	-1.85336900
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H	-5.36893000	-3.03072800	-2.28315300
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H	-5.30868300	-4.03670100	-0.79993600
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H	-3.90039100	-4.00655800	-1.91150400
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C	-5.32409600	-7.93965400	-2.20514200
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F	-5.05976300	-5.12254800	-4.22511800
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N	-4.93271400	-6.68575500	-2.21193600
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C	-6.64963400	-8.41074600	-2.76026900
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H	-7.16393600	-9.08247100	-2.05890400
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H	-7.28607800	-7.54383400	-2.96482900
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H	-6.48728600	-8.96533600	-3.69875000
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C	-4.79363000	-10.29464300	-1.65467600
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H	-3.85933600	-10.83088500	-1.88202600
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H	-5.49060000	-10.53267500	-2.46677300
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C	-5.35760000	-10.77281600	-0.31776400
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H	-6.28147000	-10.23043100	-0.06164600
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H	-5.59291900	-11.84737500	-0.37609300
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H	-4.63554800	-10.62795300	0.50004000
C	-3.20626600	-8.43047900	-1.11005500
H	-2.75749800	-7.69421100	-1.79201800
H	-2.55156200	-9.31341300	-1.08746900
C	-3.33171100	-7.82686500	0.28786700
H	-3.96895300	-6.93093600	0.26817500
H	-3.75893300	-8.54701900	1.00164900
H	-2.33551300	-7.53155700	0.65458100
N	-4.48570500	-8.86144900	-1.69044100

28

Energy = -901.28505370 a.u. #Cluster: 10

P	-5.54584000	-5.41192600	-2.84634800
O	-6.77687700	-5.49439300	-3.70248000
C	-5.36718600	-3.86398700	-1.94512700
H	-4.38781100	-3.82053600	-1.44849300
H	-5.47150300	-3.02393400	-2.64766700
H	-6.16371200	-3.80221000	-1.18835300
C	-5.60986800	-7.79507000	-1.62188100
F	-4.23853600	-5.34269400	-3.81652100
N	-5.11299800	-6.59574700	-1.81092600
C	-6.88534500	-8.29076000	-2.26517900
H	-6.71991800	-9.24718200	-2.78232200

H	-7.65954900	-8.45502100	-1.49904500
H	-7.24550900	-7.54541300	-2.98101400
C	-5.41992300	-9.97479400	-0.45872900
H	-6.50643000	-10.02278700	-0.59477700
H	-5.23475600	-10.13103100	0.61563700
C	-4.73827600	-11.07487300	-1.27098400
H	-3.65361900	-11.09943200	-1.08574700
H	-5.15258000	-12.05628100	-0.99063100
H	-4.90060300	-10.92664500	-2.35044400
C	-3.67419800	-8.19391000	-0.20305000
H	-3.47363700	-8.85625200	0.65108900
H	-3.80364000	-7.17353800	0.18595400
C	-2.50477200	-8.22547700	-1.18633500
H	-1.58385300	-7.89663600	-0.67844900
H	-2.33621700	-9.23976900	-1.57843400
H	-2.69230900	-7.54782200	-2.03152500
N	-4.95278500	-8.62453000	-0.78609900

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29

Energy = -901.72598950 a.u. #Cluster: 1

P	-1.33995500	-0.40421300	-2.15696100
F	-0.56628100	-1.06397400	-3.39883500

O	-2.07870400	-1.42425900	-1.37553100
N	1.75520700	0.42099800	0.15780400
N	-0.03425000	0.33207700	-1.30492500
C	2.74216500	-0.19480400	1.07373900
C	1.78690300	1.89767500	0.10947000
C	0.88832600	-0.28879400	-0.53234300
C	4.08678600	-0.44191400	0.40132300
C	0.83811400	2.53358100	1.12164700
C	0.87122000	-1.78511300	-0.48234300
C	-2.20948100	0.96928800	-2.88656500
H	2.31956000	-1.11612400	1.49010400
H	2.84974300	0.50499600	1.91396900
H	2.82489300	2.19138200	0.31333400
H	1.57968700	2.23106000	-0.91818500
H	4.51049100	0.49218100	0.00159700
H	4.79263100	-0.84914900	1.14102000
H	3.99452000	-1.16321000	-0.42508900
H	0.93230300	3.62854500	1.06848900
H	-0.21075000	2.26712500	0.92036800
H	1.08748500	2.21503500	2.14526100
H	1.83602800	-2.19909900	-0.17916800
H	0.09394500	-2.11134800	0.22622500

H	0.61726700	-2.18696700	-1.47062800
H	-2.98507400	0.55501000	-3.54774900
H	-2.68427000	1.55634100	-2.08660900
H	-1.51565100	1.59595500	-3.46547100
H	-0.01489700	1.35023900	-1.35117800

29

Energy = -901.72463190 a.u. #Cluster: 2

P	-1.29588900	-0.14651400	-2.37472400
F	-1.12843900	0.99892700	-3.47962100
O	-1.09440300	-1.50620500	-2.93058600
N	1.80893500	0.44662100	0.04233100
N	-0.11252500	0.36553800	-1.23057800
C	3.16436900	-0.01723900	0.41069300
C	1.32186700	1.62059000	0.79480700
C	1.10299500	-0.13702800	-0.90529500
C	3.14802300	-0.98308700	1.59001500
C	1.62097300	2.93761200	0.08308700
C	1.64056100	-1.32761500	-1.63257400
C	-2.85814300	0.25535800	-1.61301300
H	3.73925500	0.88689400	0.65574200
H	3.64299400	-0.46504900	-0.46725900
H	0.24818700	1.49669600	1.00117900

H	1.81920000	1.58944600	1.77278500
H	2.59558100	-1.90367300	1.34730500
H	4.18223600	-1.25740600	1.84793500
H	2.68458400	-0.52357300	2.47649900
H	1.11530300	2.99965700	-0.89255900
H	1.27128500	3.77428700	0.70615900
H	2.70299300	3.05567700	-0.07986000
H	2.07795100	-2.04662800	-0.92936200
H	0.85245300	-1.81098900	-2.21553900
H	2.43366200	-0.99179200	-2.32075200
H	-3.02277400	-0.43443700	-0.77259900
H	-2.85932600	1.29680000	-1.25940300
H	-3.64533800	0.11613200	-2.36902500
H	-0.38860800	1.22352300	-0.75301600

29

Energy = -901.72455750 a.u. #Cluster: 3

P	-1.30483900	-0.45640500	-2.22576900
F	-0.75197900	0.11661300	-3.61507400
O	-1.35852600	-1.93931800	-2.22903600
N	1.78323500	0.45456300	0.09090500
N	-0.17464500	0.22488800	-1.11518300
C	3.18777000	0.10173100	0.39382500

C	1.23887000	1.58862300	0.86503900
C	1.08233700	-0.18496400	-0.82165200
C	3.30478900	-0.86096200	1.56942000
C	1.44795700	2.92985100	0.16689800
C	1.66232400	-1.33898400	-1.57605700
C	-2.79677000	0.47689700	-1.94584800
H	3.69913000	1.04905100	0.61488500
H	3.65825400	-0.30430000	-0.50870600
H	0.17776600	1.39744900	1.08321600
H	1.75247700	1.57488300	1.83536400
H	4.36875000	-1.04351800	1.78367600
H	2.83995600	-0.44224800	2.47517600
H	2.82486600	-1.82615800	1.34683700
H	1.05972500	3.73564000	0.80759200
H	2.51788200	3.11542200	-0.01163600
H	0.92299600	2.97484500	-0.79954500
H	2.28227500	-1.96820700	-0.92836800
H	0.86439600	-1.95154300	-2.00798100
H	2.29172900	-0.94517100	-2.39151200
H	-2.59444000	1.55558100	-2.01617000
H	-3.52034000	0.17895900	-2.71911000
H	-3.19259100	0.22145600	-0.95197000

H	-0.50539300	1.07784600	-0.66644700
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29

Energy = -901.72440770 a.u. #Cluster: 4

P	-1.55805800	0.49073000	-2.19228200
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F	-2.57172200	-0.11036300	-1.10797000
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O	-2.02486600	1.75143600	-2.81259200
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N	1.63931700	0.61084400	0.18297900
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N	-0.17782100	0.84098600	-1.22145600
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C	2.43059500	-0.11252300	1.20224300
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C	2.19137300	1.91762800	-0.22971600
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C	0.52240400	0.12120700	-0.31577500
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C	3.53747400	-0.96091300	0.58583100
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C	1.64989300	3.07302500	0.60798700
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C	0.01774100	-1.21611700	0.12797400
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C	-1.21106900	-0.90344100	-3.25168600
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H	1.75686200	-0.72085300	1.81542800
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H	2.85319800	0.65560700	1.86483700
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H	3.28127900	1.84129800	-0.12209800
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H	2.00528100	2.06449000	-1.30380200
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H	3.12658000	-1.75424800	-0.05680400
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H	4.22466600	-0.34658500	-0.01581400
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H	4.11852300	-1.43511500	1.39123200
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H	2.12655100	4.00969000	0.28223400
H	0.56036700	3.18398400	0.49719300
H	1.87655100	2.92308300	1.67446500
H	0.77900000	-1.98856000	-0.04660900
H	-0.19554500	-1.18263800	1.20713000
H	-0.90536500	-1.49885500	-0.38092500
H	-0.45594700	-0.58488500	-3.98508700
H	-0.84238700	-1.76821800	-2.68394900
H	-2.14392200	-1.16780200	-3.77229800
H	0.15700800	1.77962800	-1.43790200

29

Energy = -901.72434280 a.u. #Cluster: 5

P	-0.90589600	-0.03704400	-2.79705400
F	-0.71885200	1.16881000	-3.82733100
O	-0.63331800	-1.37211800	-3.37964300
N	1.77541300	0.45520700	0.09438800
N	0.27420400	0.50929900	-1.65716700
C	2.49701100	-0.23511200	1.18514800
C	2.02733300	1.90710700	-0.00849700
C	0.94578400	-0.18054300	-0.70818600
C	3.89852100	-0.67016600	0.77247300
C	0.99542200	2.73579100	0.75212800

C	0.71273300	-1.65140100	-0.56126800
C	-2.50937500	0.27518500	-2.07982300
H	1.89849700	-1.08563700	1.52934500
H	2.54032100	0.47729600	2.02102200
H	3.03297900	2.07573100	0.39786000
H	2.08239600	2.18977500	-1.07054500
H	4.40224800	-1.13453900	1.63382600
H	3.86539200	-1.40448300	-0.04687400
H	4.50376400	0.18875500	0.44413400
H	-0.01727500	2.60757000	0.34025600
H	0.97541300	2.45249800	1.81544900
H	1.26264600	3.80080700	0.68243300
H	1.65786700	-2.18468600	-0.40540800
H	0.06796400	-1.82216800	0.31633000
H	0.22081700	-2.05531200	-1.45064000
H	-3.27765100	0.08867000	-2.84515200
H	-2.64756000	-0.42082500	-1.23897400
H	-2.56407700	1.31386700	-1.72421600
H	0.40523800	1.52018600	-1.68124200

29

Energy = -901.72412210 a.u. #Cluster: 6

P	-1.27019900	0.27841000	-2.46896300
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F	-1.82214300	1.76092300	-2.69203500
O	-0.72439000	-0.35628300	-3.69128500
N	1.80292800	0.54331600	0.02940900
N	-0.07680500	0.71172400	-1.29607100
C	2.99422600	-0.16892300	0.53756800
C	1.57262600	1.88366100	0.60716000
C	1.00711600	0.02092000	-0.88221100
C	2.70800100	-0.92470200	1.83037600
C	2.13660100	2.99703000	-0.27135400
C	1.29274100	-1.32963500	-1.46203300
C	-2.60328100	-0.53557400	-1.60763800
H	3.76663400	0.59688900	0.69603700
H	3.37260500	-0.84150000	-0.23943600
H	0.49755600	2.01662600	0.80169300
H	2.05557800	1.88458600	1.59244300
H	3.63538100	-1.39887500	2.18605100
H	2.34677800	-0.24647100	2.61871200
H	1.95382800	-1.71158800	1.67598800
H	3.21882700	2.86362200	-0.42098100
H	1.64978200	3.02268000	-1.25798200
H	1.97141800	3.96751600	0.22001200
H	1.36779900	-2.07540700	-0.65876700

H	0.51977700	-1.63445700	-2.17205700
H	2.25346600	-1.30295100	-1.99803200
H	-3.42687000	-0.70111400	-2.31821500
H	-2.23255300	-1.50380000	-1.23904700
H	-2.93988400	0.08482200	-0.76504100
H	-0.25958400	1.61107700	-0.85153100

29

Energy = -901.72399420 a.u. #Cluster: 7

P	-1.97977700	0.04143100	-1.23431000
F	-2.11998100	-1.52568900	-0.93048100
O	-3.05847200	0.86238800	-0.63897900
N	1.73429100	0.48729300	0.13286100
N	-0.50137900	0.42413300	-0.43675800
C	3.11738600	-0.03670800	0.09506500
C	1.56073300	1.74979200	0.88172000
C	0.73902800	-0.11330500	-0.48597700
C	3.44646100	-0.89447800	1.31142100
C	1.63316200	2.97673700	-0.02306700
C	0.96744400	-1.37512000	-1.25812900
C	-1.73656200	0.09755100	-3.00176000
H	3.77475600	0.84280700	0.04874500
H	3.26804000	-0.58850400	-0.83918600

H	0.61905700	1.71114400	1.44951100
H	2.35927200	1.77545400	1.63422400
H	3.30979500	-0.32958100	2.24625700
H	2.81068800	-1.79223500	1.35232000
H	4.49765300	-1.21525100	1.25498300
H	0.82464100	2.97917200	-0.76964500
H	1.53845000	3.88490300	0.59083500
H	2.59732900	3.01486700	-0.55234100
H	0.02936400	-1.90398100	-1.44447300
H	1.44300000	-1.13089600	-2.22203200
H	1.63326200	-2.05102400	-0.70910800
H	-2.66891100	-0.24256000	-3.47756500
H	-1.53894100	1.14305300	-3.28017700
H	-0.90248000	-0.54282400	-3.31855500
H	-0.62934700	1.26395400	0.12736800

29

Energy = -901.72364800 a.u. #Cluster: 8

P	-1.33662700	-0.32145700	-2.24413000
F	-0.90878900	-0.34651300	-3.78623200
O	-1.74557100	-1.66080600	-1.75539800
N	2.06318700	0.41211500	-0.32992400
N	0.08976200	0.31201900	-1.51364500

C	3.27427800	-0.20114000	0.25720800
C	1.93722600	1.88020100	-0.18417900
C	1.13525500	-0.31333800	-0.92183300
C	3.18240400	-0.36869100	1.76932900
C	0.90502100	2.30721200	0.85846500
C	1.23460600	-1.80448700	-0.97604100
C	-2.49250600	1.03383100	-2.16686300
H	4.11159500	0.45803700	-0.01234400
H	3.45773100	-1.16192100	-0.23457200
H	2.93281500	2.24673100	0.09341900
H	1.72174400	2.31831400	-1.17293100
H	3.08111400	0.60049400	2.27987100
H	2.32658400	-1.00278700	2.04773200
H	4.10328100	-0.84909300	2.13348900
H	1.16033200	1.90861300	1.85045300
H	0.89523500	3.40599100	0.91715700
H	-0.11167000	1.97323500	0.60348400
H	0.27894700	-2.24087300	-1.28014500
H	2.00707200	-2.08293200	-1.71143200
H	1.52423000	-2.21018100	0.00119200
H	-2.77299500	1.19903500	-1.11642300
H	-2.04554600	1.94398900	-2.59325100

H	-3.38135600	0.74765500	-2.74857300
H	0.14060200	1.32926800	-1.56111000

29

Energy = -901.72301460 a.u. #Cluster: 9

P	-1.07402300	0.24928700	-2.60364500
F	-1.11596900	1.73883600	-3.18172900
O	-0.47033200	-0.73729400	-3.53003000
N	1.46541200	0.37283800	0.44600800
N	-0.10723600	0.61599200	-1.21929400
C	2.34075100	-0.44226100	1.31576500
C	1.46814600	1.83152900	0.69821200
C	0.74539600	-0.16471800	-0.51891000
C	3.81014100	-0.36855000	0.91724300
C	2.22110800	2.63369300	-0.36199000
C	0.82727400	-1.62660400	-0.82540700
C	-2.74336400	-0.01589200	-2.03423400
H	1.98258300	-1.47670700	1.30953400
H	2.19422400	-0.06314300	2.33736000
H	0.42596900	2.17490200	0.80653700
H	1.93118600	1.97177600	1.68232400
H	4.39785900	-1.00739000	1.59390400
H	3.96005400	-0.72397300	-0.11401000

H	4.19989100	0.65726100	0.99429200
H	3.27147700	2.31507200	-0.42109600
H	1.77317400	2.53364800	-1.36154900
H	2.19639900	3.69833600	-0.08491800
H	1.86915600	-1.96869400	-0.82633600
H	0.27678600	-2.18423500	-0.05019700
H	0.38340200	-1.84086100	-1.80163100
H	-2.76723800	-0.96043500	-1.47066900
H	-3.05665500	0.81764400	-1.38969500
H	-3.40249000	-0.09110600	-2.91209100
H	-0.23512200	1.57357000	-0.89097800

29

Energy = -901.72294710 a.u. #Cluster: 10

P	-1.03426900	0.20424500	-2.66124600
F	-1.13056400	1.67643900	-3.27468400
O	-0.41923500	-0.78810200	-3.57412900
N	1.43529300	0.41403000	0.44051600
N	-0.05214300	0.63580200	-1.30603100
C	2.26038100	-0.39242200	1.36593700
C	1.44950000	1.87847100	0.65460900
C	0.74775000	-0.13822600	-0.53970300
C	3.74462800	-0.36684200	1.02014300

C	2.27930500	2.63776800	-0.37937700
C	0.81249800	-1.61047600	-0.79891000
C	-2.68412800	-0.09801500	-2.05466800
H	1.87729300	-1.41783400	1.37962900
H	2.08704900	0.02253400	2.36915700
H	0.40906100	2.24192600	0.68988800
H	1.85618600	2.03737000	1.66057500
H	4.28991200	-1.00243100	1.73438300
H	3.92295300	-0.75342500	0.00469300
H	4.15917800	0.65007200	1.08503000
H	3.32538700	2.30055300	-0.36614700
H	1.89084400	2.51520700	-1.40120100
H	2.25677900	3.71037300	-0.13456800
H	0.40387800	-1.84703300	-1.78546300
H	1.84744500	-1.97000300	-0.75052500
H	0.22356000	-2.13649300	-0.03004100
H	-3.35418400	-0.22490700	-2.91824500
H	-2.66601600	-1.02434100	-1.46115700
H	-3.01508000	0.74465800	-1.43129700
H	-0.15530000	1.61362300	-1.03439400

A230-N₂H

29

Energy = -901.70613440 a.u. #Cluster: 1

P	-1.37856000	0.53984300	-1.02214100
F	-2.03119600	1.92027000	-0.55910000
O	-0.27881100	0.75433400	-2.02424300
N	1.47631200	-0.07251800	-0.11350300
N	-0.86201800	-0.05219400	0.48012200
C	2.46611100	0.94530900	0.41700200
C	2.16158100	-1.35639100	-0.53868300
C	0.32667600	-0.31525100	0.82433800
C	1.79844400	2.24335800	0.83134600
C	1.19000400	-2.34220900	-1.16007100
C	0.68236500	-0.88645000	2.15108600
C	-2.76667700	-0.46251000	-1.50654800
H	3.17231100	1.10354500	-0.40917700
H	3.00900200	0.46884100	1.24399900
H	2.92768500	-1.03942700	-1.25874300
H	2.67048200	-1.76361700	0.34497000
H	1.21080800	2.67003000	0.00390400
H	1.13732900	2.11448200	1.70148100
H	2.58145200	2.96458300	1.10687100

H	0.44214600	-2.70283200	-0.43750000
H	0.66691000	-1.89689400	-2.01952500
H	1.75845600	-3.21340300	-1.51647400
H	-0.22942400	-0.97867200	2.75123700
H	1.14263000	-1.88037600	2.03099300
H	1.41163800	-0.25129800	2.67655900
H	-3.51490000	-0.47026300	-0.70186000
H	-3.19511000	-0.04128000	-2.42829100
H	-2.40397400	-1.48314700	-1.69952200
H	1.03975900	0.33597500	-0.97943500

29

Energy = -901.70606340 a.u. #Cluster: 2

P	-1.45295700	0.49559500	-0.87534700
F	-2.08748500	1.84653100	-0.31075900
O	-0.42126500	0.76990900	-1.93388900
N	1.46895200	-0.03838200	-0.15573800
N	-0.83236800	-0.15713600	0.56060500
C	2.42996200	1.00355000	0.38170400
C	2.19892700	-1.25707800	-0.68408800
C	0.38341000	-0.38838300	0.82409200
C	1.71901700	2.24153500	0.89614400
C	1.25429600	-2.25301100	-1.33093700

C	0.83619800	-1.01646600	2.09471200
C	-2.85895900	-0.50162400	-1.31608600
H	3.08557700	1.24131500	-0.46668100
H	3.03668200	0.51525000	1.15600300
H	2.91835300	-0.85718500	-1.41114600
H	2.76421600	-1.68953700	0.15191000
H	2.47779300	2.99010700	1.16668500
H	1.06564000	2.67588400	0.12377800
H	1.11462600	2.03615900	1.79266600
H	0.67430200	-1.78254200	-2.13883700
H	1.85173400	-3.06826200	-1.76417300
H	0.55596200	-2.69847600	-0.60604500
H	1.53888500	-0.36057400	2.63171200
H	-0.03906000	-1.21300400	2.72328900
H	1.36312700	-1.96211200	1.89089200
H	-3.34841500	-0.04512300	-2.18935900
H	-2.49972100	-1.50835100	-1.57689800
H	-3.55444400	-0.55388500	-0.46688000
H	0.96844900	0.38713100	-0.97823700

29

Energy = -901.70605970 a.u. #Cluster: 3

P	-1.44234700	0.56653800	-0.80890300
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F	-2.04604700	1.89946800	-0.17199100
O	-0.41418400	0.87698200	-1.86102900
N	1.47192500	-0.08041300	-0.15289100
N	-0.82404900	-0.17143700	0.58535600
C	2.35733600	1.03553200	0.37239200
C	2.27854700	-1.26998800	-0.62412400
C	0.38793600	-0.44855500	0.82102700
C	1.56171100	2.26833600	0.75728500
C	1.40605600	-2.31649200	-1.29204400
C	0.83853200	-1.13649100	2.06086400
C	-2.87213300	-0.37896000	-1.28648600
H	3.05297000	1.24820800	-0.45022000
H	2.93308700	0.62513900	1.21226300
H	3.00987200	-0.85184700	-1.32853500
H	2.82702600	-1.66174000	0.24266400
H	2.26913300	3.05943300	1.04550800
H	0.96225100	2.63679400	-0.08859300
H	0.89421900	2.08704800	1.61311000
H	2.05351500	-3.11379900	-1.68477300
H	0.69220200	-2.77730700	-0.59244400
H	0.84324500	-1.88261900	-2.13282400
H	1.17632900	-2.15879900	1.82428600

H	1.68522500	-0.61098600	2.52739600
H	-0.00344000	-1.19252600	2.75953100
H	-3.55958300	-0.46480800	-0.43352500
H	-3.36255300	0.13146900	-2.12868500
H	-2.53383200	-1.37642500	-1.60470300
H	0.96848300	0.31008000	-0.99082500

29

Energy = -901.70450330 a.u. #Cluster: 4

P	-1.67105800	0.35428200	-0.66025700
F	-2.46799900	1.49345500	0.12203300
O	-0.63741900	0.93548500	-1.58560800
N	1.25456200	0.04277300	0.13515200
N	-1.03437100	-0.51554500	0.64674600
C	1.87791800	1.17343900	0.94075800
C	2.27271300	-0.90081900	-0.46135700
C	0.19064800	-0.65570300	0.93294200
C	2.39095800	2.27652400	0.03325900
C	1.62442900	-1.88967700	-1.41277500
C	0.67591700	-1.48862400	2.06628500
C	-2.94716600	-0.65819700	-1.37573400
H	2.67207100	0.73207000	1.55696200
H	1.08797500	1.55310900	1.60341500

H	2.99274000	-0.25958300	-0.98542000
H	2.79626200	-1.38831100	0.37120600
H	3.19471200	1.92940700	-0.63218300
H	1.57471200	2.69361200	-0.57574000
H	2.79783000	3.08147900	0.66296800
H	1.07701500	-1.36700100	-2.21187100
H	2.41111500	-2.50304100	-1.87528800
H	0.92778400	-2.56838900	-0.89668800
H	1.14693600	-2.40674000	1.67726800
H	1.43330300	-0.95849000	2.66247800
H	-0.17747900	-1.76855200	2.69386900
H	-3.65813100	-0.96352500	-0.59562500
H	-3.45720400	-0.07292900	-2.15537900
H	-2.47379100	-1.54247900	-1.82778300
H	0.73645400	0.49380700	-0.66454300

29

Energy = -901.70442660 a.u. #Cluster: 5

P	-1.65586900	0.49066400	-0.59819900
F	-2.16769000	1.91632800	-0.09622800
O	-0.69718600	0.62398800	-1.74876200
N	1.24966200	-0.29718300	-0.10580000
N	-0.96126600	-0.08513100	0.83568100

C	2.28835100	0.77520800	0.15275200
C	1.84457300	-1.64796100	-0.45786400
C	0.25026600	-0.40592300	1.01162900
C	1.65077200	2.12485100	0.42725300
C	2.41571500	-1.66191100	-1.86421700
C	0.78112700	-0.91040600	2.30647800
C	-3.14933100	-0.44121200	-0.85770900
H	2.90322200	0.80713600	-0.75494400
H	2.91915100	0.42828800	0.98160000
H	2.60389800	-1.87777500	0.30093900
H	1.02391700	-2.37309100	-0.36710500
H	1.07696400	2.13293500	1.36641500
H	2.44891800	2.87615900	0.51460500
H	0.98449100	2.42411700	-0.39563700
H	3.27883500	-0.98983600	-1.97381000
H	2.75512100	-2.68437600	-2.08650200
H	1.64874200	-1.38661200	-2.60466700
H	1.62231600	-0.29061500	2.65395300
H	-0.02323100	-0.89511100	3.04999400
H	1.15807500	-1.93945800	2.19342900
H	-3.68607300	-0.00009500	-1.71104500
H	-2.87191600	-1.47979100	-1.09206300

H	-3.77065800	-0.40738300	0.04795400
H	0.69053900	0.02603200	-0.93904000

29

Energy = -901.70441960 a.u. #Cluster: 6

P	-1.61616500	0.56842400	-0.66550200
F	-2.16088900	1.98379700	-0.17019500
O	-0.60450500	0.72229100	-1.76717500
N	1.24864200	-0.29249700	-0.06578100
N	-0.98806500	-0.02008800	0.79395000
C	2.37666900	0.66027100	0.26264400
C	1.72217800	-1.68259600	-0.45574100
C	0.20973400	-0.36114900	1.01750800
C	1.86388500	2.06823600	0.50254700
C	2.24550800	-1.71345000	-1.88056800
C	0.68708500	-0.85358200	2.33753600
C	-3.08895700	-0.37005900	-1.00637200
H	3.04926500	0.62572800	-0.60341400
H	2.91207100	0.24664600	1.12729400
H	2.48368500	-1.98366200	0.27550500
H	0.85111000	-2.34404800	-0.34930600
H	1.28816500	2.43182300	-0.36221800
H	1.22808700	2.13272700	1.39890400

H	2.72451300	2.73619500	0.65141900
H	1.46900300	-1.39348900	-2.59214200
H	3.13567200	-1.08168700	-2.01256800
H	2.52751200	-2.74894200	-2.12185500
H	1.24754500	-1.79493500	2.23550900
H	1.36672500	-0.11398900	2.79217600
H	-0.17639400	-0.99728500	2.99636100
H	-2.79279900	-1.40308000	-1.24233800
H	-3.75106200	-0.35377100	-0.12957200
H	-3.59039100	0.07885500	-1.87694100
H	0.74360500	0.10515100	-0.90057400

29

Energy = -901.70441750 a.u. #Cluster: 7

P	-1.61870500	0.53290800	-0.66871900
F	-2.11160900	1.98711900	-0.23379200
O	-0.62775400	0.60533700	-1.79741000
N	1.25228800	-0.30753900	-0.07419000
N	-0.97293700	-0.00018800	0.80440600
C	2.35709000	0.69318100	0.18638900
C	1.76281300	-1.70257100	-0.39253000
C	0.22748600	-0.33538300	1.02442700
C	1.81052400	2.09696100	0.36923800

C	2.27079700	-1.79534000	-1.82013200
C	0.72093600	-0.77530100	2.35685700
C	-3.12459000	-0.37764700	-0.93083200
H	3.01554700	0.63570400	-0.68941200
H	2.92025300	0.33827000	1.05962600
H	2.54099600	-1.93950600	0.34471000
H	0.91339100	-2.38257000	-0.23932800
H	1.18500700	2.18689900	1.27056300
H	2.65609800	2.79169200	0.47629100
H	1.21625900	2.40795500	-0.50322300
H	1.47583900	-1.54072900	-2.53780700
H	3.13723900	-1.14234900	-1.99825300
H	2.58475300	-2.83265000	-2.00829400
H	-0.12984100	-0.85280200	3.04268700
H	1.24155400	-1.74279100	2.29063700
H	1.44124100	-0.04215200	2.75512400
H	-3.76529700	-0.29800800	-0.04165300
H	-3.63278500	0.04240200	-1.81181300
H	-2.86314700	-1.42945500	-1.12041700
H	0.72799000	0.03039200	-0.92406100

29

Energy = -901.70439960 a.u. #Cluster: 8

P	-1.65618600	0.43176400	-0.70758200
F	-2.28765300	1.82065500	-0.24050400
O	-0.64266200	0.62423100	-1.80141000
N	1.25175900	-0.23267300	-0.05692600
N	-1.01072600	-0.09655500	0.76845800
C	2.37004500	0.71705500	0.30807900
C	1.74520800	-1.60739900	-0.48411200
C	0.20352500	-0.35481500	1.01298500
C	1.85486300	2.11478800	0.59738000
C	2.25796900	-1.59256000	-1.91266300
C	0.69427200	-0.80891100	2.34199200
C	-3.06907900	-0.59502800	-1.04935700
H	3.04583100	0.71527400	-0.55611800
H	2.90573900	0.27652000	1.15905700
H	2.51517600	-1.91373400	0.23598000
H	0.88506300	-2.28460300	-0.38918300
H	1.28441400	2.51072400	-0.25690400
H	1.21287000	2.14656200	1.49101100
H	2.71462200	2.77648400	0.77608900
H	1.47008600	-1.26626100	-2.60834100
H	3.13685500	-0.94305700	-2.03442700
H	2.55474500	-2.61660100	-2.18327200

H	1.35455400	-1.68368200	2.24747100
H	1.27937800	-0.00545100	2.81925800
H	-0.16577500	-1.04754900	2.97737000
H	-3.58360000	-0.19002200	-1.93366400
H	-2.71226400	-1.61349400	-1.26333700
H	-3.74259500	-0.60154900	-0.18120200
H	0.74499700	0.17172100	-0.88703900

29

Energy = -901.70363550 a.u. #Cluster: 9

P	-2.11452500	-0.42799400	-0.80255300
F	-2.38368900	-0.42202400	-2.38086800
O	-2.59273800	-1.68880000	-0.17068400
N	1.80145600	-0.09600800	-0.28703000
N	-0.43442000	-0.14417900	-0.84687200
C	2.35170800	0.83668100	0.77519200
C	2.74452300	-1.25020200	-0.57393600
C	0.40250200	-0.53967000	0.00912400
C	1.47984100	2.06281900	0.96710700
C	2.20059500	-2.18146700	-1.63922700
C	0.21777000	-1.32226600	1.26369100
C	-2.82221000	1.12131300	-0.25824400
H	3.35659300	1.10520200	0.42344800

H	2.45641300	0.24285700	1.69283500
H	3.68169900	-0.77301400	-0.88976300
H	2.92475800	-1.75998400	0.38130900
H	1.35202000	2.61422200	0.02270300
H	0.48587200	1.81272400	1.36711300
H	1.97514400	2.72854100	1.68892700
H	1.29608300	-2.71262400	-1.30703700
H	1.96911700	-1.63603700	-2.56712800
H	2.96975400	-2.93437400	-1.86527500
H	0.14837100	-0.62050600	2.11224300
H	-0.71837900	-1.88801100	1.20048600
H	1.06161100	-1.99755900	1.45727300
H	-2.57800800	1.25799200	0.80584900
H	-2.41346800	1.95215100	-0.84992800
H	-3.91443600	1.06531500	-0.38075800
H	1.70747500	0.44673800	-1.15890600

29

Energy = -901.70341950 a.u. #Cluster: 10

P	-2.06904800	0.21172500	0.23935200
F	-2.33630600	0.59813500	1.77233000
O	-2.53050700	1.28326200	-0.68611300
N	1.88087300	-0.17513100	-0.02698200

N	-0.40379800	-0.10234000	0.36114300
C	2.28832100	0.31851800	1.34959200
C	1.95932200	-1.68799500	-0.10936000
C	0.50618900	0.32402200	-0.39456100
C	2.28510800	1.83108200	1.44908800
C	1.60704500	-2.21552400	-1.48625800
C	0.48620600	1.22220000	-1.57891100
C	-2.81212400	-1.40727700	0.08952400
H	3.28824300	-0.10072900	1.52168200
H	1.58034700	-0.14381700	2.04893500
H	2.99049600	-1.93825400	0.17253000
H	1.27619700	-2.06154800	0.66387400
H	2.66195500	2.11171500	2.44347500
H	2.94387700	2.28747500	0.69357900
H	1.27343400	2.25130600	1.34357800
H	1.75632100	-3.30521000	-1.48546300
H	0.55580700	-2.02195800	-1.74798200
H	2.25585200	-1.78310500	-2.26403100
H	1.15171000	2.08189800	-1.39411800
H	0.89375700	0.67990800	-2.44895800
H	-0.53309300	1.56699500	-1.77961700
H	-2.55437800	-1.81710800	-0.89857800

H	-2.43781200	-2.06987500	0.88188100
H	-3.90390400	-1.29527800	0.16650900
H	2.55134200	0.20874600	-0.70704900

A230-OH

29

Energy = -901.71111380 a.u. #Cluster: 1

P	-1.93121700	0.58672000	-0.55561700
F	-1.97898800	2.14084600	-0.92670800
O	-2.34345800	-0.13558500	-1.91988100
N	1.75960000	0.03271800	0.12639200
N	-0.49969800	0.23005300	-0.03544900
C	3.08929700	-0.40286800	-0.32720300
C	1.71514900	0.80469000	1.38018000
C	0.64390900	-0.21072500	-0.54941800
C	3.52212800	-1.72149200	0.30683300
C	1.69961400	2.30926300	1.12820100
C	0.70891200	-0.98003000	-1.84194200
C	-3.19282800	0.39582100	0.68223100
H	3.79037500	0.40187200	-0.06125800
H	3.09474400	-0.47141100	-1.42134000
H	0.82230700	0.49632900	1.93906300

H	2.59813400	0.51457300	1.96624300
H	2.84414100	-2.54100200	0.02216300
H	4.53762400	-1.97831300	-0.03185400
H	3.53527600	-1.64903200	1.40542100
H	2.58594100	2.62499900	0.55552600
H	0.79691900	2.60084700	0.57085200
H	1.70282000	2.84667200	2.08924800
H	1.16005800	-0.34828500	-2.62456900
H	1.32609500	-1.88255700	-1.73963700
H	-0.29687700	-1.26635000	-2.16185000
H	-2.91372200	0.98514600	1.56723000
H	-4.15244000	0.74907100	0.27712200
H	-3.26146800	-0.66970300	0.94592300
H	-3.23305200	0.07104000	-2.26370500

29

Energy = -901.71078000 a.u. #Cluster: 2

P	-2.00590200	0.33748400	-0.42261900
F	-2.75320900	-1.07585900	-0.27549400
O	-2.50569600	1.16269100	0.84729300
N	1.73631400	-0.00377700	0.18349700
N	-0.44214300	0.26388200	-0.40972200
C	2.87206600	-0.73794100	0.76135000

C	2.02841400	1.33145000	-0.36536000
C	0.49733100	-0.48001500	0.16037000
C	3.64894100	-1.53151100	-0.28532700
C	1.74708000	2.43905600	0.64564800
C	0.20880000	-1.83074600	0.76063300
C	-2.65201900	1.00770800	-1.93651800
H	2.51066700	-1.39286900	1.56281400
H	3.52156600	0.01052700	1.23834600
H	3.08615200	1.33197400	-0.66258500
H	1.42251600	1.46820100	-1.27011900
H	3.01645600	-2.30435400	-0.74890900
H	4.03057800	-0.87364700	-1.08155700
H	4.50900200	-2.02767200	0.19018800
H	0.68125600	2.45496700	0.91863600
H	2.34317100	2.29951100	1.56131800
H	2.00895200	3.41601900	0.21058900
H	0.91456900	-2.58927000	0.39594600
H	0.30775600	-1.77547100	1.85669600
H	-0.80974900	-2.14612600	0.51572900
H	-3.74965000	1.04338700	-1.87777700
H	-2.24464000	2.01960900	-2.07242600
H	-2.33722500	0.36040100	-2.76799700

H	-3.46206200	1.35570000	0.86955600
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29

Energy = -901.71065080 a.u. #Cluster: 3

P	-1.78379200	0.52195400	-1.22710700
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F	-1.90830900	1.71402200	-2.27082400
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O	-2.13123900	-0.78448000	-2.07611000
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N	1.75269600	0.11573100	0.16211700
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N	-0.29824700	0.54864100	-0.72044400
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C	2.76843600	-0.73984900	0.79416000
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C	2.12557600	1.52289900	-0.05747700
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C	0.54725800	-0.32208800	-0.18734700
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C	3.73684900	-1.34696600	-0.21702000
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C	1.69169500	2.42219300	1.09591500
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C	0.18092400	-1.76173200	0.06145500
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C	-3.04760900	0.86727700	-0.02189700
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H	2.27062300	-1.52054800	1.38152600
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H	3.31061400	-0.10793200	1.51293200
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H	3.21711100	1.54984100	-0.18393200
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H	1.66827300	1.85267400	-0.99895200
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H	4.25114400	-0.56335200	-0.79474800
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H	4.49976500	-1.93957500	0.31099000
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H	3.21273700	-2.00904700	-0.92364700
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H	0.59647300	2.41903900	1.20107900
H	2.13761100	2.09217400	2.04749800
H	2.01885200	3.45601600	0.90455000
H	-0.73526100	-2.02049900	-0.47919400
H	0.98052900	-2.44614400	-0.25013800
H	0.00765400	-1.91038500	1.13987700
H	-3.04749800	0.05054100	0.71520200
H	-2.80972300	1.81954900	0.47365500
H	-4.02609200	0.92997600	-0.52087500
H	-3.05775500	-0.87662200	-2.36904700

29

Energy = -901.71031270 a.u. #Cluster: 4

P	-2.07238100	0.46695400	-0.27095000
F	-2.74290300	-0.60345500	0.71493500
O	-2.79721400	1.83532400	0.07898800
N	1.69976900	0.15125300	0.22689100
N	-0.51753800	0.59602100	-0.03919800
C	2.86846500	-0.70259900	0.50241400
C	1.98657700	1.58308400	0.02497400
C	0.45092800	-0.29423100	0.16609300
C	3.47120300	-1.29681000	-0.76630900
C	1.91630700	2.37217800	1.32842000

C	0.13476100	-1.75596700	0.32924600
C	-2.66466700	0.00740400	-1.88286200
H	2.58856200	-1.48518600	1.21803200
H	3.60281400	-0.06526500	1.01454800
H	2.99046300	1.64698100	-0.41794000
H	1.26901700	1.97500200	-0.70558500
H	3.75538700	-0.50435300	-1.47620300
H	4.37463200	-1.87294000	-0.51379500
H	2.75912500	-1.97081200	-1.26739500
H	0.90182200	2.33417400	1.75281300
H	2.62388500	1.97543700	2.07351300
H	2.17399300	3.42571300	1.13880000
H	-0.55037100	-1.87828500	1.18089700
H	-0.39445600	-2.09809800	-0.57364000
H	1.00936800	-2.39368100	0.47727800
H	-2.27106300	0.72534400	-2.61651000
H	-2.29972500	-1.00393800	-2.11361500
H	-3.76421400	0.02504300	-1.88123700
H	-2.37324800	2.33901500	0.79959600

29

Energy = -901.71024690 a.u. #Cluster: 5

P	-2.06005300	0.27510700	0.25018500
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F	-2.71560800	-1.18048700	0.40826400
O	-2.64495800	1.10261800	1.47404000
N	1.74090600	0.03838400	0.14589100
N	-0.50017600	0.29948600	0.43076600
C	2.94467100	-0.66536500	-0.32220100
C	1.95506100	1.34329800	0.79356700
C	0.51032700	-0.43595100	-0.01437900
C	3.58841000	-1.51796000	0.76728100
C	1.83729300	2.50287400	-0.19092600
C	0.30497200	-1.76309200	-0.69704600
C	-2.70482100	0.86032600	-1.30387900
H	3.64582300	0.10781700	-0.66897500
H	2.69281700	-1.27149600	-1.20062100
H	1.22020800	1.44603900	1.60231000
H	2.95602700	1.31596800	1.24650800
H	4.50512900	-1.98635300	0.37694700
H	3.86214600	-0.90688900	1.64147500
H	2.90808800	-2.31591900	1.10357500
H	2.56301500	2.40068600	-1.01314100
H	0.82450900	2.54843000	-0.61857000
H	2.03798500	3.45301600	0.32811900
H	1.02700800	-2.51703900	-0.35934800

H	-0.70721200	-2.13350100	-0.50474900
H	0.43080000	-1.63303500	-1.78474600
H	-2.36167900	1.89416900	-1.45338200
H	-2.31625900	0.21568000	-2.10626500
H	-3.80398300	0.81904700	-1.28410700
H	-3.61115100	1.23744800	1.45560700

29

Energy = -901.70982580 a.u. #Cluster: 6

P	-2.11324700	0.19897700	0.09403300
F	-2.68449200	-1.30052000	0.12067100
O	-2.86240800	0.91936000	1.29524300
N	1.70550700	0.06436300	0.13705600
N	-0.55421100	0.27321600	0.28154500
C	2.95217100	-0.62121000	-0.23617500
C	1.85018700	1.38407800	0.77389900
C	0.49904900	-0.44429100	-0.08802900
C	3.54236800	-1.43196000	0.91398100
C	1.75992800	2.52524500	-0.23438700
C	0.37328900	-1.78799100	-0.75693300
C	-2.79690700	0.89407000	-1.39105700
H	3.65674100	0.16009100	-0.55682300
H	2.76998400	-1.25440700	-1.11253800

H	1.06962900	1.48066700	1.53944800
H	2.82431200	1.38909400	1.28257800
H	2.86173300	-2.24077100	1.22217800
H	4.49544600	-1.88317400	0.59778000
H	3.73888300	-0.79408900	1.78962100
H	0.77177500	2.54021800	-0.71801600
H	1.90923500	3.48754300	0.27952900
H	2.53245600	2.42891500	-1.01355200
H	1.04613800	-2.52935400	-0.30623700
H	-0.65488000	-2.15531500	-0.68510200
H	0.63944000	-1.69112900	-1.82217000
H	-2.48647000	1.94633700	-1.46122000
H	-2.40449600	0.32925600	-2.24921100
H	-3.89331000	0.81847300	-1.35346900
H	-2.41855700	0.82761300	2.15955500

29

Energy = -901.70974720 a.u. #Cluster: 7

P	-2.08070000	0.50498000	-0.36581500
F	-2.85744100	-0.68771100	0.37310500
O	-2.78433700	1.82016600	0.18148800
N	1.66914600	0.07535000	0.24941000
N	-0.53784300	0.52664800	-0.06623400

C	2.80953800	-0.79337600	0.57831000
C	1.98353700	1.48804600	-0.02167400
C	0.41302100	-0.35670600	0.20623600
C	3.48764900	-1.36638000	-0.66314400
C	1.87193500	2.35321100	1.22993200
C	0.12329400	-1.80739900	0.48999600
C	-2.57574000	0.35907700	-2.06520800
H	2.47466400	-1.59372400	1.24864600
H	3.51697000	-0.17889400	1.15434500
H	3.00508900	1.51678800	-0.42599900
H	1.30230500	1.84571000	-0.80365800
H	3.83807700	-0.56385500	-1.33054300
H	4.35927100	-1.96862800	-0.36419100
H	2.79933000	-2.01143500	-1.23073700
H	0.84043800	2.35374600	1.61314000
H	2.54242600	1.99006500	2.02475200
H	2.15356800	3.39057000	0.99135300
H	0.32873200	-2.02755500	1.54981000
H	-0.92644200	-2.04004900	0.28846900
H	0.76010300	-2.46347800	-0.11917800
H	-3.67148600	0.42446800	-2.13131900
H	-2.10866900	1.17460400	-2.63560200

H	-2.22757200	-0.61217200	-2.44582100
H	-2.37956800	2.18123800	0.99233200

29

Energy = -901.70962520 a.u. #Cluster: 8

P	-2.05551200	0.30794200	-0.42565300
F	-2.74749500	-1.13543500	-0.29630900
O	-2.72591600	1.14935500	0.75176600
N	1.70390200	0.02128800	0.15978800
N	-0.48882300	0.26806700	-0.38637900
C	2.86220300	-0.71073500	0.69312600
C	1.95963200	1.38336000	-0.33913900
C	0.47476200	-0.48066600	0.13356200
C	3.64442600	-1.44123300	-0.39476100
C	1.65777700	2.44536600	0.71400300
C	0.22303000	-1.86104400	0.68038900
C	-2.71445100	0.98052800	-1.92808300
H	2.52490100	-1.40795000	1.46898400
H	3.50082600	0.03086600	1.19497400
H	3.01512400	1.42073300	-0.64185400
H	1.34550800	1.53988900	-1.23525700
H	3.02323900	-2.20638500	-0.88553700
H	4.00409800	-0.74139000	-1.16499200

H	4.51968000	-1.93917000	0.05022800
H	0.59220900	2.42936700	0.98815200
H	2.25840600	2.28312000	1.62291900
H	1.89852900	3.44349400	0.31638600
H	0.34619300	-1.85220900	1.77536600
H	-0.79518900	-2.18390000	0.44474100
H	0.93398900	-2.58955600	0.26742100
H	-2.39161700	0.34505700	-2.76516500
H	-3.81165600	0.99613700	-1.86164400
H	-2.32502000	1.99999600	-2.05917900
H	-2.30346300	1.03841300	1.62434600

29

Energy = -901.70958200 a.u. #Cluster: 9

P	-2.07113000	0.23858200	-0.37636500
F	-2.70155600	-1.23847200	-0.36226500
O	-2.76395900	0.95445800	0.86901200
N	1.70836700	0.03837500	0.12397700
N	-0.50153700	0.25736400	-0.36444700
C	2.88371200	-0.66447500	0.66001500
C	1.94377900	1.38085000	-0.43437400
C	0.48255200	-0.47129400	0.14860400
C	3.64740000	-1.43501200	-0.41320400

C	1.68417800	2.48244100	0.58871600
C	0.25517700	-1.83401000	0.74791600
C	-2.77182400	1.00101900	-1.81546000
H	2.56832600	-1.32954000	1.47250300
H	3.52817300	0.10140300	1.11589900
H	2.98680400	1.40531700	-0.77911400
H	1.29466400	1.50398600	-1.31068400
H	3.02159300	-2.22387500	-0.85846400
H	3.98546300	-0.76552800	-1.21938300
H	4.53546500	-1.90837400	0.03311900
H	1.90626900	3.46423500	0.14251500
H	0.63122500	2.47699200	0.90815600
H	2.32292700	2.35647400	1.47717200
H	-0.75635200	-2.18413600	0.52267400
H	0.97985600	-2.56711100	0.36943400
H	0.37223300	-1.77573000	1.84229900
H	-3.86812600	0.96978500	-1.74020800
H	-2.42193100	2.04179300	-1.86766200
H	-2.43435200	0.44722000	-2.70325500
H	-2.31810000	0.81057100	1.72507100

29

Energy = -901.70898030 a.u. #Cluster: 10

P	-2.08963200	0.29890000	0.04800600
F	-2.76798400	-1.13919900	0.25275200
O	-2.97503400	1.27949900	0.92854500
N	1.65161000	-0.02984000	0.71190400
N	-0.58438800	0.34450000	0.50778600
C	2.87299700	-0.85479200	0.65609000
C	1.81006200	1.39846500	1.05415500
C	0.44307600	-0.49411900	0.41156800
C	3.49090200	-0.93707100	-0.73680100
C	1.83758000	2.31224100	-0.16839600
C	0.23252000	-1.91646900	-0.02973500
C	-2.44701900	0.70573900	-1.64463900
H	2.64410800	-1.85582200	1.04289500
H	3.58277200	-0.40451000	1.36260300
H	0.97840700	1.67562400	1.71547600
H	2.74326800	1.48638600	1.62551600
H	2.79160000	-1.38664100	-1.45862600
H	3.77934500	0.05764000	-1.10747200
H	4.39517200	-1.56416600	-0.69851700
H	2.68374600	2.07472300	-0.82978700
H	0.90386200	2.22512200	-0.74297600
H	1.94265100	3.35785200	0.16087900

H	-0.58316400	-2.35584000	0.56045300
H	-0.09227200	-1.89945300	-1.08318300
H	1.11869000	-2.55088000	0.04885500
H	-1.95415100	-0.03608600	-2.28991700
H	-3.53527900	0.68326500	-1.80109700
H	-2.04941200	1.70888400	-1.85479600
H	-2.69473800	1.34935200	1.86065800

A232

29

Energy = -976.46299850 a.u. #Cluster: 1

P	-6.77049800	-5.90200700	-3.36729200
O	-7.11296300	-6.17035900	-4.79053300
C	-5.91958700	-8.16387700	-2.34154100
F	-8.12772500	-5.80759700	-2.48016200
N	-5.77566700	-6.86502800	-2.52106100
C	-7.11831700	-8.90619600	-2.88206800
H	-7.13521300	-9.97718600	-2.66488900
H	-8.02205200	-8.44754200	-2.45248500
H	-7.16414200	-8.75232700	-3.97024700
C	-4.98140500	-10.26973200	-1.41311500
H	-3.92870700	-10.57902800	-1.33872500

H	-5.38641500	-10.78434300	-2.29355800
C	-5.73975600	-10.66437500	-0.14923600
H	-5.32265200	-10.15690400	0.73496800
H	-6.80532300	-10.39736400	-0.22779800
H	-5.66615100	-11.75132700	0.01216700
C	-3.85048900	-8.07641100	-1.06602200
H	-3.52678300	-8.62725100	-0.17083200
H	-4.21951000	-7.09537200	-0.74131100
C	-2.69139700	-7.91192600	-2.04467300
H	-2.32030900	-8.89032500	-2.38976000
H	-3.00694800	-7.32741400	-2.92174100
H	-1.85768200	-7.38294900	-1.55633500
N	-4.97797000	-8.81953600	-1.64696200
O	-6.18898800	-4.41689800	-3.18987400
C	-5.77077700	-3.90893200	-1.91739600
H	-6.59364800	-3.96124800	-1.18710900
H	-4.90907500	-4.47814000	-1.53788500
H	-5.48595000	-2.85970100	-2.07077600

29

Energy = -976.46242210 a.u. #Cluster: 2

P	-5.60817000	-5.77588900	-3.53117600
O	-4.66119400	-4.89067300	-4.25949300

C	-5.59285900	-8.01429800	-2.11242400
F	-6.72795100	-6.32061700	-4.57729000
N	-4.98038100	-7.05656700	-2.77978900
C	-7.09435300	-8.10962900	-1.97005300
H	-7.44767200	-9.14747500	-1.98137100
H	-7.39970600	-7.65194000	-1.01504500
H	-7.58554800	-7.56564200	-2.78265400
C	-5.37990000	-10.01344300	-0.66400000
H	-6.31447100	-9.67496000	-0.20021900
H	-4.66598500	-10.16212200	0.16019600
C	-5.58948400	-11.32188700	-1.42197100
H	-6.32909700	-11.20109500	-2.22891600
H	-4.64801700	-11.67625700	-1.87031800
H	-5.95341400	-12.10011100	-0.73302800
C	-3.37298900	-8.89095100	-1.62620000
H	-3.12673200	-8.54066800	-2.63656200
H	-3.00401000	-9.92219800	-1.52628100
C	-2.72993600	-7.98552800	-0.57938500
H	-3.07028300	-6.94711300	-0.70690400
H	-2.98091200	-8.31499000	0.44158500
H	-1.63373600	-8.00719900	-0.68507500
N	-4.83605100	-8.94145700	-1.50653600

O	-6.55241600	-5.02501600	-2.45480300
C	-7.15412600	-3.76454400	-2.78080900
H	-7.57135700	-3.35543400	-1.85140200
H	-6.40347400	-3.07084900	-3.18900400
H	-7.96187500	-3.90273700	-3.51732000

29

Energy = -976.46205250 a.u. #Cluster: 3

P	-7.09718400	-5.75386100	-2.79345900
O	-8.47132300	-6.07714000	-3.27066300
C	-6.20322500	-8.09769700	-1.88990400
F	-7.16985300	-4.68336000	-1.58423900
N	-6.03929900	-6.83680900	-2.22497500
C	-7.52066000	-8.83000700	-1.99056600
H	-7.40681600	-9.78696700	-2.51863100
H	-7.90439800	-9.04813000	-0.98095100
H	-8.24933600	-8.20639500	-2.51783700
C	-5.18481700	-10.16970600	-0.99234200
H	-6.19242900	-10.40922600	-0.63164300
H	-4.51651000	-10.26342700	-0.12257900
C	-4.75984500	-11.14122700	-2.09141200
H	-3.73951200	-10.92071000	-2.44278300
H	-4.77324300	-12.17347400	-1.70764200

H	-5.44047200	-11.08457800	-2.95548100
C	-3.84040200	-8.09018800	-1.30012200
H	-3.71111300	-7.43638100	-2.17291900
H	-3.06293000	-8.86640700	-1.34528800
C	-3.71896900	-7.28352000	-0.01008300
H	-2.72015900	-6.82348400	0.05577700
H	-4.47237600	-6.48214600	0.01488400
H	-3.85894300	-7.92639500	0.87379700
N	-5.13754800	-8.76760100	-1.41994000
O	-6.31045600	-4.89392100	-3.90198600
C	-4.97418400	-4.42167300	-3.69670300
H	-4.72468100	-3.78572800	-4.55644200
H	-4.90750100	-3.82743400	-2.77175100
H	-4.26791600	-5.26370200	-3.64036500

29

Energy = -976.46195980 a.u. #Cluster: 4

P	-7.11565200	-5.71889300	-2.65945800
O	-8.52167700	-6.01139600	-3.05702400
C	-6.20560200	-8.08349200	-1.83428600
F	-7.09628100	-4.69483100	-1.40825200
N	-6.03478100	-6.83434100	-2.20846100
C	-7.55151600	-8.76724700	-1.78131900

H	-7.84610600	-8.92902200	-0.73172400
H	-8.30353900	-8.13567700	-2.26474700
H	-7.52409200	-9.74780000	-2.27617800
C	-5.17126700	-10.17417500	-1.00060700
H	-6.13964100	-10.36383000	-0.52176500
H	-4.41281300	-10.27542300	-0.20912500
C	-4.91154900	-11.18798200	-2.11276700
H	-3.93092800	-11.01766600	-2.58453400
H	-4.91916300	-12.20918800	-1.70030900
H	-5.68441300	-11.12516900	-2.89464700
C	-3.79423400	-8.15506800	-1.50272600
H	-3.73869300	-7.51765300	-2.39517600
H	-3.05472400	-8.96030000	-1.62048700
C	-3.50104800	-7.33761600	-0.24761000
H	-2.48496400	-6.91529500	-0.30045500
H	-4.21680700	-6.50748300	-0.15194500
H	-3.56507300	-7.96336800	0.65706200
N	-5.11989000	-8.78502900	-1.46829600
O	-6.39336000	-4.82570100	-3.78449000
C	-5.04240800	-4.37080800	-3.64906200
H	-4.83553900	-3.72328100	-4.51144200
H	-4.91680200	-3.79279000	-2.71991800

H	-4.34353900	-5.22076600	-3.64650000
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29

Energy = -976.46165660 a.u. #Cluster: 5

P	-7.24748500	-5.87982600	-2.82973600
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O	-8.15385100	-6.22345000	-3.96149000
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C	-5.98501200	-8.18200200	-2.36244300
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F	-8.11362400	-5.39406700	-1.55547800
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N	-6.19734100	-6.90266100	-2.14439700
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C	-6.71252900	-8.98890600	-3.41223900
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H	-7.49183900	-8.37623000	-3.87518100
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H	-6.00619400	-9.31249300	-4.19292700
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H	-7.16326100	-9.89168300	-2.97608800
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C	-4.71628100	-10.22500300	-1.77032100
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H	-3.63717500	-10.31961300	-1.57551500
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H	-4.86665600	-10.52866700	-2.81348600
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C	-5.50254000	-11.13213900	-0.82573300
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H	-5.17910000	-12.17731800	-0.95232600
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H	-5.33754200	-10.84881200	0.22576300
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H	-6.58334400	-11.07840400	-1.02989800
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C	-4.31676700	-8.06734500	-0.58722700
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H	-4.05932600	-8.78154600	0.20887100
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H	-4.98955100	-7.31367600	-0.15944300
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C	-3.05812800	-7.40456200	-1.14093200
H	-2.37254100	-8.15128700	-1.57253700
H	-3.31741600	-6.67631500	-1.92420200
H	-2.52372400	-6.87387400	-0.33709900
N	-5.05681700	-8.80659600	-1.61717700
O	-6.43083900	-4.53424200	-3.16231100
C	-5.51553800	-3.94308900	-2.23280500
H	-5.18887900	-2.98971200	-2.66902300
H	-6.00867900	-3.75218300	-1.26665100
H	-4.64412100	-4.59559200	-2.07421800

29

Energy = -976.46164050 a.u. #Cluster: 6

P	-7.28892500	-5.85348300	-2.69703500
O	-8.34534100	-6.21518500	-3.68369200
C	-6.03565800	-8.17313800	-2.29036300
F	-7.96490100	-5.25860700	-1.35609800
N	-6.20477600	-6.88574700	-2.08280000
C	-6.85441000	-8.98212400	-3.26879300
H	-7.28270400	-9.87303600	-2.78805500
H	-7.65996000	-8.36395100	-3.67650200
H	-6.21586300	-9.32531100	-4.09821100
C	-4.76414900	-10.23075900	-1.75760100

H	-3.67517300	-10.34200200	-1.64262800
H	-4.99768600	-10.54702200	-2.78151700
C	-5.49270200	-11.10867500	-0.74205500
H	-6.58463900	-11.03832600	-0.86614500
H	-5.19757600	-12.16141900	-0.87494200
H	-5.24478300	-10.81235200	0.28937800
C	-4.24430100	-8.06510300	-0.63857100
H	-3.95100900	-8.77151800	0.15219200
H	-4.87028500	-7.28855700	-0.18186400
C	-3.00947800	-7.44218000	-1.28439300
H	-2.41202500	-6.91204000	-0.52586900
H	-2.37034600	-8.21190500	-1.74583100
H	-3.30084700	-6.72005500	-2.06200400
N	-5.06799100	-8.80423000	-1.60291500
O	-6.46971700	-4.56567100	-3.20674400
C	-5.41936200	-3.97250200	-2.43472300
H	-5.12159300	-3.05217100	-2.95447700
H	-5.77246800	-3.72193000	-1.42201500
H	-4.55743400	-4.65229400	-2.36197700

29

Energy = -976.46163340 a.u. #Cluster: 7

P	-7.23817800	-5.84484000	-2.77882700
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O	-8.30064100	-6.22093400	-3.75353800
C	-6.05546900	-8.17857100	-2.26296200
F	-7.90332900	-5.18073000	-1.46501600
N	-6.17756500	-6.87666300	-2.12397300
C	-6.92747000	-9.01320100	-3.17174100
H	-6.32511800	-9.41339500	-4.00274500
H	-7.36151700	-9.86722400	-2.63300400
H	-7.72951500	-8.39427900	-3.58513400
C	-4.83419200	-10.24457900	-1.64961300
H	-3.74550600	-10.38451500	-1.56653000
H	-5.11500600	-10.61105000	-2.64439300
C	-5.55164800	-11.03814600	-0.55955300
H	-6.64469600	-10.93859600	-0.64965100
H	-5.29434500	-12.10600500	-0.64015800
H	-5.25698100	-10.69100900	0.44337200
C	-4.21365600	-8.03847700	-0.67063200
H	-3.91122200	-8.71181300	0.14514200
H	-4.80317900	-7.22319400	-0.23297400
C	-2.98573400	-7.48293500	-1.38735300
H	-2.34853700	-6.93374100	-0.67615300
H	-2.38350700	-8.29190700	-1.83103300
H	-3.28362800	-6.79115400	-2.18965000

N	-5.08861400	-8.80239700	-1.56777400
O	-6.38799600	-4.59845100	-3.33828300
C	-5.33045800	-3.99315800	-2.58580200
H	-5.69116500	-3.66957500	-1.59665800
H	-4.49267500	-4.69424400	-2.45619900
H	-4.99455400	-3.11650900	-3.15541600

29

Energy = -976.46158550 a.u. #Cluster: 8

P	-7.17837700	-5.84440500	-2.88579600
O	-8.22316500	-6.23536600	-3.87368800
C	-6.08581300	-8.18454000	-2.22514100
F	-7.86308600	-5.11927400	-1.61485500
N	-6.14904000	-6.87185900	-2.17719900
C	-7.04231200	-9.04577600	-3.01656800
H	-7.49430500	-9.81970400	-2.38010900
H	-7.82827600	-8.42251400	-3.45342700
H	-6.50366800	-9.55603300	-3.83058700
C	-4.91903400	-10.25152800	-1.51502800
H	-3.83410300	-10.43620800	-1.48826700
H	-5.27986400	-10.68314100	-2.45635200
C	-5.59558700	-10.92154900	-0.32075100
H	-6.68719800	-10.77882500	-0.34980900

H	-5.38859200	-12.00325800	-0.32992500
H	-5.22090400	-10.51039300	0.62986900
C	-4.14567400	-8.00724700	-0.75791900
H	-3.81323600	-8.63252000	0.08382300
H	-4.67276600	-7.13876600	-0.34329000
C	-2.95059500	-7.55676300	-1.59380400
H	-3.27726500	-6.91055100	-2.42247700
H	-2.24462000	-6.98707100	-0.96890700
H	-2.41266800	-8.42028400	-2.01684200
N	-5.10685700	-8.79709000	-1.53698800
O	-6.28867400	-4.63709400	-3.46848400
C	-5.24376400	-4.02102900	-2.70705500
H	-4.84865700	-3.19657500	-3.31524700
H	-5.63708200	-3.62025200	-1.75945800
H	-4.44091700	-4.74167500	-2.49196800

29

Energy = -976.46063780 a.u. #Cluster: 9

P	-7.07928900	-5.67294200	-2.46572000
O	-8.52247000	-5.89843500	-2.75982700
C	-6.09907500	-8.14858000	-2.27690300
F	-6.92033300	-4.89006200	-1.05893100
N	-5.97329400	-6.84129400	-2.31340700

C	-7.40006300	-8.87239100	-2.53373000
H	-7.62522700	-9.58213800	-1.72495600
H	-8.21384500	-8.14577000	-2.62140400
H	-7.33515100	-9.44448400	-3.47294700
C	-4.99628800	-10.34248000	-1.97403400
H	-4.06036700	-10.67811800	-2.44712200
H	-5.81197900	-10.72123400	-2.60038400
C	-5.10333100	-10.91447800	-0.56162900
H	-4.24573000	-10.61577200	0.06017100
H	-6.02509700	-10.57131300	-0.06592400
H	-5.12316900	-12.01477200	-0.60656800
C	-3.73747900	-8.18863600	-1.70116900
H	-3.57846300	-7.40635000	-2.45786200
H	-2.93451500	-8.93068900	-1.81327800
C	-3.69988500	-7.57219300	-0.30354800
H	-2.72440900	-7.08651500	-0.14082700
H	-4.48538500	-6.81099000	-0.19419300
H	-3.83651600	-8.33642600	0.47638700
N	-4.99898600	-8.87647000	-2.01523000
O	-6.46251700	-4.58846900	-3.48032900
C	-5.10402800	-4.14323500	-3.39278700
H	-4.90052800	-3.70871700	-2.40140100

H	-4.40832100	-4.97608700	-3.57559100
H	-4.97036300	-3.37225500	-4.16310400

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Energy = -976.46057660 a.u. #Cluster: 10

P	-7.08852200	-5.80564600	-2.94235900
O	-8.09040100	-6.24382100	-3.95427400
C	-6.31236800	-8.09616400	-1.82847900
F	-7.80145100	-4.90899000	-1.80157600
N	-6.16225400	-6.81421200	-2.07927700
C	-7.49703300	-8.90809200	-2.29773500
H	-7.17838300	-9.85273000	-2.75943100
H	-8.14632400	-9.15357900	-1.44187900
H	-8.07385000	-8.32777700	-3.02510500
C	-5.43706800	-10.12403800	-0.71416100
H	-6.48824500	-10.43355400	-0.68272200
H	-5.06217700	-10.19674600	0.31832400
C	-4.63753900	-11.05275200	-1.62616700
H	-4.98885900	-10.98434700	-2.66786400
H	-3.56457200	-10.80932300	-1.60770000
H	-4.75539900	-12.09487900	-1.28962900
C	-4.17595400	-7.95416300	-0.67525100
H	-3.72914200	-8.50352100	0.16552400

H	-4.51179600	-6.97744400	-0.29932200
C	-3.14668500	-7.75448200	-1.78664000
H	-2.29726700	-7.16711100	-1.40273800
H	-2.75920300	-8.71586000	-2.15559500
H	-3.58725900	-7.20626000	-2.63186300
N	-5.36448800	-8.70968900	-1.09720600
O	-6.08664000	-4.72421400	-3.58415800
C	-5.05711500	-4.08734900	-2.81819400
H	-4.30563900	-4.82040500	-2.48984200
H	-4.58689900	-3.34218700	-3.47342100
H	-5.48357200	-3.58195900	-1.93750900

A232-N₁H

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Energy = -976.89714020 a.u. #Cluster: 1

P	-0.70692400	-2.42291900	-0.86433100
F	0.13153900	-3.77429500	-0.90009600
O	-1.78504800	-2.65539700	0.26431900
O	-1.12340900	-1.99840500	-2.21564300
N	2.22564200	-0.12741100	0.41119100
N	0.33969300	-1.40077900	0.00936900
C	3.57672500	0.36758100	0.06074200

C	1.72212400	0.30474800	1.73254900
C	1.54060600	-0.91412600	-0.38743200
C	3.53831500	1.73296600	-0.61411100
C	2.08705700	-0.67188500	2.84732300
C	2.05915700	-1.33031600	-1.72763400
C	-3.17131400	-2.97224400	-0.02126400
H	4.08172100	-0.38022600	-0.56103700
H	4.13570100	0.41665600	1.00537800
H	2.16722600	1.29053100	1.92139700
H	0.63689900	0.47228300	1.66859500
H	4.56826900	2.07412200	-0.79844600
H	3.00910700	1.69043400	-1.57844100
H	3.03919400	2.47877500	0.02340800
H	3.17780600	-0.80270900	2.91308300
H	1.72904300	-0.27146000	3.80760700
H	1.62705100	-1.66009000	2.69309400
H	1.22280600	-1.50361100	-2.41589400
H	2.71658400	-0.57421900	-2.16610200
H	2.62265100	-2.27131800	-1.61325900
H	-3.26912300	-4.05444000	-0.18225100
H	-3.51126200	-2.42064500	-0.90814800
H	-3.74226200	-2.66433400	0.86204700

H	-0.00014600	-1.18358500	0.94526800
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Energy = -976.89710670 a.u. #Cluster: 2

P	-0.84372400	-2.20649200	-1.29643400
F	-0.17894500	-3.63624600	-1.08254400
O	-2.17924600	-2.26033700	-0.46589600
O	-0.95969800	-1.82690500	-2.71504800
N	2.09019500	-0.10914300	0.29572200
N	0.16268900	-1.21407600	-0.33449300
C	3.53024100	0.20706700	0.16025900
C	1.41480300	0.50035600	1.46130200
C	1.46471700	-0.90073400	-0.54577900
C	3.76818200	1.49316000	-0.62109600
C	1.40245000	-0.42203500	2.67719400
C	2.15464500	-1.51139400	-1.72390600
C	-2.41718900	-3.07416500	0.71203800
H	4.04233300	-0.64731800	-0.29653400
H	3.91891100	0.29412100	1.18435400
H	1.95963300	1.42689900	1.68407100
H	0.40117400	0.81156400	1.16806400
H	3.40745500	1.40497700	-1.65738800
H	3.25890400	2.34652900	-0.14758700

H	4.84721600	1.70809100	-0.64610800
H	0.92810700	0.10028600	3.52136600
H	0.83813900	-1.34698500	2.48355900
H	2.42741900	-0.69528400	2.97017000
H	1.43592700	-1.67496200	-2.53596500
H	2.96304600	-0.87732700	-2.09905400
H	2.57563000	-2.48533400	-1.42304400
H	-1.73456900	-2.77724600	1.52136100
H	-2.28045300	-4.13472300	0.46420900
H	-3.45495000	-2.88012500	1.00498200
H	-0.29761400	-0.83853600	0.49351000

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Energy = -976.89688930 a.u. #Cluster: 3

P	-1.03638500	-2.07415700	-1.04681700
F	-0.28316100	-3.22158900	-1.85427100
O	-1.87528600	-2.85510300	0.03300500
O	-1.76001100	-1.12987600	-1.91358700
N	2.01266900	-0.00845200	0.34492100
N	0.22520600	-1.39601700	-0.11718500
C	3.01917400	1.01743900	-0.01510300
C	2.01320800	-0.41223900	1.76775400
C	1.16620200	-0.50836400	-0.52670700

C	4.35381100	0.40355700	-0.41837300
C	1.04191300	0.41068700	2.60916500
C	1.18266700	-0.12788000	-1.97315300
C	-1.59101500	-4.18745400	0.53214000
H	3.13344000	1.65120500	0.87484500
H	2.61048600	1.65998400	-0.80306100
H	1.80864500	-1.49057800	1.83630800
H	3.04297200	-0.28044600	2.12427900
H	4.76116300	-0.22632400	0.38724700
H	4.25225900	-0.21296700	-1.32467900
H	5.07586400	1.20824500	-0.62399100
H	0.00027300	0.27583000	2.28028300
H	1.11566000	0.09226500	3.65974300
H	1.28788300	1.48189300	2.55379200
H	2.11268400	0.36234700	-2.26775500
H	1.05798800	-1.02874300	-2.58937200
H	0.33223300	0.54069300	-2.17713900
H	-1.66067700	-4.91334400	-0.28846100
H	-2.35542400	-4.39267900	1.28988600
H	-0.59075500	-4.21674200	0.98760900
H	0.19174000	-1.64750700	0.86996100

Energy = -976.89684590 a.u. #Cluster: 4

P	-1.54160900	-1.36778600	0.14138000
F	-1.95549500	-0.53117700	-1.15113900
O	-1.13543700	-2.77043800	-0.46857600
O	-2.52503800	-1.26785000	1.23390200
N	2.19720100	-0.17208500	0.50273000
N	-0.04200900	-0.71332800	0.58192600
C	3.51916700	-0.11132900	-0.16211900
C	2.18174500	0.27873700	1.91148500
C	1.12569000	-0.62656300	-0.10646800
C	3.78845500	1.24788000	-0.79627500
C	2.38870100	-0.87010000	2.89387600
C	1.16218100	-1.07273200	-1.53347100
C	-2.08402200	-3.62550600	-1.15444200
H	3.58809300	-0.92316200	-0.89466500
H	4.25965100	-0.33156200	0.61926400
H	2.98630800	1.01940200	2.00623900
H	1.24797400	0.82680200	2.10626700
H	3.06587900	1.46586600	-1.59740100
H	3.73260500	2.05435400	-0.04924800
H	4.79996500	1.25075000	-1.22967000
H	1.57791400	-1.61174300	2.83329100

H	3.34346200	-1.38205300	2.70025400
H	2.41265700	-0.46842400	3.91786100
H	1.91076900	-0.51851700	-2.10704500
H	1.40942000	-2.14612400	-1.56715000
H	0.18671400	-0.92794000	-2.00834100
H	-2.39067900	-3.15543900	-2.09948100
H	-2.95846500	-3.80623900	-0.51375600
H	-1.55726400	-4.56595000	-1.35113800
H	-0.04910400	-0.40406200	1.55319100

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Energy = -976.89652430 a.u. #Cluster: 5

P	-0.69197300	-2.40405100	-0.86468200
F	0.19643400	-3.36508700	-1.77258700
O	-1.21598000	-3.33692600	0.29604500
O	-1.63560200	-1.60817200	-1.67274900
N	2.17534200	-0.01974400	0.37388400
N	0.49585600	-1.56294900	0.01763100
C	3.07701000	1.07906300	-0.04600500
C	2.26820000	-0.39357700	1.80198600
C	1.33848900	-0.60863800	-0.44977600
C	4.43437900	0.56902700	-0.51252400
C	1.27710600	0.37558300	2.67066500

C	1.25887800	-0.27597500	-1.90528400
C	-2.55131400	-3.90280900	0.30732200
H	3.18405600	1.73037500	0.83195200
H	2.57799500	1.67678600	-0.81714800
H	2.14359200	-1.48205100	1.89790000
H	3.30070900	-0.18202800	2.10879800
H	4.92997100	-0.02024000	0.27425900
H	4.33668700	-0.06102100	-1.40987400
H	5.07927400	1.42640300	-0.75770200
H	0.23504800	0.15533600	2.39275800
H	1.42160000	0.08974100	3.72326100
H	1.43875800	1.46053900	2.58145800
H	1.31614700	-1.20865800	-2.48537800
H	0.28494700	0.19184000	-2.11440400
H	2.06243400	0.38401800	-2.23628300
H	-3.27219400	-3.18125900	-0.10024000
H	-2.78122200	-4.12086900	1.35645300
H	-2.55765200	-4.82725700	-0.28609000
H	0.51845300	-1.80371600	1.00763500

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Energy = -976.89602130 a.u. #Cluster: 6

P	-0.06673200	-3.30853500	-0.92803300
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F	-0.19099100	-4.39776700	0.21784900
O	-1.51307000	-2.68499500	-1.04667600
O	0.48693300	-3.79016200	-2.20449300
N	2.05847600	-0.25259100	0.36435100
N	0.88879000	-2.20593400	-0.03307400
C	2.52157200	1.10239200	-0.01283600
C	2.41140100	-0.67971200	1.73509800
C	1.35354600	-1.00279400	-0.45121400
C	3.93249900	1.09367600	-0.58757600
C	1.32997800	-0.32579200	2.75279300
C	0.99571600	-0.55717100	-1.83356400
C	-2.26588500	-2.16941400	0.07712900
H	2.47728200	1.70380800	0.90568300
H	1.80129500	1.54453900	-0.71031300
H	2.64058100	-1.75572000	1.73093800
H	3.35457400	-0.17411100	1.97998200
H	4.24029800	2.12733000	-0.80637800
H	4.65146200	0.66531200	0.12741800
H	3.98043400	0.51161500	-1.52056300
H	1.14246400	0.75850500	2.76240500
H	0.38104500	-0.84084700	2.53780800
H	1.66605400	-0.62778700	3.75591800

H	1.75295100	0.10661300	-2.26076900
H	0.88739400	-1.42763700	-2.49185900
H	0.03224200	-0.02195000	-1.79524200
H	-3.19233500	-1.75995200	-0.34080500
H	-1.69716100	-1.37525000	0.58259800
H	-2.49171600	-2.98311700	0.78008100
H	1.07633300	-2.49887000	0.92462900

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Energy = -976.89598100 a.u. #Cluster: 7

P	-0.42780400	-3.24527200	-0.51166900
F	-1.04790000	-3.83854500	0.82283700
O	-1.63182500	-2.49366300	-1.20394600
O	0.25783800	-4.21489100	-1.38107800
N	2.08863900	-0.35724400	0.43148300
N	0.55246800	-2.06866400	0.25276400
C	3.11869100	0.54981500	-0.11924500
C	1.78611000	-0.17508800	1.86637200
C	1.48349800	-1.25987900	-0.30867100
C	2.53654200	1.89170700	-0.54924400
C	2.59454800	-1.11463800	2.75687200
C	1.81046000	-1.41086400	-1.76051600
C	-2.43812300	-1.48280300	-0.55434500

H	3.62972000	0.05232400	-0.95066400
H	3.86515900	0.68486500	0.67608900
H	2.01390700	0.87267800	2.10103900
H	0.70270000	-0.28841600	2.02161700
H	2.03475600	2.39775600	0.28973600
H	3.35134800	2.54155200	-0.90275800
H	1.81060800	1.77104300	-1.36767400
H	2.35497100	-0.90919100	3.81089200
H	2.36481500	-2.17115100	2.55024200
H	3.67400200	-0.95848300	2.60987100
H	1.67670200	-0.45256600	-2.28046500
H	2.86294200	-1.71540000	-1.86595100
H	1.19097900	-2.17384800	-2.23992700
H	-1.80638700	-0.63898600	-0.24098100
H	-2.95502800	-1.91619900	0.31323500
H	-3.16672300	-1.14909000	-1.30174600
H	0.35781700	-1.95317700	1.24711500

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Energy = -976.89595660 a.u. #Cluster: 8

P	-0.35289600	-3.25271200	-0.52589800
F	-0.97462900	-3.89603800	0.78441700
O	-1.56907400	-2.51878900	-1.22036600

O	0.37600400	-4.17509500	-1.41038000
N	2.09292400	-0.32644300	0.44317200
N	0.58130300	-2.06402600	0.27472400
C	3.08152000	0.62808400	-0.10930400
C	1.90140000	-0.25068700	1.90756800
C	1.43569400	-1.18343300	-0.30422800
C	2.44885700	1.96386500	-0.47843300
C	2.80023700	-1.22307100	2.66588400
C	1.58230500	-1.24677700	-1.79073300
C	-2.43655300	-1.57716800	-0.54421400
H	3.58849500	0.16553200	-0.96361600
H	3.84303300	0.75844100	0.67165400
H	2.12187100	0.78584700	2.19379500
H	0.83701700	-0.40624200	2.13849700
H	1.71064500	1.84640800	-1.28668900
H	1.94605900	2.41832000	0.38906200
H	3.23347600	2.65481900	-0.82202800
H	3.86063900	-1.02908400	2.44419300
H	2.64280700	-1.09137400	3.74681300
H	2.57726000	-2.27002500	2.40952600
H	0.58213200	-1.25805200	-2.24838200
H	2.13769300	-0.40139600	-2.20074900

H	2.08613400	-2.18742500	-2.06073300
H	-3.15192900	-1.22914200	-1.29768100
H	-1.84924600	-0.73011600	-0.16131900
H	-2.96391600	-2.07965900	0.27839100
H	0.47616500	-2.05088200	1.28834100

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Energy = -976.89503380 a.u. #Cluster: 9

P	-0.26346500	-3.28218000	-0.87494300
F	-0.44704400	-4.31869600	0.31235200
O	-1.61623700	-2.46785900	-0.90130000
O	0.11305200	-3.86311300	-2.17373800
N	2.42271200	-0.59329000	0.17820900
N	0.91183900	-2.31382700	-0.09146100
C	3.21662900	0.54980000	-0.32352500
C	2.58894800	-0.92667000	1.61166400
C	1.58947200	-1.25458300	-0.59523200
C	2.64483100	1.89847800	0.09718200
C	1.42531500	-0.46666200	2.48831100
C	1.37510400	-0.86365400	-2.02336300
C	-2.17694900	-1.77440100	0.23860300
H	3.28839800	0.47998200	-1.41332500
H	4.23301500	0.41398500	0.07324800

H	2.76213000	-2.01155400	1.69950200
H	3.52060700	-0.44396900	1.93038500
H	3.26376900	2.69844400	-0.33647200
H	1.61275800	2.02164100	-0.26574400
H	2.65037700	2.02033600	1.19017700
H	0.47414000	-0.94443300	2.21099700
H	1.64425400	-0.73304600	3.53315100
H	1.29177300	0.62230400	2.42838200
H	0.60207500	-1.47225200	-2.50118500
H	1.09017200	0.19550500	-2.08611300
H	2.30967300	-1.00552600	-2.58708500
H	-3.14071100	-1.37365400	-0.09518400
H	-1.51212000	-0.95350200	0.54342700
H	-2.32523800	-2.47564600	1.07152200
H	1.09614900	-2.58827700	0.87284000

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Energy = -976.89466440 a.u. #Cluster: 10

P	-1.45399800	-2.12418100	0.34338700
F	-2.35297000	-0.82566700	0.27097000
O	-1.50773800	-2.52175000	-1.18978700
O	-1.82276300	-3.10681300	1.37649500
N	1.97739700	-0.16149900	0.53245900

N	0.09261600	-1.48774300	0.67569800
C	2.77613700	0.93124100	-0.06776000
C	2.57907900	-0.79260400	1.72646800
C	0.80645000	-0.51635600	0.05229600
C	3.79643400	0.41624700	-1.07561800
C	2.14711000	-0.11240700	3.02285900
C	0.22359800	0.15739000	-1.14911100
C	-0.86635100	-3.72453400	-1.68355500
H	3.27638400	1.43599300	0.77030200
H	2.09953700	1.66697800	-0.51687100
H	2.34455200	-1.86724600	1.72550200
H	3.66713100	-0.72380000	1.59642200
H	4.39625000	1.26107800	-1.44642800
H	4.47983200	-0.31264700	-0.61390900
H	3.30507600	-0.06433200	-1.93536500
H	2.65596000	-0.59488300	3.87071300
H	2.42118900	0.95337000	3.01581500
H	1.06068200	-0.19144800	3.18157300
H	-0.26149500	1.09439200	-0.82896600
H	0.99933700	0.39920900	-1.88303900
H	-0.52387400	-0.47737600	-1.63358500
H	-1.17674200	-4.58939600	-1.08130000

H	0.22594800	-3.60348200	-1.64629600
H	-1.20002300	-3.84215700	-2.72056300
H	0.48068100	-1.90189300	1.52247700

A232-N₂H

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Energy = -976.87807940 a.u. #Cluster: 1

P	-1.22908900	-0.48061500	-0.77043500
F	-1.83700200	-1.93906500	-0.88528800
O	-2.47454000	0.45321000	-0.53047800
O	-0.39928100	-0.09078800	-1.94509100
N	1.69230800	0.13407600	-0.15643300
N	-0.43838700	-0.59372500	0.70751800
C	2.06900800	1.60082200	-0.02215300
C	2.91390900	-0.74844700	-0.31535400
C	0.77480200	-0.31697000	0.94272900
C	0.85151200	2.50376300	0.02767600
C	2.54371900	-2.20203800	-0.54225100
C	1.37625000	-0.39844600	2.29944800
C	-3.47606500	0.23005700	0.49243200
H	2.68798900	1.80793600	-0.90506800
H	2.70216100	1.69186500	0.86974600

H	3.44577700	-0.33028500	-1.18026500
H	3.53992400	-0.59977600	0.57414300
H	0.23530300	2.32721100	0.92227400
H	1.19838300	3.54686300	0.06139200
H	0.22503300	2.38054400	-0.86803300
H	1.87717100	-2.30880300	-1.41199700
H	3.46438200	-2.77004700	-0.73933700
H	2.05218500	-2.65070000	0.33434000
H	2.13882600	-1.19295400	2.33454100
H	1.87433800	0.54576300	2.56865400
H	0.58600000	-0.62431900	3.02366200
H	-3.01574200	0.30511000	1.48703800
H	-3.93554900	-0.75873200	0.35649900
H	-4.22599500	1.01793600	0.35889200
H	1.13432600	0.05435000	-1.03947300

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Energy = -976.87807850 a.u. #Cluster: 2

P	-1.19412400	-0.60123000	-0.75463500
F	-1.64278000	-2.12130900	-0.78806800
O	-2.53443500	0.20667700	-0.58672900
O	-0.38578400	-0.20024600	-1.94036600
N	1.68463700	0.22251400	-0.15128700

N	-0.41901100	-0.55771800	0.73538200
C	2.21640700	1.63160100	0.02673100
C	2.80200500	-0.77530700	-0.40516600
C	0.77630600	-0.20833200	0.96433900
C	1.10388400	2.64924200	0.19416900
C	2.27241000	-2.17023900	-0.67564600
C	1.37184600	-0.20565800	2.32643000
C	-3.52500200	-0.05857300	0.43697500
H	2.80116600	1.82285900	-0.88285300
H	2.90802700	1.61330600	0.87891400
H	3.33830300	-0.37204900	-1.27437600
H	3.47439500	-0.73764400	0.46178500
H	0.39878700	2.60709700	-0.65052700
H	0.54128200	2.50553400	1.12903200
H	1.55191200	3.65306100	0.22154500
H	1.76159300	-2.60159700	0.19853800
H	1.58012400	-2.17552400	-1.53083800
H	3.12418300	-2.82128500	-0.92045600
H	1.60945100	0.82326300	2.64108900
H	0.65154100	-0.64038500	3.02783600
H	2.31179000	-0.77848300	2.34805200
H	-3.08154900	0.08564300	1.43162100

H	-3.90437500	-1.08429800	0.33136300
H	-4.33244500	0.66352000	0.27102200
H	1.09111200	0.21935500	-1.01454500

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Energy = -976.87807340 a.u. #Cluster: 3

P	-1.19817100	-0.67367500	-0.69771300
F	-1.59966400	-2.20745500	-0.68179000
O	-2.55945000	0.09606100	-0.51938200
O	-0.42902600	-0.28054900	-1.91161100
N	1.67034100	0.24253600	-0.18177100
N	-0.39285300	-0.56458400	0.77338000
C	2.17346800	1.66756000	-0.05698900
C	2.80605500	-0.73652800	-0.42970300
C	0.79652800	-0.17509400	0.96615300
C	1.04239800	2.66649500	0.09668600
C	2.30882500	-2.15464400	-0.63256600
C	1.42038900	-0.10961500	2.31399100
C	-3.52085500	-0.17881700	0.52923700
H	2.74065000	1.84270400	-0.98078500
H	2.87743800	1.69035200	0.78473800
H	3.30854400	-0.35263700	-1.32740500
H	3.49936800	-0.64906600	0.41698800

H	0.49222700	2.53563500	1.04075700
H	1.47054400	3.67934000	0.09403900
H	0.32970700	2.58998000	-0.73908700
H	1.83303200	-2.56543000	0.27074400
H	1.59614100	-2.21358200	-1.46879400
H	3.17282800	-2.79070400	-0.87400700
H	2.37102300	-0.66470800	2.33544400
H	1.64597600	0.93446700	2.58406000
H	0.72393800	-0.53076700	3.04704200
H	-4.35709900	0.50898400	0.36041900
H	-3.06508100	0.00708500	1.51132400
H	-3.86400600	-1.22003000	0.45670000
H	1.05844000	0.20048200	-1.03076700

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Energy = -976.87807330 a.u. #Cluster: 4

P	-1.22366300	-0.38392400	-0.83588700
F	-1.85209200	-1.82474800	-1.03197600
O	-2.45928500	0.55575700	-0.56953600
O	-0.36532300	0.05229300	-1.97302700
N	1.70386400	0.12647800	-0.13855900
N	-0.46204000	-0.58348600	0.64850100
C	2.15398400	1.55897900	0.09078000

C	2.88349800	-0.80460600	-0.34305200
C	0.75130800	-0.34484500	0.92117600
C	0.98312600	2.51855500	0.18583400
C	2.45377800	-2.23560900	-0.60417300
C	1.31122200	-0.47023500	2.29199200
C	-3.48933100	0.28561900	0.41299500
H	2.79421600	1.78950800	-0.77103700
H	2.77899300	1.56164300	0.99333200
H	3.41969000	-0.38235800	-1.20325500
H	3.52859200	-0.71064800	0.54024200
H	0.35984200	2.48049900	-0.72004700
H	0.34877800	2.32020200	1.06316400
H	1.38042400	3.53915800	0.28514700
H	1.77185100	-2.29514500	-1.46657200
H	3.35005800	-2.83102200	-0.83077300
H	1.95925700	-2.68910500	0.26832300
H	1.55335000	0.53094200	2.68641500
H	0.56036300	-0.93637300	2.93932600
H	2.23986500	-1.05937500	2.30294900
H	-3.04496200	0.23589300	1.41646300
H	-3.99598700	-0.65886100	0.17106400
H	-4.19487400	1.12174800	0.34973300

H	1.15315100	0.12686200	-1.03021200
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Energy = -976.87650760 a.u. #Cluster: 5

P	-1.38982700	-0.49776300	-0.62285300
F	-1.78522500	-2.00481500	-0.91852100
O	-2.75490400	0.21175200	-0.28854700
O	-0.62895500	0.13708400	-1.73552000
N	1.47726500	0.29850700	0.04897000
N	-0.57936400	-0.68084700	0.83768900
C	1.75688700	1.75499200	0.39659000
C	2.73325200	-0.49338000	-0.25175500
C	0.61395800	-0.34327900	1.09443700
C	2.08350600	2.56761300	-0.84301000
C	2.42439300	-1.91215000	-0.69133800
C	1.24708900	-0.54089200	2.42483000
C	-3.71363600	-0.28437700	0.67786600
H	2.57479700	1.76076300	1.12815900
H	0.84567800	2.13275700	0.88075400
H	3.24325800	0.06438200	-1.04678600
H	3.36119800	-0.45578500	0.64800400
H	1.25876600	2.52419100	-1.57076500
H	2.21860500	3.61617300	-0.53921100

H	3.01177200	2.23429900	-1.32848800
H	1.76803100	-1.92031800	-1.57538100
H	3.36898200	-2.40749600	-0.95874600
H	1.94750500	-2.50358600	0.10514900
H	2.03058100	-1.31374800	2.35761400
H	1.72725400	0.38302600	2.78032700
H	0.48230100	-0.86906600	3.13732300
H	-4.08399200	-1.26958000	0.36232500
H	-4.53371800	0.44244000	0.69144200
H	-3.24584700	-0.35053000	1.66971500
H	0.89204500	0.31343200	-0.82094100

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Energy = -976.87649810 a.u. #Cluster: 6

P	-1.44481600	-0.45473400	-0.53290600
F	-1.98067500	-1.92062200	-0.80949200
O	-2.72418000	0.35823100	-0.10506700
O	-0.70738600	0.13210400	-1.68714600
N	1.47073700	0.25061700	0.00543000
N	-0.56001000	-0.71717500	0.87108500
C	1.75138600	1.70179000	0.37530600
C	2.72055100	-0.52374700	-0.35776800
C	0.65315500	-0.41483000	1.07244600

C	2.01826200	2.54857600	-0.85522600
C	2.40247100	-1.92735800	-0.83854300
C	1.35248600	-0.67165400	2.35877200
C	-3.66187000	-0.07912400	0.90953100
H	2.59856600	1.69821500	1.07294800
H	0.85790800	2.05876000	0.90608800
H	3.20532300	0.06402700	-1.14698200
H	3.37423100	-0.51407600	0.52411100
H	2.16098500	3.58944300	-0.52904400
H	2.92607600	2.23551300	-1.39046000
H	1.16236000	2.51937600	-1.54672700
H	1.95402600	-2.54947700	-0.04883100
H	1.71594700	-1.90494000	-1.69915800
H	3.33879600	-2.40843600	-1.15624500
H	0.61857400	-1.00098100	3.10249100
H	2.10807500	-1.46325900	2.22562600
H	1.87888400	0.22666600	2.71458400
H	-3.13926000	-0.22951700	1.86415700
H	-4.14818900	-1.01035600	0.58787700
H	-4.40242700	0.72313000	1.00398500
H	0.85166800	0.27763800	-0.84151400

Energy = -976.87648150 a.u. #Cluster: 7

P	-1.37432500	-0.65054700	-0.55859000
F	-1.86740200	-2.15565400	-0.48451800
O	-2.69637500	0.20167800	-0.48142600
O	-0.53681700	-0.36034200	-1.75644700
N	1.55411900	-0.03967200	0.02531800
N	-0.62852000	-0.49974400	0.93944500
C	2.25792500	1.30056500	0.03653400
C	2.51753200	-1.21994100	-0.03806200
C	0.58552100	-0.21477800	1.15879600
C	1.27875600	2.45652400	-0.04176200
C	3.05218900	-1.42777500	-1.44271700
C	1.15342800	-0.05746400	2.52339400
C	-3.70646400	0.04085900	0.54467100
H	2.92271100	1.28405000	-0.83588000
H	2.88245500	1.33039400	0.93867300
H	3.31526300	-1.02156500	0.68942600
H	1.94743100	-2.09846200	0.29431200
H	0.63861200	2.37361700	-0.93352500
H	0.63391400	2.52018900	0.84808400
H	1.84921300	3.39395500	-0.11186700
H	2.23227200	-1.61534400	-2.15274100

H	3.64666300	-0.57265900	-1.79534000
H	3.70636600	-2.31210200	-1.43176700
H	2.08390300	-0.63378600	2.63705700
H	1.39787700	1.00147100	2.70860500
H	0.41015200	-0.38549500	3.25836600
H	-3.27203800	0.24888200	1.53202400
H	-4.11204200	-0.97981200	0.51208600
H	-4.49216200	0.76879600	0.31280300
H	0.97150000	-0.08204200	-0.84562100

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Energy = -976.87647910 a.u. #Cluster: 8

P	-1.39738400	-0.65517900	-0.48558300
F	-2.04824700	-2.09157300	-0.33047100
O	-2.61669800	0.33997400	-0.43613800
O	-0.55164300	-0.51324700	-1.70451000
N	1.55734800	-0.13021800	0.02227800
N	-0.61455900	-0.51693000	0.99396500
C	2.14870700	1.26126600	-0.07658600
C	2.60211100	-1.23571200	0.02066400
C	0.61395800	-0.27213400	1.18103800
C	1.07032600	2.31797500	-0.22617500
C	3.16999100	-1.46410200	-1.36799000

C	1.21334200	-0.10769800	2.53096900
C	-3.63436900	0.33280600	0.59495100
H	2.80461600	1.23577400	-0.95523000
H	2.77395900	1.41201900	0.81280900
H	3.37594300	-0.95003800	0.74469100
H	2.09069400	-2.13747000	0.38522100
H	1.55581800	3.29699900	-0.34832900
H	0.44814500	2.12861500	-1.11390600
H	0.41678800	2.37549400	0.65793000
H	2.37463800	-1.72185900	-2.08418700
H	3.72318500	-0.59122600	-1.74327600
H	3.87118700	-2.31001400	-1.31561300
H	1.53394200	0.93728200	2.67637600
H	0.46079300	-0.36015700	3.28609000
H	2.10230000	-0.74419100	2.65391300
H	-4.18282500	-0.61889700	0.56818900
H	-4.30704000	1.16591000	0.36196000
H	-3.17092400	0.48056800	1.57998700
H	0.96755300	-0.27024000	-0.83370600

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Energy = -976.87647810 a.u. #Cluster: 9

P	-1.39752500	-0.66319900	-0.46868200
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F	-1.91214300	-2.15402300	-0.30755700
O	-2.70497800	0.21187700	-0.39540800
O	-0.59116900	-0.44413500	-1.70214000
N	1.55286400	-0.05388600	0.00810900
N	-0.60809700	-0.45213600	0.99894500
C	2.27636200	1.27466500	-0.05230700
C	2.49934400	-1.24950400	-0.03586400
C	0.61368300	-0.16911000	1.17329500
C	1.31319400	2.43939300	-0.18042000
C	2.95771000	-1.53935900	-1.45299100
C	1.21745700	0.04535600	2.51466100
C	-3.69327600	0.10241400	0.65840400
H	2.93502100	1.20618600	-0.92690000
H	2.90724600	1.33951100	0.84349600
H	3.33439700	-1.02117800	0.63914000
H	1.93869700	-2.10146000	0.37279500
H	1.89612500	3.36519100	-0.29116700
H	0.67091100	2.32724600	-1.06742600
H	0.67069300	2.55047700	0.70648300
H	3.60846100	-2.42591000	-1.42868300
H	2.09961800	-1.75966900	-2.10607000
H	3.53468300	-0.70840400	-1.88403700

H	1.44054800	1.11592900	2.65696700
H	0.50236100	-0.27210500	3.28165600
H	2.16383400	-0.50555300	2.62120600
H	-3.23061300	0.32492900	1.62969900
H	-4.12345900	-0.90869000	0.66203400
H	-4.46713700	0.84286900	0.42640700
H	0.94684200	-0.12392700	-0.84431500

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Energy = -976.87647590 a.u. #Cluster: 10

P	-1.37243900	-0.70701000	-0.49606900
F	-1.98166400	-2.16075700	-0.33550800
O	-2.62319000	0.24962500	-0.46660900
O	-0.51988900	-0.54805300	-1.70808000
N	1.56279200	-0.10552100	0.03405000
N	-0.60914200	-0.52920900	0.98948300
C	2.13933300	1.29124100	-0.07234400
C	2.61899900	-1.20002500	0.05409100
C	0.61030000	-0.24810900	1.18507200
C	1.05052700	2.33216400	-0.25525900
C	3.19870800	-1.43967700	-1.32772400
C	1.18858500	-0.03533400	2.53751700
C	-3.65001500	0.21239000	0.55493600

H	2.81122200	1.26263600	-0.93874600
H	2.74658500	1.46096900	0.82609300
H	3.38443100	-0.89635800	0.77960000
H	2.11455600	-2.10211900	0.42728900
H	0.44574800	2.12174400	-1.15031000
H	0.38114800	2.39330100	0.61662000
H	1.52520100	3.31571100	-0.38320600
H	3.74474400	-0.56532900	-1.71003700
H	3.90869200	-2.27715600	-1.26043200
H	2.41070900	-1.71470500	-2.04553100
H	2.13040800	-0.58777400	2.66815400
H	1.41209900	1.03557000	2.67951900
H	0.45597500	-0.34689200	3.29029200
H	-4.35764500	1.00999900	0.30207000
H	-3.20325200	0.39690300	1.54148500
H	-4.15470600	-0.76346900	0.53908800
H	0.98283500	-0.26095800	-0.82617600

A232-OH

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Energy = -976.88232120 a.u. #Cluster: 1

P	-1.66008200	-0.69779900	-0.75219900
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F	-2.25610700	-1.26568200	0.60779300
O	-2.70374500	0.37183700	-1.23557700
O	-1.75438100	-1.89652500	-1.77431200
N	1.90687400	0.25372400	0.12429200
N	-0.23315900	-0.09065900	-0.56365200
C	3.18500200	-0.12716600	0.75051200
C	1.78696500	1.66210100	-0.29751800
C	0.89150000	-0.57950200	-0.03374900
C	4.22025100	-0.59211400	-0.26815900
C	1.17050300	2.53675500	0.78913800
C	0.99011000	-2.01812000	0.39196800
C	-2.79541200	1.69959800	-0.65707200
H	2.99973600	-0.89349500	1.51263300
H	3.54349200	0.76304000	1.28678400
H	2.80021200	2.00452000	-0.54968900
H	1.18129500	1.69289300	-1.21139900
H	3.88647500	-1.50463500	-0.78586700
H	4.40910300	0.18545900	-1.02460200
H	5.16961900	-0.81085900	0.24414900
H	1.76703100	2.50393600	1.71438200
H	1.13139900	3.58131200	0.44345900
H	0.14575000	2.20899300	1.01830200

H	0.48227000	-2.13063700	1.36450000
H	0.46133300	-2.64523700	-0.33865800
H	2.01691700	-2.38295600	0.48750700
H	-1.84323200	2.22919300	-0.79507900
H	-3.04310800	1.62522300	0.41099800
H	-3.60077700	2.20719100	-1.19939400
H	-2.64702100	-2.25890600	-1.93807700

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Energy = -976.88227570 a.u. #Cluster: 2

P	-1.49592000	0.17667000	-1.07927000
F	-1.61872800	-1.06056900	-2.07209000
O	-2.42460000	-0.19345600	0.13285200
O	-2.22007000	1.35506800	-1.83687700
N	2.10488600	0.38075000	0.10265700
N	-0.01420500	0.51319000	-0.71351200
C	3.19599700	-0.20925100	0.89830900
C	2.40897700	1.66693500	-0.55312200
C	0.90610800	-0.16534300	-0.02036100
C	4.10709300	-1.10594100	0.06663200
C	2.02589000	2.86119100	0.31456300
C	0.57788100	-1.48482900	0.62205700
C	-3.84014500	-0.49874400	0.02238900

H	2.77075000	-0.75067300	1.75156500
H	3.76263300	0.63423600	1.31751900
H	3.48714200	1.66632900	-0.76548400
H	1.87491100	1.69375400	-1.51055700
H	4.54298200	-0.55259400	-0.77956300
H	4.93120200	-1.47844100	0.69424100
H	3.55599000	-1.97149800	-0.33267300
H	2.30631100	3.79432100	-0.19804600
H	0.94123800	2.87782400	0.49737500
H	2.54699200	2.83326200	1.28448300
H	1.45565200	-2.06410000	0.92112200
H	-0.04759700	-1.29715600	1.50993400
H	-0.01292000	-2.08791400	-0.08188500
H	-3.98655500	-1.34063200	-0.66812700
H	-4.38208500	0.38934600	-0.32984400
H	-4.16781400	-0.77249300	1.03132200
H	-1.68318400	1.82223900	-2.50419200

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Energy = -976.88220500 a.u. #Cluster: 3

P	-1.62667300	-0.65598500	-1.01324000
F	-2.21921400	-1.69777300	0.03560800
O	-2.73818500	0.44821900	-1.13894600

O	-1.61367100	-1.42486100	-2.38905000
N	1.89277300	0.25639300	0.11485700
N	-0.23633200	-0.07315900	-0.61225800
C	3.15272600	-0.14603700	0.76056800
C	1.82923400	1.64487100	-0.37460900
C	0.85588900	-0.55726100	-0.02171700
C	4.19585700	-0.62987400	-0.24307400
C	1.25550800	2.59474600	0.67199800
C	0.94637800	-1.96521700	0.50389900
C	-2.90975700	1.50954400	-0.16521900
H	2.94530500	-0.91385100	1.51493400
H	3.52232900	0.73573000	1.30393500
H	2.85384000	1.93519700	-0.64584300
H	1.22142500	1.65717000	-1.28736600
H	4.41961900	0.14756100	-0.98993300
H	5.12939400	-0.87468600	0.28625900
H	3.85242300	-1.53109800	-0.77372200
H	1.85998100	2.58678100	1.59266900
H	1.24929800	3.62188500	0.27562200
H	0.22266000	2.31594800	0.92888500
H	1.03438200	-1.94804800	1.60156900
H	0.05498100	-2.54202400	0.23961400

H	1.83235700	-2.47746200	0.10382400
H	-3.14669800	1.08088900	0.81857200
H	-3.74793100	2.11531200	-0.52686400
H	-1.99382500	2.11354700	-0.11195300
H	-2.48526300	-1.69497300	-2.73759800

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Energy = -976.88170360 a.u. #Cluster: 4

P	-1.81345700	-0.52449300	-0.29217500
F	-2.47696900	-0.25855700	1.12439200
O	-2.66885900	0.32841600	-1.29822500
O	-2.13875800	-2.03609600	-0.61443000
N	1.88847400	0.19159900	0.17236900
N	-0.31578400	-0.10761200	-0.28394400
C	3.22253300	-0.23852500	0.62088300
C	1.74808200	1.60963800	-0.20527100
C	0.84275400	-0.61971000	0.12418300
C	4.13159600	-0.63533100	-0.53846200
C	1.22201400	2.46303600	0.94413800
C	0.98707000	-2.06173000	0.52672700
C	-2.51100400	1.76070600	-1.45898000
H	3.11515800	-1.06049500	1.33846600
H	3.65246400	0.60765200	1.17651200

H	2.74101500	1.95383800	-0.52516500
H	1.07609300	1.66638000	-1.07130600
H	3.72649000	-1.50142500	-1.08414500
H	4.25560200	0.19541800	-1.25017300
H	5.12581000	-0.90484800	-0.15039600
H	0.21339400	2.13915500	1.24049000
H	1.88549700	2.39983300	1.82095800
H	1.16951000	3.51641600	0.62826200
H	1.07221100	-2.12648700	1.62404300
H	0.10779300	-2.63191500	0.20988000
H	1.88495900	-2.51786900	0.09006500
H	-1.47587500	1.99043000	-1.74560100
H	-2.77325600	2.27251300	-0.52250400
H	-3.20362300	2.05061300	-2.25695500
H	-3.08212200	-2.28906700	-0.62221700

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Energy = -976.88142560 a.u. #Cluster: 5

P	-1.84864300	-0.36928700	-0.02048700
F	-2.41045400	0.39776700	1.25105000
O	-2.69869400	0.18569400	-1.22152200
O	-2.29637000	-1.87078800	0.17893800
N	1.89990200	0.18859800	0.14558700

N	-0.32958300	-0.09234500	-0.18229200
C	3.23557100	-0.22080100	0.60757800
C	1.79478000	1.52691100	-0.46323000
C	0.82329900	-0.57178200	0.27596300
C	4.07515600	-0.84044500	-0.50566900
C	1.32795500	2.57936500	0.53698700
C	0.93110000	-1.92811500	0.91759800
C	-2.47543000	1.49525100	-1.80343000
H	3.12940500	-0.91185200	1.45202500
H	3.72129300	0.68404100	1.00114300
H	2.78881000	1.77558700	-0.85928700
H	1.10016600	1.46152800	-1.31073500
H	3.61071400	-1.76285200	-0.88743300
H	4.19956400	-0.14122700	-1.34707400
H	5.07436600	-1.09054900	-0.11738800
H	0.32091300	2.34187400	0.91063400
H	2.01649000	2.64593200	1.39401700
H	1.29275500	3.56469700	0.04700000
H	1.11249900	-1.81078300	1.99838500
H	0.00084200	-2.48717700	0.77611400
H	1.76411800	-2.50632800	0.49559700
H	-1.44733900	1.56175900	-2.18437400

H	-2.65789200	2.27439600	-1.05006800
H	-3.19547200	1.58525600	-2.62435700
H	-3.25100500	-2.03284200	0.31014800

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Energy = -976.88133880 a.u. #Cluster: 6

P	-1.70628100	-0.63957500	-0.72409500
F	-2.47871300	-1.00857000	0.61289300
O	-2.62107200	0.42807100	-1.42583000
O	-1.78059200	-1.94155700	-1.61378300
N	1.87896400	0.21122600	0.21309000
N	-0.27372000	-0.09063600	-0.44424800
C	3.18100500	-0.22489100	0.74245200
C	1.74388700	1.64766100	-0.09036600
C	0.85893200	-0.61259000	0.02558900
C	4.19240600	-0.51706100	-0.36215100
C	1.12581800	2.42498200	1.06707900
C	1.00174800	-2.07275800	0.36104700
C	-2.65779300	1.82112800	-1.02381700
H	3.03466600	-1.10036000	1.38569600
H	3.54195700	0.58547700	1.39255000
H	2.75143400	2.02150300	-0.31816900
H	1.13296100	1.74801400	-0.99628400

H	4.35546700	0.36710700	-0.99748800
H	5.15717300	-0.79791800	0.08731200
H	3.85447100	-1.34612400	-1.00304100
H	0.10295900	2.07501800	1.27007100
H	1.72557800	2.31542900	1.98429000
H	1.08192900	3.49492900	0.81120400
H	0.16308700	-2.64579200	-0.04921200
H	1.93719300	-2.49130500	-0.03276500
H	1.00904500	-2.19555500	1.45647200
H	-3.03288100	1.90222000	0.00601100
H	-3.34605300	2.31543900	-1.71837400
H	-1.65249500	2.25670200	-1.10177000
H	-2.67226900	-2.29873000	-1.79294700

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Energy = -976.88130370 a.u. #Cluster: 7

P	-1.52998100	0.24996400	-1.02282700
F	-1.60936500	-0.60003600	-2.36056500
O	-2.44122700	-0.52498900	-0.00194800
O	-2.31157000	1.57871000	-1.36545100
N	2.10186500	0.38604100	0.10811400
N	-0.04867200	0.50109300	-0.61758800
C	3.20337200	-0.17293600	0.90808800

C	2.42185100	1.57174100	-0.70679200
C	0.87537500	-0.11571400	0.11561400
C	4.07027500	-1.14530300	0.11339900
C	2.10675800	2.87325800	0.02369800
C	0.56685300	-1.32117900	0.96191500
C	-3.84656700	-0.82224300	-0.21684300
H	2.79173100	-0.65370100	1.80290700
H	3.80266900	0.68037500	1.25798600
H	3.49104600	1.51087600	-0.95240500
H	1.85606800	1.50437900	-1.64426900
H	4.89587100	-1.50409700	0.74703300
H	3.48727900	-2.01693000	-0.22198000
H	4.50633400	-0.65889100	-0.77291900
H	2.39888300	3.72945800	-0.60381900
H	1.03010800	2.95082800	0.23650600
H	2.66040100	2.93917400	0.97344600
H	1.29545800	-2.12462300	0.78835800
H	0.61442100	-1.04590300	2.02783200
H	-0.43906000	-1.69430000	0.74682100
H	-4.41627600	0.11507400	-0.27216800
H	-4.16389000	-1.41376300	0.64889100
H	-3.96574100	-1.40332400	-1.14152500

H	-1.79545700	2.25844300	-1.83809100
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Energy = -976.88118060 a.u. #Cluster: 8

P	-1.64419800	0.62679100	-0.38396400
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F	-1.89515300	0.96747500	-1.91400800
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O	-2.40211700	-0.73257000	-0.15272600
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O	-2.48214500	1.71546600	0.39510300
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N	2.12030200	0.35299300	0.06571000
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N	-0.12471100	0.67474600	-0.06603000
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C	3.34428800	-0.46357500	0.10046600
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C	2.30444800	1.81415000	0.12390400
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C	0.90593200	-0.16625000	-0.03697200
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C	3.81659900	-0.75075100	1.52265400
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C	2.32654800	2.44647300	-1.26406900
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C	0.73022500	-1.65803900	-0.11671500
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C	-3.81336000	-0.94354000	-0.42301800
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H	4.11004100	0.09782300	-0.45435400
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H	3.17439400	-1.39313900	-0.45524100
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H	1.49265600	2.23545300	0.73038600
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H	3.25054000	1.99517900	0.65227100
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H	4.75852800	-1.31948700	1.49015000
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H	3.99902400	0.18258900	2.07749300
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H	3.07301400	-1.34348000	2.07757600
H	2.50420700	3.52934400	-1.17451000
H	3.12950100	2.01678300	-1.88345700
H	1.36541800	2.29396900	-1.77742400
H	1.06707600	-2.01409700	-1.10412500
H	1.32375500	-2.17407700	0.64951900
H	-0.32458200	-1.92162500	0.00880000
H	-4.00731800	-1.99843100	-0.20004700
H	-4.02419200	-0.73099200	-1.48003300
H	-4.41432600	-0.29594700	0.22954300
H	-2.05558100	2.58824900	0.48453400

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Energy = -976.88117160 a.u. #Cluster: 9

P	-1.62059200	0.44351400	-0.65890300
F	-1.82702700	-0.20400600	-2.09657000
O	-2.37421000	-0.52661600	0.32259200
O	-2.47757800	1.76668600	-0.69596700
N	2.10642200	0.40406100	0.05594500
N	-0.11774400	0.70657900	-0.31845800
C	3.35685000	-0.37351400	0.12736500
C	2.23151800	1.84990800	0.32051400
C	0.92940200	-0.12242300	-0.23928800

C	3.63003900	-0.91160900	1.52788200
C	2.47512900	2.64942800	-0.95505600
C	0.76823600	-1.59485900	-0.49438400
C	-3.77784400	-0.88156700	0.20726700
H	4.16112100	0.30540600	-0.18907300
H	3.32390100	-1.18071900	-0.61401900
H	1.31449600	2.18441100	0.82003300
H	3.06649200	1.97181700	1.02460900
H	4.60011500	-1.43167700	1.54112600
H	3.66739700	-0.09497300	2.26546400
H	2.84993400	-1.62355700	1.83895400
H	1.62287400	2.55464300	-1.64452300
H	2.60173500	3.71386500	-0.70387200
H	3.38609500	2.30913300	-1.47201300
H	1.62748800	-2.20069900	-0.19585500
H	-0.11908300	-1.94958900	0.04922600
H	0.58167100	-1.74331300	-1.57066300
H	-4.39679200	0.01901400	0.31813000
H	-3.97715700	-1.58579500	1.02243900
H	-3.96064700	-1.35993600	-0.76463700
H	-2.04342600	2.53786800	-1.10684800

Energy = -976.87993120 a.u. #Cluster: 10

P	-1.58943200	0.43692400	-0.74598200
F	-1.60653700	-0.37696200	-2.11084500
O	-2.52827600	-0.38137200	0.21219900
O	-2.36141200	1.77158300	-1.07824900
N	1.97435000	0.43469100	0.56661600
N	-0.14058500	0.69709400	-0.22172800
C	3.08789900	-0.33743700	1.14291100
C	2.19619700	1.87824800	0.34656000
C	0.81322000	-0.11398100	0.23948200
C	4.14522600	-0.72969600	0.11496500
C	2.46484000	2.23867700	-1.11207900
C	0.59905800	-1.59220100	0.42879600
C	-3.91828500	-0.69341200	-0.07072000
H	2.68375900	-1.22483900	1.64263900
H	3.53017300	0.29206400	1.92877200
H	1.30809100	2.41127400	0.71312100
H	3.04725200	2.16308100	0.97894300
H	4.61975500	0.15515600	-0.33459700
H	4.93006200	-1.32322600	0.60852300
H	3.70652700	-1.33709800	-0.69211900
H	2.63085200	3.32449500	-1.19073700

H	3.35922600	1.72633100	-1.49585000
H	1.60723900	1.97613800	-1.74776600
H	1.44871800	-2.17307700	0.04678700
H	0.48717100	-1.81578900	1.50222200
H	-0.30982300	-1.92256400	-0.08592500
H	-4.25630600	-1.33174400	0.75294900
H	-3.99178900	-1.23135000	-1.02577500
H	-4.50428900	0.23500000	-0.10326400
H	-1.82406800	2.47547500	-1.48843000

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Energy = -1015.71101200 a.u. #Cluster: 1

P	-5.38755600	-5.15871500	-0.61065000
O	-6.73124500	-4.52690000	-0.72633000
C	-5.69730000	-7.76701900	-0.71366700
F	-4.90869100	-5.15287800	0.93998700
N	-5.09167300	-6.67132600	-1.12200700
C	-6.76742100	-7.75511700	0.35356200
H	-6.29218700	-7.85031400	1.34383300
H	-7.29672300	-6.79445800	0.31783200
H	-7.50152300	-8.56096600	0.24327500

C	-5.84333900	-10.23997000	-0.81447400
H	-6.12961700	-10.18516400	0.24327200
H	-5.00673400	-10.95324700	-0.86722100
C	-7.00840400	-10.73009300	-1.67051200
H	-7.32850000	-11.72901600	-1.33491500
H	-7.86980200	-10.04776600	-1.59684000
H	-6.71811500	-10.80230100	-2.73051400
C	-4.28989300	-8.96985500	-2.29424400
H	-4.42405600	-8.08725400	-2.93268800
H	-4.48056100	-9.86113400	-2.90968700
C	-2.87331400	-9.00424600	-1.72686000
H	-2.66827900	-8.09655900	-1.14022300
H	-2.72578300	-9.88255400	-1.07816000
H	-2.14059900	-9.05836800	-2.54743000
N	-5.32023200	-8.93906800	-1.24787900
O	-4.26168600	-4.23831300	-1.28314600
C	-2.87413900	-4.64159000	-1.35877200
H	-2.68134100	-5.45031500	-0.63695500
H	-2.28825000	-3.76333200	-1.04773000
C	-2.52076700	-5.07044500	-2.76781400
H	-3.10593600	-5.95553200	-3.05785600
H	-2.72450900	-4.25932200	-3.48451900

H	-1.44995300	-5.32367600	-2.82433500
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Energy = -1015.70942700 a.u. #Cluster: 2

P	-4.72936100	-5.53699400	0.03740000
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O	-5.88011600	-4.94008400	0.77261300
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C	-5.58746500	-8.00138600	-0.51643000
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F	-3.42995400	-5.58985400	0.99807500
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N	-4.72403000	-7.01541800	-0.61968600
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C	-6.85029700	-7.93131300	0.30957500
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H	-6.99698400	-6.90887500	0.67148200
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H	-7.72734200	-8.24354200	-0.27442800
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H	-6.76691600	-8.60627500	1.17651500
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C	-6.18787500	-10.32432700	-1.13385200
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H	-6.72355900	-10.35202300	-0.17718400
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H	-5.52845900	-11.20578200	-1.14239800
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C	-7.16840000	-10.38871000	-2.30292700
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H	-6.63676800	-10.38382700	-3.26761700
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H	-7.76261000	-11.31427500	-2.24534100
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H	-7.86062200	-9.53232400	-2.28849900
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C	-4.10351500	-9.25235800	-1.98764900
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H	-3.93442100	-8.29004600	-2.48862200
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H	-4.29607600	-10.00544800	-2.76552000
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C	-2.88303800	-9.63985000	-1.15682200
H	-2.66718400	-8.86565200	-0.40542400
H	-3.04536400	-10.59830000	-0.63799600
H	-2.00083900	-9.74798100	-1.80766400
N	-5.32267800	-9.14121500	-1.17740700
O	-4.21021900	-4.53203700	-1.10414100
C	-3.09009900	-4.84376900	-1.95932900
H	-3.36969200	-5.68125800	-2.61807000
H	-2.24047300	-5.16888100	-1.33654300
C	-2.74016500	-3.60529500	-2.75495900
H	-3.59562300	-3.28108000	-3.36840600
H	-2.45442500	-2.77776600	-2.08683400
H	-1.89355800	-3.82086500	-3.42558200

32

Energy = -1015.70919000 a.u. #Cluster: 3

P	-4.51641800	-5.45795100	0.28957400
O	-5.61877600	-4.92432000	1.13945800
C	-5.42663900	-7.86114600	-0.42826900
F	-3.16347600	-5.59055700	1.16528600
N	-4.55010600	-6.88328800	-0.47514000
C	-6.68214300	-7.82588600	0.41124800
H	-7.57001600	-8.06591500	-0.19067800

H	-6.61323000	-8.57188900	1.21891800
H	-6.79934300	-6.83323200	0.85697200
C	-6.06806500	-10.12908700	-1.19250400
H	-6.60931200	-10.20289600	-0.24170200
H	-5.42289400	-11.01937300	-1.24960800
C	-7.04398400	-10.10948500	-2.36680200
H	-6.50832400	-10.05607000	-3.32776000
H	-7.65231300	-11.02768400	-2.36587800
H	-7.72360500	-9.24508200	-2.30430400
C	-3.96731400	-9.03911800	-1.98222800
H	-3.78751000	-8.05257600	-2.42866600
H	-4.17035400	-9.74461900	-2.80083000
C	-2.75083200	-9.48763300	-1.17645600
H	-2.52678300	-8.76028300	-0.38204700
H	-2.92389100	-10.47240200	-0.71339500
H	-1.86997700	-9.56782500	-1.83311900
N	-5.18400700	-8.95977000	-1.16394500
O	-4.06214900	-4.36020700	-0.79154200
C	-3.05604500	-4.61313400	-1.79828700
H	-2.44708300	-5.48314600	-1.50875700
H	-2.40310000	-3.72694900	-1.80117900
C	-3.70273400	-4.82360200	-3.15198800

H	-2.92625300	-4.95969500	-3.92182200
H	-4.34302400	-5.71859000	-3.13922500
H	-4.31842600	-3.95340000	-3.42899600

32

Energy = -1015.70907200 a.u. #Cluster: 4

P	-4.14079600	-5.50727600	0.28680400
O	-5.02549800	-5.01258000	1.37974100
C	-5.19165300	-7.88842100	-0.30352600
F	-2.62539000	-5.64649700	0.83131000
N	-4.33321700	-6.91199700	-0.49278000
C	-6.24432100	-7.88413900	0.78016200
H	-6.01502600	-8.65882000	1.52926600
H	-6.25820500	-6.90853700	1.27575700
H	-7.23987500	-8.10173900	0.36840900
C	-6.00788100	-10.11906600	-1.00440100
H	-6.32397100	-10.23961700	0.03885800
H	-5.40605800	-11.00807600	-1.24803200
C	-7.22018000	-10.03283800	-1.92921900
H	-7.85208500	-9.16740900	-1.67484500
H	-6.90978400	-9.93362300	-2.98136300
H	-7.83021500	-10.94522100	-1.83741500
C	-4.11217600	-9.00409200	-2.18187300

H	-4.00894800	-7.99628900	-2.60376800
H	-4.50475100	-9.65986600	-2.97256900
C	-2.76092200	-9.51169100	-1.68558600
H	-2.35418300	-8.83796600	-0.91651400
H	-2.84934900	-10.52237600	-1.25551500
H	-2.04427400	-9.55717600	-2.52104000
N	-5.12138100	-8.95659800	-1.11650500
O	-3.95132600	-4.37318600	-0.83518600
C	-3.24543500	-4.60048800	-2.07593700
H	-2.57246100	-5.46502900	-1.97014100
H	-2.62649500	-3.70481100	-2.23765600
C	-4.22458500	-4.80409000	-3.21435600
H	-4.83107900	-5.70672700	-3.04524800
H	-4.89886600	-3.93815600	-3.30689400
H	-3.67774200	-4.92241200	-4.16360900

32

Energy = -1015.70893800 a.u. #Cluster: 5

P	-4.68557500	-5.56699900	0.58616100
O	-5.92473700	-5.00884200	1.19786300
C	-5.52787200	-7.71026200	-0.72988300
F	-3.53398700	-5.70097600	1.70501200
N	-4.59342600	-7.03514100	-0.09687300

C	-6.93128000	-7.19353600	-0.94311200
H	-7.68784500	-7.96871900	-0.76501900
H	-7.11562300	-6.34940500	-0.27027300
H	-7.03886400	-6.84711700	-1.98422600
C	-6.13941600	-9.73500900	-2.01831600
H	-5.54571500	-10.23938500	-2.79589500
H	-6.84557500	-9.08408300	-2.54849400
C	-6.88284700	-10.76647500	-1.17247800
H	-7.52746100	-11.38602600	-1.81561900
H	-6.17857300	-11.43377700	-0.65102000
H	-7.51662700	-10.27820700	-0.41572300
C	-3.86170800	-9.46262200	-1.04366100
H	-3.95725900	-10.55841700	-1.02386000
H	-3.50072700	-9.13869200	-0.05923300
C	-2.88564600	-9.03177300	-2.13531900
H	-2.75310900	-7.94021700	-2.13086400
H	-1.90288600	-9.50050000	-1.96838900
H	-3.24304100	-9.33530700	-3.13240500
N	-5.20878100	-8.91304200	-1.23709400
O	-4.01726400	-4.49115700	-0.40676500
C	-2.90591400	-4.81282300	-1.27385300
H	-2.36809600	-5.68918700	-0.88080700

H	-2.22760600	-3.94757900	-1.22658000
C	-3.38721700	-5.05430100	-2.69033500
H	-2.52634100	-5.24157100	-3.35186900
H	-4.05364600	-5.92910500	-2.73479600
H	-3.93346700	-4.17656100	-3.06994700

32

Energy = -1015.70889200 a.u. #Cluster: 6

P	-4.86867200	-5.37638900	0.35285500
O	-6.15491800	-4.82926100	0.87008200
C	-5.53634500	-7.68537100	-0.76125000
F	-3.73913800	-5.30265200	1.49955600
N	-4.67327900	-6.90840700	-0.14316900
C	-6.93471500	-7.25006200	-1.13139400
H	-7.67735600	-8.03552300	-0.94081200
H	-7.20306900	-6.35612400	-0.55820600
H	-6.96757500	-7.00370200	-2.20554000
C	-5.98558300	-9.85985100	-1.85743600
H	-5.32097000	-10.41852500	-2.53414000
H	-6.67378800	-9.29861100	-2.50139700
C	-6.75183600	-10.82580200	-0.95644300
H	-6.06339400	-11.41061100	-0.32631600
H	-7.44693900	-10.28533800	-0.29484400

H	-7.33513700	-11.53030600	-1.56997300
C	-3.79525200	-9.39223900	-0.76218100
H	-3.85366200	-10.48376900	-0.63832500
H	-3.52235900	-8.95782500	0.20793000
C	-2.75460200	-9.02920200	-1.81812900
H	-2.65889100	-7.93777100	-1.91057200
H	-1.77237800	-9.44054800	-1.53638100
H	-3.02654000	-9.44028800	-2.80356900
N	-5.14215500	-8.92214700	-1.10799700
O	-4.24058100	-4.38505700	-0.74937100
C	-3.08032300	-4.73216900	-1.53907000
H	-2.49505300	-5.50769300	-1.02125100
H	-2.46677400	-3.81993700	-1.58786700
C	-3.49229000	-5.18853300	-2.92420500
H	-4.08833000	-6.11228400	-2.87322300
H	-4.08946400	-4.41189100	-3.42719600
H	-2.59676100	-5.38892200	-3.53383600

32

Energy = -1015.70887900 a.u. #Cluster: 7

P	-5.29099300	-5.18116200	-0.48851100
O	-6.63646200	-4.61307700	-0.78330900
C	-5.65353100	-7.80093100	-0.53061800

F	-4.91870900	-4.94510400	1.07014100
N	-4.91240700	-6.73695200	-0.75483900
C	-7.02794800	-7.73956200	0.09517100
H	-7.41416200	-6.71623600	0.03278900
H	-7.73761600	-8.41403700	-0.40111200
H	-6.96553100	-8.03255700	1.15606300
C	-5.85414300	-10.26518500	-0.59359300
H	-6.51733900	-10.13434000	0.26998100
H	-5.09418100	-11.00113700	-0.29060100
C	-6.63912700	-10.78961900	-1.79440500
H	-5.97545400	-11.00624700	-2.64475500
H	-7.15762300	-11.72200700	-1.52077000
H	-7.39405600	-10.05873800	-2.12458400
C	-3.83808000	-9.08460100	-1.51510100
H	-3.45716600	-10.10278300	-1.35315000
H	-3.15807000	-8.38509700	-1.00932800
C	-3.89160500	-8.76602000	-3.00815300
H	-4.51667900	-9.48861000	-3.55350400
H	-4.29604200	-7.75749500	-3.17591900
H	-2.87534500	-8.80208600	-3.43169300
N	-5.14686500	-9.00492600	-0.85012200
O	-4.14336200	-4.32013100	-1.20307800

C	-2.73747500	-4.63385300	-1.07507200
H	-2.59053100	-5.37248700	-0.27221400
H	-2.24264700	-3.69893100	-0.76996500
C	-2.18903300	-5.14204700	-2.39203800
H	-2.67369100	-6.08790300	-2.67424500
H	-2.35741400	-4.40607300	-3.19398100
H	-1.10484200	-5.31687700	-2.30315300

32

Energy = -1015.70819700 a.u. #Cluster: 8

P	-4.89719000	-5.35851500	0.07379300
O	-6.09952700	-4.83306800	0.78165000
C	-5.68470600	-7.74427900	-0.80180800
F	-3.62292300	-5.28136300	1.06084700
N	-4.75198200	-6.87251100	-0.48514100
C	-7.16462100	-7.44971300	-0.72677800
H	-7.72136800	-8.27234600	-0.25873600
H	-7.32623600	-6.53119200	-0.15324800
H	-7.56385200	-7.30789500	-1.74438500
C	-6.23844300	-9.99276900	-1.67975200
H	-5.76064700	-10.51769300	-2.52105100
H	-7.14001900	-9.51974900	-2.08794200
C	-6.59982400	-10.98576500	-0.57743500

H	-7.11620100	-10.48495100	0.25642100
H	-7.26670800	-11.76533800	-0.97809200
H	-5.70061600	-11.47960400	-0.17654600
C	-3.87460100	-9.29970900	-1.30835600
H	-3.79367100	-10.38599000	-1.15410800
H	-3.36142300	-8.80424200	-0.47441600
C	-3.23774000	-8.90175300	-2.63711900
H	-3.74859500	-9.38562100	-3.48495200
H	-3.28171000	-7.81206600	-2.77964200
H	-2.18026300	-9.20942900	-2.65513200
N	-5.29987100	-8.95645900	-1.23569500
O	-4.44406900	-4.34766400	-1.09384000
C	-3.55413900	-4.70213400	-2.17377200
H	-3.61283900	-3.85474400	-2.87191500
H	-3.95117800	-5.59401500	-2.68337700
C	-2.12731400	-4.92637000	-1.71023200
H	-2.05210500	-5.81429400	-1.06511400
H	-1.47759900	-5.08276600	-2.58601100
H	-1.75614900	-4.05280200	-1.15178700

32

Energy = -1015.70815600 a.u. #Cluster: 9

P	-4.99579600	-5.37493900	0.06497100
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O	-6.26573500	-4.80558300	0.60001600
C	-5.76014100	-7.72393500	-0.92959600
F	-3.88989900	-5.40107800	1.24150800
N	-4.83957100	-6.87051000	-0.53702800
C	-7.23944600	-7.41715100	-0.93467400
H	-7.58556400	-7.28082100	-1.97213500
H	-7.82378100	-8.23460500	-0.49116700
H	-7.42494300	-6.49403700	-0.37649000
C	-6.28462000	-9.94885500	-1.88195700
H	-5.76598600	-10.46593800	-2.70376100
H	-7.15760300	-9.45998400	-2.33137200
C	-6.71651900	-10.95578200	-0.81809700
H	-7.36642800	-11.72249400	-1.26844000
H	-5.84550400	-11.46451800	-0.37581700
H	-7.27494200	-10.46374400	-0.00637800
C	-3.93921000	-9.28925100	-1.36443400
H	-3.87852800	-10.37884100	-1.22463900
H	-3.46956200	-8.81374800	-0.49409000
C	-3.22250800	-8.87762000	-2.64759100
H	-3.24749700	-7.78543100	-2.77528800
H	-2.16883300	-9.19633000	-2.60959900
H	-3.68808000	-9.34297500	-3.53116000

N	-5.36230200	-8.93035500	-1.36837800
O	-4.31585500	-4.35170900	-0.97417700
C	-3.27256300	-4.70991100	-1.90544500
H	-3.17098100	-3.83182500	-2.55932900
H	-3.61919100	-5.55586600	-2.51918400
C	-1.95758200	-5.03331200	-1.22188200
H	-1.64548000	-4.20700800	-0.56421900
H	-2.03655300	-5.95078400	-0.62021700
H	-1.17692400	-5.18787200	-1.98362300

32

Energy = -1015.70779700 a.u. #Cluster: 10

P	-5.21287400	-5.17858500	-0.33458300
O	-6.43566500	-4.33136100	-0.35279900
C	-5.92462700	-7.63252400	-0.96281400
F	-4.81676100	-5.54258500	1.19773700
N	-5.13220300	-6.59563600	-1.12577900
C	-7.05386600	-7.67690400	0.04263400
H	-8.02416500	-7.68849800	-0.47882400
H	-6.99855600	-8.57933400	0.66749200
H	-7.02961800	-6.79925400	0.69675200
C	-6.54868500	-9.92350800	-1.65366100
H	-6.67303000	-10.30720600	-2.67746900

H	-7.55192500	-9.65622600	-1.30086900
C	-5.94375400	-11.00472300	-0.75960900
H	-6.62525600	-11.86860300	-0.70874600
H	-4.97727500	-11.35732900	-1.15011300
H	-5.78502300	-10.63015500	0.26400100
C	-4.63519700	-8.69943400	-2.72687000
H	-4.63679000	-7.71941300	-3.22444400
H	-4.87645100	-9.46074200	-3.48211600
C	-3.25857300	-8.96908300	-2.12196300
H	-2.49449000	-8.93341200	-2.91479500
H	-3.00722300	-8.20653800	-1.37119600
H	-3.21296200	-9.96021500	-1.64668500
N	-5.73264900	-8.70758200	-1.74845800
O	-3.92372100	-4.34394200	-0.79134800
C	-2.61501900	-4.94445100	-0.92862900
H	-2.58586000	-5.90359600	-0.38877500
H	-1.91409900	-4.25615800	-0.43229800
C	-2.26522700	-5.12693100	-2.39108200
H	-2.30470900	-4.16339000	-2.92319500
H	-1.24567100	-5.53409500	-2.48394300
H	-2.96620400	-5.82539900	-2.87122400

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33

Energy = -1016.14525300 a.u. #Cluster: 1

P	-0.52414500	-6.16445000	-0.04431600
F	0.25900500	-6.63875800	-1.33711200
O	-0.11913500	-7.34264500	0.92846700
O	-1.94141300	-5.81585700	-0.24639000
N	2.06992400	-3.48430100	1.26237700
N	0.35515900	-4.78093500	0.42695700
C	1.18772400	-2.30271600	1.36787000
C	3.45450000	-3.28012700	1.74423700
C	1.64860600	-4.64421500	0.80954100
C	0.40725800	-2.27708200	2.67960300
C	4.37287600	-2.73407000	0.65764300
C	2.56088100	-5.82784900	0.73737700
C	-0.84813100	-7.62297500	2.16851300
C	-0.58544700	-6.57234800	3.22564300
H	1.83946900	-1.42320800	1.28694900
H	0.52499800	-2.26461500	0.49055500
H	3.83262200	-4.22120200	2.15917000
H	3.38082800	-2.57487000	2.58358000
H	1.09243900	-2.27813900	3.54079000

H	-0.19985800	-1.36051000	2.72109100
H	-0.26664100	-3.14248200	2.77117300
H	4.48049200	-3.44798200	-0.17335400
H	3.99039000	-1.78459400	0.25250900
H	5.36930800	-2.54781600	1.08595200
H	2.20219500	-6.56173000	0.01062900
H	3.57389700	-5.52553000	0.45190900
H	-1.91692500	-7.70247700	1.92169300
H	-0.47870800	-8.61105400	2.47048100
H	0.49364800	-6.46201300	3.41436500
H	-0.99757600	-5.59317900	2.93528500
H	-1.07286800	-6.87909000	4.16414200
H	2.60217600	-6.30823700	1.72855100
H	-0.25190000	-3.96411700	0.48472500

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Energy = -1016.14512700 a.u. #Cluster: 2

P	0.61100000	-7.09216400	1.84652100
F	1.39771400	-7.72199200	3.06912800
O	-0.84405800	-6.99232200	2.44874400
O	0.84581600	-7.79592600	0.57027600
N	2.37219500	-3.56617700	1.54372700
N	1.10604100	-5.45883900	1.91642300

C	1.39941900	-2.70994000	2.25344600
C	3.57393800	-2.86705600	1.03678900
C	2.20140100	-4.86071000	1.38707900
C	1.65225700	-2.65639100	3.75761600
C	3.35170300	-2.25420600	-0.34103000
C	3.21101800	-5.69057400	0.65943900
C	-2.05120400	-7.15814300	1.63178700
C	-2.33866700	-5.91698300	0.81722900
H	1.48894500	-1.70951200	1.81035300
H	0.38023300	-3.05041000	2.01909300
H	4.41998200	-3.56319600	1.03600200
H	3.80721300	-2.08886200	1.77675000
H	2.66469200	-2.28136700	3.97138600
H	0.92536000	-1.97279000	4.22122400
H	1.54225200	-3.64638500	4.22616800
H	4.25858300	-1.70977000	-0.64491400
H	3.14234300	-3.02767300	-1.09578200
H	2.51233600	-1.54212900	-0.33122200
H	2.79082900	-6.66312800	0.38606600
H	3.54903200	-5.18461000	-0.25256700
H	-1.91537800	-8.04701100	0.99902000
H	-2.83951700	-7.36259200	2.36718100

H	-2.42435200	-5.03123300	1.46559600
H	-1.55008800	-5.73716000	0.06919400
H	-3.29163600	-6.05043700	0.28151800
H	4.08274400	-5.84595400	1.31606800
H	0.46350300	-4.88552900	2.46229600

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Energy = -1016.14509400 a.u. #Cluster: 3

P	0.63197700	-7.10209900	1.78777200
F	1.44830600	-7.76921400	2.97019100
O	-0.80861700	-7.02499900	2.42709900
O	0.83731200	-7.76446100	0.48428900
N	2.37095400	-3.56148300	1.54535200
N	1.12458100	-5.47035600	1.89986600
C	1.40707600	-2.72876800	2.29423800
C	3.55794600	-2.84218500	1.03203300
C	2.20463900	-4.85291600	1.36142200
C	1.68875000	-2.70905100	3.79408200
C	3.30375100	-2.19732400	-0.32540500
C	3.20403100	-5.65911000	0.59492300
C	-2.03577800	-7.18174400	1.63936100
C	-2.35645200	-5.92246800	0.86613500
H	1.48247400	-1.71752600	1.87373700

H	0.38596300	-3.07041800	2.07038600
H	4.40806200	-3.53245500	0.99699700
H	3.80106600	-2.08124500	1.78656100
H	1.59511800	-3.71021700	4.24182800
H	2.70227900	-2.33115500	3.99686300
H	0.96608500	-2.04205400	4.28738800
H	2.46040400	-1.49137200	-0.28130000
H	4.20085200	-1.63966300	-0.63401800
H	3.08408400	-2.95372100	-1.09430700
H	4.08484200	-5.83234800	1.23478800
H	2.78117300	-6.62397200	0.29903900
H	-1.90895700	-8.05206100	0.97953900
H	-2.80162500	-7.41363000	2.39015500
H	-2.43141900	-5.05448300	1.53919800
H	-1.59038900	-5.71676000	0.10177400
H	-3.32268800	-6.05085800	0.35354800
H	3.52868900	-5.12662400	-0.30656200
H	0.49116200	-4.91442900	2.47363000

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Energy = -1016.14492000 a.u. #Cluster: 4

P	0.65948900	-7.11163500	2.05523400
F	1.30401000	-7.58300500	3.42253300

O	-0.85710300	-7.01352300	2.48117800
O	1.05942000	-7.93018600	0.89391600
N	2.30758100	-3.55083000	1.55747000
N	1.10624100	-5.46395400	2.01084800
C	1.28760000	-2.70221400	2.20773800
C	3.48794500	-2.82952400	1.03241800
C	2.19137600	-4.85783100	1.46839400
C	1.50529200	-2.57546000	3.71324000
C	3.26758000	-2.30772600	-0.38270600
C	3.24449700	-5.68486300	0.80348900
C	-1.95948000	-7.17354300	1.52734100
C	-2.08566500	-5.97373700	0.61441200
H	1.34948400	-1.71884500	1.72387400
H	0.28763400	-3.09126300	1.96578300
H	4.36350600	-3.48600600	1.08769000
H	3.67163600	-2.00060500	1.72993200
H	1.42993600	-3.54890700	4.22165100
H	2.49572300	-2.14725500	3.92978500
H	0.73964700	-1.90657500	4.13380200
H	3.10639200	-3.13237300	-1.09364100
H	2.39849600	-1.63380900	-0.42943400
H	4.15644200	-1.74304800	-0.70234400

H	4.10772800	-5.77318800	1.48366700
H	2.86466400	-6.68585000	0.57889400
H	-1.79036000	-8.10429500	0.96669400
H	-2.84171700	-7.29957800	2.16736300
H	-2.19778300	-5.04534700	1.19561900
H	-1.20945000	-5.87835400	-0.04623800
H	-2.97693000	-6.09758500	-0.02043700
H	3.58303100	-5.21413500	-0.12684500
H	0.43878800	-4.87612200	2.50928500

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Energy = -1016.14488300 a.u. #Cluster: 5

P	1.25059000	-7.38645700	2.27249500
F	1.06102400	-7.52526000	3.84295700
O	-0.20423000	-7.53385000	1.68378700
O	2.24270300	-8.29737200	1.67634700
N	2.16550400	-3.64611700	1.42718100
N	1.64190500	-5.71944800	2.28859900
C	1.87256800	-2.99088600	2.71950200
C	2.56310100	-2.73586200	0.33049400
C	2.04393400	-4.94278600	1.25271400
C	0.38648000	-2.68857700	2.89349100
C	4.05906600	-2.44539700	0.33271800

C	2.30079700	-5.58484500	-0.07293000
C	-1.34785900	-6.69725800	2.05599200
C	-1.69932800	-5.76343200	0.92104900
H	2.26756200	-3.61142600	3.53771500
H	2.46134800	-2.06508200	2.73678600
H	1.98472100	-1.81305200	0.47800600
H	2.23597500	-3.16204300	-0.62431400
H	-0.22076300	-3.60630000	2.90628000
H	0.23498700	-2.16212900	3.84751400
H	0.02294000	-2.04350100	2.07949800
H	4.64450100	-3.36060100	0.15563800
H	4.28898300	-1.72584700	-0.46756800
H	4.37968400	-2.00724100	1.29029200
H	1.41362400	-5.44702400	-0.71294900
H	3.16522600	-5.13281200	-0.57195000
H	-2.15814700	-7.40690200	2.27002700
H	-1.11622400	-6.14992700	2.98173100
H	-2.61115200	-5.20509100	1.18510800
H	-0.89612900	-5.03462200	0.73377800
H	-1.89100900	-6.32742900	-0.00419900
H	2.48713900	-6.65690200	0.05055800
H	1.46613200	-5.26569300	3.18425300

Energy = -1016.14485200 a.u. #Cluster: 6

P	0.59392700	-7.11561600	1.79869000
F	1.33710100	-7.78047600	3.02915000
O	-0.87715000	-7.02155200	2.36179000
O	0.86168900	-7.79039000	0.51328700
N	2.36455800	-3.58916500	1.58563300
N	1.09760200	-5.48803500	1.91943100
C	1.36474300	-2.73916700	2.26449000
C	3.57945500	-2.88350600	1.12078200
C	2.20377300	-4.88368000	1.42005100
C	1.57265400	-2.68002800	3.77508800
C	3.40171200	-2.26963800	-0.26309500
C	3.23592700	-5.70734500	0.71824600
C	-2.06132900	-7.10709700	1.50055600
C	-2.27714000	-5.82503000	0.72794900
H	1.45958900	-1.73899000	1.82186400
H	0.35608900	-3.08908800	2.00079000
H	4.42852900	-3.57548100	1.14912300
H	3.78298700	-2.10522200	1.86922400
H	2.57322900	-2.29136000	4.01790900
H	0.82366200	-2.00506900	4.21555500

H	1.46198700	-3.67019800	4.24297700
H	4.31553200	-1.71968900	-0.53430400
H	3.22297700	-3.04284500	-1.02582800
H	2.55839500	-1.56250700	-0.28106500
H	4.07901500	-5.87900000	1.40764800
H	2.82124400	-6.67311800	0.41392400
H	-1.93774700	-7.97515300	0.83703500
H	-2.88048800	-7.31000300	2.20180800
H	-2.34674500	-4.96156100	1.40754500
H	-1.46277300	-5.64771400	0.00757700
H	-3.21927900	-5.90034500	0.16263400
H	3.61374900	-5.19047500	-0.17137800
H	0.44817400	-4.92262600	2.46551600

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Energy = -1016.14462100 a.u. #Cluster: 7

P	0.74907300	-7.16944400	1.13306400
F	1.98311100	-8.11383000	1.43915100
O	-0.16665900	-7.49510000	2.37712200
O	0.22328200	-7.29805100	-0.23950600
N	2.31919500	-3.55048800	1.32461600
N	1.36970800	-5.63706700	1.55965100
C	2.05524000	-3.22149000	2.74130700

C	2.95973900	-2.47652600	0.53391200
C	1.98423300	-4.70542700	0.79124500
C	0.64272100	-2.68713900	2.96184900
C	4.47964000	-2.49603700	0.65007900
C	2.25830800	-4.99363000	-0.65047800
C	-1.62816800	-7.38809500	2.33157600
C	-2.07927400	-5.94707200	2.41935200
H	2.26708700	-4.10415800	3.36325800
H	2.80173800	-2.46999600	3.02844900
H	2.55091800	-1.53134600	0.91782000
H	2.63637600	-2.55801300	-0.50976000
H	0.46879200	-1.78527700	2.35567300
H	-0.12275600	-3.43376600	2.70259200
H	0.51871200	-2.42120300	4.02221700
H	4.90149800	-3.42616900	0.23984600
H	4.89562900	-1.64842400	0.08478000
H	4.80225500	-2.40040100	1.69808100
H	2.08540000	-6.04554200	-0.89092100
H	1.58248400	-4.38652900	-1.27386400
H	-1.97697700	-7.87576300	1.40979100
H	-1.96202800	-7.97877200	3.19389400
H	-3.17910100	-5.91597000	2.46514200

H	-1.67882800	-5.46273400	3.32314900
H	-1.75935900	-5.37178000	1.53629500
H	3.29234100	-4.72778600	-0.90334900
H	1.22132100	-5.41814600	2.54456900

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Energy = -1016.14444100 a.u. #Cluster: 8

P	0.28045200	-6.49110500	1.47804800
F	0.90563200	-7.04517400	2.83296800
O	-1.21873000	-6.16304700	1.84499300
O	0.59178400	-7.37078200	0.33313100
N	2.46483600	-3.22367900	1.28883800
N	0.88312800	-4.89843500	1.45015300
C	1.43927300	-2.17085200	1.44328400
C	3.85877300	-2.73546000	1.18573300
C	2.16723800	-4.50300100	1.27381400
C	1.15605600	-1.83730500	2.90522100
C	4.24966800	-2.38679600	-0.24521400
C	3.21449300	-5.55713300	1.10176400
C	-2.32702000	-7.05374000	1.48835900
C	-2.34764700	-8.28172600	2.37094500
H	1.82171800	-1.28951500	0.91199600
H	0.52959800	-2.47463800	0.90517800

H	4.53225100	-3.48308600	1.61956500
H	3.91655500	-1.84907300	1.83265900
H	0.74684600	-2.70161000	3.45050500
H	2.07234900	-1.50533500	3.41639500
H	0.42003100	-1.02082700	2.95188800
H	3.57717200	-1.62558200	-0.66947800
H	5.27253900	-1.98080700	-0.25086900
H	4.22501400	-3.27404900	-0.89619100
H	3.62046500	-5.82093400	2.09254000
H	2.77636700	-6.45513200	0.65030000
H	-3.21882800	-6.42956200	1.62545200
H	-2.22979300	-7.30939500	0.42304000
H	-3.24183700	-8.88033400	2.13643700
H	-1.46195600	-8.91324400	2.19697500
H	-2.38367600	-8.00059800	3.43443500
H	4.03421400	-5.21444900	0.46319800
H	0.16868600	-4.19476800	1.63453900

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Energy = -1016.14431100 a.u. #Cluster: 9

P	-0.90231500	-5.92132600	0.32401700
F	-0.47069800	-6.03381000	-1.19427500
O	-0.30973600	-7.29391500	0.84206900

O	-2.31531800	-5.58747100	0.57366500
N	1.99336200	-3.40659900	1.29212800
N	0.10093200	-4.65803600	0.87979100
C	1.20366900	-2.35837800	1.97371300
C	3.44218600	-3.12865200	1.17347200
C	1.44454900	-4.49403100	0.79781900
C	0.62209300	-1.33735500	0.99948900
C	4.21941600	-3.55945300	2.41167100
C	2.26317100	-5.54111800	0.11191500
C	-0.68297100	-7.87390800	2.13545800
C	0.05080600	-7.20420000	3.27669800
H	0.42404000	-2.83657900	2.58483400
H	1.88475700	-1.87212700	2.68390600
H	3.53127800	-2.04474900	1.01491300
H	3.82636400	-3.60982000	0.26732500
H	0.07708300	-0.56782300	1.56626200
H	1.42156800	-0.84363000	0.42658500
H	-0.07750500	-1.80243000	0.28832600
H	5.27866500	-3.28870000	2.28596200
H	3.84213700	-3.05608300	3.31491100
H	4.15462400	-4.64731600	2.56716200
H	3.24612800	-5.64992000	0.58113600

H	1.75977400	-6.51204500	0.14090900
H	-1.77497500	-7.79468900	2.24046700
H	-0.41189200	-8.93259600	2.03672100
H	-0.25933800	-6.15475300	3.39877500
H	-0.18029200	-7.73726100	4.21225200
H	1.13973200	-7.23670300	3.11770600
H	2.40454900	-5.24725700	-0.94138000
H	-0.45019300	-3.90843700	1.29620100

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Energy = -1016.14428800 a.u. #Cluster: 10

P	-0.89869500	-5.50624300	0.93865700
F	-0.42229200	-6.35813900	-0.32444000
O	-0.49668200	-6.41782300	2.16496000
O	-2.27290300	-4.99267100	0.79794800
N	2.25497600	-3.16947500	1.32362600
N	0.24459800	-4.25503100	1.00906600
C	1.59672100	-1.84569700	1.29773000
C	3.71520400	-3.14041200	1.56608300
C	1.59149100	-4.29383300	1.17433800
C	1.06266400	-1.43332600	2.66645000
C	4.51339300	-2.96565900	0.28010400
C	2.28360500	-5.61968700	1.20520700

C	-1.26966300	-7.59518600	2.57295400
C	-0.87285700	-8.81532600	1.77142500
H	2.35307500	-1.13242900	0.94536800
H	0.80898400	-1.84959400	0.53052600
H	4.00678000	-4.04848100	2.10530600
H	3.89145500	-2.30005600	2.25184600
H	1.87298600	-1.40835000	3.41062400
H	0.62666000	-0.42568700	2.59500700
H	0.28249600	-2.12245000	3.02434700
H	4.22334700	-2.04396900	-0.24708900
H	5.58409000	-2.89802600	0.52528300
H	4.36598700	-3.81675300	-0.40226300
H	1.71676300	-6.36850700	0.64434000
H	3.28842300	-5.55421400	0.77609600
H	-1.03589500	-7.70934400	3.63909900
H	-2.33859700	-7.35604000	2.46977100
H	-1.40673300	-9.69337100	2.16775600
H	-1.13531200	-8.70427700	0.70860200
H	0.20928700	-9.00034300	1.85264700
H	2.36570200	-5.95665300	2.25127500
H	-0.21340700	-3.34411800	0.98795500

A234-N₂H

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Energy = -1016.12624800 a.u. #Cluster: 1

P	0.56812600	-0.33747800	-1.74583700
F	0.68415500	0.19880600	-3.23251600
O	2.05416100	-0.47349400	-1.24977700
O	-0.23095500	-1.59105300	-1.63607700
N	-1.85402900	-0.17100600	0.09886400
N	-0.06860900	1.02515000	-0.99499400
C	-3.27907400	-0.11591200	-0.42132300
C	-1.79938800	-0.52020400	1.57396800
C	-1.07224000	1.06843500	-0.22482900
C	-3.32693800	0.16560100	-1.91102100
C	-0.37464500	-0.64801800	2.08037700
C	-1.53999900	2.31984700	0.42593400
C	3.02525200	0.62481800	-1.21354600
C	3.12993400	1.18159000	0.18768200
H	-3.69838700	-1.10237700	-0.18310500
H	-3.81365500	0.63721400	0.17164800
H	-2.34242900	-1.47118400	1.65474800
H	-2.37298400	0.24799100	2.10937600
H	-2.96104100	1.17414000	-2.15660400

H	-2.73558100	-0.57252200	-2.47356300
H	-4.37260600	0.09708200	-2.24426700
H	0.18928600	-1.39709800	1.50314700
H	0.17172000	0.30671800	2.04607500
H	-0.40821900	-0.97789500	3.12881200
H	-1.36349100	2.26722100	1.51278100
H	-0.97862500	3.16478500	0.01242500
H	3.96722400	0.17173800	-1.54996800
H	2.72617000	1.39038400	-1.94440600
H	3.40384300	0.39092500	0.90277400
H	3.91103300	1.95781200	0.20981000
H	2.17886200	1.63559600	0.50437900
H	-2.61900700	2.47310400	0.27564300
H	-1.38453700	-0.94730800	-0.42588100

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Energy = -1016.12623300 a.u. #Cluster: 2

P	0.60685800	-0.52241300	-1.61412800
F	0.69228900	-0.17171100	-3.15724100
O	2.10089500	-0.58335500	-1.12889400
O	-0.17320400	-1.76250600	-1.33813400
N	-1.89061100	-0.13075400	0.09252100
N	-0.02712200	0.91677400	-1.02016100

C	-3.32665300	-0.03227500	-0.38652000
C	-1.80792600	-0.42175800	1.57991600
C	-1.05436400	1.05376300	-0.29319500
C	-3.41832700	0.24106700	-1.87578100
C	-0.37772400	-0.63839000	2.03861600
C	-1.48041300	2.36345600	0.26560800
C	3.04284900	0.53883300	-1.18361800
C	3.16416400	1.17683900	0.18109200
H	-3.77060800	-1.00257800	-0.12739100
H	-3.81907500	0.74037800	0.21776700
H	-2.41750300	-1.32396200	1.72205100
H	-2.30017000	0.41108700	2.09884000
H	-4.47678100	0.20359800	-2.17154600
H	-3.02902200	1.23531200	-2.14257600
H	-2.87058600	-0.51909500	-2.45388300
H	-0.39370300	-0.91285300	3.10332100
H	0.10067200	-1.45769800	1.48122100
H	0.23846800	0.26780500	1.93561400
H	-1.29010000	2.37844900	1.35226000
H	-0.89376500	3.15824000	-0.20813300
H	3.98864000	0.09130200	-1.51691200
H	2.70602600	1.25361900	-1.94857300

H	3.92506800	1.97219800	0.14278500
H	2.20799200	1.62313700	0.49360200
H	3.47338100	0.43395000	0.93212200
H	-2.55487100	2.54424400	0.11847600
H	-1.46144700	-0.95129500	-0.39839800

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Energy = -1016.12623000 a.u. #Cluster: 3

P	0.63786500	-0.42504300	-1.64816600
F	0.80214800	0.01833300	-3.16074400
O	2.10618900	-0.52398200	-1.09401300
O	-0.15826900	-1.67497100	-1.48627500
N	-1.88721600	-0.14462200	0.03577500
N	-0.02260600	0.97805500	-0.99951200
C	-3.32675900	-0.03249400	-0.42766700
C	-1.79466500	-0.52695700	1.50321000
C	-1.06265800	1.06804100	-0.28317600
C	-3.43087800	0.30493400	-1.90279200
C	-0.36209600	-0.76728800	1.94116500
C	-1.51416000	2.34528600	0.32763400
C	3.06892900	0.58183800	-1.07574400
C	3.12230900	1.20253300	0.30131500
H	-3.76369300	-1.01572800	-0.20872900

H	-3.81904300	0.70959400	0.21399100
H	-2.40099300	-1.43826900	1.59042300
H	-2.28742400	0.26942700	2.07661700
H	-4.49110100	0.27454400	-2.19286400
H	-3.04738300	1.31121600	-2.12956000
H	-2.88320600	-0.42741600	-2.51594200
H	0.11464200	-1.55363400	1.33721100
H	0.25254400	0.14423800	1.88877500
H	-0.37395500	-1.10172800	2.98871900
H	-0.92144200	3.16606500	-0.09094100
H	-2.58543800	2.52649000	0.15972400
H	4.02448600	0.12072900	-1.35867100
H	2.79071000	1.31120900	-1.85048200
H	3.37254300	0.44639300	1.06098500
H	3.90004600	1.98229300	0.31562400
H	2.15931700	1.66627300	0.56283900
H	-1.35294200	2.30772600	1.41841300
H	-1.45247300	-0.92967800	-0.50641000

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Energy = -1016.12622900 a.u. #Cluster: 4

P	0.59104000	-0.39075000	-1.63822900
F	0.59568200	0.10417100	-3.14512300

O	2.10955100	-0.48010800	-1.24265600
O	-0.16902500	-1.65833100	-1.44478500
N	-1.88550400	-0.16898500	0.13310700
N	-0.02525000	0.97978900	-0.88469200
C	-3.25073500	-0.07999500	-0.53017800
C	-1.99298400	-0.49467700	1.60995300
C	-1.04667400	1.04508900	-0.13954800
C	-3.14781100	0.17547500	-2.02143200
C	-0.63408400	-0.69521400	2.25431800
C	-1.49255500	2.30324400	0.51521500
C	3.05613100	0.63662400	-1.32590900
C	3.26625300	1.24282500	0.04228800
H	-3.72429400	-1.04776500	-0.31866800
H	-3.81527400	0.70113000	-0.00506800
H	-2.59398100	-1.41312900	1.64856600
H	-2.57209900	0.31180800	2.07823500
H	-2.71467600	1.16130300	-2.24825200
H	-2.54733800	-0.60047100	-2.51938500
H	-4.16180800	0.14952500	-2.44625900
H	-0.03545300	0.22826300	2.27479400
H	-0.78702300	-1.01875300	3.29411900
H	-0.05897800	-1.47492700	1.73127600

H	-0.92500000	3.14122600	0.09582400
H	-2.57163600	2.46877800	0.38058800
H	3.97600300	0.19034500	-1.72662600
H	2.67986300	1.37100100	-2.05301500
H	3.61689800	0.48200900	0.75625600
H	4.02925400	2.03418100	-0.02675600
H	2.33495100	1.68848100	0.42305500
H	-1.30151100	2.24872000	1.59962100
H	-1.38860900	-0.96747600	-0.32990300

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Energy = -1016.12622800 a.u. #Cluster: 5

P	0.58259700	-0.42316900	-1.65120400
F	0.59939000	0.03854700	-3.16836900
O	2.09765200	-0.51077900	-1.24230600
O	-0.18539800	-1.68258000	-1.43569200
N	-1.87739700	-0.15685800	0.13891500
N	-0.03185200	0.96717900	-0.93271100
C	-3.25864300	-0.08634900	-0.49118000
C	-1.94846900	-0.44805800	1.62541500
C	-1.04760900	1.05190200	-0.18182800
C	-3.19325800	0.13300600	-1.99027500
C	-0.57334100	-0.61421700	2.24427900

C	-1.49593600	2.32925500	0.43255600
C	3.04285800	0.60859000	-1.30739700
C	3.24290500	1.19712600	0.06996700
H	-3.72462900	-1.04946400	-0.24474500
H	-3.81094600	0.70651900	0.02928600
H	-2.53597600	-1.37306200	1.69892500
H	-2.52789400	0.36168000	2.08753000
H	-2.77092500	1.11501100	-2.25148300
H	-2.59988300	-0.65161600	-2.48319900
H	-4.21697000	0.09161200	-2.38977200
H	-0.69851400	-0.91400600	3.29480300
H	0.00158500	-1.39815100	1.72725300
H	0.01086200	0.31841700	2.22749200
H	-0.91678300	3.15239600	-0.00002100
H	-2.57138800	2.49697200	0.27160100
H	3.96583300	0.16894300	-1.70825200
H	2.66879200	1.35142700	-2.02694600
H	3.59145300	0.42770300	0.77570200
H	4.00367500	1.99179500	0.01634200
H	2.30779900	1.63444600	0.45132400
H	-1.32663600	2.30406600	1.52156200
H	-1.38962900	-0.96487600	-0.31684100

Energy = -1016.12622700 a.u. #Cluster: 6

P	0.62849500	-0.47875100	-1.61898800
F	0.74539300	-0.08967400	-3.15082600
O	2.11251100	-0.55185500	-1.10482000
O	-0.15659900	-1.72534500	-1.39065500
N	-1.88541900	-0.13766300	0.07283400
N	-0.01980000	0.94468600	-1.00326000
C	-3.33111800	-0.02721900	-0.36830200
C	-1.76972900	-0.47844200	1.54958200
C	-1.06135100	1.06171100	-0.29333400
C	-3.45658000	0.18510600	-1.86473600
C	-0.32745600	-0.63170000	1.99421400
C	-1.53809300	2.36606700	0.23696200
C	3.06003200	0.56686300	-1.13047900
C	3.16104400	1.18934100	0.24301400
H	-3.78970600	-0.97527900	-0.05763600
H	-3.79011700	0.78026800	0.21667900
H	-2.32774600	-1.41765300	1.65978900
H	-2.30174300	0.30485100	2.10510400
H	-4.52362400	0.17761200	-2.13035000
H	-3.03566600	1.14965200	-2.18722900

H	-2.95504900	-0.62101200	-2.42212900
H	-0.32496200	-0.94661300	3.04787900
H	0.19381100	-1.40295700	1.40770200
H	0.23622600	0.31086300	1.92519400
H	-0.76487900	3.12242300	0.06279300
H	-2.46037800	2.67021700	-0.28470600
H	4.00953100	0.11933700	-1.45307600
H	2.73899200	1.29174100	-1.89277000
H	2.20195000	1.63711800	0.54421600
H	3.45393000	0.43715800	0.99136300
H	3.92618800	1.98139900	0.22599300
H	-1.77333200	2.30291700	1.30984100
H	-1.46142800	-0.94175900	-0.44913300

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Energy = -1016.12508500 a.u. #Cluster: 7

P	0.71488600	-0.09599900	-1.19527800
F	0.89488400	0.55769100	-2.62999200
O	2.16008600	-0.13410700	-0.57848400
O	0.03158300	-1.42020300	-1.23427900
N	-2.01129900	-0.20889800	0.17720100
N	-0.10132200	1.14416500	-0.40616900
C	-3.36511100	-0.07093400	-0.49501500

C	-2.12654000	-0.81624200	1.56353100
C	-1.22098600	1.06791600	0.17970200
C	-3.26293900	0.52573100	-1.88666800
C	-0.76682100	-1.09536200	2.17686500
C	-1.81835200	2.20134600	0.93333400
C	3.07916800	1.00758300	-0.52240100
C	3.98774900	1.02007200	-1.73092900
H	-3.76131700	-1.09463100	-0.52591100
H	-4.00233000	0.52053800	0.17509300
H	-2.69785100	-1.74213000	1.41521200
H	-2.73427100	-0.13132800	2.16928900
H	-4.25869700	0.49268800	-2.35195800
H	-2.93304100	1.57554900	-1.86983600
H	-2.56798500	-0.05213500	-2.51563500
H	-0.91927100	-1.58867700	3.14771300
H	-0.17262400	-1.76661600	1.53895600
H	-0.19019200	-0.17494800	2.35589800
H	-1.79842800	1.97741200	2.01303700
H	-1.22533400	3.10307900	0.74546300
H	2.48757800	1.93041300	-0.43319500
H	3.63698300	0.85925200	0.41129900
H	4.54786300	0.07578700	-1.80936600

H	3.41548800	1.17430400	-2.65767500
H	4.70990700	1.84543100	-1.62818200
H	-2.86780300	2.37201400	0.65310300
H	-1.45033100	-0.88535500	-0.39398900

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Energy = -1016.12491400 a.u. #Cluster: 8

P	0.71764500	-0.15407400	-1.17148200
F	0.92582600	0.47204900	-2.61486900
O	2.15565300	-0.21857300	-0.54061300
O	-0.00162600	-1.45910000	-1.20070900
N	-2.00760300	-0.17814800	0.21332900
N	-0.07642900	1.12264300	-0.41849900
C	-3.27869600	-0.10051500	-0.61473000
C	-2.28594700	-0.63118500	1.63394400
C	-1.20673600	1.09068700	0.15017900
C	-2.99488300	0.24351300	-2.06444900
C	-1.01654500	-0.75845900	2.45448000
C	-1.83527400	2.28648400	0.76995000
C	3.09844800	0.90353000	-0.48017900
C	4.03325700	0.87661800	-1.66807000
H	-3.73365100	-1.09533400	-0.51981500
H	-3.93963500	0.62667300	-0.12534300

H	-2.79022700	-1.60007600	1.52197700
H	-3.00270000	0.07881300	2.06657700
H	-3.94391600	0.21349000	-2.61919800
H	-2.56976900	1.25204700	-2.18146600
H	-2.30828200	-0.48600600	-2.51954600
H	-1.27723200	-1.18233700	3.43504500
H	-0.29512100	-1.43274600	1.96740100
H	-0.52916900	0.21324700	2.62627800
H	-1.14256600	3.13124600	0.69069300
H	-2.77497800	2.53359800	0.24990200
H	2.52610500	1.84058900	-0.41844500
H	3.63190200	0.75751500	0.46807100
H	4.77021300	1.68851600	-1.56319800
H	4.57499400	-0.08025000	-1.71820400
H	3.48423600	1.02630000	-2.60958500
H	-2.08464200	2.10481500	1.82634800
H	-1.40932700	-0.91216400	-0.23504100

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Energy = -1016.12458600 a.u. #Cluster: 9

P	0.76535200	-0.04160200	-1.78373900
F	1.00211600	0.62341700	-3.20212300
O	2.20678500	-0.31398700	-1.21764500

O	-0.10009300	-1.25431700	-1.84209400
N	-1.83712500	0.14002800	-0.21475400
N	0.16171800	1.27630500	-0.93370500
C	-3.19147800	0.46855700	-0.82448300
C	-1.92969500	-0.46565000	1.17199500
C	-0.91095200	1.31796400	-0.26206500
C	-3.86821100	-0.77603800	-1.36890900
C	-0.56973700	-0.90030300	1.68616100
C	-1.32532300	2.50333100	0.53271700
C	3.20814800	0.71979400	-0.94052500
C	3.23660900	1.02697600	0.53920700
H	-3.78641500	0.96337200	-0.04614300
H	-2.99711700	1.18825300	-1.63158900
H	-2.60871100	-1.32090800	1.06785200
H	-2.41154700	0.27913500	1.81856600
H	-4.81371400	-0.47321400	-1.84259300
H	-3.24221000	-1.26251100	-2.13270900
H	-4.10383200	-1.50397800	-0.57910900
H	-0.09650000	-1.62074500	1.00208100
H	0.11355400	-0.04958100	1.83299900
H	-0.70687300	-1.39184500	2.66013900
H	-2.36144700	2.79813600	0.30950200

H	-1.27546100	2.26622500	1.60844700
H	4.15554700	0.28952900	-1.29158200
H	2.98279100	1.60972000	-1.54624200
H	2.28208100	1.46349300	0.87003600
H	3.43262200	0.11441000	1.12266400
H	4.04095200	1.75106900	0.74372700
H	-0.64188900	3.33200900	0.31732200
H	-1.39661600	-0.58363500	-0.83267400

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Energy = -1016.12449500 a.u. #Cluster: 10

P	0.70241200	-0.11123800	-1.75971900
F	0.82713600	0.53884300	-3.20019100
O	2.18871900	-0.36078900	-1.30956600
O	-0.15266700	-1.33217100	-1.73633700
N	-1.83676700	0.10874500	-0.08574000
N	0.15097400	1.21233400	-0.88223900
C	-3.12611100	0.40975900	-0.84289700
C	-2.07740200	-0.36801600	1.33092700
C	-0.89325000	1.27058900	-0.16833100
C	-3.75418800	-0.86279200	-1.37968900
C	-0.79007100	-0.79007700	2.01462500
C	-1.27181000	2.47171100	0.62142400

C	3.22318900	0.67533300	-1.24403300
C	3.40361800	1.14470600	0.18127800
H	-3.78574200	0.94923300	-0.15133800
H	-2.84952700	1.08353400	-1.66541500
H	-2.77373600	-1.21071300	1.23801400
H	-2.59400600	0.44333200	1.86003300
H	-4.65987000	-0.59083100	-1.94147100
H	-3.06456900	-1.37918600	-2.06444200
H	-4.04870200	-1.55383500	-0.57651200
H	-1.03640700	-1.18855100	3.00940600
H	-0.27683800	-1.57879100	1.44307200
H	-0.09450600	0.05195500	2.15159400
H	-1.09587900	2.28062000	1.69326600
H	-0.64757000	3.31550400	0.30704300
H	4.12647200	0.18905600	-1.63597400
H	2.95019100	1.49828600	-1.92093100
H	3.64974300	0.29992200	0.84258500
H	4.23178700	1.86987800	0.21989700
H	2.49228400	1.63670900	0.55302400
H	-2.33729800	2.71720300	0.50122700
H	-1.36628100	-0.66685500	-0.61185900

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Energy = -1016.12987900 a.u. #Cluster: 1

P	1.21802100	1.02068200	0.65097700
F	1.27233900	1.03262400	2.24342800
O	2.09615400	-0.20953800	0.23464600
N	-2.37450800	0.39547900	-0.39981000
N	-0.24053800	1.01708000	0.08411200
C	-2.51314700	1.60661300	-1.22962100
C	-3.53976100	-0.50603000	-0.37518300
C	-1.24447600	0.14895800	0.24309000
C	-2.01557900	1.38605400	-2.65442000
C	-4.53253500	-0.14816000	0.72597000
C	-1.08920300	-1.08631600	1.08699000
C	3.49873300	-0.41619800	0.62693600
C	4.42655000	0.06055200	-0.46605000
H	-3.57888900	1.87485200	-1.22345700
H	-1.95676600	2.41727800	-0.74387700
H	-3.19392500	-1.54253200	-0.28334100
H	-4.01409000	-0.42388700	-1.36339100
H	-0.94043300	1.15293300	-2.65956300
H	-2.55776900	0.56112100	-3.14292800

H	-2.17596600	2.29978100	-3.24722800
H	-4.07967400	-0.25999200	1.72329400
H	-4.88316700	0.89010900	0.62004000
H	-5.40698600	-0.81395300	0.66510000
H	-0.58357800	-1.86027900	0.48575600
H	-0.45192700	-0.86055000	1.95199100
H	-2.03862000	-1.48991300	1.45177300
H	3.67611100	0.09810800	1.58264300
H	3.57430700	-1.49839700	0.79359200
H	4.20982500	-0.45415400	-1.41445400
H	4.33607800	1.14617900	-0.61798300
H	5.46504400	-0.16558600	-0.17681400
O	2.02404600	2.31102700	0.23058000
H	1.53586800	3.15361900	0.29817100

33

Energy = -1016.12935300 a.u. #Cluster: 2

P	1.39093400	0.64937600	1.36339300
F	1.95084800	-0.81568400	1.63108500
O	2.56086800	1.39362200	0.62893300
N	-2.01487400	0.23052700	-0.26525500
N	0.07380300	0.65126000	0.52363800
C	-1.70633400	1.07186500	-1.43732500

C	-3.34758300	-0.39746800	-0.25411900
C	-1.11273500	0.06223000	0.68816100
C	-0.98543000	0.29392400	-2.53339800
C	-4.40812400	0.49745600	0.37839500
C	-1.39868700	-0.77755700	1.90144900
C	2.74047300	1.39586700	-0.82749500
C	3.15542700	0.03647600	-1.34394700
H	-2.66374400	1.46770400	-1.80345400
H	-1.09767700	1.91843500	-1.09668000
H	-3.28728900	-1.36804600	0.25251200
H	-3.59758700	-0.61049600	-1.30325000
H	-1.58522300	-0.56531700	-2.87239700
H	-0.81067600	0.95286400	-3.39795600
H	-0.01238700	-0.07413800	-2.17624000
H	-5.39223500	0.00887000	0.31169500
H	-4.18535600	0.68712600	1.43992400
H	-4.46949200	1.46635500	-0.14101300
H	-0.87034400	-1.73928600	1.79285500
H	-0.99104400	-0.27010400	2.78693500
H	-2.46112300	-0.97445700	2.06899000
H	1.79937200	1.74104600	-1.27895200
H	3.51717300	2.15339500	-0.98992100

H	4.06016100	-0.32188600	-0.82983900
H	2.35257000	-0.70651700	-1.21672800
H	3.37317300	0.11597800	-2.42062500
O	1.26164900	1.29401200	2.79924800
H	2.08303000	1.37013100	3.32235400

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Energy = -1016.12861100 a.u. #Cluster: 3

P	1.35684800	0.99658900	-0.10499800
F	1.52273300	2.21462200	0.90324400
O	2.09751400	-0.19773500	0.59466100
N	-2.38112200	0.41174300	-0.42333200
N	-0.13573000	0.75746800	-0.50004900
C	-2.46965700	0.82879500	-1.83455500
C	-3.65639800	0.08631000	0.23739100
C	-1.21131300	0.38056400	0.19570500
C	-2.58928800	2.34212600	-1.98182700
C	-4.07265100	-1.36597000	0.02738600
C	-1.12282400	-0.03874000	1.63776000
C	3.48572700	-0.15985100	1.08172700
C	4.42275700	-0.74917000	0.05347900
H	-1.57845000	0.45661800	-2.35453500
H	-3.34722100	0.32301500	-2.26069500

H	-4.40809800	0.76780200	-0.18664900
H	-3.58277500	0.33034800	1.30371800
H	-2.69110600	2.60263400	-3.04669000
H	-3.47360900	2.72537500	-1.44894000
H	-1.69414400	2.84414100	-1.58551600
H	-3.34271600	-2.05852000	0.47422000
H	-5.05136500	-1.54071700	0.49994300
H	-4.16256600	-1.60246300	-1.04411500
H	-1.85673000	-0.80792400	1.90252400
H	-0.11792000	-0.42258800	1.85082400
H	-1.29855000	0.84429500	2.27524300
H	3.73887400	0.88010000	1.33412400
H	3.46104800	-0.74872700	2.00752300
H	5.44179800	-0.77106300	0.47113200
H	4.12853300	-1.77940600	-0.19841800
H	4.43670500	-0.14467500	-0.86538500
O	2.24339700	1.39984300	-1.34825600
H	1.82983500	2.03272500	-1.96567400

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Energy = -1016.12859900 a.u. #Cluster: 4

P	1.36835200	0.96062300	-0.29082900
F	1.58405200	2.40692000	0.32919500

O	2.10091600	-0.01142700	0.70091700
N	-2.39147400	0.42224100	-0.40900000
N	-0.14211500	0.70275200	-0.57108100
C	-2.53779400	0.97183500	-1.76820100
C	-3.63635000	0.04967100	0.28223400
C	-1.19384800	0.30988700	0.14579400
C	-2.60557800	2.49549900	-1.76737700
C	-4.07886800	-1.37553000	-0.03474800
C	-1.06169700	-0.23789000	1.54064100
C	3.50759300	0.09572500	1.11808700
C	4.38713900	-0.77121700	0.24753600
H	-1.69052300	0.62002100	-2.36999800
H	-3.45554700	0.53900800	-2.18978500
H	-4.40010800	0.77179000	-0.04088200
H	-3.50733000	0.19420100	1.36147700
H	-1.67279100	2.92700100	-1.37448300
H	-2.75047100	2.86018200	-2.79607500
H	-3.44663200	2.85564700	-1.15427900
H	-3.33554900	-2.11002800	0.31170900
H	-5.03447700	-1.58572800	0.46959800
H	-4.22434100	-1.51533700	-1.11710400
H	-1.69148500	-1.12378600	1.69105400

H	-0.01916800	-0.50184100	1.74553900
H	-1.37874100	0.53240200	2.26309400
H	3.80001400	1.15533500	1.08878300
H	3.50134100	-0.23712600	2.16378600
H	4.05317800	-1.81953600	0.27614500
H	4.38356100	-0.42160100	-0.79512200
H	5.42010600	-0.72485600	0.62712900
O	2.23798500	0.97428100	-1.61027100
H	1.83218800	1.42844500	-2.37251400

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Energy = -1016.12853300 a.u. #Cluster: 5

P	1.60296600	-0.83196600	-0.66059500
F	2.04951500	-0.23466900	-2.06281700
O	2.72231600	-0.35963200	0.33560500
N	-1.98932800	0.30544200	-0.17405300
N	0.19409900	-0.30203900	-0.28383300
C	-1.56502600	1.65296600	0.24619800
C	-3.43737700	0.08127900	-0.30446900
C	-1.08469200	-0.62550600	-0.43974200
C	-1.20609000	2.53735500	-0.94386300
C	-4.08904100	-0.31318200	1.01720200
C	-1.51926900	-1.99025100	-0.89816100

C	2.68607000	0.90517800	1.07562600
C	2.83295400	2.10074500	0.16099200
H	-2.39564300	2.08562300	0.82040400
H	-0.70719000	1.54509500	0.92216900
H	-3.61773500	-0.67706500	-1.07537800
H	-3.86709800	1.02049600	-0.68240400
H	-0.36891200	2.10416800	-1.51089300
H	-2.06584900	2.65947700	-1.62111400
H	-0.90416000	3.53398000	-0.58672200
H	-5.17455500	-0.42641400	0.87373000
H	-3.68754400	-1.26833400	1.38991400
H	-3.92363100	0.45570400	1.78773100
H	-1.91562700	-1.92431500	-1.92450200
H	-0.66817600	-2.67857600	-0.89404300
H	-2.31230900	-2.39514700	-0.25519600
H	1.74578900	0.93187600	1.64506000
H	3.52596700	0.81705600	1.77594700
H	2.91126400	3.01121600	0.77561200
H	3.74120500	2.01661600	-0.45488400
H	1.95975000	2.21442600	-0.49938100
O	1.77416400	-2.39505600	-0.82893700
H	2.67473200	-2.71898300	-1.02423500

Energy = -1016.12849300 a.u. #Cluster: 6

P	1.22910800	1.14224000	0.53300700
F	1.25959500	1.64501600	2.03988600
O	2.10021200	-0.16247400	0.52693000
N	-2.37188100	0.37570700	-0.42076600
N	-0.23173000	1.01399900	-0.00209100
C	-2.57924800	1.63184600	-1.16346400
C	-3.51484600	-0.55032900	-0.37706600
C	-1.20314800	0.11369500	0.14577300
C	-2.12521200	1.52385500	-2.61574600
C	-4.48584300	-0.22864600	0.75540700
C	-1.00717500	-1.17960300	0.89062800
C	3.50947800	-0.23970900	0.94235200
C	4.41565100	-0.17189400	-0.26472900
H	-3.65202500	1.86235600	-1.10590800
H	-2.03410800	2.42914200	-0.64340400
H	-3.14436300	-1.57918500	-0.29952400
H	-4.01904300	-0.47130200	-1.35126400
H	-1.04360000	1.33119500	-2.67367800
H	-2.65649500	0.71367700	-3.13967700
H	-2.33784500	2.46808800	-3.14055200

H	-5.34053400	-0.92117700	0.71553000
H	-4.00094400	-0.33282000	1.73835400
H	-4.87301300	0.79831200	0.66801500
H	-0.06684500	-1.16520500	1.45142400
H	-1.83434600	-1.37204200	1.58674100
H	-0.96641800	-2.01518600	0.17313200
H	3.70882300	0.56637000	1.66336700
H	3.58382900	-1.20230500	1.46437200
H	4.17716600	-0.97595500	-0.97745400
H	4.32464400	0.79869700	-0.77415000
H	5.45940100	-0.29658800	0.06438500
O	2.06270000	2.23332400	-0.24868200
H	1.57959200	3.05446500	-0.46017700

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Energy = -1016.12847500 a.u. #Cluster: 7

P	1.44080800	1.04892400	1.26854600
F	1.77756600	-0.34589300	1.96103800
O	2.67077600	1.33911600	0.33940300
N	-2.08387000	0.76635600	-0.13032800
N	0.09082000	1.02735800	0.48003000
C	-1.71167200	1.17566800	-1.49981200
C	-3.50411300	0.46922000	0.12317900

C	-1.15157700	0.67007300	0.80721600
C	-1.07490300	0.05315100	-2.31563200
C	-3.91891200	-0.93200500	-0.31644700
C	-1.51637800	0.20629700	2.19228700
C	2.77406400	0.88003800	-1.05047500
C	2.93164700	-0.62143300	-1.13443900
H	-2.63173600	1.53116900	-1.98211100
H	-1.02075600	2.02551700	-1.41768200
H	-4.08313500	1.22942600	-0.42104900
H	-3.71358000	0.62003900	1.18821100
H	-0.16015300	-0.31685800	-1.83191200
H	-1.76682700	-0.79083900	-2.45060200
H	-0.80370600	0.43834600	-3.31093100
H	-3.79534900	-1.06913600	-1.40081900
H	-3.32574800	-1.70179300	0.20162000
H	-4.98067200	-1.08981100	-0.07205300
H	-2.22361500	-0.63198500	2.17187700
H	-0.61999800	-0.11163700	2.73637500
H	-1.98292600	1.03787100	2.74584100
H	1.88092800	1.23490300	-1.58421000
H	3.65541100	1.40991000	-1.43229200
H	3.09280500	-0.90478000	-2.18634600

H	3.79623200	-0.96130500	-0.54425000
H	2.02881800	-1.14232000	-0.77891800
O	1.49550900	2.09754900	2.44659600
H	2.35578200	2.19642900	2.89905800

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Energy = -1016.12830500 a.u. #Cluster: 8

P	1.45489400	0.99502600	1.17402700
F	1.91271300	-0.24599700	2.05646400
O	2.67562900	1.27448100	0.22849700
N	-1.99565100	0.27801400	-0.25382100
N	0.14545900	0.70703600	0.37290300
C	-1.53920700	0.16537200	-1.65119500
C	-3.44320300	0.13476800	-0.02733200
C	-1.13000500	0.52984600	0.71645300
C	-1.45598300	1.52273900	-2.34169400
C	-3.87068300	-1.32009100	0.13930100
C	-1.60650500	0.64837400	2.13899700
C	2.83896500	0.67430500	-1.10016300
C	3.12165900	-0.80860400	-1.01303600
H	-0.56140000	-0.33189500	-1.65047800
H	-2.25283800	-0.49237900	-2.16628300
H	-3.94119800	0.58562800	-0.89807100

H	-3.73362300	0.73568800	0.84248900
H	-2.43240000	2.03214100	-2.33514600
H	-0.71774400	2.16898800	-1.84438100
H	-1.14770800	1.38568500	-3.38970300
H	-4.96380800	-1.37067000	0.25887400
H	-3.59482800	-1.92048500	-0.74134200
H	-3.40406000	-1.77410600	1.02728900
H	-2.37954100	-0.09148700	2.37879900
H	-0.77062400	0.51894000	2.83589100
H	-2.03188700	1.65371900	2.29505400
H	1.92910000	0.89167000	-1.67753700
H	3.68054800	1.22999100	-1.53206900
H	3.33187700	-1.19199900	-2.02381000
H	3.99702300	-1.00598400	-0.37573500
H	2.25652800	-1.36144600	-0.61490800
O	1.36652200	2.19734300	2.19344600
H	2.18352000	2.42295300	2.67919000

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Energy = -1016.12770900 a.u. #Cluster: 9

P	1.38781600	0.36902200	-0.84494400
F	1.82106000	1.87312800	-0.56308900
O	2.16090900	-0.48869100	0.21862200

N	-2.37455600	0.40995200	-0.37346000
N	-0.16306900	0.27177100	-0.87400500
C	-2.60851000	1.02526300	-1.69214000
C	-3.55255200	0.24096400	0.49240300
C	-1.14934500	0.06554900	-0.00543600
C	-2.34241800	2.52739400	-1.68032400
C	-4.29904800	-1.06130400	0.21938200
C	-0.91214600	-0.54150400	1.35028100
C	3.62008800	-0.53027100	0.39566500
C	4.07766800	0.54447600	1.35495800
H	-1.96127200	0.52210100	-2.42183900
H	-3.65186400	0.81322500	-1.96318000
H	-4.20485600	1.10638400	0.30542700
H	-3.24154500	0.30512200	1.54177800
H	-1.28935000	2.73338200	-1.43733100
H	-2.55885100	2.94957700	-2.67391300
H	-2.98170800	3.03817700	-0.94310000
H	-5.19107900	-1.11637800	0.86207900
H	-4.62839400	-1.11873200	-0.82964900
H	-3.66473300	-1.93581000	0.43159000
H	0.10010300	-0.95419200	1.40544300
H	-1.01816800	0.23683800	2.12380400

H	-1.63836000	-1.33598100	1.56692800
H	3.80929200	-1.53891500	0.78420500
H	4.08989500	-0.43974800	-0.59423600
H	3.89038200	1.54977900	0.95002700
H	3.56612300	0.44744300	2.32467600
H	5.16095200	0.43444600	1.52099700
O	2.05790600	0.02927100	-2.23463600
H	1.61117000	0.40582400	-3.01601500

33

Energy = -1016.12770700 a.u. #Cluster: 10

P	1.39900700	0.73424200	-0.38772400
F	1.69095600	1.87158900	0.68692100
O	2.09419400	-0.55502200	0.17457600
N	-2.38401600	0.41943200	-0.44559800
N	-0.13109900	0.61564900	-0.69009000
C	-2.54388400	0.77282800	-1.86827300
C	-3.63011300	0.20427900	0.31011300
C	-1.17729200	0.33954400	0.09263800
C	-2.58812400	2.28185300	-2.08556200
C	-4.12511600	-1.23584600	0.22591500
C	-0.99622500	-0.02243300	1.54098400
C	3.53917100	-0.82060600	0.21402800

C	4.24967500	0.06228100	1.21493000
H	-1.71230200	0.32393900	-2.42507000
H	-3.47524700	0.29969200	-2.20920200
H	-4.37357900	0.89302600	-0.11617200
H	-3.48100500	0.51590100	1.35071300
H	-2.74528600	2.49661300	-3.15388300
H	-3.41249400	2.74214100	-1.51852500
H	-1.64194800	2.74786700	-1.77263600
H	-4.29086400	-1.53789000	-0.81980700
H	-3.40101800	-1.93211400	0.67666400
H	-5.07977300	-1.32958400	0.76587200
H	-1.83713500	-0.57988300	1.96400100
H	-0.08455500	-0.62469400	1.65024400
H	-0.86006100	0.90672000	2.11972800
H	3.59527500	-1.88128300	0.48833100
H	3.92776700	-0.69472100	-0.80650600
H	4.23303000	1.11956900	0.91035000
H	3.79539800	-0.03042200	2.21312900
H	5.30193800	-0.25617900	1.28041300
O	2.23940100	1.15853600	-1.65358100
H	1.82686100	1.83254000	-2.22595200

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Energy = -1107.93392500 a.u. #Cluster: 1

P	3.29544100	0.37161300	1.61750000
O	4.42329200	-0.27242800	0.84943800
N	-0.06429500	-0.03294200	-0.26391300
N	1.77771100	0.43830600	0.99917700
C	-0.89952600	0.69287800	0.69862900
C	-0.76215000	-0.64145100	-1.39967700
C	1.26439200	-0.14410900	-0.05722700
C	-1.36281100	-0.19589500	1.85056300
C	-0.93545200	0.31519300	-2.57773600
C	2.06730600	-0.93739300	-1.06385000
C	3.67919500	2.02807300	2.21252600
H	-1.76317200	1.09417500	0.14769100
H	-0.32055100	1.54287700	1.08157100
H	-0.23278000	-1.54955700	-1.71307100
H	-1.74646100	-0.97269200	-1.03418000
H	-0.50201000	-0.56504900	2.42703100
H	-2.01748600	0.37216300	2.53072400
H	-1.92966600	-1.06418600	1.47756600
H	-1.48543200	1.22047500	-2.27524800

H	0.04009400	0.62692800	-2.98293000
H	-1.50317600	-0.17576000	-3.38395700
H	1.85153600	-0.61391400	-2.09165200
H	3.13433700	-0.81980000	-0.85235600
H	1.80991300	-2.00597300	-0.98663800
H	3.85535800	2.67751100	1.34209200
H	2.84628500	2.42534800	2.80837400
H	4.59350900	1.98590400	2.82259200
O	3.06025400	-0.38687200	3.09299000
C	2.30411600	-1.52843100	3.19603500
C	2.41329400	-2.57360200	2.26862300
C	1.40635700	-1.62362200	4.26532600
C	1.60386800	-3.70444400	2.40834700
H	3.13382900	-2.49342400	1.45372900
C	0.61266500	-2.76511700	4.40343200
H	1.33633800	-0.79279300	4.97051600
C	0.70126700	-3.80648800	3.47233700
H	1.68651900	-4.51461100	1.67908900
H	-0.08823200	-2.83511700	5.23933500
H	0.07263400	-4.69383400	3.57785200

39

Energy = -1107.93231400 a.u. #Cluster: 2

P	3.44094900	-0.35189900	0.89569800
O	4.43488500	-0.49582000	-0.22385900
N	-0.20380300	-0.08595500	-0.37306100
N	1.82730200	-0.39668100	0.61362200
C	-0.82909800	-0.81623800	0.73485200
C	-1.10188000	0.45951600	-1.39320100
C	1.13666300	0.06958600	-0.39381600
C	-1.07698800	0.05557700	1.96329400
C	-1.46390000	-0.55168300	-2.47927800
C	1.75548000	0.79655800	-1.56718800
C	3.75697400	1.08623200	1.94762900
H	-0.17662100	-1.65776800	1.00204400
H	-1.77690100	-1.23021800	0.35977100
H	-2.01234800	0.79928900	-0.87494300
H	-0.65176100	1.35700700	-1.83597100
H	-0.12509600	0.43862900	2.35989400
H	-1.72909400	0.91087400	1.72300900
H	-1.56543400	-0.53683200	2.75351800
H	-1.93696100	-1.44718600	-2.04608000
H	-2.17306300	-0.10315300	-3.19294500
H	-0.56986000	-0.87278100	-3.03677000
H	1.32391200	0.47877800	-2.52566700

H	1.58543500	1.88095300	-1.46354000
H	2.83461300	0.60730900	-1.57919800
H	3.62342400	1.99543400	1.34155500
H	3.06045900	1.11329800	2.79714200
H	4.79332800	1.04308800	2.31463400
O	3.65451400	-1.64602400	1.91928800
C	2.69878200	-2.08080400	2.81074900
C	1.80808400	-3.08887800	2.42613700
C	2.64441000	-1.54129300	4.10004300
C	0.85239200	-3.54986500	3.33439400
H	1.87133200	-3.49214600	1.41405700
C	1.68243600	-2.00660300	5.00277300
H	3.35661800	-0.76556800	4.38789300
C	0.78195500	-3.00761100	4.62346900
H	0.15447500	-4.33439600	3.03060000
H	1.63974400	-1.58286400	6.00947500
H	0.03095200	-3.36792000	5.33062700

39

Energy = -1107.93220800 a.u. #Cluster: 3

P	3.38833300	-0.87063000	0.70149400
O	4.28735500	-1.14517200	-0.47216200
N	-0.19458300	0.14338300	-0.34143700

N	1.77682600	-0.64615700	0.49319100
C	-0.91346300	-0.60916400	0.69231300
C	-1.00619400	0.97181100	-1.23630900
C	1.15163700	0.06818300	-0.40617800
C	-0.97243800	0.11996200	2.03235700
C	-1.56159200	0.20073400	-2.43220800
C	1.85788100	0.83630900	-1.50203900
C	3.98683100	0.46834100	1.76324300
H	-0.41531500	-1.57931400	0.81794300
H	-1.92849100	-0.79769000	0.31221400
H	-1.83232800	1.38284500	-0.63528300
H	-0.41673000	1.83423100	-1.57225900
H	-1.54816600	-0.47396900	2.75999200
H	0.04070000	0.26686400	2.43469300
H	-1.45828900	1.10386500	1.93121600
H	-2.17057100	-0.65614300	-2.10325100
H	-2.20000400	0.85838500	-3.04321000
H	-0.74912700	-0.18125200	-3.07027700
H	2.88375600	0.46402100	-1.60078900
H	1.34904500	0.74031200	-2.47033500
H	1.89175900	1.90721100	-1.24251400
H	3.96451300	1.40430300	1.18424000

H	3.34994600	0.57839400	2.65172800
H	5.02195400	0.25329900	2.06767100
O	3.43086800	-2.21285600	1.68080200
C	2.52897700	-2.44785000	2.69599800
C	2.78758400	-1.97013700	3.98500300
C	1.37804600	-3.19993600	2.43665200
C	1.87919000	-2.23640700	5.01500600
H	3.69885100	-1.39906100	4.17228500
C	0.47690400	-3.46236400	3.47086300
H	1.20163200	-3.56389900	1.42339900
C	0.72070900	-2.97810000	4.76190000
H	2.08190700	-1.86132800	6.02150800
H	-0.42393400	-4.04620600	3.26495000
H	0.01233100	-3.18287600	5.56824100

39

Energy = -1107.93083600 a.u. #Cluster: 4

P	3.54050000	0.34579600	1.28009400
O	4.59918900	0.47400900	0.21797300
N	-0.05897700	0.01293700	-0.02235500
N	1.94321600	0.50856400	0.95352100
C	-0.72070800	0.19937100	1.27343100
C	-0.91669400	-0.37730400	-1.14357400

C	1.27920600	0.13283000	-0.11427700
C	-1.07343200	1.65754800	1.55174300
C	-1.18284400	-1.88118000	-1.19368800
C	1.92957700	-0.16050900	-1.44729800
C	3.83195500	1.41887400	2.70073500
H	-0.05506100	-0.19217200	2.05353800
H	-1.62961100	-0.42016600	1.26728700
H	-1.86467900	0.17250900	-1.03609600
H	-0.46794600	-0.03431400	-2.08372000
H	-0.16259900	2.27272500	1.60324300
H	-1.72745400	2.06502200	0.76398800
H	-1.60361000	1.74253500	2.51383600
H	-1.64789900	-2.23459000	-0.26010800
H	-1.86471600	-2.11598600	-2.02614200
H	-0.24899000	-2.44521800	-1.34136100
H	1.67452300	-1.17183100	-1.79632300
H	1.57935100	0.55358900	-2.20897400
H	3.01606500	-0.06766600	-1.35032700
H	3.09624100	1.22042700	3.49257400
H	4.84836400	1.23796500	3.07982000
H	3.74692300	2.46768500	2.37809600
O	3.66326200	-1.19359300	1.94122000

C	2.55947400	-1.90450000	2.35503700
C	2.14234600	-1.83525300	3.68825500
C	1.86392800	-2.69750400	1.43578500
C	1.01548700	-2.55541700	4.09649100
H	2.70099000	-1.21261500	4.39032800
C	0.73676600	-3.41056400	1.85042400
H	2.20875700	-2.73617300	0.40075800
C	0.30620100	-3.34003000	3.18017200
H	0.68816400	-2.49830500	5.13790700
H	0.18874700	-4.01942100	1.12706800
H	-0.57770100	-3.89613500	3.50156900

39

Energy = -1107.93000500 a.u. #Cluster: 5

P	3.30599300	0.54670000	1.54388800
O	4.49369900	0.73708300	0.63987600
N	0.02841700	-0.13285200	-0.38411700
N	1.77521400	0.47636900	0.95405200
C	-0.90294400	0.45479200	0.58472700
C	-0.57079300	-0.77174200	-1.55869200
C	1.35488000	-0.09628600	-0.14943400
C	-1.27667300	-0.51567600	1.70242900
C	-0.85442300	0.20866400	-2.69491200

C	2.27258700	-0.72928600	-1.17192900
C	3.22184900	1.77121700	2.86615700
H	-1.79905900	0.76843500	0.02886900
H	-0.43593400	1.35510100	1.00445100
H	0.07723100	-1.58682200	-1.90362300
H	-1.50700100	-1.24599600	-1.22558000
H	-1.73446300	-1.43216100	1.29678700
H	-0.38864100	-0.80138800	2.28334700
H	-2.00263600	-0.04531400	2.38477800
H	-1.34249000	-0.31453500	-3.53237300
H	-1.52340200	1.01807900	-2.36233300
H	0.07606400	0.66484000	-3.06797400
H	3.30999300	-0.46258400	-0.94425600
H	2.16884000	-1.82583800	-1.13989400
H	2.03081100	-0.40114100	-2.19234400
H	3.06339400	2.76397400	2.41840400
H	2.39222700	1.54615200	3.55057800
H	4.17375600	1.76854100	3.41685600
O	3.53097200	-0.89855600	2.36036100
C	2.50026000	-1.67315100	2.84181000
C	2.00098400	-2.71629000	2.05420500
C	1.98010400	-1.44016500	4.11979900

C	0.97280400	-3.52411900	2.54627500
H	2.42635300	-2.88294300	1.06301400
C	0.94938900	-2.25172700	4.60332800
H	2.38892100	-0.62852200	4.72483100
C	0.44105200	-3.29359900	3.81985600
H	0.58250900	-4.33619400	1.92749400
H	0.54229800	-2.06719900	5.60086400
H	-0.36583400	-3.92392500	4.20107400

39

Energy = -1107.92891400 a.u. #Cluster: 6

P	3.22443500	-0.35595600	1.00228000
O	4.28800500	-0.44811600	-0.05734900
N	-0.26928400	0.15978800	-0.60154500
N	1.65468600	-0.07546700	0.61372400
C	-1.01175300	0.47036700	0.62353400
C	-1.04924600	0.15206400	-1.84266800
C	1.05272900	-0.11010700	-0.55056800
C	-1.62447900	-0.77237000	1.26596600
C	-1.15002200	1.52908800	-2.49645600
C	1.74928800	-0.44674600	-1.85041000
C	3.61834800	0.83534800	2.30183000
H	-1.79913900	1.19273400	0.35950600

H	-0.32466200	0.96435700	1.32177400
H	-0.62281200	-0.57741000	-2.54225600
H	-2.05426200	-0.21936700	-1.59057600
H	-0.84282600	-1.49792700	1.53538300
H	-2.16877600	-0.49686800	2.18330700
H	-2.33477600	-1.26548600	0.58316300
H	-0.15720800	1.90297200	-2.79203400
H	-1.77978700	1.47353200	-3.39852300
H	-1.60196100	2.26263300	-1.81013400
H	1.52913300	0.29550000	-2.63034600
H	2.82950800	-0.49389400	-1.68125000
H	1.40180300	-1.42711700	-2.21498000
H	3.58603500	1.84409200	1.86344600
H	2.90478200	0.78117000	3.13503200
H	4.63533200	0.63055800	2.66749000
O	3.23310900	-1.82691000	1.78696700
C	2.57623300	-2.21356800	2.92642000
C	1.41098500	-1.59409700	3.39990600
C	3.12003200	-3.30602300	3.61763400
C	0.80305500	-2.07225000	4.56569600
H	0.98144300	-0.75987600	2.84727200
C	2.50040600	-3.77621100	4.77684400

H	4.02827700	-3.77271800	3.23007200
C	1.33882200	-3.16099600	5.25966300
H	-0.10624200	-1.58455300	4.92704100
H	2.93145000	-4.62901400	5.30800500
H	0.85564900	-3.52921500	6.16779000

39

Energy = -1107.92878900 a.u. #Cluster: 7

P	3.16297000	-0.69819900	0.87979600
O	4.19125100	-0.84285200	-0.20826000
N	-0.29078500	0.24635900	-0.59824300
N	1.58772700	-0.42024500	0.51244900
C	-1.10816500	-0.27168600	0.50300000
C	-1.01020100	0.89304500	-1.69887400
C	1.05330100	0.13084800	-0.54818000
C	-1.26348200	0.72973000	1.64498700
C	-1.49122700	-0.09270400	-2.76210500
C	1.85347200	0.67012800	-1.71281300
C	3.62746700	0.49307200	2.15932100
H	-0.64361800	-1.19688500	0.86909200
H	-2.09194000	-0.53456600	0.08667000
H	-1.86970100	1.42111800	-1.25744000
H	-0.37543100	1.66722100	-2.14745600

H	-0.28250000	0.98575000	2.07271300
H	-1.74390600	1.65809100	1.29645400
H	-1.88817400	0.30039500	2.44442700
H	-0.64213000	-0.59927500	-3.24721700
H	-2.14296500	-0.86362300	-2.32132800
H	-2.06585200	0.43758400	-3.53794900
H	2.88804900	0.32157600	-1.63242900
H	1.43564700	0.35044100	-2.67718100
H	1.84271000	1.77218600	-1.69102900
H	3.63547000	1.49482300	1.70370300
H	2.91991600	0.48449500	2.99959500
H	4.63815900	0.24914500	2.51926300
O	3.12789900	-2.15456900	1.67882100
C	2.51366900	-2.48106200	2.86220200
C	3.10521200	-3.51053600	3.60778800
C	1.34278500	-1.86288000	3.32356500
C	2.52788200	-3.91977000	4.81131700
H	4.01671400	-3.97702000	3.22768200
C	0.77895500	-2.27802200	4.53460700
H	0.87934400	-1.07769300	2.72862400
C	1.36245700	-3.30411500	5.28371000
H	2.99565400	-4.72394900	5.38546300

H	-0.13344200	-1.79081200	4.88888300
H	0.91312100	-3.62360400	6.22702200

39

Energy = -1107.92877100 a.u. #Cluster: 8

P	3.19745700	-0.42105300	0.98134800
O	4.26919800	-0.43043000	-0.07355900
N	-0.29491000	0.21702400	-0.57150700
N	1.61710500	-0.24105600	0.58473800
C	-1.08173100	-0.24099200	0.57790100
C	-1.04977000	0.71407300	-1.72459100
C	1.05334800	0.17725300	-0.52018200
C	-1.27321300	0.84357700	1.63518800
C	-1.48630600	-0.39603600	-2.67886400
C	1.82105000	0.63974800	-1.73824600
C	3.52825900	0.73885900	2.32865700
H	-0.57687700	-1.11260000	1.01519000
H	-2.05584800	-0.57895500	0.19453800
H	-1.93177400	1.24246700	-1.33041900
H	-0.45566800	1.46769500	-2.25615300
H	-1.79352400	1.71967200	1.21564600
H	-1.87626700	0.45551300	2.47151400
H	-0.30149700	1.17243200	2.03294500

H	-0.61473500	-0.91001800	-3.11385200
H	-2.10262200	-1.14666400	-2.15912800
H	-2.08467800	0.02577400	-3.50193800
H	1.72517100	1.73238500	-1.84665600
H	2.87846600	0.38410400	-1.61757700
H	1.43423400	0.17820900	-2.65751600
H	4.54743900	0.56175300	2.70323700
H	3.46212200	1.76002600	1.92379400
H	2.80523000	0.62739600	3.14796200
O	3.25772400	-1.91387000	1.71226300
C	2.59772800	-2.37635100	2.82212900
C	3.17336300	-3.48036500	3.46784700
C	1.40398500	-1.82397400	3.30891100
C	2.55919000	-4.02840200	4.59524200
H	4.10279900	-3.89425000	3.07054900
C	0.80269600	-2.37962100	4.44347800
H	0.94803100	-0.98135400	2.79212000
C	1.37064800	-3.47980700	5.09212700
H	3.01613400	-4.88923900	5.09059000
H	-0.12749000	-1.94296100	4.81698200
H	0.89184200	-3.90802400	5.97594300

Energy = -1107.92876800 a.u. #Cluster: 9

P	3.20094300	-0.38529100	0.98451200
O	4.26925000	-0.37897100	-0.07384100
N	-0.30260500	0.21841000	-0.55703300
N	1.61842200	-0.20866000	0.59625700
C	-1.08069300	-0.22986800	0.60212300
C	-1.06646400	0.69506700	-1.71281600
C	1.04607500	0.18817200	-0.51226200
C	-1.27362300	0.86603100	1.64726200
C	-1.50092100	-0.43045100	-2.64973700
C	1.80449600	0.63671400	-1.74130000
C	3.53087500	0.76386600	2.34090600
H	-0.56838600	-1.09312700	1.04721600
H	-2.05468500	-0.57849500	0.22806500
H	-1.94965800	1.22347400	-1.32131000
H	-0.47979100	1.44504700	-2.25764900
H	-1.80043300	1.73444200	1.21985300
H	-1.87138400	0.48449500	2.49039900
H	-0.30221100	1.20466100	2.03748000
H	-0.62841400	-0.94556200	-3.08152500
H	-2.11095200	-1.17721500	-2.11715600
H	-2.10516000	-0.02325700	-3.47588800

H	2.86455800	0.39208800	-1.62101400
H	1.41702100	0.15720100	-2.65107900
H	1.69927700	1.72662400	-1.86716700
H	2.81219600	0.64134300	3.16245400
H	4.55263600	0.58847000	2.70920400
H	3.45779100	1.78859200	1.94631700
O	3.27298400	-1.88462000	1.70152600
C	2.61234200	-2.36684400	2.80230400
C	3.18422700	-3.48675800	3.42371400
C	1.42266600	-1.81888500	3.30404000
C	2.57077900	-4.05468700	4.54159400
H	4.11052200	-3.89687800	3.01530100
C	0.82191900	-2.39484700	4.42877600
H	0.96821900	-0.96395900	2.80651800
C	1.38637600	-3.51072900	5.05325200
H	3.02504100	-4.92766700	5.01781500
H	-0.10499900	-1.96137700	4.81396000
H	0.90807500	-3.95461000	5.92958300

AMP-N₁H

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Energy = -1108.37496400 a.u. #Cluster: 1

P	3.40687200	0.20274600	1.33486000
O	4.42352100	0.42484200	0.27191000
N	-0.11532700	0.01185000	-0.51103800
N	1.75931800	0.35205100	0.79445800
C	-0.99054000	0.68437300	0.47103100
C	-0.80419000	-0.53315200	-1.70030200
C	1.18348500	-0.12488900	-0.32988500
C	-1.47992200	-0.26111700	1.56495900
C	-0.97025400	0.50493200	-2.80415100
C	2.03303800	-0.83216900	-1.33905500
C	3.42627800	1.29153600	2.75588600
H	-1.83815500	1.08900000	-0.09700200
H	-0.46640100	1.55826400	0.88608300
H	-0.26076900	-1.41500400	-2.05714600
H	-1.78351700	-0.88909400	-1.35029500
H	-2.16664500	0.28166600	2.23167700
H	-2.02256500	-1.11387000	1.12929600
H	-0.65037100	-0.65527500	2.17053000
H	-1.53153400	1.38184700	-2.44664300
H	0.00553400	0.84741300	-3.18160200
H	-1.52888300	0.05920200	-3.64118200
H	1.76455000	-0.53121300	-2.35863400

H	3.09093900	-0.61073800	-1.16702600
H	1.87169200	-1.91856800	-1.24402100
H	3.30262300	2.32590400	2.40307300
H	2.62721400	1.03483100	3.46583100
H	4.40588900	1.18042400	3.24308700
O	3.50279200	-1.33515300	1.87128000
C	2.60861300	-1.90871500	2.77221900
C	1.51210400	-2.62168000	2.28405400
C	2.84410200	-1.78934200	4.14336300
C	0.62719600	-3.21262900	3.19048500
H	1.36118100	-2.71694300	1.20783700
C	1.95250400	-2.38491600	5.04019800
H	3.71914600	-1.23999000	4.49539600
C	0.84181400	-3.09239000	4.56751000
H	-0.23466100	-3.76886800	2.81428500
H	2.13031900	-2.29470500	6.11453300
H	0.14649600	-3.55403600	5.27239900
H	1.14243500	0.79175300	1.47505800

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Energy = -1108.37495100 a.u. #Cluster: 2

P	3.35512800	0.34580600	1.41596800
O	4.38463000	0.61541900	0.37653000

N	-0.09395000	-0.05483200	-0.53162800
N	1.71602900	0.39033200	0.83335900
C	-1.03632300	0.56167100	0.42366600
C	-0.71100900	-0.64175500	-1.74031300
C	1.20466600	-0.11065400	-0.31199100
C	-1.49325400	-0.40894500	1.50975200
C	-0.90880300	0.38301800	-2.85120000
C	2.12520800	-0.75196800	-1.30242100
C	3.28134800	1.45275200	2.82078600
H	-1.89350900	0.90869600	-0.16763500
H	-0.58004000	1.46905300	0.84722100
H	-0.10185000	-1.48742700	-2.07830600
H	-1.67591400	-1.05858400	-1.41870900
H	-0.65862100	-0.74673300	2.14193600
H	-2.23214500	0.09145700	2.15342100
H	-1.96773800	-1.29688000	1.06488400
H	0.05425900	0.78522000	-3.20120900
H	-1.41388000	-0.09753600	-3.70283200
H	-1.53360000	1.22363400	-2.51247700
H	3.16242900	-0.47072700	-1.09593900
H	2.02654400	-1.84719500	-1.22534100
H	1.86866600	-0.45339900	-2.32564600

H	3.11980800	2.47477400	2.44783700
H	2.47500100	1.17012400	3.51237600
H	4.25089300	1.39479900	3.33652000
O	3.52600200	-1.17771300	1.97428500
C	2.62212600	-1.80905600	2.82531500
C	2.75069800	-1.65004900	4.20652300
C	1.62424100	-2.61721700	2.27770900
C	1.84955100	-2.30376500	5.05194900
H	3.55207300	-1.02674500	4.60717900
C	0.72905600	-3.26561400	3.13307000
H	1.55831800	-2.74017100	1.19569800
C	0.83601800	-3.10738600	4.51875500
H	1.94374500	-2.18341300	6.13387000
H	-0.05607500	-3.89676400	2.71015300
H	0.13306900	-3.61475200	5.18351100
H	1.05312600	0.77070500	1.50669400

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Energy = -1108.37494700 a.u. #Cluster: 3

P	3.34625400	0.35650500	1.39708600
O	4.36906500	0.63148400	0.35220300
N	-0.10899800	-0.06508700	-0.53492400
N	1.70422100	0.39254900	0.82212400

C	-1.05095700	0.55375000	0.41914400
C	-0.72764900	-0.66063300	-1.73862300
C	1.19034200	-0.11637000	-0.31855000
C	-1.50817100	-0.41445800	1.50721400
C	-0.93096300	0.35728500	-2.85473900
C	2.10971700	-0.76208400	-1.30719500
C	3.27325000	1.46376000	2.80166800
H	-1.90767800	0.90043300	-0.17312200
H	-0.59443100	1.46167000	0.84112200
H	-0.11715900	-1.50668800	-2.07323400
H	-1.69063800	-1.07804800	-1.41211800
H	-1.98521300	-1.30217100	1.06466400
H	-0.67277800	-0.75248900	2.13832000
H	-2.24519300	0.08829500	2.15117800
H	0.03011900	0.76043300	-3.20906000
H	-1.43644100	-0.12963700	-3.70249200
H	-1.55754100	1.19789200	-2.51933300
H	2.01591200	-1.85700900	-1.21998800
H	1.84822600	-0.47348600	-2.33198500
H	3.14659700	-0.47496400	-1.10733100
H	3.10488200	2.48439200	2.42791500
H	2.47170200	1.17812600	3.49754500

H	4.24560600	1.41151200	3.31268000
O	3.52780000	-1.16640100	1.95369400
C	2.64028800	-1.79571500	2.82353300
C	1.62975800	-2.60239200	2.29738000
C	2.79796000	-1.63573600	4.20160900
C	0.75121300	-3.24815800	3.17189700
H	1.54075500	-2.72652100	1.21718900
C	1.91335100	-2.28701500	5.06616800
H	3.60848700	-1.01340000	4.58496000
C	0.88731800	-3.08901000	4.55488400
H	-0.04378600	-3.87807400	2.76594300
H	2.03026500	-2.16592500	6.14577500
H	0.19727600	-3.59429200	5.23456100
H	1.04314800	0.77585600	1.49556000

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Energy = -1108.37432300 a.u. #Cluster: 4

P	3.46564700	0.43784700	1.45963200
O	4.51347000	0.61934200	0.41930500
N	-0.01500100	-0.11412600	-0.37602200
N	1.83094800	0.49266300	0.86961100
C	-0.93831200	0.49489000	0.60337000
C	-0.66048400	-0.76738500	-1.53360700

C	1.29313000	-0.10272600	-0.21748400
C	-1.25595900	-0.43690400	1.76986400
C	-0.98464100	0.21638300	-2.65185100
C	2.19562400	-0.74407700	-1.22510900
C	3.42379700	1.62400900	2.79950400
H	-1.85228100	0.74838600	0.05130100
H	-0.52264900	1.45518000	0.94429900
H	-0.01822700	-1.57952500	-1.89101200
H	-1.57664200	-1.23632900	-1.14737600
H	-0.36307400	-0.67528300	2.36507100
H	-1.98959900	0.04942500	2.43004700
H	-1.68797100	-1.38171400	1.40746100
H	-1.49884900	-0.31676900	-3.46587300
H	-1.64756400	1.02063300	-2.29757300
H	-0.07037200	0.67369700	-3.05998700
H	1.94283400	-0.39684200	-2.23562400
H	3.24093000	-0.49805700	-1.01590300
H	2.06396900	-1.83677200	-1.19703200
H	3.33713300	2.63316700	2.37083400
H	2.58392500	1.42823200	3.48088200
H	4.37387400	1.53259200	3.34600700
O	3.58337000	-1.05333800	2.11731800

C	2.54379100	-1.73114900	2.74795000
C	1.85558700	-2.71178600	2.03088500
C	2.22477100	-1.44777600	4.07718300
C	0.81997300	-3.41194200	2.65480700
H	2.13891400	-2.92034300	0.99807000
C	1.18284300	-2.15151700	4.68935600
H	2.79153600	-0.69368500	4.62567400
C	0.47766100	-3.13029100	3.98142400
H	0.27597500	-4.17753000	2.09667200
H	0.92572700	-1.93279700	5.72857100
H	-0.33661100	-3.67508900	4.46454400
H	1.17872600	0.91548800	1.52812800

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Energy = -1108.37430500 a.u. #Cluster: 5

P	3.62643100	0.00446900	1.15134100
O	4.55310800	0.00488600	-0.01241900
N	-0.09102000	0.04640300	-0.25974300
N	1.96038600	0.31104400	0.76060100
C	-0.77553400	0.78670000	0.82004500
C	-0.96722500	-0.46114100	-1.33583900
C	1.20988500	-0.16593600	-0.25628700
C	-1.12522100	-0.10008500	2.01234900

C	-1.22477700	0.58184800	-2.41724900
C	1.86884100	-0.93079800	-1.36118200
C	3.93326300	1.20013200	2.44809300
H	-1.68424600	1.21328500	0.37627900
H	-0.15849100	1.64839900	1.11642100
H	-0.52790300	-1.37197100	-1.75743600
H	-1.90680600	-0.76018700	-0.85002100
H	-1.76303800	-0.94036900	1.69938500
H	-0.22945800	-0.51247800	2.49862200
H	-1.67673100	0.49571400	2.75501400
H	-0.29163600	0.86982700	-2.92497000
H	-1.91330900	0.16442300	-3.16757300
H	-1.68604300	1.48859900	-1.99670400
H	1.55370800	-0.53864600	-2.33705000
H	2.95755100	-0.85794000	-1.28115700
H	1.56851400	-1.98882500	-1.30516600
H	3.94003200	2.20580300	2.00295300
H	3.16731700	1.13762400	3.23424100
H	4.92181400	0.97481100	2.87456000
O	3.59042900	-1.47689800	1.83922500
C	2.53519100	-1.98419600	2.59199900
C	1.62603500	-2.84289700	1.97089300

C	2.41677600	-1.65742200	3.94397200
C	0.57166800	-3.37452900	2.71773500
H	1.75440400	-3.08909100	0.91562000
C	1.35457600	-2.19201900	4.67997100
H	3.15217200	-1.00116400	4.41256300
C	0.43043000	-3.04707900	4.07042100
H	-0.14464900	-4.04445600	2.23635300
H	1.25393300	-1.93859500	5.73804600
H	-0.39799400	-3.46028200	4.65027900
H	1.46353800	0.82121700	1.48913600

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Energy = -1108.37297600 a.u. #Cluster: 6

P	2.76088200	-1.01481300	1.23536900
O	3.89917000	-1.19300200	0.29314900
N	-0.21416700	0.39226400	-1.01194200
N	1.26558800	-0.63292600	0.43102200
C	-1.35849000	-0.34626700	-0.44167000
C	-0.55215700	1.35829400	-2.07807100
C	1.02116700	0.22520900	-0.57870600
C	-1.92985600	0.32779000	0.80321000
C	-0.61033400	0.70981200	-3.45642100
C	2.15686000	0.99930500	-1.17143100

C	2.96327900	0.20845800	2.53134300
H	-1.05599500	-1.38567100	-0.24275900
H	-2.11778000	-0.40271200	-1.23249200
H	-1.52863200	1.78406300	-1.80656400
H	0.16595200	2.18558600	-2.05511500
H	-2.80201900	-0.24219900	1.15707600
H	-1.19255300	0.37001100	1.61952400
H	-2.25574100	1.35431500	0.57653900
H	-1.34557800	-0.10917900	-3.48195400
H	-0.91116900	1.46287600	-4.20062300
H	0.37046700	0.30485600	-3.74958200
H	2.06771500	1.06088400	-2.26216000
H	2.14223700	2.02294300	-0.76248700
H	3.11101400	0.52632800	-0.91914100
H	2.06352000	0.25871300	3.16010900
H	3.83983300	-0.05548300	3.14047100
H	3.13554500	1.17866900	2.04213200
O	2.23287600	-2.39202100	1.92064500
C	2.17907900	-2.64263600	3.28999100
C	0.94687600	-2.55327700	3.93835300
C	3.34061900	-3.00758000	3.97130800
C	0.88075500	-2.83781100	5.30533600

H	0.06011600	-2.26302900	3.37093800
C	3.26171100	-3.28600000	5.33906900
H	4.28680700	-3.07092600	3.42964300
C	2.03514300	-3.20247700	6.00719200
H	-0.07932900	-2.77176800	5.82293800
H	4.16535800	-3.57147100	5.88296700
H	1.97864400	-3.42264600	7.07577700
H	0.46850600	-1.10830100	0.85033600

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Energy = -1108.37297200 a.u. #Cluster: 7

P	2.21412900	-0.43932700	1.78684400
O	3.58996600	-0.41428300	1.21431000
N	-0.22879200	0.11667300	-1.30112600
N	0.95023300	-0.43975900	0.60117900
C	-1.34582800	-0.77398000	-0.92810800
C	-0.41195700	0.87222000	-2.55783300
C	0.85154100	0.24588500	-0.55524300
C	-2.34281200	-0.10160500	0.01208500
C	0.01281100	0.07116800	-3.78354500
C	1.95970000	1.16641500	-0.96105700
C	1.82438800	0.85094100	2.96956900
H	-0.93944800	-1.70330600	-0.50091400

H	-1.83743200	-1.06664800	-1.86502800
H	-1.47984800	1.12783000	-2.61008100
H	0.13340600	1.82017700	-2.49094600
H	-3.16993200	-0.79649000	0.22126800
H	-1.87804400	0.17849700	0.96988900
H	-2.76168400	0.80608300	-0.44854400
H	-0.55120700	-0.87113000	-3.85863800
H	-0.18445600	0.66171700	-4.69107900
H	1.08675100	-0.16857900	-3.75156300
H	2.18851900	1.05743200	-2.02797200
H	1.64526700	2.20677600	-0.77809100
H	2.86429300	0.95742100	-0.38225600
H	1.95168800	1.82329900	2.47132400
H	0.79071500	0.73647600	3.32494300
H	2.52807700	0.77731200	3.81193300
O	1.73035100	-1.84692400	2.45408900
C	2.19182900	-2.26629600	3.70051300
C	3.55829800	-2.44026100	3.93294600
C	1.24279700	-2.53080400	4.68856600
C	3.97605100	-2.88688100	5.19045500
H	4.27499300	-2.22955400	3.13768700
C	1.67452700	-2.98494200	5.93770100

H	0.18422400	-2.37985200	4.46844800
C	3.03933600	-3.16134400	6.19234800
H	5.04287100	-3.02463100	5.38285500
H	0.93826700	-3.19775200	6.71665700
H	3.37234800	-3.51378400	7.17135800
H	0.15998500	-1.02001200	0.87837700

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Energy = -1108.36798600 a.u. #Cluster: 8

P	3.53955900	0.52680400	1.58975400
O	4.57516700	0.77624200	0.55119500
N	0.03342200	-0.07352100	-0.11966300
N	1.89489900	0.65654300	1.03944400
C	-0.84299600	0.11696400	1.05363800
C	-0.64203000	-0.56287700	-1.33989200
C	1.33201800	0.14290400	-0.07985600
C	-1.40551500	1.53241900	1.15158700
C	-0.78610100	-2.08106500	-1.35598400
C	2.19557000	-0.14281300	-1.26733400
C	3.55140200	1.58744700	3.03051500
H	-0.29215900	-0.17342300	1.96039900
H	-1.65625800	-0.61326800	0.95139500
H	-1.62802600	-0.07793500	-1.36110900

H	-0.09565700	-0.20518800	-2.21963700
H	-1.97728000	1.78939300	0.24697100
H	-2.08248300	1.59296600	2.01686500
H	-0.61167000	2.28390400	1.28287100
H	0.19527400	-2.57831000	-1.35784700
H	-1.35126700	-2.43987700	-0.48269900
H	-1.33023700	-2.38192400	-2.26393500
H	1.94158800	0.57086900	-2.06761400
H	3.25235400	-0.01333200	-1.01625600
H	2.01826300	-1.15829900	-1.64383000
H	2.72971500	1.33315100	3.71516400
H	4.51505800	1.43526900	3.53859500
H	3.46518000	2.63367300	2.70300400
O	3.62439200	-1.01539200	2.13574600
C	2.51493300	-1.77855500	2.48856200
C	1.98116300	-1.68268500	3.77451500
C	1.95411900	-2.62669900	1.53172300
C	0.85277000	-2.44258400	4.09848000
H	2.44555100	-1.02017700	4.50722100
C	0.82509500	-3.37909900	1.86574000
H	2.40022500	-2.68398900	0.53710300
C	0.26989800	-3.28572800	3.14640700

H	0.42699300	-2.37069000	5.10217600
H	0.37661600	-4.03580900	1.11699200
H	-0.61539100	-3.87185100	3.40331600
H	1.25176400	0.93472100	1.77959500

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Energy = -1108.36797400 a.u. #Cluster: 9

P	3.52671600	0.50194100	1.58882200
O	4.58217200	0.76130900	0.57318700
N	0.05003900	-0.07728100	-0.18388200
N	1.89247800	0.64696200	1.01026100
C	-0.84996800	0.12208300	0.96966600
C	-0.60078300	-0.57700500	-1.41319900
C	1.34818100	0.13541000	-0.11903300
C	-1.41284300	1.53875500	1.04481600
C	-0.74220000	-2.09562300	-1.41775100
C	2.23453200	-0.15572900	-1.28860400
C	3.51309100	1.54394900	3.04309300
H	-0.31836200	-0.16039300	1.89017300
H	-1.66108800	-0.60909000	0.85692600
H	-1.58680400	-0.09377200	-1.45811800
H	-0.03774000	-0.22632500	-2.28521100
H	-0.61985500	2.28939200	1.18574300

H	-1.96662700	1.78902000	0.12725800
H	-2.10637100	1.60710900	1.89631400
H	-1.26472800	-2.40681500	-2.33485800
H	0.23978700	-2.59136300	-1.39209200
H	-1.32699500	-2.44670600	-0.55423100
H	3.28607900	-0.01944100	-1.01992900
H	2.06788300	-1.17447900	-1.66143300
H	1.99217300	0.55097400	-2.09863500
H	2.68404600	1.27857800	3.71431700
H	4.47114800	1.39138400	3.56146400
H	3.42510300	2.59324500	2.72575700
O	3.59843800	-1.05041500	2.10509500
C	2.48980700	-1.77870700	2.52843100
C	2.06328100	-1.69365400	3.85450000
C	1.82421400	-2.58508100	1.60259200
C	0.93658500	-2.42088500	4.25181700
H	2.61019700	-1.06749100	4.56186600
C	0.69731600	-3.30344100	2.00955600
H	2.19118400	-2.64094200	0.57635500
C	0.24880200	-3.21966800	3.33217400
H	0.59548700	-2.35870900	5.28798500
H	0.16781100	-3.92717100	1.28579200

H	-0.63432000	-3.78021900	3.64707300
H	1.23805400	0.92847400	1.73926300

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Energy = -1183.11292200 a.u. #Cluster: 1

P	-2.14080800	-0.58604900	-0.30602700
O	-1.95467600	-1.76518700	-1.41646200
O	-2.69169800	-1.08795200	0.99054900
N	1.47223700	0.69530900	-0.31200900
N	-0.76584600	0.27289500	-0.40116200
C	2.87570900	0.33502100	-0.08435400
C	1.21977000	2.03390500	-0.86069900
C	0.44208600	-0.13838000	-0.08943400
C	3.39188700	0.77525700	1.28334700
C	1.10270900	2.03781600	-2.38279500
C	0.72327600	-1.51063800	0.47974200
C	-2.98206300	-2.75004200	-1.57270000
H	3.46212200	0.81363400	-0.88355500
H	3.00189300	-0.74634000	-0.22062700
H	0.29660400	2.42071600	-0.40988700
H	2.04890400	2.67918000	-0.53538500

H	3.27974600	1.86282300	1.41700000
H	2.84365500	0.27192400	2.09530100
H	4.46040600	0.52693300	1.38166500
H	2.01674800	1.64086900	-2.85315000
H	0.24519400	1.43107700	-2.70765900
H	0.95026000	3.06660000	-2.74563800
H	-0.17670700	-1.88504100	0.98291900
H	0.97728600	-2.20424500	-0.33834600
H	1.55017100	-1.50988700	1.19967600
H	-2.57391800	-3.54881700	-2.20611600
H	-3.86726000	-2.31178900	-2.06254900
H	-3.27607800	-3.16290500	-0.59562500
O	-3.25730100	0.42340300	-0.96900400
C	-2.97067400	1.25807400	-2.03299900
C	-2.67420500	0.73964000	-3.29748700
C	-3.01208400	2.63833000	-1.81899000
C	-2.41407100	1.61849200	-4.35320700
H	-2.63738200	-0.34036400	-3.44254000
C	-2.75507200	3.50822300	-2.88225800
H	-3.23965200	3.01228700	-0.81869900
C	-2.45345500	3.00237800	-4.15177300
H	-2.17885000	1.21470100	-5.34129600

H	-2.78659000	4.58786300	-2.71465800
H	-2.24917200	3.68437400	-4.98056800

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Energy = -1183.11140400 a.u. #Cluster: 2

P	-2.25183300	-1.08501900	-0.68680600
O	-2.55514400	-1.95829400	-2.02123500
O	-2.68839800	-1.76400800	0.57302200
N	1.22551600	0.54012200	-0.45390000
N	-0.71917000	-0.56801400	-0.89936900
C	2.12858100	1.33288600	0.38659000
C	1.67050400	0.28390000	-1.82898200
C	0.02399000	0.09856300	-0.04308500
C	3.17394800	0.48161400	1.10381700
C	1.12921400	1.31469600	-2.81670700
C	-0.41197600	0.42409900	1.36709300
C	-1.81639400	-3.16065300	-2.25044400
H	1.54231500	1.91728800	1.10647800
H	2.62077200	2.06467800	-0.27214600
H	2.77033700	0.29274200	-1.82248600
H	1.34599600	-0.72506400	-2.11434700
H	3.78020400	-0.09039100	0.38373000
H	3.85140600	1.12596900	1.68601600

H	2.69740200	-0.23252900	1.79372400
H	1.44022000	2.33390400	-2.53639300
H	1.51207300	1.10685100	-3.82856500
H	0.03112600	1.28290200	-2.84797800
H	-1.26570400	-0.20525400	1.64100400
H	0.39416300	0.26808200	2.09581700
H	-0.71814100	1.48178400	1.42049500
H	-2.24265700	-3.63945900	-3.14206000
H	-1.90508300	-3.84516500	-1.39120200
H	-0.75200600	-2.93604600	-2.42690000
O	-3.24064500	0.19534000	-0.97523700
C	-2.89114400	1.21490100	-1.84350000
C	-2.93450600	1.01531300	-3.22626800
C	-2.51338900	2.44842000	-1.30785200
C	-2.59178100	2.06872100	-4.07845600
H	-3.22443500	0.03832200	-3.61511600
C	-2.17562500	3.49627700	-2.16909800
H	-2.48372700	2.57001100	-0.22315800
C	-2.21192500	3.30995800	-3.55517700
H	-2.62086700	1.91590600	-5.16035000
H	-1.87725600	4.46157000	-1.75228400
H	-1.94286200	4.12916800	-4.22614400

Energy = -1183.11050100 a.u. #Cluster: 3

P	-2.30944400	-1.22615600	-0.74923800
O	-2.56173800	-2.62821400	-1.49452900
O	-2.97481400	-1.23233300	0.59078200
N	1.20293200	0.31904400	-0.84899100
N	-0.72817700	-0.89447000	-0.94309000
C	2.10753000	1.31198400	-0.26256400
C	1.62059000	-0.27003300	-2.12603900
C	0.01031600	-0.00575800	-0.31731200
C	1.88415200	2.71683200	-0.82066700
C	2.32899500	-1.61021600	-1.94923700
C	-0.39605500	0.66388400	0.97514600
C	-2.02165200	-2.90897800	-2.79002400
H	3.13562000	0.97826600	-0.47101200
H	1.99916700	1.30961200	0.82872700
H	0.72824600	-0.38827700	-2.75417200
H	2.28547200	0.45439500	-2.61876800
H	0.86710300	3.07549900	-0.60061400
H	2.60549200	3.41908500	-0.37395900
H	2.02054400	2.73641200	-1.91346800
H	1.65535600	-2.34624300	-1.48508400

H	2.64937200	-2.00228800	-2.92765800
H	3.22274300	-1.50495800	-1.31337700
H	0.34992900	0.46624500	1.75975900
H	-0.46834700	1.75348500	0.84617900
H	-1.36325700	0.27235000	1.30474600
H	-2.39925000	-3.89676600	-3.08646400
H	-0.92199900	-2.92495300	-2.75757400
H	-2.35219000	-2.15523200	-3.52165800
O	-3.06812200	-0.20025300	-1.81720000
C	-2.74884600	1.14335800	-1.75066500
C	-1.88107900	1.68512900	-2.70340300
C	-3.27328300	1.93633500	-0.72565500
C	-1.53962200	3.03766800	-2.62922000
H	-1.47379800	1.03711600	-3.48158800
C	-2.92480100	3.28848600	-0.65913500
H	-3.93616200	1.48069000	0.01180100
C	-2.05699400	3.84193200	-1.60678200
H	-0.85670200	3.46271000	-3.36890900
H	-3.33141600	3.91079000	0.14207800
H	-1.78271000	4.89791300	-1.54862200

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Energy = -1183.11050000 a.u. #Cluster: 4

P	-2.33365800	-1.18318000	-0.74610400
O	-2.62499300	-2.57626200	-1.49360000
O	-2.98338100	-1.17955600	0.60151800
N	1.21641500	0.27440900	-0.87696900
N	-0.74724900	-0.88665200	-0.95511200
C	2.14683500	1.25274700	-0.30663000
C	1.61719300	-0.34406700	-2.14551800
C	0.01516100	-0.00997000	-0.34130200
C	1.95976400	2.65402000	-0.88678300
C	2.28342800	-1.70311300	-1.95039300
C	-0.37356300	0.69078200	0.93988900
C	-2.10252400	-2.86592400	-2.79434800
H	3.16563300	0.88898000	-0.51026200
H	2.03941200	1.27064000	0.78455400
H	0.72253000	-0.44275500	-2.77388100
H	2.30472200	0.35301100	-2.64643800
H	2.09301100	2.65194200	-1.98013700
H	0.95377600	3.04356900	-0.66902900
H	2.70148300	3.34343800	-0.45369100
H	2.59367800	-2.11710100	-2.92303500
H	3.17866300	-1.61745100	-1.31364300
H	1.58639500	-2.41210100	-1.47889700

H	-0.42568800	1.77905900	0.79036400
H	-1.34684400	0.32459400	1.28058900
H	0.37128100	0.49444200	1.72579500
H	-1.00331800	-2.90673100	-2.77136200
H	-2.42257900	-2.10348100	-3.52162600
H	-2.50472700	-3.84436700	-3.08944400
O	-3.08182200	-0.13765800	-1.80231000
C	-2.75107100	1.20201500	-1.71544900
C	-1.85166100	1.74374600	-2.63843300
C	-3.29647900	1.99064100	-0.69801400
C	-1.49958400	3.09224600	-2.54195700
H	-1.42859400	1.09905000	-3.41086300
C	-2.93785800	3.33875700	-0.60962000
H	-3.98333800	1.53414500	0.01661400
C	-2.03832300	3.89219500	-1.52738800
H	-0.79175300	3.51708600	-3.25790100
H	-3.36121700	3.95796100	0.18530800
H	-1.75605600	4.94498300	-1.45195500

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Energy = -1183.11037400 a.u. #Cluster: 5

P	-2.31892100	-0.96387400	-0.48524200
O	-2.46830000	-2.51618700	-0.88953300

O	-3.02277700	-0.71231200	0.81083500
N	1.26672400	0.45321900	-0.52500400
N	-0.77049200	-0.54662600	-0.75112200
C	2.29279200	1.20534000	0.20351200
C	1.58206900	0.09924600	-1.91373700
C	0.07259800	0.12440500	-0.00003100
C	3.31986300	0.30442800	0.88582400
C	1.07525500	1.14479200	-2.90428000
C	-0.22216100	0.55850500	1.41700000
C	-1.90297800	-3.04934800	-2.09058500
H	1.81334300	1.86936600	0.93299100
H	2.78978900	1.86170500	-0.52712800
H	2.67468000	-0.00651500	-1.98538000
H	1.13555300	-0.87984500	-2.12899100
H	4.09161500	0.91694500	1.37812300
H	2.84503000	-0.33171300	1.64920100
H	3.81910300	-0.35135000	0.15501500
H	1.35303500	0.86061500	-3.93181200
H	-0.01976400	1.22916900	-2.85353200
H	1.51191400	2.13446000	-2.69426800
H	-1.16530500	0.11393700	1.74819000
H	0.58666700	0.26512300	2.10055000

H	-0.31626300	1.65553800	1.45878400
H	-0.80369500	-3.00195400	-2.05958900
H	-2.26584300	-2.49692600	-2.97148700
H	-2.22460900	-4.09727900	-2.15858500
O	-3.11930700	-0.28384300	-1.76870300
C	-2.86938300	1.00208700	-2.18845200
C	-2.78859200	1.23456200	-3.56474300
C	-2.70608300	2.05327500	-1.27787800
C	-2.53370500	2.52659900	-4.03142000
H	-2.91652200	0.39595900	-4.25238200
C	-2.43721200	3.33875300	-1.75575400
H	-2.79589600	1.85970300	-0.20741800
C	-2.34880400	3.58160600	-3.13058500
H	-2.46867800	2.70660200	-5.10756000
H	-2.30151500	4.15698200	-1.04384900
H	-2.14012900	4.58894300	-3.49843500

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Energy = -1183.11027100 a.u. #Cluster: 6

P	-1.90185500	-1.10506200	-0.64978500
O	-1.78343700	-2.20050400	-1.84536900
O	-2.45586200	-1.68145900	0.61583000
N	1.41847400	0.79529400	-0.23687300

N	-0.47180400	-0.35615900	-0.77894600
C	2.38768000	1.37605700	0.69703100
C	1.68912600	0.99770600	-1.66528500
C	0.32155800	0.12068400	0.15224600
C	3.57412100	0.45465200	0.97357200
C	1.00041400	2.24388200	-2.21561800
C	0.07136200	-0.03690100	1.63444600
C	-2.88502500	-3.08508600	-2.07568700
H	1.88166900	1.64637200	1.63174400
H	2.73715700	2.32076000	0.25287200
H	2.78009200	1.07247900	-1.78445900
H	1.35064000	0.10530000	-2.20680600
H	4.10128100	0.19665400	0.04151900
H	4.29106700	0.95416100	1.64405000
H	3.24684200	-0.48117900	1.45325100
H	-0.09144500	2.15872800	-2.12047700
H	1.33038200	3.14904300	-1.68064500
H	1.24253300	2.37098200	-3.28259400
H	-0.77611200	-0.71086600	1.79434600
H	0.95752400	-0.43409600	2.14918800
H	-0.16353200	0.94277100	2.08058600
H	-3.19115100	-3.57849100	-1.14042700

H	-2.54894600	-3.83876900	-2.79990700
H	-3.74440900	-2.53476400	-2.49305300
O	-3.02081000	-0.02703900	-1.21454500
C	-2.78007300	0.89550400	-2.21178700
C	-3.00953600	2.24277300	-1.91823600
C	-2.35409300	0.50665200	-3.48694800
C	-2.81449500	3.20901100	-2.90921700
H	-3.33595900	2.51595900	-0.91262200
C	-2.15543600	1.48180000	-4.46779700
H	-2.16967800	-0.54744800	-3.69596000
C	-2.38486800	2.83334200	-4.18635800
H	-2.99397200	4.26201000	-2.67738700
H	-1.81827000	1.17927200	-5.46265800
H	-2.22805400	3.59006700	-4.95869800

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Energy = -1183.10969200 a.u. #Cluster: 7

P	-1.78452000	-0.20968000	-0.99181900
O	-2.28361000	-1.53537100	-1.77158300
O	-2.73891500	0.10085200	0.11477500
N	1.92728900	0.05049000	-0.06409300
N	-0.19578800	-0.45578500	-0.73670000
C	2.96160100	0.93431900	0.48481000

C	2.38250900	-1.25069800	-0.56833100
C	0.63150400	0.39183700	-0.16332300
C	3.23346900	0.68816000	1.96686200
C	2.71079400	-1.21896300	-2.05880400
C	0.19895200	1.74286200	0.36089300
C	-1.56957800	-2.05360400	-2.89782800
H	2.68175000	1.98016300	0.30703600
H	3.87588500	0.75950000	-0.10249100
H	3.26967300	-1.53537000	0.01652600
H	1.59617400	-1.98935200	-0.36611700
H	3.53097200	-0.35703200	2.14654200
H	4.05010700	1.34057100	2.31400800
H	2.34007400	0.89904400	2.57544100
H	3.07294100	-2.20610700	-2.38732300
H	1.81586000	-0.96517500	-2.64638700
H	3.49559700	-0.47705200	-2.27751800
H	0.40267200	2.51459500	-0.39953100
H	-0.87844600	1.72933200	0.56320900
H	0.72342000	2.02398000	1.28211700
H	-2.14375300	-2.90974100	-3.27626600
H	-0.56244500	-2.38218700	-2.59992800
H	-1.48330000	-1.29249400	-3.68985500

O	-1.77762200	0.96578600	-2.16237300
C	-2.91214400	1.65784300	-2.53094800
C	-2.81016700	3.04771100	-2.64581800
C	-4.11846900	1.00534200	-2.81222200
C	-3.92248200	3.79022000	-3.05111600
H	-1.85705800	3.52863100	-2.41569200
C	-5.22661200	1.75985600	-3.20792500
H	-4.18312400	-0.07992700	-2.72238600
C	-5.13536100	3.15064000	-3.33080900
H	-3.84015600	4.87632500	-3.14308800
H	-6.16939800	1.25134700	-3.42596100
H	-6.00519600	3.73322200	-3.64344200

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Energy = -1183.10964500 a.u. #Cluster: 8

P	-1.74193500	-0.14003700	-0.92397100
O	-2.19541200	-1.25836500	-1.99643100
O	-2.66446700	-0.18990400	0.25351400
N	1.96770100	0.06915700	0.04289000
N	-0.13429700	-0.31536100	-0.75931100
C	2.95619000	0.76720400	0.87181300
C	2.49165600	-0.92810200	-0.89789000
C	0.64982100	0.33116900	0.07512900

C	3.28832200	0.01989000	2.16135500
C	2.75805400	-0.34208500	-2.28217000
C	0.14662600	1.37811000	1.04292700
C	-1.49024900	-1.45675800	-3.22570700
H	2.60069900	1.78205500	1.08963500
H	3.86230700	0.88593000	0.25821000
H	3.41837700	-1.33184700	-0.46408600
H	1.76722900	-1.75015300	-0.96475100
H	4.06553900	0.56238700	2.72233800
H	2.39984300	-0.07525200	2.80516500
H	3.66588200	-0.99222700	1.94644800
H	1.82557200	0.03742400	-2.72585900
H	3.48439900	0.48492700	-2.23065800
H	3.16926800	-1.11708700	-2.94839400
H	-0.92861600	1.23960800	1.20402900
H	0.65629900	1.33256000	2.01329100
H	0.31238500	2.38110000	0.61641200
H	-1.48382800	-0.53537300	-3.82947100
H	-2.01988800	-2.24666400	-3.77484500
H	-0.45309000	-1.76950700	-3.03285500
O	-1.84847400	1.27184000	-1.78397900
C	-2.99773600	1.70606200	-2.41321500

C	-2.83805500	2.34685500	-3.64700700
C	-4.27108600	1.54450700	-1.85325300
C	-3.95935800	2.83155500	-4.32425100
H	-1.83251900	2.45651500	-4.05876400
C	-5.38590100	2.02656400	-2.54644800
H	-4.37258900	1.04880700	-0.88771200
C	-5.23857000	2.67055700	-3.77921000
H	-3.83131500	3.33314800	-5.28697700
H	-6.38048500	1.89879100	-2.11098900
H	-6.11519800	3.04608900	-4.31241400

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Energy = -1183.54876700 a.u. #Cluster: 1

P	-2.31085500	-1.08552900	-2.11007100
O	-2.03660400	-1.67401500	-3.56104100
O	-3.17788400	-1.85364400	-1.18730200
N	1.13548400	0.29887400	-0.78914200
N	-0.79562000	-0.84292100	-1.33373500
C	2.32032300	1.11456400	-1.13123100
C	1.00163300	-0.05859000	0.63794400
C	0.25282900	-0.06360500	-1.69428300

C	2.06628200	2.60495300	-0.92987800
C	1.61884000	-1.41602600	0.96346600
C	0.41368200	0.33696700	-3.12640600
C	-1.68166000	-3.06545000	-3.73093700
H	2.62286600	0.89479100	-2.16111100
H	3.13391600	0.76482800	-0.48061300
H	1.50158700	0.73798000	1.20403700
H	-0.06078600	-0.00934600	0.91890500
H	1.78889800	2.82467700	0.11233200
H	2.98413800	3.16413900	-1.16609900
H	1.25924500	2.96716300	-1.58465000
H	1.11661000	-2.23485200	0.42538900
H	2.68722300	-1.43265300	0.69968800
H	1.52587800	-1.60589800	2.04323000
H	1.27899700	-0.20481800	-3.54176400
H	-0.46347100	0.07533300	-3.72234700
H	0.60672100	1.41266700	-3.21564300
H	-0.65462800	-3.23293300	-3.37449000
H	-1.74604500	-3.26988800	-4.80586200
H	-2.38372800	-3.70634900	-3.17940500
O	-2.76838900	0.39399300	-2.56142300
C	-2.66575300	1.49238800	-1.70203300

C	-3.11757200	1.42637700	-0.38274900
C	-2.08303300	2.64808200	-2.22072500
C	-2.96272700	2.54893800	0.43622100
H	-3.57865500	0.51186500	-0.00621600
C	-1.94267900	3.76480400	-1.39223000
H	-1.74369300	2.66001200	-3.25766300
C	-2.37553700	3.71625600	-0.06275700
H	-3.30761600	2.50629800	1.47206900
H	-1.48543000	4.67395800	-1.78970100
H	-2.25733700	4.58866800	0.58388400
H	-0.82065700	-1.19102100	-0.37671900

41

Energy = -1183.54828300 a.u. #Cluster: 2

P	-2.08447000	-1.01182300	-2.49395900
O	-1.94902700	-0.57162100	-4.01762500
O	-2.46923400	-2.40828600	-2.19209100
N	1.08776900	-0.03945400	-0.33743200
N	-0.54788400	-0.51575400	-1.89061600
C	1.78762000	0.85515300	-1.28301900
C	1.69428200	-0.14407900	1.00634900
C	-0.01989100	-0.67503800	-0.65508800
C	1.20181100	2.26482900	-1.29696900

C	2.78771100	-1.20397600	1.06982300
C	-0.71988400	-1.55544500	0.33100100
C	-1.32625200	-1.42376400	-5.00790300
H	1.78366400	0.39819200	-2.28411800
H	2.83892500	0.87554200	-0.96883900
H	2.10126900	0.85085000	1.23568700
H	0.90498800	-0.33676300	1.74136400
H	1.79550800	2.89553200	-1.97536900
H	0.15891500	2.27535600	-1.64429800
H	1.23381500	2.71112200	-0.29170500
H	2.38474300	-2.20773400	0.86539100
H	3.58834900	-0.99628500	0.34331600
H	3.23159200	-1.20698800	2.07687100
H	-0.00329700	-2.19597000	0.85936900
H	-1.23527100	-0.92506900	1.07371900
H	-1.45647400	-2.18638200	-0.17602700
H	-1.59906000	-1.00936400	-5.98535200
H	-1.70234700	-2.45157900	-4.91180100
H	-0.23374700	-1.40594800	-4.88182800
O	-3.12091700	0.06174200	-1.89457400
C	-2.80927500	1.40567800	-1.66180300
C	-2.66710900	2.28980100	-2.73115700

C	-2.66464100	1.82229700	-0.33894000
C	-2.36890200	3.62859800	-2.45927000
H	-2.78423100	1.92831900	-3.75350200
C	-2.37017300	3.16405200	-0.08186500
H	-2.78135400	1.09706000	0.46852000
C	-2.22027500	4.06758100	-1.13926900
H	-2.25241500	4.33104200	-3.28797000
H	-2.25304900	3.50092500	0.95078300
H	-1.98570300	5.11463600	-0.93450100
H	-0.06128500	0.11405400	-2.52636300

41

Energy = -1183.54825300 a.u. #Cluster: 3

P	-2.32976500	-0.87542600	-1.82212200
O	-2.31499400	-2.05144700	-2.88353700
O	-3.05273900	-1.22033200	-0.57925200
N	1.25458100	-0.08521800	-0.37812800
N	-0.70118300	-0.37744500	-1.56089100
C	1.59642200	1.12000400	-1.16320600
C	2.21855900	-0.44431000	0.68436000
C	0.14759100	-0.76698000	-0.58239800
C	0.91623300	2.37580100	-0.62336200
C	3.35160000	-1.32243400	0.16659500

C	-0.19889500	-1.96038100	0.25135500
C	-1.63650400	-1.97798700	-4.15519000
H	1.36096100	0.94478600	-2.22395100
H	2.68826000	1.21977500	-1.11636800
H	2.60820400	0.50597400	1.07534800
H	1.68037700	-0.92387400	1.50957500
H	1.20505300	2.55253600	0.42377700
H	1.23033400	3.24363300	-1.22194000
H	-0.18000300	2.30444700	-0.67521200
H	4.06137900	-1.51990500	0.98416600
H	2.97228500	-2.28708300	-0.20421000
H	3.89880400	-0.82713100	-0.65032000
H	-0.64684700	-1.62461000	1.20036900
H	-0.92353500	-2.59751500	-0.26439500
H	0.69580600	-2.55175800	0.47486600
H	-2.08409500	-1.18932600	-4.77604300
H	-1.76950900	-2.95629600	-4.63156200
H	-0.56529700	-1.77846100	-4.00381000
O	-2.84155100	0.37896800	-2.69969600
C	-2.77691800	1.70098400	-2.24555200
C	-3.26401700	2.05467200	-0.98624000
C	-2.20273500	2.63948900	-3.10232400

C	-3.16082800	3.38819800	-0.57880800
H	-3.70779900	1.29638400	-0.34007700
C	-2.11386500	3.96989900	-2.68336100
H	-1.82906400	2.31917800	-4.07679500
C	-2.58808100	4.34603200	-1.42207300
H	-3.53448100	3.67632800	0.40669200
H	-1.66469700	4.71323600	-3.34618200
H	-2.51116200	5.38575700	-1.09606600
H	-0.39309500	0.38287800	-2.16509000

41

Energy = -1183.54824500 a.u. #Cluster: 4

P	-2.39111900	-0.90829800	-1.50486800
O	-2.50518600	-2.12439100	-2.51391200
O	-2.94482700	-1.20549700	-0.16625800
N	1.34406100	-0.04221300	-0.57638300
N	-0.74575000	-0.39887700	-1.47836300
C	1.56845900	1.12422700	-1.45594300
C	2.44326200	-0.34904000	0.36447500
C	0.22480000	-0.73405600	-0.59740700
C	0.97019500	2.40505100	-0.87988000
C	3.49711800	-1.26077800	-0.25276800
C	0.00196000	-1.87700600	0.34174700

C	-1.97670400	-2.10283900	-3.85675800
H	1.18045200	0.90537500	-2.46207100
H	2.65529000	1.22053900	-1.57376800
H	2.88078000	0.61857400	0.64749300
H	2.02214100	-0.78175500	1.27871000
H	1.18905300	3.24398700	-1.55690800
H	-0.12131100	2.33176100	-0.76765900
H	1.40837600	2.62900400	0.10442400
H	4.30863900	-1.42041800	0.47331600
H	3.07186100	-2.24058800	-0.51905100
H	3.93142300	-0.81243400	-1.15965700
H	-0.25982100	-1.48374400	1.33719200
H	-0.81587000	-2.51667200	-0.00152200
H	0.91168300	-2.48152800	0.43462800
H	-2.49008400	-1.33451100	-4.45174700
H	-2.16626700	-3.09719100	-4.27753500
H	-0.89471400	-1.90527700	-3.83574000
O	-3.02498600	0.30789200	-2.35551500
C	-2.89303300	1.64950400	-1.98221600
C	-2.44248900	2.53771100	-2.95809000
C	-3.19592800	2.06997200	-0.68627600
C	-2.29245200	3.88656500	-2.62475500

H	-2.21113000	2.16459500	-3.95757200
C	-3.03348500	3.42143600	-0.36672800
H	-3.54532700	1.34881100	0.05370500
C	-2.58381800	4.33005100	-1.33032700
H	-1.93928600	4.59118600	-3.38132900
H	-3.26329300	3.76279300	0.64542900
H	-2.45985300	5.38421100	-1.07234600
H	-0.51803000	0.32490800	-2.15882700

41

Energy = -1183.54820100 a.u. #Cluster: 5

P	-2.24840500	-0.75255900	-2.23991300
O	-2.21316400	-1.46670200	-3.65386000
O	-2.85134200	-1.58868500	-1.17977100
N	1.32962900	-0.19589400	-0.69171400
N	-0.65176500	-0.21933400	-1.87241200
C	2.38977100	-0.83380600	0.11944800
C	1.49750600	1.25568500	-0.91587400
C	0.28891300	-0.86287400	-1.14259000
C	3.57368100	-1.28509500	-0.72729900
C	0.75458700	2.09237400	0.12221500
C	0.10877400	-2.32137500	-0.85912700
C	-1.64050100	-0.87226700	-4.83786800

H	1.95644500	-1.66514100	0.68628800
H	2.70138000	-0.08057000	0.85645800
H	2.57643000	1.45254900	-0.87411200
H	1.19072300	1.50638500	-1.94180100
H	4.01165200	-0.44066500	-1.28129800
H	4.35096600	-1.70488200	-0.07098600
H	3.27544700	-2.05847300	-1.45169300
H	0.94384600	3.15871500	-0.07087200
H	-0.33201900	1.92627700	0.08184000
H	1.10746700	1.85505600	1.13729900
H	1.07191800	-2.84176500	-0.83892900
H	-0.38172200	-2.44268700	0.11983700
H	-0.52425900	-2.78599100	-1.62215500
H	-1.71443300	-1.62881900	-5.62775500
H	-0.58515900	-0.61596000	-4.66238500
H	-2.20647800	0.02687500	-5.11865800
O	-2.92115000	0.67356400	-2.58575700
C	-2.90784400	1.75133500	-1.69355000
C	-3.36385900	1.60434400	-0.38274600
C	-2.41836000	2.96660000	-2.17099600
C	-3.31834200	2.71190400	0.46935900
H	-3.73980900	0.63908200	-0.04118000

C	-2.38560700	4.06609500	-1.30868500
H	-2.06680200	3.03560300	-3.20223100
C	-2.83163800	3.94083500	0.01123600
H	-3.66857900	2.60929700	1.49918500
H	-2.00326600	5.02290800	-1.67205800
H	-2.79908100	4.80105300	0.68368300
H	-0.46076200	0.74804800	-2.12963500

41

Energy = -1183.54772600 a.u. #Cluster: 6

P	-1.85930600	-0.41245200	-1.28374600
O	-2.02453100	-0.07777800	-2.83587300
O	-2.65826700	-1.53508700	-0.74032000
N	2.05712400	-0.30767300	-0.74105800
N	-0.20317800	-0.70697000	-0.97635100
C	3.27813700	0.50394300	-0.93902100
C	2.23897800	-1.53750800	0.05776600
C	0.88633300	0.06077500	-1.21587400
C	4.08002000	0.05807500	-2.15584900
C	1.92922200	-1.32133600	1.53663200
C	0.73513200	1.32739700	-1.99825500
C	-2.12077600	-1.13058600	-3.82060300
H	3.86903100	0.39141900	-0.01938100

H	2.99949200	1.56162600	-1.00447200
H	1.63111900	-2.34495400	-0.37589900
H	3.28368300	-1.84497400	-0.07915100
H	3.50653300	0.19424200	-3.08550000
H	4.99938500	0.65904100	-2.22427700
H	4.36753400	-1.00152900	-2.07686200
H	0.87885600	-1.03302200	1.69513600
H	2.11707200	-2.25581900	2.08620800
H	2.57333800	-0.53521000	1.95904700
H	1.58192200	1.46780400	-2.67931900
H	-0.18653500	1.31946400	-2.58619300
H	0.70156800	2.17990100	-1.30087200
H	-2.85517600	-1.88220700	-3.49952700
H	-1.13568100	-1.59908100	-3.96173800
H	-2.44833200	-0.65318000	-4.75151800
O	-2.01852500	1.04972200	-0.63301500
C	-3.09503900	1.89981000	-0.90057200
C	-4.41039800	1.43971900	-0.82607400
C	-2.79534400	3.22523900	-1.21054400
C	-5.45031300	2.33970200	-1.07779900
H	-4.61232600	0.39790800	-0.57083400
C	-3.84603500	4.11501700	-1.45104600

H	-1.75212700	3.54239000	-1.25963300
C	-5.17299000	3.67509100	-1.38841900
H	-6.48442400	1.99090700	-1.02424900
H	-3.62312400	5.15707500	-1.69284900
H	-5.99085600	4.37342300	-1.58031300
H	-0.07640400	-1.56928400	-0.44884000

41

Energy = -1183.54745900 a.u. #Cluster: 7

P	-1.80045800	0.42648300	-0.99461600
O	-2.24764300	-0.83350500	-1.86394600
O	-2.53073700	0.49660000	0.28933200
N	1.97284700	-0.51950500	-0.34121500
N	-0.08615700	0.35378900	-0.91173200
C	2.84384400	-1.54438800	0.27485400
C	2.67568700	0.54434300	-1.08785700
C	0.66064800	-0.57351400	-0.27102700
C	3.33312100	-1.13557700	1.65889000
C	2.80665600	0.22094600	-2.57375300
C	-0.04769400	-1.66224500	0.47234400
C	-1.71313300	-1.11980000	-3.17392900
H	3.68900800	-1.67670400	-0.41489800
H	2.30944000	-2.50071800	0.29987200

H	2.16225300	1.50187600	-0.91587000
H	3.66548700	0.64726800	-0.62466800
H	4.01897500	-1.90544400	2.04369000
H	3.87699500	-0.17915200	1.62255000
H	2.49526700	-1.03193700	2.36532900
H	3.35511800	-0.72189500	-2.71995200
H	1.82384900	0.12992300	-3.06138800
H	3.36466300	1.02726100	-3.07277500
H	0.52480200	-1.99636100	1.34310600
H	-1.02744500	-1.30897400	0.81500100
H	-0.19619900	-2.51898800	-0.20553200
H	-1.91517500	-0.28312000	-3.85795300
H	-2.22488500	-2.02390000	-3.52364300
H	-0.63016900	-1.30345600	-3.11242300
O	-1.83523500	1.72169600	-1.95682400
C	-2.98019400	2.50226100	-2.13946200
C	-4.20293000	1.91759600	-2.47243600
C	-2.83820700	3.88245100	-2.00682500
C	-5.31137000	2.74641300	-2.67058500
H	-4.28817400	0.83459300	-2.57936100
C	-3.95286900	4.69878600	-2.21763400
H	-1.86423500	4.29877300	-1.74302300

C	-5.19032200	4.13419200	-2.54633500
H	-6.27401800	2.29894700	-2.92928300
H	-3.85170500	5.78228300	-2.11889600
H	-6.05982000	4.77581200	-2.70650300
H	0.38490400	1.07793100	-1.45168200

41

Energy = -1183.54736900 a.u. #Cluster: 8

P	-2.23769700	-1.15077900	-2.25973200
O	-1.94062600	-1.18018300	-3.82290800
O	-2.90881000	-2.31671800	-1.64438200
N	0.76405600	0.15624200	-0.09959500
N	-0.66610000	-0.78065700	-1.65262400
C	1.23006000	0.38434700	1.28456300
C	1.53665100	0.84951900	-1.15096100
C	-0.29030300	-0.58385800	-0.36478500
C	0.64189500	1.65859800	1.88128600
C	2.63859200	-0.02563300	-1.74171800
C	-1.07567700	-1.23303600	0.72990700
C	-1.43168000	-2.36538500	-4.47926000
H	2.32615600	0.44344900	1.23636600
H	0.98590400	-0.49206300	1.89479400
H	0.84386200	1.22041900	-1.92101700

H	1.96598900	1.74350500	-0.68051900
H	1.05390900	1.80958000	2.89039400
H	0.89366300	2.53917100	1.27123900
H	-0.45395000	1.59698600	1.95841100
H	3.33448600	-0.35861200	-0.95688500
H	2.23018900	-0.91645800	-2.24341200
H	3.20518800	0.55716700	-2.48320700
H	-1.40878000	-0.48667400	1.46348300
H	-1.93956000	-1.76760400	0.32430600
H	-0.43181000	-1.96120400	1.24747300
H	-1.99267100	-3.25029500	-4.14848200
H	-0.36234600	-2.48708300	-4.25197100
H	-1.57273200	-2.20657300	-5.55464100
O	-3.06228800	0.22149700	-2.07420900
C	-2.44767100	1.47911900	-2.11045800
C	-2.08784000	2.04344800	-3.33359000
C	-2.20013400	2.12631300	-0.90042300
C	-1.45262500	3.28922200	-3.33655500
H	-2.29403200	1.50572300	-4.26008500
C	-1.56130600	3.36913900	-0.91743600
H	-2.49621300	1.65056400	0.03642600
C	-1.18454100	3.95040800	-2.13289800

H	-1.16213600	3.74144700	-4.28785800
H	-1.35270000	3.87897500	0.02579200
H	-0.68135800	4.91996000	-2.14238700
H	-0.06022400	-0.39094100	-2.37350200

41

Energy = -1183.54730800 a.u. #Cluster: 9

P	-1.80420300	0.26563200	-1.39552500
O	-1.83424000	-0.45957800	-2.81604600
O	-2.80379500	-0.30244700	-0.46525300
N	1.85672900	-0.72894100	-0.31697100
N	-0.16141700	0.23116800	-0.89487500
C	2.73075100	-1.89167900	-0.04717400
C	2.52808900	0.58768400	-0.30181300
C	0.57847900	-0.86056900	-0.59825200
C	2.86851300	-2.18227300	1.44238700
C	2.98947700	1.01947100	-1.69139100
C	-0.08927700	-2.19923800	-0.63836300
C	-0.97736600	-0.07945900	-3.91394000
H	3.70667600	-1.64654900	-0.48911900
H	2.34925900	-2.76049000	-0.59517300
H	1.85771900	1.32902200	0.15833100
H	3.38263000	0.49233400	0.38035500

H	3.26723400	-1.31054400	1.98349200
H	1.89950700	-2.45453200	1.88831800
H	3.56492200	-3.02242100	1.58527800
H	2.14160900	1.13282500	-2.38421300
H	3.50617500	1.98794900	-1.61732000
H	3.68950200	0.28435000	-2.11647800
H	0.04283900	-2.63630100	-1.64187000
H	0.33381900	-2.88536600	0.10205200
H	-1.16189600	-2.09181200	-0.43873500
H	-1.22858600	-0.74839400	-4.74512600
H	0.07952800	-0.20758800	-3.63718200
H	-1.16738200	0.96512300	-4.19926900
O	-1.83197100	1.85832300	-1.65545300
C	-3.01578800	2.59069400	-1.78131700
C	-3.14272800	3.73769400	-0.99972500
C	-4.00787700	2.20102200	-2.68218700
C	-4.29530600	4.51765400	-1.12844300
H	-2.34355200	4.00573600	-0.30622700
C	-5.15945000	2.98607200	-2.79291900
H	-3.88180300	1.30298100	-3.28963700
C	-5.30561700	4.14337500	-2.02131900
H	-4.40352900	5.42076700	-0.52294800

H	-5.94353800	2.68940200	-3.49361000
H	-6.20627700	4.75420900	-2.11638700
H	0.28693100	1.14573500	-0.88701200

41

Energy = -1183.54667000 a.u. #Cluster: 10

P	-1.69799800	0.18162700	-1.69001100
O	-1.74390800	-0.06897100	-3.26565000
O	-2.52953900	-0.79099500	-0.95155000
N	2.03316400	-0.62610100	-0.71823100
N	-0.03620500	0.24267000	-1.25793300
C	2.99787400	-1.73728900	-0.56047700
C	2.51864200	0.69846600	-0.27655200
C	0.81867700	-0.80299800	-1.19083900
C	3.90612600	-1.89234700	-1.77386000
C	2.15532000	0.99886000	1.17487400
C	0.32126100	-2.14001900	-1.64290500
C	-1.05907500	0.77249400	-4.21821700
H	2.44907900	-2.66030100	-0.34187400
H	3.58348200	-1.50298000	0.33932600
H	3.60828500	0.68927600	-0.40934700
H	2.14005700	1.46849300	-0.96478800
H	4.63710100	-2.69225100	-1.58143000

H	3.32923500	-2.15728100	-2.67325900
H	4.45968300	-0.96291900	-1.97758100
H	2.57512600	1.97578500	1.45767700
H	1.06553600	1.03571300	1.32518200
H	2.57266100	0.23459100	1.84789600
H	-0.34025900	-2.01538300	-2.50960400
H	1.13389300	-2.81511100	-1.92241500
H	-0.26531200	-2.59370400	-0.82801500
H	-1.24209500	0.33091400	-5.20464700
H	0.02036900	0.78639600	-4.00737100
H	-1.46524000	1.79321600	-4.17897600
O	-1.96207300	1.75589200	-1.44582000
C	-3.23597700	2.29014100	-1.23596900
C	-3.40158700	3.13102500	-0.13678400
C	-4.28416700	2.01309800	-2.11455400
C	-4.65266100	3.71315700	0.08491500
H	-2.55573200	3.31968000	0.52687000
C	-5.53274900	2.59448700	-1.87400200
H	-4.12699000	1.35893000	-2.97431700
C	-5.71994900	3.44463800	-0.77923800
H	-4.79255800	4.37638100	0.94197100
H	-6.36154700	2.38257300	-2.55370900

H	-6.69717700	3.89875500	-0.59996500
H	0.27201400	1.15243700	-0.91987700

AEOP

43

Energy = -1222.35929500 a.u. #Cluster: 1

P	-1.83117400	0.36123100	-0.27056800
O	-2.25013100	-1.09976200	0.29366900
O	-2.02064900	1.44898700	0.74071100
N	1.46073700	0.58913100	-2.24091100
N	-0.39955500	0.10605200	-1.01224800
C	2.39041200	1.49007300	-2.92933800
C	1.72730300	-0.84825700	-2.37264900
C	0.38449300	1.01219500	-1.55459700
C	3.61613100	1.83863700	-2.08800300
C	0.96434300	-1.47917400	-3.53481200
C	0.12938000	2.49980400	-1.47019300
C	-2.02279000	-1.44822500	1.67398900
C	-0.56211700	-1.74887500	1.95713600
H	2.69864300	0.98534300	-3.85778200
H	1.85925800	2.39868500	-3.23846400
H	1.45335100	-1.33545000	-1.42804900

H	2.81209000	-0.96703700	-2.51075500
H	3.32821800	2.37700300	-1.17126100
H	4.16555000	0.93045500	-1.79386900
H	4.30052600	2.48000100	-2.66532800
H	1.21795900	-2.54805500	-3.61746700
H	-0.12030200	-1.39164100	-3.38124300
H	1.22136300	-0.99316800	-4.48970800
H	-0.28350900	2.85580900	-2.42834300
H	-0.59802400	2.70143400	-0.67622600
H	1.04655700	3.06712300	-1.26551000
H	-2.38857600	-0.62899900	2.31356000
H	-2.65113400	-2.33264500	1.85387500
H	-0.18588100	-2.53237800	1.28065600
H	0.05988300	-0.84934900	1.82692600
H	-0.44739400	-2.09793600	2.99584200
O	-2.93851800	0.54617400	-1.47501200
C	-2.81428600	-0.07536100	-2.70397900
C	-3.04756100	-1.44795200	-2.83213000
C	-2.47272300	0.70027500	-3.81440200
C	-2.93440300	-2.04503000	-4.09059200
H	-3.30288300	-2.03042800	-1.94579500
C	-2.36593000	0.09384900	-5.06937400

H	-2.29110800	1.76854100	-3.68032700
C	-2.59455400	-1.27894200	-5.21154700
H	-3.11226500	-3.11853000	-4.19419200
H	-2.09681700	0.69873800	-5.93897200
H	-2.50581400	-1.75138800	-6.19266900

43

Energy = -1222.35888900 a.u. #Cluster: 2

P	-1.39325800	0.62492000	-0.40612700
O	-1.10108700	-0.79942000	0.32913600
O	-1.66636000	1.73172000	0.56267000
N	1.82901500	0.86035600	-2.47229300
N	-0.25782300	0.73761800	-1.56409900
C	3.29451100	0.88099900	-2.41834400
C	1.22500900	0.82331800	-3.81046000
C	1.04011500	0.83240700	-1.38459800
C	3.87623200	2.28974500	-2.50616700
C	0.92744000	-0.59586800	-4.28778900
C	1.67683400	0.88396800	-0.01450100
C	-1.69620800	-1.10064400	1.60878600
C	-3.17111000	-1.44366800	1.49722400
H	3.63467500	0.37283200	-1.50733400
H	3.65356100	0.26936900	-3.26009100

H	1.92528300	1.32306200	-4.49589500
H	0.30012200	1.41420200	-3.78423200
H	4.97657500	2.24396000	-2.51672000
H	3.54603500	2.79667600	-3.42651400
H	3.56376800	2.90299600	-1.64624900
H	0.19369700	-1.08082500	-3.62826200
H	0.50766400	-0.56986800	-5.30588700
H	1.84278200	-1.20908400	-4.31120600
H	0.96560800	1.32442600	0.69555200
H	1.90739000	-0.14050400	0.32038000
H	2.60122700	1.47234500	0.00930600
H	-1.11986000	-1.95226800	1.99873400
H	-1.54392600	-0.24174400	2.28142000
H	-3.75437400	-0.57897400	1.14556700
H	-3.33148500	-2.27990200	0.79875200
H	-3.55716100	-1.73898500	2.48599800
O	-2.76474000	0.37160700	-1.28049400
C	-2.79245400	-0.38157000	-2.43858200
C	-2.46128500	-1.74070200	-2.43019200
C	-3.18870500	0.24873300	-3.62107600
C	-2.52771600	-2.46800000	-3.62193600
H	-2.14328600	-2.21034500	-1.49935100

C	-3.25596700	-0.48909900	-4.80635100
H	-3.43413300	1.31245300	-3.59725400
C	-2.92448400	-1.84854700	-4.81211700
H	-2.26506300	-3.52902700	-3.61741300
H	-3.56492900	0.00462400	-5.73130500
H	-2.97403200	-2.42233300	-5.74063300

43

Energy = -1222.35872100 a.u. #Cluster: 3

P	-1.83905900	0.26647100	-0.13382800
O	-2.46611100	-1.19254700	0.19043400
O	-1.93949700	1.21371500	1.01995700
N	1.43587600	0.35433100	-2.12907900
N	-0.40591100	-0.05805000	-0.84659600
C	2.37787100	1.22124200	-2.84253000
C	1.60932200	-1.09144800	-2.31389900
C	0.40419900	0.81732100	-1.40030600
C	1.94819200	1.49699000	-4.28275300
C	2.42225300	-1.73091800	-1.19170500
C	0.24494000	2.31491000	-1.26851400
C	-2.26318500	-1.80991500	1.47755600
C	-0.86881600	-2.39228100	1.62452100
H	2.50469400	2.16050900	-2.29069800

H	3.35739000	0.71943900	-2.82662600
H	2.10748500	-1.24025600	-3.28302900
H	0.61339900	-1.54908100	-2.37411400
H	1.84570600	0.55973400	-4.85208300
H	0.98090400	2.02218500	-4.31633900
H	2.70031000	2.12317500	-4.78781000
H	1.91030100	-1.61101800	-0.22521000
H	2.55069900	-2.80809100	-1.38354100
H	3.42255500	-1.27491900	-1.11719500
H	1.15216400	2.76246700	-0.83557300
H	0.07974000	2.77877800	-2.25168500
H	-0.59665000	2.55123200	-0.60917400
H	-2.46635700	-1.06562000	2.26440200
H	-3.02906500	-2.59642800	1.54302300
H	-0.79232000	-2.93600900	2.57970500
H	-0.64936600	-3.09328600	0.80395600
H	-0.10338600	-1.60103000	1.61620100
O	-2.85822300	0.75535800	-1.33520300
C	-2.66553700	0.42298100	-2.66283700
C	-2.70776100	-0.90936500	-3.08666800
C	-2.43341700	1.45638100	-3.57363100
C	-2.50473200	-1.20276700	-4.43752300

H	-2.88624900	-1.69844600	-2.35460700
C	-2.23638400	1.15222100	-4.92413900
H	-2.40185000	2.48569900	-3.21148400
C	-2.26682500	-0.17668300	-5.35971200
H	-2.53152000	-2.24343300	-4.77070300
H	-2.05134600	1.96014700	-5.63658400
H	-2.10633300	-0.41273500	-6.41432200

43

Energy = -1222.35801100 a.u. #Cluster: 4

P	-2.01930000	0.51859900	-0.31806400
O	-2.08431700	-0.29769400	1.06680900
O	-2.57864600	1.89326500	-0.12412500
N	1.40164100	0.54049900	-2.09984100
N	-0.55875300	0.23949000	-0.97582600
C	2.44985600	1.34936100	-2.72869300
C	1.57157400	-0.91563800	-2.17002700
C	0.31173600	1.06432500	-1.50916300
C	3.62156200	1.63751100	-1.79223200
C	0.86016700	-1.52404400	-3.37627400
C	0.15859400	2.56747300	-1.50884200
C	-1.56430700	-1.63853200	1.19896900
C	-0.21795000	-1.62497500	1.89474300

H	2.79816700	0.79455000	-3.61329900
H	2.01699300	2.28404900	-3.10548800
H	1.18756500	-1.35287900	-1.23974500
H	2.65189800	-1.11794300	-2.21453300
H	4.39857100	2.20896900	-2.32401200
H	3.29580800	2.22591500	-0.92007300
H	4.07517600	0.70309100	-1.42554700
H	1.03795400	-2.61069400	-3.41291700
H	-0.22436400	-1.35446200	-3.31490700
H	1.22930000	-1.08563800	-4.31736200
H	-0.01024300	2.92524200	-2.53721000
H	-0.70255000	2.84861500	-0.89530200
H	1.06338800	3.06015100	-1.12625200
H	-2.31066700	-2.19549800	1.78606600
H	-1.49557900	-2.10988800	0.20647200
H	-0.29407200	-1.14354700	2.88252300
H	0.14090900	-2.65688900	2.03824900
H	0.52253600	-1.07770400	1.29216600
O	-3.02533200	-0.43714600	-1.22930800
C	-2.93409100	-0.49486800	-2.60044300
C	-3.04914500	-1.74918000	-3.20766000
C	-2.73753300	0.65512400	-3.37489900

C	-2.95880400	-1.85307800	-4.59791000
H	-3.19845000	-2.62955200	-2.57914700
C	-2.63414400	0.53731500	-4.76363800
H	-2.67274800	1.62989700	-2.88832400
C	-2.74280200	-0.71333000	-5.38088800
H	-3.04667200	-2.83464800	-5.07068100
H	-2.47227600	1.43473500	-5.36626400
H	-2.66255000	-0.79938700	-6.46705100

43

Energy = -1222.35706800 a.u. #Cluster: 5

P	-2.00283100	0.38511200	-0.39929000
O	-2.05166500	-0.52291000	0.93044600
O	-2.49831700	1.76385800	-0.08919700
N	1.47946900	0.44669000	-2.05365500
N	-0.59354800	0.11462500	-1.16820700
C	2.74440400	1.17050600	-2.21150300
C	1.35766300	-0.82219400	-2.78131600
C	0.46470700	0.88237700	-1.28485500
C	2.77037700	2.06643600	-3.44843200
C	1.77043300	-2.02880700	-1.94260900
C	0.61938700	2.21043900	-0.58171500
C	-1.49575500	-1.85500100	0.97479100

C	-0.14840800	-1.84698200	1.66915100
H	2.94640900	1.75467600	-1.30520500
H	3.54291600	0.41513500	-2.27374400
H	1.98980100	-0.74496000	-3.67837700
H	0.31657100	-0.92722500	-3.11311000
H	1.99804800	2.84895100	-3.38780900
H	3.75275500	2.55613100	-3.53882200
H	2.59469500	1.48238200	-4.36558700
H	1.70421700	-2.94805600	-2.54602800
H	2.80794600	-1.92899000	-1.58518200
H	1.10982800	-2.13895900	-1.07084500
H	1.02526100	2.98383200	-1.24716400
H	-0.35427700	2.53513300	-0.19992300
H	1.31350800	2.09599000	0.26699300
H	-2.22398000	-2.46984300	1.52553300
H	-1.41482100	-2.25915600	-0.04603800
H	-0.23756500	-1.44047800	2.68884300
H	0.24621500	-2.87347200	1.73637600
H	0.57352300	-1.23385000	1.10868500
O	-3.06840500	-0.46956600	-1.33387000
C	-3.09141200	-0.32644900	-2.70424700
C	-3.08855300	-1.48740100	-3.48303300

C	-3.12908800	0.93706500	-3.30607900
C	-3.12754700	-1.38190000	-4.87603700
H	-3.05133000	-2.45892300	-2.98578000
C	-3.15974200	1.03034300	-4.70033400
H	-3.13534800	1.82916200	-2.67751900
C	-3.15971800	-0.12447100	-5.49007200
H	-3.12597700	-2.28973900	-5.48489100
H	-3.18653300	2.01666700	-5.17080100
H	-3.18521300	-0.04522000	-6.57949300

43

Energy = -1222.35687600 a.u. #Cluster: 6

P	-1.56997900	0.85517400	-0.22936200
O	-1.69912100	0.08489600	1.17688000
O	-1.89353600	2.30446900	-0.04283900
N	1.74477100	0.32154700	-2.13263200
N	-0.19547500	0.34040300	-0.93188400
C	2.87083900	0.95213300	-2.82787600
C	1.70354200	-1.14494400	-2.16277700
C	0.76358200	1.01357500	-1.52410600
C	4.11310500	1.08796400	-1.94992000
C	0.87844500	-1.67525800	-3.33277300
C	0.82603300	2.52265000	-1.57519100

C	-1.57811400	-1.34956900	1.29710300
C	-2.93289900	-1.97313100	1.56776000
H	3.09578400	0.33014300	-3.70799600
H	2.56289600	1.93028500	-3.21651200
H	1.28882700	-1.49804500	-1.21010700
H	2.74227000	-1.50073400	-2.22831800
H	3.91873400	1.73968300	-1.08363400
H	4.44185300	0.10643200	-1.57328600
H	4.94012500	1.52475800	-2.53166800
H	1.28562800	-1.32689000	-4.29560800
H	0.88998100	-2.77692400	-3.33671800
H	-0.16618300	-1.34152100	-3.25573400
H	1.80980300	2.89319400	-1.25548400
H	0.65608200	2.86617700	-2.60829500
H	0.04590400	2.94379700	-0.93428500
H	-1.12158600	-1.76092500	0.38396500
H	-0.88191700	-1.53032500	2.13063600
H	-3.38214800	-1.55120300	2.48077500
H	-3.61597700	-1.79324300	0.72421100
H	-2.82403300	-3.06088700	1.70624300
O	-2.74892400	0.05829900	-1.08402700
C	-2.70802200	-0.05679100	-2.45443200

C	-2.38331700	1.03169100	-3.27275200
C	-3.00915900	-1.30255700	-3.01301200
C	-2.34054700	0.85826100	-4.65888500
H	-2.17277600	2.00288400	-2.82139000
C	-2.97739800	-1.46049400	-4.40084900
H	-3.25228600	-2.13565100	-2.35035800
C	-2.63572200	-0.38485600	-5.22854500
H	-2.07866000	1.70636000	-5.29668400
H	-3.21022900	-2.43539600	-4.83676800
H	-2.60209500	-0.51447000	-6.31281800

43

Energy = -1222.35639200 a.u. #Cluster: 7

P	-0.93492200	-0.17212900	0.08929500
O	-1.13780200	-1.75696200	0.35891200
O	-0.92854500	0.63782400	1.34877200
N	1.83004200	0.61533700	-2.45102100
N	0.29266100	-0.20319300	-0.97674500
C	2.60083200	1.68227300	-3.09704200
C	2.01647400	-0.73813700	-2.98682600
C	0.95103600	0.82893900	-1.45634700
C	3.99650900	1.85444200	-2.50195600
C	1.00114300	-1.07467900	-4.07600000

C	0.75727800	2.24553000	-0.96568900
C	-1.85025300	-2.20658800	1.52993800
C	-3.35244500	-2.02178900	1.40901300
H	2.67292800	1.42451400	-4.16479800
H	2.03842600	2.62281200	-3.04867100
H	1.93472100	-1.44961900	-2.15525800
H	3.04204800	-0.79546600	-3.38042300
H	3.94282800	2.14929600	-1.44218400
H	4.57349300	0.91863100	-2.56888700
H	4.54682300	2.63502600	-3.05053400
H	-0.02193100	-1.04667400	-3.67586800
H	1.06682100	-0.36187900	-4.91361900
H	1.19122000	-2.08485100	-4.47225600
H	0.22548500	2.23311300	-0.00802600
H	1.71120500	2.77309200	-0.83549500
H	0.15515300	2.80776000	-1.69815800
H	-1.59063600	-3.27069000	1.62894400
H	-1.45998900	-1.67116300	2.40983900
H	-3.74419500	-2.53081600	0.51448800
H	-3.84797300	-2.44949200	2.29527500
H	-3.61862100	-0.95548300	1.34847900
O	-2.27437900	0.27933500	-0.77625400

C	-2.43864400	-0.03672200	-2.11070000
C	-2.36639600	0.99502700	-3.05066900
C	-2.69361600	-1.35215900	-2.51205200
C	-2.55895500	0.70834300	-4.40507500
H	-2.15718300	2.01028400	-2.70734600
C	-2.88155900	-1.62851400	-3.86901300
H	-2.73048000	-2.14402800	-1.76345500
C	-2.81682900	-0.60286000	-4.81895700
H	-2.50156900	1.51518300	-5.14013900
H	-3.07847500	-2.65617900	-4.18501900
H	-2.96362800	-0.82572900	-5.87842300

AEOP-N₁H

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Energy = -1222.79672000 a.u. #Cluster: 1

P	0.46784900	-1.29347900	-1.41693900
O	-0.66589800	-1.89708700	-2.35872500
O	1.77639400	-1.98878100	-1.38209400
N	0.26045100	2.41055700	-2.79264000
N	0.71127900	0.33349400	-1.89118000
C	-0.65714200	3.46551400	-3.27708100
C	1.69742400	2.69452500	-2.98957800

C	-0.17533900	1.28550300	-2.26624300
C	-0.91087100	4.54210700	-2.22863600
C	2.22157400	2.15055700	-4.31580700
C	-1.63761500	1.01900600	-2.09601200
C	-0.35200000	-2.59949600	-3.59824300
C	0.14130000	-1.65293400	-4.67268500
H	-0.17972700	3.89574100	-4.16859800
H	-1.59001600	3.00221000	-3.61671000
H	2.26604200	2.30611500	-2.13212400
H	1.80500900	3.78618700	-2.94778400
H	-1.41346000	4.12662300	-1.34171400
H	0.03010300	5.01331600	-1.90557500
H	-1.55540400	5.32342000	-2.65910300
H	3.28303900	2.41924700	-4.42347600
H	2.13477300	1.05480600	-4.36880400
H	1.66768200	2.58359600	-5.16253000
H	-2.19256400	1.94054200	-1.89626500
H	-2.02801900	0.56145000	-3.01924100
H	-1.80379600	0.32464300	-1.26712500
H	0.38788800	-3.38135700	-3.37132200
H	-1.29844000	-3.07923400	-3.87976200
H	0.26773200	-2.20809800	-5.61513600

H	-0.57988000	-0.83838100	-4.84235800
H	1.11526600	-1.21409500	-4.40511100
O	-0.33560900	-1.09607100	-0.03368100
C	-0.90301900	-2.19188800	0.62967600
C	-2.28989700	-2.23052900	0.76314000
C	-0.08283400	-3.18791100	1.16047300
C	-2.86951200	-3.29799900	1.45490800
H	-2.89763900	-1.43467000	0.32884400
C	-0.67728000	-4.25263400	1.84452500
H	0.99910300	-3.12353000	1.03633100
C	-2.06698400	-4.30975300	1.99415400
H	-3.95549400	-3.33853000	1.56867200
H	-0.04616700	-5.03939100	2.26481900
H	-2.52536500	-5.14307800	2.53174400
H	1.70461200	0.52748500	-2.00981500

44

Energy = -1222.79667700 a.u. #Cluster: 2

P	0.97468000	-2.14707700	-2.20851300
O	0.02551300	-2.92582900	-3.21788600
O	2.43164600	-2.39854500	-2.27426200
N	0.11172700	1.66630900	-1.88395300
N	0.47056000	-0.52500500	-2.51159200

C	0.53565500	2.94413600	-1.27500600
C	-1.26701300	1.63854700	-2.41479300
C	0.89777500	0.61225100	-1.91060400
C	0.09968300	3.05409100	0.18236100
C	-1.32717000	1.92759200	-3.91191700
C	2.26736900	0.64979900	-1.31142000
C	0.48406700	-3.39093200	-4.52651800
C	0.63273800	-2.24936400	-5.50923300
H	1.62188000	3.04578800	-1.37418200
H	0.08406700	3.74162100	-1.88152700
H	-1.83008700	2.39513700	-1.85386500
H	-1.72517900	0.67104000	-2.15951900
H	-0.99276200	2.96527800	0.28169700
H	0.56546500	2.27131600	0.79954900
H	0.40237700	4.03544300	0.57769300
H	-0.79673300	1.16369900	-4.50141400
H	-2.37862700	1.94126700	-4.23555800
H	-0.88189800	2.90852800	-4.13702300
H	2.75634800	-0.32515300	-1.39697900
H	2.87490400	1.38943600	-1.85589000
H	2.22077400	0.95372800	-0.25684600
H	1.42977800	-3.93364100	-4.38224200

H	-0.28904500	-4.10395600	-4.84023800
H	1.43495400	-1.55932400	-5.20367500
H	0.89358000	-2.65650800	-6.49872200
H	-0.30723800	-1.68325400	-5.60234600
O	0.34959300	-2.47005800	-0.75640200
C	-0.84320400	-1.89380600	-0.30483900
C	-2.06833900	-2.35185100	-0.78877800
C	-0.76068100	-0.85168200	0.61803700
C	-3.24012400	-1.73681100	-0.33720400
H	-2.09440200	-3.16674900	-1.51355300
C	-1.93932600	-0.24378300	1.05881400
H	0.21784000	-0.52034200	0.97055500
C	-3.17873200	-0.68245100	0.58059000
H	-4.20651100	-2.08385800	-0.71079200
H	-1.88405700	0.58031000	1.77372100
H	-4.09801300	-0.20208400	0.92337600
H	-0.42628400	-0.48553500	-2.99391000

44

Energy = -1222.79665800 a.u. #Cluster: 3

P	0.65243700	-1.13504100	-1.18703600
O	-0.18480700	-2.03397300	-2.20105600
O	2.03566600	-1.56109900	-0.86886000

N	0.04870100	2.36639900	-2.93347200
N	0.69597200	0.45383100	-1.82095900
C	-0.94949800	3.22324200	-3.60872400
C	1.43053000	2.88889100	-2.93402800
C	-0.26791500	1.20436000	-2.40160400
C	-1.51207900	4.29798800	-2.68550500
C	2.24900700	2.36242600	-4.11017300
C	-1.67380300	0.69453200	-2.45640100
C	0.44881000	-2.76921700	-3.29072700
C	0.80906600	-1.85533500	-4.44319400
H	-0.43196800	3.67734000	-4.46554800
H	-1.74490900	2.59307500	-4.02062900
H	1.90488200	2.66428400	-1.96732100
H	1.34833400	3.98243600	-2.97815300
H	-2.21540000	4.92844300	-3.25035900
H	-2.05063600	3.85401100	-1.83430000
H	-0.71291500	4.94471600	-2.29221600
H	1.77303600	2.62870300	-5.06611500
H	3.25194800	2.81400900	-4.08490500
H	2.36246900	1.26831000	-4.07212500
H	-1.90800800	0.40205500	-3.49225200
H	-1.81390200	-0.17457100	-1.81112000

H	-2.37804900	1.47759800	-2.14938100
H	1.33081500	-3.28822900	-2.88739400
H	-0.30028200	-3.51749900	-3.58078100
H	1.59378600	-1.13717200	-4.15845800
H	1.19121000	-2.46057300	-5.27997900
H	-0.07294500	-1.29619600	-4.79237900
O	-0.40004100	-0.94803200	0.01756100
C	-0.99299700	-2.02560900	0.68229800
C	-0.23062900	-3.10490400	1.13206500
C	-2.36841400	-1.95673700	0.89927200
C	-0.87457800	-4.14430600	1.81040100
H	0.84625300	-3.12539100	0.95688400
C	-2.99614000	-2.99900400	1.58687700
H	-2.92774100	-1.09430700	0.53181400
C	-2.25330800	-4.09484700	2.04042000
H	-0.28822800	-4.99557200	2.16467200
H	-4.07343600	-2.95391800	1.76405300
H	-2.74880400	-4.90909500	2.57420500
H	1.64606000	0.82169600	-1.81017700

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Energy = -1222.79660500 a.u. #Cluster: 4

P	1.10828600	-1.51023700	-2.74447200
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O	0.24049000	-1.97301500	-3.99575800
O	2.57482400	-1.70553200	-2.79808700
N	0.10865400	2.16199100	-1.72619100
N	0.51852300	0.10123800	-2.67876700
C	0.40709900	3.25093900	-0.77167300
C	-1.08582200	2.36416800	-2.57227600
C	0.83532800	1.06724300	-1.78716500
C	1.25269400	4.35485700	-1.39564800
C	-2.32986300	1.71037000	-1.97658300
C	2.00941400	0.86241300	-0.88179100
C	0.68753700	-3.03903600	-4.88898500
C	0.56151200	-4.40224700	-4.24325100
H	-0.56550400	3.64224900	-0.44133800
H	0.89251300	2.82698300	0.11423300
H	-0.87646800	2.00195000	-3.58990800
H	-1.22234300	3.44917300	-2.66508200
H	1.40778400	5.15464900	-0.65569000
H	2.23772800	3.97542900	-1.70777200
H	0.75402000	4.79250400	-2.27409000
H	-2.22369400	0.61850100	-1.90305100
H	-2.53316400	2.10624600	-0.97030300
H	-3.19671800	1.92968900	-2.61764200

H	2.60735600	0.00486200	-1.20625300
H	2.65118500	1.75293200	-0.88248400
H	1.65719100	0.69431600	0.14778100
H	0.03781000	-2.93985100	-5.76801700
H	1.72380400	-2.82153700	-5.18740400
H	-0.47276200	-4.59357400	-3.91885400
H	0.84520700	-5.17528800	-4.97465300
H	1.23048300	-4.49674500	-3.37331700
O	0.48950300	-2.20409900	-1.41982900
C	-0.79783900	-1.95358100	-0.93706600
C	-1.92330800	-2.34209300	-1.66515700
C	-0.91161300	-1.32036300	0.30065900
C	-3.19051300	-2.07919200	-1.13573600
H	-1.80666800	-2.83543800	-2.62986200
C	-2.18422500	-1.06653300	0.81931200
H	-0.00839900	-1.03713900	0.84394500
C	-3.32494400	-1.44221900	0.10231300
H	-4.07782700	-2.37671700	-1.69953400
H	-2.28104900	-0.56918800	1.78722600
H	-4.31852900	-1.23891000	0.50810300
H	-0.26014100	0.26755300	-3.31469500

Energy = -1222.79656500 a.u. #Cluster: 5

P	1.04330400	-2.11306100	-2.18390000
O	0.11595100	-2.93160100	-3.18158000
O	2.50641400	-2.32670400	-2.24606500
N	0.08147400	1.67958900	-1.89832400
N	0.49819600	-0.50775100	-2.50718300
C	0.47023300	2.97127000	-1.29509700
C	-1.29303700	1.61463300	-2.43653700
C	0.89350600	0.64521100	-1.91338200
C	0.02266200	3.07971900	0.15887600
C	-1.35036600	1.89116000	-3.93602700
C	2.25823800	0.72155700	-1.30673800
C	0.57934400	-3.39479200	-4.48912100
C	0.55692700	-2.28232300	-5.51518400
H	1.55431400	3.09854600	-1.38813100
H	0.00322400	3.75371900	-1.90940000
H	-1.87714700	2.36175400	-1.88452500
H	-1.72882600	0.63826000	-2.17593700
H	0.29947000	4.07042300	0.54979800
H	-1.06793100	2.96543300	0.25239100
H	0.50303700	2.31203100	0.78378400
H	-2.39963600	1.87869600	-4.26664900

H	-0.92547700	2.88011600	-4.16536400
H	-0.79864300	1.13533300	-4.51616900
H	2.85042300	1.47250400	-1.85248900
H	2.19759400	1.03084900	-0.25439400
H	2.77157200	-0.24148200	-1.38316300
H	1.58673900	-3.81792000	-4.36381400
H	-0.11521000	-4.20458000	-4.74711800
H	1.28389300	-1.49273300	-5.26779900
H	0.82433500	-2.69447200	-6.50089300
H	-0.44556600	-1.83229000	-5.58594400
O	0.42590200	-2.43384800	-0.72814200
C	-0.78413200	-1.88748100	-0.28556000
C	-1.99427000	-2.38545900	-0.76788200
C	-0.73449000	-0.83465100	0.62740000
C	-3.18466100	-1.80040700	-0.32533000
H	-1.99478900	-3.20780600	-1.48463200
C	-1.93151000	-0.25707400	1.05939000
H	0.23301900	-0.47149300	0.97889800
C	-3.15639000	-0.73596000	0.58236800
H	-4.13947700	-2.17909500	-0.69794400
H	-1.90220900	0.57508200	1.76645200
H	-4.09014900	-0.27918000	0.91822800

H	-0.39830400	-0.49600500	-2.99197600
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Energy = -1222.79650500 a.u. #Cluster: 6

P	1.21853200	-1.93597300	-1.75915500
O	0.51360200	-2.93150200	-2.77887700
O	2.69590700	-1.94851200	-1.67093700
N	-0.02476100	1.79842000	-2.18013300
N	0.51100700	-0.44248600	-2.25237200
C	0.18323500	3.18604200	-1.71445300
C	-1.20211600	1.58888500	-3.04830700
C	0.76592900	0.81192700	-1.81453400
C	0.96769300	4.02396600	-2.71723600
C	-2.43608000	1.15526200	-2.26100500
C	1.93253300	1.04499500	-0.90786400
C	1.15477200	-3.37793100	-4.01542400
C	1.03083800	-2.34433800	-5.11409800
H	-0.81895100	3.60747400	-1.55326600
H	0.67576300	3.16451800	-0.73612900
H	-0.94495700	0.87070300	-3.84115400
H	-1.38358600	2.54306000	-3.55923200
H	0.46044000	4.05520900	-3.69368000
H	1.05150300	5.05498200	-2.34151900

H	1.98267100	3.62443400	-2.86526300
H	-2.69257900	1.90320500	-1.49572600
H	-3.28853400	1.05834300	-2.94981000
H	-2.28772700	0.18788400	-1.76010200
H	2.48801000	1.94200200	-1.20661200
H	1.56397400	1.19053100	0.12061500
H	2.60923000	0.18498200	-0.92667300
H	2.20505800	-3.61313400	-3.78940300
H	0.62983900	-4.30823300	-4.26779900
H	1.59071600	-1.42770600	-4.87082200
H	1.44533800	-2.75838900	-6.04675900
H	-0.02390000	-2.08073400	-5.28959200
O	0.51143400	-2.25827800	-0.34935900
C	-0.81460000	-1.93417900	-0.04420600
C	-1.04037400	-0.91385700	0.87905400
C	-1.86562600	-2.63026800	-0.64213400
C	-2.35673600	-0.58295300	1.21205700
H	-0.18937000	-0.39090900	1.31962900
C	-3.17755200	-2.28569200	-0.30272800
H	-1.65228400	-3.42090000	-1.36249400
C	-3.42576100	-1.26531600	0.62164400
H	-2.54469800	0.21678500	1.93227500

H	-4.00960800	-2.82085700	-0.76650300
H	-4.45348100	-1.00051700	0.88044800
H	-0.30719300	-0.57322400	-2.84517100

44

Energy = -1222.79648600 a.u. #Cluster: 7

P	0.97150100	-2.09147600	-2.09467000
O	0.12071500	-2.83557100	-3.21337800
O	2.43743000	-2.29563800	-2.07477200
N	0.16886700	1.78022700	-1.92593900
N	0.43884700	-0.47126300	-2.34443100
C	0.54797300	3.04978400	-1.27020000
C	-1.03945200	1.84144800	-2.77512200
C	0.84398000	0.66659700	-1.73553700
C	1.41862600	3.92907000	-2.16032900
C	-2.30521900	1.45308700	-2.01490900
C	2.04646900	0.62866700	-0.84620900
C	0.69045900	-3.22488500	-4.50276600
C	0.83160200	-2.04047200	-5.43422000
H	-0.39460100	3.55762700	-1.02201500
H	1.04389000	2.82705400	-0.31899500
H	-0.88713000	1.21935300	-3.66983000
H	-1.10895200	2.87439800	-3.13953500

H	1.63266400	4.87344800	-1.63721100
H	2.37541800	3.43807700	-2.39505000
H	0.91020900	4.16953000	-3.10670200
H	-2.44760400	2.10360000	-1.13893000
H	-3.17490000	1.57080400	-2.67852000
H	-2.27679700	0.40998000	-1.66853100
H	1.71980000	0.68452400	0.20471200
H	2.60689100	-0.29865900	-0.99978300
H	2.70667500	1.48067500	-1.04942900
H	1.65645400	-3.71558500	-4.31419700
H	-0.01536100	-3.97016000	-4.89129000
H	-0.13340100	-1.52737000	-5.56884100
H	1.56917700	-1.31613600	-5.05423500
H	1.17823200	-2.39393200	-6.41804700
O	0.27056100	-2.52255800	-0.71070100
C	-0.99645400	-2.09042100	-0.30629500
C	-2.14001300	-2.55501500	-0.95566300
C	-1.07050600	-1.20255700	0.76655600
C	-3.38992200	-2.11002500	-0.51413300
H	-2.04566300	-3.24738800	-1.79305900
C	-2.32654400	-0.76925900	1.19987100
H	-0.15078500	-0.86071700	1.24500000

C	-3.48642300	-1.21976100	0.56060600
H	-4.29320100	-2.46399400	-1.01661900
H	-2.39544800	-0.07196800	2.03808500
H	-4.46639200	-0.87545900	0.89887000
H	-0.39412400	-0.41996200	-2.92841900

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Energy = -1222.79567300 a.u. #Cluster: 8

P	1.09128800	-1.60811300	-2.84625800
O	0.12508000	-2.12939300	-3.99846600
O	2.54421000	-1.85612700	-2.98392800
N	0.09665600	2.02353700	-1.79369000
N	0.54505400	0.02085100	-2.85211600
C	0.46933600	3.16585400	-0.93300800
C	-1.26099800	2.07901600	-2.37151800
C	0.90848000	1.01089400	-2.00140900
C	-0.01445000	2.98933200	0.50242300
C	-1.28609300	2.71910000	-3.75635000
C	2.24786300	0.94177100	-1.33913600
C	0.45874500	-3.29506700	-4.81266000
C	0.24783300	-4.58718800	-4.05299400
H	1.55531400	3.30574500	-0.97468400
H	0.01677100	4.05637900	-1.39139200

H	-1.87212400	2.65846700	-1.66751800
H	-1.68300000	1.06323200	-2.37665300
H	0.24766900	3.88619900	1.08360900
H	-1.10655300	2.85992200	0.54452900
H	0.45409200	2.11631500	0.98086300
H	-0.70045700	2.14001000	-4.48709300
H	-2.32586700	2.77041700	-4.11238400
H	-0.88108400	3.74175900	-3.72103000
H	2.15598700	1.07443200	-0.25348600
H	2.74952300	-0.00597400	-1.55845300
H	2.87788300	1.75519600	-1.73293500
H	-0.20925100	-3.21546100	-5.68003000
H	1.49863500	-3.18661600	-5.15486500
H	0.44777400	-5.43705500	-4.72442500
H	0.93342100	-4.66420800	-3.19436100
H	-0.78761000	-4.66800300	-3.68836200
O	0.53994000	-2.18449200	-1.43360900
C	-0.67459700	-1.76537300	-0.88148800
C	-1.88480200	-2.19156000	-1.42879200
C	-0.63062400	-0.90701400	0.21702700
C	-3.07776400	-1.73381800	-0.86082300
H	-1.88793600	-2.86197600	-2.28854000

C	-1.82988200	-0.45491700	0.77380400
H	0.33505100	-0.59861600	0.62140700
C	-3.05413700	-0.86407000	0.23479400
H	-4.03159900	-2.05962500	-1.28264300
H	-1.80244100	0.22468400	1.62857300
H	-3.99029800	-0.50646400	0.66961800
H	-0.30748700	0.14574000	-3.39635800

ADPP

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Energy = -1217.61563800 a.u. #Cluster: 1

P	-0.40051400	-2.10246600	0.75948100
O	0.78669100	-1.66544300	-0.28358100
O	-0.64142600	-0.66115000	1.46925900
O	0.03341800	-3.09531200	1.79449200
N	-1.69822200	-2.43885600	-0.17787200
N	-2.07690000	-4.60817300	0.64990200
C	1.02715400	-2.35447100	-1.45762700
C	-0.72832900	0.57938400	0.86121600
C	1.19938800	-1.60528500	-2.62366200
C	-0.29136000	1.67080400	1.61735900
C	1.11144300	-3.75023000	-1.47752700

C	-1.24181700	0.75833000	-0.42761100
C	1.46509700	-2.26542900	-3.82632700
C	-0.36843300	2.95693100	1.07741600
C	1.36717700	-4.39940000	-2.68894100
C	-1.30632600	2.05075900	-0.95788600
C	-2.34768200	-3.58562700	-0.16123000
C	1.54641600	-3.66228100	-3.86435100
C	-0.87268300	3.15240000	-0.21325600
C	-3.46890600	-3.76254500	-1.14726000
H	1.11806400	-0.51769900	-2.57302700
H	0.10574800	1.49595800	2.61936400
H	0.98114800	-4.31469200	-0.55210000
H	-1.59336700	-0.10169800	-0.99744600
H	1.60218000	-1.68284900	-4.74087600
H	-0.02706200	3.80976100	1.66964600
H	1.43051700	-5.49027200	-2.70920400
H	-1.70552800	2.19279600	-1.96547600
H	1.74894400	-4.17472800	-4.80774500
H	-0.92863100	4.15842900	-0.63565500
H	-4.14440000	-2.89703900	-1.08538700
H	-4.03330400	-4.68921700	-0.97803800
H	-3.04327100	-3.77636500	-2.16319900

H	-1.31706600	-4.51646400	1.32753000
H	-2.61714800	-5.46425300	0.60739500

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Energy = -1217.61489800 a.u. #Cluster: 2

P	0.16917700	-2.62099200	0.72642300
O	0.12277300	-3.03755800	-0.87861600
O	0.43560400	-0.99913900	0.65496800
O	1.28204700	-3.25600200	1.48128200
N	-1.33143100	-2.84675400	1.28949500
N	-2.68746300	-2.82680600	-0.63387000
C	1.14975900	-2.85004000	-1.78840900
C	-0.54877200	-0.14076800	0.18504800
C	2.49842000	-2.91562800	-1.42348300
C	-1.52523000	0.32884200	1.06719000
C	0.77515800	-2.59965300	-3.11240400
C	-0.54558900	0.24209300	-1.15798900
C	3.47574500	-2.71856900	-2.40440700
C	-2.51917300	1.18761000	0.59072400
C	1.76270200	-2.41224600	-4.08206800
C	-1.54220300	1.10490100	-1.62338500
C	-2.49735900	-2.83562800	0.68572000
C	3.11678300	-2.46723900	-3.73220400

C	-2.53247500	1.57503000	-0.75405800
C	-3.73117400	-2.79717400	1.54560000
H	2.76738300	-3.12192400	-0.38765700
H	-1.50289500	0.00576600	2.10896700
H	-0.28543700	-2.54842100	-3.36692200
H	0.22959500	-0.13863400	-1.82459600
H	4.53054300	-2.76700400	-2.12180800
H	-3.28790600	1.55413900	1.27558100
H	1.46941100	-2.21654400	-5.11660000
H	-1.54470500	1.40684400	-2.67372600
H	3.88759600	-2.31588100	-4.49151200
H	-3.31281100	2.24484400	-1.12313600
H	-3.92433400	-1.74632600	1.81937400
H	-3.55289400	-3.35975700	2.47084900
H	-4.61456500	-3.19065600	1.02379900
H	-1.89212500	-2.85020800	-1.26749400
H	-3.62314300	-2.82690800	-1.02289800

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Energy = -1217.61467900 a.u. #Cluster: 3

P	-0.68061600	-2.28474600	0.71003800
O	0.67914900	-2.20093900	-0.19634300
O	-1.66211600	-1.19620600	-0.01941600

O	-0.32263400	-1.96341800	2.13043400
N	-1.43571700	-3.68962000	0.36351900
N	-1.49632400	-4.51507800	2.56767100
C	0.72766400	-1.97104900	-1.56240100
C	-1.25680700	0.08458100	-0.36191600
C	-0.08607200	-2.66845200	-2.45850000
C	-1.66692600	0.56430400	-1.60807300
C	1.63246700	-1.00527900	-2.00983600
C	-0.47233000	0.86621800	0.49079300
C	0.00292700	-2.37487100	-3.82288600
C	-1.27683400	1.84253700	-2.01105500
C	1.71719900	-0.72720100	-3.37538500
C	-0.08059700	2.14137900	0.07058000
C	-1.73802800	-4.60741700	1.25991400
C	0.89915400	-1.40613900	-4.28608600
C	-0.47727400	2.63307300	-1.17690400
C	-2.39913900	-5.86489000	0.76595300
H	-0.78354900	-3.41736700	-2.08170000
H	-2.26910400	-0.07928200	-2.25181900
H	2.24387300	-0.47222400	-1.27938000
H	-0.17092200	0.47156500	1.46188000
H	-0.63664100	-2.91190800	-4.52810000

H	-1.59143300	2.21841600	-2.98789500
H	2.41977700	0.03214500	-3.72780500
H	0.53912600	2.75433300	0.73006800
H	0.96102000	-1.18099900	-5.35341300
H	-0.16630200	3.62996700	-1.49809100
H	-2.69888300	-6.53250300	1.58468500
H	-1.69820600	-6.39506900	0.10220400
H	-3.27959400	-5.59538100	0.16438000
H	-1.04116800	-3.67569200	2.93164900
H	-1.76413000	-5.25917600	3.20101400

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Energy = -1217.61391000 a.u. #Cluster: 4

P	-0.04207200	-2.02477000	0.57553000
O	1.24026600	-2.77680100	-0.10324000
O	0.34655700	-0.47737300	0.18873300
O	-0.03848800	-2.28876400	2.04515300
N	-1.36147400	-2.29800800	-0.34599700
N	-3.21713600	-3.41214600	-1.04971900
C	1.42839900	-2.84303900	-1.47600000
C	-0.56829600	0.55470300	0.26451700
C	0.97216500	-3.96483100	-2.17156600
C	-0.62296700	1.45030300	-0.80656400

C	2.09840200	-1.80825600	-2.13284800
C	-1.39256000	0.72025700	1.38298600
C	1.19376600	-4.05033100	-3.54905500
C	-1.51204600	2.52718700	-0.75464200
C	2.31404400	-1.90378600	-3.51082300
C	-2.28387100	1.79656300	1.41874100
C	-2.17027300	-3.32546100	-0.22860000
C	1.86294200	-3.02162700	-4.22173400
C	-2.34715100	2.70283900	0.35480500
C	-1.99566700	-4.44691900	0.76285900
H	0.45038800	-4.75545900	-1.62869000
H	0.02880500	1.28878400	-1.66757500
H	2.43955300	-0.94446200	-1.56068600
H	-1.32344000	0.01380400	2.21185800
H	0.83970100	-4.92623900	-4.09850900
H	-1.55535700	3.22977300	-1.59084700
H	2.83879600	-1.09801500	-4.03047100
H	-2.93003300	1.92774400	2.29051300
H	2.03381000	-3.09162200	-5.29866300
H	-3.04380100	3.54375700	0.39034500
H	-2.86775100	-5.11302900	0.79119100
H	-1.80360500	-4.02632500	1.75882500

H	-1.10567700	-5.03253700	0.48072300
H	-3.36902500	-2.69311800	-1.75088000
H	-3.86589500	-4.18918700	-1.00189400

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Energy = -1217.61388700 a.u. #Cluster: 5

P	0.12287900	-2.20412500	0.44450500
O	1.14119200	-1.77092400	-0.76761500
O	0.07144500	-0.77863600	1.24291800
O	0.68635300	-3.24799300	1.35110300
N	-1.29052500	-2.42326000	-0.34227200
N	-3.44397500	-3.11103700	-0.60326300
C	1.27603200	-2.51249800	-1.92483600
C	-0.49727300	0.36350700	0.69801400
C	1.29326000	-1.81941800	-3.13787400
C	-1.83577900	0.65539600	0.96919500
C	1.41984100	-3.90377300	-1.88933500
C	0.28519500	1.21876100	-0.08151700
C	1.45999300	-2.52913600	-4.33001500
C	-2.39752300	1.82581500	0.45088900
C	1.57713500	-4.60295800	-3.08952100
C	-0.28678000	2.38635100	-0.59516900
C	-2.36594700	-2.97595500	0.16950200

C	1.59923900	-3.92174400	-4.31133600
C	-1.62673900	2.69252100	-0.33211000
C	-2.48765500	-3.45611200	1.59278700
H	1.17124600	-0.73435900	-3.13112900
H	-2.42130600	-0.03365800	1.58100400
H	1.41425700	-4.42110500	-0.92842900
H	1.32644700	0.95958400	-0.27765700
H	1.47495900	-1.98889600	-5.28009200
H	-3.44439900	2.05947400	0.66048800
H	1.68815100	-5.69008300	-3.06508100
H	0.32060700	3.06018500	-1.20485800
H	1.72552000	-4.47369100	-5.24573800
H	-2.06962000	3.60602600	-0.73620300
H	-1.62050900	-4.08285000	1.84059200
H	-3.41982700	-4.00896100	1.76664800
H	-2.45800700	-2.58181900	2.26312900
H	-3.41717700	-2.78480100	-1.56477400
H	-4.29970200	-3.52621800	-0.25417500

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Energy = -1217.61352000 a.u. #Cluster: 6

P	0.01281900	-1.85898100	0.50700900
O	1.13633600	-2.71753000	-0.31153400

O	0.33916400	-0.37916600	-0.11585300
O	0.30487300	-1.97354900	1.96587300
N	-1.47918300	-2.18229400	-0.07143200
N	-3.41232600	-3.37005600	-0.26669000
C	1.24293600	-2.93291800	-1.67044600
C	-0.50882300	0.70168300	0.02842500
C	2.22656200	-3.84831700	-2.06272700
C	-1.15439900	0.97610900	1.23892200
C	0.44642300	-2.29159800	-2.62693000
C	-0.67891500	1.53343700	-1.08144300
C	2.41619400	-4.12368700	-3.41815700
C	-1.98541300	2.09677700	1.32740400
C	0.64754200	-2.57866000	-3.98137900
C	-1.50509500	2.65553800	-0.97681100
C	-2.18121600	-3.25122200	0.22933800
C	1.62747400	-3.49003300	-4.38535200
C	-2.16388700	2.93953700	0.22505400
C	-1.68155400	-4.38058600	1.09319500
H	2.83192600	-4.33252200	-1.29360400
H	-0.99545400	0.32091800	2.09703000
H	-0.32663500	-1.58701400	-2.32471400
H	-0.16141900	1.28974400	-2.01151100

H	3.18594300	-4.83937600	-3.71814200
H	-2.49267800	2.31302700	2.27112800
H	0.02389200	-2.07816600	-4.72665600
H	-1.63813200	3.30809500	-1.84349100
H	1.77547800	-3.70627700	-5.44594700
H	-2.81226600	3.81547300	0.30267200
H	-2.45814200	-5.12964300	1.29418600
H	-1.30106800	-3.96866400	2.03834900
H	-0.83325600	-4.86754900	0.58625400
H	-3.78789800	-2.63888800	-0.86355400
H	-3.98879400	-4.18003500	-0.07069100

35

Energy = -1217.61349800 a.u. #Cluster: 7

P	-0.39139800	-2.24753300	0.48930000
O	0.74838500	-3.16861700	-0.23385900
O	0.25399700	-0.77707800	0.17108500
O	-0.42753600	-2.59422600	1.94047200
N	-1.76301300	-2.24849800	-0.39831400
N	-3.79006100	-3.01832300	-1.09153300
C	1.27088200	-3.04704700	-1.50650000
C	-0.47257300	0.39354400	0.27827000
C	2.49682000	-3.68437300	-1.72677900

C	-0.37780100	1.31139800	-0.77039200
C	0.63409000	-2.35016900	-2.54021700
C	-1.25338300	0.66561200	1.40642400
C	3.09039200	-3.62471600	-2.98942100
C	-1.07148100	2.52154500	-0.68471700
C	1.24290300	-2.29498900	-3.79832900
C	-1.94903100	1.87605500	1.47598400
C	-2.70170200	-3.16517100	-0.33630200
C	2.46771300	-2.92789100	-4.03119500
C	-1.86069800	2.80705200	0.43536800
C	-2.63294800	-4.40069900	0.52372400
H	2.96955400	-4.21889500	-0.90019600
H	0.23629400	1.06407200	-1.63865200
H	-0.32673900	-1.86653000	-2.36619400
H	-1.30332100	-0.06428400	2.21633800
H	4.04790100	-4.12457300	-3.15680400
H	-0.99802700	3.24291300	-1.50261300
H	0.74564200	-1.74974600	-4.60477800
H	-2.56111900	2.09230900	2.35532300
H	2.93400600	-2.87959900	-5.01802600
H	-2.40435900	3.75271500	0.49731600
H	-1.80304000	-5.03286700	0.16934600

H	-3.56454200	-4.98038400	0.49602000
H	-2.39775800	-4.10866400	1.55631900
H	-3.87959600	-2.20627900	-1.69512900
H	-4.53744200	-3.70245100	-1.08356600

ADPP-N₁H

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Energy = -1218.05076800 a.u. #Cluster: 1

P	0.46371100	-2.62321500	-0.15173000
O	1.42638800	-1.81831200	-1.15308400
O	-0.98084800	-2.23081800	-0.71566300
O	0.76078200	-2.48268600	1.29738600
N	0.51772700	-4.25656800	-0.63980800
N	1.28655700	-5.18930100	1.34143200
C	2.67866500	-1.31494800	-0.77732500
C	-1.35692800	-0.91098900	-1.00161200
C	3.71261100	-2.18410600	-0.43291400
C	-1.99981100	-0.68531300	-2.21652700
C	2.84731500	0.06771100	-0.79115100
C	-1.10986500	0.11837300	-0.09309800
C	4.95592100	-1.64292300	-0.09230900
C	-2.40805200	0.61427500	-2.52922900

C	4.09800600	0.59422000	-0.45548900
C	-1.51455800	1.41503600	-0.42517200
C	0.92323600	-5.31669000	0.09498900
C	5.15131000	-0.25759300	-0.10446100
C	-2.16364900	1.66552600	-1.63851700
C	0.94788200	-6.64792500	-0.57426800
H	3.54668800	-3.26325900	-0.43447600
H	-2.16936100	-1.52031200	-2.89867100
H	2.00567000	0.70926600	-1.05871000
H	-0.61299600	-0.09099800	0.85604800
H	5.77559800	-2.31148400	0.18138500
H	-2.91477800	0.80439600	-3.47838100
H	4.24607700	1.67675700	-0.46423500
H	-1.32296300	2.23103500	0.27558800
H	6.12584900	0.15895600	0.16059600
H	-2.47999400	2.68043300	-1.88995300
H	1.63685000	-6.60458400	-1.43250700
H	-0.05774500	-6.87777400	-0.95941400
H	1.26955300	-7.43289400	0.12035900
H	1.25861400	-4.26927100	1.79643400
H	1.58346700	-6.00555200	1.86914000
H	0.25523900	-4.45505800	-1.60661000

Energy = -1218.05075400 a.u. #Cluster: 2

P	0.40323500	-2.47317200	-0.37651200
O	1.43536400	-1.41145800	-0.99963000
O	-0.91284200	-2.14928300	-1.22170400
O	0.33059200	-2.53879200	1.10679800
N	0.82892100	-3.98565700	-1.03747600
N	1.11085500	-5.17431700	0.93558500
C	2.70533700	-1.22151800	-0.43505800
C	-1.46482700	-0.86022300	-1.29035900
C	2.84025200	-0.38674900	0.67267600
C	-1.87078500	-0.20447000	-0.12841700
C	3.79657100	-1.85928300	-1.02190000
C	-1.61369700	-0.29163300	-2.55300900
C	4.11679600	-0.18289400	1.20403500
C	-2.44189700	1.06669100	-0.24441200
C	5.06768400	-1.64500100	-0.48008300
C	-2.19363100	0.97617400	-2.65286600
C	1.14978200	-5.11590400	-0.36647300
C	5.22911800	-0.80937800	0.63040300
C	-2.60573400	1.65712900	-1.50179200
C	1.56000200	-6.29883400	-1.17534000

H	1.95751200	0.08960400	1.10250400
H	-1.74357000	-0.68360300	0.84375600
H	3.64326000	-2.50694800	-1.88715800
H	-1.27751700	-0.84082600	-3.43428200
H	4.24048500	0.46993100	2.07143100
H	-2.76377300	1.59357700	0.65698100
H	5.93420000	-2.13555200	-0.92987200
H	-2.31923300	1.43383100	-3.63701700
H	6.22432400	-0.64561600	1.05024700
H	-3.05601200	2.64889200	-1.58528200
H	1.73892700	-7.17200100	-0.53697100
H	2.47896500	-6.04847000	-1.72897900
H	0.77353700	-6.52592600	-1.91140600
H	0.83525700	-4.34860200	1.48033500
H	1.36020300	-6.03524900	1.41490900
H	0.88451200	-4.04105800	-2.05561800

36

Energy = -1218.05071600 a.u. #Cluster: 3

P	1.21743100	-2.60809400	-0.17099800
O	2.80589700	-2.78148800	-0.19384200
O	1.03873900	-1.32123000	-1.11479400
O	0.50102800	-2.58944400	1.13130200

N	0.74399900	-3.94719800	-1.11397800
N	-0.79064300	-4.89014600	0.34894700
C	3.67218900	-1.74379600	0.18782000
C	-0.21044200	-0.70274500	-1.27179600
C	3.65423000	-1.26277900	1.49647000
C	-0.65441500	0.19390500	-0.30163700
C	4.55122800	-1.24909800	-0.77253100
C	-0.95572000	-0.99095400	-2.41340100
C	4.55084800	-0.24850100	1.84708300
C	-1.88684200	0.82572200	-0.48982400
C	5.44624100	-0.24048000	-0.40472200
C	-2.18621900	-0.35038900	-2.58862300
C	-0.16506600	-4.89770200	-0.79522300
C	5.44640900	0.26180700	0.90151100
C	-2.65227900	0.55585700	-1.62999700
C	-0.43600300	-5.95783900	-1.80753000
H	2.95274200	-1.67809100	2.22188600
H	-0.03983200	0.38672500	0.57915800
H	4.52534600	-1.65310900	-1.78610200
H	-0.57044200	-1.70336400	-3.14525400
H	4.54848800	0.13972800	2.86834400
H	-2.24883900	1.53279600	0.26035600

H	6.14380100	0.15604000	-1.14632700
H	-2.78196500	-0.56354800	-3.47935600
H	6.14632000	1.05203200	1.18275700
H	-3.61450400	1.05347100	-1.77144000
H	0.51072100	-6.44622400	-2.08508600
H	-0.85207600	-5.48650300	-2.71222700
H	-1.14126800	-6.70181100	-1.41937000
H	-0.60193300	-4.14819700	1.03351800
H	-1.46978600	-5.61542700	0.56388100
H	1.18478800	-4.03651400	-2.03093500

36

Energy = -1218.05070000 a.u. #Cluster: 4

P	1.45690300	-2.55248900	-0.65678500
O	2.97917000	-2.15063800	-0.93105100
O	0.74644900	-1.11390900	-0.71162400
O	1.13064200	-3.42172700	0.50444400
N	1.05955500	-3.31792300	-2.12631500
N	0.29030400	-5.33823400	-1.28364000
C	3.67361100	-1.25512900	-0.10117300
C	-0.61473200	-0.96360600	-0.40636900
C	3.88882500	-1.56597700	1.24115700
C	-1.51964700	-0.83942800	-1.45859200

C	4.15628200	-0.08246400	-0.67724500
C	-1.01557400	-0.91671900	0.92765900
C	4.61238000	-0.66400700	2.02748800
C	-2.87276700	-0.65364900	-1.15932500
C	4.88389600	0.80546500	0.12013300
C	-2.37167400	-0.73229600	1.21145500
C	0.54098200	-4.55622300	-2.29623400
C	5.11108400	0.51833900	1.47083800
C	-3.29956300	-0.60026200	0.17206300
C	0.25970000	-4.99652100	-3.69235400
H	3.49861700	-2.49653200	1.65637600
H	-1.16077900	-0.88615400	-2.48845700
H	3.96010500	0.12078600	-1.73149900
H	-0.27321800	-1.02301900	1.72032100
H	4.78877400	-0.89338800	3.08106800
H	-3.59480800	-0.55115700	-1.97291200
H	5.27183700	1.72789500	-0.31858700
H	-2.70260300	-0.69121500	2.25193700
H	5.67864700	1.21689100	2.08999200
H	-4.35796000	-0.45492500	0.40057000
H	-0.14447700	-6.01545600	-3.71055400
H	1.18966000	-4.95062100	-4.28015200

H	-0.46255400	-4.30051700	-4.14750300
H	0.47842200	-5.01772900	-0.32637300
H	-0.09943900	-6.26366500	-1.44043900
H	1.21612000	-2.78038600	-2.98028000

36

Energy = -1218.05069900 a.u. #Cluster: 5

P	1.28324500	-2.50160500	0.04315000
O	2.85837600	-2.73494700	-0.07388000
O	1.04330900	-1.43112800	-1.13167000
O	0.68106700	-2.18338000	1.36427400
N	0.70085900	-3.98968600	-0.55191000
N	-0.88272400	-4.43186600	1.08594600
C	3.77667900	-1.67215600	-0.07584600
C	-0.22675700	-0.87087100	-1.33485800
C	3.85078400	-0.80446900	1.01319800
C	-1.03854300	-1.40893100	-2.33175900
C	4.61104900	-1.54533700	-1.18359500
C	-0.62867500	0.21033200	-0.55284700
C	4.79473700	0.22678600	0.98160400
C	-2.29444600	-0.83591600	-2.55417700
C	5.55473300	-0.51431400	-1.19666300
C	-1.88690300	0.77239800	-0.78624400

C	-0.28820000	-4.75131100	-0.02958300
C	5.64664200	0.37284700	-0.11821700
C	-2.71930500	0.25195000	-1.78375200
C	-0.68180700	-5.97543200	-0.78327800
H	3.18328500	-0.93837400	1.86624200
H	-0.68400600	-2.25940500	-2.91706900
H	4.51290000	-2.24532800	-2.01523700
H	0.03720500	0.59648100	0.22056300
H	4.86383800	0.91597700	1.82655000
H	-2.94217100	-1.24476600	-3.33328800
H	6.21760600	-0.40318500	-2.05808600
H	-2.21694500	1.62171000	-0.18331200
H	6.38373500	1.17894900	-0.13521400
H	-3.70179700	0.69567100	-1.96078000
H	-1.03758400	-5.68021600	-1.78307200
H	-1.46975400	-6.52671300	-0.25638300
H	0.20200800	-6.61889700	-0.91493600
H	-0.60174500	-3.58650200	1.59680500
H	-1.62259100	-5.02292200	1.45462400
H	1.10406800	-4.32203600	-1.42925800

36

Energy = -1218.05066400 a.u. #Cluster: 6

P	0.45426700	-2.51271200	-0.72467500
O	1.40661500	-1.21956000	-0.67637600
O	-0.70650500	-1.99864400	-1.69421300
O	0.09954900	-3.13331700	0.57869000
N	1.24287700	-3.63085000	-1.74145600
N	1.31265800	-5.44715800	-0.29763200
C	2.54212800	-1.19067800	0.14708200
C	-1.44200500	-0.83391900	-1.41757300
C	2.39537000	-0.92277200	1.50688600
C	-1.34087600	0.22480200	-2.31669600
C	3.78852900	-1.41124200	-0.43604300
C	-2.26024600	-0.77632500	-0.29014700
C	3.54197900	-0.86924600	2.30446200
C	-2.09207200	1.37917900	-2.07810800
C	4.92655800	-1.35313500	0.37411900
C	-3.00045600	0.38791300	-0.06176300
C	1.59949000	-4.90211000	-1.44689000
C	4.80526600	-1.08316500	1.74163500
C	-2.91953300	1.46343300	-0.95263200
C	2.35084200	-5.65980500	-2.48698900
H	1.39961700	-0.76195900	1.92295000
H	-0.68269000	0.13593600	-3.18273100

H	3.85538300	-1.62198400	-1.50506000
H	-2.31447300	-1.62845100	0.38936300
H	3.44495200	-0.65859700	3.37220800
H	-2.02568500	2.21759500	-2.77560100
H	5.91132000	-1.52111700	-0.06833100
H	-3.64612800	0.44901200	0.81750100
H	5.69744500	-1.03918300	2.37063700
H	-3.50258700	2.36900500	-0.77002000
H	2.52613900	-6.69558000	-2.17343300
H	3.31534800	-5.15664400	-2.66201900
H	1.78535100	-5.64440000	-3.43130200
H	0.80480500	-4.90991700	0.41500000
H	1.59265500	-6.40515500	-0.10623700
H	1.51628100	-3.29583800	-2.66656600

36

Energy = -1218.05039800 a.u. #Cluster: 7

P	0.71676800	-1.77942500	1.01465800
O	2.15634200	-1.33998700	1.54371000
O	0.32854200	-0.54864300	0.06372800
O	-0.21019800	-2.17680800	2.10223600
N	0.95297500	-3.06725300	-0.09216900
N	-0.17854700	-4.73761100	1.05369600

C	3.25271800	-1.07742800	0.70644800
C	-0.76921900	-0.58971000	-0.80949700
C	4.15578400	-2.10828200	0.45348500
C	-2.05989100	-0.76331600	-0.31168700
C	3.41932100	0.20250400	0.18130300
C	-0.51321800	-0.42862800	-2.16950900
C	5.26511300	-1.84251000	-0.35513200
C	-3.12670600	-0.77554200	-1.21568200
C	4.53391400	0.45321100	-0.62410600
C	-1.59075100	-0.43721300	-3.05954000
C	0.51960000	-4.34327100	0.02526400
C	5.45489800	-0.56540000	-0.89363600
C	-2.89590500	-0.61205300	-2.58555700
C	0.86861100	-5.28459500	-1.07637500
H	3.98560100	-3.09550900	0.88688500
H	-2.21957800	-0.88501400	0.76056500
H	2.68653500	0.97942900	0.40325300
H	0.51548700	-0.30056600	-2.51161600
H	5.98300200	-2.63957300	-0.56248100
H	-4.14438300	-0.91091200	-0.84190400
H	4.68057400	1.45176900	-1.04253800
H	-1.40631400	-0.31009000	-4.12893400

H	6.32359000	-0.36269200	-1.52430900
H	-3.73459000	-0.62040800	-3.28555600
H	1.96368900	-5.31917800	-1.18678900
H	0.44619300	-4.90094600	-2.01861200
H	0.48160700	-6.29088000	-0.87787900
H	-0.43345300	-4.06766100	1.78900100
H	-0.49652600	-5.70101200	1.11560800
H	1.47058400	-2.86138600	-0.94829300

36

Energy = -1218.05039200 a.u. #Cluster: 8

P	0.54530100	-2.22560000	0.91841900
O	1.48787100	-0.96518600	0.61099900
O	-0.90232600	-1.55776800	0.93747400
O	0.81895800	-3.05999300	2.11376900
N	0.66342000	-3.15742400	-0.51618100
N	0.99423600	-5.24397500	0.44293500
C	2.84316000	-1.11660700	0.27903500
C	-1.43370700	-0.77513100	-0.10007900
C	3.25094700	-0.68247100	-0.98043100
C	-2.25026300	-1.39165800	-1.04618200
C	3.73348600	-1.66825500	1.19915600
C	-1.15725100	0.59035100	-0.13389100

C	4.60017900	-0.80110000	-1.32538800
C	-2.80695600	-0.60810200	-2.06190000
C	5.07908000	-1.78512100	0.83717200
C	-1.72173900	1.36050900	-1.15443700
C	0.86514400	-4.49147800	-0.61402400
C	5.51385500	-1.35282900	-0.42017500
C	-2.54386200	0.76465200	-2.11768200
C	0.93967600	-5.07353700	-1.98391800
H	2.51532500	-0.26264600	-1.66903900
H	-2.44137200	-2.46431200	-0.97974400
H	3.37492200	-1.99745200	2.17550600
H	-0.51165100	1.03187000	0.62637100
H	4.93589100	-0.46337300	-2.30876000
H	-3.44987800	-1.07610000	-2.81106400
H	5.78972300	-2.21567400	1.54662300
H	-1.51575700	2.43275400	-1.19481000
H	6.56691800	-1.44584400	-0.69555200
H	-2.98142600	1.37246600	-2.91301600
H	1.74296900	-4.56919700	-2.54363200
H	-0.00950100	-4.88111600	-2.50844900
H	1.13234900	-6.15193100	-1.94721400
H	0.96124900	-4.82411500	1.37963400

H	1.14687800	-6.24383800	0.34143200
H	0.60632200	-2.65735500	-1.40491600

36

Energy = -1218.05036900 a.u. #Cluster: 9

P	0.56508100	-2.13587200	0.93954700
O	1.52870800	-0.91099900	0.56004400
O	-0.86657000	-1.43423200	0.95818200
O	0.84696900	-2.92541500	2.16313900
N	0.62993400	-3.12853700	-0.45764100
N	0.95650500	-5.17745500	0.58008100
C	2.87753800	-1.10989000	0.22573800
C	-1.40895100	-0.70842900	-0.11470900
C	3.28229500	-0.76087400	-1.06087700
C	-2.26358500	-1.36651200	-0.99718600
C	3.76505600	-1.62325000	1.17043300
C	-1.10327900	0.64485500	-0.24646200
C	4.62563700	-0.92815600	-1.40872300
C	-2.82910800	-0.63901800	-2.04901200
C	5.10463100	-1.78948900	0.80555100
C	-1.67723500	1.35889600	-1.30199000
C	0.81485900	-4.46783400	-0.50463200
C	5.53632100	-1.44298300	-0.47912100

C	-2.53714700	0.72037800	-2.20285100
C	0.85708200	-5.10635700	-1.85062600
H	2.54910400	-0.36803800	-1.76775200
H	-2.47614600	-2.42767300	-0.85488500
H	3.40900400	-1.88522100	2.16776700
H	-0.42827600	1.12029400	0.46632000
H	4.95904400	-0.65742500	-2.41335300
H	-3.50131000	-1.14022900	-2.74940900
H	5.81295600	-2.19089500	1.53415800
H	-1.44867700	2.42089400	-1.41899400
H	6.58473100	-1.57412900	-0.75670400
H	-2.98149100	1.28439100	-3.02620000
H	1.02730000	-6.18644500	-1.77320700
H	1.66309300	-4.64197300	-2.44028800
H	-0.09474100	-4.91417500	-2.37029500
H	0.94757900	-4.71858300	1.49891100
H	1.09732300	-6.18227300	0.51796100
H	0.55793500	-2.66393600	-1.36487400

36

Energy = -1218.05035200 a.u. #Cluster: 10

P	0.69010100	-2.49060700	0.90455400
O	2.08289500	-2.21714600	1.63166800

O	0.24035400	-1.00847900	0.49218100
O	-0.22934200	-3.33548800	1.70524300
N	1.03624900	-3.22702700	-0.60519200
N	-0.06887000	-5.24135500	-0.28428400
C	3.14175700	-1.48857300	1.06645800
C	-0.80422000	-0.75874800	-0.41038600
C	3.17476900	-0.10419600	1.22285900
C	-0.49854100	-0.02969900	-1.55766900
C	4.14328000	-2.18426600	0.39190400
C	-2.09403600	-1.21437800	-0.14097400
C	4.25259800	0.60293600	0.68277900
C	-1.52449700	0.25599800	-2.46262400
C	5.21460200	-1.46279900	-0.14421100
C	-3.10827800	-0.92558300	-1.05939700
C	0.65524100	-4.45336000	-1.02944000
C	5.27038600	-0.07248500	-0.00034100
C	-2.82743700	-0.19198900	-2.21678100
C	1.09460700	-4.87350600	-2.38991900
H	2.36802800	0.40041700	1.75614100
H	0.52780900	0.30129300	-1.72682400
H	4.07810700	-3.26956100	0.29460400
H	-2.29447400	-1.78149000	0.76920100

H	4.29444600	1.68863500	0.79776300
H	-1.30121900	0.82863200	-3.36591700
H	6.00828000	-1.99356200	-0.67529000
H	-4.12438000	-1.27623500	-0.86357500
H	6.10958500	0.48656600	-0.42067500
H	-3.62529500	0.03155100	-2.92871700
H	2.19533000	-4.87580200	-2.42690000
H	0.73414100	-4.13794000	-3.12600300
H	0.71132200	-5.86940000	-2.64028700
H	-0.37661100	-4.92967000	0.64446200
H	-0.34227500	-6.15775500	-0.62855200
H	1.57776200	-2.68152000	-1.27781500

ANMP

41

Energy = -1312.26407700 a.u. #Cluster: 1

P	2.74622200	-0.71943500	0.24239700
O	2.87485000	-2.03834800	0.96007000
N	-0.85758300	0.58515000	0.12547700
N	1.28951900	-0.12232600	-0.20438100
C	-0.56219000	1.80669800	-0.63104400
C	-2.22078100	0.46256900	0.65116400

C	0.10968800	-0.32575400	0.34038400
C	-0.75263500	1.62633500	-2.13424600
C	-2.40254000	1.15151700	2.00307000
C	-0.23810800	-1.54323900	1.16613000
C	3.83670400	-0.54029300	-1.17552200
H	0.47096300	2.10004100	-0.40819200
H	-1.22560000	2.59655200	-0.24869900
H	-2.89563200	0.90977700	-0.09456700
H	-2.49612500	-0.59706700	0.71818300
H	-0.05621100	0.86774100	-2.52217300
H	-1.78139300	1.30991500	-2.37025100
H	-0.55821700	2.57574000	-2.65819200
H	-1.79315100	0.67049400	2.78254700
H	-2.11210000	2.21269000	1.95256700
H	-3.45828800	1.10048900	2.31225500
H	-0.99738300	-2.14377500	0.64035000
H	0.65874000	-2.15244200	1.31289200
H	-0.65348200	-1.25801300	2.14276000
H	4.87254000	-0.71820400	-0.85160500
H	3.55808400	-1.29613200	-1.92490200
H	3.74234400	0.46479700	-1.60797200
O	3.35078400	0.53692600	1.21630900

C	2.48841700	1.11076700	2.09974300
C	1.92541900	0.35651900	3.14173600
C	2.12748000	2.45392700	1.91659600
C	0.96595100	0.92902600	3.96877800
H	2.22831900	-0.68306200	3.26865900
C	1.17061700	3.03228300	2.74149400
H	2.58097300	3.01687700	1.09959900
C	0.58612300	2.25519900	3.74660000
H	0.49608500	0.35575100	4.76674200
H	0.85102100	4.06363500	2.59866200
N	-0.47676500	2.83497500	4.56426100
O	-0.81148300	3.99250000	4.34319000
O	-0.99518800	2.13228100	5.42368300

41

Energy = -1312.25989200 a.u. #Cluster: 2

P	2.24696900	-0.72559800	0.66067100
O	2.56496900	-2.19028100	0.75827600
N	-1.50490900	-0.13693400	-0.09449500
N	0.75053100	-0.18291100	0.28450700
C	-1.43040800	1.29362900	-0.40837300
C	-2.83669300	-0.74512600	-0.18017200
C	-0.39683700	-0.82188200	0.25099400

C	-1.69152900	2.17304200	0.81220600
C	-3.18448900	-1.22674100	-1.58746200
C	-0.55352600	-2.28755000	0.58836400
C	3.38545300	0.18118300	-0.40533700
H	-2.17273200	1.49895700	-1.19450200
H	-0.43640300	1.49850500	-0.82453500
H	-2.91326200	-1.56830100	0.54054500
H	-3.56117200	0.01609100	0.14697500
H	-2.69784200	1.99674000	1.22456200
H	-0.95357700	1.97365900	1.60294300
H	-1.61902700	3.23676700	0.53487700
H	-3.13527800	-0.40007700	-2.31369400
H	-2.49381700	-2.01718800	-1.92083500
H	-4.20782300	-1.63387200	-1.60368600
H	0.43435600	-2.74209900	0.71033600
H	-1.11466800	-2.39202800	1.53098000
H	-1.11167300	-2.82235400	-0.19272900
H	4.41488000	-0.07135900	-0.11202200
H	3.21240600	-0.14476200	-1.44214600
H	3.23353400	1.26708500	-0.34027900
O	2.56995200	-0.09835200	2.19258300
C	2.46755900	1.16260500	2.66797000

C	3.01592400	1.38818900	3.94573400
C	1.85353100	2.22012100	1.97122200
C	2.95605600	2.64847100	4.52238600
H	3.48713400	0.55367500	4.46776400
C	1.79376400	3.48416600	2.54770200
H	1.40404600	2.04144400	0.99658300
C	2.34365100	3.69018200	3.81545900
H	3.37672900	2.83636200	5.50943500
H	1.31650200	4.31110800	2.02338800
N	2.27584700	5.01745400	4.41646600
O	1.73039900	5.91463600	3.78380900
O	2.76746300	5.17642700	5.52808100

41

Energy = -1312.25984800 a.u. #Cluster: 3

P	2.24414400	-0.71690800	0.60061600
O	2.58426400	-2.17614300	0.70316900
N	-1.53934200	-0.15419800	0.00408200
N	0.72326100	-0.19139800	0.31830000
C	-1.51208100	1.31183000	-0.01514900
C	-2.85407300	-0.77806500	-0.17391300
C	-0.40236200	-0.85389200	0.18954000
C	-1.70145100	1.91334500	1.37536800

C	-3.22392500	-0.98066100	-1.64195100
C	-0.50339700	-2.36169900	0.23579800
C	3.31724400	0.18912600	-0.53317000
H	-2.31111500	1.64843100	-0.69258700
H	-0.55410100	1.63060700	-0.44479500
H	-2.88621000	-1.73046200	0.36885500
H	-3.59144900	-0.12270400	0.31435300
H	-0.90357800	1.57988300	2.05515100
H	-1.66814300	3.01314400	1.32132300
H	-2.67261500	1.62128000	1.80614100
H	-3.21263700	-0.02432300	-2.18825000
H	-2.52087900	-1.66764700	-2.13859800
H	-4.23634100	-1.40727300	-1.72062700
H	-1.07755200	-2.67263000	1.12323000
H	-1.02472400	-2.75079900	-0.65036300
H	0.49974600	-2.79408200	0.29723200
H	3.09867000	-0.15313200	-1.55606800
H	3.15576900	1.27400000	-0.47516600
H	4.36280400	-0.04722900	-0.28670600
O	2.63569800	-0.06524900	2.10481700
C	2.52049100	1.19414500	2.58152300
C	1.88232600	2.24493500	1.89599100

C	3.08608900	1.42627300	3.85079900
C	1.81777900	3.50787500	2.47414400
H	1.41594300	2.06323700	0.93029700
C	3.02094000	2.68526300	4.42951200
H	3.57520700	0.59695400	4.36462200
C	2.38539500	3.72011000	3.73302200
H	1.32267800	4.32937700	1.95792000
H	3.45487100	2.87717000	5.41001400
N	2.31219300	5.04627200	4.33529900
O	2.81847600	5.21047800	5.43966800
O	1.74797700	5.93784200	3.71110900

41

Energy = -1312.25980900 a.u. #Cluster: 4

P	2.20259800	-0.79494900	0.85222100
O	2.48568300	-2.25911100	1.02806900
N	-1.49334800	-0.14561700	-0.08223500
N	0.70557400	-0.23905400	0.51296600
C	-1.52984200	1.25910700	0.33887700
C	-2.72856900	-0.69204900	-0.65127500
C	-0.35545400	-0.85464400	0.05020600
C	-1.03076900	2.21483500	-0.74165400
C	-3.70064000	-1.20562100	0.40907600

C	-0.36764100	-2.30676800	-0.36941400
C	3.35546500	0.03121700	-0.26621100
H	-0.92108900	1.35969600	1.24701400
H	-2.57054900	1.49333900	0.60729500
H	-3.19828600	0.11340400	-1.23699600
H	-2.48185200	-1.48575100	-1.36710200
H	-1.64607900	2.14098500	-1.65277400
H	-1.07807200	3.25405500	-0.37943800
H	0.01247400	1.98868900	-1.00838900
H	-3.26340300	-2.04134400	0.97774500
H	-3.96792400	-0.40898600	1.12125100
H	-4.62724300	-1.56098400	-0.06869400
H	-0.40985200	-2.37485300	-1.46871000
H	0.54712500	-2.79361500	-0.01668200
H	-1.24188900	-2.83714700	0.03209300
H	4.38179000	-0.21939900	0.04031800
H	3.17623400	-0.35273200	-1.28208500
H	3.22000100	1.12133100	-0.26494500
O	2.54363000	-0.09167400	2.34159100
C	2.41223000	1.18325000	2.77159600
C	2.90136500	1.44833600	4.06579100
C	1.83082000	2.21982100	2.01660500

C	2.81674600	2.72516900	4.60155500
H	3.34746800	0.63011500	4.63368900
C	1.74685200	3.50046800	2.55190500
H	1.42539600	2.01537700	1.02881700
C	2.23850400	3.74514200	3.83668500
H	3.19192700	2.94209300	5.60093100
H	1.29677100	4.31127200	1.98029700
N	2.14487100	5.08972200	4.39356000
O	2.58294400	5.28214500	5.52222000
O	1.63202300	5.96781200	3.70878100

41

Energy = -1312.25931600 a.u. #Cluster: 5

P	2.17609400	-0.84448200	0.83156200
O	2.35799800	-2.31468400	1.07759800
N	-1.36017600	-0.05528600	-0.52847500
N	0.77359400	-0.22769800	0.26269600
C	-1.32001200	1.38656500	-0.25094200
C	-2.59238300	-0.59794300	-1.10926100
C	-0.29872800	-0.82184000	-0.20345000
C	-1.55771000	1.73520500	1.21753400
C	-3.69676300	-0.86187900	-0.08671900
C	-0.40156900	-2.31355100	-0.42776900

C	3.50965900	-0.10279600	-0.13324200
H	-2.08405600	1.85808000	-0.88534900
H	-0.33972500	1.76731100	-0.57171000
H	-2.94223300	0.12756700	-1.85987700
H	-2.35661700	-1.51745600	-1.65781300
H	-0.81818300	1.23683400	1.85969700
H	-1.45514300	2.82217100	1.36405500
H	-2.56529500	1.43752600	1.54440100
H	-4.57549700	-1.29356500	-0.59161900
H	-3.36011200	-1.57109000	0.68597100
H	-4.01434000	0.06597800	0.41251400
H	-0.41649100	-2.53078400	-1.50799900
H	0.46310500	-2.80908700	0.02424000
H	-1.32503600	-2.72016600	0.00778300
H	3.45326400	-0.50617900	-1.15562600
H	3.43005900	0.99186900	-0.17347400
H	4.46961400	-0.39227900	0.31921100
O	2.34580200	-0.12228400	2.34277000
C	2.31641600	1.17932000	2.70832000
C	2.74369700	1.46111900	4.02048300
C	1.88496200	2.22476400	1.87094800
C	2.74597300	2.76548700	4.49320300

H	3.07225400	0.63429600	4.65240800
C	1.89011900	3.53282900	2.34192600
H	1.52077500	2.00462400	0.86987600
C	2.31939600	3.79463800	3.64561900
H	3.07446900	2.99686300	5.50570600
H	1.55572000	4.35259200	1.70739400
N	2.32059000	5.16882000	4.13432100
O	2.69580500	5.37609800	5.28274900
O	1.94669000	6.05557200	3.37489400

ANMP-N₁H

42

Energy = -1312.70570700 a.u. #Cluster: 1

P	1.38106700	-2.01185000	1.36786500
O	0.31388000	-2.73477000	2.11367500
N	-0.37801500	1.08679900	-0.31406400
N	0.77400400	-0.85054100	0.22517600
C	0.77132100	1.65411100	-1.04581200
C	-1.58794000	1.93849300	-0.30462100
C	-0.34021400	-0.07790900	0.30120100
C	0.77855500	1.26514500	-2.52121200
C	-1.58367500	2.94223700	0.84379400

C	-1.53830600	-0.57732700	1.04499700
C	2.58510600	-2.96310500	0.46143800
H	1.70171700	1.36055500	-0.54023600
H	0.70098600	2.74408600	-0.93152700
H	-1.60575400	2.45773700	-1.27261000
H	-2.47830000	1.30065200	-0.27306300
H	-0.14345700	1.59981900	-3.02021800
H	1.63414500	1.74651000	-3.01811500
H	0.86951200	0.17608700	-2.65337100
H	-2.45625400	3.60558600	0.74588700
H	-1.64233600	2.44089900	1.82066600
H	-0.67654500	3.56588300	0.83138600
H	-1.89136700	0.17324800	1.76314800
H	-2.34414000	-0.76403200	0.31725700
H	-1.30827100	-1.50982300	1.56544900
H	3.13094000	-3.58210300	1.18919700
H	2.05011500	-3.61092400	-0.24779200
H	3.28672500	-2.30310700	-0.06806100
O	2.33752700	-1.04837500	2.30663300
C	1.83294400	0.14117300	2.78970400
C	0.72384800	0.15133200	3.64326200
C	2.43580700	1.32852800	2.36016600

C	0.18229300	1.37178000	4.03770700
H	0.28335700	-0.79000500	3.97201100
C	1.89761400	2.54869000	2.75409700
H	3.30035400	1.27922900	1.69667100
C	0.76625600	2.55119800	3.57329900
H	-0.69380300	1.41452100	4.68318200
H	2.32741300	3.49009900	2.41516300
N	0.15402100	3.83484200	3.93185500
O	-0.86181300	3.81654300	4.61318800
O	0.68112700	4.85857300	3.51923800
H	1.51482800	-0.51150600	-0.38963800

42

Energy = -1312.70505100 a.u. #Cluster: 2

P	1.40774900	-1.73892400	1.14765400
O	0.82017600	-3.08458700	0.92542700
N	-0.87208700	0.90021400	-0.72024600
N	0.76741000	-0.49079400	0.12864100
C	0.11479200	1.96491800	-1.00023400
C	-2.26903200	1.23743800	-1.07533200
C	-0.53388400	-0.23912000	-0.15295000
C	0.75836500	1.82152600	-2.37599100
C	-3.01577900	1.87101200	0.09229300

C	-1.54187400	-1.27344200	0.23391100
C	3.17347100	-1.53820100	0.94541200
H	0.86112800	1.98146500	-0.19264000
H	-0.42837900	2.91589300	-0.92391000
H	-2.20752600	1.93137900	-1.92403500
H	-2.77693300	0.33887300	-1.44379400
H	1.44830500	2.66236900	-2.54232700
H	1.32876200	0.88416300	-2.46466200
H	-0.00546200	1.83911200	-3.16818800
H	-3.10921900	1.16831100	0.93444000
H	-2.49748000	2.77452100	0.44875800
H	-4.02694500	2.15907400	-0.23294900
H	-1.66776500	-1.24309300	1.32873800
H	-2.51657800	-1.10847900	-0.22923600
H	-1.16036500	-2.26881500	-0.02191300
H	3.43687200	-1.81640400	-0.08573700
H	3.48795900	-0.50457600	1.14912700
H	3.66483700	-2.22367800	1.65126500
O	1.01737300	-1.22030700	2.65773700
C	1.28190600	0.03997700	3.15212000
C	0.31896500	1.04711600	3.01865600
C	2.49477000	0.27584400	3.80887300

C	0.57744900	2.31298400	3.53612700
H	-0.63032400	0.83817800	2.52522000
C	2.75603800	1.53981700	4.33000000
H	3.22030500	-0.53244700	3.91019900
C	1.79437300	2.54151600	4.18159900
H	-0.15202400	3.11660600	3.44603200
H	3.69078800	1.75422300	4.84614500
N	2.06854500	3.87686300	4.72726400
O	3.13554600	4.05661500	5.29686800
O	1.21578200	4.74179400	4.58485000
H	1.45525900	0.20004300	-0.16624400

42

Energy = -1312.70486100 a.u. #Cluster: 3

P	0.45689200	-1.78626200	1.96461300
O	-0.61057900	-2.80408100	2.14577600
N	-0.91260300	0.84513200	-0.68717000
N	0.19071500	-0.66581300	0.66567700
C	0.33740000	1.21495500	-1.38243300
C	-2.11973100	1.58003900	-1.12188500
C	-0.95003300	-0.05295500	0.27623700
C	1.12341600	2.29416500	-0.64223600
C	-2.78667000	0.94163100	-2.33464100

C	-2.23421000	-0.38966400	0.96701000
C	2.11871400	-2.35783100	1.63293000
H	0.04414200	1.56593300	-2.38010700
H	0.93897300	0.30908300	-1.55090700
H	-2.81335900	1.65876900	-0.27756800
H	-1.78762300	2.60222000	-1.35246300
H	2.01163100	2.56430300	-1.23270900
H	0.51028500	3.19779600	-0.50517600
H	1.45838700	1.95217600	0.34786100
H	-3.64986600	1.55356300	-2.63756900
H	-2.09348800	0.88219700	-3.18777200
H	-3.14458500	-0.07407100	-2.10696700
H	-2.12402400	-1.30779900	1.55184600
H	-2.50795500	0.43796300	1.64153700
H	-3.04395200	-0.52298000	0.23933200
H	2.09646000	-2.97005900	0.71930800
H	2.81489100	-1.51642100	1.50627300
H	2.43161500	-2.97592200	2.48706700
O	0.51511700	-0.82248100	3.29234200
C	1.21481700	0.36217200	3.38466800
C	2.56689900	0.34279300	3.74425800
C	0.54282100	1.56552100	3.14493000

C	3.26421400	1.54352300	3.84373300
H	3.06201700	-0.60735400	3.94844700
C	1.23555400	2.76817900	3.24493200
H	-0.51603100	1.55264400	2.88564000
C	2.58913800	2.73854100	3.58609000
H	4.31822600	1.56136800	4.11736100
H	0.74092100	3.71991800	3.05692300
N	3.32538100	4.00543600	3.68063000
O	4.51263100	3.95985500	3.97008100
O	2.71427900	5.04222000	3.46386600
H	1.04444300	-0.39942500	0.17720600

42

Energy = -1312.70478400 a.u. #Cluster: 4

P	1.38018800	-0.80145100	1.24068100
O	0.66776100	-1.54185000	2.31906900
N	-1.33601000	0.69741300	-1.21862000
N	0.39981200	-0.35198600	-0.10834400
C	-0.83122300	0.25985400	-2.53660400
C	-2.54510900	1.54940800	-1.25617200
C	-0.73453000	0.38270900	-0.09034200
C	0.21585300	1.21260300	-3.10777500
C	-3.83282800	0.73411800	-1.26745500

C	-1.25970600	0.84984100	1.23154800
C	2.79356200	-1.57168500	0.46552300
H	-1.70470400	0.20366400	-3.19919400
H	-0.45255600	-0.76977600	-2.45544000
H	-2.51690300	2.24868300	-0.41299200
H	-2.46070900	2.15634600	-2.16851700
H	0.52439900	0.85719200	-4.10235500
H	-0.19710200	2.22702800	-3.21599800
H	1.11053900	1.26892600	-2.46881100
H	-4.69306800	1.41580100	-1.34837400
H	-3.86077600	0.04403700	-2.12463500
H	-3.94263800	0.14520800	-0.34391900
H	-0.91814000	0.18389500	2.03147100
H	-0.88250800	1.86696600	1.42770300
H	-2.35418000	0.87415900	1.24200400
H	2.47015700	-2.50152300	-0.02552400
H	3.24818000	-0.88637100	-0.26406600
H	3.51690100	-1.80824900	1.25956700
O	1.88118400	0.70030100	1.69679200
C	2.12246300	1.11844700	2.98085000
C	1.82115100	2.45674200	3.26509700
C	2.66733500	0.27513100	3.95867500

C	2.06672100	2.96320900	4.53608300
H	1.39618000	3.08403100	2.48008700
C	2.90716200	0.77886700	5.23341800
H	2.90182300	-0.76513300	3.73289500
C	2.60469000	2.11451900	5.50739400
H	1.84122000	3.99988200	4.78244400
H	3.32951700	0.14680100	6.01340000
N	2.85862300	2.64000700	6.85087600
O	3.30822500	1.87510200	7.69383000
O	2.60810600	3.81861300	7.06551700
H	0.76620800	-0.64249900	-1.01282000

42

Energy = -1312.70450200 a.u. #Cluster: 5

P	1.13609600	-1.55632300	1.22833800
O	0.44387600	-2.87135800	1.22538400
N	-1.20071500	0.85429600	-0.89235000
N	0.45340100	-0.41170000	0.11641700
C	-0.26998800	1.36741800	-1.91809900
C	-2.57422100	1.40053500	-0.96158400
C	-0.83359700	-0.00448500	0.03625100
C	0.46268400	2.63135000	-1.47538900
C	-3.47009800	0.61097500	-1.90818200

C	-1.80367200	-0.52225300	1.05157800
C	2.88246300	-1.49974600	0.84852900
H	-0.87627200	1.56768800	-2.81152800
H	0.42757200	0.56707200	-2.20448400
H	-2.99301700	1.44407100	0.05015000
H	-2.47119200	2.44050100	-1.30108300
H	-0.24961200	3.43267600	-1.22724600
H	1.09937600	2.45037900	-0.59652700
H	1.10422700	2.98254800	-2.29726700
H	-3.60629200	-0.42493600	-1.56194300
H	-4.45836400	1.09273900	-1.95835600
H	-3.05050200	0.58463600	-2.92555800
H	-1.82575000	0.17101100	1.90874100
H	-2.81438400	-0.60627400	0.64079700
H	-1.48596100	-1.50979500	1.40427600
H	3.27950400	-0.47665500	0.90690200
H	3.39177400	-2.14269500	1.58154500
H	3.03069300	-1.90577100	-0.16312800
O	0.92391200	-0.86687400	2.69987500
C	1.51644100	0.23520100	3.26343900
C	1.80779400	1.39617500	2.53561400
C	1.78939200	0.15649000	4.63577700

C	2.38569300	2.48292500	3.18636400
H	1.57968200	1.46732000	1.47363000
C	2.36139900	1.24195100	5.28817100
H	1.54807800	-0.76204200	5.17265200
C	2.65582100	2.39344000	4.55238100
H	2.62130800	3.39658200	2.64245200
H	2.58457500	1.20459100	6.35360500
N	3.26330000	3.53972700	5.23455400
O	3.51155400	4.53835100	4.57252000
O	3.49231900	3.44117800	6.43235200
H	1.11597100	-0.02193900	-0.55259800

42

Energy = -1312.70448200 a.u. #Cluster: 6

P	1.12634300	-1.58416800	1.22358800
O	0.41134700	-2.88697200	1.23044900
N	-1.18512100	0.86552400	-0.87896700
N	0.45534500	-0.42992100	0.11501300
C	-0.25643100	1.35784300	-1.91689900
C	-2.54858700	1.43806600	-0.93409100
C	-0.82432300	0.00226100	0.04777400
C	0.50426000	2.60957100	-1.48704000
C	-3.47062000	0.66319500	-1.86757700

C	-1.79199100	-0.49399100	1.07609900
C	2.86943900	-1.56321800	0.82698500
H	-0.86899100	1.56629400	-2.80416800
H	0.42276500	0.54368600	-2.20836300
H	-2.95464700	1.49223400	0.08229600
H	-2.42929500	2.47500600	-1.27746300
H	-0.19056700	3.42464000	-1.23425500
H	1.14741400	2.42015900	-0.61468800
H	1.14272000	2.94589500	-2.31747900
H	-3.62097300	-0.36926200	-1.51695600
H	-4.45051000	1.16275000	-1.90619400
H	-3.06451300	0.62679900	-2.89006800
H	-1.49315300	-1.49001100	1.42154200
H	-1.78393300	0.19700900	1.93530400
H	-2.81037700	-0.55230500	0.68040700
H	3.28965000	-0.54921100	0.88377300
H	3.37173100	-2.21932300	1.55310000
H	2.99850400	-1.96967500	-0.18714700
O	0.93797600	-0.88918600	2.69561700
C	1.51864300	0.22242600	3.25156900
C	1.83531900	1.36903300	2.51156400
C	1.75190800	0.16859100	4.63267800

C	2.39720800	2.46604000	3.15922300
H	1.63903600	1.42286300	1.44245100
C	2.30814400	1.26407000	5.28159900
H	1.49180500	-0.73906100	5.17913500
C	2.62700900	2.40133500	4.53385100
H	2.65110700	3.36900700	2.60578600
H	2.50002200	1.24573100	6.35357700
N	3.21689900	3.55873500	5.21238600
O	3.48593000	4.54505000	4.54005100
O	3.41120500	3.48141100	6.41785800
H	1.11757300	-0.05993900	-0.56535000

42

Energy = -1312.70441100 a.u. #Cluster: 7

P	0.30746900	-1.86203600	2.14824200
O	-0.88387600	-2.70928100	2.41491400
N	-0.73980900	0.84532100	-0.57151200
N	0.15872000	-0.76984000	0.80839200
C	0.56631800	1.09006000	-1.21869000
C	-1.85163000	1.68955700	-1.05792000
C	-0.90100000	-0.03979600	0.39082300
C	1.43366300	2.07128900	-0.43446300
C	-2.52138900	1.11200800	-2.29963400

C	-2.23621300	-0.24271900	1.03542600
C	1.85414700	-2.69117500	1.80180600
H	0.34629300	1.48330400	-2.21939300
H	1.07760800	0.12926600	-1.38329900
H	-2.57362100	1.83694800	-0.24734100
H	-1.41419900	2.67481100	-1.27304000
H	1.70530800	1.67770600	0.55513000
H	2.36160800	2.26129500	-0.99408800
H	0.91116300	3.02918800	-0.29233100
H	-3.30618500	1.80322300	-2.64256900
H	-1.79922400	0.98026900	-3.11999700
H	-2.98671600	0.13743800	-2.08673200
H	-2.22148900	-1.12764100	1.67830900
H	-2.48639900	0.64247400	1.64128700
H	-3.01495200	-0.36553100	0.27151800
H	2.65404000	-1.96969200	1.58098100
H	2.11906600	-3.27776600	2.69361100
H	1.70380500	-3.36305400	0.94412000
O	0.57380700	-0.85814200	3.42208000
C	1.17642200	0.37942700	3.35849900
C	2.57155600	0.48321600	3.37626300
C	0.36364300	1.51700400	3.30014700

C	3.16279100	1.74220200	3.31016100
H	3.18543200	-0.41584400	3.44431700
C	0.94992400	2.77678300	3.23396300
H	-0.72108200	1.40272400	3.30353600
C	2.34305000	2.86975300	3.23287100
H	4.24586800	1.85625600	3.31489300
H	0.34272500	3.67891400	3.17618100
N	2.96593600	4.19619700	3.14286700
O	4.18645300	4.26133800	3.17662800
O	2.23220400	5.16867900	3.03597100
H	1.04403600	-0.59515100	0.33504300

42

Energy = -1312.70439400 a.u. #Cluster: 8

P	0.34866700	-1.80969500	2.11218700
O	-0.78895900	-2.73604300	2.34781300
N	-0.80918200	0.81746000	-0.64095500
N	0.16003400	-0.73395700	0.76361100
C	0.48616800	1.11106700	-1.28999300
C	-1.95721500	1.60435900	-1.13873600
C	-0.93130900	-0.06048100	0.33383800
C	1.31308800	2.13207300	-0.51239400
C	-2.59732800	0.98163800	-2.37418000

C	-2.25452100	-0.31293400	0.98530100
C	1.96019700	-2.52370000	1.80621700
H	0.25082100	1.48749900	-2.29354900
H	1.03589300	0.17039700	-1.44709000
H	-2.68607500	1.72893700	-0.33043500
H	-1.56513000	2.60601000	-1.36548800
H	2.23431500	2.35283500	-1.07194200
H	0.75279700	3.07015300	-0.38158300
H	1.59601400	1.75879400	0.48237000
H	-3.01528400	-0.01179300	-2.15024500
H	-3.41388100	1.63055400	-2.72551300
H	-1.86848400	0.87550700	-3.19236900
H	-2.52633400	0.55800600	1.60298900
H	-3.03645800	-0.45459500	0.22837900
H	-2.20487500	-1.20289600	1.61974500
H	2.71029800	-1.74741300	1.59829700
H	2.24696300	-3.08822500	2.70543400
H	1.87846400	-3.20720500	0.94826800
O	0.49669100	-0.78984300	3.39077100
C	1.16058800	0.41815400	3.38072300
C	2.54865600	0.45613600	3.55165000
C	0.41380300	1.59173500	3.22944500

C	3.20287100	1.68510800	3.54816600
H	3.10706600	-0.46979300	3.69401700
C	1.06316500	2.82200500	3.22780100
H	-0.66895400	1.53032800	3.11433500
C	2.45085800	2.84954500	3.38014900
H	4.28266700	1.74800500	3.67527900
H	0.50965400	3.75160500	3.10437100
N	3.14098000	4.14536600	3.36575400
O	2.46799400	5.15246000	3.19735100
O	4.35385700	4.15216300	3.52121800
H	1.03669300	-0.53034600	0.28596200

42

Energy = -1312.70430800 a.u. #Cluster: 9

P	0.42154100	-1.85599100	2.03464600
O	-0.69452300	-2.81140000	2.25727100
N	-0.81354400	0.84397200	-0.61118800
N	0.19630100	-0.74622400	0.71945800
C	0.46779700	1.17388700	-1.27023400
C	-1.97889900	1.63431400	-1.06097300
C	-0.90944900	-0.07077700	0.33217100
C	1.30225200	2.16904900	-0.46753900
C	-2.62979000	1.05241000	-2.31056900

C	-2.21959700	-0.36483900	0.99260100
C	2.04284200	-2.52884500	1.68887600
H	0.21165500	1.58946300	-2.25296900
H	1.01941100	0.24374400	-1.47578200
H	-2.69698000	1.71480000	-0.23773900
H	-1.60348800	2.64967400	-1.25221200
H	2.21054600	2.42006000	-1.03539200
H	0.73736700	3.09624600	-0.28808800
H	1.60803000	1.75880500	0.50556200
H	-3.46112700	1.70265700	-2.62259700
H	-1.91309000	0.99005800	-3.14383800
H	-3.02986500	0.04477200	-2.11986600
H	-2.50103800	0.48270100	1.63761700
H	-3.00703900	-0.49890500	0.23971000
H	-2.14710800	-1.27213700	1.59967500
H	2.77538700	-1.73282800	1.49367600
H	2.35142200	-3.11266100	2.56836000
H	1.96255500	-3.18963600	0.81315000
O	0.56460500	-0.86816800	3.33933700
C	1.18811700	0.36132200	3.35067800
C	2.57891000	0.44188200	3.47826000
C	0.39761700	1.51242800	3.26307600

C	3.19079800	1.69239100	3.49413900
H	3.17316200	-0.46783500	3.57185300
C	1.00461700	2.76408000	3.28098200
H	-0.68566000	1.41630100	3.18154300
C	2.39487500	2.83479000	3.38920400
H	4.27158500	1.78882500	3.58762400
H	0.41598800	3.67718500	3.20610700
N	3.04067700	4.15331900	3.39250600
O	4.25732100	4.19689100	3.50721800
O	2.32929800	5.14138800	3.27801000
H	1.06179200	-0.51818600	0.23264400

42

Energy = -1312.70056000 a.u. #Cluster: 10

P	1.23808300	-0.63143700	1.32160900
O	0.53811900	-1.57139700	2.24311400
N	-1.44869300	0.60177800	-1.30755300
N	0.34007900	-0.20020900	-0.08494700
C	-0.74231900	0.37102300	-2.58429500
C	-2.78616800	1.22288900	-1.42732200
C	-0.91313700	0.30473700	-0.14216600
C	0.15962600	1.53952000	-2.97275800
C	-3.88892600	0.19357900	-1.64580200

C	-1.64743700	0.54630100	1.13952500
C	2.82826600	-1.12885600	0.67326400
H	-1.51875800	0.21250900	-3.34405200
H	-0.18781400	-0.57717600	-2.52149000
H	-2.97709200	1.83685800	-0.53979600
H	-2.72439300	1.91490000	-2.27895900
H	-0.42338100	2.46841700	-3.06442200
H	0.95853000	1.70332900	-2.23310400
H	0.62852200	1.32806600	-3.94540000
H	-3.97713200	-0.48730800	-0.78544800
H	-4.84982000	0.71404300	-1.77647800
H	-3.70026000	-0.40879600	-2.54767900
H	-2.72045800	0.35994900	1.02712500
H	-1.25937400	-0.10725500	1.92807700
H	-1.50056400	1.59619000	1.44202900
H	3.23766500	-0.34861500	0.01616100
H	3.49573000	-1.28365300	1.53434100
H	2.70847600	-2.07702200	0.12860100
O	1.44341000	0.88674700	1.92421500
C	1.95304500	1.23449900	3.15072700
C	2.47140500	2.53321300	3.24852300
C	1.94592800	0.37199300	4.25642300

C	2.99028600	2.97852100	4.45800600
H	2.46095000	3.17708600	2.36779200
C	2.47056800	0.81701200	5.46654800
H	1.52477100	-0.62862000	4.16857800
C	2.98579600	2.11158500	5.55479800
H	3.40026400	3.98251000	4.55875800
H	2.47786900	0.16898300	6.34206800
N	3.53572600	2.57421000	6.83085700
O	3.53341300	1.79647300	7.77603800
O	3.97185500	3.71630700	6.89022300
H	0.85261500	-0.30390200	-0.95876100

ANMOP

42

Energy = -1387.44036100 a.u. #Cluster: 1

P	-0.06050100	-1.07841300	-4.35722500
O	0.29682500	0.09588800	-5.39133700
O	0.48587600	-2.38137300	-4.84454900
N	0.16360300	-0.46414500	-0.58940400
N	0.21023500	-0.48734500	-2.87131300
C	0.35165900	-1.05368500	0.74034300
C	-0.33574300	0.91567800	-0.62522900

C	0.38888000	-1.12757200	-1.73488200
C	-0.92672200	-1.67294900	1.30385100
C	0.78763800	1.94345900	-0.72178600
C	0.86175600	-2.55947000	-1.64800300
C	-0.10969000	1.45266600	-5.17602500
H	0.70611800	-0.24866000	1.40183800
H	1.15669800	-1.79757800	0.70124000
H	-1.01356000	1.00673900	-1.48263900
H	-0.92747600	1.07182000	0.28857700
H	-0.75096300	-2.02333200	2.33295100
H	-1.74912000	-0.94061100	1.32815000
H	-1.25642100	-2.53261100	0.70140600
H	0.36859900	2.96223800	-0.72313300
H	1.48006400	1.85994300	0.13128100
H	1.36018000	1.80339800	-1.65110900
H	1.85387500	-2.59493800	-1.17098900
H	0.17641800	-3.16983700	-1.04379500
H	0.93986700	-2.98253800	-2.65435200
H	0.21457200	2.02509100	-6.05509400
H	0.36262000	1.86056600	-4.27007600
H	-1.20436400	1.51855400	-5.07759900
O	-1.73887700	-1.04503900	-4.46492400

C	-2.45233300	-1.40892300	-3.35859500
C	-3.19870200	-0.43382000	-2.68386900
C	-2.39034800	-2.72539500	-2.87932500
C	-3.84708900	-0.76039800	-1.49854300
H	-3.22770600	0.58216300	-3.08005700
C	-3.03468800	-3.05741600	-1.69297600
H	-1.81023200	-3.46743200	-3.42934100
C	-3.74007700	-2.06517300	-1.00797200
H	-4.40740400	-0.01391700	-0.93734700
H	-2.97973800	-4.06566100	-1.28495700
N	-4.35586700	-2.39297100	0.27739100
O	-4.22992700	-3.53391800	0.70454500
O	-4.95595400	-1.50761200	0.87359100

42

Energy = -1387.44013800 a.u. #Cluster: 2

P	-0.86702300	-0.69236000	-3.07791500
O	-1.11574700	0.67734700	-3.89246600
O	-0.78373200	-1.83575300	-4.03395500
N	1.73881500	-0.67833300	-0.26849700
N	0.28718400	-0.34071300	-1.99598100
C	2.36452600	-1.47102600	0.79603100
C	2.12406600	0.73701600	-0.33854900

C	0.82624000	-1.16640500	-1.12198900
C	3.71399000	-2.05738700	0.38917300
C	1.17826800	1.63993100	0.44882500
C	0.44154500	-2.62408400	-1.01808500
C	-1.26437200	1.93720200	-3.22738200
H	1.67546700	-2.26192500	1.11743800
H	2.48676200	-0.80238800	1.66169700
H	3.14885900	0.81549500	0.05271100
H	2.14504100	1.03350900	-1.39504900
H	4.41450300	-1.26464300	0.08268900
H	4.16030900	-2.59790600	1.23861800
H	3.60530600	-2.76193800	-0.45032100
H	0.15943000	1.58454200	0.03730100
H	1.14427400	1.34994000	1.51124600
H	1.51955400	2.68562900	0.39072300
H	1.29937100	-3.26978700	-0.79401800
H	-0.30227100	-2.75037300	-0.21408200
H	-0.00723700	-2.95202300	-1.96296200
H	-0.33419700	2.21214700	-2.70828900
H	-2.08981900	1.89884400	-2.49908000
H	-1.49435600	2.68117800	-4.00125200
O	-2.22192500	-0.81327100	-2.09973900

C	-3.45413700	-1.19124600	-2.53270500
C	-4.27530400	-1.84946700	-1.60272100
C	-3.91920100	-0.92786100	-3.83278700
C	-5.55681000	-2.24555600	-1.96298600
H	-3.88734300	-2.04132900	-0.60099300
C	-5.19928200	-1.32979400	-4.19740200
H	-3.28570000	-0.40453200	-4.54806500
C	-6.00560300	-1.98385000	-3.26170400
H	-6.20804800	-2.75747600	-1.25569600
H	-5.58121900	-1.13603000	-5.19897600
N	-7.35063100	-2.40246200	-3.64909300
O	-7.72487900	-2.16557800	-4.79132400
O	-8.04269300	-2.97181600	-2.81366900

42

Energy = -1387.43946200 a.u. #Cluster: 3

P	-0.18787100	-1.37516200	-4.11068800
O	0.46410700	-0.36156100	-5.17384000
O	0.10082100	-2.78871600	-4.49988400
N	0.56010300	-0.63875100	-0.40413800
N	0.08546200	-0.77494200	-2.62946800
C	1.05295300	-1.16143100	0.87443800
C	0.03175600	0.73107900	-0.38679300

C	0.54884200	-1.35213900	-1.54225100
C	2.51329600	-0.80218800	1.14024600
C	-1.47860900	0.76664900	-0.16654000
C	1.05882500	-2.77330700	-1.49661800
C	0.34145300	1.06034900	-5.05203800
H	0.90903300	-2.24802400	0.90787900
H	0.40902300	-0.74234600	1.66261200
H	0.55260900	1.27221800	0.41663400
H	0.29121800	1.21233700	-1.33835200
H	3.17566800	-1.24290100	0.37879000
H	2.66086100	0.28932400	1.13350300
H	2.82066100	-1.18218600	2.12720800
H	-1.82960600	1.80975100	-0.12026200
H	-2.00389000	0.26282900	-0.99017100
H	-1.75380900	0.27119400	0.77823300
H	2.05830000	-2.82265500	-1.04263400
H	0.38126300	-3.39240400	-0.88688800
H	1.09240300	-3.18646000	-2.50905800
H	0.80566200	1.49775200	-5.94577700
H	0.86021000	1.42003600	-4.15067300
H	-0.71808800	1.35621000	-5.00573700
O	-1.79723600	-0.98814100	-4.36235700

C	-2.75308200	-1.19319100	-3.41941200
C	-2.75199400	-2.33243800	-2.59703200
C	-3.75739100	-0.22199700	-3.29080700
C	-3.73535500	-2.48216400	-1.62628100
H	-1.98563600	-3.09688800	-2.73004100
C	-4.74976800	-0.37484500	-2.33052700
H	-3.73434100	0.65323500	-3.94203700
C	-4.72196300	-1.50013300	-1.50052000
H	-3.74884000	-3.35225900	-0.97120400
H	-5.53366300	0.37128600	-2.20690900
N	-5.75221900	-1.65365200	-0.47481500
O	-6.62702000	-0.79951100	-0.40156700
O	-5.69216900	-2.62838200	0.26449500

42

Energy = -1387.43936300 a.u. #Cluster: 4

P	-0.18097300	-1.58034700	-3.68200700
O	-0.22352800	-0.08661300	-4.32323100
O	0.73238200	-2.51279500	-4.40812500
N	0.77370000	-0.76296800	-0.06156600
N	-0.11789300	-1.33301400	-2.08172000
C	1.83481600	-0.26424200	0.82063200
C	-0.52581900	-1.02831000	0.56884600

C	0.92656000	-0.94267300	-1.38284900
C	2.61400200	-1.38304700	1.50783700
C	-1.45862200	0.17914100	0.52317700
C	2.27292400	-0.66160400	-2.00871200
C	-0.31256200	0.06947000	-5.74585100
H	1.34972100	0.37668900	1.57252200
H	2.50726100	0.38956000	0.25122300
H	-0.98511000	-1.88404600	0.05761500
H	-0.32723200	-1.32391700	1.60961500
H	3.14232000	-2.01010400	0.77247100
H	3.35943400	-0.95485300	2.19624300
H	1.94209300	-2.03168600	2.09163900
H	-2.40799300	-0.05916400	1.02857700
H	-1.01003400	1.04868100	1.02983900
H	-1.68459600	0.45471500	-0.51688900
H	3.11134500	-0.93578600	-1.35758100
H	2.35930700	-1.22330100	-2.94680000
H	2.35104300	0.41395000	-2.23791100
H	-1.32692900	-0.18008400	-6.09720300
H	0.41892700	-0.57824900	-6.25224700
H	-0.09567300	1.12194700	-5.97051000
O	-1.72245400	-2.15261800	-3.89868700

C	-2.82824400	-1.71485100	-3.23351400
C	-3.75657000	-2.68809000	-2.83410600
C	-3.06357900	-0.35482700	-2.97334200
C	-4.91565400	-2.31089600	-2.16648100
H	-3.54752200	-3.73709300	-3.04992900
C	-4.21943900	0.02525800	-2.30148000
H	-2.33945500	0.39294600	-3.29390500
C	-5.13215700	-0.95513400	-1.90191400
H	-5.64596600	-3.05126400	-1.84269000
H	-4.42027800	1.07322900	-2.08298100
N	-6.34243600	-0.55252900	-1.18851500
O	-6.51027100	0.63922700	-0.96006400
O	-7.13286600	-1.42523400	-0.85070800

42

Energy = -1387.43927000 a.u. #Cluster: 5

P	-0.14604800	-1.12605500	-3.77870800
O	-0.15167300	0.46132300	-4.12776300
O	0.75348500	-1.92744000	-4.66226700
N	0.74771200	-1.13431100	-0.04749900
N	-0.10250500	-1.17403800	-2.16169400
C	1.82615400	-1.01464800	0.93989400
C	-0.61652800	-1.24188000	0.48519800

C	0.94912600	-1.11060700	-1.37458100
C	2.33395600	-2.36657100	1.43554800
C	-1.29936200	0.11607300	0.62776500
C	2.36268000	-0.98360900	-1.89269800
C	-0.26714400	0.88036700	-5.49408500
H	1.42577100	-0.42828800	1.78084700
H	2.64538800	-0.42058900	0.51624600
H	-1.19510700	-1.88975900	-0.18560900
H	-0.54632700	-1.74315400	1.46181500
H	2.77311900	-2.95248200	0.61285200
H	3.10690700	-2.21888700	2.20606600
H	1.51734900	-2.95759000	1.87942300
H	-1.39660100	0.60518900	-0.35238300
H	-2.30935600	-0.01263300	1.04825100
H	-0.73123100	0.78050700	1.29848400
H	3.07449400	-1.59216100	-1.32081400
H	2.39545500	-1.29532600	-2.94311100
H	2.68351400	0.06913100	-1.82712300
H	-0.01840000	1.94909200	-5.52770200
H	-1.29734600	0.73109600	-5.85598500
H	0.42930000	0.31590900	-6.13258400
O	-1.69823000	-1.60671900	-4.11861500

C	-2.80971000	-1.27887300	-3.40309900
C	-3.00496200	-0.00360500	-2.84724300
C	-3.78742600	-2.27537900	-3.26021400
C	-4.16818900	0.26398600	-2.13516200
H	-2.24475800	0.76623200	-2.97135600
C	-4.95555100	-2.00824700	-2.55637400
H	-3.60917000	-3.25665700	-3.70283300
C	-5.13070200	-0.73992600	-1.99444100
H	-4.33681600	1.24284800	-1.68849100
H	-5.72408700	-2.76968400	-2.42978200
N	-6.34985900	-0.45697300	-1.24002600
O	-7.19793300	-1.33723100	-1.15926000
O	-6.46741000	0.64704100	-0.72216700

42

Energy = -1387.43923800 a.u. #Cluster: 6

P	-0.19312300	-1.39067600	-3.75862500
O	-0.09413300	0.17642200	-4.18498100
O	0.66326700	-2.28675600	-4.59110400
N	0.72438800	-1.12020900	-0.04867400
N	-0.15274800	-1.38960800	-2.13768400
C	1.75562500	-0.69822400	0.90676400
C	-0.54496300	-1.58387500	0.52645800

C	0.87390600	-1.06291700	-1.38113900
C	2.63792800	-1.85036800	1.38052300
C	-1.56504800	-0.45975300	0.68713000
C	2.19288300	-0.59943000	-1.95458900
C	-0.11088900	0.53411400	-5.57346200
H	1.23141100	-0.24484900	1.76164500
H	2.35960000	0.10249100	0.46196100
H	-0.94555600	-2.37154500	-0.12428700
H	-0.31264200	-2.03697500	1.50150700
H	3.35659900	-1.48997500	2.13319900
H	2.03310500	-2.64855000	1.83885000
H	3.20400500	-2.28741000	0.54303500
H	-1.17161400	0.34659900	1.32664600
H	-1.83156400	-0.03546900	-0.29132900
H	-2.48346600	-0.84914500	1.15445900
H	2.34506200	-1.07299700	-2.93306200
H	2.15932000	0.49203500	-2.10450600
H	3.05059300	-0.83639900	-1.31576900
H	-1.12895600	0.43408200	-5.98350400
H	0.57733700	-0.10620600	-6.14556000
H	0.21041600	1.58157300	-5.64243100
O	-1.77033300	-1.79105200	-4.07845900

C	-2.84871900	-1.35680700	-3.36658900
C	-2.98759700	-0.02262200	-2.95051200
C	-3.84739500	-2.30004600	-3.08205500
C	-4.11823600	0.36021800	-2.23827200
H	-2.20758100	0.70186300	-3.18114300
C	-4.98161200	-1.91938900	-2.37461800
H	-3.71253300	-3.32975300	-3.41694100
C	-5.10204100	-0.59121600	-1.95487000
H	-4.24432100	1.38761000	-1.89936100
H	-5.76558900	-2.63743900	-2.13758500
N	-6.28553200	-0.18724700	-1.19768300
O	-6.36019300	0.97484700	-0.81774700
O	-7.14708000	-1.02948000	-0.97692000

42

Energy = -1387.43922800 a.u. #Cluster: 7

P	-0.15525800	-1.24110700	-3.77382600
O	-0.16672200	0.32502600	-4.20817400
O	0.74412700	-2.08566200	-4.61627300
N	0.74598600	-1.04000400	-0.04983400
N	-0.10627800	-1.20352100	-2.15668600
C	1.82236700	-0.84805700	0.92828200
C	-0.61583200	-1.14835600	0.48945300

C	0.94527500	-1.07996700	-1.37667700
C	2.35918500	-2.16246400	1.48972100
C	-1.33008400	0.19935700	0.55464500
C	2.35430600	-0.95225500	-1.90652300
C	-0.28578500	0.66993000	-5.59445200
H	1.41044700	-0.22886300	1.73966100
H	2.62846900	-0.25840000	0.47414300
H	-1.17903100	-1.84642400	-0.14305500
H	-0.53475200	-1.59186300	1.49276500
H	3.13094400	-1.96006400	2.24894900
H	1.55620900	-2.74696900	1.96591500
H	2.80832400	-2.78015300	0.69613200
H	-0.77827400	0.91394800	1.18624400
H	-1.43724000	0.62880400	-0.45194400
H	-2.33750100	0.07153800	0.98157500
H	2.39213400	-1.33804100	-2.93202200
H	2.64488200	0.11128000	-1.92005100
H	3.08522200	-1.49703300	-1.29618500
H	-0.05311900	1.73907700	-5.68376700
H	-1.31306200	0.48667300	-5.94923000
H	0.41971700	0.08311400	-6.20211400
O	-1.70721900	-1.74430000	-4.07919700

C	-2.81112300	-1.38577100	-3.36584500
C	-3.01920400	-0.07617000	-2.90274100
C	-3.76558000	-2.38613000	-3.12663500
C	-4.17170200	0.22373600	-2.18616200
H	-2.27600400	0.69485100	-3.10122200
C	-4.92280000	-2.08797400	-2.41708400
H	-3.57778300	-3.39473100	-3.49831300
C	-5.11032800	-0.78422300	-1.94790000
H	-4.35004100	1.23034400	-1.81046300
H	-5.67299100	-2.85152200	-2.21546400
N	-6.31756200	-0.46749400	-1.18713800
O	-6.44793500	0.67172800	-0.75608900
O	-7.14240300	-1.35641900	-1.01369400

42

Energy = -1387.43921600 a.u. #Cluster: 8

P	-0.16679700	-1.83229800	-3.56316900
O	0.04397000	-0.38298500	-4.27077500
O	0.65145800	-2.91862700	-4.17978700
N	0.66962000	-0.91457700	0.06041100
N	-0.17009100	-1.52038900	-1.97250200
C	-0.66197800	-1.10454600	0.64961300
C	1.71592800	-0.42127700	0.96362300

C	0.86397400	-1.15201500	-1.24593500
C	-1.54480100	0.13446100	0.52383900
C	2.43042500	-1.54029100	1.71720500
C	2.24434700	-0.95849200	-1.82997100
C	0.07273800	-0.29162700	-5.70134200
H	-0.51365400	-1.36689300	1.70757700
H	-1.13544400	-1.96135900	0.15342700
H	2.42998600	0.18938500	0.39684500
H	1.22657800	0.26212800	1.67408600
H	-2.51706000	-0.04575700	1.00936700
H	-1.07789800	1.00754800	1.00735000
H	-1.72941200	0.37362400	-0.53319900
H	3.16750100	-1.11323800	2.41522100
H	1.71619800	-2.14278700	2.30021800
H	2.95955800	-2.21224500	1.02332000
H	2.36250600	0.09114900	-2.14523900
H	3.04760500	-1.19935600	-1.12453900
H	2.35383400	-1.59773600	-2.71498400
H	0.46266100	0.70268600	-5.95537200
H	-0.94283000	-0.40497300	-6.11395100
H	0.72737400	-1.06798800	-6.12519500
O	-1.75615500	-2.19583000	-3.86537800

C	-2.83111900	-1.57114000	-3.30749100
C	-3.91710200	-2.38112800	-2.94245900
C	-2.88551200	-0.17965500	-3.12413100
C	-5.05545500	-1.80925800	-2.38714300
H	-3.84671300	-3.45906000	-3.09638400
C	-4.02065800	0.39488200	-2.56413500
H	-2.03956600	0.44073600	-3.41658600
C	-5.09254300	-0.42428600	-2.19888300
H	-5.90711000	-2.42089300	-2.09228800
H	-4.08294000	1.47080200	-2.40690000
N	-6.28244400	0.18272700	-1.60546700
O	-7.21800700	-0.54940600	-1.30690300
O	-6.28899000	1.39545600	-1.43327200

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43

Energy = -1387.87775700 a.u. #Cluster: 1

P	-0.44531000	-1.09331600	-4.26782800
O	-0.40745200	0.41818200	-4.75776400
O	0.29714000	-2.11575500	-5.03459900
N	0.42206500	-1.47602500	-0.42439200
N	0.01679400	-0.90181100	-2.62165700

C	0.66037400	-2.45776600	0.65603800
C	0.34932900	-0.06499300	0.00996900
C	0.25863800	-1.84279500	-1.67705000
C	2.14355800	-2.64503200	0.95301500
C	-1.08100300	0.38743000	0.29135000
C	0.31074900	-3.28279000	-2.07675400
C	0.81914500	1.04709100	-5.20471200
H	0.18072400	-3.40638700	0.39090200
H	0.12980300	-2.07249300	1.53814400
H	0.96314700	0.01166800	0.91658400
H	0.84453800	0.57099900	-0.73859400
H	2.67719200	-3.05842500	0.08359500
H	2.61896700	-1.69207400	1.23163900
H	2.25888200	-3.34407800	1.79517400
H	-1.70726300	0.36227300	-0.61155400
H	-1.54987700	-0.25219500	1.05408400
H	-1.06487500	1.42108000	0.66774200
H	0.39503700	-3.37730200	-3.16365200
H	1.16451300	-3.78683300	-1.60769900
H	-0.61404200	-3.78035400	-1.74187600
H	0.52061800	1.96028500	-5.73198200
H	1.36049100	0.37428300	-5.88371000

H	1.44550100	1.29753000	-4.33627300
O	-2.03018600	-1.40566500	-4.20335400
C	-2.88727700	-0.88507700	-3.24712700
C	-3.36742500	-1.74958800	-2.26016700
C	-3.25416800	0.46270600	-3.28983000
C	-4.22734200	-1.25544700	-1.28379800
H	-3.05336700	-2.79447200	-2.26098100
C	-4.11355800	0.95958100	-2.31331600
H	-2.85934900	1.10933000	-4.07358400
C	-4.58354700	0.09394300	-1.32377800
H	-4.61227200	-1.89802900	-0.49341200
H	-4.41548400	2.00589600	-2.30925700
N	-5.47242600	0.62402300	-0.28074600
O	-5.77998500	1.80590600	-0.33473500
O	-5.85696200	-0.14411600	0.58924800
H	-0.03685700	0.06752300	-2.31125200

43

Energy = -1387.87718900 a.u. #Cluster: 2

P	-1.39650600	-1.42713000	-2.58446200
O	-0.76521000	-0.72028500	-3.86271100
O	-1.81406400	-2.81681900	-2.86340400
N	1.68118800	-1.45631900	-0.12543400

N	-0.28877400	-1.18447500	-1.29923200
C	3.07459400	-1.93611000	0.01103500
C	1.17934000	-0.63448200	0.99549600
C	0.95139600	-1.71493200	-1.18741300
C	3.16204800	-3.26698900	0.74807600
C	1.40359400	0.85880800	0.77300300
C	1.45915900	-2.55490200	-2.31685600
C	-0.32420900	0.65591900	-3.87622500
H	3.61320700	-1.15051500	0.55892600
H	3.53173200	-1.99154200	-0.98370100
H	0.11837700	-0.87104500	1.16583000
H	1.71152300	-0.97707700	1.89251300
H	2.64811000	-4.06717600	0.19361400
H	4.21965100	-3.54858000	0.86376500
H	2.71400300	-3.19744500	1.75128400
H	2.47424900	1.07854300	0.64407500
H	0.86467800	1.22612400	-0.11398700
H	1.03996100	1.41360200	1.65081100
H	0.62364900	-3.07276900	-2.80361900
H	1.94793700	-1.89936600	-3.05647300
H	2.17929800	-3.30535700	-1.97835900
H	0.10067000	0.83054000	-4.87125700

H	0.44421700	0.81766400	-3.10615800
H	-1.17848600	1.32620500	-3.70537200
O	-2.51532400	-0.41816000	-1.97743400
C	-3.81315200	-0.31387900	-2.43534800
C	-4.78683000	-0.00232300	-1.48175500
C	-4.13594700	-0.48273300	-3.78663600
C	-6.11038400	0.14516200	-1.88245800
H	-4.49435900	0.12046700	-0.43798300
C	-5.46212700	-0.34496600	-4.18635000
H	-3.36453000	-0.70919500	-4.52389200
C	-6.43055600	-0.03205700	-3.23093800
H	-6.89196300	0.38876300	-1.16407300
H	-5.74693800	-0.47044800	-5.23002200
N	-7.82616200	0.11916900	-3.65712400
O	-8.08950000	-0.05968400	-4.83814400
O	-8.65638400	0.41764000	-2.80995100
H	-0.63399500	-0.57493600	-0.55960800

43

Energy = -1387.87670100 a.u. #Cluster: 3

P	-1.41865600	-1.45006500	-2.54231100
O	-0.80256100	-1.14134700	-3.97860000
O	-1.99176300	-2.80812400	-2.45864700

N	1.65568000	-1.42126500	-0.09043400
N	-0.21727100	-1.04908100	-1.38830400
C	2.85395500	-2.19491800	0.30552600
C	1.35874400	-0.24146700	0.74944200
C	0.89182200	-1.77040500	-1.10142400
C	4.12709000	-1.65466300	-0.33419100
C	0.37586000	-0.55810800	1.87314100
C	1.18727100	-2.96856000	-1.94784600
C	-0.19441200	0.12288600	-4.32653600
H	2.69449400	-3.25191400	0.06470300
H	2.90794800	-2.12855900	1.40100500
H	2.31913900	0.09756100	1.15849100
H	1.00148000	0.57704600	0.10734000
H	4.09122600	-1.74414500	-1.43084500
H	4.28393100	-0.59598100	-0.07679000
H	4.99056900	-2.22922500	0.03377000
H	-0.59932600	-0.88641600	1.48246500
H	0.77236200	-1.34933400	2.52718100
H	0.21780800	0.34605000	2.47976800
H	0.62668300	-3.83123200	-1.55304500
H	0.86163900	-2.79079200	-2.98021900
H	2.25354300	-3.20967500	-1.96181900

H	0.12659000	0.02987300	-5.37035800
H	0.67425100	0.31529600	-3.68038100
H	-0.92894400	0.93464600	-4.22719900
O	-2.38468000	-0.20090800	-2.15955900
C	-3.71074700	-0.10266500	-2.53208000
C	-4.59515800	0.40951500	-1.57877600
C	-4.14100800	-0.47193400	-3.81127700
C	-5.93903200	0.55607900	-1.90634400
H	-4.21961600	0.68487300	-0.59225400
C	-5.48706500	-0.33318900	-4.13712900
H	-3.43398600	-0.85434100	-4.54872400
C	-6.36695800	0.17845100	-3.18154000
H	-6.65438000	0.95104700	-1.18633200
H	-5.85597700	-0.61202100	-5.12317700
N	-7.78541400	0.32427700	-3.52795300
O	-8.13959200	-0.00446800	-4.65153300
O	-8.54263600	0.76633500	-2.67526200
H	-0.44572600	-0.24222200	-0.80989600

43

Energy = -1387.87652400 a.u. #Cluster: 4

P	-0.55053400	-0.79920300	-4.11517200
O	0.43742400	0.09006900	-4.97052200

O	-0.68743200	-2.18524400	-4.60823200
N	0.66510400	-1.46117300	-0.42677800
N	-0.08268700	-0.68386100	-2.46446600
C	1.39438400	-2.41769000	0.43589100
C	-0.07167500	-0.40208300	0.29527900
C	0.63404300	-1.57498900	-1.73645200
C	2.80314500	-1.94267400	0.76876500
C	-1.52376000	-0.78602700	0.56729400
C	1.36020100	-2.67269500	-2.44743500
C	0.78358000	1.45558200	-4.64912700
H	1.40029000	-3.40210000	-0.04514400
H	0.79102700	-2.51948900	1.34852300
H	0.46929300	-0.23508300	1.23563900
H	0.00706000	0.54376800	-0.26071900
H	2.78493300	-0.95848800	1.26159100
H	3.27545000	-2.66169800	1.45507500
H	3.42502800	-1.86609200	-0.13640400
H	-2.01254600	0.02445900	1.12803400
H	-2.08540900	-0.94562100	-0.36449700
H	-1.57818300	-1.70619500	1.16841100
H	1.64164400	-2.35356000	-3.45658200
H	2.26434900	-2.96650100	-1.90596400

H	0.69621200	-3.54714300	-2.53819500
H	1.22132400	1.50811700	-3.64150200
H	-0.10928200	2.09329300	-4.71012600
H	1.52375600	1.76670500	-5.39524900
O	-1.88020600	0.13256800	-4.06405000
C	-2.96806400	-0.11840900	-3.24674200
C	-3.52353500	0.98030800	-2.58528900
C	-3.48135500	-1.41046700	-3.08951500
C	-4.61200700	0.78665100	-1.74095600
H	-3.08981000	1.97047000	-2.73195800
C	-4.56636600	-1.60539800	-2.23925500
H	-3.03174500	-2.24779300	-3.62360400
C	-5.11490900	-0.50603900	-1.57654100
H	-5.06505100	1.62003900	-1.20580800
H	-4.98827000	-2.59803200	-2.08868500
N	-6.25503200	-0.71579600	-0.67603700
O	-6.67280200	-1.85631300	-0.53423200
O	-6.72905700	0.26062700	-0.11274300
H	-0.48134900	0.11011300	-1.96447000

43

Energy = -1387.87652100 a.u. #Cluster: 5

P	-0.56552400	-0.82821900	-4.12413100
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O	0.42030400	0.05609500	-4.98709800
O	-0.70451900	-2.21683100	-4.60903000
N	0.67036300	-1.44982200	-0.43268300
N	-0.09339600	-0.70216700	-2.47558900
C	1.39458400	-2.40175400	0.43925400
C	-0.03950200	-0.36508400	0.27835800
C	0.62255300	-1.58742900	-1.73975300
C	2.81384900	-1.94260500	0.74918900
C	-1.49415100	-0.71786100	0.57702100
C	1.32872600	-2.70647500	-2.43740200
C	0.76699800	1.42365900	-4.67487500
H	1.38107000	-3.39431900	-0.02448000
H	0.79924200	-2.47862000	1.35956500
H	0.51594700	-0.19053100	1.20886700
H	0.04983700	0.56885800	-0.29615000
H	2.81610600	-0.95006400	1.22526800
H	3.28255300	-2.65698600	1.44278100
H	3.42698400	-1.89132300	-0.16368400
H	-2.07337300	-0.88172600	-0.34313800
H	-1.55602100	-1.62725400	1.19365000
H	-1.95953000	0.10999500	1.13229600
H	1.60107900	-2.41144700	-3.45619700

H	2.23593000	-2.99893000	-1.90040800
H	0.65462000	-3.57546400	-2.50307000
H	-0.12582100	2.06106600	-4.73956100
H	1.50687200	1.72971500	-5.42337700
H	1.20534400	1.48285500	-3.66787900
O	-1.89507400	0.10409100	-4.07517400
C	-2.97664600	-0.13669900	-3.24649100
C	-3.52835100	0.97059400	-2.59638800
C	-3.48759100	-1.42688100	-3.06758400
C	-4.61052100	0.78776100	-1.74160600
H	-3.09656000	1.95897200	-2.75980600
C	-4.56612800	-1.61102900	-2.20671400
H	-3.04141100	-2.27122300	-3.59346100
C	-5.11088800	-0.50292400	-1.55550600
H	-5.06049100	1.62809400	-1.21480900
H	-4.98591700	-2.60186600	-2.03924500
N	-6.24388800	-0.70108900	-0.64341300
O	-6.65616400	-1.84051000	-0.47867900
O	-6.71775200	0.28327200	-0.09400200
H	-0.48656300	0.09901700	-1.98281500

43

Energy = -1387.87641400 a.u. #Cluster: 6

P	-0.58992800	-1.02250600	-4.10587300
O	0.41874600	-0.24384600	-5.04105600
O	-0.77579400	-2.43919900	-4.48249800
N	0.66665700	-1.39957100	-0.38963500
N	-0.10645800	-0.78740500	-2.47335000
C	1.39628500	-2.28808100	0.54349600
C	-0.03916900	-0.26714100	0.24926900
C	0.61199700	-1.62393000	-1.68424600
C	2.82221600	-1.81648600	0.79806300
C	-1.49233800	-0.59815800	0.57930600
C	1.30932300	-2.78244200	-2.32307100
C	0.81472500	1.13164200	-4.84655400
H	1.36859100	-3.31312800	0.15799200
H	0.81311900	-2.28957200	1.47459700
H	0.52152800	-0.03081600	1.16281300
H	0.04733800	0.62600200	-0.38718700
H	3.42182600	-1.83947600	-0.12486200
H	2.83609400	-0.79051200	1.19687500
H	3.29675900	-2.47882800	1.53785000
H	-2.07969100	-0.81524700	-0.32476500
H	-1.55058000	-1.46863500	1.25007900
H	-1.95149900	0.26258800	1.08783800

H	1.69712000	-2.48607600	-3.30550200
H	2.14001200	-3.14644000	-1.71339900
H	0.58547100	-3.59768300	-2.47759500
H	1.54938400	1.35188500	-5.62959400
H	1.27406800	1.25678100	-3.85510900
H	-0.05824800	1.79144800	-4.94728900
O	-1.88773600	-0.04573000	-4.11867300
C	-2.97535600	-0.20339400	-3.27704600
C	-3.48282000	0.95406700	-2.68038000
C	-3.53435000	-1.46314500	-3.03585800
C	-4.56907600	0.85354500	-1.81700500
H	-3.01442600	1.91646200	-2.89132700
C	-4.61683000	-1.56471500	-2.16647600
H	-3.12131800	-2.34778400	-3.52076700
C	-5.11755100	-0.40673500	-1.56889600
H	-4.98569700	1.73448900	-1.33069800
H	-5.07385400	-2.52961200	-1.95167400
N	-6.25521700	-0.51792200	-0.64785700
O	-6.69457800	0.50951300	-0.15120500
O	-6.70559300	-1.63246400	-0.42337000
H	-0.49597400	0.04517100	-2.03331100

Energy = -1387.87564400 a.u. #Cluster: 7

P	-0.68167000	-1.14084800	-3.95384300
O	0.31211200	-0.33023100	-4.87610700
O	-0.83747400	-2.55582400	-4.35522600
N	0.87371500	-1.23249200	-0.30831600
N	-0.19933000	-0.89338600	-2.32129900
C	1.80987500	-1.95661600	0.57964200
C	0.25395500	-0.02660400	0.27859900
C	0.63326500	-1.62591400	-1.54055700
C	1.09662400	-2.96520100	1.47259500
C	1.05304300	1.24074900	-0.01237000
C	1.28601300	-2.84599800	-2.10560700
C	0.68567700	1.04966200	-4.66806800
H	2.31294500	-1.18853300	1.18353400
H	2.58504600	-2.43407800	-0.02991600
H	-0.78557800	0.05121100	-0.07211100
H	0.19141800	-0.20526400	1.35996600
H	0.61484400	-3.75657400	0.87824500
H	1.82908200	-3.43413500	2.14691800
H	0.32684700	-2.47628800	2.08913000
H	0.55982700	2.09775700	0.47011700
H	2.07496000	1.15902000	0.38768500

H	1.11920200	1.44467400	-1.09212100
H	0.74199600	-3.19556600	-2.98788200
H	2.31709400	-2.58868000	-2.40050300
H	1.32704800	-3.65201300	-1.36468400
H	1.16158500	1.16878200	-3.68367700
H	-0.20084600	1.69468800	-4.74322700
H	1.40136600	1.29494600	-5.46104600
O	-1.99762200	-0.19391800	-3.96688000
C	-3.16909100	-0.41261400	-3.26695000
C	-3.61765900	-1.69965000	-2.94892400
C	-3.89256900	0.72808800	-2.90514400
C	-4.81172900	-1.84271200	-2.24755200
H	-3.04427800	-2.57490100	-3.25417600
C	-5.08929100	0.58403100	-2.21163900
H	-3.50686900	1.71360000	-3.17006600
C	-5.53116600	-0.70163800	-1.88897000
H	-5.18873200	-2.82975800	-1.98328900
H	-5.67614800	1.45234900	-1.91541900
N	-6.78999000	-0.85741100	-1.15180900
O	-7.14304700	-1.98865000	-0.84911800
O	-7.42346600	0.15217700	-0.87666500
H	-0.56380300	-0.02932500	-1.92122400

Energy = -1387.87562100 a.u. #Cluster: 8

P	-0.64587700	-1.15111300	-3.96630700
O	0.35260500	-0.34730800	-4.88906100
O	-0.79837100	-2.56948200	-4.35656400
N	0.84182500	-1.23169200	-0.29169000
N	-0.17464600	-0.89001200	-2.33261400
C	1.74791100	-1.96043500	0.62319600
C	0.21817800	-0.01747300	0.27346000
C	0.62854500	-1.62899200	-1.52774600
C	1.00318800	-2.95694000	1.50390300
C	1.03033300	1.24322900	-0.01096500
C	1.28119500	-2.86015400	-2.06791500
C	0.72215200	1.03533300	-4.69353400
H	2.24378700	-1.19396300	1.23501500
H	2.53279900	-2.44972000	0.03580800
H	-0.81404100	0.06298300	-0.09845600
H	0.13348700	-0.18702900	1.35470000
H	0.22327300	-2.45778200	2.09914600
H	0.52870400	-3.74729200	0.90240400
H	1.71477800	-3.42892400	2.19816500
H	0.53391000	2.10632500	0.45712800

H	2.04430200	1.15759400	0.40810900
H	1.11777900	1.44025100	-1.09053800
H	0.76950900	-3.19889700	-2.97329500
H	2.32916200	-2.62265500	-2.31575600
H	1.27381900	-3.66755900	-1.32707200
H	1.44345700	1.27304100	-5.48373500
H	1.19046100	1.16644600	-3.70695800
H	-0.16493200	1.67782300	-4.78242800
O	-1.96265900	-0.20542900	-3.99559800
C	-3.13360200	-0.41608900	-3.29229200
C	-3.57866500	-1.69939500	-2.95473200
C	-3.85956700	0.72800900	-2.94665500
C	-4.77134300	-1.83514800	-2.24959900
H	-3.00333900	-2.57768500	-3.24743600
C	-5.05489200	0.59119600	-2.24920200
H	-3.47684900	1.71048800	-3.22672100
C	-5.49305400	-0.69062400	-1.90678500
H	-5.14556700	-2.81907900	-1.97017100
H	-5.64350100	1.46227000	-1.96481900
N	-6.74999300	-0.83841300	-1.16487400
O	-7.10181200	-1.96638100	-0.84856000
O	-7.38311600	0.17389000	-0.89928300

H	-0.53215300	-0.01630100	-1.94762200
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43

Energy = -1387.87561100 a.u. #Cluster: 9

P	-0.65480200	-0.62074800	-4.01416100
O	0.30275000	0.40611500	-4.73912600
O	-0.73674500	-1.93235400	-4.69257100
N	0.83087700	-1.40841500	-0.42587700
N	-0.19550100	-0.68724200	-2.35805800
C	1.81851400	-2.22172200	0.31725600
C	0.06377100	-0.44297100	0.38980400
C	0.66821500	-1.52003300	-1.72667400
C	1.19906900	-3.47266000	0.92926400
C	0.70667100	0.94122700	0.42145000
C	1.44206800	-2.51718600	-2.52647000
C	0.60570700	1.72927200	-4.24496600
H	2.22544300	-1.56532500	1.09921700
H	2.65179200	-2.46912700	-0.34987200
H	-0.97361200	-0.41057400	0.02393000
H	0.01254600	-0.86590900	1.40126500
H	0.81565100	-4.15107600	0.15185900
H	1.96474100	-4.00848700	1.51043300
H	0.37020700	-3.21726300	1.60700200

H	0.75019100	1.40057600	-0.57835800
H	0.11457300	1.59909400	1.07491600
H	1.73064700	0.88642200	0.82065100
H	1.57621700	-3.45438200	-1.97604500
H	0.93038700	-2.72478800	-3.47167500
H	2.43590000	-2.09286300	-2.74766600
H	-0.31168600	2.33237500	-4.19710100
H	1.31149900	2.16812600	-4.95940700
H	1.07064700	1.66431300	-3.25021300
O	-2.01650700	0.24457000	-3.85512100
C	-3.14774100	-0.17480400	-3.17722700
C	-3.78455800	0.77536600	-2.37364700
C	-3.63595900	-1.47960300	-3.30479500
C	-4.93515600	0.41681700	-1.67873200
H	-3.36899300	1.78136700	-2.30018200
C	-4.78429200	-1.83984200	-2.60481800
H	-3.12211400	-2.19741600	-3.94418700
C	-5.41709200	-0.88858700	-1.80263900
H	-5.45464700	1.13167600	-1.04209800
H	-5.19203000	-2.84702500	-2.67929800
N	-6.62730400	-1.27215800	-1.06591700
O	-7.17487700	-0.42195100	-0.37821800

O	-7.02722500	-2.42261000	-1.17677100
H	-0.62006300	0.04671600	-1.79310700

43

Energy = -1387.87557800 a.u. #Cluster: 10

P	-0.63317700	-0.58432200	-3.99194400
O	0.35045300	0.45645500	-4.66029700
O	-0.70538300	-1.87461500	-4.71134800
N	0.82610800	-1.43334500	-0.40786900
N	-0.21723500	-0.70238600	-2.32740800
C	1.82835100	-2.24106700	0.32165500
C	0.04527800	-0.49183000	0.42252800
C	0.66447500	-1.52671800	-1.71002900
C	1.23126400	-3.51154200	0.91496600
C	0.66751900	0.90130400	0.47326100
C	1.45717500	-2.49372900	-2.52853900
C	0.66002500	1.75667500	-4.11178400
H	2.22494500	-1.58973100	1.11310000
H	2.66494300	-2.46335900	-0.35014200
H	-0.99286400	-0.46971500	0.05827100
H	0.00111700	-0.93026100	1.42770800
H	0.39807800	-3.28058100	1.59613900
H	0.85984300	-4.18496700	0.12744500

H	2.00617200	-4.04228900	1.48849900
H	0.06638300	1.54092700	1.13650000
H	1.69262700	0.85607100	0.87072300
H	0.70276600	1.37503900	-0.52007700
H	2.43988300	-2.04383200	-2.74886500
H	1.61526500	-3.43615100	-1.99369100
H	0.94478200	-2.69811000	-3.47419800
H	-0.25431700	2.36171900	-4.03675000
H	1.36638500	2.22177700	-4.80883800
H	1.12651700	1.64739600	-3.12174100
O	-1.99310700	0.28481500	-3.84167900
C	-3.14294800	-0.14355300	-3.20161500
C	-3.79392300	0.79204700	-2.39237900
C	-3.63450600	-1.44257100	-3.36969600
C	-4.96226900	0.42432600	-1.73277200
H	-3.37527600	1.79388100	-2.28670100
C	-4.80078600	-1.81202000	-2.70513100
H	-3.10911800	-2.14892700	-4.01247500
C	-5.44748800	-0.87537600	-1.89687500
H	-5.49306800	1.12764300	-1.09257600
H	-5.21146500	-2.81512400	-2.81148000
N	-6.67641400	-1.26866900	-1.19704700

O	-7.23344100	-0.43204600	-0.50029600
O	-7.08139500	-2.41298000	-1.34585300
H	-0.66499000	0.00665100	-1.74865200

ANEOP

45

Energy = -1426.68835100 a.u. #Cluster: 1

P	-1.01584200	2.10245400	-2.58760500
O	-2.08835100	2.68572700	-1.52691800
O	-0.25302300	3.16880100	-3.30522200
N	1.13661600	-0.88732200	-1.50981000
N	-0.26708400	0.89093500	-1.79425600
C	2.12585400	-1.87315000	-1.95920500
C	0.61705000	-1.06317900	-0.14796400
C	0.66570400	0.10053800	-2.28739800
C	3.55689800	-1.49429500	-1.58514600
C	-0.64211800	-1.92607000	-0.11389000
C	1.20205400	0.22654900	-3.69507900
C	-1.79823200	3.87273500	-0.75655600
C	-0.86122000	3.58568200	0.40167100
H	1.85444000	-2.83341100	-1.49486500
H	2.03073000	-2.02061300	-3.04201600

H	0.41094000	-0.07005000	0.27032800
H	1.41831000	-1.52200300	0.44991700
H	4.25138600	-2.28831700	-1.90153200
H	3.85981100	-0.55480500	-2.07342200
H	3.66013800	-1.36378500	-0.49640000
H	-0.98420600	-2.05478300	0.92523000
H	-1.45103400	-1.45331900	-0.68914000
H	-0.45132300	-2.92551700	-0.53673200
H	0.69756500	-0.50853900	-4.34392900
H	0.99611400	1.23230000	-4.07804200
H	2.28238700	0.04474600	-3.75189500
H	-1.37761900	4.63635100	-1.42968400
H	-2.77597700	4.22650500	-0.39944200
H	-1.26269100	2.78292500	1.03987500
H	0.13375600	3.27967200	0.04228700
H	-0.74069200	4.49296500	1.01491400
O	-2.04389200	1.37496200	-3.67144600
C	-2.66189800	0.17591600	-3.46658300
C	-2.56634500	-0.78412800	-4.48419200
C	-3.38536200	-0.09251500	-2.29401300
C	-3.18781800	-2.01857300	-4.33260600
H	-1.99406500	-0.54801400	-5.38264200

C	-4.00427000	-1.32707000	-2.13706000
H	-3.44960700	0.66684400	-1.51514000
C	-3.89707300	-2.27779900	-3.15629400
H	-3.12213800	-2.78163600	-5.10701900
H	-4.56679100	-1.56137900	-1.23435500
N	-4.54338200	-3.57870300	-2.98627700
O	-4.44808900	-4.39500200	-3.89424500
O	-5.14918300	-3.79145000	-1.94343400

45

Energy = -1426.68822600 a.u. #Cluster: 2

P	-0.83422800	0.95852100	-2.86458600
O	-1.46948900	2.28490900	-2.20974500
O	-0.79437900	1.09969400	-4.35101700
N	2.27482900	-0.57203700	-1.23086400
N	0.46632900	0.61256900	-1.96181600
C	3.20269900	-1.70913900	-1.24639700
C	2.45715000	0.40362100	-0.14827400
C	1.27526900	-0.41620500	-2.11197900
C	4.49293300	-1.41482400	-2.00776600
C	1.59589700	0.09089300	1.07286700
C	1.10723700	-1.44231900	-3.20858000
C	-1.41702000	2.61004200	-0.80290400

C	-2.30016200	1.71091900	0.04179200
H	3.42871600	-1.95060500	-0.19675700
H	2.69592500	-2.59026600	-1.65932500
H	2.21624200	1.39964400	-0.54134200
H	3.52387000	0.39664700	0.11929700
H	5.01261800	-0.54193200	-1.58222800
H	5.17145200	-2.28014600	-1.94693400
H	4.28988600	-1.20869100	-3.07039300
H	1.78968600	0.82699300	1.86904000
H	0.52735600	0.13375700	0.81459700
H	1.82089400	-0.91131800	1.47136200
H	2.06615500	-1.80507800	-3.59750000
H	0.54570200	-2.30638600	-2.81677400
H	0.53732000	-1.00302400	-4.03575000
H	-0.36919000	2.56136700	-0.47029000
H	-1.75289800	3.65554600	-0.74874000
H	-2.30548600	2.07769500	1.08054800
H	-3.33569200	1.71164300	-0.33334700
H	-1.93048400	0.67511000	0.04497300
O	-1.89096700	-0.26760700	-2.42213000
C	-3.13276200	-0.45459700	-2.93522200
C	-3.88974900	0.58121500	-3.51135700

C	-3.65862100	-1.75479200	-2.84781700
C	-5.16124000	0.30916500	-4.00308200
H	-3.48847100	1.59208400	-3.56519300
C	-4.93107100	-2.02621700	-3.33235000
H	-3.04928600	-2.53913000	-2.39585700
C	-5.67098700	-0.98901400	-3.91048500
H	-5.76509400	1.09588800	-4.45362700
H	-5.35459300	-3.02806000	-3.27374800
N	-7.00813300	-1.26784500	-4.42597000
O	-7.63632000	-0.34787700	-4.93641500
O	-7.44141300	-2.40963100	-4.32514500

45

Energy = -1426.68796800 a.u. #Cluster: 3

P	-0.80236700	0.57472400	-3.22776500
O	-1.55413700	1.95320700	-2.88175400
O	-0.70111900	0.41233800	-4.71089400
N	2.34644500	-0.36394400	-1.25726800
N	0.48860600	0.51026600	-2.25159700
C	3.33777200	-1.41557000	-1.00462900
C	2.44271900	0.83750100	-0.41820100
C	1.36177300	-0.47156200	-2.16212300
C	4.63982700	-1.20461400	-1.77320100

C	1.56105600	0.75676600	0.82512500
C	1.28471500	-1.72322600	-3.00582100
C	-1.54641000	2.58730000	-1.58332900
C	-2.36107200	1.83154900	-0.55025800
H	3.53254900	-1.41708200	0.07874900
H	2.90003200	-2.39406600	-1.23696500
H	2.16430600	1.70531400	-1.02984600
H	3.49942600	0.95204800	-0.13579100
H	5.09060200	-0.23014200	-1.52782700
H	5.36358400	-1.99192000	-1.51024200
H	4.46995100	-1.23997200	-2.86080600
H	1.69125800	1.66248500	1.43831700
H	0.50044000	0.67889300	0.54414900
H	1.82547900	-0.11599100	1.44346500
H	0.69248300	-1.52311500	-3.90651100
H	2.27403100	-2.08532200	-3.31125800
H	0.78882900	-2.52250200	-2.43094200
H	-0.50261600	2.70396100	-1.25512400
H	-1.96949700	3.58630200	-1.76218900
H	-3.39133900	1.66762000	-0.90288200
H	-1.91128700	0.85425700	-0.32099100
H	-2.40185200	2.41870800	0.38099700

O	-1.80570900	-0.58773700	-2.55280800
C	-3.11295400	-0.78103100	-2.86566900
C	-3.89227100	-1.44653900	-1.90401000
C	-3.68649300	-0.35515500	-4.07676200
C	-5.23895600	-1.68444700	-2.14257800
H	-3.42140100	-1.76484700	-0.97263800
C	-5.03678900	-0.58767000	-4.31374500
H	-3.06680700	0.13798700	-4.82494000
C	-5.80065700	-1.24770900	-3.34731700
H	-5.85943300	-2.19594400	-1.40787200
H	-5.50292100	-0.26665900	-5.24454900
N	-7.21807300	-1.49016300	-3.60190300
O	-7.86722300	-2.08038400	-2.74637400
O	-7.69407100	-1.09273500	-4.65865600

45

Energy = -1426.68795100 a.u. #Cluster: 4

P	-0.56674700	1.76117100	-2.62528500
O	-1.00366200	2.22963300	-1.13229200
O	0.06592800	2.85193000	-3.42608000
N	1.65890300	-1.22336900	-1.72416600
N	0.10891400	0.29911300	-2.42424700
C	2.88203200	-1.63643200	-1.02578200

C	0.82748300	-2.30216200	-2.27311300
C	1.26255800	0.05387700	-1.83903100
C	4.07995600	-1.79041900	-1.95923500
C	-0.23341200	-2.78608700	-1.28824900
C	2.13794400	1.14669300	-1.26985900
C	-1.43355900	3.58573000	-0.87517300
C	-2.85808900	3.83184700	-1.33738200
H	3.10066300	-0.92443200	-0.22017700
H	2.65947500	-2.59496200	-0.53313200
H	1.50376200	-3.12505200	-2.54831100
H	0.35462600	-1.93372200	-3.19222400
H	3.86610600	-2.51444000	-2.76128600
H	4.34584600	-0.82954400	-2.42717800
H	4.95324200	-2.15318000	-1.39470100
H	-0.93000500	-1.97299800	-1.03821300
H	-0.81303300	-3.60990400	-1.73410900
H	0.22547600	-3.15569800	-0.35727600
H	3.20714700	0.91243900	-1.32095300
H	1.95803700	2.07718400	-1.82263400
H	1.86906600	1.31461000	-0.21406300
H	-1.34061000	3.71139200	0.21306600
H	-0.73136700	4.27720400	-1.36673000

H	-2.93952100	3.76236400	-2.43279400
H	-3.54856100	3.10053000	-0.88870600
H	-3.17590800	4.84188300	-1.03311900
O	-1.99465500	1.38169200	-3.38076000
C	-2.80571900	0.33050200	-3.07961700
C	-3.02835700	-0.10462000	-1.76249200
C	-3.45040300	-0.29855500	-4.15580100
C	-3.88311400	-1.17561000	-1.52887400
H	-2.53277400	0.39691000	-0.93286300
C	-4.30966700	-1.36583800	-3.92486600
H	-3.25927400	0.06092900	-5.16815800
C	-4.51306300	-1.79755600	-2.61049400
H	-4.06574200	-1.53368700	-0.51664900
H	-4.81519400	-1.87056400	-4.74718900
N	-5.40589600	-2.92720900	-2.36142400
O	-5.55577700	-3.30285900	-1.20506800
O	-5.96262600	-3.44755100	-3.32054200

45

Energy = -1426.68691700 a.u. #Cluster: 5

P	-1.13706500	1.95434200	-2.85530300
O	-2.01542100	2.64338500	-1.67758200
O	-0.45624500	2.95256400	-3.73643300

N	1.17412600	-0.88163700	-1.63809500
N	-0.37952000	0.69972800	-2.16392200
C	2.52452100	-1.45216400	-1.63053200
C	0.14093900	-1.64228600	-0.92352800
C	0.85864500	0.27338500	-2.25149300
C	3.33351300	-1.05015700	-0.39884700
C	-0.60764800	-2.61004200	-1.83646100
C	1.94896000	1.00876900	-2.99465300
C	-1.50836100	3.79272400	-0.96715600
C	-0.43528800	3.41931900	0.03950400
H	2.41195800	-2.54638500	-1.66979800
H	3.05085200	-1.16536500	-2.54908200
H	-0.55789700	-0.92804600	-0.47029800
H	0.64002000	-2.18801000	-0.10911400
H	3.49031300	0.03934100	-0.36412700
H	2.82148400	-1.35295800	0.52816800
H	4.31983500	-1.53984600	-0.41970800
H	0.07983300	-3.34287100	-2.28869400
H	-1.36821800	-3.16205600	-1.26222000
H	-1.11987300	-2.06658800	-2.64304800
H	2.80718600	1.20896500	-2.33713700
H	2.30959600	0.39960400	-3.83829800

H	1.55641900	1.95333700	-3.38335700
H	-1.12923200	4.52295200	-1.70000600
H	-2.38524200	4.22950700	-0.46790800
H	-0.80116600	2.64482900	0.73175100
H	0.46948600	3.03925800	-0.46042200
H	-0.15224500	4.30729500	0.62697400
O	-2.35890900	1.24207600	-3.71644700
C	-2.99371000	0.08443600	-3.37756400
C	-3.20348600	-0.85430200	-4.39773100
C	-3.44367600	-0.16568700	-2.07116900
C	-3.84582600	-2.05450100	-4.11474800
H	-2.84304200	-0.63230200	-5.40339700
C	-4.07530300	-1.36851500	-1.78223000
H	-3.28295500	0.57972900	-1.29303100
C	-4.26546900	-2.30263500	-2.80506300
H	-4.00909900	-2.80292000	-4.88907300
H	-4.41946300	-1.59252900	-0.77348100
N	-4.90875100	-3.57721900	-2.49344300
O	-5.13454300	-4.35241900	-3.41455200
O	-5.18960600	-3.81292400	-1.32447700

45

Energy = -1426.68671200 a.u. #Cluster: 6

P	-0.58505700	1.98653700	-1.93546100
O	-1.35253700	2.32217700	-0.54862000
O	0.11302700	3.16869400	-2.52797100
N	1.53665500	-1.20588000	-1.62166800
N	0.09684600	0.56106200	-1.59653200
C	2.81967200	-1.85756200	-1.90355600
C	0.50197500	-2.04540600	-1.00460500
C	1.27841800	0.08135200	-1.91115100
C	3.77460900	-1.83114300	-0.71196900
C	-0.40017200	-2.71019100	-2.04120400
C	2.36178600	0.89312600	-2.58201300
C	-1.90299000	3.63774100	-0.31591600
C	-3.21276600	3.85490900	-1.05185400
H	2.59683100	-2.89710500	-2.18846000
H	3.28369900	-1.39214400	-2.78168000
H	-0.09089800	-1.41725000	-0.32806800
H	1.01611400	-2.80371600	-0.39574700
H	3.32345600	-2.31440800	0.16899200
H	4.70165400	-2.37144200	-0.96043200
H	4.03985800	-0.79782200	-0.43850300
H	0.18086400	-3.35591400	-2.71916200
H	-1.15807600	-3.33351300	-1.54107700

H	-0.92429400	-1.95379500	-2.64246300
H	3.30487200	0.83808200	-2.01997000
H	2.55237700	0.50226500	-3.59411700
H	2.04513400	1.93767100	-2.66158900
H	-2.04604900	3.69538600	0.77267000
H	-1.15473200	4.39089500	-0.60857100
H	-3.63596500	4.83153500	-0.76753000
H	-3.06386300	3.84928000	-2.14217000
H	-3.94362300	3.07223100	-0.79468900
O	-1.81556200	1.59443300	-2.99393500
C	-2.56126500	0.45641000	-2.94493300
C	-3.09360600	-0.04336800	-1.74462200
C	-2.80212600	-0.20260400	-4.15980100
C	-3.84387100	-1.21245500	-1.76103700
H	-2.90402600	0.48111000	-0.80931200
C	-3.55844500	-1.36857800	-4.18074400
H	-2.37579800	0.20839500	-5.07628300
C	-4.06520200	-1.86614900	-2.97689600
H	-4.25715400	-1.62555000	-0.84183800
H	-3.74776600	-1.90141600	-5.11161900
N	-4.83739800	-3.10666200	-2.98772800
O	-5.23772700	-3.54855900	-1.91756800

O	-5.04645000	-3.64947700	-4.06582900
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45

Energy = -1426.68666000 a.u. #Cluster: 7

P	-1.08206300	2.13648500	-2.57428100
O	-2.07317700	2.68753400	-1.42048300
O	-0.37061900	3.22616600	-3.31056400
N	1.10758400	-0.90106900	-1.71702100
N	-0.29835600	0.88785900	-1.87970300
C	2.15285900	-1.80693400	-2.20440100
C	0.48911800	-1.25294600	-0.43283600
C	0.67920900	0.17384600	-2.39899300
C	3.53849800	-1.46519100	-1.66207500
C	-0.77540100	-2.09074700	-0.60461600
C	1.32675100	0.48237700	-3.72931800
C	-1.69601900	3.81428000	-0.60021000
C	-0.70418400	3.42706600	0.48119100
H	1.86488700	-2.82372900	-1.89635000
H	2.15303100	-1.80948800	-3.30124100
H	0.26135900	-0.32353900	0.10473500
H	1.24251000	-1.80272100	0.15001500
H	3.54823100	-1.48160800	-0.56078800
H	4.27543800	-2.20064100	-2.02119500

H	3.85907800	-0.46473500	-1.99282800
H	-1.18192200	-2.36855200	0.38070900
H	-1.54351200	-1.52341800	-1.14747600
H	-0.56634300	-3.01774700	-1.16204500
H	2.41989500	0.38999500	-3.68676600
H	0.95569600	-0.22343300	-4.49060300
H	1.06775200	1.50122000	-4.03716500
H	-1.28783800	4.60458100	-1.25025400
H	-2.63739700	4.17822200	-0.16407600
H	-1.09697200	2.59951200	1.09257000
H	0.25665900	3.11129000	0.04569200
H	-0.51597100	4.29033200	1.13928800
O	-2.19057000	1.44053300	-3.59319500
C	-2.76304700	0.22532600	-3.33404500
C	-3.70833100	0.08648900	-2.30780200
C	-2.39379300	-0.86987700	-4.12525300
C	-4.28143400	-1.15716500	-2.06686600
H	-3.97072300	0.95408700	-1.70226000
C	-2.96533800	-2.11577100	-3.88933600
H	-1.64996800	-0.73133500	-4.91141200
C	-3.90077700	-2.24403800	-2.85932600
H	-5.01296300	-1.29556700	-1.27187500

H	-2.68790600	-2.98570300	-4.48288400
N	-4.48993400	-3.55773900	-2.59405700
O	-4.14798600	-4.49742200	-3.30042400
O	-5.29558100	-3.65490600	-1.67740600

45

Energy = -1426.68664900 a.u. #Cluster: 8

P	-1.31699900	1.93992700	-2.69283300
O	-1.38319900	3.18821300	-1.68288300
O	-1.04005000	2.40977100	-4.08519000
N	1.19104600	-0.73003400	-1.51317100
N	-0.49792900	0.72018900	-1.99900100
C	2.57972800	-1.20017300	-1.55702100
C	0.27153400	-1.49218300	-0.65912600
C	0.75149400	0.35065600	-2.17881500
C	2.80783700	-2.29437600	-2.59733900
C	0.17719000	-0.92827400	0.75603500
C	1.72274800	1.09384800	-3.06475100
C	-1.46758200	3.02111600	-0.24830700
C	-0.10542000	3.19525800	0.39253700
H	3.24859300	-0.34875600	-1.73348900
H	2.82218100	-1.57672200	-0.55146600
H	0.63452300	-2.53024900	-0.63667800

H	-0.71652600	-1.49290900	-1.13711900
H	2.60714600	-1.92405000	-3.61483000
H	3.85225500	-2.64127000	-2.55563900
H	2.15280600	-3.16022800	-2.41245200
H	-0.22647200	0.09445500	0.73950500
H	-0.49073900	-1.55502800	1.36791200
H	1.16558500	-0.90693000	1.24237100
H	1.16875100	1.75870300	-3.73630100
H	2.39446300	1.70394600	-2.43844800
H	2.34267800	0.41283000	-3.66206800
H	-2.17337500	3.78972800	0.10049300
H	-1.89619300	2.03454200	-0.01411600
H	0.59037800	2.41266100	0.05405000
H	0.32044400	4.17882300	0.13966300
H	-0.19654600	3.12633800	1.48830800
O	-2.88938100	1.40721500	-2.52205700
C	-3.30790700	0.18495800	-2.94185300
C	-4.32901100	-0.43169100	-2.20205700
C	-2.76747100	-0.44580300	-4.07596500
C	-4.80732700	-1.67842200	-2.58526400
H	-4.72989200	0.08034400	-1.32581000
C	-3.23960400	-1.69623700	-4.45762500

H	-1.99396100	0.05600600	-4.65802200
C	-4.25282700	-2.30119400	-3.70829700
H	-5.59607400	-2.17623700	-2.02270700
H	-2.83537900	-2.20469400	-5.33201800
N	-4.74657700	-3.61664500	-4.10938300
O	-5.64104900	-4.12626900	-3.44521300
O	-4.24346000	-4.14997100	-5.09078900

45

Energy = -1426.68662800 a.u. #Cluster: 9

P	-1.21673300	2.11662600	-2.75628600
O	-1.26318100	3.38574000	-1.77546600
O	-0.96882600	2.55439100	-4.16398100
N	1.07075400	-0.77525800	-1.63804800
N	-0.37427100	0.94392200	-2.01851100
C	2.18848600	-1.66045800	-1.98022300
C	0.40690800	-1.02955400	-0.35334800
C	0.63117200	0.20991600	-2.43938200
C	3.52162600	-1.17931300	-1.41090900
C	-0.80851600	-1.94184600	-0.50119500
C	1.31236300	0.40144000	-3.77362700
C	-1.39514800	3.25975700	-0.34059600
C	-0.04812600	3.41183100	0.33673900

H	1.94322500	-2.65723400	-1.58300700
H	2.24979500	-1.77122700	-3.06960900
H	0.11075000	-0.06526300	0.07868800
H	1.15281300	-1.48246500	0.31585000
H	3.47297100	-1.08488700	-0.31457500
H	4.31842800	-1.89866600	-1.65714300
H	3.79990200	-0.19897300	-1.82828900
H	-1.56914200	-1.47362800	-1.14202600
H	-0.52680500	-2.91052300	-0.94429000
H	-1.25937500	-2.13496700	0.48514300
H	1.12356800	-0.47224100	-4.41751800
H	0.91265900	1.29203600	-4.26740400
H	2.40033800	0.50082100	-3.65347800
H	-2.08865700	4.05736800	-0.03436000
H	-1.85957700	2.29253600	-0.09491900
H	0.41378600	4.37605000	0.07228100
H	-0.17360300	3.37515500	1.43081800
H	0.63136800	2.60026100	0.03563100
O	-2.79411400	1.58971100	-2.54978800
C	-3.17288900	0.31329300	-2.81773600
C	-4.13182600	-0.26784700	-1.97390800
C	-2.63687600	-0.41254200	-3.89533200

C	-4.54430500	-1.57650000	-2.19106500
H	-4.53036900	0.31863800	-1.14465500
C	-3.03820500	-1.72604700	-4.10799400
H	-1.91670300	0.06035500	-4.56388200
C	-3.98488000	-2.29592600	-3.25207200
H	-5.28094700	-2.05020800	-1.54355000
H	-2.63044200	-2.31042100	-4.93174600
N	-4.40232600	-3.67892500	-3.47279300
O	-3.88654100	-4.29929000	-4.39455900
O	-5.24810000	-4.15445800	-2.72511400

45

Energy = -1426.68614000 a.u. #Cluster: 10

P	-0.89365000	0.19352600	-3.11029500
O	-1.44035400	1.65432400	-2.68846900
O	-0.79412300	0.11403500	-4.60165800
N	2.38091900	-0.66228300	-1.28443600
N	0.29748100	-0.22307600	-2.09818700
C	3.84457600	-0.71795200	-1.36568700
C	1.78799900	-1.02475900	0.00874400
C	1.59467600	-0.28685400	-2.30686200
C	4.37235200	-2.11046800	-1.70344200
C	1.58797000	0.18027100	0.92361200

C	2.24933800	0.05711100	-3.62411100
C	-1.31593900	2.22052600	-1.36646200
C	-2.19639000	1.53291900	-0.33981800
H	4.19892300	0.01990700	-2.09572300
H	4.23303500	-0.39280900	-0.38831400
H	2.45982200	-1.75753100	0.47953400
H	0.82950000	-1.52323100	-0.18376200
H	5.47364500	-2.10439600	-1.70448200
H	4.03620400	-2.85308200	-0.96277700
H	4.02802800	-2.43744300	-2.69714700
H	2.54217400	0.69622500	1.11620000
H	0.88769500	0.89875100	0.47336600
H	1.17420300	-0.14510600	1.89113100
H	2.75270600	1.03431800	-3.54187100
H	3.00401900	-0.68730500	-3.91055000
H	1.48673100	0.11972600	-4.40713800
H	-0.25694700	2.18913200	-1.06558900
H	-1.60474900	3.27452100	-1.48799800
H	-3.24802500	1.52473900	-0.66630300
H	-1.87491100	0.49528200	-0.16765000
H	-2.13308000	2.07591400	0.61660800
O	-2.08238500	-0.82172100	-2.52420900

C	-3.39918500	-0.74581600	-2.84961300
C	-3.86813000	-0.17018900	-4.04380300
C	-4.30189500	-1.28907200	-1.91962200
C	-5.23514200	-0.13217400	-4.29520300
H	-3.15807400	0.22879400	-4.76715200
C	-5.66660400	-1.25644700	-2.17235300
H	-3.91051500	-1.72787500	-1.00050400
C	-6.12149100	-0.67309600	-3.35987500
H	-5.62122300	0.30906400	-5.21335300
H	-6.38129700	-1.66867900	-1.46129000
N	-7.55617200	-0.63025400	-3.62923200
O	-7.93506500	-0.11375300	-4.67370000
O	-8.31622200	-1.11253200	-2.79778500

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46

Energy = -1427.12566200 a.u. #Cluster: 1

P	-0.98781700	2.13396000	-3.16124100
O	-1.90165300	2.91496200	-2.12498200
O	-0.12850600	2.90717200	-4.08317100
N	0.82808300	-0.96675700	-1.58138400
N	-0.18691500	1.04269900	-2.09527400

C	1.77521700	-2.06952300	-1.85234500
C	0.03179100	-1.10822800	-0.34474800
C	0.68083100	0.04647500	-2.40572000
C	1.09756800	-3.24929400	-2.54282500
C	0.67090100	-0.40398400	0.84885400
C	1.46655700	0.13598200	-3.67446700
C	-1.54838300	4.23748300	-1.60399100
C	-0.43513100	4.15650300	-0.58233400
H	2.61142500	-1.68603600	-2.44689600
H	2.18676600	-2.36933800	-0.87829100
H	-0.05571500	-2.18555600	-0.15492800
H	-0.99116100	-0.75308200	-0.53764300
H	0.71590100	-2.96817600	-3.53563400
H	1.82981100	-4.06089400	-2.66944800
H	0.25651100	-3.63601300	-1.94715500
H	1.68515100	-0.78952400	1.03220900
H	0.73532900	0.68444800	0.69627100
H	0.06166500	-0.58971600	1.74592200
H	1.31199600	-0.76021600	-4.29061400
H	1.19266900	1.02997300	-4.24284700
H	2.53731500	0.20103000	-3.42620100
H	-1.27877100	4.87678500	-2.45721100

H	-2.48394800	4.60667800	-1.16515400
H	0.50746400	3.81895900	-1.04135800
H	-0.26491100	5.15700400	-0.15471400
H	-0.69916300	3.46859000	0.23599100
O	-2.03770000	1.17962900	-3.94915200
C	-2.55394000	0.01701000	-3.39861100
C	-2.05413600	-1.20272100	-3.86079800
C	-3.52368500	0.08350900	-2.39449800
C	-2.50482700	-2.38547000	-3.28332300
H	-1.30184400	-1.21207500	-4.65065600
C	-3.98126500	-1.09915700	-1.81896200
H	-3.89343600	1.05283700	-2.05856800
C	-3.45470900	-2.31388000	-2.26313200
H	-2.11820200	-3.35158200	-3.60363400
H	-4.72652000	-1.08656400	-1.02487900
N	-3.90531400	-3.55931100	-1.62835900
O	-4.79307000	-3.48868400	-0.79107600
O	-3.36459000	-4.60278000	-1.96653100
H	-0.63100000	1.00819400	-1.17861300

46

Energy = -1427.12565800 a.u. #Cluster: 2

P	-0.94058800	2.14290000	-3.16618100
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O	-1.84785700	2.94229500	-2.13835600
O	-0.05982500	2.89866700	-4.08228700
N	0.81161700	-0.98975000	-1.57716500
N	-0.16645900	1.03685800	-2.09531500
C	1.74079300	-2.10886800	-1.84366900
C	0.00253400	-1.12140400	-0.34768500
C	0.68839500	0.02777900	-2.40027900
C	1.04778500	-3.27281200	-2.54580800
C	0.64534100	-0.43601100	0.85484800
C	1.48640200	0.10738700	-3.66195500
C	-1.46329100	4.24758600	-1.59613500
C	-0.38060700	4.11965300	-0.54676400
H	2.59012000	-1.73869900	-2.42812900
H	2.13671200	-2.42045000	-0.86687500
H	-0.10806600	-2.19773600	-0.16443600
H	-1.01148400	-0.74518500	-0.54666900
H	0.68149700	-2.98031600	-3.54115800
H	1.76567900	-4.09771200	-2.66860300
H	0.19361200	-3.64572900	-1.96006700
H	0.73016200	0.65196400	0.70939600
H	0.02623900	-0.61633100	1.74626700
H	1.65103100	-0.84093700	1.04361200

H	1.31851600	-0.78268800	-4.28358600
H	1.23480400	1.00926800	-4.22808400
H	2.55617600	0.14914800	-3.40495300
H	-1.14980000	4.88434300	-2.43614900
H	-2.39682100	4.64488300	-1.17800200
H	0.56253200	3.75641600	-0.98453400
H	-0.18982200	5.10950200	-0.10334900
H	-0.68855000	3.43204300	0.25633500
O	-2.00399600	1.20854600	-3.95975000
C	-2.54336600	0.05452700	-3.41329000
C	-2.06344800	-1.17314600	-3.87557800
C	-3.51513800	0.13638600	-2.41223700
C	-2.53572100	-2.34863800	-3.30063400
H	-1.30862100	-1.19440400	-4.66281700
C	-3.99467900	-1.03898500	-1.83953200
H	-3.86921500	1.11144800	-2.07603500
C	-3.48713700	-2.26200600	-2.28306300
H	-2.16454500	-3.32082600	-3.62086000
H	-4.74192300	-1.01456400	-1.04758800
N	-3.95932800	-3.50020200	-1.64984900
O	-4.85364700	-3.41639800	-0.82080900
O	-3.42879300	-4.55119000	-1.98085700

H	-0.62058200	1.00470800	-1.18348800
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46

Energy = -1427.12556600 a.u. #Cluster: 3

P	-0.83108300	1.96634900	-3.19205600
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O	-1.67560500	2.80806600	-2.14474700
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O	0.08252900	2.67692300	-4.11202800
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N	1.06114500	-1.07856900	-1.52299300
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N	-0.10882200	0.81169000	-2.13939400
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C	1.99626400	-2.19256200	-1.78989500
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C	0.44715700	-1.07605100	-0.17887100
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C	0.77528500	-0.17224400	-2.43198600
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C	3.41209100	-1.88659500	-1.31540100
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C	-0.91475200	-1.76542500	-0.15823400
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C	1.39114800	-0.21481000	-3.79439300
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C	-1.24083600	4.11441900	-1.64418400
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C	-0.12911000	3.98061700	-0.62683600
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H	1.58702100	-3.06565100	-1.26234000
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H	1.97275600	-2.43265700	-2.85859100
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H	0.39247500	-0.04138700	0.19111700
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H	1.15315900	-1.59256300	0.48385200
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H	3.83713000	-1.02536400	-1.85334100
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H	3.43305600	-1.66781100	-0.23674000
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H	4.05311700	-2.76196400	-1.49967300
H	-1.29460500	-1.78498100	0.87404500
H	-1.65093600	-1.24026400	-0.78335000
H	-0.83355300	-2.80202300	-0.51827000
H	2.46018000	-0.44971300	-3.73212300
H	0.89681600	-1.00144000	-4.38774200
H	1.26750600	0.74714400	-4.30169700
H	-0.93838600	4.72458600	-2.50752500
H	-2.15034700	4.54454300	-1.20612600
H	0.10557000	4.97544800	-0.21676600
H	-0.43132500	3.32402100	0.20383800
H	0.78760700	3.57682500	-1.08498800
O	-1.94499300	1.10504400	-3.99200500
C	-2.71031900	0.10217700	-3.42011500
C	-2.47051100	-1.21308800	-3.82606200
C	-3.69379800	0.41372200	-2.47662400
C	-3.21974400	-2.24508800	-3.26875000
H	-1.69372500	-1.41509600	-4.56504000
C	-4.44306700	-0.61719800	-1.91604800
H	-3.85754800	1.45063500	-2.18355800
C	-4.19193400	-1.93079400	-2.31745100
H	-3.05163800	-3.28219700	-3.55516100

H	-5.21255400	-0.41277600	-1.17295500
N	-4.97099800	-3.01913400	-1.71202400
O	-4.72666800	-4.16422700	-2.06415200
O	-5.82236000	-2.72458100	-0.88553600
H	-0.52615600	0.81536500	-1.20920000

46

Energy = -1427.12556500 a.u. #Cluster: 4

P	-0.83656700	1.96578300	-3.19067500
O	-1.68638500	2.80545500	-2.14597500
O	0.07586000	2.67914100	-4.10980800
N	1.06095900	-1.07272600	-1.51679000
N	-0.11195900	0.81493700	-2.13559700
C	1.99957700	-2.18422300	-1.78176700
C	0.44381700	-1.07184100	-0.17413200
C	0.77497400	-0.16707900	-2.42633500
C	3.41355800	-1.87448400	-1.30424800
C	-0.91678600	-1.76390700	-0.15702200
C	1.39360400	-0.20814000	-3.78758100
C	-1.25847100	4.11540800	-1.64878100
C	-0.13376200	3.99215000	-0.64452700
H	1.59161800	-3.05839400	-1.25500900
H	1.97888800	-2.42442500	-2.85048900

H	0.38612800	-0.03739100	0.19600200
H	1.14932300	-1.58700500	0.49016600
H	3.43144100	-1.65528400	-0.22561700
H	4.05722400	-2.74827300	-1.48678300
H	3.83766200	-1.01232600	-1.84144200
H	-1.29878400	-1.78485200	0.87444600
H	-1.65270000	-1.23953900	-0.78315000
H	-0.83294300	-2.80007200	-0.51766100
H	2.46290500	-0.44123100	-3.72353100
H	0.90169300	-0.99546100	-4.38204800
H	1.26881200	0.75364200	-4.29491000
H	-0.97208400	4.72929300	-2.51497500
H	-2.16716900	4.53605200	-1.19997500
H	0.78155300	3.59800700	-1.11373000
H	0.09574000	4.98917300	-0.23686600
H	-0.41942900	3.33230600	0.18942000
O	-1.94524000	1.09900500	-3.99181600
C	-2.70737500	0.09288900	-3.42146200
C	-2.46264900	-1.22114600	-3.82850700
C	-3.69277000	0.40010000	-2.47853200
C	-3.20866900	-2.25630000	-3.27275500
H	-1.68459900	-1.41960700	-4.56711200

C	-4.43916700	-0.63398300	-1.91989800
H	-3.86002600	1.43611900	-2.18423200
C	-4.18300700	-1.94631100	-2.32221200
H	-3.03649000	-3.29255300	-3.55982100
H	-5.21022700	-0.43292200	-1.17750800
N	-4.95888900	-3.03798000	-1.71868000
O	-4.70667800	-4.18222500	-2.06787700
O	-5.81560800	-2.74679600	-0.89651000
H	-0.53026300	0.81833700	-1.20581200

46

Energy = -1427.12556300 a.u. #Cluster: 5

P	-0.80789300	1.95771100	-3.23409100
O	-1.65414800	2.81358500	-2.20066000
O	0.10217400	2.65457800	-4.16794800
N	1.07986400	-1.07408400	-1.53793000
N	-0.08051700	0.81831900	-2.16802400
C	2.00738900	-2.19583300	-1.79888800
C	0.46941200	-1.05800100	-0.19235500
C	0.79671800	-0.17396300	-2.45389600
C	3.42680900	-1.89485400	-1.33207600
C	-0.89294500	-1.74630400	-0.16158700
C	1.40853400	-0.23231500	-3.81759400

C	-1.22777700	4.12715700	-1.71159200
C	-0.36286200	3.99693400	-0.47754100
H	1.59487500	-3.06214800	-1.26280100
H	1.97851800	-2.44459900	-2.86543600
H	0.41616600	-0.01986100	0.16776500
H	1.17665100	-1.56872500	0.47357300
H	3.45332600	-1.66799700	-0.25521500
H	4.06157200	-2.77564300	-1.51213200
H	3.85521700	-1.04046700	-1.87817000
H	-0.81336400	-2.78664600	-0.51096600
H	-1.27007900	-1.75494300	0.87183000
H	-1.63026000	-1.22720500	-0.79033700
H	2.47697100	-0.47026300	-3.75600200
H	0.91043100	-1.02306000	-4.40225400
H	1.28656900	0.72489700	-4.33401700
H	-0.70545900	4.64247800	-2.53042300
H	-2.16732200	4.65445300	-1.50223300
H	-0.88746800	3.43786000	0.31266700
H	0.58606100	3.48605300	-0.70456300
H	-0.12716100	5.00243300	-0.09469900
O	-1.92176900	1.08233000	-4.01896900
C	-2.68393100	0.08595400	-3.43192000

C	-2.45050600	-1.23285800	-3.82984300
C	-3.65860700	0.40660100	-2.48210200
C	-3.19719300	-2.25892700	-3.25815400
H	-1.68040100	-1.44244300	-4.57370800
C	-4.40467100	-0.61844100	-1.90668600
H	-3.81784500	1.44581100	-2.19495500
C	-4.16006600	-1.93552900	-2.30054600
H	-3.03403200	-3.29857000	-3.53818800
H	-5.16698500	-0.40650800	-1.15834300
N	-4.93604100	-3.01760500	-1.68020000
O	-4.70400600	-4.16507200	-2.03286600
O	-5.77294500	-2.71572400	-0.84167100
H	-0.49436400	0.83275700	-1.23637600

46

Energy = -1427.12556200 a.u. #Cluster: 6

P	-0.81304700	1.94925200	-3.22857800
O	-1.67391900	2.80699800	-2.20795200
O	0.11396700	2.64544300	-4.14616400
N	1.05597800	-1.06935100	-1.48767500
N	-0.10636200	0.80986500	-2.14913200
C	1.99545200	-2.18638100	-1.72467500
C	0.42539700	-1.04400300	-0.15136400

C	0.78200500	-0.17781700	-2.41473000
C	3.40529600	-1.87078300	-1.23867500
C	-0.93639700	-1.73376700	-0.13476600
C	1.41527800	-0.24152600	-3.76840100
C	-1.24425600	4.11745000	-1.71353600
C	-0.17835900	3.98848700	-0.64774100
H	1.58112700	-3.05120900	-1.18758100
H	1.98482500	-2.44423900	-2.78942400
H	0.36585800	-0.00284600	0.19949200
H	1.12349700	-1.54832500	0.52890800
H	3.41289800	-1.63367000	-0.16371600
H	4.04932800	-2.74839700	-1.40034800
H	3.83596300	-1.01825100	-1.78591300
H	-0.85093000	-2.77585200	-0.47754400
H	-1.32715800	-1.73726000	0.89361300
H	-1.66625400	-1.21923300	-0.77595400
H	1.29354600	0.71105300	-4.29337600
H	2.48454500	-0.47032900	-3.68911700
H	0.93149400	-1.04056800	-4.35378100
H	-0.89788800	4.70765800	-2.57421500
H	-2.16570900	4.56670800	-1.32206000
H	-0.52508600	3.35235100	0.18146200

H	0.75087900	3.56329600	-1.05884400
H	0.05314600	4.98786700	-0.24698300
O	-1.91532000	1.07572500	-4.03118100
C	-2.68601200	0.07923800	-3.45551700
C	-3.67840800	0.40116000	-2.52483600
C	-2.44211800	-1.24058800	-3.84393900
C	-4.43279100	-0.62345000	-1.95958900
H	-3.84511300	1.44125400	-2.24499700
C	-3.19615300	-2.26635800	-3.28163800
H	-1.65832800	-1.45058600	-4.57326200
C	-4.17743700	-1.94150600	-2.34328700
H	-5.20943500	-0.41065600	-1.22636300
H	-3.02500900	-3.30669200	-3.55427500
N	-4.96178000	-3.02314900	-1.73275000
O	-5.82537900	-2.71894000	-0.92258400
O	-4.70938500	-4.17253600	-2.06449200
H	-0.53580400	0.82578200	-1.22464200

46

Energy = -1427.12490600 a.u. #Cluster: 7

P	-1.24619800	0.96994500	-2.64081400
O	-2.02433600	1.01666800	-1.25491200
O	-1.27294300	2.17735200	-3.49706300

N	2.20413000	-0.49151700	-1.37001200
N	0.37338600	0.53578500	-2.32275200
C	2.84277000	-1.47115000	-0.46408600
C	3.13645500	0.39979200	-2.09018700
C	0.89775500	-0.40462000	-1.50142000
C	3.24885000	-2.75025400	-1.18678900
C	3.37973400	1.70959600	-1.34502000
C	-0.01066200	-1.31333600	-0.73425300
C	-2.12626300	2.24134900	-0.46343400
C	-0.81950600	2.56956900	0.22741800
H	3.72255900	-0.96635300	-0.04078700
H	2.16836300	-1.67934700	0.37375900
H	2.76196800	0.56753100	-3.11073700
H	4.07367400	-0.15968100	-2.20604600
H	3.93837900	-2.53700400	-2.01794700
H	3.76189200	-3.41843500	-0.47864800
H	2.37178700	-3.27923300	-1.58979300
H	2.45353900	2.29372700	-1.23129200
H	3.79303700	1.51687200	-0.34341100
H	4.10432900	2.31709000	-1.90747100
H	-1.04010800	-1.25841400	-1.09253600
H	0.33313200	-2.35224700	-0.81031300

H	0.00379300	-1.01829800	0.32716400
H	-2.45415400	3.05222700	-1.13028300
H	-2.92796400	2.02693400	0.25485100
H	-0.47324200	1.72148900	0.83827200
H	-0.03270800	2.82772800	-0.49879400
H	-0.96847600	3.43753300	0.88835800
O	-1.80138200	-0.42363700	-3.25313800
C	-3.13463700	-0.70545900	-3.47674900
C	-3.53755500	-2.02584400	-3.25710500
C	-4.02930800	0.27132800	-3.92805800
C	-4.86154400	-2.38119400	-3.49182200
H	-2.80891500	-2.75756800	-2.90543700
C	-5.35655300	-0.08186200	-4.15454100
H	-3.68755100	1.29101800	-4.11029700
C	-5.75451400	-1.40195600	-3.93465800
H	-5.20769700	-3.40124000	-3.33099300
H	-6.07914200	0.65366000	-4.50524900
N	-7.15265500	-1.77289600	-4.17877500
O	-7.47711100	-2.93902700	-4.00233400
O	-7.92435000	-0.89792400	-4.54631600
H	1.01658200	1.15262300	-2.81767100

Energy = -1427.12482100 a.u. #Cluster: 8

P	-1.14807900	0.76070300	-2.94370900
O	-1.98057300	1.18278600	-1.65679000
O	-1.07476500	1.71542600	-4.07279300
N	2.17635400	-0.46641500	-1.18204300
N	0.43332900	0.35531900	-2.44605600
C	2.73338400	-1.22035800	-0.03752300
C	3.17438300	0.20268500	-2.04257400
C	0.88164200	-0.37675300	-1.39849300
C	3.11858100	-2.64614800	-0.41559400
C	3.42170900	1.65027900	-1.62736800
C	-0.09641100	-1.04934900	-0.48755200
C	-2.05398700	2.56865800	-1.19685200
C	-0.81197100	2.96047700	-0.42522300
H	3.61333300	-0.65524600	0.30030700
H	2.01378600	-1.20354600	0.78831900
H	2.86094600	0.12138700	-3.09395400
H	4.09719600	-0.38595000	-1.96144500
H	3.57238600	-3.14180200	0.45590200
H	2.23866700	-3.22926700	-0.72749900
H	3.85193500	-2.65649300	-1.23649000
H	4.19914900	2.08451400	-2.27351500

H	2.51316100	2.26472600	-1.72063300
H	3.76930200	1.70189800	-0.58448400
H	0.21309200	-2.08258100	-0.28746200
H	-0.12625500	-0.50349600	0.46898800
H	-1.10300900	-1.06143200	-0.90981200
H	-2.21560100	3.21223700	-2.07391500
H	-2.95317300	2.59350700	-0.56784700
H	-0.63022000	2.26090700	0.40522800
H	0.07811300	2.98017600	-1.07366600
H	-0.94924300	3.96982300	-0.00691900
O	-1.75380700	-0.71669900	-3.22227900
C	-3.09661200	-0.97708900	-3.41656200
C	-3.91953900	-0.09890200	-4.13033200
C	-3.58507000	-2.17457900	-2.88616200
C	-5.26159100	-0.42352400	-4.30629700
H	-3.51171500	0.82104600	-4.55118000
C	-4.92433500	-2.50308500	-3.06824000
H	-2.91071100	-2.83302900	-2.33676300
C	-5.74570000	-1.61988000	-3.77365500
H	-5.92994100	0.23805900	-4.85574900
H	-5.33669500	-3.42751600	-2.66617300
N	-7.16012300	-1.96053500	-3.96186800

O	-7.86388200	-1.17387600	-4.57995400
O	-7.56516000	-3.01429700	-3.49105300
H	1.12435900	0.81855700	-3.03438700

46

Energy = -1427.12481700 a.u. #Cluster: 9

P	-0.84163200	0.52267900	-3.18024000
O	-1.60329500	1.43635900	-2.12500200
O	-0.46771700	1.12102100	-4.48167400
N	1.95264100	-0.92934600	-0.78576800
N	0.55234700	-0.10789700	-2.42370200
C	3.14331800	-0.74084100	-1.64037400
C	2.22510700	-1.46072300	0.56759900
C	0.73795600	-0.61429000	-1.18127200
C	3.70988400	0.67269300	-1.53608700
C	2.26514800	-2.98413300	0.59523300
C	-0.43200900	-0.78078100	-0.26320800
C	-1.34684300	2.87047000	-2.00742700
C	-0.06754300	3.14340100	-1.24555900
H	3.88295500	-1.48148400	-1.31002700
H	2.89363500	-1.01065400	-2.67683500
H	1.47871500	-1.06599000	1.26533300
H	3.19349700	-1.03912200	0.87122300

H	3.99080700	0.90451800	-0.49759300
H	4.60967600	0.75029100	-2.16437400
H	2.98426600	1.42749800	-1.87563900
H	3.02948500	-3.37645200	-0.09294100
H	2.51484200	-3.32089200	1.61279400
H	1.29157100	-3.41539700	0.31636300
H	-0.40319700	-1.76506000	0.22015300
H	-0.38251400	-0.00651500	0.51902400
H	-1.38150800	-0.67869500	-0.79179600
H	-1.32279500	3.29840200	-3.02039600
H	-2.22892000	3.25663700	-1.48054800
H	-0.08502300	2.65226300	-0.26031100
H	0.81665500	2.79232300	-1.80046200
H	0.03741000	4.22871800	-1.09201900
O	-1.79199200	-0.79012900	-3.18263900
C	-3.14391800	-0.76621000	-3.46606900
C	-3.95383100	-1.63174500	-2.72530800
C	-3.67094000	0.06332200	-4.46228900
C	-5.32043200	-1.67051800	-2.98135300
H	-3.50334800	-2.26219100	-1.95742100
C	-5.03970700	0.03092800	-4.71306300
H	-3.01602100	0.71731200	-5.03944900

C	-5.84513900	-0.83469800	-3.97044900
H	-5.97993200	-2.33240200	-2.42173300
H	-5.48325200	0.66410000	-5.48019400
N	-7.28720600	-0.86892400	-4.23872100
O	-7.97430800	-1.64529300	-3.58972000
O	-7.73048400	-0.11913100	-5.09752100
H	1.37023000	0.00790000	-3.02066400

46

Energy = -1427.12395600 a.u. #Cluster: 10

P	-1.12874300	0.89999900	-2.94329400
O	-1.81969300	1.43024400	-1.61139700
O	-1.07123600	1.81384500	-4.10618500
N	2.16848500	-0.75760500	-1.51552700
N	0.44641300	0.36216100	-2.56596100
C	2.70504500	-1.71357500	-0.52141100
C	3.17237200	-0.17101700	-2.42731600
C	0.88645200	-0.47433500	-1.59470500
C	3.20804800	-1.02064600	0.73932900
C	3.33975100	-0.97852100	-3.71132300
C	-0.10002100	-1.07829800	-0.64576700
C	-1.72677900	2.82352100	-1.18026600
C	-0.43861600	3.07826600	-0.42787400

H	1.93768800	-2.46164700	-0.29354800
H	3.52288300	-2.24746300	-1.02515100
H	4.11521800	-0.13679000	-1.86601200
H	2.90594600	0.87667500	-2.62959700
H	2.39092100	-0.50694700	1.26843400
H	3.64158200	-1.77223500	1.41632100
H	3.98850900	-0.28121100	0.50328300
H	3.63735900	-2.01372800	-3.48589100
H	2.41120900	-1.00470000	-4.30186300
H	4.12712600	-0.51874000	-4.32714300
H	0.32211300	-1.15695800	0.36160600
H	-1.01234800	-0.47843300	-0.59271300
H	-0.36238300	-2.08905000	-0.99868900
H	-1.82098600	3.46433800	-2.06921000
H	-2.61022900	2.96760600	-0.54483200
H	-0.44261100	4.10996600	-0.04255100
H	-0.33880100	2.38848400	0.42440800
H	0.43956700	2.96175200	-1.08192700
O	-1.87593700	-0.52711100	-3.11586700
C	-3.24632900	-0.69486300	-3.11240500
C	-3.73331800	-1.85089000	-2.49610900
C	-4.10151600	0.23250400	-3.71804700

C	-5.10384000	-2.08822700	-2.48203500
H	-3.03274200	-2.54760200	-2.03376500
C	-5.47351100	0.00008300	-3.69659900
H	-3.69661400	1.11835200	-4.20962700
C	-5.95585700	-1.15640000	-3.08034000
H	-5.51628200	-2.97881200	-2.00977600
H	-6.16754700	0.70167900	-4.15730200
N	-7.40214800	-1.40163100	-3.06315700
O	-8.13322900	-0.56661200	-3.57757700
O	-7.80488500	-2.42880900	-2.53515600
H	1.12615400	0.73470100	-3.22758800

Cartesian coordinates of transition states (TS) for studied NAs and simulants were optimized at the PCM(H₂O)/B3LYP-D3(BJ)/def2-SVP level .

Dominant hydrolysis reaction pathways

PATH4

A230

34

P	-5.49238396163334	-5.26961565392808	-2.56226926766634
O	-7.00308874649247	-5.01621037368712	-2.92521310972405
C	-4.42070896778555	-3.83695327117383	-2.24510395959149

H	-5.03507137010565	-3.01191013003311	-1.86026387156339
H	-3.66922036128056	-4.10953438206972	-1.49105470788014
H	-3.92028864942689	-3.53732606640699	-3.17412648959119
C	-5.37011628533848	-7.75298894489205	-1.58596050003971
F	-5.02660042604783	-5.38715694289288	-4.16011163596782
N	-4.82713689370603	-6.72020457148346	-2.16729459002907
C	-6.84899914262095	-7.89459138596841	-1.30207222043778
H	-7.02440446416970	-7.88364170976001	-0.21560276285510
H	-7.40039012415711	-7.06243782293945	-1.74491309152635
H	-7.24355916965841	-8.83965691446820	-1.70152520751217
C	-5.04969528805980	-10.00583171747031	-0.58566479475761
H	-5.94895638248917	-9.78879850474205	0.00418924025687
H	-4.28267837111508	-10.32609681315861	0.13661202208093
C	-5.32471993698971	-11.12602366948603	-1.58792791772662
H	-5.64447011693343	-12.03859434916600	-1.06007184451581
H	-6.12023205708577	-10.83950167406881	-2.29386429520003
H	-4.42113577932747	-11.36705890374601	-2.17017517509284
C	-3.12032866064688	-8.67989565739116	-1.44144054121747
H	-2.95649491403555	-8.17408412717687	-2.40264616401385
H	-2.72938225179086	-9.70446376444150	-1.53072477172794
C	-2.40049184739887	-7.92963233401326	-0.32281415898610
H	-2.76947714364898	-6.89502383229299	-0.25428023590368

H	-2.55941468951210	-8.42179062600011	0.65028293056305
H	-1.31648553890742	-7.89893331238915	-0.51804633099755
N	-4.56418669990186	-8.77609689099379	-1.21408766283620
O	-6.04247861510413	-5.08561017398567	-0.58325654302689
H	-5.44071240016688	-4.55263901785276	-0.04482171335553
H	-7.19765829939515	-4.67167322108349	-0.57991167550012
O	-8.27319831678714	-4.38427843231151	-0.99005498624851
H	-7.72720598928250	-4.69687505005529	-2.06924340614170
H	-8.86315213899804	-5.11423175847105	-0.74727556126776

A232

35

P	-6.43073869427019	-5.75845841459059	-3.21931784113436
O	-7.78521110252016	-5.85786189633762	-3.98859977383778
C	-5.81732065483480	-8.18506095265853	-2.31083761554738
F	-7.11516844822624	-4.93710516851215	-1.93669066732662
N	-5.77041211813100	-6.88598940233867	-2.21744385629817
C	-6.74505056062044	-8.93725712116707	-3.23907658551613
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H	-7.45778644575175	-8.24621069406093	-3.69764893766981
C	-4.96678128073818	-10.37920897013936	-1.50935666713286
H	-3.91854279064769	-10.68556086501759	-1.36733146630686

H	-5.26347391707792	-10.76407719530433	-2.49314835719206
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H	-6.90120446778887	-10.72201136793599	-0.56130043392351
H	-5.75288672157330	-12.08121173823832	-0.41556248370748
C	-4.03845201778777	-8.22991365990670	-0.64810528369248
H	-3.79170202195522	-8.91693460623236	0.17487990867269
H	-4.53833693072089	-7.35355838284484	-0.21300980614723
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H	-2.07292243389240	-7.30528043711712	-0.69262991526963
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C	-5.19927300690485	-3.39987069690238	-2.69193338713611
H	-6.10683569996841	-2.78522438415742	-2.60692349484252
H	-4.88443648004891	-3.71663311983825	-1.68615810034411
H	-4.39679626211467	-2.80718464398713	-3.15325314976240
O	-5.52105919333413	-6.56827222860506	-4.71272253868783
H	-4.77916364801882	-5.99669215285604	-4.96326088305785
H	-6.33276095472585	-6.70177770814496	-5.63616022948393
O	-7.37601516758960	-6.69448357059672	-6.19267172537391

H	-7.74451010999979	-6.28356259303487	-5.17693700044241
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H	-7.67567355081549	-7.61565674005618	-6.25155793795436
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A234

38

P	-5.44804753888247	-5.22796193635727	-1.26725541673884
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O	-6.59333864509094	-4.51466820078214	-0.48685322436710
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C	-5.64074332574123	-7.85378059300095	-0.90575050119504
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F	-4.51981877494503	-5.43154516596616	0.13780196171662
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C	-6.34908738265109	-7.72869031541755	0.42617524217829
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H	-7.15455443074059	-8.46825004614408	0.52829290850933
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H	-5.63371247094509	-7.88931581520005	1.24818393348018
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H	-6.77534302974620	-6.72593178519574	0.53099338280275
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C	-5.58437782586321	-10.31376968975822	-0.55431752045686
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H	-5.57923237256041	-10.07734802735087	0.51713566103673
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H	-4.73571426007134	-10.99665735933673	-0.71700030395331
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H	-7.75694232876205	-10.35103585376554	-0.75411932912207
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H	-5.00881967072053	-8.53613810782846	-3.31302083521157
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C	-3.10558265450788	-9.14705827541020	-2.47779910159728
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H	-2.69908433515841	-9.88865662694297	-1.77118679170298
H	-2.62490619799228	-9.30886537966897	-3.45601162113690
N	-5.31456417010411	-9.09959315443152	-1.32675565798370
O	-4.30458611261600	-4.30863641128351	-1.97490818234826
C	-3.00396082241458	-4.01949975712751	-1.43750519382885
H	-3.08421886701517	-3.72655015045031	-0.38142939014257
H	-2.65962960415899	-3.14433919893124	-2.01043823821373
C	-2.04255789934665	-5.18161153893434	-1.61115641336264
H	-2.36713152922736	-6.04248760124722	-1.00954201554415
H	-1.99105175708754	-5.48959069419671	-2.66762499843051
H	-1.03172101718721	-4.88758444843038	-1.28514984214227
O	-6.36220056151775	-4.99782718405999	-2.89481329384395
H	-7.50066788642075	-4.59549113230357	-2.65374121674886
H	-6.35389793195455	-5.86076601395623	-3.33921989815289
O	-8.40810079819908	-4.16258956108705	-2.02027043737724
H	-7.67358758830502	-4.25168593361249	-1.16765001477088
H	-8.46173657431945	-3.21618645185874	-2.23106272229061

ADPP

P	-0.68936121811734	-2.18867893890242	0.85732977346076
O	0.53441838370346	-3.06584610243618	-0.01516047053649
O	0.13035446620182	-0.79875576012900	0.50989515431459
O	-0.32486768814830	-2.94288608035264	2.16133505601271
N	-1.93185491826257	-2.50125451648637	-0.20733824418992
N	-3.33941372767610	-3.80409748968549	-1.44257808753121
C	0.98908253016569	-2.87583496955295	-1.27327128005728
C	-0.31055906488766	0.50136724343161	0.47088391120010
C	2.15697750729590	-3.58111002805054	-1.62440206072957
C	-1.35817406424690	0.89420922950726	-0.36972141626710
C	0.38060268534482	-2.05254998578505	-2.23946274088486
C	0.38078286689809	1.44515735931661	1.23491751241983
C	2.70265244333322	-3.46790908261894	-2.90333365628549
C	-1.71279144890634	2.24358306321981	-0.43603711749294
C	0.94027187694701	-1.94299684968438	-3.51644908038074
C	0.02146112507119	2.79397916220284	1.15675320110671
C	-2.40444131273695	-3.68233743903394	-0.48623097976208
C	2.09945882087094	-2.64435736420969	-3.86202231649008
C	-1.02649239205902	3.19896724813390	0.32318599608497
C	-1.98451855320702	-4.95998295365334	0.19959461938162
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H	-1.89459492179292	0.14176623363506	-0.94926802033259

H	-0.53235609132137	-1.51256370712544	-1.99983457863222
H	1.19480668855830	1.10890958057729	1.88058144221485
H	3.60961847159071	-4.02652909938348	-3.15145988161603
H	-2.53368800870487	2.55031592803489	-1.08958754066391
H	0.45292200347402	-1.29752724118103	-4.25289714808362
H	0.56442639733087	3.53124812083922	1.75398048613319
H	2.52646752631932	-2.55277144291044	-4.86365090114300
H	-1.30739747380443	4.25326484818582	0.26480375521413
H	-0.91244768952641	-5.12440515188766	0.02071186351771
H	-2.55547319660768	-5.82744308970851	-0.15626817035235
H	-2.11695715576167	-4.85159288345224	1.28542442676939
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H	-3.75981635443105	-4.69919847330060	-1.65756255960435
O	-1.94080676834241	-1.12138690539211	1.81755824939706
H	-2.08506041718697	-1.60455752030247	2.96453252211838
H	-2.76778589279219	-1.09037648411704	1.31226867521799
O	-1.87271467406245	-2.29625586290019	3.88134650130031
H	-1.07770332346919	-2.72034177757619	3.21669147477874
H	-1.41687321585805	-1.75191973536016	4.54429847815199

AMP

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P	3.20761283192963	0.73435931525647	1.50367529214711
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C	-0.65921220286576	-0.84059851513685	-1.51703221659310
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C	-1.33225170029044	-0.67872661970083	1.74382591702455
C	-0.95346231947796	0.12004124059938	-2.66681419876842
C	2.23232417349963	-0.46505811250139	-1.22422044654176
C	3.31517865077565	1.68751318860611	3.04005141628660
H	-1.92554826646942	0.62560010487651	0.11131144444014
H	-0.57691709068445	1.24158193142190	1.08785819338364
H	-0.00991784244959	-1.66141496370502	-1.84854442737031
H	-1.59094064576548	-1.31592002473232	-1.17465768254829
H	-1.75845598514893	-1.60206415282927	1.31955892040045
H	-0.42806055063892	-0.94457259246482	2.30773903006092
H	-2.06896213269401	-0.25484887644395	2.44504961619252
H	-1.44701626243014	-0.41497316376556	-3.49371271288251
H	-1.62015542177208	0.93342275898796	-2.33886543774753
H	-0.02602489693065	0.57235709973201	-3.05235865593620
H	2.86763274931354	0.39666389555499	-1.47224720402248
H	2.89433038497808	-1.25161347656030	-0.83299724445225

H	1.75819383906102	-0.82453476169251	-2.14122925327937
H	3.58147399000031	2.72755720299771	2.83202658072502
H	2.33183661156906	1.64835121093634	3.53002829656782
H	4.05851651077074	1.20429920956350	3.68747801618774
O	3.43552892385243	-0.81070733668333	2.25149152367258
C	2.44776849809513	-1.60118741613332	2.75410961927270
C	1.98276311724130	-2.68715383507270	1.99649629909671
C	1.92833261791151	-1.38620326803252	4.04027924527492
C	1.01198456149180	-3.54523107027175	2.51806245309186
H	2.39448519561757	-2.84503522037470	0.99757238371819
C	0.95336084850352	-2.24636524070309	4.55412042977564
H	2.29685574264753	-0.54762585494934	4.63369441189699
C	0.49019110208196	-3.32906195072350	3.79848483500799
H	0.65715916056840	-4.38663089595537	1.91675658327950
H	0.55506577854100	-2.06846590893129	5.55677292805588
H	-0.27198249013483	-3.99868108288873	4.20421962988287
O	4.51763674531372	2.11637188874826	-1.19582088523632
H	4.65757710461077	1.25085514700676	-0.20760811631857
H	5.26991850410828	2.72632276727140	-1.19334500692004
O	2.99892562220357	2.62164942423483	0.56692280609779
H	3.71003354364318	2.53539687767298	-0.41934652383391
H	2.07171838817144	2.69607826435810	0.29870680746617

AMOP

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P	-2.63445442037786	-1.23212546678870	-0.90219496475462
O	-2.40236220980604	-2.66356841611967	-1.68443761375537
O	-2.91022983298520	-1.25908208489872	0.64556475208367
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C	2.08935043897519	-1.13125151434974	-2.46238969464348
C	-0.45219388724171	0.38521066303065	1.11611887087084
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H	0.27736681139337	0.00161492049146	-2.82269503082692
H	1.74588593559280	0.99451856258071	-2.72883987175724
H	0.76109959460048	3.05631620180715	0.06881017575548
H	2.53035970399542	3.29060805489825	0.14582571542188
H	1.72497373347591	3.02045788277446	-1.42309535532175
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H	0.32010355977164	-0.07093443592134	1.75586457069069
H	-0.38901073276865	1.47488047176025	1.24256366935011
H	-1.43222109029873	0.03092386369830	1.44129785069547
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H	-0.64640449739960	-2.66467654639184	-2.82344214376319
O	-3.27693568659683	0.05517487570398	-1.76684139305351
C	-2.66894092291243	1.28702911918500	-1.82157925501518
C	-2.05025457706259	1.69878076871170	-3.00528528779226
C	-2.72712004977643	2.14095322609629	-0.71575421918719
C	-1.48097011786043	2.97250624843992	-3.07772790198225
H	-2.01508453261961	1.01015050880415	-3.85160064137123
C	-2.15091081287662	3.41147199396382	-0.79435343255097
H	-3.21644102984023	1.79538495693182	0.19680732257347
C	-1.52540722730273	3.83119783914102	-1.97305734744777
H	-0.99263409166363	3.29371324281727	-4.00134847904912
H	-2.18953614243735	4.07557402380644	0.07292831560163
H	-1.07164876191145	4.82336079048479	-2.03051391720013
O	-4.49183252999197	-1.82643226328130	-1.20081719767725
H	-4.42187268772534	-2.77154823405106	-1.40361471340622

H	-5.07085213601999	-1.73883456852443	-0.11158811647904
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H	-4.04408659930645	-1.41892556148810	1.00303517608143
H	-5.37198339635747	-2.48510834242947	1.40555059298815

AEOP

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P	-0.61065617489061	-0.27430932185533	0.17217792241554
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N	1.86832127464565	0.59800120712113	-2.66595470656040
N	0.48059314877666	-0.24766256181703	-1.05809106683599
C	2.54063058375974	1.68702905667254	-3.37519069667398
C	2.08551640549899	-0.75272929392096	-3.18601639365673
C	1.05763221789086	0.78748655058417	-1.59525119071769
C	3.97037122081804	1.92912324248750	-2.89328827745515
C	1.02935223443387	-1.17206640056881	-4.20612625014352
C	0.87598198568498	2.20468938033962	-1.09773674185211
C	-1.85438168029212	-2.23367401374772	1.47784915204485
C	-3.29718224407427	-1.76278415368171	1.52895164511826
H	2.54370776983446	1.42540389027733	-4.44508351934592
H	1.94596547620918	2.60536533022344	-3.29152973413276
H	2.08910289549368	-1.44867650122360	-2.33613229594685

H	3.08838547073607	-0.77464229862474	-3.63928392920407
H	3.98646172919959	2.23217575874275	-1.83451398120264
H	4.58273143064671	1.01933970681556	-2.99786756138568
H	4.44212502073324	2.72762728917873	-3.48793839120445
H	0.02990721497146	-1.18966120759790	-3.74972065979657
H	1.00534691085267	-0.47709584218857	-5.06108533602625
H	1.25220755638264	-2.17956970007422	-4.59301013239656
H	0.33050112115272	2.20728813270483	-0.14811012405070
H	1.84154008475346	2.70889882506875	-0.95222218069595
H	0.29964392185215	2.78952817096830	-1.83162565781027
H	-1.79827008158251	-3.33220241978501	1.45862351098936
H	-1.29412270120605	-1.88663005936029	2.36047967324999
H	-3.85334392612149	-2.10462619422824	0.64217344776161
H	-3.78901497493686	-2.17093431428070	2.42659939619602
H	-3.34834637728206	-0.66495985568329	1.57252523455477
O	-1.93669925532688	0.31987022531057	-0.78210383636427
C	-2.17771643032292	-0.00807400289564	-2.07786823999290
C	-2.14339678283965	1.01271993717241	-3.04161794606552
C	-2.50758604217383	-1.31522998294250	-2.47593607860112
C	-2.43644102626662	0.73460742102901	-4.37913621293562
H	-1.88679733034606	2.02432154372216	-2.71959608266119
C	-2.79592499436622	-1.58539496362021	-3.81610201259531

H	-2.52195058644291	-2.10705227231160	-1.72780128302745
C	-2.76315256089345	-0.56670793976321	-4.77563897156983
H	-2.40444876105448	1.54128419238696	-5.11674538194658
H	-3.04892216847697	-2.60700635045556	-4.11354594670128
H	-2.98880338910912	-0.78571239794121	-5.82218577832979
O	0.87743396610272	-0.85454333652031	1.31293631225417
H	1.08049090454197	-1.79214788119208	1.18184829487102
H	0.66743147227668	-0.48026408236683	2.48191659007297
O	0.14875217226332	0.13326765896522	3.33322585369329
H	-0.47167114657732	0.56226374965888	2.40579075315565
H	0.77236201630641	0.82057496648394	3.61491517068725

ANMP

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P	-4.27678302898492	2.15613313593040	-0.14876053948208
O	-3.96974924863886	1.04885873797052	0.92097553584964
N	-7.84378975855554	3.66332995087960	0.03046803367787
N	-5.72675034871171	2.91862692308510	-0.39121699051892
C	-7.53523125710555	4.90539315141018	-0.68040284097244
C	-9.19176764856483	3.54873206906391	0.58992811892937
C	-6.88464159656210	2.71741963829561	0.17473079669912
C	-7.75241916275018	4.79511101202060	-2.18745883050885
C	-9.32684592425938	4.19437421583242	1.96906587360372

C	-7.24711304098551	1.47265878072762	0.95465474334138
C	-2.98939842903927	2.56603872246645	-1.35634555861914
H	-6.49155532758642	5.16822033397367	-0.46339617228166
H	-8.17338161619700	5.69581990915919	-0.25730681602764
H	-9.88093676726906	4.03147919607374	-0.12055179802943
H	-9.48776507191193	2.49299661752633	0.62993375748278
H	-7.08650256036245	4.03230858408380	-2.61864897870355
H	-8.79403298039973	4.52025316861786	-2.41990977098008
H	-7.53630488162193	5.75885410239710	-2.67605058514196
H	-8.70608837484054	3.67764598078982	2.71578967606671
H	-9.01542419767222	5.25069111956997	1.94580384855145
H	-10.37505885812896	4.15422277496211	2.30521790443650
H	-8.02503945626510	0.91114461275343	0.41348451469020
H	-6.37433059819121	0.82605194856664	1.06861791257045
H	-7.64047921022439	1.71971386701353	1.94988837182048
H	-2.22212802343074	3.19440235372666	-0.89047554147732
H	-2.56041035118046	1.63296667859945	-1.74018189365538
H	-3.46356902243262	3.10762640992630	-2.18709256572655
O	-3.69906202351570	3.52014143590186	0.89900596128821
C	-4.48263118465587	4.04688342084951	1.83840334348324
C	-5.09681949479097	3.25555439976577	2.83582108734724
C	-4.73335303495414	5.43729286673355	1.81677418359740

C	-5.98568923309662	3.82341916334111	3.73642287705652
H	-4.87916234762812	2.18881057812309	2.86014554920425
C	-5.61907933659175	6.01101999775396	2.71626497502661
H	-4.24621828050966	6.04024241680599	1.04831181185529
C	-6.25831625382261	5.19418244976353	3.65856358059839
H	-6.48462039288158	3.21631589969337	4.49096814760840
H	-5.84773015878526	7.07565202099848	2.68288034033662
N	-7.24772681472501	5.77352430067294	4.54852155462262
O	-7.45568405461696	6.98197131517825	4.48570398323829
O	-7.84815729546088	5.02862763180858	5.31930453807546
O	-4.84450660731456	0.76571762212079	-1.42612052144603
H	-5.70535569756906	1.00470350052070	-1.80065445339034
H	-4.87691872223798	-0.31651470428790	-0.80124270475436
O	-4.73113154914854	-1.06147509448165	0.09017703273702
H	-4.29246360709570	-0.11544151699564	0.62694185288553
H	-3.98897116872549	-1.64484720968880	-0.13366387496517

ANMOP

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P	-0.23238544807977	-1.73751927435796	-3.57933391654506
O	0.06441264386504	-0.08399199652865	-3.81300272227545
O	0.75799264147046	-2.25954758413196	-4.66723126423460
N	0.77910721649887	-0.91606542830017	0.05991554281172

N	-0.11362924009884	-1.58470569176152	-1.93793214465342
C	1.88080687249609	-0.49483454055942	0.92851242054864
C	-0.52815199403584	-1.07380194611873	0.70164788960746
C	0.92305919191094	-1.16593476413235	-1.26230529228160
C	2.57993711531181	-1.66227648849690	1.62342960430474
C	-1.33016486270630	0.22568322052149	0.72747375087497
C	2.29308429047728	-0.95994418317424	-1.87097187909824
C	0.07180812220022	0.47229793580938	-5.11235944163310
H	1.45719980151174	0.18919445559235	1.67998527475922
H	2.59996024075820	0.09978324930608	0.35114010238032
H	-1.08080850992269	-1.85143187079190	0.15929893079376
H	-0.35527647384341	-1.43680210463029	1.72659550279143
H	3.36301201112303	-1.28624963064576	2.30087200324055
H	1.86629190907077	-2.25147183390735	2.22082042422475
H	3.05246854627073	-2.33684703399888	0.89210448304213
H	-0.79800725435055	1.01252863906875	1.28579619432929
H	-1.51400143511840	0.58945340014081	-0.29367479469927
H	-2.30533043233005	0.06211442529909	1.21334777296804
H	2.32682901569780	-1.38956231506183	-2.87727878458442
H	2.51098904536469	0.11699474310113	-1.94526727759892
H	3.08169899966996	-1.42381299064355	-1.26325949720608
H	-0.89583990277144	0.32445376827106	-5.62519671392285

H	0.86542774931881	0.03077774384962	-5.73838147804505
H	0.25255713927707	1.55415034428578	-5.01490941478424
O	-1.78498835478655	-1.64405182355967	-4.20955587620557
C	-2.87723720025361	-1.38583853043904	-3.44776315016889
C	-2.95734218502389	-0.22302318323595	-2.66320236629405
C	-3.94457608654742	-2.29564699082050	-3.48668647823893
C	-4.10094591845175	0.02590783974184	-1.91509750490162
H	-2.11534670057249	0.46843384963720	-2.65536257092016
C	-5.09394581924164	-2.04731578780672	-2.74471641004330
H	-3.84872937533607	-3.19503819624549	-4.09616865959172
C	-5.15714517316643	-0.89015197674102	-1.96181423286438
H	-4.18490824627415	0.91857359102405	-1.29684370509061
H	-5.93393978385917	-2.74077540538056	-2.75562432602790
N	-6.35787881217742	-0.63140170503218	-1.17019228489173
O	-6.38848413653083	0.37848432760725	-0.47685912885339
O	-7.27913996641080	-1.43654944150215	-1.23388328472064
O	-0.76291808849852	-3.56274448813792	-3.17668948713207
H	-0.48622677909408	-3.73434053459710	-2.26362311969150
H	-0.16209759066745	-4.32358832082854	-3.99033335450024
O	0.54488237113376	-4.63404453181551	-4.85481792527296
H	0.76613296435525	-3.48297354935557	-4.88798423774016
H	-0.02605963763287	-4.81813482051638	-5.61821804196475

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P	-0.62735035996351	1.46526240715618	-2.98783579495329
O	-1.69595349951046	2.41026808926591	-2.19785061228433
O	-0.88668120173906	1.33180577323952	-4.51568635647066
N	2.13502299884343	-0.62785284490819	-1.28763496959972
N	0.59372814887265	0.86647421527387	-2.06833430933268
C	2.94708753472168	-1.84335751482359	-1.37618148605049
C	2.29724758092296	0.17976010075469	-0.07666155053262
C	1.27188845144309	-0.23284790082833	-2.25234044822961
C	4.34569556603607	-1.59450004608172	-1.93848732782296
C	1.29454152810813	-0.18004795166972	1.01717795157501
C	1.15947361680659	-1.09509010073156	-3.49022227795847
C	-1.63845338846682	2.62565994481332	-0.77297942824173
C	-2.33642397808882	1.52869260615039	0.00951996347588
H	3.01888931676830	-2.25942625881206	-0.35917881471978
H	2.41820995171556	-2.59627672234061	-1.97378699563607
H	2.19275984761901	1.23665296097300	-0.35592037673112
H	3.32589753862839	0.02991861704799	0.28469498381107
H	4.89195631591080	-0.85712456441645	-1.32911145129179
H	4.92576746699647	-2.53099458928280	-1.94130314752717
H	4.29739629652950	-1.21528331724193	-2.97147510826055

H	1.47386497272087	0.43366809000595	1.91442453093128
H	0.26488671409464	0.00210013206094	0.67669476666306
H	1.38344925249514	-1.23988577852144	1.30547960578346
H	2.14610071634709	-1.38151306038529	-3.87834635545239
H	0.60667655849680	-2.01743207641693	-3.25146355229435
H	0.61154890923931	-0.55939943747436	-4.27179988771077
H	-0.58668912674043	2.72681145011171	-0.46297508046013
H	-2.13434690974956	3.59471383076816	-0.61340311781795
H	-2.33318492396250	1.78479568644332	1.08121228278147
H	-3.38097824021494	1.41837695460385	-0.32051632776084
H	-1.82861339015981	0.56367777736424	-0.12361644860669
O	-1.59946584731402	-0.02582076991264	-2.60528419862880
C	-2.84473649913507	-0.29787771653710	-2.95096115052844
C	-3.69867681140493	0.58494227335977	-3.66120717599982
C	-3.35307621795801	-1.56599140314133	-2.56613035808847
C	-4.99708153798952	0.20779452678372	-3.96857585931294
H	-3.33120173835190	1.56064999388613	-3.96832857792880
C	-4.64930018557195	-1.94213450110827	-2.87196788451357
H	-2.69072675668300	-2.23947372108609	-2.01853302944448
C	-5.47273743258823	-1.05097968540378	-3.57661900376646
H	-5.65664561295180	0.88233010207781	-4.51397003193525
H	-5.03816279006820	-2.91575672806432	-2.57540568803528

N	-6.82900217363115	-1.43676400750188	-3.90271725440449
O	-7.53227923756348	-0.64418732491842	-4.52663120018331
O	-7.22692950317470	-2.54345271979885	-3.54365439849862
O	0.42800108059858	3.01890380538111	-3.22607228265473
H	-0.16767151792518	3.78300960045123	-3.15553288776621
H	0.81151686269341	2.98955105919076	-4.46332348720117
O	0.79934929252807	2.68399241598735	-5.56519996459411
H	-0.03149315016831	1.98835485808040	-5.26230207936486
H	1.58176042193893	2.12781124017631	-5.71756674642473

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P	-5.72664220375532	-5.39167342287123	-2.66813295720057
O	-7.21812531816592	-5.23934157547810	-2.89229555404167
C	-4.73464070953923	-3.92430534941093	-2.30116484871155
H	-5.03193387713869	-3.13402588499426	-3.00661437302482
H	-4.91349593448093	-3.61183038208676	-1.26861804545430
H	-3.67348533363270	-4.16584593834270	-2.45660258253495
C	-5.46529085649394	-7.83968378911779	-1.60349550681941
F	-5.16357259909455	-5.50577529536827	-4.27271743079400
N	-4.97443370465678	-6.75790199438500	-2.14859496721960
C	-6.93821530930098	-8.08041445355583	-1.36530691045067

H	-7.14857676212362	-8.11539289663353	-0.28469558841818
H	-7.52408936549675	-7.27174051445899	-1.81115454703596
H	-7.25826658750329	-9.03881273667918	-1.79889695814120
C	-5.02947750274698	-10.07462279402771	-0.60828892681862
H	-5.94923395176324	-9.91419140425206	-0.03288434368117
H	-4.25591724732949	-10.35257802039238	0.12396786551958
C	-5.22002506384914	-11.20449845546358	-1.62033521953401
H	-5.49282413089457	-12.13624748106281	-1.09927896307032
H	-6.01999484086985	-10.96387983552512	-2.33780007728930
H	-4.29356815628478	-11.38881199702637	-2.18690518115132
C	-3.16469951382473	-8.64782261074847	-1.43511936213651
H	-3.01235185922484	-8.11610145449006	-2.38354278012137
H	-2.73076965056972	-9.65253026758422	-1.54458524326091
C	-2.48314884810247	-7.89876091812228	-0.29137471583282
H	-2.89156753302721	-6.88146575777018	-0.19546859990458
H	-2.62715989632039	-8.42432996190671	0.66615901867087
H	-1.40001717779170	-7.82209640960069	-0.47981447769486
N	-4.60571514870995	-8.81391490970374	-1.22375582884794
O	-6.18963744482245	-4.99838538260643	-0.13735981293816
H	-6.78252647248565	-5.69801010633437	0.16964291793835

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P	-6.60124847509738	-5.71277656649762	-2.79547719655931
O	-7.58654988793810	-5.84153478912499	-3.92650465914899
C	-5.79266896935773	-8.16885724110955	-2.15702002075919
F	-7.59919279564928	-5.30270959776167	-1.50646365694869
N	-5.77305134256431	-6.86944065573115	-1.99910527677493
C	-6.66310611422678	-8.89138791508620	-3.15827826340395
H	-6.03893025555732	-9.35420975000868	-3.93841946248782
H	-7.24534208097335	-9.68829920768217	-2.67419099902686
H	-7.34736806061983	-8.18677604298199	-3.63988862261037
C	-4.90697759474488	-10.38061481835831	-1.45851735973513
H	-3.85831525564910	-10.66040509216859	-1.27433931036430
H	-5.13331278228426	-10.70674982047003	-2.48081060303318
C	-5.81927997296617	-11.08559071604648	-0.45508091853474
H	-5.58062048873101	-10.78478052626961	0.57739262262951
H	-6.87794309374195	-10.85032319574848	-0.64624788908268
H	-5.68959314828522	-12.17714422045878	-0.53098932651477
C	-4.11100013199081	-8.27877133638929	-0.38793251150778
H	-3.95335242759702	-9.00200707541805	0.42551527849243
H	-4.64200594598732	-7.41565781376363	0.03438972793229
C	-2.77106052326905	-7.84309611890819	-0.97819445350944
H	-2.14148784865927	-7.38927699224756	-0.19582705430410
H	-2.22619666741870	-8.70320475103813	-1.39913405894272

H	-2.92036648641472	-7.10103149720197	-1.77708249172910
N	-4.98169222746120	-8.91884229352428	-1.37864805503400
O	-5.73401269536037	-4.35097992392529	-2.69629887804730
C	-5.63466258492952	-3.44855502077241	-3.80600695535421
H	-4.99857008119138	-2.61805375618910	-3.47127238249688
H	-5.17140667750841	-3.96944866201614	-4.65488149370594
H	-6.62630924365338	-3.05780388437732	-4.08324959369118
O	-4.78374972491390	-6.23500666704065	-4.59055247612956
H	-4.25241841525810	-6.86107905168345	-4.08055365961704

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P	-5.07365439427693	-5.21545249403551	-0.29660113635861
O	-6.24160007837491	-4.54432836697641	0.37131407640069
C	-5.61647943423338	-7.80847455574223	-0.59936997161199
F	-3.93435567142892	-5.23529018642970	0.95162760616573
N	-4.84438272413566	-6.76351458124580	-0.74286304942093
C	-6.92386531941857	-7.79375357252195	0.15470889133445
H	-6.81878891464693	-8.35125577350691	1.09974965828821
H	-7.20620718622546	-6.76267434041021	0.38755642276951
H	-7.73002652623330	-8.26372434457451	-0.42560609816972
C	-5.94339033987339	-10.23919974680223	-0.98670150634292
H	-6.52226821121638	-10.22257690833743	-0.05525942242712

H	-5.19652560459487	-11.03934818192509	-0.86659954291747
C	-6.85076464544533	-10.54603078226268	-2.17735514560507
H	-7.34487939616003	-11.52024000703944	-2.03331191833378
H	-7.63071713261417	-9.77690520296731	-2.29168828701852
H	-6.27359809086239	-10.59243263735158	-3.11441723368749
C	-3.94665239306023	-9.04548519064486	-1.87837810308980
H	-3.83464429253013	-8.11403751353018	-2.44781482961067
H	-4.03527341454220	-9.86879507870350	-2.60203248806862
C	-2.73567760728258	-9.26270178797640	-0.97261678500355
H	-2.62218825562375	-8.42449733146263	-0.26901015834172
H	-2.83671191449265	-10.19463875503018	-0.39366713237999
H	-1.81757660088481	-9.33410666011222	-1.57775175434988
N	-5.20777324767304	-8.98033197924684	-1.13317158320625
O	-4.21776092778311	-4.24332546957030	-1.25822391962831
C	-2.96413442343563	-4.64193320151052	-1.85783491588431
H	-2.52944804023199	-5.47597629635057	-1.28670171330820
H	-2.29828529686253	-3.77197024886514	-1.75062227718747
C	-3.13745944950145	-5.01460898683632	-3.31764404135018
H	-3.77544247446360	-5.90363613993591	-3.42650341196731
H	-3.58822591013767	-4.18542398891877	-3.88509439838546
H	-2.15142211116217	-5.23887985801537	-3.75689479465922
O	-6.65026999434980	-5.28728968560504	-2.36440053621811

H	-6.08169397624158	-5.77437614555563	-2.97597350042581
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ADPP

37

P	-1.07663104660385	-2.08007906246296	0.27086803207368
O	0.59386255474923	-2.28926772587390	-0.03087976247263
O	-1.25557190471246	-0.68537052085152	-0.59084422163769
O	-1.03564302103532	-2.01556238585351	1.77464263693548
N	-1.64519072446046	-3.21461518310521	-0.76862622262608
N	-2.62787583803551	-5.14106538315090	-1.48313572282576
C	1.14751680993388	-2.40088362463861	-1.27927606944390
C	-1.07426567129949	0.58099872200724	-0.09753067106335
C	1.40994508776254	-3.67148403660799	-1.80978355124611
C	-1.94454092007853	1.57335752626671	-0.56656238482580
C	1.50400270068069	-1.25241420323168	-1.99957085520701
C	-0.03904053370286	0.90717935957321	0.78920860656198
C	2.02688499456862	-3.79085378029214	-3.05876937510049
C	-1.78040787992815	2.89553506526729	-0.14436927159339
C	2.11970781736490	-1.38024668797376	-3.24948913717941
C	0.10971282495024	2.23312499915259	1.21064324297966
C	-2.26464836928151	-4.31995474469557	-0.47824482126003
C	2.38248463665022	-2.64692498060259	-3.78553545950290
C	-0.75537733288212	3.23188828121233	0.74893635504294

C	-2.61660000867284	-4.76951978275031	0.91500329137476
H	1.12390573920384	-4.55452308011714	-1.23490645632971
H	-2.74080224518750	1.29435145159515	-1.25941771663825
H	1.30282604029633	-0.26861824631259	-1.57321866583886
H	0.64246099700927	0.13312339372325	1.14118835929271
H	2.23015619261734	-4.78448429085144	-3.46749969877812
H	-2.46169885198946	3.66649097193987	-0.51401041531210
H	2.39808307610759	-0.48142137221831	-3.80643625695971
H	0.91687546949324	2.48506513587674	1.90350207703077
H	2.86495447411246	-2.74260572307151	-4.76150667109009
H	-0.63103053942912	4.26545392381762	1.08099368537577
H	-1.69510393208999	-4.93171697469646	1.49428725699560
H	-3.20680768106653	-5.69566990741734	0.91194019886037
H	-3.17916659922553	-3.95367879166381	1.39099643312788
H	-2.41271018294078	-4.89442159388574	-2.44405335545114
H	-3.09894048814103	-6.01925517264881	-1.30294517023441
O	-3.53465361653325	-1.70070229759104	0.55786063730565
H	-3.54227702820402	-0.87995527786695	1.06966511965980

AMP

41

P	3.29938475060222	0.66363534439922	1.49218058024167
O	4.57917238912189	0.66824093780112	0.66991548607742

N	-0.00414158943837	-0.20312809424327	-0.36489641250801
N	1.75342186699576	0.46686053575035	0.93554422194330
C	-0.93794174633077	0.38820521310850	0.59480486199014
C	-0.60062564187979	-0.89006645911453	-1.51089954319256
C	1.33526855801305	-0.11915054055776	-0.14925430236930
C	-1.30385646786337	-0.55978956213096	1.73558627544177
C	-0.95546520235777	0.04946667007345	-2.66391353502104
C	2.24645851171190	-0.71798220530458	-1.19803689466697
C	3.31217943587815	1.61742365002668	3.03482687903761
H	-1.84098824645243	0.68131769916414	0.03853953020312
H	-0.48347352498898	1.30425187893729	0.99504393982008
H	0.07188851555517	-1.68434302792973	-1.85745012762079
H	-1.50874889143021	-1.39857472480956	-1.15018253235443
H	-1.76454292355248	-1.48364674458278	1.35074983467455
H	-0.41272958350292	-0.83582163242765	2.31537155997270
H	-2.02588008503978	-0.07650783685734	2.41374167690908
H	-1.43675657209771	-0.51555738632343	-3.47849132986922
H	-1.65524790902157	0.83406785047575	-2.33492983453245
H	-0.05595014029818	0.53937798131179	-3.06853856921543
H	3.28540824544506	-0.44942259503788	-0.98287311890525
H	2.16172307644191	-1.81638591441479	-1.19251061348591
H	1.98802677049300	-0.36875958880858	-2.20790976064766

H	3.60184881030876	2.65124704870704	2.82563213818021
H	2.30847135076185	1.60331708687971	3.48111427529495
H	4.02269239155014	1.13958576177108	3.72427729385087
O	3.46915513418992	-0.92668412050641	2.22417015894849
C	2.45115149013760	-1.67218332452503	2.73712686898381
C	1.93889063672354	-2.74377551888946	1.98847736050026
C	1.94280095119589	-1.42550122090526	4.02308883762103
C	0.93143416798051	-3.55532285520318	2.51702843049814
H	2.34133406798952	-2.92937888698318	0.99068862553809
C	0.93210974404048	-2.23980605970524	4.54450331565615
H	2.34581239081971	-0.59867197027197	4.61002935919997
C	0.42087421959322	-3.30795714940505	3.79723150394217
H	0.53960353431917	-4.38475125455267	1.92185468262307
H	0.54277457536137	-2.03750995186637	5.54620769833030
H	-0.36967990122943	-3.94049912168918	4.20852147288450
O	2.84073346351706	2.95311967855166	0.64057720253623
H	2.17578726673676	2.76860033008815	-0.03661392651083

AMOP

42

P	-2.33497588830096	-1.12450382089174	-0.73402014752738
O	-2.73693785714413	-2.42818151897929	-1.60821353568262
O	-3.20395374100174	-0.91759493723749	0.48225116578867

N	1.21863937511942	0.39767502639486	-0.91098980552211
N	-0.77167035022890	-0.71615301731701	-1.00360010665139
C	2.15379426063901	1.37149685466021	-0.34613646486660
C	1.65521771339993	-0.30465126907450	-2.11933879465986
C	-0.01999956215469	0.16489941807828	-0.40825416643839
C	2.06979352644277	2.74583232000985	-1.01135108762136
C	2.27434531157105	-1.66914890776022	-1.82016580796088
C	-0.43175468364732	0.93982930288216	0.82145242487919
C	-1.94990911586619	-2.86514913359080	-2.71595095216827
H	3.16718669577738	0.95764905373098	-0.46600413327364
H	1.98817837046365	1.45924639429698	0.73455089972780
H	0.78884921479788	-0.41685859353018	-2.78476904236716
H	2.38481481910971	0.34025022570640	-2.63085792662818
H	1.07821781592750	3.19961525176881	-0.86393223061298
H	2.82798198476973	3.42022004428518	-0.58169090021615
H	2.25284160920385	2.67337847913726	-2.09518294818598
H	1.53897674690514	-2.33217345740725	-1.34041320602896
H	2.61430335784284	-2.14708495177635	-2.75328602148236
H	3.14334296365873	-1.56892419060688	-1.15035547849282
H	0.21207952173879	0.67557480173985	1.67505807373759
H	-0.34479343144359	2.02333563077288	0.65581633307008
H	-1.46738392776768	0.70460017988617	1.08391327812395

H	-2.50404370510882	-3.68494651370059	-3.19302631376629
H	-0.97033517639854	-3.23236922871119	-2.37394754572606
H	-1.80142257163324	-2.05069667683573	-3.44250105074813
O	-3.02313850611502	-0.03137893697928	-1.90288942320247
C	-2.75913552385889	1.30668735588105	-1.80526296904082
C	-1.74528319573182	1.87417447079246	-2.59157841571245
C	-3.49858139106991	2.11759550479657	-0.93112066314219
C	-1.47291140512619	3.24184380368638	-2.50087358079445
H	-1.17045375709591	1.22975120039335	-3.25890862707622
C	-3.22021715284250	3.48549407567892	-0.84521517748403
H	-4.28053406072517	1.66275739415496	-0.32080321205664
C	-2.20552312320603	4.05341422803745	-1.62562720584523
H	-0.67694201166623	3.67438514710245	-3.11263213907878
H	-3.79940051961908	4.11148945303563	-0.16073789790712
H	-1.98737987219017	5.12181018445109	-1.55262089741387
O	-1.17709172347729	-2.82488567787363	0.64210896427724
H	-0.30769871394729	-2.84567168908810	0.21983994577743

AEOP

45

P	-0.82961338574127	-0.17885828362095	0.15382412661083
O	-1.23018079283480	-1.74832103146226	0.28862268840222
O	-1.08839472687262	0.73048511203446	1.33472490811522

N	1.82079733261239	0.63640769381454	-2.53853959217125
N	0.32089244251985	-0.17638691407546	-1.01736065503585
C	2.56789276582890	1.70702959043389	-3.20138859174637
C	2.01131719584275	-0.71445561440913	-3.07124464160943
C	0.96726898168970	0.84477750748804	-1.50530794955754
C	3.98727799850866	1.87783518515847	-2.65949410986651
C	0.98745322726631	-1.07795095126523	-4.14528114473916
C	0.82169937617866	2.26042006099847	-0.99432381676976
C	-1.84983622850130	-2.26713806410755	1.47566067673930
C	-3.35811053215406	-2.08051416511935	1.46761746198363
H	2.60356473469300	1.46221763139404	-4.27445382122868
H	2.01073349815027	2.64888601380044	-3.12493139466505
H	1.95502005038851	-1.42473707269364	-2.23586453277954
H	3.03051128313071	-0.76544992465342	-3.48244553480965
H	3.97434459607434	2.16428338870559	-1.59628510054972
H	4.56293532678721	0.94371425275384	-2.75657348571234
H	4.51550316411595	2.66397539333845	-3.22268697151868
H	-0.03199690810973	-1.05401382765838	-3.73701208061774
H	1.03641659736627	-0.37479632094849	-4.99203377331018
H	1.18528857535278	-2.09092949940319	-4.53154408794241
H	0.24078018012997	2.26735836190030	-0.06622035255013
H	1.79817360282041	2.72703494434742	-0.80307936333373

H	0.29367056676011	2.87769358975543	-1.73877610199128
H	-1.59190421192586	-3.33686053800437	1.49293554107962
H	-1.39306872980149	-1.79729886138351	2.36011045280656
H	-3.80741172321571	-2.54270803099154	0.57479038951661
H	-3.79367117526479	-2.55868559282482	2.36033931100324
H	-3.63010773320139	-1.01400886372490	1.48192892804771
O	-2.16279124750681	0.32699077946361	-0.82742482732550
C	-2.33846725207492	-0.00821715460625	-2.13903417925296
C	-2.18572321427171	0.98801231266854	-3.11466594878773
C	-2.71970135753698	-1.30370097395245	-2.52125190715338
C	-2.41617500561753	0.69294284028375	-4.46146870386608
H	-1.88276615089985	1.98978333222614	-2.80220923603517
C	-2.94426570503050	-1.59146450502618	-3.87125787058130
H	-2.83202771583354	-2.07224180588360	-1.75624221339896
C	-2.79637123065603	-0.59798258972247	-4.84757492772503
H	-2.29215717397960	1.47648726712978	-5.21402668362376
H	-3.24018088898252	-2.60314905441667	-4.16246868613306
H	-2.97292595240081	-0.82939510940553	-5.90093931339386
O	1.12496125549946	-0.87608376011864	1.50233952721168
H	0.80421629069760	-0.57561674821722	2.36275758826541

ANMP

P	2.71882694680997	-0.77496182205345	0.20689551164630
O	2.95602829432477	-1.96238304146429	1.12148656676681
N	-0.91871591984499	0.51518861263443	0.17114939043335
N	1.25317569331754	-0.11675928033670	-0.13339132057149
C	-0.62561022841504	1.80671443739128	-0.45589481548645
C	-2.29247193518813	0.31921713096236	0.63984489606265
C	0.06894307921570	-0.39251494048674	0.34516831986867
C	-0.75953674192230	1.77072700837327	-1.97671785870637
C	-2.53443771012557	0.89577214944021	2.03545299160019
C	-0.27827648247276	-1.68002673077978	1.05502486159411
C	3.91564427387370	-0.47113578815614	-1.10841604545529
H	0.39074781374963	2.10417180774391	-0.16784802777845
H	-1.32140014163192	2.54441062581332	-0.02933386858113
H	-2.95698014836171	0.80742862414516	-0.08949080302788
H	-2.54398505435452	-0.74825225303060	0.61347748301643
H	-0.04857005180836	1.05280667038394	-2.41252039605509
H	-1.77839004942076	1.47919945841343	-2.27856468221115
H	-0.55012036020248	2.76646659990911	-2.40021831707404
H	-1.92244681088251	0.38071735442304	2.79084947920955
H	-2.28362570968573	1.96753564196133	2.07120032535906
H	-3.59472178737101	0.78216340969227	2.31238339938642
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H	-0.80547409538818	-1.49437773887132	2.00078080937309
H	4.89507905150881	-0.30769996748597	-0.63576537672327
H	3.93689731645050	-1.33833544187301	-1.77446359075223
H	3.62449770142500	0.43041504742368	-1.66483537900560
O	3.29006093742675	0.61035247551037	1.16916124419896
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C	1.68601267788326	0.49059228032213	2.96030115371531
C	2.38892593059906	2.62555280233537	2.01746878223799
C	0.79459405296443	1.14937832119987	3.79326380930397
H	1.77266656669583	-0.59476722547806	2.99694800089710
C	1.50246868107676	3.29038629391017	2.85221956694544
H	3.00507695566794	3.17842255180650	1.30640336751185
C	0.69596707054770	2.54593392313189	3.72627112803435
H	0.16899682909184	0.59106374206597	4.48855196807345
H	1.41249275333448	4.37572367704319	2.81827566567756
N	-0.26568171820335	3.22884718565505	4.56421456289874
O	-0.33954772713252	4.45689230039177	4.50026887323117
O	-0.98187408877334	2.55844154305968	5.30910270844320
O	1.98168143115896	-2.49168792949830	-1.66614624895886
H	1.10955234017690	-2.78579627848749	-1.36834162731668

ANMOP

P	-0.03455464894260	-0.76585345711765	-3.79207907754279
O	-0.80346444958937	0.53555228640382	-4.38153833103505
O	0.85963306519119	-1.53219085795953	-4.72967873603259
N	0.67724137550217	-0.64730914497835	-0.00839535959151
N	0.04249720851300	-0.52489361693665	-2.19113066054111
C	1.54634926154061	-1.07851377016021	1.08927366462336
C	-0.48211185568515	0.17395811429141	0.35630051632057
C	0.88471158691053	-0.97814750866422	-1.30123380349748
C	1.05562073052091	-2.35173606233659	1.77839266320006
C	-0.20983917981836	1.67122848649495	0.22586465711911
C	2.07134534622359	-1.85305218353783	-1.62534790381518
C	-0.72313969186519	0.84989792245607	-5.77373628898997
H	1.58726514434944	-0.24998491898972	1.81289064001781
H	2.57033914219139	-1.21040000896584	0.71867181999137
H	-1.32530525751713	-0.11724337096707	-0.28355943009983
H	-0.74872798984494	-0.07610801833747	1.39347460102860
H	1.72065925660493	-2.60601111016552	2.61916735066441
H	0.03726188267297	-2.21958224029981	2.17669425210749
H	1.04334667452919	-3.20201605609424	1.07867983277047
H	0.62726550381871	1.97915032207505	0.87272931803879
H	0.03822857862086	1.93181571716524	-0.81371468763470

H	-1.10179237522502	2.24550773815630	0.52403819983945
H	2.04253782587634	-2.14706539049387	-2.67875524375011
H	3.00713020587257	-1.30117336982786	-1.44701516455082
H	2.08555972234302	-2.75551181734236	-0.99742300139173
H	-1.10038978672096	0.02009859421995	-6.39204364687043
H	0.31442165510324	1.08253700798987	-6.05699725984897
H	-1.35413153996167	1.73477329258577	-5.93063077543168
O	-1.40447337252037	-1.84943161577448	-3.79823783929933
C	-2.54672174037009	-1.75318039813630	-3.10784051285359
C	-3.03346878239507	-0.55407491117146	-2.54003267484453
C	-3.30216965792591	-2.94000482810285	-2.97006837684552
C	-4.23553583708169	-0.55145099232980	-1.84693996226894
H	-2.46798892171819	0.36776166061726	-2.64794396290541
C	-4.50310806345798	-2.93937214765991	-2.27864372825403
H	-2.91724770751612	-3.85951628277536	-3.41458341873646
C	-4.96631787926995	-1.74095907449440	-1.71331662840564
H	-4.61375280691097	0.37103470027362	-1.40716298364644
H	-5.08167421823031	-3.85606011356617	-2.16794325847782
N	-6.21479035967023	-1.73163571223677	-0.98655487558373
O	-6.60796052222803	-0.67083456757094	-0.49697176911669
O	-6.84610763391781	-2.78503860937473	-0.87954889777726
O	1.93646772137002	0.93623269716454	-3.68997863913545

H	2.30512239062845	0.87158361647411	-4.58149061694665
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ANEOP

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P	-0.72571373322777	0.75007898143622	-3.16206052666410
O	-1.46331520356041	2.07252796337559	-2.60109961790906
O	-0.81380820215470	0.62180415301938	-4.65927424129764
N	2.28782652394627	-0.67233750497715	-1.21951587465878
N	0.40748424296614	0.26765781503498	-2.10038801378521
C	3.46722592518239	-1.54052044103118	-1.25669949992471
C	2.01995457878124	0.01191541234291	0.04876769144140
C	1.45469317715827	-0.49416425655535	-2.26855766728916
C	4.75606877793172	-0.78529227941724	-1.58028701965153
C	1.06193576819462	-0.76648089106912	0.94907854930912
C	1.77800920279887	-1.20842656787782	-3.55899056785475
C	-1.32302125366602	2.57523744575889	-1.25725378569063
C	-2.12517856103843	1.77595897709469	-0.24556487077935
H	3.54902024882818	-2.01930743991068	-0.26865858319870
H	3.30552068014401	-2.35293843157648	-1.97580321199612
H	1.60918374838527	1.00465079388316	-0.17665712330563
H	2.98588272358769	0.15720281918052	0.55419571012924
H	4.93672626517873	0.01999673275427	-0.85084257830200
H	5.61542740195367	-1.47403609673657	-1.54816485534141

H	4.71136227378660	-0.33571998266325	-2.58455823626802
H	0.90906419768309	-0.22576078080190	1.89694350903665
H	0.08398647796872	-0.88978840504898	0.46075842693719
H	1.46386386083033	-1.76463038452628	1.18524088923485
H	2.82491430005532	-1.05576457846029	-3.85606516459704
H	1.61615190660323	-2.29212836350740	-3.43910991588893
H	1.12492429354533	-0.84638820801374	-4.35927070823174
H	-0.25512457120963	2.59414716025597	-0.99398342001912
H	-1.68349395853591	3.61281259317754	-1.31074071079404
H	-2.06622424709145	2.27199964890112	0.73698899178554
H	-3.18422789904848	1.71694363673889	-0.54082207345254
H	-1.73239378641795	0.75484774962772	-0.14090921020940
O	-1.89190017836102	-0.42794729156362	-2.59692166603867
C	-3.18461129748698	-0.51463948493874	-2.91161977541222
C	-3.88240801452105	0.43420392172403	-3.69372554926658
C	-3.88060072815718	-1.63721386170242	-2.40400320488060
C	-5.23428670078378	0.26014288350327	-3.95503014575602
H	-3.36407440208427	1.30478312819180	-4.08886209520006
C	-5.22978254525150	-1.81116771923738	-2.66258978592270
H	-3.33103197521849	-2.36283574298973	-1.80191532133357
C	-5.90663343692377	-0.85829878172949	-3.44146316841921
H	-5.77536504473359	0.99022017915644	-4.55646871703060

H	-5.76432490936021	-2.67562958338685	-2.26973331445482
N	-7.31324388651476	-1.03194539044312	-3.71618813013154
O	-7.89245264883440	-0.18850014818064	-4.40420493396665
O	-7.89001146914541	-2.01867306556760	-3.25344624308643
O	1.17073973264272	2.42916201811054	-3.66445647286653
H	1.65484247517481	2.39291440864510	-2.82842445699797

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P	-1.66420278501866	-0.34441157306538	-2.21162051243298
F	-0.58006414213243	-1.02052012017831	-3.22641983255991
O	-2.22207665659347	-1.14869691927388	-1.03153233995077
N	1.65081851805217	0.36785503190699	0.11556302274022
N	-0.20634809939110	0.33506287791236	-1.26843259465559
C	2.63035233931710	-0.29378634138193	0.99488792900024
C	1.75062260838632	1.83367380468253	0.04597526618288
C	0.70236251654085	-0.30346367036026	-0.54332192173473
C	3.95544032697554	-0.58264067500357	0.29678600211213
C	0.84048557161675	2.53912021411889	1.04936768880319
C	0.66061467189025	-1.80143217231238	-0.44111554830795
C	-2.19651849036500	1.32488650440671	-2.68295157955232
H	2.19083841546193	-1.21086056198135	1.40422514297219

H	2.78659887385244	0.37950049444051	1.85068598453843
H	2.80152367811280	2.09117318168952	0.23606963343077
H	1.54676604621994	2.16177765726239	-0.98520154992611
H	4.40919181624572	0.34166761554984	-0.09353015467474
H	4.66072693888832	-1.03301089873388	1.01234988932017
H	3.82140089809713	-1.28145172622316	-0.54352156219430
H	0.97838309166585	3.62858504702746	0.97353032498446
H	-0.22093362309184	2.31311717416702	0.86398875558682
H	1.08377191255100	2.23155135192603	2.07824178290731
H	1.67023846959045	-2.22527457390795	-0.49625435086500
H	0.21401883403959	-2.08846358306618	0.52370543340480
H	0.05237511527481	-2.23181792170696	-1.23844950841474
H	-1.90590795958247	2.07470634071522	-1.93678840294370
H	-1.72633566923411	1.56320613196448	-3.64998115133696
H	-3.28462223174893	1.31406138864147	-2.80878888462738
H	-0.11028551434379	1.34585394169632	-1.30301982686138
O	-2.92482139466459	-1.03051147905561	-3.37767081770578
H	-3.49878513147946	-2.07802969147405	-2.83196993215851
H	-2.57564383330736	-1.17571739539795	-4.27169353963431
O	-3.78624353919430	-2.77035354753929	-1.98986100535672
H	-3.33822513616007	-3.62125252797200	-2.14264731331670
H	-3.15202643647139	-2.20554037947364	-1.35402852677302

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P	-0.14865713515156	-3.26395373934903	-1.21230924740269
F	1.20814405728421	-4.13880925414686	-1.40446635618220
O	-0.90543570119143	-3.56101990865843	0.18277342928277
O	-0.60684428509464	-2.29990413445947	-2.29796400270466
N	2.22373951530504	-0.27443268099073	0.18158082993035
N	0.81785639876687	-2.05563594099102	-0.24855850644111
C	3.20205746697710	0.74558556855755	-0.23382494573255
C	1.77317579643573	-0.19189502501134	1.58022545116101
C	1.73486769072562	-1.18929041623392	-0.65727006562830
C	4.64045880995573	0.35270527700084	0.08696740681342
C	0.47335403572163	0.59476349405248	1.73759296146671
C	2.21616701474108	-1.22508751314390	-2.07871739476591
C	-2.08800546085017	-4.34667878633220	0.38502743331063
H	2.92976327222401	1.67196344719185	0.29341232330398
H	3.07788088458957	0.95375682374029	-1.30275108091302
H	1.68276696762269	-1.20848592233265	1.99367942954071
H	2.58178605285181	0.28882804573367	2.14687620687478
H	5.32027644564429	1.17019968019584	-0.19899532397471
H	4.77042059298106	0.16143385557852	1.16362150234141
H	4.93888379598246	-0.55399085886879	-0.46200041975466

H	0.59002640002160	1.61984773611656	1.35314389448882
H	-0.35883671247196	0.11664846221477	1.19838124758464
H	0.20300845138924	0.65408270082823	2.80296165215446
H	1.97191619010792	-2.17911236479186	-2.55009121603525
H	1.72565165891832	-0.42167315886340	-2.65003750167206
H	3.30114589607597	-1.07536001804159	-2.12895003141891
H	-2.41882103899066	-4.12086846828638	1.40743688142774
H	-1.86650113838148	-5.41821137412626	0.29324557853978
H	-2.87409613734912	-4.07067018440758	-0.33039523584826
H	0.52235736908202	-2.00267740823846	0.72140081453755
O	-0.98362688310073	-4.68109059687165	-2.01054213096530
H	-0.51029773661805	-5.52653476456744	-1.94170859775639
H	-1.41174242713848	-4.37636832759444	-3.14845520893426
O	-1.69690472920721	-3.69565716437667	-4.05331465892195
H	-2.66471740645950	-3.58853888365996	-4.05749431894467
H	-1.31564897139902	-2.88931219686647	-3.53587779876189

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39

P	0.59391407543111	-7.09906390611200	1.09030694583861
F	2.08488720391026	-7.73125157482511	1.23678233800530
O	-0.17728641009010	-6.95835230560836	2.49937017720055
O	0.04319837021638	-6.72517860215710	-0.27916377025556

N	2.40715085511305	-3.45916440791749	1.19261948555938
N	1.29830090765376	-5.46430379137653	1.49048629299596
C	1.91661269438101	-2.93720519078129	2.47813027642007
C	3.22341511042404	-2.52781799289124	0.39409804069151
C	2.09196320270229	-4.68464899488420	0.76919571263885
C	0.50904962908619	-2.35148196768150	2.38344804258263
C	4.70181994569355	-2.56409465575110	0.76756986648859
C	2.62902321240241	-5.17571296871708	-0.54384538983997
C	-1.25215330650895	-7.78087157399624	3.00971660632538
C	-1.87724688777652	-7.03514161803712	4.16862258608061
H	1.97435603167613	-3.73330186076592	3.23674568240229
H	2.62917203611556	-2.16622256587214	2.80118582777558
H	2.80856826020638	-1.52368028579242	0.56575301188346
H	3.07820883870471	-2.74008408083656	-0.67159152217001
H	0.47873731268698	-1.52802938905197	1.65319848610315
H	-0.22803021891368	-3.11004153516454	2.07805942565787
H	0.20628899110360	-1.95408512860457	3.36427726880034
H	5.14146919327132	-3.55302245842876	0.56457205523804
H	5.25146263059970	-1.81359907770790	0.17857842044903
H	4.84795526009941	-2.33480939271338	1.83469387982703
H	2.58733156289858	-6.26565430298108	-0.59945415935802
H	2.01825523519872	-4.76510019047921	-1.36305462444169

H	-1.98014567971765	-7.96527462404391	2.20700046634932
H	-0.83797528293272	-8.74874543091239	3.32602855293560
H	-2.69343617769187	-7.63946542156859	4.59473564020676
H	-1.13545862172650	-6.84540321879948	4.96016059422093
H	-2.29313704155758	-6.07099914220163	3.83692469745730
H	3.66698070543253	-4.85489276314893	-0.68757025895858
H	0.94616630498562	-5.09497856063293	2.36836734323528
O	0.05148124773035	-8.83754769802751	0.92178767343245
H	0.65965608514496	-9.49117506950789	1.30439527712689
H	-0.36425639158013	-9.07408909376835	-0.23842985667709
O	-0.71584613706573	-8.85283339073547	-1.32839600705685
H	-0.49660840644789	-7.85664819870355	-1.17012229325448
H	-1.68690434085934	-8.92134956881427	-1.35051779191657

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P	0.10548362296754	-2.58955254802042	0.12736025416061
O	1.37718926973412	-1.62452617338237	0.57683012040980
O	-0.66652392304429	-2.05104177248074	-1.21923436345123
O	-0.33626642348493	-3.81586910241077	0.93950690708609
N	1.13785325084776	-3.53281381159142	-1.05102258110061
N	1.48738692294354	-5.54033885497847	0.04866966678717
C	2.71534841436254	-1.96876925820870	0.48298266745063

C	-1.50924431263515	-0.96059624792087	-1.34933615389875
C	3.51303359640195	-1.33142436592462	-0.46839814345445
C	-0.96236272655879	0.31319711038641	-1.51343387670009
C	3.24690663546926	-2.91809240089001	1.35794019289279
C	-2.88811831668134	-1.16934231894968	-1.38821963010852
C	4.86905706720647	-1.65981754826324	-0.54768275396705
C	-1.81872474670218	1.39983253822128	-1.71366216445961
C	4.60261054992346	-3.24414975589412	1.26520902755821
C	-3.73485874285724	-0.07683133035994	-1.59354123582834
C	1.74825311239721	-4.70621478803222	-0.93573949368466
C	5.41555214791697	-2.61834587402190	0.31372462059686
C	-3.20428996248295	1.20860562245163	-1.75442084660132
C	2.80449215880930	-5.05932010950433	-1.93722430264912
H	3.06231358750154	-0.59786254919638	-1.13986829832617
H	0.12169889370484	0.44058613059275	-1.47866472490148
H	2.59466508663415	-3.39975387923826	2.08880620801378
H	-3.27954392318124	-2.17956899981187	-1.25343256803967
H	5.50016142066581	-1.16732111855564	-1.29152940411363
H	-1.39850605031800	2.40071496697209	-1.84020373315859
H	5.02386420820847	-3.99218303252240	1.94125268757240
H	-4.81628712006135	-0.23168795868741	-1.62539740998228
H	6.47490726678354	-2.87618500689399	0.24429789677859

H	-3.87029191730493	2.06016215613309	-1.91268454956870
H	3.73056618758852	-4.53204616922558	-1.65392691033140
H	2.51172079915515	-4.72054636710601	-2.94074728213428
H	2.99757208486742	-6.13961516508120	-1.94966504143979
H	0.76415393065642	-5.26579672029843	0.72171188540519
H	1.97924711756219	-6.42367157999954	0.11951230422681
H	1.41200799477383	-3.00381135550517	-1.87599234970919
O	-0.88532623601152	-1.47176507558306	1.15140197772286
H	-1.28017558835943	-2.05010321801023	2.21419193474320
H	-0.45790673241844	-0.61327781971602	1.30695642069624
O	-1.51584666040670	-2.90895086700545	2.94717296741966
H	-0.91506540758763	-2.83026732744909	3.71013263738844
H	-1.07197153698597	-3.56667205403754	2.29655244069962

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P	3.64054336191181	0.51844199260008	1.19342428809612
O	4.00556160369018	0.74312005884576	-0.28854202200001
N	-0.20152116485115	-0.12630985037304	-0.21133277106081
N	1.79753029870364	0.37477940356136	0.84465908223931
C	-0.97477263532094	0.71092141094873	0.71822060341886
C	-0.99134975577757	-0.80668809311261	-1.25119197419508
C	1.12614614346914	-0.25021059802634	-0.11418311893827

C	-1.37003423844995	-0.03346008916615	1.99154026643905
C	-1.22057460726761	0.06460132740887	-2.48272165958776
C	1.84567430721365	-1.12085436437486	-1.10244132426783
C	3.37253747244451	1.90709645837234	2.34189362735618
H	-1.86948074311351	1.04559431860597	0.17597770941146
H	-0.40461177396899	1.62504002173960	0.94578371628335
H	-0.50333162345040	-1.74904749434856	-1.52383861180836
H	-1.95192734868832	-1.07852635621039	-0.78943054808019
H	-1.97174269715170	-0.92375481098826	1.75127795237976
H	-0.48806340456284	-0.36311088873585	2.55939622009384
H	-1.97095468488386	0.62542714599207	2.63695422055252
H	-0.26994146529674	0.31534712568976	-2.97801235356662
H	-1.85449534986808	-0.47328047116521	-3.20459708151509
H	-1.72858212213920	1.00458889997546	-2.21605414718073
H	1.44933112751847	-2.14422164965476	-1.04954153517172
H	1.68682973273588	-0.74764717233941	-2.12440942062356
H	2.91737298709459	-1.13246193183292	-0.90239115156756
H	4.06859068251202	2.69662436843544	2.02822130288355
H	2.34706901005056	2.29420620067807	2.33721438259166
H	3.65346078479336	1.58475086467991	3.35418475697447
O	3.68268189059678	-1.00776704736743	1.86474732868432
C	2.63292883674840	-1.73946896368709	2.38339352147944

C	2.24952149015063	-2.91447396046873	1.73377378101228
C	2.01717547149455	-1.34637154870626	3.57538218664082
C	1.22045659937439	-3.69221667778657	2.27268819957305
H	2.76070927561983	-3.20762874122620	0.81588443128835
C	0.98957956266790	-2.13048974323599	4.10577521459005
H	2.34044480534016	-0.43269275749196	4.07730173083701
C	0.58430558278534	-3.30143480906483	3.45552448281532
H	0.91575732703412	-4.60921113935045	1.76220170195967
H	0.50213955181499	-1.82080126591492	5.03340922456006
H	-0.22209908634845	-3.90933230273057	3.87211213426814
H	1.21935090809749	0.87162170899898	1.51485709321274
O	6.41066298321882	0.44440097265796	-0.47206092588417
H	6.59964796128787	-0.47642036371248	-0.72350774538955
H	5.35459143304073	0.58696791571206	-0.63144294410562
O	5.42902608857856	0.55885355925293	1.69656217458054
H	6.17535644419498	0.44349645820215	0.63963826276340
H	5.61245264695512	-0.10493534128541	2.38006719795716

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O	1.72182348683733	-1.42021557100045	1.67495488176679
H	1.45140321419629	-2.27828262483622	2.04601322615095
H	2.76626766844333	-1.36481645815031	1.74686540690982

O	2.50460778495158	-1.65767378043684	-0.55643729041307
H	1.85114013355388	-1.54241533126947	0.54242005198681
H	2.08869826626698	-1.34882134431659	-1.37713803425466
P	4.21597901082843	-1.10750416430297	-0.36087110907486
O	4.59515652114553	-2.31332543396089	-1.37427361711325
O	4.12271085890971	-1.23922776273632	1.16377130414224
N	8.11344893169485	-0.11375446083214	0.46912432432346
N	5.95665127430590	-0.44256355788702	-0.29922946996776
C	8.23957086088035	1.16215858643341	-0.25298214145505
C	9.28848557601386	-0.51356098610673	1.26262092164502
C	6.99170664794872	-0.83620385426085	0.43074253061290
C	7.66628419157041	2.33932473124646	0.53198789351503
C	10.31448267811766	-1.29187857248774	0.44475706272841
C	6.91788154907590	-2.11732257457643	1.21085407520876
C	5.75564880958948	-2.41201237939666	-2.20619304074513
H	7.77166879106573	1.07425358028141	-1.24592553921834
H	9.31014826479502	1.31339885954215	-0.44635897862605
H	9.73244398406319	0.41349195592780	1.65440891370779
H	8.95949603340066	-1.08833912980629	2.13599540861943
H	7.80464028362181	3.26952637677759	-0.03894028882278
H	6.59017219225331	2.21538371805830	0.72113184928043
H	8.17988952261059	2.44620674613239	1.50001270876789

H	11.18953557468496	-1.52510312799786	1.07093107524308
H	9.89274094885569	-2.23840549114551	0.07235389967223
H	10.65954053745208	-0.70492882524135	-0.42079419565042
H	6.80498292055070	-1.89363937774577	2.28277731644079
H	6.05942822459262	-2.71655879402938	0.90017010949645
H	7.83547810841316	-2.70261777708539	1.07308550412807
H	5.96023527940386	-1.46528715354133	-2.72570201347579
H	5.52554656763405	-3.19035747693880	-2.94635872345159
H	6.64132123861465	-2.71479589743556	-1.62969157034559
O	3.79695679288813	0.23926142432509	-1.23475709165442
C	3.99233118673228	1.54349731856544	-0.82392831125938
C	4.56101378451498	2.43317408032393	-1.73943989603699
C	3.61051417544416	1.96701813497834	0.45329709881987
C	4.74493471611731	3.76870879052079	-1.37047147145487
H	4.85155671292324	2.06794050852766	-2.72665668297131
C	3.80823236430876	3.30320388991382	0.81128432617019
H	3.16422917529939	1.25608117373084	1.14918432113372
C	4.37254718751444	4.20702907560233	-0.09563154150745
H	5.18838196234699	4.46731334941013	-2.08415178027519
H	3.51361423172146	3.63863803315299	1.80876067592295
H	4.52328275384223	5.25005972955068	0.19179358359622
H	6.11828591000332	0.38118192452330	-0.87168492221538

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P	1.07983244823260	-1.80208257098099	-2.89285676267390
O	0.07631430058880	-1.99486355686489	-4.15844812286891
O	2.48186579330871	-1.19046666717173	-3.01443330075166
N	-0.06831089151685	2.01027217297542	-1.81421021920982
N	0.26758042963965	-0.14743332725921	-2.58403427876246
C	0.24103410955016	3.13378301607001	-0.91415672840701
C	-1.16971026125265	2.24195433381022	-2.76018021820297
C	0.59946908503992	0.85352268417947	-1.78115690803116
C	1.21340111065644	4.13526950582465	-1.53021438183729
C	-2.51688620120211	1.75670757476188	-2.22909973254795
C	1.72073330475245	0.68957659345652	-0.79784641406229
C	0.44918582234874	-1.49486660948967	-5.46514964737092
C	1.47767306788047	-2.37416290192254	-6.15198766863777
H	-0.71623928785071	3.62225415149264	-0.68017351464697
H	0.62855159225373	2.74596464723234	0.03494909945787
H	-0.92203470871174	1.77157063911529	-3.72408246817657
H	-1.20115677351835	3.32287713881896	-2.95359829493296
H	1.37400520402027	4.97229298886283	-0.83307882058141
H	2.18832373127275	3.66857293799034	-1.73930932784684
H	0.81867113483943	4.54684761430974	-2.47247666354439

H	-2.51467183591165	0.67247579752953	-2.04540499384153
H	-2.76704352966763	2.26190579762437	-1.28324897607962
H	-3.30837154622162	1.98197652947904	-2.96025361064743
H	2.19506921814713	-0.28694682709572	-0.90438221973872
H	2.48326590767997	1.46610745337620	-0.95088918780096
H	1.32877050911127	0.79362765826626	0.22397565526057
H	-0.49312165161076	-1.46734194495543	-6.03031021737124
H	0.81545627963769	-0.45948786287590	-5.36454474381701
H	1.11851021426966	-3.41199577532455	-6.22464345973210
H	1.66096562451299	-1.99307088275479	-7.16918921325311
H	2.43068303631582	-2.37234875630534	-5.60383004932769
O	0.38996918519068	-2.45404309852820	-1.54403132104139
C	-0.75258693477918	-2.01993923702348	-0.89324029152567
C	-1.99807571748081	-2.13793528280099	-1.51477910948119
C	-0.63733061392994	-1.53324880688722	0.40898053363232
C	-3.14437043432975	-1.74594482382319	-0.81919993121965
H	-2.05602494139188	-2.52382106257655	-2.53394837666327
C	-1.79143000934948	-1.14373325896984	1.09553626752357
H	0.34906353728228	-1.46569210808970	0.87027675579886
C	-3.04531619806761	-1.24555405930028	0.48421747357429
H	-4.12098269011096	-1.83019571109031	-1.30203346660415
H	-1.70683141615947	-0.75826639585061	2.11454854646097

H	-3.94438834336731	-0.93740756271436	1.02281347609065
H	-0.56257259171678	-0.01291393125966	-3.15352758068894
O	4.07946355772641	-3.05908591105298	-3.10733917022890
H	4.46403985797062	-3.17697655078116	-3.99372032078817
H	3.63051400973456	-2.10851310366942	-3.08879864584319
O	1.74332373435796	-3.47543657898016	-3.14127511074360
H	3.02672212677346	-3.50527844313276	-3.11284243288806
H	1.23499864505262	-4.17063562564408	-2.69532190538011

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P	1.35146637335300	-2.28583683357749	1.47693682633569
O	-0.02727794233727	-2.79066055095404	1.93343933154735
N	-0.34652245045826	1.10918281347682	-0.24556032538374
N	0.68035548795119	-0.86982243593734	0.38647731060273
C	0.86428569963227	1.60393112753626	-0.91635163033740
C	-1.52098496045142	1.99304777026249	-0.34223826436684
C	-0.38006482279236	-0.06816746946778	0.39081679515550
C	0.99066320308547	1.11553291796652	-2.35778645490248
C	-1.57379939819796	3.03958801562526	0.76716470362640
C	-1.65071478864635	-0.48157572423947	1.07006867871565
C	2.26341105776500	-2.94982810411239	0.05154322447554
H	1.74735709522492	1.32987669166491	-0.32072796891429

H	0.81804253726097	2.70115988708788	-0.88547777425591
H	-1.46554512668804	2.48263259709667	-1.32540766801939
H	-2.43469930584684	1.38743840582393	-0.35242528397622
H	0.11729719711481	1.42413935930082	-2.95283362432831
H	1.89215354159693	1.54728844492370	-2.81883646929032
H	1.07054521132867	0.01840560042466	-2.40888531648885
H	-2.41190646499929	3.72962483292463	0.58410103309561
H	-1.72317872907566	2.57476585952201	1.75241452217323
H	-0.64570371431146	3.63107862413373	0.80580345624785
H	-2.01199146010552	0.30948791171506	1.73875857859433
H	-2.42219851842912	-0.66150785055129	0.30443845492162
H	-1.48234612407883	-1.40419899765375	1.62720691803868
H	2.19454878304850	-4.04306981871748	0.11081173789397
H	1.86222221107395	-2.58632495114388	-0.90125256956629
H	3.31981539075955	-2.66036025465342	0.15702504600438
O	2.22100809011895	-1.12657553411024	2.33947790628239
C	1.70275911454712	0.06191090727077	2.76163969358395
C	0.54531457296282	0.09151779815464	3.55195700638277
C	2.35859648564499	1.24457740263811	2.39695076214936
C	0.00842504972926	1.31561392721779	3.93376674450872
H	0.06814584281936	-0.84511182076473	3.84126548035452
C	1.82548979507586	2.47048766569727	2.77755019833584

H	3.26474256816838	1.18647804246622	1.79224457198807
C	0.64551827348780	2.49009971596670	3.52606138947449
H	-0.90272317141457	1.36866707013709	4.52788126910603
H	2.29839803405975	3.40624807037329	2.48318016342230
N	0.04388145046226	3.77898742514439	3.86794759976022
O	-1.00690498525210	3.77686136949626	4.49663674714612
O	0.61154791931349	4.79804315125245	3.49642638549634
H	1.45509398077296	-0.50294915365141	-0.16317536239490
O	0.38870105175634	-4.16027573052366	3.91160435106373
H	0.30798161084553	-3.62973024516988	4.72448380983015
H	-0.04289480021075	-3.59084014631534	3.12280070546993
O	2.23833955935442	-3.49238794018392	2.53824781434842
H	1.38590024949739	-3.96280115111753	3.47561534516695
H	3.05618932548381	-3.11641869245531	2.90149415092597

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P	-0.25820754552970	-1.14746225256498	-4.40683164472430
O	0.03832536763410	0.44307521586368	-4.52307103063101
O	0.80229383346601	-2.23705981790527	-4.54640586035077
N	0.34725663588943	-1.34705467576671	-0.36640341952096
N	-0.01033376534528	-0.87836053196801	-2.60282682463573
C	0.40185955543170	-2.27301678439899	0.77803934402715

C	0.62701789324931	0.06256993742526	-0.05212483201556
C	0.05312861829176	-1.74983809213520	-1.60407831236884
C	1.81258390766832	-2.78121280101408	1.05891855941716
C	-0.64005682314974	0.86851263985338	0.22621280502006
C	-0.23250529443987	-3.20207078260636	-1.85091032079675
C	0.17836962727987	1.22192710789309	-5.71840291519210
H	-0.28847692292077	-3.10642132727505	0.60617391592986
H	0.01167517383408	-1.72241642099312	1.64655136310747
H	1.28426247571558	0.06720309200869	0.82791948131340
H	1.21847376917899	0.50639381878726	-0.86726930729860
H	2.20354710261138	-3.36413844836944	0.21084307291046
H	2.50505797639100	-1.94736153215445	1.25340394021301
H	1.80134906133825	-3.43001415732083	1.94837474450286
H	-1.30191558832938	0.89990215143052	-0.65140642019859
H	-1.20392547865241	0.43053252801948	1.06436566438820
H	-0.37148145112002	1.90207313762672	0.49295258771492
H	-0.39757111996269	-3.39589449395077	-2.91153733208859
H	0.61181210430560	-3.81911167013276	-1.51365874604828
H	-1.12337550866361	-3.50314892445086	-1.28124459933350
H	0.53021256813007	2.20749318769303	-5.38566989020735
H	-0.78512137160617	1.32571584797245	-6.23492576752182
H	0.91423762388790	0.77244384832176	-6.39800140376069

O	-1.86453273683944	-1.56248316975597	-4.17426633874117
C	-2.70912965544584	-1.09678347019735	-3.20694289909694
C	-3.44080943193428	-2.03869307895294	-2.47309379877210
C	-2.88388034524291	0.27784366042656	-2.99261244819716
C	-4.33952707845687	-1.60847638206188	-1.50245926608924
H	-3.29346256378745	-3.10100609709292	-2.67075427207018
C	-3.77875235519081	0.71142596177741	-2.02147499812190
H	-2.31200248217531	0.99684029108676	-3.57951514469459
C	-4.49226946511609	-0.23719653278962	-1.28385461607901
H	-4.91533089469523	-2.32063201346918	-0.91296882252350
H	-3.92701321462083	1.77292739579539	-1.82859831550563
N	-5.42723437484543	0.21988905168689	-0.25381363478932
O	-5.53742307640914	1.42489918280880	-0.06874035150352
O	-6.05251553428815	-0.62489750522516	0.37345968919351
H	0.16424342520612	0.09652909049497	-2.37866077420972
O	0.65451955921106	-3.07723212439537	-6.88003588814157
H	1.39665493804773	-2.76157331236805	-7.42546605741585
H	0.93683125481154	-2.94283922025716	-5.89355350650738
O	-0.68845353671596	-1.24412818254777	-6.18089084629946
H	-0.09548903317866	-2.19288907541425	-6.74698812203146
H	-1.64032233291750	-1.16792840943723	-6.35715989025421

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P	-2.13190032352087	6.21327497186993	-7.66695479927557
O	-2.74510424235943	6.83650494387906	-6.30260165198931
O	-0.72554783919849	6.49320361508210	-8.19580063177677
N	-0.58271836168219	2.85921324482282	-5.90647374603573
N	-1.64481893120074	4.79499662705784	-6.59609322746113
C	0.20603047481755	1.64276052469016	-6.16784657194755
C	-1.00087210440895	3.05568568940315	-4.50991114063622
C	-0.91022900532448	3.72383436409880	-6.86861067680108
C	1.69678763709880	1.84109487605332	-5.91136089359166
C	-2.40851116690558	2.53043106770607	-4.23711188493618
C	-0.45906193790312	3.45627836381551	-8.27441678352360
C	-3.13961184538924	8.20421473011178	-6.04650150201291
C	-1.95422264873778	9.14826005994110	-6.07366093333019
H	-0.19670949750718	0.85919041234902	-5.50934207031617
H	0.02611224224549	1.30538242239033	-7.19462676852098
H	-0.90804918452793	4.12146656377350	-4.24954517845209
H	-0.26812195264392	2.53142104934615	-3.88188007015267
H	1.88271732160211	2.16247138739473	-4.87467620010781
H	2.23019198126541	0.89203155047357	-6.07560020618310
H	2.12115992238404	2.59819754742724	-6.58878004211563
H	-2.65964452034772	2.67336376350552	-3.17500977591963

H	-3.16116484260945	3.05544420043105	-4.84286943260452
H	-2.47478865112666	1.45564695664426	-4.46681291817118
H	0.63097642449189	3.32249660203053	-8.30645970390135
H	-0.92624264860340	2.52980647328563	-8.63884539154284
H	-0.72431770595977	4.28141018099958	-8.93681980849255
H	-3.91310539437595	8.50208722835295	-6.76547375826163
H	-3.58875926673862	8.16124351568433	-5.04408921920246
H	-1.52253780419933	9.21395304004442	-7.08236653537350
H	-2.27920602769506	10.15661184812909	-5.77193588963879
H	-1.17150274004125	8.81147683507290	-5.37615419672185
O	-3.18399832617640	5.24813181528024	-8.54225928927184
C	-3.89883309599151	4.17778574879852	-8.08362132173228
C	-3.84148948827964	2.99069397639422	-8.82418227004678
C	-4.70809679120807	4.27746557966608	-6.94292286328283
C	-4.57780244077983	1.88496930280009	-8.41167266940331
H	-3.21476551312958	2.94676763575068	-9.71562057319520
C	-5.44407606381029	3.17420868152685	-6.52692578191688
H	-4.74739735105182	5.21271437192783	-6.38426919679234
C	-5.36511613136965	1.98851657324056	-7.26236097332940
H	-4.54283103980008	0.94720795584812	-8.96447439802403
H	-6.07324744529069	3.22201088593768	-5.63927907384639
N	-6.12891341542680	0.82215858988982	-6.81500812721593

O	-6.04355514863902	-0.20879196213154	-7.46933278592213
O	-6.81427169313064	0.93363029843853	-5.80693804048024
H	-1.94910469747074	4.91671272022955	-5.63476511983346
O	-0.94405558964958	8.29022278823561	-9.88656336545893
H	-0.62636578692399	9.15329354016820	-9.56837925148005
H	-0.56280592970587	7.56698308250926	-9.24459590458732
O	-2.85095981250626	7.56685448588140	-8.66729743452031
H	-1.99382732568141	8.08601157393032	-9.43073974174152
H	-3.70745032487607	7.34449399981111	-9.06660872892150

PATH10

A230-H⁺

44

P	-1.53260669174080	0.13624349578477	-2.12256464185735
F	-0.27306397689690	-0.50976590125835	-2.89733642349175
O	-1.65213017582162	-0.22022439996173	-0.65418530296119
N	2.43382504600279	1.91611957471008	-0.70893027907260
N	0.21003682449047	1.46628483314632	-1.31190764808197
C	3.83385252970160	2.15067987859249	-1.07100393937200
C	2.11671623969954	1.95186822882592	0.71991383562515
C	1.45718368356697	1.66675582969114	-1.62421630376733
C	4.18577287197068	3.63203711864897	-1.19623995901685
C	2.01524615518558	0.55927629762967	1.34495156419087

C	1.84762724909496	1.61651435422357	-3.08053667887014
C	-2.09785175146044	1.70446353043849	-2.81414807193337
H	4.06602082556272	1.62205506381272	-2.00380198041278
H	4.45635468521200	1.67964017352459	-0.29373996474855
H	2.90609950820797	2.53279227728785	1.21772078263369
H	1.18351015483388	2.51856422478760	0.87465520893266
H	3.98409474870308	4.16908273977082	-0.25553236027409
H	5.25516783297442	3.75131470365918	-1.43332154339528
H	3.59931844584697	4.11157789476961	-1.99600801597169
H	1.80369154733287	0.63878685437141	2.42304820982390
H	1.20848263676839	-0.02801467935095	0.87972257559392
H	2.96033346867364	0.00787485908481	1.21794364243285
H	2.39440615601934	2.52230286360676	-3.37966505214445
H	2.49703068933873	0.74966818783598	-3.27970669820721
H	0.94792010378107	1.52279461615874	-3.69565544729825
H	-3.16314694046052	1.60505185709150	-3.06346719443397
H	-1.92744279386548	2.51089221615253	-2.09505687026959
H	-1.52254414533739	1.90635390830242	-3.72942061502663
H	0.01671158349363	1.48792470138605	-0.31266493426473
O	-2.64051610781930	-0.80523974817349	-2.92036757359868
H	-2.55473038346411	-1.79709208634797	-2.73986122148297
O	-5.18921821870227	-0.52553578874978	-2.25326738170122

H	-5.72932726624027	-0.94527504519058	-2.94318243909417
H	-5.26346321769985	-1.22685627349510	-1.10425090730617
H	-4.24341984819470	-0.59526521828772	-2.57109362057284
O	-2.67293788658507	-3.34717590535647	-2.29368133501668
H	-2.65799435703810	-3.21401574749441	-1.31822113157093
H	-3.59789900118081	-3.57968902382714	-2.47589957225523
O	-5.26464513766042	-1.78512890943492	-0.15427614392027
H	-5.72418897908837	-2.63065921119571	-0.30499906104049
H	-4.27395586819789	-2.01602187407112	0.07694485534083
O	-2.83316448758305	-2.31198326689661	0.21599286171235
H	-2.32315593435636	-1.47718742350842	-0.06463316264072
H	-2.51079981706754	-2.57637552069357	1.09203173878602

A232-H⁺

45

P	-5.93772526137818	2.28114264642280	-9.78775192688105
F	-5.96331353304191	1.41422932414796	-8.45119085907543
O	-6.83852505293989	3.58472761632397	-9.59299284640806
O	-4.64714587137521	2.39486869105656	-10.54184978953782
N	-4.01764043004003	5.35890214658865	-6.66254687398326
N	-4.56439349139348	3.64397644381847	-8.18958453302664
C	-4.34740175919022	6.16196827903469	-5.48414086804609
C	-2.75654550594341	5.67669304472995	-7.32895121721073

C	-4.83005922784493	4.37191607965231	-7.15087114917839
C	-5.04488962688362	7.47862741501446	-5.82518781487575
C	-1.60196428612401	4.77383907427032	-6.89300619432589
C	-6.12808548550850	4.11003909009206	-6.42376045278788
C	-8.26892411611761	3.58198113137223	-9.76971676619686
H	-3.40706069545696	6.36303187399312	-4.94596308152367
H	-4.96622947216597	5.57146204927665	-4.79688718502762
H	-2.89808538111373	5.62419724891161	-8.42112190271757
H	-2.51798320167505	6.72738633507401	-7.10687630821230
H	-5.23521528565956	8.06045572094860	-4.90891620467087
H	-4.42430061574984	8.09409559845861	-6.49623382234453
H	-6.00950720716001	7.29570341683420	-6.32452741325541
H	-1.43520772355558	4.85266805148380	-5.80679504799954
H	-1.81233286664997	3.71957218642666	-7.13159091033994
H	-0.67084524586305	5.06330679266334	-7.40592560809811
H	-6.75581977038879	5.01280423822522	-6.37917416013098
H	-6.67380460860111	3.31824629314815	-6.94485960076995
H	-5.93990519538948	3.78493951717023	-5.38869016464431
H	-8.53136874960483	3.38394578084925	-10.81836041715965
H	-8.60529962527459	4.58613470121703	-9.48251603007369
H	-8.74295872187899	2.83239382010486	-9.12021832311450
H	-3.67622733209113	3.86101827716534	-8.64041201490975

O	-6.94203159407869	1.27327434056500	-10.57544860305947
H	-6.98344214017398	1.39810752105471	-11.59254241117089
O	-6.38051446748217	-1.35407909561523	-10.73953348026379
H	-7.16620896666318	-1.76327292159371	-11.13919188708145
H	-5.36684001739017	-1.31048871724927	-11.65101829618661
H	-6.64411961307217	-0.41633175321525	-10.54954136682684
O	-6.96401533399806	1.39057241698997	-13.13968383884863
H	-5.99132895164096	1.41760332527561	-13.29296767265224
H	-7.21459081213651	0.48866341830397	-13.39923191113115
O	-4.53567874371437	-1.24184936870240	-12.36060184123185
H	-4.82640474478572	-1.64470794159030	-13.19872771899939
H	-4.35488916284490	-0.23646203775202	-12.55565726472865
O	-4.26751324138762	1.22519865578048	-12.82080198850089
H	-4.31864848339814	1.71461625421961	-11.94096595266132
H	-3.48663147117169	1.55122372905249	-13.29612902012679

A234-H⁺

48

P	-0.40198194982558	-2.56613428037150	2.13588152292889
F	0.59741583997548	-3.63220719400059	2.77455304773383
O	-1.81284655383966	-2.61329856061881	2.87510889267666
O	0.14790047368908	-1.24317356502782	1.69001738628607
N	-0.50308471029038	-0.78199465391417	6.45927478322578

N	0.13944408490694	-1.54974709171461	4.32261995937643
C	-0.06498971078377	0.58764453721094	6.19754155270421
C	-1.11506404034832	-1.02689065027791	7.76657942506620
C	-0.37572691270539	-1.74447345227670	5.49777604405467
C	1.42983988560707	0.79702179319831	6.44097091210825
C	-2.60699286524673	-0.69617751655743	7.80403842133820
C	-0.86772324743798	-3.13410800806358	5.82572139955987
C	-2.84522198622029	-3.60979866331097	2.63393122487292
C	-3.91868915213320	-3.04583933577150	1.72739940502838
H	-0.33173181781527	0.86488613331058	5.16416566244196
H	-0.64954671565221	1.25445685797937	6.84820688996500
H	-0.57501454287198	-0.41390793733960	8.50595998959694
H	-0.94936196073677	-2.07041019434220	8.06196315664139
H	1.69206148614722	0.55793969825431	7.48409084423362
H	2.03272675442494	0.15471465850816	5.78022051779726
H	1.70826618127819	1.84542415023757	6.24812860446138
H	-3.16930457479636	-1.33029076295142	7.10040944448448
H	-3.01080907235411	-0.86075992719563	8.81599850337252
H	-2.78620338871634	0.35662626543247	7.53291467848771
H	-0.67684232262183	-3.79009857984349	4.97169547829136
H	-0.34593565105035	-3.54048264926906	6.70560530456776
H	-2.38992964986952	-4.51477761170278	2.20955380632058

H	-3.23943702251851	-3.85039463456793	3.63144056305360
H	-4.72274963477630	-3.78875543658179	1.60188991321675
H	-4.35528238891018	-2.13311336117000	2.16256151784808
H	-3.50810623482220	-2.80320625004116	0.73608268146161
H	-1.94593506134584	-3.13627447640660	6.04646765764639
H	0.44562833097858	-0.59324582957121	4.14817270309897
O	-0.66705673831268	-3.49073734450015	0.81471126022292
H	-1.18542867590557	-3.01730121546056	0.07379769223683
O	1.43757922549709	-4.24210447392527	-0.67947645444128
H	1.14350025811523	-4.98275764286865	-1.23600799428605
H	1.56277985167917	-3.12146858027020	-1.43247511342579
H	0.68801941056166	-4.07500110886792	-0.04926977377325
O	-1.88644900206564	-2.24699776778195	-1.09470482344129
H	-1.29447560003497	-1.46151630954757	-1.15384716513667
H	-1.72422191504615	-2.73525860782206	-1.91826260180896
O	1.65445989983580	-2.18972275575719	-2.00657543621801
H	1.24235013562105	-2.33252085723481	-2.87777400792714
H	1.09953491892681	-1.45355996558643	-1.52791824929582
O	0.19009753478850	-0.52455257532341	-0.79997488993872
H	0.22396711934076	-0.71731789525979	0.18929897559140
H	0.31915474768070	0.42979783896327	-0.92039809230684

ADPP-H⁺

P	-0.02106450344778	-2.35994503020930	-0.02985464465539
O	1.20842302876499	-1.34766966571919	-0.32923593467011
O	-1.04505846913233	-2.46482829775659	-1.28383031792119
O	0.13906346220173	-3.59540758189429	0.82108113014253
N	1.24506704282775	-3.68288903531189	-1.68037034092980
N	2.19829088614830	-5.22650954923397	-0.27476438253462
C	2.56133814842628	-1.63695626341984	-0.25987149013320
C	-1.60088426893617	-1.34508261585288	-1.89571427889036
C	3.11655379716629	-2.13158926246463	0.92045201206047
C	-0.85824441149910	-0.64701804315883	-2.84939347649045
C	3.35105024961380	-1.36027544812171	-1.37601548471903
C	-2.90837711067724	-0.97845733149077	-1.57499506884911
C	4.49292406600102	-2.37310447303477	0.97101567083368
C	-1.44674930158318	0.44130617150266	-3.50037859969640
C	4.72495614772794	-1.60059413769714	-1.31163765265909
C	-3.48623632058341	0.10927763366713	-2.23581545438453
C	2.13245139481205	-4.60402421469833	-1.47287282417720
C	5.29901318447516	-2.11376536988953	-0.14166742152572
C	-2.75944034198427	0.82000114406266	-3.19794410546687
C	3.15737971064520	-5.02020162231083	-2.49875140934008
H	2.47741664649967	-2.30950674992149	1.78593843166114

H	0.16322237953767	-0.95920092395712	-3.07359267640318
H	2.87949152276471	-0.97562269793749	-2.28186757169305
H	-3.44401299591086	-1.53452006711288	-0.80387330231658
H	4.93525849345876	-2.76428106038921	1.89063407238469
H	-0.87444315675231	0.99348832957141	-4.24995616308258
H	5.34955085807471	-1.39175463026396	-2.18370009653284
H	-4.51009172287599	0.40468440263568	-1.99295589297305
H	6.37362479825546	-2.30592896920712	-0.09736885430882
H	-3.21561578864957	1.67010237952511	-3.71083070777338
H	3.34782209707353	-6.10326452655001	-2.45701483139933
H	4.10482390473771	-4.49886982950495	-2.28277952101709
H	2.83318522022338	-4.74435761202110	-3.51117718528808
H	1.60329992707540	-4.85756625426068	0.46529772885166
H	2.98930841652808	-5.81282087038164	-0.04385269750626
H	1.29563985316421	-3.30691051089150	-2.62679099389808
O	-0.82005203037787	-1.24829505330484	0.87146650409681
H	-1.74132486505502	-1.56782406003315	1.15859862534186
O	0.51731384764372	-0.91393305127304	3.17008338687423
H	0.50731885333084	-0.00172645778412	3.50340981966123
H	-0.15397429760904	-1.77489476896896	3.98292561428913
H	0.03394685484924	-0.90087902957839	2.30037913864824
O	-3.11057981913979	-2.19408749708296	1.65813826617379

H	-2.78043838064228	-2.99456169098483	2.12643424462135
H	-3.49089525052050	-1.63740266954719	2.35639979913926
O	-0.69678561410340	-2.52504288166742	4.56591798516506
H	-1.48634738028652	-2.09264125881418	4.93901468837750
H	-1.03565796054408	-3.23944508418924	3.89093282954761
O	-1.51047022015967	-4.10622657758419	2.77434091583292
H	-0.84947103526213	-4.00791978694648	2.02236110787509
H	-1.61658279629521	-5.05530826854135	2.94836062965728

AMP-H⁺

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P	5.20312196272007	0.92324329196392	2.46957173114994
O	5.20979736525306	1.10590633077186	0.96157108606181
N	0.67604048010345	0.00790159439038	2.08619064398026
N	2.88196826748964	0.81309613058156	2.10917495494706
C	0.65015048570503	-0.12319461738955	0.62936070199303
C	-0.56644837874458	-0.32527371208510	2.78868955764342
C	1.80158298443404	0.42726304560948	2.72322666721215
C	0.30130573582256	1.17914381594774	-0.09115590538982
C	-0.71541853444983	-1.81747142997566	3.07999274558154
C	1.79425227140978	0.45331279135674	4.23062094084735
C	4.79411090732011	2.29102101736733	3.57839389027873
H	-0.08870106406295	-0.89955911685473	0.38205923556549

H	1.62287915639822	-0.51321538078163	0.28970630553447
H	-0.62848678050696	0.25689385300043	3.71685065429778
H	-1.40160460155565	0.02090163362457	2.15917710938677
H	-0.68609957770765	1.54930789243289	0.22793781135445
H	1.04430712419553	1.96434667887390	0.11868966253905
H	0.27155969146461	1.01713195518943	-1.18029900226081
H	0.08006454212159	-2.17220649591102	3.75280087361722
H	-1.68866626351644	-2.01659905638895	3.55621351184485
H	-0.66073555680250	-2.40979065559353	2.15286999615311
H	1.19689916955201	1.30484571060914	4.59478252076055
H	1.37024182886901	-0.46509766946905	4.65652741292362
H	2.81934462232732	0.56841847907152	4.59554179455213
H	3.83664781315839	2.74134251723220	3.30782806857753
H	4.76247705632293	1.90589812911544	4.60765267600566
H	5.61430582843142	3.01893394810036	3.49896090409164
O	4.96702772339456	-0.58013285267109	3.11164949660791
C	4.24332583144655	-1.62111360989983	2.57467178989512
C	4.33497811732446	-1.96483501445426	1.22142704828111
C	3.44958090654020	-2.36863385941371	3.44786541636585
C	3.58916735091549	-3.04398853388775	0.74071791317496
H	4.97689123063200	-1.38795566377099	0.55832911028475
C	2.71654174570466	-3.45189801615796	2.95703574377010

H	3.40833883303439	-2.08710592956682	4.50089789636519
C	2.77338438343719	-3.78795401595839	1.60047156064426
H	3.65160276562277	-3.30568186604685	-0.31867888631270
H	2.09104570687950	-4.03093643141020	3.64081883070123
H	2.19195510320525	-4.62948347989056	1.21672753668769
H	2.82404719092386	0.79662311616255	1.09315324964030
O	6.83292452858807	0.90088820700390	2.90895651637968
H	7.29021278648329	0.05973112935974	2.57643492649771
O	8.28586553075632	2.71680232546645	1.92332036864293
H	9.03799026184049	2.88893523088480	2.51715098889454
H	8.67176288879199	2.25683121575109	0.98304489755256
H	7.68666504086552	2.00022578808963	2.37930266712933
O	7.99718560082196	-1.16179569715641	1.80252470384561
H	7.70636309708359	-0.94193524466273	0.88524477448067
H	8.95181605866972	-0.98673807185864	1.79396104661615
O	9.06522077864291	1.66201595858100	-0.13503114749941
H	9.82353575082259	1.09051303517463	0.07266892321688
H	8.32751844124633	1.03242648185063	-0.39520566355530
O	7.05759193900908	0.00163562849358	-0.46280021233301
H	6.29045883955563	0.45472876466361	0.01311472528710
H	6.71399503200938	-0.33978927546507	-1.30234077051024

AMOP-H⁺

P	-2.43832849042293	-1.03581900186062	-1.43711759161259
O	-1.66161211315500	-2.14301298635313	-2.30781683127281
O	-2.37425578732875	-1.16448904926347	0.06255079448019
N	1.87808942446215	0.20405179496616	-0.44980833322241
N	-0.28562091722242	-0.12395225420879	-1.29226546046503
C	2.00609010163994	1.52148463237610	-1.07453228467627
C	3.01973262312412	-0.24418956220006	0.35194936097571
C	0.74283118391846	-0.53136088346798	-0.60588477160805
C	1.36185570904352	2.64155706055596	-0.25756983188677
C	4.10972016162783	-0.92457994126812	-0.47442618084595
C	0.68424679831188	-1.88471663528785	0.05748898677202
C	-1.21693884387767	-1.89310004988637	-3.64422871378223
H	1.58043442178146	1.48659736682798	-2.09109671279432
H	3.07960440025167	1.71931608710295	-1.20714629376513
H	3.43068197619177	0.64214792556135	0.86113633031390
H	2.66802593098509	-0.91174581203387	1.14820858925352
H	1.50930910112287	3.61165291373781	-0.75730973678777
H	0.27949145556148	2.48404299777527	-0.14143481007594
H	1.81286721907593	2.69789739654178	0.74590308114106
H	4.95836771963576	-1.20377714247859	0.17033371043841
H	3.72846507817903	-1.83778342019526	-0.95814480690567

H	4.48771851132406	-0.25361447537550	-1.26240132990658
H	0.61237521957065	-1.77196741262108	1.15085722074611
H	-0.19749663910563	-2.42407425728392	-0.29443333933259
H	1.58422838182841	-2.47594846849434	-0.16171149896380
H	-2.06452166216567	-1.62509481998055	-4.29405746019756
H	-0.76025071969937	-2.82488643320708	-4.00186366639706
H	-0.46907889985160	-1.08650066913449	-3.64764713262897
O	-2.65704499899319	0.37506909335027	-2.23074059904232
C	-2.42998941531499	1.65303374031225	-1.76363496766374
C	-1.92332673406256	2.58097826162478	-2.67676214297419
C	-2.73548206676518	2.02354126933245	-0.45072979319717
C	-1.72521021638723	3.90305941683596	-2.26965246852482
H	-1.69166642731606	2.25482711340261	-3.69261036923354
C	-2.52606338211019	3.34762507084764	-0.05627637390965
H	-3.12476689317748	1.28162279679484	0.24610391964208
C	-2.02447746978891	4.29090166953914	-0.95955397021542
H	-1.33039589145414	4.63129674076530	-2.98234061200645
H	-2.76069064154376	3.64205647419406	0.96972343874316
H	-1.86421932825664	5.32379360633345	-0.64220413905538
H	-0.15811818572184	0.80170143953972	-1.69531612411285
O	-3.98650399514576	-1.51096278202030	-1.85297486757887
H	-4.22924509148016	-2.43320528966654	-1.50969072758099

O	-5.76854190006031	0.08109356579284	-0.97059413656898
H	-6.52274096589621	0.14405186907730	-1.58219721138075
H	-6.10405870816753	-0.44360825939307	0.00074225436297
H	-5.07352084000100	-0.54127807601385	-1.40144045307215
O	-4.75693240825401	-3.75820523343345	-0.77266993444662
H	-4.57031303254518	-3.47659360198743	0.15447754346149
H	-5.72554288916688	-3.73061529601009	-0.83136474094434
O	-6.38653720144496	-1.05354021390997	1.07602091557670
H	-7.04164834825888	-1.74216743113018	0.87065395528588
H	-5.55027006149962	-1.55406960550617	1.34500383992193
O	-4.18645228564330	-2.37291413858172	1.48065054677455
H	-3.44906742964705	-1.88028693763101	1.00563611113675
H	-3.84338453670400	-2.63782016330315	2.34791981960928

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P	-0.95610908978988	2.27534499438407	-2.94499458482593
O	-1.33459558993925	2.49109094894291	-1.40327711383742
O	0.35369802232304	2.61665374053158	-3.56619861035822
N	1.45510385664878	-1.49958647881623	-1.29498534866950
N	0.29125749304401	0.51694308011527	-1.66825860723855
C	2.27685315481081	-2.60184648633961	-1.79642125773770
C	1.04708080663147	-1.58158712923953	0.10601968011702

C	1.05520725263702	-0.44955847383045	-2.07337930330856
C	3.77009597100493	-2.41863217536414	-1.52781426795650
C	-0.33854178051781	-2.19872191605140	0.29484304774490
C	1.52614247253632	-0.41624986105218	-3.50774407389033
C	-1.97393682928469	3.68236630988904	-0.87273045575310
C	-1.04864541889151	4.88111879930630	-0.90965989700375
H	1.91972475941706	-3.52610769169659	-1.31405086715369
H	2.09591935633870	-2.73525279640770	-2.87038698078325
H	1.08755621542265	-0.57559987928833	0.55530504756517
H	1.80297101455811	-2.17857927063417	0.63765524176055
H	3.96833052827235	-2.30658795547519	-0.44971382208103
H	4.33458093187920	-3.29382257320840	-1.88803714927344
H	4.15707580131128	-1.52379796600973	-2.04057918284534
H	-0.59244089084750	-2.25369271338400	1.36558044240048
H	-1.11256525601773	-1.60539520921921	-0.21301773123098
H	-0.37035197499162	-3.21928326504376	-0.11858215891496
H	2.61417589654711	-0.55716221430414	-3.58326849387640
H	1.04605612659722	-1.21738414315466	-4.09188117868116
H	1.25446392655330	0.55426536360602	-3.93484830260965
H	-2.90691312270753	3.86976220879392	-1.42188450036628
H	-2.22686364075768	3.40438810412555	0.15994660848065
H	-0.81843106954709	5.17081874721044	-1.94625027458476

H	-1.53282127904934	5.73680093315939	-0.41271161419494
H	-0.10546326595708	4.66128580423413	-0.38572829204467
O	-1.66744024720015	0.89686318872493	-3.51677418457674
C	-2.26977614100491	-0.15705367262027	-2.85368212131252
C	-2.00793014106500	-1.44112390807211	-3.33602242178082
C	-3.16821965465514	0.04698303131039	-1.80391497053317
C	-2.64617137214378	-2.53764369945739	-2.75258786244607
H	-1.31093855786927	-1.56778779256912	-4.16583398514971
C	-3.79296870979591	-1.06015134449499	-1.22216948417621
H	-3.37990131762040	1.05455762278348	-1.45077257332830
C	-3.53762590671080	-2.35273091450959	-1.69078141678892
H	-2.43963211258041	-3.54232382046941	-3.12954085810203
H	-4.49304611138160	-0.90427537297539	-0.39754684079162
H	-4.03114591337263	-3.21176382070359	-1.23053248437652
H	-0.03120761688612	0.42099557413893	-0.70677048789158
O	-2.05917052306756	3.32218848567512	-3.61172439864995
H	-1.81605356251404	3.54910165171183	-4.57573704200648
O	-4.44894233726669	2.46479760170389	-3.92073503085820
H	-5.05289700107885	3.22442561547854	-3.99975047814113
H	-4.42757341021755	1.90011651774987	-4.90835451698234
H	-3.51110518374698	2.84132508372684	-3.75346777759506
O	-1.64489820130200	3.65010416165541	-6.14141472554926

H	-1.54390025086286	2.69933357907241	-6.37595077906461
H	-2.52127261693753	3.87829256851553	-6.49228051648985
O	-4.36152032697290	1.23741706628186	-6.01478937937239
H	-4.63886065621837	1.81406988444791	-6.74696324651604
H	-3.40016837647010	1.02145900035016	-6.19394924626765
O	-1.75042942788988	0.89915213513350	-6.27422972025519
H	-1.49613179919704	0.71172200104816	-5.34550098658076
H	-1.31082690220619	0.23073874058389	-6.82366846326552

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P	1.35600264933106	-2.59207381812281	1.21980353194681
O	-0.14368852329740	-2.82055558058412	1.18593289188733
N	0.69963288330979	0.74454191474829	-1.97405743840949
N	0.82821493991395	-1.02652673635023	-0.43615471991125
C	-0.76161481539013	0.68952810413693	-2.04116443638010
C	1.34935193786390	1.73328283266891	-2.83879695686135
C	1.38856334812292	-0.10932110970779	-1.17027419517920
C	-1.43648434772427	1.45920937258147	-0.90620189061945
C	1.59880748616485	1.21986974710915	-4.25587659348722
C	2.89030449694486	0.01650066772148	-1.13106042547401
C	2.45728668322142	-3.29686855469846	-0.02695446132951
H	-1.08989746812594	-0.36260908840582	-2.05021558685270

H	-1.06244027594912	1.10550224634082	-3.01329918814258
H	0.69863772389400	2.62138143694563	-2.86709214676754
H	2.28987482034689	2.06235700214731	-2.38045661901880
H	-1.12997473307146	2.51726718975497	-0.91681701009433
H	-2.53206424192818	1.41589613893975	-1.01174434041621
H	-1.16863527470833	1.03788059148632	0.07342283446784
H	2.04843668182694	2.01272424864489	-4.87482376657127
H	2.28410439123962	0.35751254009985	-4.24906765607613
H	0.65758977215478	0.90602731193159	-4.73502751522856
H	3.32940251067378	-0.20940099147208	-2.11475217647645
H	3.19482761135727	1.03593033031513	-0.85532846915768
H	3.29873769107141	-0.67747390363685	-0.39142781691947
H	2.45496704658942	-4.38455525058221	0.13290601232671
H	2.12276059626798	-3.04631912447460	-1.03613203380902
H	3.47350623200613	-2.91687067772775	0.14976214962028
O	1.95690196585440	-1.23529696322047	1.97696510322575
C	1.31185807480187	-0.04987581777078	2.15419060973611
C	-0.02471301049112	0.01099925309091	2.57988025746662
C	2.05365585650545	1.12372028521916	1.96038051641370
C	-0.62611678136970	1.24857714518301	2.77395206183502
H	-0.58393944686376	-0.90593287963771	2.75146074035168
C	1.45437754493521	2.36250100519896	2.15136959702693

H	3.09579013100659	1.04854043844814	1.65050323015489
C	0.11493399852974	2.41172501383878	2.54782825779022
H	-1.66439428807224	1.32128559044328	3.09443215941745
H	2.00796057003400	3.28649934726316	1.99034312592390
N	-0.52814435434617	3.71145468917522	2.72675629356002
O	-1.70788003476937	3.73295387720308	3.05589304799312
O	0.14111568012349	4.71951053708471	2.53580505217631
H	-0.18740138662869	-1.06654198948880	-0.49196549318557
O	1.92528947432232	-3.58043272428460	2.45499820641793
H	1.58417895860421	-3.28051115860999	3.36216575727007
O	1.20842591684025	-6.01558086120002	2.38596066581650
H	1.87598214430046	-6.56721208185979	2.83078003399153
H	0.25732439153844	-6.02578906081421	2.99836200735571
H	1.55603575590074	-5.04371983581440	2.39819837948309
O	0.82540109504589	-2.91984339442878	4.72594276298766
H	-0.10346151059311	-3.01514736748500	4.40585184855265
H	0.94552141000999	-3.66969953110388	5.33032153274167
O	-0.84579710509375	-5.96222606088425	3.68438858494207
H	-0.62145009973049	-6.02889072125532	4.62808889646908
H	-1.20380972021653	-5.03029217762764	3.56575115469185
O	-1.44580716823745	-3.43105235212469	3.33639569003029
H	-1.02099582507558	-3.19303708726451	2.45278404735832

H	-2.33371967897154	-3.04179170708298	3.34137448493845
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P	-0.46946980592955	-1.34611322564826	-4.49938805948869
O	0.08692887948688	0.15760920347688	-4.65790617557770
O	0.45917458605681	-2.53005184483597	-4.63798371621769
N	0.86921565394369	-1.58419943062128	-0.12171241985764
N	0.38704193828493	-1.08553467845667	-2.36261735941667
C	0.91343916450824	-2.53337076194819	0.99479168195415
C	1.23599957112774	-0.20397186066370	0.20004896655259
C	0.49379240489918	-1.93629135736093	-1.37927184028048
C	2.30243699918099	-3.12111594484464	1.23551540224088
C	0.03404006110148	0.67410706857142	0.54736580587158
C	0.16752562254684	-3.38498525498091	-1.63612290547504
C	1.45336307275037	0.53649997730830	-4.43250886195389
H	0.18117932609320	-3.33230676050240	0.82627113144625
H	0.57152027969531	-1.99520921366065	1.89299259024158
H	1.93630703687190	-0.24029655076842	1.04716913950221
H	1.80424844635475	0.22518745886965	-0.64081801305441
H	2.64673099571830	-3.69909561731712	0.36354743557334
H	3.04095811623148	-2.32782028515867	1.43313574540680
H	2.28367833385711	-3.79261731370911	2.10869642110077

H	-0.65717278640560	0.75732545789752	-0.30252175517170
H	-0.52372402400185	0.25569201735563	1.39993250047089
H	0.36745081968745	1.68821825480045	0.81830584826079
H	0.05435210294732	-3.54000703072286	-2.71192218193052
H	0.95796512288630	-4.04812555020224	-1.25779123383257
H	-0.76991689629024	-3.65772427641902	-1.12644253019939
H	1.50151984322637	1.24306385811538	-3.59196753511335
H	1.80795342779952	1.02914793797872	-5.34884144957101
H	2.07672173969606	-0.34069086765261	-4.21707560129390
O	-1.84934864552865	-1.51139815219752	-3.61394997980859
C	-2.34710188933781	-0.72939751345153	-2.61862159414497
C	-2.93673747113539	-1.38029605021948	-1.52666466929262
C	-2.34066595862886	0.67081527220993	-2.70425315283887
C	-3.50941979654180	-0.63324302245946	-0.50459688683337
H	-2.93104800961793	-2.47019667872660	-1.49161911891743
C	-2.91415314406887	1.42034565513262	-1.68375204392547
H	-1.88090604423208	1.16098465157254	-3.56194663456250
C	-3.48922567458423	0.76132939699106	-0.59365250453196
H	-3.96273709721403	-1.11623035786688	0.35987047873615
H	-2.91701237912260	2.50874658144708	-1.72197551141438
N	-4.06855313219700	1.55240559393228	0.49044430129059
O	-4.04177633622335	2.77293784099245	0.39370491518121

O	-4.55088238774096	0.95745427077794	1.44613107896962
H	0.55943550849105	-0.12220365205851	-2.08373040545615
O	-1.37330901201865	-1.32418333444842	-5.88451387291223
H	-0.81147076559209	-1.33213908333197	-6.72467328688440
O	-3.14215622799517	-3.22429276591944	-6.23124903130284
H	-3.81977677206742	-2.90191376795214	-6.84884281776715
H	-2.38391301934741	-4.09960715433260	-6.82935278120449
H	-2.53895518789566	-2.44059646227395	-6.05390650852451
O	0.03921927201693	-1.57476047294721	-8.07602274309949
H	0.43976264966010	-2.43675757649612	-7.81962245768457
H	-0.60380141235658	-1.81372891900509	-8.76288835321819
O	-1.67206962468616	-4.83026417765929	-7.31433281191468
H	-1.78256273148959	-4.75813062508986	-8.27919513708207
H	-0.70794991486531	-4.51970167661890	-7.10676493528437
O	0.63395816288853	-3.90676436915798	-6.81079204399838
H	0.60570728500493	-3.42408446060276	-5.92172066381964
H	1.40778972410104	-4.49197239914050	-6.80062185794145

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P	-0.94215396984388	2.28026392503315	-2.94384891271094
O	-1.32143964010550	2.49649499719909	-1.40346474891515
O	0.37135146528428	2.59386472963167	-3.56999901998450

N	1.40608495910892	-1.51955783580079	-1.31172002182885
N	0.25291017375099	0.50216802652783	-1.68526057016626
C	2.21491592905425	-2.63115678784010	-1.81575697773922
C	1.01657479570587	-1.59166194886951	0.09570068380069
C	1.01117350792396	-0.47057534122624	-2.09112606365616
C	3.71133706038783	-2.46056570109297	-1.55785499217871
C	-0.37639924977370	-2.18311560480150	0.31000257471493
C	1.47962163179997	-0.44368050531363	-3.52627401454463
C	-2.01271880822947	3.66265352114211	-0.87642932163008
C	-1.13056749487493	4.89319033338639	-0.89573388876359
H	1.85180695755368	-3.54991811984476	-1.32764361412501
H	2.02497849280126	-2.76601776966914	-2.88781441846546
H	1.08156997247724	-0.58569233991666	0.54226394386385
H	1.77019370933628	-2.20105889542825	0.61585343120847
H	3.91867874077771	-2.34870889295638	-0.48148446867355
H	4.26471419419881	-3.34169222713857	-1.92063208828237
H	4.10302104871049	-1.57044057814194	-2.07511053533991
H	-0.60035724915583	-2.25757014349406	1.38602252219412
H	-1.14823166515901	-1.55558440140965	-0.15656432745730
H	-0.44906152725846	-3.19132547754306	-0.12780911177423
H	2.56800542230688	-0.58307955440173	-3.59899991140632
H	1.00352348415053	-1.24912300380500	-4.10721823266772

H	1.20910097610054	0.52428731847099	-3.95922648197711
H	-2.94417777775488	3.81683519390736	-1.43767588441628
H	-2.26854225697623	3.36887786435951	0.15104439950108
H	-0.89589885050435	5.19455387592216	-1.92792532773375
H	-1.65327059358176	5.72866146634019	-0.40342236317080
H	-0.18860896645269	4.70572302845585	-0.35733550581501
O	-1.68590263844580	0.90484243224324	-3.52732473022950
C	-2.25145503695796	-0.14830230561131	-2.86471728260121
C	-1.99292871673682	-1.43009525885788	-3.36659151508745
C	-3.11727243431869	0.03849723737253	-1.77899845124359
C	-2.56636858125654	-2.53926307728617	-2.75816292439197
H	-1.33354291812445	-1.54413371806350	-4.22719327073624
C	-3.69581301122230	-1.06971487417119	-1.17029529778264
H	-3.33378387003667	1.04037189278112	-1.41508448641942
C	-3.40656708803718	-2.34603133191710	-1.65894452375786
H	-2.36339536006705	-3.54666652804781	-3.11839290933693
H	-4.36473201413330	-0.95395776330873	-0.31870146439931
N	-3.98048499044094	-3.51163397052259	-0.98855253281680
O	-3.65328353188488	-4.62365815948224	-1.38393675842244
O	-4.75538953433092	-3.32159427108200	-0.05983004841732
H	-0.06125742235926	0.41670371991705	-0.72002229222547
O	-2.03266642995522	3.33003569088378	-3.61388846219231

H	-1.78599208961427	3.56192934736756	-4.57760231538170
O	-4.42657852915737	2.45035200596254	-3.92971089572792
H	-5.04578400182438	3.19911913257910	-3.99132181139349
H	-4.39846582318147	1.89138524283498	-4.93635471907803
H	-3.49932265647721	2.84093759857006	-3.76254704815013
O	-1.60680993287986	3.68265962350046	-6.13260281364514
H	-1.50600446382778	2.73576271443974	-6.38156954724549
H	-2.47897814665933	3.91975250267109	-6.48814167821998
O	-4.32476043910979	1.24922783853380	-6.03244480947400
H	-4.61255891468722	1.82875449702976	-6.75859619273685
H	-3.36047286264113	1.04618441903802	-6.21543422860951
O	-1.71366700823314	0.93027166532949	-6.30695226122976
H	-1.44486193725753	0.71933250560901	-5.38951075328227
H	-1.28156408790035	0.27638204000483	-6.87976072762550

PATH11

A230-H⁺

31

P	-1.47418072676601	-0.49027110253701	-2.04120778154974
F	-0.59818745091258	-1.19922715699748	-3.19455439408121
O	-2.16702825161145	-1.45235050832255	-1.13420859302113
N	1.73795366718932	0.41322792949322	0.17230063689213
N	-0.12672471000365	0.24586518644913	-1.18357283243816

C	2.78139456162994	-0.16579321520704	1.04380647588828
C	1.77053169844897	1.88301519061978	0.04647740413767
C	0.82619042677303	-0.33168322832565	-0.42926231660409
C	4.09745104651775	-0.39732142442312	0.30834060705544
C	0.86048844384935	2.57912094504076	1.05620490009535
C	0.84354239721212	-1.82085928570238	-0.26713446078596
C	-2.23516701415440	0.99166452608523	-2.69303268778325
H	2.40578764072362	-1.09250916720179	1.49102990521743
H	2.92004836104734	0.54587600278539	1.86991373617854
H	2.81440375684282	2.18576092550700	0.19922506668212
H	1.52760940475319	2.16652312531002	-0.98849949245226
H	4.48802916764272	0.53991907186144	-0.11710284422717
H	4.84474434533608	-0.78813654557855	1.01600086312266
H	3.97930573473964	-1.12602384643280	-0.50796129108510
H	0.95808962417309	3.66951820580838	0.94217614351130
H	-0.19661644217710	2.31090819050624	0.90797734188246
H	1.14523331474802	2.31227388697675	2.08522386886166
H	1.85872657075308	-2.21181365485056	-0.40837923415570
H	0.51018604572119	-2.08058429303665	0.75027979039856
H	0.17389039930143	-2.31136925282663	-0.97687106649774
H	-3.09970380217483	0.67728754927139	-3.28779651824532
H	-2.53169898454492	1.61366457792662	-1.83447816345213

H	-1.50231297055738	1.53006884286233	-3.31209104227942
H	-0.08364228212431	1.25824752120583	-1.28179780761093
O	-3.32640672153333	-1.27260771120345	-3.99570569122482
H	-3.42056704084280	-2.22775043506386	-4.12136831242949

A232-H⁺

32

P	-1.42523380405647	-1.92830485748290	0.74950438228802
F	-1.36441799005382	-2.33701999636279	2.28547654283370
O	-2.03584614668975	-0.47459054125004	0.62497095262988
O	-1.90062734325913	-2.92562990554682	-0.23463897204107
N	2.29015832931138	-0.98464620917449	-0.27253150469803
N	0.28780703837478	-1.66681931882130	0.65485131160039
C	3.10456163783673	-0.41284178311922	-1.36639734747476
C	3.02432171996897	-1.26879911469275	0.97705313623375
C	0.99365401063432	-1.18860423314532	-0.39244788593889
C	3.78838212820263	-1.48594424398557	-2.20675985529961
C	2.97977319581580	-0.09798084522970	1.95699591712122
C	0.27525446376924	-0.86598462968368	-1.66531922734410
C	-1.75686793285663	0.59770007489043	1.55619873025635
H	3.85007269261659	0.23525775684031	-0.88495587659797
H	2.47586076024773	0.24019473672037	-1.98193416796334
H	2.63685312587403	-2.19612790263687	1.42380505480468

H	4.05973778424840	-1.48824097560588	0.68658403771036
H	4.41924442462281	-1.00194241941252	-2.96810522558213
H	4.43231968410952	-2.12879171039370	-1.58711448677802
H	3.05260096175690	-2.12312255434262	-2.72082358087783
H	3.41345487475845	0.80546125875811	1.50254185772763
H	1.95109843805801	0.13303415227377	2.27320544335652
H	3.56738417107619	-0.35161177794849	2.85223811075737
H	0.86231362013365	-1.16912378816563	-2.53977676313010
H	-0.69322058592202	-1.37322062485191	-1.71034297350160
H	0.10697510813772	0.22223269081653	-1.71698004010659
H	-2.16417154700605	1.50616565053214	1.09843223671981
H	-0.67224704205930	0.70362707587322	1.70551908050663
H	-2.26108895827437	0.39207636759020	2.51031307520261
H	0.78777509337844	-1.84544876268356	1.52344956423494
O	-4.12062746000882	-2.21270175215354	1.88611815139906
H	-4.63396445274595	-1.75531181760577	1.20552032195113

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35

P	0.55329320918627	-6.96344690245229	0.87315096124464
F	1.83295321013552	-7.90873298740447	0.79196103563107
O	-0.14519351295858	-7.34514782552837	2.23530379643745
O	-0.17023895414032	-6.74310404809393	-0.40160462493665

N	2.38756622898465	-3.47541215007701	1.28749943216609
N	1.32492640523304	-5.51793599050427	1.42625156911329
C	2.00786654755656	-3.13085898124426	2.67256422536290
C	3.15033455336049	-2.43701858245721	0.56303558979858
C	2.04065261453167	-4.61596019470607	0.72416421861259
C	0.60180776556024	-2.54034773068825	2.76092119881345
C	4.64930842352505	-2.52042901764521	0.83166299757475
C	2.42322523793397	-4.91776304094309	-0.69155413256611
C	-1.59016265745010	-7.51014261544879	2.40155156740584
C	-2.24805578963279	-6.17817761746582	2.68939937384365
H	2.12608291758138	-4.01596393323909	3.31490903052964
H	2.75104224049624	-2.40565077621035	3.02727070678651
H	2.74830646333437	-1.47131260232493	0.90062829790335
H	2.93067404174843	-2.50927772182895	-0.50786065254866
H	0.52333346902256	-1.63510183933584	2.14036032327128
H	-0.16600615592902	-3.25647459924624	2.43095533875499
H	0.38906313079168	-2.26508346176304	3.80500876491247
H	5.06772097204427	-3.47384879297248	0.47463474716396
H	5.15837575656586	-1.69941910257103	0.30385580357879
H	4.86952433745172	-2.42494929002816	1.90600805970451
H	2.28264306780098	-5.97500628982686	-0.93244672668187
H	1.79662101752696	-4.32342793231655	-1.37566267225368

H	-1.98273964734977	-7.99638863668826	1.49904943892747
H	-1.68451346497268	-8.20791834267658	3.24313506370745
H	-3.32227210188847	-6.34072093564160	2.87324512813976
H	-1.81087584442625	-5.70496855391275	3.58210619285407
H	-2.14725612817993	-5.48795055327993	1.83707528198743
H	3.47395403699568	-4.65813984856548	-0.87001703057887
H	1.10951911028351	-5.30730610403414	2.39888957735260
O	-0.27680352629728	-9.76155143769899	0.42644180678412
H	-1.23693381442599	-9.84300696117929	0.33884232120304

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38

P	0.47771335469318	-3.12168667555466	-0.99331972035956
O	1.41895697328625	-1.86204036516655	-1.31039888427035
O	-0.80834609011682	-2.92650266082096	-1.91719982860711
O	0.37535630341754	-3.68317240693795	0.38372146248411
N	1.25033883669900	-4.34838961353055	-1.95994657254231
N	1.72204475391235	-5.94827797217873	-0.34559615240638
C	2.52359328086940	-1.54372224883946	-0.50986670092423
C	-1.45047386184743	-1.79693757811447	-2.42056986289356
C	2.31864275711679	-0.85203775421665	0.68281652210359
C	-0.77764782807135	-0.91637965549206	-3.26640033757103
C	3.79317572497338	-1.90445692487933	-0.95920324486780

C	-2.80362384631723	-1.64199260048141	-2.12267187611051
C	3.43782374757923	-0.50697999332177	1.44812840532978
C	-1.48147441645529	0.16602897766079	-3.80531475910626
C	4.90184281979062	-1.54993178560461	-0.18197020341139
C	-3.49574396145405	-0.55825718500667	-2.67169402665280
C	1.78554743364956	-5.51912944918438	-1.58247937677082
C	4.72627860499791	-0.85363357234447	1.02015751256094
C	-2.83702833469341	0.35043525028744	-3.50919099691609
C	2.48012939859956	-6.33245289529740	-2.62549023271453
H	1.28890045935672	-0.60815561418838	0.96094992242454
H	0.27773650898820	-1.07096580661785	-3.49220221310828
H	3.90339884573738	-2.44986066842872	-1.89856636161715
H	-3.29663141465156	-2.36010197221082	-1.46522156335145
H	3.30199457315204	0.03684527526676	2.38658237100505
H	-0.96331514654652	0.86642354917389	-4.46515583253571
H	5.90551619698961	-1.82162406040267	-0.51849266638003
H	-4.55556716382556	-0.42460395721547	-2.44080781477252
H	5.59519976909981	-0.58012859986667	1.62377715073444
H	-3.38050644680210	1.19782911077083	-3.93391623800058
H	2.78400389837489	-7.30867561780368	-2.22975523805368
H	3.37142646354403	-5.78260642280180	-2.96794129529047
H	1.81359788247778	-6.47225272756919	-3.48983648194940

H	1.25266734931050	-5.37851045715456	0.36609801762316
H	2.13024817043809	-6.84400155368135	-0.09570554924505
H	1.36145327190230	-4.12158049054758	-2.94847290273075
O	-0.80516086963021	-0.90647607026099	0.41894488889440
H	-1.61059799854460	-0.63005680743787	-0.03778932000021

AMP-H⁺

42

P	3.41813233790999	0.56995181608159	1.31080859323779
O	4.32121910017487	0.88405852642224	0.15673812276368
N	-0.15514708335724	-0.11113937978620	-0.41434168743283
N	1.72731379761163	0.58428532721195	0.72884755318383
C	-1.04917811981734	0.52003538057973	0.57526945444901
C	-0.82857409400449	-0.80387118600453	-1.52935880653875
C	1.16380503960478	-0.06799290544507	-0.29919926466478
C	-1.27950428416586	-0.35544670036258	1.80594484545144
C	-1.21089706655251	0.14486062839062	-2.66140082213535
C	2.03377482080015	-0.73997855350056	-1.31724192763965
C	3.15389336420555	1.74550500758881	2.65005036849543
H	-1.99955875691197	0.71228375395940	0.06160951386110
H	-0.65363515376756	1.51128004218557	0.84498126114525
H	-0.18696139921646	-1.61377840815251	-1.89246922993294
H	-1.72337058389829	-1.28000466265924	-1.10317646184307

H	-1.70529467830012	-1.32747342552154	1.51533758723517
H	-0.34989769071790	-0.54428951200329	2.36178902718029
H	-1.98877550998955	0.14695151300174	2.48095058595383
H	-0.31968042755762	0.61095399996181	-3.10876218979672
H	-1.73933067873160	-0.41747874752644	-3.44666380946493
H	-1.87920155629700	0.94376356496785	-2.30462711915952
H	1.88240547080583	-1.82916962033051	-1.28630736984783
H	1.77064945772582	-0.39163594515085	-2.32567403012224
H	3.08711331652442	-0.51489243358966	-1.13335186185213
H	2.86024813037670	2.69296456815521	2.17216272199227
H	2.33998509679496	1.40259997581351	3.30432605161822
H	4.08913965095766	1.84332671478855	3.20708455318425
O	3.49171169893329	-1.01415843932930	1.72801346285060
C	2.56126831967876	-1.66483538447599	2.52734000618667
C	1.76173366479686	-2.64802893602749	1.93925688351757
C	2.46210249756697	-1.37675868036300	3.89139282447336
C	0.83540353016758	-3.33912578452455	2.72538560279692
H	1.86956226570819	-2.86768759538170	0.87646965365212
C	1.52586987282886	-2.06919264160326	4.66645671409661
H	3.11620652652713	-0.62903126766944	4.34108163705847
C	0.70927377011777	-3.04795153549407	4.08823749117457
H	0.20504303538184	-4.10416621109673	2.26558738140680

H	1.44186200267102	-1.84369866711234	5.73254253631408
H	-0.02059196519753	-3.58416136247583	4.69939872900390
H	1.08301011872116	1.02668154900579	1.37917131342711
O	5.65626283709782	0.47595741052998	2.83765823860457
H	6.16721811479317	-0.29576191305757	2.55537411611557

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43

P	-2.43786655744744	-0.86738721903529	-1.34926774650360
O	-2.28349317525136	-2.17390127293168	-2.24502337508983
O	-2.88695835557510	-1.07827625924545	0.05286886463526
N	1.38273003156220	0.01554866167690	-0.54718492830022
N	-0.77921183713853	-0.26360384359677	-1.29267844020906
C	1.52995377151520	1.26554801406055	-1.31836730262998
C	2.56369174494148	-0.39186082731375	0.23967356882460
C	0.25794083316653	-0.68140771766082	-0.55039697761667
C	0.95621832206401	2.47839787304060	-0.58897848748461
C	3.56093523638071	-1.19937488637591	-0.58585622465291
C	0.13391247865724	-1.92994012726888	0.26634407781052
C	-1.82462059621705	-2.13925612182761	-3.61139869851668
H	1.07961139120446	1.13836124533610	-2.31465013635178
H	2.60435495954247	1.39898090653261	-1.49707180901652
H	3.02479542851713	0.53584365868363	0.60762423480957

H	2.23486322194339	-0.94839679878573	1.12429529662249
H	1.12586214933577	3.37994373892665	-1.19659099889521
H	-0.12604385325217	2.38485089998224	-0.41747218197500
H	1.45301940843279	2.61617727619560	0.38318603048487
H	4.43848275788144	-1.44120937344208	0.03330963741153
H	3.11478855991465	-2.14190123289149	-0.93885974608834
H	3.90645745587899	-0.62960400270756	-1.46228763003875
H	0.06118193621803	-1.66786978416287	1.33378003362156
H	-0.75767682923325	-2.49821413743707	-0.00993784138190
H	1.01594508964122	-2.56780297642128	0.12730779292673
H	-2.58997678153371	-1.67660667390913	-4.25005941952507
H	-1.66747834292351	-3.18342078447221	-3.90619139943837
H	-0.87824219268906	-1.58286461264839	-3.68633936680367
O	-2.96340126464183	0.31836553491584	-2.31648956969840
C	-2.81921960605862	1.67217746241511	-2.02310224265010
C	-2.24099228496794	2.47789587952292	-3.00595776799292
C	-3.24703406901750	2.19924665447716	-0.80239561219820
C	-2.08530190256116	3.84502634123587	-2.75623301043029
H	-1.91529093175359	2.02882749781955	-3.94646662177089
C	-3.07912865900282	3.56733688579658	-0.56545018112123
H	-3.69786173823467	1.54900416729849	-0.05160175857254
C	-2.50070336513372	4.39222249260365	-1.53713286394346

H	-1.63132083457105	4.48216453666706	-3.51907354779896
H	-3.40650319276096	3.98905646468709	0.38803620741787
H	-2.37209428573226	5.45960655159294	-1.34319414789139
H	-0.60505208008808	0.54215159745843	-1.88827430206823
O	-5.05817080585007	-1.41074091327823	-1.93575712058352
H	-5.23947414516213	-2.21624254551348	-1.43135603732644

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P	-2.46906535038024	-0.85281203188787	-1.29764276131542
O	-2.32882681524296	-2.17455081207584	-2.16892160058595
O	-2.90065101138227	-1.03029870385492	0.11540868218673
N	1.36643914453971	0.01087307882520	-0.54174773807141
N	-0.80342256092352	-0.25959311849090	-1.26780619082350
C	1.51471267313634	1.25582166846184	-1.32060534358029
C	2.55033381875162	-0.39837672791753	0.23948855358861
C	0.23747931469531	-0.67996209835716	-0.53363815077104
C	0.95397030644896	2.47631196055141	-0.59376178136003
C	3.53803266789156	-1.21611784860546	-0.58742029174336
C	0.11277551663607	-1.92490076139561	0.28866205149451
C	-1.87480231778865	-2.17465445510184	-3.55084020577777
H	1.05580233022593	1.12564182993858	-2.31257920083854
H	2.58842497801992	1.38203185734796	-1.50850725090603

H	3.01891287330669	0.52896371989017	0.59882275748446
H	2.22436756880603	-0.94757670492408	1.12981123387138
H	1.12248314518394	3.37311139773651	-1.20866272436123
H	-0.12708301150166	2.38955634422575	-0.41146424844725
H	1.46044122461952	2.61767612951468	0.37289038658197
H	4.41878508856375	-1.45801358694394	0.02718591770343
H	3.08514613897501	-2.15883705101307	-0.93118268995290
H	3.88011606641440	-0.65373399772617	-1.46995035548173
H	0.03391983941205	-1.65744324927179	1.35432530680736
H	-0.77595719320004	-2.49652063389918	0.00992413279408
H	0.99632409911025	-2.56205060814762	0.15745471804392
H	-2.68287061851918	-1.75600783686336	-4.16926627333939
C	-1.54981070751617	-3.59917614584124	-3.93736061454409
H	-0.99046280415684	-1.52308949717938	-3.63406954277512
O	-2.99564832823692	0.32646536372295	-2.27425224820485
C	-2.82839254268555	1.68212546919022	-2.00393697896060
C	-2.25227127087096	2.46439079275508	-3.00700222183796
C	-3.23156155413228	2.23453034361098	-0.78595875160346
C	-2.07377557846394	3.83286899738190	-2.78111010079475
H	-1.94623872209813	1.99613070817811	-3.94475396370476
C	-3.04113437210435	3.60361053633597	-0.57302428497736
H	-3.68085000489725	1.60248313625409	-0.01885379423373

C	-2.46441794285739	4.40491414065717	-1.56525630881030
H	-1.62131536345030	4.45134553572382	-3.56005739264952
H	-3.34903334986361	4.04481201368518	0.37811322141165
H	-2.31783961356566	5.47318677813144	-1.38988515627085
H	-0.63182836303704	0.54457766749227	-1.86599296542330
O	-5.08321237910579	-1.40513572161737	-1.86031494188054
H	-5.19829464840629	-2.28340407041008	-1.47122962589870
H	-1.22021401584519	-3.62247668958554	-4.98805099722742
H	-2.43522683141236	-4.24576206312080	-3.83685455155003
H	-0.74052952309252	-4.00265505538056	-3.30933571326483

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P	1.31299789741550	-2.04377140756490	1.38555026067000
O	0.14679536304115	-2.72908488691824	2.02454110175048
N	-0.40524213582754	1.14496422376755	-0.31016503568133
N	0.69498471578958	-0.80440004997797	0.26786352305779
C	0.77855956468885	1.68216448140019	-1.00590639644680
C	-1.60301980144308	2.00818275843531	-0.36055200511102
C	-0.40118646459705	-0.01998334316172	0.31797183330121
C	0.86400084172559	1.23433862611028	-2.46355886004442
C	-1.62629118291723	3.03942694177749	0.76392569066262
C	-1.63054732590821	-0.48713753991233	1.03151088250163

C	2.44680027797755	-2.86866144119929	0.27132059420246
H	1.68293266879404	1.41330144798283	-0.44216240488057
H	0.70450065228668	2.77601605179008	-0.94516310660432
H	-1.58474956353041	2.50619854020046	-1.33975926786530
H	-2.50259227287765	1.38282236221728	-0.34518327692926
H	-0.03450926381851	1.54170588575177	-3.01960643631882
H	1.74022872849458	1.70252379496317	-2.93711873791298
H	0.96788591310177	0.14202787743272	-2.55217058342966
H	-2.48888567368623	3.70898116120247	0.62545503619858
H	-1.71714201738870	2.55948249639281	1.74866609269516
H	-0.71173418938273	3.65200660029974	0.76368934503412
H	-2.02874327187910	0.29532849740070	1.68859041602690
H	-2.39726239943442	-0.72912464987671	0.27744491843979
H	-1.41621847579466	-1.38708910203904	1.61164253426949
H	2.98891645497623	-3.62575904673255	0.84700345253845
H	1.83745078505700	-3.31988446646908	-0.52598392602613
H	3.13570655652909	-2.12761424377806	-0.15933263881132
O	2.21500096306558	-1.02292791605819	2.32739223126774
C	1.72340455301877	0.18312825394733	2.75974151978922
C	0.59390146927468	0.24707870103650	3.58599645221901
C	2.38635697460804	1.34523427403573	2.34484393088895
C	0.10101554781016	1.48981101325351	3.97187382314877

H	0.10076375359220	-0.66995362448940	3.90880140916702
C	1.89842458262044	2.58813405603327	2.73021807082894
H	3.26293599542355	1.26052373680848	1.70102018287362
C	0.75356675499865	2.64528049122239	3.53231825904027
H	-0.78572580717754	1.56477318826045	4.60003427473884
H	2.38498439929725	3.50499857098274	2.39994104780143
N	0.21107168399885	3.94928541749353	3.90019034047805
O	-0.82387416965303	3.98559450702179	4.55875693951029
O	0.80788783563211	4.95508915962321	3.52791244762478
H	1.44334679463283	-0.45675705709407	-0.32957990218915
O	2.83710673634215	-3.78192153067404	2.93562057793617
H	2.68803150112306	-3.66567516089845	3.88489187958881

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P	-0.04050349894754	-1.00901039934529	-4.10784735304546
O	-0.00559110209799	0.54574764563866	-4.42745842609015
O	0.87922072463354	-1.98140723684535	-4.75460294621105
N	0.58068630544278	-1.31582816049924	-0.18313385273152
N	0.33156270559900	-0.77916441813967	-2.41580867392746
C	0.60395020521925	-2.27522450737694	0.94038992779580
C	0.78686942709695	0.09768359564203	0.18879361618696
C	0.35845023799170	-1.69402277674073	-1.42811073985486

C	2.01661360521000	-2.74080488110057	1.27873013024548
C	-0.53098192979671	0.83437147898323	0.42025048945614
C	0.11233314592945	-3.13432958987652	-1.75697171300504
C	0.50829833772857	1.14375169896304	-5.64488898989113
H	-0.05116578867143	-3.12185102932101	0.70720039392768
H	0.15162295721514	-1.75665662187225	1.79729658620560
H	1.39145495738880	0.09485831831166	1.10474062132135
H	1.40587598057082	0.59086198494295	-0.57469651094903
H	2.47378006597168	-3.27858443444556	0.43416502424223
H	2.66510609639371	-1.89079767309416	1.54120936871641
H	1.97776481056235	-3.42150302067879	2.14301690920245
H	-1.14964854838285	0.86241871598648	-0.48873736234281
H	-1.11241148780394	0.34809712797457	1.21824323102739
H	-0.32024873690361	1.87007412596290	0.72670524459361
H	0.19950097497628	-3.31383533484311	-2.83174412485047
H	0.83070134089397	-3.78188767113049	-1.24026003933018
H	-0.90201653328527	-3.41441794355759	-1.43103170618793
H	0.33477439913056	2.22065693956093	-5.53303537290850
H	-0.04602879524481	0.72333764368689	-6.49150592102622
H	1.58591848812270	0.94127914494927	-5.72148054939470
O	-1.55475361881341	-1.59835460762466	-3.94928527697220
C	-2.58389662722731	-1.10734533212531	-3.19194224761988

C	-3.50689528686405	-2.05524236947605	-2.72749023313417
C	-2.73473719877321	0.25509621786261	-2.90039679627086
C	-4.58405803784103	-1.64417056265918	-1.95324865456940
H	-3.36185273276427	-3.10779876160681	-2.97453438111964
C	-3.81024027742886	0.66722025839908	-2.11987568448723
H	-2.02254961410124	0.98717429241659	-3.27744051264343
C	-4.72174570051678	-0.28366382359845	-1.65188459529310
H	-5.30754526194884	-2.36708139722658	-1.57821155027847
H	-3.94216791459770	1.72077092427316	-1.87651251247562
N	-5.84360464734828	0.15220287279781	-0.82925997113939
O	-5.93904908690909	1.34559797448819	-0.55585786068844
O	-6.64662353886532	-0.69236760243376	-0.44198756314939
H	0.51139319152332	0.19221408465742	-2.17345721104138
O	-1.30128495965240	-0.89955181383008	-6.64224305100159
H	-1.88736703281450	-1.62200307604922	-6.38030915929015

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P	-0.62231202598016	1.95206190846021	-2.95504560394536
O	-1.41227645278660	2.67493848610325	-1.78625949878292
O	0.42151088808115	2.62632785600289	-3.77126951485415
N	1.10871153941888	-1.22862663069396	-1.29029818785888
N	0.05384766717578	0.73467773742806	-1.89876844803213

C	1.86273703361936	-2.46126732526609	-1.59850373239431
C	0.73127669127905	-1.05583377939968	0.12620699394533
C	0.76646091617064	-0.36068446382101	-2.22402277473910
C	3.36303756985311	-2.29615588197524	-1.37944561737899
C	-0.67622812659557	-1.57110774721199	0.41884435540917
C	1.14710814764601	-0.58892333981176	-3.65452915900332
C	-1.56400377845436	4.12251329440788	-1.62125748685121
C	-0.37478909666080	4.70008612945398	-0.88464253888311
H	1.45888044005369	-3.24143386091795	-0.93796201530919
H	1.63888848909608	-2.77510103680470	-2.62390852167259
H	0.85072697759536	0.00032571277723	0.41007071178894
H	1.47348986830955	-1.60802520777743	0.71642751204238
H	3.58321816740688	-2.00235031326671	-0.34160981883629
H	3.86781342310621	-3.25386630962652	-1.57886280963903
H	3.78468478276592	-1.53467553184448	-2.05304688505469
H	-0.89209654250864	-1.45253172170322	1.49139462587027
H	-1.44015242983431	-1.02082771121343	-0.14906860432650
H	-0.76059732323805	-2.63838771010804	0.16385658020929
H	2.19618053272712	-0.89937119790385	-3.73307394576618
H	0.51790400393175	-1.38816492408391	-4.07695356852298
H	1.01159810456473	0.31916879861298	-4.24779934023754
H	-1.71813654823168	4.54087591880951	-2.62326243548205

H	-2.49106611004410	4.22477202750477	-1.04179876052848
H	0.55176718139926	4.58589300467093	-1.46859657458855
H	-0.54472853989454	5.77642855980690	-0.71978506917768
H	-0.23771139851452	4.21829872979976	0.09603994009435
O	-1.58183453263656	0.99233331259502	-3.86380849566476
C	-2.43565039953589	0.01093555378157	-3.43630103196717
C	-2.57180370515088	-1.09808853558514	-4.28311715601344
C	-3.15398736224777	0.10030860348122	-2.23638075606918
C	-3.42090748055778	-2.13696282820042	-3.92376398587476
H	-2.00063317245767	-1.13518844045682	-5.21177014134789
C	-4.00035403096732	-0.94218692005102	-1.87263395128595
H	-3.05302786095047	0.97294995803144	-1.59283757724541
C	-4.12333692045956	-2.05049924449025	-2.71576198423841
H	-3.53420369960869	-3.01028257691150	-4.56506239502948
H	-4.56320803043532	-0.89557758477924	-0.94116826770871
N	-5.00563717790257	-3.14439616344390	-2.32685239000040
O	-5.12223978679361	-4.09999107835803	-3.08917558494677
O	-5.59423059433807	-3.06629547625906	-1.25201543682884
H	-0.19309976264715	0.87373637818195	-0.92156521691606
O	-2.43148914463242	3.63236652160586	-4.37227736295369
H	-2.43597039013535	3.01250505044996	-5.11400807340326

Other hydrolysis reaction pathways

PATH1

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P	-5.67759734375359	-5.39319093802926	-3.24992719923464
O	-7.17263926231072	-5.53525698889391	-3.37850064680656
C	-4.48445642506533	-5.79763303735362	-4.57111762195439
H	-3.52863061952798	-5.30655405006643	-4.33418110140045
H	-4.32838938235255	-6.88462341258078	-4.60079121007893
H	-4.85521259557591	-5.41788799973974	-5.53001468556302
C	-5.44740866683164	-7.81876698047424	-2.00898195511987
F	-5.72474592108783	-3.69545004162046	-4.16467447498971
N	-5.12477906781838	-6.56405491484411	-2.08416807401652
C	-6.41819516989222	-8.51634110809561	-2.94188476325803
H	-7.26381947872119	-8.93777877114954	-2.37658043630019
H	-6.82478871521932	-7.80226941375477	-3.66312542188044
H	-5.92644625785345	-9.34713210077473	-3.46992713653716
C	-5.14357563120938	-10.01441440713259	-0.85940612323198
H	-6.16358580923699	-10.24394790676923	-1.19173112474393
H	-5.12404551631529	-10.22291315338089	0.22247591360849
C	-4.13829223561522	-10.91427876917276	-1.57902637293896
H	-4.35884445807034	-11.97451867809648	-1.37506484837885
H	-4.17569303543559	-10.75835952307155	-2.66883022114024

H	-3.11006431820907	-10.70928782378715	-1.24029326324721
C	-3.90405267041584	-7.99011602994894	-0.12051124029341
H	-3.28919948209288	-7.27602834160638	-0.68626808247204
H	-3.23968533903018	-8.79385736414697	0.23155091950523
C	-4.55970545959104	-7.28794424782947	1.06751013268863
H	-5.19634051723694	-6.46008916842535	0.72048545028452
H	-5.18336137495149	-7.98845189417156	1.64651857075745
H	-3.79221010061437	-6.87567447074490	1.74268364228384
N	-4.87542827610566	-8.58827786786184	-1.03557478744452
O	-5.04609395999482	-4.24516899072681	-2.00620536829925
H	-4.59557186716764	-4.86811389295768	-1.38777685751401
H	-4.46612557189848	-3.40229138711048	-2.33494596145119
O	-3.89390247346937	-2.37639646682237	-3.10832248721692
H	-4.56801880487622	-2.65043306753809	-3.79471421197039
H	-4.19863219245287	-1.51472979132100	-2.77997795164527

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P	-5.30860246743884	-5.17220262533930	-1.69613876094668
O	-6.31316713335735	-4.60657025516515	-2.67723586987502
C	-5.72723645335491	-7.71410280283942	-0.90245004333791
F	-4.24486918011125	-5.54137834008117	0.00580761814195
N	-5.38344217138777	-6.80265525081678	-1.76783597675605

C	-6.35485379580542	-7.41249375831249	0.43924371763469
H	-6.63070501351567	-6.35669832672136	0.50189827418298
H	-7.24872945965186	-8.02870610879212	0.60845011279033
H	-5.63461112834631	-7.62528208099274	1.24365637980964
C	-5.88778788296776	-10.13186699284753	-0.35158135336207
H	-5.82917860894887	-9.81167714592803	0.69605227292308
H	-5.10967592933310	-10.90108307426441	-0.47764565149317
C	-7.26260387255927	-10.72442598803636	-0.65635660020447
H	-7.45788264612990	-11.58630440206278	0.00131325020997
H	-8.05992003340253	-9.98136027132188	-0.49727265777455
H	-7.32206123648905	-11.07178640340359	-1.70003513868794
C	-4.92765540297449	-9.35984205882261	-2.51615860021882
H	-5.28930703199749	-8.64524067218026	-3.26791541375793
H	-5.29863464126172	-10.35663160958926	-2.79819134576997
C	-3.40125314527543	-9.35340551965639	-2.47392955984921
H	-3.02394917873472	-8.34708840208860	-2.23780814362241
H	-3.02236966047485	-10.05566298691226	-1.71400040486896
H	-2.99184883190845	-9.65400637433709	-3.45165661084888
N	-5.53250083795958	-9.01342499088038	-1.22744691452419
O	-3.90486017367451	-4.56870631683300	-2.23460305080318
C	-2.58568258543804	-4.96989771350061	-1.86662834403493
H	-1.94180697370488	-4.73550804809423	-2.72737268479882

H	-2.53743608263160	-6.04454526043411	-1.64765385390612
H	-2.24103776853626	-4.41016412774730	-0.98612217470273
O	-6.03359891005800	-4.10603147837360	-0.34148074060304
H	-5.36083298457980	-3.64069582558934	0.33669761713350
H	-6.58899730652761	-3.47047350234672	-0.83226536314008
O	-4.24906056204174	-3.38005080272372	1.21078194051654
H	-3.96305659385279	-4.29216643690144	0.90207903271180
H	-3.64120431556800	-2.76585404606367	0.76789504183271

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P	-5.27603199091842	-5.15957525373103	-1.76716283323602
O	-6.29197928715207	-4.58830264384185	-2.73306980710979
C	-5.71594050812838	-7.68323547114230	-0.92514927735367
F	-4.20151876138357	-5.50635929025447	-0.07633135245825
N	-5.37646694575790	-6.79022324368046	-1.81101285354331
C	-6.33576155000827	-7.35495412445369	0.41383792803606
H	-6.60281261189777	-6.29619517659545	0.46109536155861
H	-7.23541846984796	-7.95958449668425	0.59474290957338
H	-5.61632863674046	-7.56392346910321	1.22001974923647
C	-5.88171140270705	-10.09074775618888	-0.33055141777312
H	-5.82848235064606	-9.75162125826169	0.71138308849195
H	-5.10337245921967	-10.86239025926697	-0.43889743799329

C	-7.25542398251740	-10.68777352431859	-0.63150764680613
H	-7.45521594660139	-11.53713826557762	0.04094923553694
H	-8.05264650418333	-9.94092383125519	-0.49052334591388
H	-7.30957115617427	-11.05427534025241	-1.66895170254183
C	-4.90858746904937	-9.35728751044419	-2.50372457405781
H	-5.27953069816281	-8.66823680009176	-3.27469357807136
H	-5.26214670557175	-10.36691149313354	-2.76088666218289
C	-3.38248819224380	-9.32378273911108	-2.45673968235802
H	-3.02333948989735	-8.30629357664583	-2.24114419843139
H	-2.99509947555192	-10.00295225914189	-1.68022342706150
H	-2.96436286177640	-9.63887170955571	-3.42621470103525
N	-5.52193167712503	-8.98875634551177	-1.22501609694094
O	-3.87747570372164	-4.59427024920396	-2.35300997382205
C	-2.54098131094186	-5.02810115562661	-2.04840053273261
H	-2.05808579591402	-5.20040987687742	-3.02433019113326
H	-2.57373211659461	-5.97602822843365	-1.49919196090103
C	-1.80776475023912	-3.96036299380972	-1.26179291989071
H	-1.76904829903185	-3.01350763316376	-1.82376223380766
H	-2.32788673290164	-3.78340864664124	-0.31092365528344
H	-0.77520974375260	-4.28046421353975	-1.04812964783829
O	-5.99672384267301	-4.08540231925535	-0.41015900210047
H	-5.42614134119749	-3.71360455767141	0.38926761110769

H	-6.54200834027031	-3.42290929178545	-0.87321983898464
O	-4.49005579277101	-3.61110265082334	1.51118547217228
H	-4.10354995452188	-4.43128857376129	1.08982739417753
H	-3.82903314220643	-2.91201477116297	1.38664480147174

PATH2

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34

P	-6.16851929062342	-5.53166371998360	-1.70221923983957
O	-7.64783599102288	-5.29100128137563	-1.44041088507389
C	-4.99347684425383	-4.21582883577926	-2.68281014928912
H	-5.69216156824291	-3.44771041659009	-2.32904352481907
H	-4.21513334251555	-4.76316794521479	-2.12604931718405
H	-4.91038967602779	-4.31092102818878	-3.76522740404678
C	-5.57560834217141	-8.07410683209875	-1.25158665719311
F	-6.37975168504985	-6.17619003776509	-3.28829214098452
N	-5.20483609335079	-6.82635102701318	-1.25236157380595
C	-6.99907362013935	-8.54107776951726	-1.47474986528210
H	-7.36338399003306	-9.10366297110517	-0.60170885366207
H	-7.65649797874463	-7.68093131994436	-1.63245772279006
H	-7.05923989748134	-9.20714790489756	-2.34856377074535
C	-4.92388433395182	-10.46128481448792	-0.95441532284949
H	-5.95543714379382	-10.62016533462909	-0.61650799568778

H	-4.27809410645777	-10.89628385488418	-0.17483077584181
C	-4.68748644946660	-11.17529255492081	-2.28515034010038
H	-4.87647531025552	-12.25549451191284	-2.17812966874635
H	-5.35649996135753	-10.78394533901952	-3.06775747660295
H	-3.64817811234186	-11.04313418386293	-2.62595648849739
C	-3.24273409259383	-8.63181349625423	-0.80333411366275
H	-3.00683001769437	-7.81238348511162	-1.49644255955480
H	-2.60994993007441	-9.48936727678462	-1.07722063018288
C	-2.95985635294982	-8.20038012493553	0.63458126390564
H	-3.55992782360533	-7.31499676719950	0.89277583133221
H	-3.20165428241856	-9.00828986243939	1.34419352874049
H	-1.89455179643110	-7.94572376808937	0.75656573135041
N	-4.63627596612761	-9.02853816960501	-1.01195046887145
O	-5.60092572768674	-4.60000439140664	-0.28061063012356
H	-6.42786770518777	-4.28923272333488	0.11970696896416
H	-4.37285175449127	-3.31527153828052	-0.33592513478764
O	-3.73733012861095	-2.72778212181748	-0.83040811511638
H	-4.25899772714373	-3.36638075201890	-2.09184461570097
H	-4.10977995770233	-1.83355383953082	-0.74915688325059

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P	-5.88277784114688	-5.96338318778567	-3.81464341528166
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O	-6.92107467832671	-6.00692303755395	-4.91228874719991
C	-5.59398507676811	-8.26684551019300	-2.52811360604775
F	-7.01086764482163	-5.80648642688049	-2.52176250690955
N	-5.06976570770477	-7.15390177569231	-2.95803127812272
C	-6.97664128771674	-8.75638899033125	-2.90345804509936
H	-6.91684361421012	-9.73638506002766	-3.40077352553267
H	-7.60523606488931	-8.87571167229665	-2.00834713247453
H	-7.45662681668215	-8.04828117255282	-3.58561780526968
C	-5.30230481791667	-10.35168577472584	-1.19686835195760
H	-4.42749403743660	-11.02076200529433	-1.16868927102590
H	-6.00997823417406	-10.80719990148098	-1.90047652112133
C	-5.92805558186616	-10.25288075748821	0.19397781807705
H	-5.22027500215039	-9.81667976396580	0.91688178849386
H	-6.83219184090669	-9.62392009461252	0.17778934838889
H	-6.21124958368685	-11.25409268580959	0.55635331318558
C	-3.50392151249734	-8.63680370247528	-1.32418536835987
H	-3.28293781021520	-9.09391169375957	-0.34781804289254
H	-3.51229158628051	-7.54702974417889	-1.18805076268651
C	-2.44219287803413	-9.03093878703965	-2.34938525440169
H	-1.44251411125398	-8.71786310796409	-2.00747623093841
H	-2.42489161278218	-10.12228355667258	-2.50191674956840
H	-2.64482223482354	-8.54722308473030	-3.31703417822624

N	-4.84912045871948	-9.06147431028555	-1.71620035630104
O	-5.31942682469917	-4.35936014485598	-3.29474284051736
C	-5.96432632858999	-3.51612391842462	-2.32264226740565
H	-5.39457644524650	-2.57633664305866	-2.30989946225413
H	-7.00818543427768	-3.32406461224275	-2.60207213106497
H	-5.92557315407932	-3.99521712370443	-1.33828158108392
O	-4.48560501489278	-5.89060913633648	-4.91689611960334
H	-3.71837758772639	-6.23901721358566	-4.43381428953244
H	-4.19024247436126	-4.43935203236348	-5.43265517698096
O	-4.24492284370000	-3.43629310945642	-5.22201278126501
H	-4.80078069724867	-3.74730662751513	-4.19509130391780
H	-4.91497916016789	-3.06807763465919	-5.82458916510236

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P	-5.49123353238060	-5.30210764711900	-1.60039499561050
O	-6.57445806808236	-4.37631592045140	-1.09440785502104
C	-5.81545641876376	-7.84389640640599	-0.91771337609961
F	-4.65745750897831	-5.41149189240286	-0.09502347830386
N	-5.38170562802610	-6.96397357787914	-1.77551173686545
C	-6.69911469450902	-7.50778010951605	0.26532613173571
H	-6.12521948198366	-7.59328340035728	1.20133226638713
H	-7.06456126794878	-6.47914070982763	0.17603116589699

H	-7.56000192541558	-8.18735337151908	0.33331831100427
C	-5.90939380642476	-10.22781356786457	-0.21373883746235
H	-6.06750689167697	-9.83874251474076	0.80010938349830
H	-5.07563275460557	-10.94339836163972	-0.13627341111023
C	-7.16415721199914	-10.94094357115403	-0.71574040235580
H	-7.42577487075081	-11.77294249523826	-0.04251416913058
H	-8.02107241356982	-10.25007505262405	-0.75972948298264
H	-7.00645881658947	-11.35455814951678	-1.72457832099801
C	-4.59507476587527	-9.51386133857568	-2.20799637008625
H	-4.88728969466749	-8.92284612676572	-3.08725053922937
H	-4.78381348373031	-10.57259427507495	-2.44036405478474
C	-3.11620909890450	-9.29168010357478	-1.89681927723812
H	-2.92305709409702	-8.22608224060271	-1.70174069958515
H	-2.80605128742250	-9.87184684194602	-1.01259133471115
H	-2.49307180686550	-9.60695535313301	-2.74925300591891
N	-5.46907388610335	-9.14444078148282	-1.09296300053301
O	-3.99292519653828	-4.56324787612260	-2.19602900528262
C	-2.80916287443047	-4.25874063451529	-1.41254081641585
H	-2.49496491010919	-5.18484888114513	-0.91789320213940
H	-3.07523952516718	-3.52634029566602	-0.63708292416982
C	-1.73984256401844	-3.73120214463586	-2.34740928823644
H	-1.50120461791439	-4.47000651073448	-3.12863464158949

H	-2.05144359072701	-2.79195725631651	-2.83160820474592
H	-0.82397534967477	-3.52789523357778	-1.77107331999981
O	-6.00135588287937	-5.20742534242520	-3.30760071293873
H	-5.43392220154414	-3.94653860362514	-4.03733758234430
H	-5.66470627541387	-6.00005046534685	-3.75638040493427
O	-4.67720476536566	-3.25133428280982	-4.07969469684929
H	-4.18617416227269	-3.82392814496044	-3.13237236789338
H	-4.15432967457363	-3.47084351870617	-4.87071774295621

PATH3

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P	-6.12546874959316	-5.47615178149572	-1.96830421907904
O	-7.56075215025466	-5.24264683355688	-1.57838604026964
C	-5.02864699150888	-4.25156905214133	-2.73969714909109
H	-4.96794872879506	-4.43914656102574	-3.81820781680968
H	-5.43781393878309	-3.25451823770683	-2.53344845228747
H	-4.03441763456777	-4.32351154647694	-2.28069325503680
C	-5.52757736476851	-8.03514596444768	-1.27382377691980
F	-6.33440535086051	-6.34018385619840	-3.39449057037341
N	-5.18051299259388	-6.74988489851953	-1.26221651697207
C	-6.94807894134396	-8.45056986928478	-1.55408285973916
H	-7.31782327558879	-9.07021199891164	-0.72448764176432

H	-7.59610597408992	-7.57534077585879	-1.64470014009940
H	-7.00556440097093	-9.04876790953297	-2.47402141537363
C	-4.97061109147455	-10.41740689777387	-0.97979969546365
H	-5.98937251373721	-10.54448308807521	-0.59601099092733
H	-4.30286093068391	-10.88627063613168	-0.24307672784487
C	-4.81295016096238	-11.09478048583183	-2.33884384843124
H	-5.03127327144173	-12.16967041887198	-2.24268564609560
H	-5.50230340098037	-10.66970424378537	-3.08414119048873
H	-3.78517614026012	-10.98905585160478	-2.71967464240345
C	-3.19795837724111	-8.69492747871881	-0.81463743877703
H	-2.95666569922117	-7.75393811071795	-1.32432647305321
H	-2.64227903194925	-9.49331453129802	-1.32882575689605
C	-2.79669987320915	-8.62729431196624	0.65560782293828
H	-3.24934106369826	-7.74885782201501	1.13371819726463
H	-3.08763100200753	-9.54235484825194	1.19500031417745
H	-1.70241780224658	-8.52430624078672	0.72891680532466
N	-4.62701061903792	-8.98522517699732	-1.01130806407645
O	-5.52207804884346	-4.39520084115850	-0.22718194168738
H	-6.15039679399298	-4.68584716962381	0.45061346779335
H	-4.50621530465399	-4.81598902172026	0.04537233640673
O	-3.44915152295555	-5.56434573454633	0.11800987268728
H	-4.25943901439923	-6.34608913905403	-0.69001569116278

H	-2.73255784328436	-5.17341666591291	-0.40286585546908
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P	-6.47558852813277	-6.08367706426344	-3.70664486055207
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C	-5.67729597571604	-8.36014743948416	-2.48480630721362
F	-7.50281767498068	-6.22665567093418	-2.36163003488506
N	-5.35079332280295	-7.18371025575620	-2.99221784684344
C	-7.00472590549758	-9.01548664860183	-2.77691412398413
H	-6.83951585495935	-10.01946065216208	-3.19377622884252
H	-7.59562970558843	-9.12580437084145	-1.85655634337244
H	-7.57190711510872	-8.42710144140240	-3.50283096009392
C	-5.09246939891711	-10.34522705468776	-1.12935276709874
H	-4.13669288337823	-10.88737752052762	-1.07789541696929
H	-5.73205218536928	-10.91773040511748	-1.81089689051710
C	-5.72349601025553	-10.26095370231994	0.25869864711177
H	-5.07796082774387	-9.70439348778030	0.95622462967611
H	-6.70349115168033	-9.76074600042299	0.22386835166253
H	-5.86857135569706	-11.27444641940431	0.66437789921857
C	-3.50871908631973	-8.44995966617147	-1.33136690892221
H	-3.29961943049161	-8.77625524758359	-0.30176603643979
H	-3.60286092698780	-7.35669970113741	-1.30319378598021

C	-2.37515640758685	-8.87681605060962	-2.26054262353688
H	-1.42273237473667	-8.45660133017452	-1.90070361259359
H	-2.27554211493360	-9.97342595670259	-2.28755871615959
H	-2.54371846389196	-8.50638976080467	-3.28094471500598
N	-4.80557573441919	-9.02499483136862	-1.70878193056588
O	-6.04951651952648	-4.56368035389702	-3.27296674894459
C	-6.40973409428858	-3.94271517737116	-2.04123406655105
H	-6.07014926360129	-4.53408602860694	-1.17732832102335
H	-5.90430235993568	-2.96626137997598	-2.03291636375801
H	-7.49614249297400	-3.79214153883605	-1.96365940501293
O	-5.14181922134156	-5.74927850136784	-5.03259989283771
H	-5.23460434489344	-6.45941159333291	-5.68730728545729
H	-4.07113955221341	-5.82336194203692	-4.48126317359601
O	-3.23769423782487	-6.09182495716356	-3.64181719580482
H	-4.14308076158956	-6.69070927339496	-3.14638063831426
H	-3.11061853534493	-5.29186697925165	-3.10764122662437

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P	-5.60185937267205	-5.28992462881145	-0.99468434031108
O	-6.80000720489257	-4.61106355708535	-0.39477123289550
C	-5.82266911204185	-7.97901119417875	-0.82569154104175
F	-4.81262538128614	-5.69927474358085	0.44751495496095

N	-5.48723369108686	-6.92043725916209	-1.54974034784540
C	-6.63831955594082	-7.84366415197102	0.43585086041570
H	-5.99895372974994	-7.99838872032580	1.31769821271842
H	-7.08065037179912	-6.84468041124726	0.49551049464442
H	-7.44368188892643	-8.58897683527219	0.45695038356394
C	-5.79439618176592	-10.41916546241988	-0.45855078957951
H	-5.90143228388278	-10.17033235376474	0.60336709462298
H	-4.92220928009072	-11.08626102583493	-0.53075397369570
C	-7.04357945659982	-11.12055539197841	-0.98402982288426
H	-7.22202800121425	-12.04484586307932	-0.41270749300094
H	-7.93184582806725	-10.47686635069842	-0.88696465284648
H	-6.92992646645549	-11.39122511685846	-2.04553142179618
C	-4.65333644081871	-9.41600276445653	-2.43039351483739
H	-5.07000222975477	-8.81525528166766	-3.24770151878544
H	-4.78523502716640	-10.46676034652511	-2.72088129970409
C	-3.17366855929501	-9.10462984763244	-2.22350641403444
H	-3.02057523691934	-8.04647389728706	-1.96735857350374
H	-2.75221534367843	-9.72623894841900	-1.41797048168005
H	-2.61746915249416	-9.31491303746289	-3.15010391189368
N	-5.45798595308873	-9.20495340797159	-1.21778224142047
O	-4.30853519456365	-4.45451517221353	-1.52794455657752
C	-2.94485958771875	-4.77330918065116	-1.19498209214724

H	-2.86687250701221	-5.83699729571537	-0.92686062696911
H	-2.64667041949057	-4.18414870678512	-0.31242636870016
C	-2.08645610197117	-4.45744570905588	-2.40264699097867
H	-2.42082719788066	-5.05895456589937	-3.26174709461480
H	-2.15927076277481	-3.39133587441952	-2.67065452419456
H	-1.03114305949313	-4.69111708526651	-2.18945157843690
O	-6.26423243961848	-4.97070122889469	-2.82040982833873
H	-5.53275131931243	-5.57351426449043	-3.50214905582701
H	-6.15800605752873	-4.02287248025832	-2.99678026240917
O	-4.72290693767758	-6.46953080222320	-3.85842011443859
H	-5.03633011370653	-6.90931200549930	-2.71742861401907
H	-5.16392555156330	-6.99828403093582	-4.53980672151866

PATH6

A230-H⁺

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P	-0.02209119641633	-1.44804916910440	-2.89714129412899
F	1.56571504515899	-2.19494759138792	-3.27426392184139
O	-0.64769527312918	-2.71426158604576	-2.37455387860712
N	2.78797057419296	0.05912901648127	-0.43827637325042
N	0.97720972598638	-0.45209329617635	-1.78416184691384
C	3.82025670474558	-0.29349884953864	0.55471121902686
C	2.75727567506994	1.47699109275084	-0.83897764023831

C	1.94987663096554	-0.83486877136378	-0.94540139292879
C	5.16943232284516	-0.59639992573083	-0.08931292965807
C	1.79546856029330	2.31120355991520	0.00401573339217
C	2.03787280969551	-2.27330864121747	-0.53055584796808
C	-1.36729877206489	-0.18036134839360	-2.82292524059595
H	3.47237479135766	-1.14203144311551	1.15388564577293
H	3.90234793851486	0.56214041193345	1.24031321493138
H	3.78315085568107	1.85523130120605	-0.73551741417656
H	2.51666814113794	1.53846153688884	-1.91078459092165
H	5.53708913151115	0.26349401243241	-0.67042614204989
H	5.90805454186970	-0.81847837331581	0.69614354175100
H	5.10546801421226	-1.46661689054134	-0.76004050786096
H	1.84660221639054	3.36335782008475	-0.31462555687268
H	0.75436189914094	1.96970934429168	-0.10453538213875
H	2.06495416801984	2.25991313127617	1.07007583398207
H	1.94555432901871	-2.33776449692664	0.56398407208193
H	1.23339733864243	-2.85275146873057	-0.98978241979755
H	3.00924382147673	-2.69936396744347	-0.81704969771402
H	-2.22080582638320	-0.53878373780271	-3.41835644006467
H	-1.68436837267357	-0.08974538621639	-1.77419872467070
H	-1.05518591553972	0.80831700656205	-3.19641627123149
H	0.83374538852694	0.54715166908985	-1.90289233091854

O	0.07524079077737	-1.21908096890985	-4.65175467854642
H	0.65425093741157	-2.14113310184796	-5.32287515005889
H	-0.72609344784408	-0.82348299815959	-5.03604049088630
O	1.31968668742197	-3.01790570995023	-5.63928062828132
H	1.73696105627244	-3.13586829673064	-4.74773778528514
H	0.75967170771345	-3.80280988426308	-5.78987868333178

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P	-4.99186007182914	-5.16701003721556	-1.86561770090401
O	-5.70591028002769	-4.86527872652325	-3.17122557173390
C	-5.63300233578143	-7.81785753270357	-0.87457770258854
F	-4.32226347013449	-5.54136843264860	-0.23755219678782
N	-5.47961898666540	-6.86206334340236	-1.80653273525610
C	-5.96106015816246	-7.46774540869055	0.54672138960555
H	-6.23501316206480	-6.41423048892629	0.62379617997205
H	-6.79965874950774	-8.08485279779380	0.89508577959215
H	-5.09552662658779	-7.65742577622915	1.19865754659660
C	-5.81098964453471	-10.20484250588845	-0.31383795607637
H	-5.56130268315224	-9.88615718649510	0.70406417222066
H	-5.08978901142897	-10.99110347188585	-0.58024443454053
C	-7.23924209570171	-10.73258087826259	-0.39467817568888
H	-7.35254484347550	-11.59251999511790	0.28308064755947

H	-7.96613742525864	-9.95996193792512	-0.09950653016405
H	-7.48379385991589	-11.06606489275957	-1.41510825915398
C	-5.21470807413258	-9.47522663030806	-2.62717122602850
H	-5.82803095230775	-8.90286725659042	-3.34055895638435
H	-5.52154267031556	-10.52190834756695	-2.74676052477989
C	-3.72332069927580	-9.31764823309214	-2.91166222925951
H	-3.40293435893796	-8.26873443430319	-2.82545530883922
H	-3.13082812884712	-9.92429115383654	-2.20979760187321
H	-3.50793509386496	-9.66004820557496	-3.93508544917264
N	-5.56729472813865	-9.08817933576530	-1.24633856146862
O	-3.45332425886107	-4.87591966327215	-2.32348085378290
C	-2.26061283982647	-4.89715706721124	-1.53797054493392
H	-1.44341814565823	-4.62780601095530	-2.22234589192260
H	-2.07272228416078	-5.89505813603170	-1.11723188375343
O	-5.77390761690523	-3.97156181940154	-0.92453453934505
H	-5.30426984243660	-3.55009990354788	0.31715345776657
H	-6.33139280500728	-3.45397642814675	-1.53323683480936
O	-4.77037144334064	-3.56577699169189	1.25352184326446
H	-4.25546033988235	-4.39883917994875	1.08543002095102
H	-4.13250464180799	-2.82492613584073	1.27758619969736
H	-5.60596536993339	-7.15193050925991	-2.77462128176029
H	-2.30720330213080	-4.16251814518664	-0.72091828621819

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P	-4.97165274645066	-5.13415057201611	-1.90706679214856
O	-5.69966187336561	-4.83762342189431	-3.20555695874748
C	-5.62249282181487	-7.76794644351461	-0.86521315306159
F	-4.26868521148340	-5.50737524679076	-0.24240333254342
N	-5.47966141792150	-6.81772630668123	-1.80505303973758
C	-5.95299673498682	-7.41079985338098	0.55304321433620
H	-6.25914402946929	-6.36550687319817	0.61656099920110
H	-6.77503676084965	-8.04282386865633	0.91325672242542
H	-5.08088143186712	-7.56927070751447	1.20421129386814
C	-5.78516274483570	-10.15253794667481	-0.29004283829116
H	-5.53661442714737	-9.82708311320824	0.72597982389237
H	-5.05972134720805	-10.93608483707521	-0.55265032038455
C	-7.21069743103717	-10.68804162468837	-0.36821254831609
H	-7.31958933509243	-11.54514568558372	0.31380681794337
H	-7.94152742526850	-9.91762880489531	-0.07698183018596
H	-7.45340068323460	-11.02777291583043	-1.38699629280295
C	-5.19343773055862	-9.43328579370986	-2.60784061610948
H	-5.81345681106148	-8.87231396630979	-3.32451902799204
H	-5.49061525137790	-10.48363258810907	-2.71906743387988
C	-3.70407835868086	-9.26414357013770	-2.89595859989093

H	-3.39359197060639	-8.21136219353855	-2.82222650201638
H	-3.10486487206783	-9.85727266618258	-2.18830550347282
H	-3.48709712490424	-9.61594738729490	-3.91583377080116
N	-5.54761525754202	-9.03962969171748	-1.22897162727514
O	-3.43472517088088	-4.92097398245751	-2.39133994040709
C	-2.18619900734814	-4.97636169143349	-1.67930104355274
H	-1.43693213618628	-5.18476835089628	-2.45868255603751
H	-2.19140981019722	-5.81596391588521	-0.97316825121244
C	-1.88103609466871	-3.66168899609397	-0.98728755478403
H	-1.89022342661275	-2.83048929858593	-1.71003590326376
H	-2.62171785600455	-3.44873870802627	-0.20412864733928
H	-0.88472672780045	-3.70340408682138	-0.51861542898724
O	-5.70766463684829	-3.92535522645628	-0.96661806287135
H	-5.43362467457189	-3.61745321832483	0.42946380241196
H	-6.30341412640170	-3.44214679428821	-1.56740793414008
O	-5.02014969556508	-3.80880723489598	1.38025587340642
H	-4.46232554610271	-4.59178262427140	1.08380153114338
H	-4.42246903504421	-3.07882783329222	1.63651000769028
H	-5.61043825693475	-7.11929095966763	-2.76923857606592

PATH7

A230-H⁺

P	-2.35070633645703	-0.15273466860388	-1.17208201549327
F	-2.10772821343266	-1.58562107246441	-0.43627421435286
O	-2.98395837025389	0.96684840394213	-0.39958479692388
N	1.55203680698658	0.31415517614695	0.09422225447934
N	-0.62672235832641	0.31110078213974	-0.66051824287407
C	2.84427230571106	-0.34182036134724	0.35848593918710
C	1.43829596482472	1.70898881894753	0.55065108295086
C	0.53203955096453	-0.31369074901990	-0.49405212231868
C	3.88122795747962	-0.06257615495711	-0.72455803280472
C	0.75788044871532	1.83585775285096	1.91261686717520
C	0.70815771230461	-1.73007071596109	-0.95545260239760
H	2.68602250718125	-1.41879310052527	0.48617584309711
H	3.19321326361957	0.03544545981306	1.33121487109612
H	2.45881121625059	2.11183144843683	0.59518524649665
H	0.91699586744826	2.30026653794734	-0.21861689958180
H	4.05654476689167	1.01863755059738	-0.83828261162599
H	4.83709863086263	-0.53667337719212	-0.45288413891162
H	3.56064700113376	-0.46376258429169	-1.69853996683100
H	0.73613025397316	2.89327581465419	2.21743846967106
H	-0.27840044982365	1.46532533315052	1.88746947009733
H	1.30955440233765	1.26649652427400	2.67651478896763
H	0.70969252053137	-2.40179090670375	-0.08254430686195

H	-0.09864795131579	-2.04244286399238	-1.62006866208606
H	1.66392651628967	-1.84670274346197	-1.48097632588819
H	-0.69283825226679	1.26606456588995	-0.31807770426461
O	-3.64765728422366	-0.79702361411701	-2.04063269688995
H	-4.41788187305847	-0.84276925068873	-1.44821434940269
O	-1.80642281624010	-2.41437705172194	-3.14039354717534
H	-2.76547092591150	-2.50010148294731	-2.96529304791779
H	-1.67854165206640	-2.62689315774008	-4.08255548369217
C	-1.60487957785291	0.22535034070472	-3.09587035942130
H	-0.52040668712910	0.31816257136981	-3.23403487067131
H	-1.95892096161487	1.21494826374650	-2.75527093002043
H	-2.18050871130713	0.09544062682897	-4.03036808113789
H	-1.70015527222562	-1.04757211570472	-2.96486882367323

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P	-6.18552590324629	-6.03092599803830	-4.08237003136842
O	-7.29447298059507	-6.16288279149985	-5.07969265913578
C	-5.64827088354543	-8.38516771491776	-2.64230719925360
F	-7.09247801413109	-6.11272300773544	-2.66536633072833
N	-5.25866330365446	-7.37630120187461	-3.44574313753491
C	-7.07149196619631	-8.85095024312629	-2.66923960646236
H	-7.08954497502772	-9.91783549537655	-2.93810358557417

H	-7.54060837720663	-8.74049531855840	-1.68193986513783
H	-7.64684157483367	-8.29457846617138	-3.41314081589454
C	-5.07617024831485	-10.18542656954098	-1.07676879654831
H	-4.17527765058023	-10.81494837245913	-1.06876690109568
H	-5.86029316384085	-10.76256373117190	-1.57998528774467
C	-5.49122991566856	-9.81997392551814	0.34468360106729
H	-4.70092815568441	-9.25213944662241	0.85937011682509
H	-6.41267624327420	-9.21837247593544	0.35115091184299
H	-5.67695124912728	-10.74187336728752	0.91656926367813
C	-3.35869569811348	-8.51895991639513	-1.79076842824769
H	-3.01948499833243	-8.75908490162647	-0.77419968100109
H	-3.36105711841265	-7.42196762463461	-1.87051480111963
C	-2.43427518587518	-9.15739398642296	-2.82436147417699
H	-1.40732189987683	-8.79477846433259	-2.66689709385876
H	-2.43190289433303	-10.25360765108202	-2.72522785746455
H	-2.73221049597320	-8.90654350005832	-3.85448967494996
N	-4.75131683341959	-8.99784389196495	-1.89126189419371
O	-5.87572344626699	-4.31116786911260	-3.51283466365959
C	-6.73687385630977	-3.55600668280515	-2.62940105201148
H	-6.41230860826890	-2.50966781337755	-2.70060245641397
H	-7.76565874378197	-3.65953457298511	-2.99023287760415
H	-6.65131981533448	-3.92727440347288	-1.60118512475194

O	-4.80278799987342	-5.74853074116726	-5.01204922070126
H	-5.00164877301655	-5.08306727085899	-5.69035794079692
H	-3.16570915071965	-4.75026153197638	-3.83080921059884
O	-3.43713982093505	-4.11473933428055	-3.14246227555836
H	-4.83431698001232	-4.15586197378023	-3.32490853977730
H	-3.19063840899083	-4.53708735720249	-2.30125007756829
H	-4.26902966722580	-7.30011838662858	-3.66289233248001

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P	-4.91214754028547	-5.01180279472625	-2.48250559198601
O	-4.69997069152367	-5.07689270982421	-3.96174085865963
C	-5.29704228528671	-7.60182285794369	-1.19834739982214
F	-6.39861176409231	-4.94059391904800	-1.80851234122583
N	-5.05735700455354	-6.83738651700982	-2.25497545465951
C	-5.39677838812377	-6.97760829855844	0.16425344972892
H	-6.28915668797456	-7.33751697284157	0.69228045197569
H	-4.51272800010602	-7.25430082905593	0.75978919985331
H	-5.45096266676898	-5.88874901114142	0.10824620381612
C	-5.63001973540927	-9.81572656190618	-0.16996468456595
H	-5.18336767387951	-9.36637651255877	0.72426050236394
H	-5.05774402206432	-10.73262607783883	-0.37374941765903
C	-7.10209660403953	-10.14364360185537	0.05777493087591

H	-7.19939451693914	-10.83912664661115	0.90570121057152
H	-7.68171447257829	-9.23577759640303	0.28585293828692
H	-7.54530589576422	-10.62241920465634	-0.82929129679178
C	-5.31774943672189	-9.58703009506500	-2.63228301769597
H	-5.82316345460606	-8.96960064540945	-3.39074358525254
H	-5.90175407125718	-10.51478017003536	-2.56386015475596
C	-3.87577719683391	-9.89470159277445	-3.03030043657402
H	-3.27686029629302	-8.97663947911966	-3.12989578955748
H	-3.39365113909690	-10.54103921160920	-2.28070429031849
H	-3.86283450035544	-10.41951231395720	-3.99773476788436
N	-5.41788180856055	-8.92337803965282	-1.32314367556118
O	-3.39120433304891	-5.15754286180553	-1.50703674359139
C	-2.35393407856402	-6.16877896372280	-1.68090569885580
H	-2.51413481143372	-6.96258649906563	-0.93753840060207
C	-0.99710323299518	-5.51503704894404	-1.53873418022941
H	-2.49791084819575	-6.58546375055983	-2.68501637890813
O	-4.81572216978171	-3.38600242179033	-2.08013525317519
H	-4.05739799833739	-2.97658378463815	0.00907426845917
H	-4.02632735199559	-3.00743782579875	-2.50222078297188
O	-3.38577703574910	-3.58789693517496	0.36776296119244
H	-3.29694042005432	-4.47426279587278	-0.65501617577447
H	-2.57456476196836	-3.05737649063773	0.45639319498583

H	-4.95921404451926	-7.28346758485438	-3.16288058455587
H	-0.86673165965419	-4.71680305769605	-2.28505361748412
H	-0.21719280048739	-6.27577695755769	-1.69804405692970
H	-0.85805460010019	-5.09131136227820	-0.53188467606163

PATH8

A230-H⁺

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P	-5.69253665107994	-5.58724011854590	-2.03137859390446
O	-7.07917536764481	-5.31776520166456	-2.55462465599045
C	-4.11566813715368	-4.92403223925347	-2.66111372336745
H	-3.32911777358114	-5.07486092593796	-1.90621957520130
H	-3.83960571129912	-5.42623403792455	-3.59426947818824
H	-4.24555949003422	-3.84299335310345	-2.80076200639350
C	-5.75212601331903	-8.17724318049879	-0.76098766808182
F	-5.39501382673489	-7.03890054865591	-2.92393528367547
N	-5.64135482218880	-6.80344874531691	-0.50743826099824
C	-7.14133374797158	-8.71162849513333	-0.77812906276480
H	-7.62165606500679	-8.47401866397154	0.18512347965572
H	-7.68588441923671	-8.15384912836486	-1.55831305664703
H	-7.22056434995939	-9.78366333276081	-0.96986010574262
C	-4.77320790595782	-10.32289081881888	-1.37132425024147
H	-5.54433594574381	-10.81427063707802	-0.76714904092388

H	-3.81274040493729	-10.77304325598667	-1.09153316379369
C	-5.03316256522835	-10.47567960280557	-2.86568976686798
H	-5.03570822768162	-11.54537722924801	-3.12310026849565
H	-6.00469483850207	-10.04492039210275	-3.14891388738296
H	-4.24948378477564	-9.97849053872287	-3.45679557807553
C	-3.32526198375687	-8.33254737316384	-0.99905981857136
H	-3.37812405969860	-7.25989166215353	-1.19334884178208
H	-2.81868857207055	-8.78201526364561	-1.86428613820087
C	-2.57294265038128	-8.62969810249458	0.29267791711639
H	-3.07058714310471	-8.16578586929536	1.15789494343675
H	-2.49187282192852	-9.71162120733758	0.47561317056412
H	-1.55561911855059	-8.21814633070774	0.21434311827560
N	-4.69230447823451	-8.89479217214464	-0.98294735314665
O	-5.65185559458798	-4.35326011143727	-0.75434696102679
H	-6.56328182746439	-4.06665651110344	-0.57989810038536
H	-4.68492207306185	-4.70969872979887	0.51456567638327
O	-4.25551050742527	-5.46349646360101	1.04315827772052
H	-4.75945552864191	-6.28614477706998	0.35856638918672
H	-3.29608196173008	-5.42264514007255	0.87442572139791
H	-6.49766042132556	-6.50746738007814	-0.02545987388720

A232-H⁺

P	-6.38963652435519	-6.20288544770384	-2.90587775766900
O	-7.74641486824504	-6.76327458183589	-2.57497677655561
C	-5.15718423718985	-8.66696467890198	-2.60063187773415
F	-5.85940948447931	-6.11351746012346	-1.27299730172775
N	-4.84582393065049	-7.36794235203637	-2.99843666169255
C	-6.08328242158827	-9.43542492113380	-3.48282437116470
H	-5.54494971116687	-10.29092296269669	-3.92167600291756
H	-6.93779319460654	-9.82106861147948	-2.91090809314997
H	-6.44643737261892	-8.79588810067766	-4.29136086711982
C	-4.94807572773699	-10.56547736710858	-1.09662204686322
H	-4.03036040955493	-10.95019498716346	-0.63145798177483
H	-5.13908083156037	-11.17196446619338	-1.98853848256994
C	-6.11964869752262	-10.61900973760438	-0.12183500825479
H	-5.91328780136976	-10.03087911792984	0.78510317606822
H	-7.04283714114040	-10.23732682253584	-0.58296438530526
H	-6.28620744660100	-11.66452427108406	0.17745093963145
C	-3.75781433677966	-8.42133941525756	-0.60095697452687
H	-3.92435285308384	-8.84424704379606	0.39793142722976
H	-4.10865789471326	-7.38277797462400	-0.55877352558239
C	-2.28976429988142	-8.53593789634009	-0.99691243969508
H	-1.67861887898446	-8.00036631010521	-0.25535471509350
H	-1.96684960622451	-9.58775260724695	-1.01721405870796

H	-2.09850902088747	-8.09350966747586	-1.98661309063001
N	-4.64744883497313	-9.17683577140984	-1.51560126755388
O	-5.89842848115153	-4.68095971169400	-3.16282136631801
C	-5.51834408668208	-3.73691182224301	-2.15385000719370
H	-4.56265486160315	-4.01925880158875	-1.69067119613025
H	-5.40649211733552	-2.77549740538571	-2.67351050773748
H	-6.28819076804881	-3.64859977331630	-1.37512235157049
O	-6.48956343006495	-6.38695418910698	-4.62496376070351
H	-7.40029510278913	-6.65744319102182	-4.82047244700744
H	-5.12507743981075	-6.75454501490064	-5.52155102584677
O	-4.22644753844078	-7.18508119722499	-5.40518581308395
H	-3.55684994269255	-6.49168437705302	-5.54986659523109
H	-4.39640564802600	-7.33082987653715	-4.21627402511726
H	-4.13454505744011	-6.93770206746286	-2.40305076070050

A234-H⁺

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P	-6.33908547957790	-6.25531186721933	-3.07493954848157
O	-7.71856440822637	-6.64021917897259	-2.61154590465183
C	-5.23778691246443	-8.76717934252029	-2.61192360729049
F	-5.69172559638615	-6.04523114678484	-1.51346717474506
N	-4.89167877466346	-7.53160295172493	-3.15439003809383
C	-6.26704990381007	-9.55744133647027	-3.34790589550679

H	-5.79869752223235	-10.46096288071977	-3.77148803663054
H	-7.07833040551769	-9.87071864612634	-2.67762316802741
H	-6.67920027779748	-8.96055525959242	-4.16595114137400
C	-4.98717283703472	-10.53640297760561	-0.96250126420111
H	-4.05003240558053	-10.92349204247214	-0.53957890699391
H	-5.27595443277905	-11.20616042568157	-1.77997230763301
C	-6.07513451684849	-10.45377376503764	0.10273055071705
H	-5.77431792715023	-9.79629643259919	0.93221444281828
H	-7.01981334533504	-10.07697027849724	-0.31706847682546
H	-6.25195376642344	-11.46078042577229	0.50910019010705
C	-3.67215271087538	-8.41357716085573	-0.75969347293534
H	-3.76627079224259	-8.74103136947082	0.28360407170179
H	-3.97995023711475	-7.36047230852568	-0.78229332810714
C	-2.24922337004446	-8.62701747684813	-1.26411027194120
H	-1.55669203422715	-8.05941280074182	-0.62493215439161
H	-1.96929085484522	-9.69033214641623	-1.21871499452489
H	-2.12575468039147	-8.27803894605617	-2.30086180259130
N	-4.66564733686488	-9.20442861590038	-1.52616971895096
O	-5.69629214717400	-4.80554112773370	-3.39913212322127
C	-5.76846117264629	-4.09344980980616	-4.65227044600043
H	-5.14205521557321	-4.61241581995859	-5.39292005436523
H	-6.80393102444626	-4.09446635509731	-5.02247418095843

O	-6.58826734568765	-6.63981616167952	-4.75969858385359
H	-7.53885511933388	-6.79307471918663	-4.87553802157781
H	-5.32709936857153	-7.20691447932519	-5.71812132268662
O	-4.44114935112907	-7.66128268413010	-5.60318539405127
H	-3.75507904224493	-7.03225015301646	-5.89287273211064
H	-4.52618422297698	-7.64828187821560	-4.40215659042984
H	-4.11904670720872	-7.08979477056110	-2.65256076603691
C	-5.27335937792108	-2.68502637719024	-4.39940094824492
H	-5.90724495845812	-2.17344518558099	-3.65815593292271
H	-4.23692694287003	-2.69423976182078	-4.02684228785748
H	-5.30054447532467	-2.10942393408580	-5.33810165712940

Reaction path of intermediate in protonation of NAs

A230-R-TS1

31

P	-1.42272486331431	-0.51788418440536	-2.12062104736057
F	-0.10942645288921	-1.07096965696392	-2.94451633963136
O	-1.83383906933381	-1.31289112062869	-0.90202754151280
N	2.08252582955903	0.67312440067267	0.44342186332742
N	0.21163151310553	0.42907340976636	-0.94727088776644
C	3.13319687953026	0.10049577492693	1.29383870146333
C	2.08086946071147	2.13407165098631	0.33377984370230
C	1.16032334448273	-0.08234629434877	-0.20725875041620

C	4.46090277422013	-0.09712320304248	0.56328601975472
C	1.13391318536663	2.81249161472318	1.32500540945246
C	1.24581563985337	-1.57903920661652	-0.05665339034943
C	-1.80865677979062	1.22548757854437	-2.46734566076042
H	2.78548561414093	-0.84745688192439	1.72112538270544
H	3.26969558627993	0.78537981250572	2.14515189637003
H	3.11120358858783	2.47541177723149	0.50762272764341
H	1.84097248113131	2.42481738386388	-0.70165721191485
H	4.83412819143085	0.85381787984482	0.15087550642192
H	5.22009055993633	-0.48643688718962	1.26059948256952
H	4.35567107893846	-0.81321409608412	-0.26655153212255
H	1.19706406842605	3.90725656371090	1.21920517992327
H	0.08817167756235	2.51173036662882	1.15653914169434
H	1.40396739850603	2.55096589116490	2.36026094862396
H	2.24706927408143	-1.94591386112571	-0.32401554733368
H	1.04795449653389	-1.87066372864564	0.98659991689791
H	0.49990665229611	-2.06078409620540	-0.69168025130560
H	-2.74346082962273	1.27811738407616	-3.03740621160711
H	-1.90798118072322	1.76872690923133	-1.51931082461002
H	-0.98909761616954	1.66643998165399	-3.05227498993097
H	0.22594010148002	1.44538765176185	-0.98925624829625
O	-2.47131423559910	-1.07832099626346	-3.32490126443572

H	-2.53471146871813	-2.04631385784958	-3.30490172119605
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A230-R-TS2

31

P	-1.33394765037838	0.29845545986849	-1.98295141884606
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F	-0.92839933567092	0.07776102453644	-3.92786004341830
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O	-1.59606132993311	0.33516481878658	-0.46200173590249
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N	1.46315673507288	0.17909879803261	-0.05425456811769
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N	0.28398151627159	-0.42128655869544	-1.99363934101048
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C	2.29294922178511	-0.20778795434648	1.10552036430151
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C	1.24715115005751	1.63369146159944	-0.20736076301651
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C	1.11916665252935	-0.70692192132356	-0.97050207719572
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C	3.78404966843180	0.04829396926369	0.89741847272093
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C	0.42346865951959	2.28518733246236	0.89556739182699
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C	1.68180540057315	-2.09846977196425	-0.93537103510575
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C	-1.52680856595068	2.03165053431283	-2.51985407681591
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H	2.10115016818722	-1.26005818342771	1.34176023874638
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H	1.92555228926186	0.37234878649287	1.96207035178048
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H	2.25315419439435	2.08182326137047	-0.23817990664423
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H	0.79782567023738	1.80652027556549	-1.18773522402556
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H	3.99283842727912	1.11459446772306	0.72487403860971
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H	4.33006910434846	-0.26069135332918	1.80196977361113
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H	4.17868829873396	-0.52437330589328	0.04448429068889
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H	0.29630484616034	3.35095081225224	0.64910441882744
H	-0.56534937071677	1.81438915204826	0.95494999709261
H	0.92521698468529	2.23049195442562	1.87333999972935
H	2.74567056908439	-2.12424885050706	-0.67212112208699
H	1.12100462897658	-2.68414609182571	-0.18642710793993
H	1.53559413761430	-2.58272271299060	-1.90902315648373
H	-2.38295445240580	2.08803672261422	-3.20655940701338
H	-1.70750323965059	2.65576231350776	-1.63520544554060
H	-0.63197518262768	2.36893095979396	-3.05792456983217
H	0.39770642520307	-1.02490397748865	-2.80472419092055
O	-2.50272451231189	-0.78338690309709	-2.45727692638655
H	-2.96272110876144	-1.02258451976739	-1.63360722163280

A232-R-TS1

32

P	-0.26801044844770	-3.76079705689504	-1.23888489904766
F	0.68157056333363	-4.49964582545854	-0.14690055568344
O	-1.55320236596723	-3.18878102762396	-0.46423321926105
O	0.31636185476150	-3.21365022439102	-2.50147122705958
N	2.07784936190174	-0.09909405740312	0.54977758619717
N	0.89673356293189	-2.03365672483965	-0.07571905014753
C	2.56812912297309	1.25020055161164	0.25017426810559
C	2.42951970879721	-0.62907094017746	1.86770721385313

C	1.34770207685216	-0.83784516290495	-0.33182186470622
C	3.99635742348806	1.26666085212839	-0.29454755852356
C	1.33524044135904	-0.41480337919665	2.91502085584397
C	1.02827835933455	-0.22348622645497	-1.67078904582115
C	-1.91314428291711	-1.83206640122458	-0.16096667321241
H	2.51538661933801	1.83186993750032	1.18388336407464
H	1.88418312115432	1.74387771568380	-0.45084566275936
H	2.68277079475000	-1.69779954877326	1.77886511146335
H	3.35514932269931	-0.12868849266920	2.18694292244937
H	4.32603049149800	2.30436381233916	-0.46460185985355
H	4.69706180551846	0.79884283215491	0.41534735906030
H	4.06165749811306	0.72263207770711	-1.24979356254018
H	1.11932419234377	0.65851361717324	3.03640240677776
H	0.40015133764596	-0.92200849658675	2.63040558796005
H	1.65839281497943	-0.81286296616946	3.89028492864279
H	1.92967397195405	0.16535541519446	-2.16563233947409
H	0.57170710211245	-0.98804555062474	-2.30593102269648
H	0.32445877323773	0.61569115330579	-1.54819188622164
H	-3.00402060476770	-1.84085103983460	-0.03778264475850
H	-1.63937707900955	-1.15826360043049	-0.98283339920253
H	-1.42794733419733	-1.50536955951330	0.76632609970031
H	1.12309447271343	-2.36846441237036	0.85950876396499

O	-0.98278870543485	-5.16464846113271	-1.73192966002680
H	-1.46086117304941	-5.62685125012398	-1.02387777709768

A232-R-TS2

32

P	-0.30458468222372	-3.29468946508192	-1.22241447341884
F	-0.35735297394225	-3.81111156534958	0.84259196648586
O	-1.89426654214924	-3.10095839919360	-1.01170302203829
O	-0.14755224432465	-2.94282295340146	-2.69820062247170
N	2.04268321496495	-0.36780602975174	0.17774809451907
N	0.67352607831239	-2.12324674707930	-0.37431622657751
C	2.70841759951448	0.92164987586219	-0.09115592331123
C	2.24447261973440	-0.90509555349418	1.53636559825872
C	1.29884592030430	-0.98681221065890	-0.73079930403608
C	4.15899869328177	0.75119552599369	-0.53255278975253
C	1.14000732547844	-0.48738884026633	2.50625883921839
C	1.14171378769589	-0.39198290059983	-2.09340130106688
C	-2.73736634390327	-3.14048079619379	0.14536964629034
H	2.65555575452470	1.49872576404275	0.84299802562933
H	2.13082004431497	1.48054825274539	-0.83540403717519
H	2.34739363000413	-1.99856997380920	1.48116180908894
H	3.21573365019182	-0.52763050541757	1.88221647543390
H	4.61684549124550	1.74218867172035	-0.67576407783988

H	4.74564925535728	0.20984658988240	0.22559585852961
H	4.22508384451860	0.19844810991553	-1.48192611189586
H	1.07710043420613	0.60922459623508	2.57565177548388
H	0.15530238867444	-0.87080164897877	2.19815040362722
H	1.36441830805327	-0.88425348355404	3.50816780866231
H	2.11379379247938	-0.08756067874522	-2.50152776628955
H	0.66277543970562	-1.11819415199942	-2.75518084856157
H	0.50485729015082	0.50479276560311	-2.01663035471760
H	-3.73945425487465	-2.87635303691227	-0.22103116435384
H	-2.40887266758528	-2.40929028763984	0.89511028684008
H	-2.75037128953909	-4.14287950556551	0.59024759431191
H	0.71394178820176	-2.41711348470846	0.60181964295747
O	0.28245268928927	-4.82573072806042	-1.16121622614723
H	0.53071195833776	-5.03772720553906	-2.07929957568325

A234-R-TS1

35

P	0.20958670896199	-7.14336513964499	0.71482003755812
F	1.70690594591377	-7.72656327880374	0.58119141948669
O	-0.07979309347802	-7.02052416621234	2.28738869199182
O	-0.27468933465127	-6.21601486213526	-0.35556558812032
N	2.60085701200205	-3.14911905143880	1.34117458808533
N	1.55965452032235	-5.25999113205231	1.47216552262582

C	2.17908966717818	-2.75460006936008	2.68547712645607
C	3.40227811360313	-2.16726331562887	0.60472902242600
C	2.26399681627155	-4.37055742120326	0.83460276291531
C	0.77024911502136	-2.15903185000122	2.72554266956740
C	4.89329379329400	-2.22849923552159	0.93760130950729
C	2.73767849628281	-4.70773284540566	-0.55830119865126
C	-1.26167838408883	-7.54928356464594	2.95417843055303
C	-2.51595196072917	-6.78547611776324	2.58164392473857
H	2.25660264763319	-3.61975079011327	3.36345661784279
H	2.90572795776976	-2.01759205117811	3.05719860946162
H	3.00438229194077	-1.16940841708977	0.84899597788655
H	3.24522190505350	-2.29804391610539	-0.47288697156964
H	0.70864735705335	-1.26576068609989	2.08390272097007
H	0.01700139535999	-2.88328235722024	2.37827838580857
H	0.51123619422921	-1.86177159715644	3.75447452288477
H	5.32111401911889	-3.20519553558071	0.66166297570992
H	5.43784463297992	-1.44493837030654	0.38612108327092
H	5.06690445151248	-2.06944824762818	2.01388250944044
H	2.48860839578598	-5.74902370967723	-0.78182321922027
H	2.24597414224135	-4.06375335303163	-1.30454937689972
H	-1.35234664486279	-8.61989754300357	2.72670201466537
H	-1.02656859444957	-7.43263683558647	4.02095293303333

H	-3.36026231444341	-7.16152309163270	3.18180599979970
H	-2.39744780847535	-5.70995732341734	2.78574000014583
H	-2.76948561328650	-6.91929034513306	1.51841356499185
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H	1.24710644277370	-4.96903205192996	2.39657515077721
O	-0.54002867768811	-8.59195737382364	0.46199966338707
H	-0.88946917246013	-8.64673979648241	-0.44139795010458

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P	0.23016988547022	-6.79415746605609	0.70937256778442
F	0.31596647754519	-6.78176970433915	2.83140996598863
O	-1.34450979991089	-6.54295607835441	0.95456943908685
O	0.29966613664701	-6.82069099231950	-0.81526518238778
N	2.57361018429644	-3.57790136315027	1.20412429673639
N	1.23188833699771	-5.43892111328967	1.17496468748889
C	2.76159742624195	-3.68711607216464	2.66276370107267
C	3.21843525241506	-2.40721693905103	0.57769994581872
C	1.84713061195944	-4.44580039493796	0.50911456073895
C	1.63127286701109	-3.02906083628593	3.45266423057153
C	4.67804323051252	-2.66287845791914	0.21355597312480
C	1.70872091001193	-4.27805919125513	-0.97007375592274
C	-2.20887215887064	-6.57356772998281	2.11044628976763

C	-2.54523476862938	-7.99016638255438	2.53307576390865
H	2.88765215081240	-4.74502100884170	2.93494969287664
H	3.71871616449659	-3.20110089833548	2.89257673764694
H	3.14192731591655	-1.58609045979296	1.30484750178338
H	2.63855533246517	-2.09966105931147	-0.29929456020354
H	1.54546160620478	-1.96292660959976	3.19337624323824
H	0.66117616145316	-3.51106516514366	3.25802927314205
H	1.84347782941242	-3.10673746602285	4.52992988524763
H	4.76986613114528	-3.46375739101912	-0.53589465751841
H	5.11657955057661	-1.74422508371506	-0.20612508626805
H	5.26645978402351	-2.94825172235281	1.09930577824982
H	1.26781129551123	-5.18177230954389	-1.39889799994864
H	1.03876198210209	-3.42520850297459	-1.16936665026145
H	-1.74918333567820	-6.00560530240522	2.92640060951368
H	-3.11272593157834	-6.04618236503862	1.76955787112470
H	-3.28567737516790	-7.96153427418728	3.34962838353362
H	-2.98091261180556	-8.55821645245345	1.69552571837004
H	-1.65056525247221	-8.51625419257225	2.89521574553804
H	2.68092814959639	-4.06553215779395	-1.43147894687264
H	1.28689349618391	-5.45135077488972	2.19373786102178
O	0.84612818833687	-8.26341655684935	1.10769844466363
H	1.04425990676736	-8.69173672549574	0.25535718134467

