

Supporting Information:

Halogen Bonded Supramolecular Capsules:
A Challenging Test Case for Quantum Chemical Methods

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Computational Details

General Remarks

Our procedure to obtain the target binding free energy ΔG_a involves three subsequent steps. First, the electronic binding energy in the gas phase ΔE is computed for equilibrium structures. The molecules of interest (e.g. host, guest and complex) are optimised in the gas phase on an affordable level including a dispersion correction. Our default level for the geometry optimisations was up to now the TPSS meta-GGA density functional¹ together with the triple-zeta (TZ) basis set def2-TZVP² and the D3 dispersion correction with Becke-Johnson damping^{3,4} (D3(BJ)).⁵ Here, we also employ the composite density functional based method PBEh-3c⁶ that uses the modified double-zeta (DZ) basis set def2-SVP² (dubbed def2-m-SVP) together with the D3-dispersion correction including three-body contributions (D3^{ATM}) and the geometrical counter-poise correction (gCP).⁷

Single-point energies are obtained by employing a hybrid-functional like PW6B95⁸-D3 together with a large quadruple-zeta (QZ) basis set, e.g. def2-QZVP.² The gas phase binding energy ΔE is calculated in the supermolecular approach

$$\Delta E = E(\text{complex}) - E(\text{host}) - E(\text{guest}), \quad (1)$$

where E is the total electronic energy of the species involved. At a QZ basis set level, basis set superposition errors (BSSE) diminish to typically less than 2% of ΔE and can be ignored⁹ for (hybrid)GGA functionals. In addition to the two-body dispersion interaction $\Delta E_{disp}^{(2)}$, the Axilrod-Teller-Muto-type three-body dispersion (ATM) energy $\Delta E_{disp}^{(3)}$ is also included.^{10,11} The three-body dispersion contribution to ΔE was found to be usually positive and to contribute significantly with 2-3 kcal/mol for typical supramolecular systems.¹² We disregard many-body dispersion effects beyond the three-body term, see Refs.¹³⁻¹⁷ for examples and further discussion. Note that $\Delta E_{disp}^{(3)}$ varies in methodologically different approaches,^{14,18} and we decided to use the efficient D3 method for its computation without any empirical adjustments. The total electronic interaction energy ΔE thus comprises the

pure electronic DFT energy ΔE_{el}^{DFT} , two-body $\Delta E_{disp}^{(2)}$, and three-body dispersion energy $\Delta E_{disp}^{(3)}$:

$$\Delta E = \Delta E_{el}^{DFT} + \Delta E_{disp}^{(2)} + \Delta E_{disp}^{(3)} \quad (2)$$

Second, the sum of thermostatistical corrections from energy to free energy G_{RRHO}^T are obtained for each molecule in the gas phase at a given temperature T and normal pressure of 1 atm, including the zero-point vibrational energy. Since low-lying vibrational frequencies are inaccurate in the harmonic approximation, a modified rigid-rotor-harmonic-oscillator scheme is used.¹² In this approach vibrational modes below 100 cm^{-1} are treated within a rigid-rotor model with smooth interpolation to the standard harmonic regime, for additional details, see Ref.¹² Its good performance has been verified repeatedly also for computing reaction thermochemistry, see e.g. Refs.^{19–21} The computation of the harmonic frequencies is carried out with semiempirical methods like our recently developed minimal basis set Hartree-Fock (HF-3c) method.²² HF-3c is a fast quantum chemical procedure with three atom-pairwise correction terms: the (D3(BJ)) dispersion correction, the gCP correction,⁷ and an additional short-range term to correct for basis set incompleteness effects. It yields very reasonable structures and interaction energies for typical supramolecular systems and can therefore be used for pre-optimisations or screening applications.

Third, a continuum solvation model like COSMO-RS^{23,24} is used in a black-box manner to calculate the solvation free energy $\delta G_{solv}^T(X)$ of each gas phase species at the temperature T in solvent X . The resulting values implicitly contain the conversion to standard state conditions.

The final binding free energy ΔG_{bind} is the sum of the three contributions:

$$\Delta G_{bind} = \Delta E + \Delta G_{RRHO}^T + \Delta \delta G_{solv}^T(X) \quad (3)$$

Technical Details

Geometry optimisations of all capsules, hemispheres, guest molecules, and host-guest complexes were done employing the composite density functional based method PBEh-3c.⁶ For the study on the influence of the geometry on single-point energies some molecules were reoptimised on the TPSS¹-D3 level of theory employing the TZ basis set def2-TZVP.² In all DFT and HF-3c calculations the D3 dispersion correction²⁵ with Becke-Johnson (BJ) damping³⁻⁵ was used. All DFT and HF-3c energies include the ATM three-body contributions to the D3 dispersion energy. For the capsules except for the fluorine one, no restrictions regarding symmetry were made. The fluorine capsule was optimised in C_4 symmetry to prevent dissociation.

Single-point calculations for gas phase interaction energies were conducted at the PW6B95⁸-D3 level together with the QZ basis set def2-QZVP' with discarded g- and f-functions on the non-hydrogen and hydrogen atoms, respectively.² For such a large basis set the BSSE almost vanishes (remaining BSSE at this level is typically 1-2% of ΔE , see Ref.⁹) and hence, no special treatment, e.g. such as a computationally demanding counter-poise correction, is required. For iodine the pseudopotentials from the Stuttgart/Cologne group were used.²⁶

All DFT and HF-3c calculations were performed using the TURBOMOLE 7.0.2 program package.^{27,28} The resolution-of-identity (RI) approximation for the Coulomb integrals²⁹ was applied in all cases using matching default auxiliary basis sets.³⁰ For the integration of the exchange-correlation contribution the numerical quadrature grids m3 in case of PBEh-3c and m4 in case of PW6B95-D3 were employed. For the geometry optimisations as well as for the single-point energies the default convergence criteria were used (10^{-7} E_h for energies and 10^{-5} E_h/Bohr for gradients). For the constrained geometry optimization of the PES the guest coordinates were fixed and further, the spatially closer C-atoms of the terminal methyl groups at the bottom of the RA4 container were frozen to prevent a shift of the whole capsules.

Computations of the HF-3c harmonic vibrational frequencies were performed analytically using the aoforce code of TURBOMOLE 7.0.2. The HF-3c vibrational frequencies were scaled with a factor of 0.86.²² For the bromine capsule a small imaginary frequency $< i10\text{ cm}^{-1}$ was obtained and inverted to the corresponding positive value in order to minimize the error resulting from missing low-lying modes. The same was done for the thermostistical corrections involved in the potential surface of free energy for imaginary frequencies $< i20\text{ cm}^{-1}$

The COSMO-RS solvation model^{23,24} was used as implemented in COSMOtherm 2014³¹ employing the 2012 BP86/def-TZVP parametrisation. To obtain the solvation free energies the standard procedure with two single point calculations (one in the gas phase and one in an ideal conductor) on the default BP86^{32,33}/def-TZVP³⁴ level of theory were performed on the optimised gas-phase geometries and then used as input for COSMOtherm.

All visualisations of molecules were done with USCF Chimera version 1.8.1³⁵ and all graphs were plotted with Gnuplot 4.6.³⁶

References

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Cartesian Coordinates

Cartesian coordinates (in Å) and SCF energies (in a.u.) of the optimized capsules, the individual hemispheres, and the host-guest complexes on the PBEh-3c level of theory.

I-capsule				O	-12.6938122	-4.8474484	0.7891330
				C	-16.4741777	3.5096062	0.3821437
380				H	-16.8658568	4.1115997	-0.4374218
Energy = -12605.82788284				H	-16.8802058	2.5046692	0.2666752
C	-13.2161428	2.2493899	-3.3385968	C	-16.4683734	-0.4074394	3.5070684
C	-14.3365992	3.0995800	-0.9193790	H	-16.8579924	0.4110640	4.1118290
C	-14.3236555	1.5707417	-2.8378555	H	-16.8579322	-1.3422483	3.9092995
C	-12.6984483	3.3451723	-2.6732307	C	-16.4766633	-3.5202641	-0.4218556
C	-13.2321727	3.7481988	-1.4633035	H	-16.8673321	-3.9210045	-1.3568358
C	-14.8537419	2.0253602	-1.6349920	H	-16.8819887	-2.5148770	-0.3078723
H	-11.8935270	3.9087416	-3.1195029	C	-16.4566812	0.3966548	-3.5468353
H	-15.7151012	1.5102538	-1.2299977	H	-16.8441232	1.3317092	-3.9505320
O	-12.6865124	4.8329957	-0.8171076	H	-16.8714194	0.2816241	-2.5454111
C	-11.4830722	4.6363905	-0.1961313	H	-16.8799024	-0.2917199	2.5044015
C	-11.4779162	4.4766825	1.2087902	H	-16.8714702	-4.1216547	0.3966491
C	-11.4511258	1.2072874	-4.4631802	H	-16.8451755	-0.4216654	-4.1525644
C	-11.4595241	-0.1970846	-4.6282054	H	-16.8672812	3.9105378	1.3160223
O	-12.6624691	-0.8141492	-4.8415247	C	-9.1127580	-4.2859024	-1.1926174
C	-13.2337698	3.3268769	2.2408293	C	-9.1377904	-4.4443518	0.1962817
C	-14.3357139	0.8981503	3.0875732	C	-9.1114655	4.2670095	1.1742914
C	-12.7082257	2.6616568	3.3330965	C	-9.1326591	4.4258478	-0.2146240
C	-14.3373339	2.8186553	1.5611381	C	12.5124670	3.7721034	-1.3915705
C	-14.8585926	1.6116363	2.0147016	C	13.6030794	1.6135963	-2.7958037
C	-13.2323979	1.4467605	3.7341552	C	13.6198161	3.1188373	-0.8594473
H	-11.9046805	3.1115259	3.8958250	C	11.9736559	3.3832487	-2.6040234
H	-15.7176850	1.2013821	1.5000084	C	12.4977366	2.3013352	-3.2883971
C	-13.2215096	-1.4603511	-3.7631627	C	14.1334476	2.0517728	-1.5870724
C	-14.3354660	-2.8315486	-1.5943177	H	11.1660386	3.9516263	-3.0401466
C	-12.7000847	-2.6759538	-3.3606493	H	14.9953838	1.5317993	-1.1898895
C	-14.3265966	-0.9108056	-3.1204044	O	11.9462725	1.9448881	-4.4975242
C	-14.8539056	-1.6238997	-2.0494392	C	10.7421052	1.2951120	-4.4603979
C	-13.2303068	-3.3409858	-2.2705016	C	10.7429607	-0.1103050	-4.6147505
H	-11.8950124	-3.1264160	-3.9207088	C	10.7795850	4.7085452	-0.1114384
H	-15.7143657	-1.2128691	-1.5376710	C	10.7758601	4.5461755	1.2941628
O	-12.6776631	0.8001697	4.8145438	O	11.9820870	4.5324316	1.9394138
O	-12.6812400	-4.5428646	-1.8901110	C	12.4918035	-1.4003024	-3.7463725
C	-11.4745304	0.1822283	4.6047519	C	13.6148435	-2.8100377	-1.6096407
C	-11.4666781	-1.2220315	4.4388965	C	11.9678914	-2.6212229	-3.3621574
C	-11.4792241	-4.4934065	-1.2335557	C	13.6020695	-0.8636996	-3.1020706
C	-11.4884069	-4.6525858	0.1714055	C	14.1314470	-1.5942127	-2.0446960
C	-13.2287876	-2.2629911	3.3086938	C	12.5081555	-3.3091559	-2.2908613
C	-14.3425411	-3.1123423	0.8860886	H	11.1607567	-3.0623484	-3.9273332
C	-14.3341561	-1.5833886	2.8045367	H	14.9952512	-1.1938577	-1.5303540
C	-12.7099859	-3.3592688	2.6449662	C	12.5073449	3.3095475	2.2874035
C	-13.2403283	-3.7619209	1.4334036	C	13.5965351	0.8634253	3.1015283
C	-14.8609005	-2.0375806	1.6000433	C	11.9615426	2.6211810	3.3556800
H	-11.9069967	-3.9235837	3.0937730	C	13.6156798	2.8097994	1.6095748
H	-15.7205571	-1.5217526	1.1923787	C	14.1301525	1.5936657	2.0460596
O	-12.6675415	-1.8797845	4.5039959	C	12.4835466	1.3998914	3.7413751
C	-14.9410846	-0.4122587	3.5540527	H	11.1516438	3.0614269	3.9175896
H	-14.6738861	-0.5320148	4.6035692	H	14.9956518	1.1929800	1.5348507
C	-14.9472639	3.5647946	0.3891900	O	11.9781790	-4.5305473	-1.9443236
H	-14.6857166	4.6157838	0.5084744	O	11.9289524	0.7370090	4.8114052
C	-14.9292492	0.4000659	-3.5891004	C	10.7716673	-4.5405149	-1.2989864
H	-14.6586466	0.5193406	-4.6378008	C	10.7756345	-4.7031939	0.1064603
C	-14.9498016	-3.5770532	-0.4242626	C	10.7316196	0.1106766	4.6105941
H	-14.6889871	-4.6283212	-0.5426921	C	10.7318730	-1.2954177	4.4587640
C	-9.1281492	0.2099052	4.3559740	C	12.5070471	-3.7702929	1.3896318
C	-9.1042849	-1.1776242	4.1863464	C	13.5968125	-1.6134890	2.7965390
C	-9.1137771	-0.2260298	-4.3736729	C	13.6159820	-3.1180275	0.8598558
C	-9.0893087	1.1615716	-4.2047534	C	11.9658718	-3.3812550	2.6009697
O	-12.6513946	1.8657609	-4.5320963	C	12.4896959	-2.3000845	3.2866913
O	-12.6817052	4.5278499	1.8619757	C	14.1293973	-2.0518008	1.5887754

H	11.1566899	-3.9486892	3.0353358	F	-5.6799132	-1.7262602	1.8907274
H	14.9926040	-1.5324791	1.1934790	F	-3.0251744	-1.7385813	1.7351901
O	11.9797163	-4.8571269	0.7321485	C	-10.3092926	4.6359482	-0.9201613
C	14.2321131	-3.5694363	-0.4507512	H	-10.3006410	4.8018483	-1.9875170
H	13.9761209	-4.6202880	-0.5817327	C	-10.2974609	4.3166735	1.9034279
C	14.2085241	0.4502141	-3.5585140	H	-10.2837746	4.2373483	2.9812321
H	13.9400022	0.5797506	-4.6064424	C	-10.3031880	0.9099812	4.5915727
C	14.2351888	3.5692614	0.4519308	H	-10.2948821	1.9768548	4.7604854
H	13.9800813	4.6203167	0.5829937	C	-10.2864112	-1.9114270	4.2553055
C	14.2012146	-0.4504091	3.5604073	H	-10.2701970	-2.9885363	4.1683316
H	13.9298870	-0.5791968	4.6076976	C	-10.3165595	-4.6533550	0.8986232
C	8.3938858	-4.4932901	-1.2866150	H	-10.3110440	-4.8189740	1.9660480
C	8.4179693	-4.6402727	0.1027208	C	-10.2967174	-4.3349883	-1.9250179
C	8.3993052	4.5059323	1.2821031	H	-10.2799722	-4.2558620	-3.0027858
C	8.4212692	4.6522273	-0.1070020	C	-10.2887095	-0.9255832	-4.6114412
O	11.9842912	4.8601444	-0.7366113	H	-10.2805919	-1.9925850	-4.7795815
O	11.9400937	-0.7365256	-4.8174686	C	-10.2708710	1.8960474	-4.2769217
O	11.9368069	-1.9437602	4.4952371	H	-10.2542473	2.9732106	-4.1906110
C	15.7358256	0.4434327	-3.5145474	C	-7.0946313	4.1422699	0.4973545
H	16.1252360	1.3814321	-3.9091170	C	-7.0948619	-0.4891847	4.0111081
H	16.1500274	0.3179542	-2.5141941	C	-7.0979286	-4.1599450	-0.5101348
C	15.7584697	-3.5068029	-0.4427396	C	-7.0805902	0.4719263	-4.0256015
H	16.1534651	-3.8948775	-1.3811164	C	6.3610753	4.5314269	0.6285539
H	16.1526696	-4.1173191	0.3691352	C	6.3497865	0.6046293	-4.1265225
C	15.7286180	-0.4446980	3.5204127	C	6.3360180	-0.6106285	4.1425042
H	16.1151251	0.3685158	4.1340693	C	6.3576212	-4.5133523	-0.6274395
H	16.1455584	-0.3207471	2.5210142	C	9.6017423	4.7763954	-0.8263371
C	15.7614658	3.5051143	0.4455085	H	9.5935984	4.9315919	-1.8953391
H	16.1557970	3.8932174	1.3841585	C	9.5932671	4.4650899	1.9995385
H	16.1571921	4.1148720	-0.3661892	H	9.5881563	4.3874189	3.0778778
H	16.1606449	-2.5018883	-0.3147781	C	9.5631572	1.9968536	-4.3153987
H	16.1163178	-1.3825126	3.9170955	H	9.5586100	3.0748865	-4.2359903
H	16.1627928	2.4997463	0.3184761	C	9.5661291	-0.8294300	-4.6063072
H	16.1233459	-0.3693373	-4.1281457	H	9.5542437	-1.8985853	-4.7598239
C	8.3824138	0.1126923	4.4087906	C	9.5542175	0.8287385	4.6042253
C	8.3622755	-1.2780956	4.2783514	H	9.5389244	1.8987772	4.7510438
C	8.3940269	-0.1164349	-4.4030242	C	9.5535971	-1.9989622	4.3181288
C	8.3731798	1.2745414	-4.2713852	H	9.5505602	-3.0770711	4.2397831
C	-2.8179156	4.0572145	0.5539615	C	9.5980362	-4.7685439	0.8213611
C	-3.5525055	3.0678635	1.1831565	H	9.5893875	-4.9245593	1.8901921
C	-4.9344795	3.0694164	1.1416177	C	9.5884910	-4.4569525	-2.0039607
C	-5.6324253	4.0664646	0.4734688	H	9.5846691	-4.3839238	-3.0826596
C	-4.8863237	5.0415628	-0.1748244	N	7.0906193	-4.4172668	-1.7132350
C	-3.5059921	5.0365636	-0.1392540	N	7.0651666	-1.7028974	4.1193510
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F	-2.9447200	-2.1004134	-1.8498805	N	-7.8175862	-0.6341798	-4.2587905
F	-5.6009154	-2.1038111	-1.7616330	H	-7.5136911	-1.6286202	-4.2538647
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C	-4.8398781	-0.2393621	-4.8100259	N	7.1074490	-4.6518975	0.4910254
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C	4.8727720	-0.5612535	4.0009591	H	6.7861796	-6.2407274	4.0300707
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C	4.6048568	2.0135674	-6.0438849	H	-5.4077161	-3.8584619	-4.3825977
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H	5.7833855	2.2379304	-0.7510165	H	-5.3596925	-4.3090212	3.7604032
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C	3.9851296	-1.3339282	-3.7612966	C	1.0539850	-0.7570764	-4.5775975
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C	3.4664817	-2.5631879	-3.3975356	C	1.0273728	0.7591696	4.5820636
C	5.0935747	-0.8048355	-3.1075836	H	1.0160251	1.8250802	4.7563313
C	5.6244798	-1.5503900	-2.0612487	C	1.0275178	-2.0586149	4.2323607
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H	2.6610748	-2.9978871	-3.9699310	C	1.0901148	-4.7874249	0.7455176
H	6.4861447	-1.1549039	-1.5394007	H	1.0793339	-4.9679530	1.8105261
C	3.9873072	3.2738748	2.3569063	C	1.0874338	-4.4193716	-2.0721602
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C	3.4427884	2.5702985	3.4155155	N	-1.4107350	-4.4311626	-1.7938455
C	5.0960393	2.7842501	1.6720455	N	-1.4506206	-1.7520148	3.9552025
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H	6.4755996	1.1682105	1.5741737	H	-1.7084526	4.7462008	-1.3909550
O	3.4781203	-4.4919416	-2.0082163	N	-1.4168933	-0.4564633	-4.2118838
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C	2.2691719	-4.5121648	-1.3656490	N	-1.4017343	-4.7154524	0.4041204
C	2.2698848	-4.7014819	0.0353191	H	-1.7062265	-4.7495772	1.3815935
C	2.2035835	0.0381226	4.6019507	N	-1.4409220	0.4533698	4.2035250
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C	5.1072015	-3.1255566	0.8205347	C	-4.2619518	5.5323523	1.6035317
C	3.4545456	-3.4252677	2.5529705	C	-5.7948141	3.9211296	0.0368391
C	3.9717031	-2.3540439	3.2585952	H	-6.4333698	3.2900756	-0.5749948
C	5.6163157	-2.0718713	1.5705243	C	-3.6135946	0.5762627	-3.8025956
H	2.6450239	-4.0022469	2.9737726	C	-4.1468053	-0.1564824	-2.7402058
H	6.4789409	-1.5427567	1.1867934	C	-4.4705610	1.2226398	-4.6961740
O	3.4744379	-4.8665216	0.6598666	C	-5.5340507	-0.2135811	-2.6423597
C	5.7271914	-3.5506070	-0.4971490	H	-5.9903515	-0.7759602	-1.8325265
H	5.4747687	-4.5998211	-0.6472203	C	-3.6334279	-0.5840437	3.7836939
C	5.6962286	0.5181684	-3.5416317	C	-4.1630644	0.1478501	2.7189231
H	5.4247982	0.6657096	-4.5864355	C	-4.4933551	-1.2325311	4.6729131
C	5.7173825	3.5622288	0.5275431	C	-3.6184340	-4.6505457	-0.7415174
H	5.4620793	4.6109429	0.6762343	C	-4.4053090	-3.8438591	0.0850503
C	5.6777975	-0.5066555	3.5717945	C	-4.2420766	-5.5407125	-1.6265808
H	5.4010210	-0.6546897	4.6151211	C	-5.7867470	-3.9330582	-0.0678520
C	-0.1091946	-4.4805860	-1.3606843	H	-6.4299115	-3.3036110	0.5408057
C	-0.0891652	-4.6576965	0.0256889	C	-3.2971653	-0.8163055	-1.6982934
C	-0.1254391	4.4807359	1.3597665	H	-2.8855682	-1.7671803	-2.0355897
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O	3.4681268	4.8735315	-0.6417058	H	-3.8884882	-1.0205131	-0.8082774
O	3.4263721	-0.6536740	-4.8182714	C	-3.9730332	2.0198599	-5.8633057
O	3.4078286	-2.0157509	4.4669286	H	-4.7943093	2.2827626	-6.5284032
C	7.2236881	0.5134692	-3.5012221	H	-3.4939212	2.9448603	-5.5436661
H	7.6105439	1.4589258	-3.8803481	H	-3.2354001	1.4673478	-6.4456473
H	7.6400080	0.3717195	-2.5039041	C	-3.8515400	2.9070934	-1.1409981
C	7.2533189	-3.4831108	-0.4847492	H	-3.6342089	3.4319240	-2.0719065
H	7.6516782	-3.8536974	-1.4288235	H	-2.9293179	2.4199325	-0.8253283
H	7.6479900	-4.1058354	0.3176337	H	-4.5741798	2.1311362	-1.3859721
C	7.2054462	-0.4988911	3.5396263	C	-3.5201953	6.5085803	2.4680608
H	7.5881883	0.3034376	4.1698241	H	-3.0089038	6.0255218	3.2985815
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C	7.2436922	3.4977519	0.5234825	H	-4.2094733	7.2431927	2.8827225
H	7.6361439	3.8691316	1.4697112	C	-3.4936107	-6.5152447	-2.4872574
H	7.6415027	4.1212383	-0.2767516	H	-4.1791395	-7.2510599	-2.9059702
H	7.6515095	-2.4790199	-0.3388810	H	-2.9785960	-6.0309595	-3.3147524
H	7.5921386	-1.4435884	3.9208060	H	-2.7349519	-7.0536426	-1.9195344
H	7.6446640	2.4944485	0.3798410	C	-3.8519897	-2.9152135	1.1206775
H	7.6114437	-0.2881087	-4.1293082	H	-3.6388741	-3.4398499	2.0526702
C	-0.1411105	0.0548165	4.3331761	H	-2.9289239	-2.4262340	0.8103087
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C	-0.1172468	-0.0552062	-4.3346926	C	-3.9998638	-2.0290406	5.8422446
C	-0.1391379	1.3329721	-4.1720600	H	-4.8238121	-2.2936814	6.5033406
C	-2.1619462	4.5769561	0.7057889	H	-3.5174317	-2.9530450	5.5247330
C	-2.1556171	0.6533757	-3.9858730	H	-3.2661059	-1.4752261	6.4282263

C	-3.3098667	0.8100926	1.6814430	H	-11.7858159	-3.1036171	-3.9407038
H	-2.4658911	0.1836547	1.3896502	H	-15.6049331	-1.2032825	-1.5466729
H	-3.8970841	1.0125095	0.7883050	O	-12.5667025	0.7705321	4.8175223
H	-2.9029014	1.7622095	2.0208389	O	-12.5729912	-4.5321024	-1.9187507
C	-5.6520467	5.5190347	1.6276276	C	-11.3638080	0.1540103	4.6045388
H	-6.1792607	6.1953222	2.2935057	C	-11.3559198	-1.2495194	4.4298626
N	-6.4059529	4.7298588	0.8818972	C	-11.3713679	-4.4884700	-1.2618253
N	-6.3803620	-0.4021304	3.4454306	C	-11.3811697	-4.6570604	0.1423262
N	-6.3916119	-4.7429291	-0.9163044	C	-13.1183824	-2.2833732	3.2931005
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C	-5.8585076	-1.0996873	4.4397289	C	-14.2238140	-1.6004874	2.7936564
H	-6.5640705	-1.5847648	5.1072767	C	-12.6003482	-3.3760019	2.6228122
C	-5.6320442	-5.5303794	-1.6580943	C	-13.1317160	-3.7712461	1.4092505
H	-6.1542393	-6.2076905	-2.3268785	C	-14.7511201	-2.0470933	1.5865904
C	-5.5499382	0.2018856	2.6142840	H	-11.7978368	-3.9436522	3.0683083
H	-6.0034995	0.7635021	1.8023856	H	-15.6109484	-1.5286939	1.1825778
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H	-6.5399002	1.5703290	-5.1406797	C	-14.8305150	-0.4341492	3.5507206
O	-2.1901161	-3.0994821	-4.1553247	H	-14.5629005	-0.5602966	4.5993715
H	-1.9330670	-3.6297655	-3.3676513	C	-14.8383315	3.5614955	0.4095374
O	-1.5044566	4.4219128	-3.1939489	H	-14.5774504	4.6119023	0.5351906
H	-1.5726800	3.4704366	-3.4413433	C	-14.8192553	0.4215568	-3.5882794
O	-2.2169725	3.0953303	4.1434636	H	-14.5483458	0.5471395	-4.6361508
H	-1.9573966	3.6262588	3.3570304	C	-14.8412277	-3.5741036	-0.4471230
O	-1.5125854	-4.4252585	3.1855367	H	-14.5812477	-4.6248222	-0.5720111
H	-1.5842437	-3.4740117	3.4328496	C	-9.0173770	0.1830097	4.3574687
C	-3.5273102	-3.3783891	-4.5057424	C	-8.9934486	-1.2033286	4.1790190
H	-3.8296778	-2.6794593	-5.2856009	C	-9.0039741	-0.1995658	-4.3774186
H	-3.6435563	-4.3906843	-4.9043535	C	-8.9795356	1.1869131	-4.2001687
H	-4.2191521	-3.2599877	-3.6660213	O	-12.5413449	1.8930433	-4.5218640
C	-1.9392501	5.2085416	-4.2756802	O	-12.5730424	4.5166704	1.8878851
H	-3.0154346	5.1163890	-4.4608148	O	-12.5866936	-4.8537773	0.7583899
H	-1.7319559	6.2541712	-4.0495316	C	-16.3651959	3.5055543	0.4022605
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C	-3.5555582	3.3731979	4.4893027	H	-16.7708111	2.5011763	0.2807014
H	-4.2443096	3.2549660	3.6470206	C	-16.3578068	-0.4290880	3.5044732
H	-3.8602903	2.6735504	5.2675970	H	-16.7471159	0.3856863	4.1144083
H	-3.6738352	4.3851451	4.8882097	H	-16.7471193	-1.3662821	3.9013000
C	-1.9515772	-5.2132704	4.2645614	C	-16.3680219	-3.5162467	-0.4443336
H	-3.0289895	-5.1237045	4.4437182	H	-16.7589702	-3.9109535	-1.3817366
H	-1.7405695	-6.2583316	4.0392241	H	-16.7727393	-2.5113555	-0.3240579
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Br-capsule

380

Energy = -21706.88227638

C	-13.1063430	2.2694045	-3.3259731	C	-9.0047485	-4.2847518	-1.2186430
C	-14.2274000	3.1044899	-0.9018223	C	-9.0305203	-4.4526600	0.1690526
C	-14.2137599	1.5874754	-2.8296473	C	-9.0030502	4.2649869	1.1977746
C	-12.5890848	3.3613898	-2.6540632	C	-9.0248729	4.4328488	-0.1899897
C	-13.1234015	3.7569079	-1.4419108	C	12.4222088	3.7660152	-1.4126170
C	-14.7440637	2.0344924	-1.6240389	C	13.5103800	1.5994641	-2.8064523
H	-11.7846968	3.9282598	-3.0971567	C	13.5291707	3.1142518	-0.8775695
H	-15.6054727	1.5168144	-1.2224571	C	11.8823039	3.3709613	-2.6226010
O	-12.5788387	4.8384916	-0.7891389	C	12.4052042	2.2853673	-3.3020538
C	-11.3753120	4.6398843	-0.1698095	C	14.0414769	2.0430656	-1.6000303
C	-11.3696168	4.4711647	1.2343505	H	11.0741171	3.9370775	-3.0605614
C	-11.3413202	1.2343504	-4.4574560	H	14.9027878	1.5239437	-1.2003505
C	-11.3496902	-0.1693361	-4.6309277	O	11.8522934	1.9228362	-4.5086255
O	-12.5523491	-0.7850947	-4.8473722	C	10.6475091	1.2736202	-4.4651142
C	-13.1242441	3.3128700	2.2593965	C	10.6472590	-0.1325319	-4.6097972
C	-14.2252941	0.8789405	3.0917655	C	10.6904063	4.7101604	-0.1368539
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C	-14.7487036	1.5987926	2.0234360	C	12.3977171	-1.4194018	-3.7389036
C	-13.1217831	1.4237550	3.7410957	C	13.5243304	-2.8183660	-1.5967370
H	-11.7948225	3.0881919	3.9130118	C	11.8751824	-2.6388807	-3.3481987
H	-15.6082204	1.1917143	1.5069484	C	13.5091309	-0.8797114	-3.0990377
C	-13.1114817	-1.4377934	-3.7727599	C	14.0403520	-1.6048323	-2.0388162
C	-14.2261986	-2.8217313	-1.6124553	C	12.4170417	-3.3213533	-2.2741937
C	-12.5904019	-2.6559636	-3.3776442	H	11.0671155	-3.0826916	-3.9098797
C	-14.2166245	-0.8919368	-3.1270621	H	14.9048306	-1.2017151	-1.5277560
C	-14.7442665	-1.6112909	-2.0604833	C	12.4181276	3.3205913	2.2682506
C	-13.1211824	-3.3273526	-2.2916523	C	13.5060824	0.8782972	3.0952030

C	11.8715702	2.6377092	3.3396873	C	-2.7104053	0.4299101	-3.6538888
C	13.5263215	2.8168011	1.5931330	C	-3.4894894	1.0932633	-2.7198052
C	14.0404108	1.6028734	2.0361427	C	-4.8677718	1.1004496	-2.8244598
C	12.3926844	1.4180413	3.7317512	C	-5.5160718	0.4519698	-3.8675314
H	11.0611211	3.0806773	3.8986269	C	-4.7241531	-0.2184594	-4.7901058
H	14.9058077	1.1991212	1.5271589	C	-3.3477318	-0.2360764	-4.6876489
O	11.8884150	-4.5410914	-1.9207840	F	-2.9165340	1.7305973	-1.7076405
O	11.8372357	0.7608631	4.8046801	F	-5.5705459	1.7313804	-1.8917454
C	10.6818461	-4.5485978	-1.2748496	F	-5.2919843	-0.8400279	-5.8184416
C	10.6861361	-4.7055024	0.1308741	F	-2.6423334	-0.8816493	-5.6048253
C	10.6400542	0.1326246	4.6056948	C	-2.7223927	-0.4570678	3.6504672
C	10.6409227	-1.2739931	4.4620000	C	-3.3609841	0.2104039	4.6825086
C	12.4177681	-3.7651901	1.4080787	C	-4.7378163	0.1967607	4.7806123
C	13.5064407	-1.6003322	2.8035570	C	-5.5287566	-0.4710714	3.8553354
C	13.5260099	-3.1146533	0.8745061	C	-4.8791748	-1.1200794	2.8134161
C	11.8765171	-3.3698381	2.6173649	C	-3.5006214	-1.1167044	2.7130609
C	12.3996926	-2.2848545	3.2975296	F	-2.6565916	0.8526757	5.6027018
C	14.0387610	-2.0442235	1.5977332	F	-5.3070823	0.8189480	5.8077662
H	11.0670966	-3.9349503	3.0542618	F	-5.5808488	-1.7484101	1.8781274
H	14.9010845	-1.5258775	1.1992048	F	-2.9263265	-1.7551137	1.7023496
O	11.8908798	-4.8559522	0.7571065	C	-10.2018417	4.6459853	-0.8940806
C	14.1421459	-3.5717843	-0.4341712	H	-10.1935823	4.8190600	-1.9602839
H	13.8866418	-4.6233800	-0.5601062	C	-10.1889019	4.3084362	1.9277108
C	14.1146965	0.4318054	-3.5634015	H	-10.1749484	4.2221635	3.0049666
H	13.8446061	0.5554695	-4.6116386	C	-10.1925530	0.8817927	4.5966664
C	14.1456397	3.5702558	0.4314189	H	-10.1843578	1.9475944	4.7721651
H	13.8913439	4.6220953	0.5577014	C	-10.1756610	-1.9377387	4.2425492
C	14.1103776	-0.4331103	3.5613441	H	-10.1594902	-3.0142408	4.1483776
H	13.8384571	-0.5562263	4.6091692	C	-10.2096885	-4.6646459	0.8698361
C	8.3041773	-4.5027354	-1.2623091	H	-10.2046863	-4.8374676	1.9361050
C	8.3281493	-4.6451306	0.1275388	C	-10.1885535	-4.3271606	-1.9518929
C	8.3109365	4.5153283	1.2586651	H	-10.1715026	-4.2406985	-3.0290850
C	8.3318001	4.6565764	-0.1309879	C	-10.1789509	-0.8978718	-4.6190583
O	11.8952965	4.8580319	-0.7636044	H	-10.1709116	-1.9638483	-4.7935187
O	11.8438904	-0.7609004	-4.8119373	C	-10.1611329	1.9219979	-4.2675325
O	11.8462749	-1.9221464	4.5037880	H	-10.1445756	2.9985831	-4.1743502
C	15.6420882	0.4254535	-3.5215348	C	-6.9865868	4.1463113	0.5192334
H	16.0308368	1.3612281	-3.9220543	C	-6.9844309	-0.5133919	4.0064113
H	16.0575976	0.3059383	-2.5209877	C	-6.9903151	-4.1655921	-0.5343785
C	15.6684710	-3.5082307	-0.4266328	C	-6.9713629	0.4958074	-4.0221075
H	16.0636240	-3.9006266	-1.3631730	C	6.2715484	4.5430284	0.6074984
H	16.0631652	-4.1144301	0.3882600	C	6.2558766	0.5876490	-4.1069000
C	15.6378199	-0.4277636	3.5219548	C	6.2453594	-0.5923767	4.1276472
H	16.0242249	0.3888055	4.1312482	C	6.2672208	-4.5254310	-0.6041289
H	16.0550782	-0.3093623	2.5220088	C	9.5120405	4.7763226	-0.8513936
C	15.6718674	3.5048327	0.4242967	H	9.5034443	4.9268444	-1.9210733
H	16.0671794	3.8968999	1.3609144	C	9.5051338	4.4760533	1.9754130
H	16.0675946	4.1104141	-0.3905509	H	9.5002499	4.4021431	3.0540185
H	16.0699685	-2.5024117	-0.3036758	C	9.4692453	1.9770187	-4.3213534
H	16.0252666	-1.3634948	3.9238321	H	9.4655002	3.0555255	-4.2485051
H	16.0721919	2.4985094	0.3016602	C	9.4699129	-0.8508926	-4.5926633
H	16.0289222	-0.3909063	-4.1308317	H	9.4566828	-1.9211586	-4.7381801
C	8.2910996	0.1328215	4.3987160	C	9.4622227	0.8501725	4.5931615
C	8.2715726	-1.2586943	4.2756904	H	9.4460297	1.9211149	4.7332540
C	8.2988817	-0.1361133	-4.3895999	C	9.4630206	-1.9787162	4.3227079
C	8.2790495	1.2558544	-4.2677953	H	9.4604730	-3.0571866	4.2494364
C	-2.7120400	4.0587073	0.5751073	C	9.5085388	-4.7691013	0.8463305
C	-3.4458737	3.0667434	1.2053348	H	9.5003048	-4.9205769	1.9158321
C	-4.8270474	3.0721597	1.1615815	C	9.4984345	-4.4683977	-1.9799021
C	-5.5245876	4.0703515	0.4946981	H	9.4939957	-4.3994889	-3.0588678
C	-4.7772821	5.0454931	-0.1523404	N	7.0011468	-4.4303828	-1.6895180
C	-3.3972320	5.0424171	-0.1186787	N	6.9751462	-1.6845871	4.1136700
F	-2.8263627	2.0982132	1.8652107	N	6.9830673	1.6812042	-4.0990675
F	-5.4840297	2.0920821	1.7699643	N	7.0095270	4.4474181	1.6900491
F	-5.3932139	6.0332617	-0.7930706	N	-7.7090603	4.0896240	1.6126193
F	-2.7367378	6.0101591	-0.7370689	N	-7.6890574	1.5930925	-3.9821038
C	-2.7159447	-4.0623453	-0.5758813	N	-7.7027241	-1.6101939	3.9638995
C	-3.4517554	-3.0736140	-1.2087209	N	-7.7096506	-4.1091304	-1.6298184
C	-4.8329059	-3.0845089	-1.1698610	N	-7.7207979	0.5914967	4.2470909
C	-5.5286569	-4.085630	-0.5054551	H	-7.4169744	1.5860224	4.2485415
C	-4.7796608	-5.0579335	0.1437630	N	-7.7302492	-4.3748429	0.5741003
C	-3.3994370	-5.0492190	0.1150082	H	-7.4218759	-4.3571837	1.5675445
F	-2.8338543	-2.1022954	-1.8659738	N	-7.7079721	-0.6088121	-4.2634728
F	-5.4915363	-2.1065875	-1.7798951	H	-7.4051073	-1.6035856	-4.2638393
F	-5.3940302	-6.0481050	0.7823094	N	-7.7234993	4.3549982	-0.5913651
F	-2.7370556	-6.0142585	0.7356544	H	-7.4125189	4.3381559	-1.5839929

N	7.0193433	4.6729904	-0.5142177	O	6.4272581	-3.2123084	-4.1522163
H	6.7178306	4.6748677	-1.4936779	H	6.5985343	-3.6908472	-3.3090041
N	6.9959006	-0.5301107	-4.2829115	O	6.9046576	4.3528620	-3.2969483
H	6.6775673	-1.5134204	-4.2532215	H	6.8458484	3.4080697	-3.5683579
N	7.0172743	-4.6585489	0.5150382	O	6.6663063	3.2556210	4.1867424
H	6.7186889	-4.6615231	1.4955777	H	6.7257665	3.7078000	3.3136098
N	6.9867983	0.5252122	4.3019971	O	6.9084569	-4.3523718	3.2942572
H	6.6817551	1.5096922	4.2838044	H	6.8407470	-3.4116979	3.5773975
Br	-0.8627705	-0.4615013	3.5456579	C	5.2731207	-3.7300908	-4.7719836
Br	-0.8558839	-4.0995481	-0.6687004	H	5.0491457	-3.1177989	-5.6454011
Br	-0.8513269	0.4228763	-3.5405318	H	5.4192984	-4.7576898	-5.1188224
Br	-0.8526732	4.1080590	0.6762972	H	4.3963839	-3.7087290	-4.1163241
C	4.8001878	4.5190892	0.6116497	C	6.4571846	5.1645559	-4.3557232
C	4.0950329	3.6214310	-0.1942184	H	5.3833404	5.0585621	-4.5455967
C	4.0937183	5.3861178	1.4549381	H	6.6452941	6.2060392	-4.0966682
C	2.7096876	3.6058657	-0.0721994	H	6.9886839	4.9527294	-5.2884566
H	2.1264016	2.9102863	-0.6686067	C	5.8788489	4.0214629	5.0663903
C	4.7938691	0.5273936	-3.9540278	H	4.8445150	4.1284705	4.7228751
C	4.2294518	-0.2030852	-2.9056801	H	5.8569512	3.5195388	6.0334203
C	3.9640844	1.1992580	-4.8557214	H	6.2937395	5.0220836	5.2236958
C	2.8410522	-0.2273700	-2.8223660	C	6.4932043	-5.1870131	4.3482176
H	2.3577595	-0.7828315	-2.0241534	H	5.4184005	-5.1143889	4.5476500
C	4.7830492	-0.5413594	3.9767346	H	6.7093150	-6.2199531	4.0769744
C	4.2082885	0.2200566	2.9556546	H	7.0259717	-4.9692196	5.2788087
C	3.9606701	-1.2612903	4.8484431	O	-7.2702925	4.1930525	-3.2377641
C	4.7960213	-4.4956581	-0.6038103	H	-7.3660188	3.2500117	-3.5170501
C	4.0964847	-3.5890902	0.1967256	C	-6.2369571	4.7927461	-3.9795764
C	4.0851696	-5.3686296	-1.4374865	H	-6.1862381	5.8479543	-3.7140524
C	2.7109490	-3.5673071	0.0745580	H	-5.2559999	4.3487047	-3.7752178
H	2.1309175	-2.8656445	0.6670466	H	-6.4192378	4.7260854	-5.0560760
C	5.0457305	-0.8861192	-1.8518362	O	-7.3077855	-3.2711991	-4.2012215
H	5.3767917	-1.8769406	-2.1618807	H	-7.3949014	-3.5940808	-3.2716989
H	5.9349254	-0.3133642	-1.5876031	C	-6.3111867	-4.0153113	-4.8578043
H	4.4539650	-1.0145758	-0.9480245	H	-6.2768918	-3.7052773	-5.9014114
C	4.4919525	1.9896126	-6.0141171	H	-5.3145889	-3.8595464	-4.4295042
H	3.6865306	2.2562084	-6.6966973	H	-6.5244880	-5.0878547	-4.8334177
H	4.9706519	2.9119681	-5.6870010	O	-7.2823088	-4.2102635	3.2211208
H	5.2375856	1.4301995	-6.5789027	H	-7.3789289	-3.2671026	3.4997248
C	4.7423636	2.6799636	-1.1592377	C	-6.2505670	-4.8093243	3.9656485
H	4.9665111	3.1670512	-2.1080744	H	-6.1979051	-5.8642985	3.6995753
H	5.6737100	2.2573882	-0.7831764	H	-5.2694725	-4.3641017	3.7645293
H	4.0678916	1.8581319	-1.3868114	H	-6.4361405	-4.7435670	5.0416405
C	4.7527678	6.4426114	2.2900313	O	-7.3159604	3.2529822	4.1856104
H	5.2752088	6.0233149	3.1473984	H	-7.3994860	3.5754104	3.2555985
H	5.4891474	7.0062514	1.7178129	C	-6.3198191	3.9953585	4.8448587
H	4.0114980	7.1475413	2.6640406	H	-6.2898359	3.6862885	5.8888846
C	4.7406336	-6.4422448	-2.2536264	H	-5.3221460	3.8367706	4.4201361
H	3.9931920	-7.1298437	-2.6469532	H	-6.5305021	5.0683772	4.8186780
H	5.3004112	-6.0405259	-3.0956358				
H	5.4448223	-7.0225132	-1.6574691				
C	4.7494521	-2.6512420	1.1618492	Br-RA4			
H	4.9625286	-3.1397323	2.1126193				
H	5.6878719	-2.2403768	0.7906265	180			
H	4.0836137	-1.8209783	1.3849458	Energy = -16601.67168999			
C	4.4930328	-2.0823810	5.9831985	C	4.6709224	4.8790310	-0.2787778
H	3.6897015	-2.3646986	6.6619868	C	3.8768857	3.9682170	0.4054876
H	4.9672523	-2.9973920	5.6305368	C	4.5223407	2.9432505	1.0845674
H	5.2425794	-1.5401024	6.5590146	C	5.8997759	2.8452740	1.0952152
C	5.0106449	0.9711876	1.9378351	C	6.6788045	3.7677368	0.4168547
H	5.9166824	0.4372003	1.6508430	C	6.0495720	4.7849543	-0.2808473
H	4.4181733	1.1266061	1.0385925	C	2.4201805	4.1110526	0.4384412
H	5.3097974	1.9566277	2.2947965	N	1.6829862	4.3219409	-0.6718619
C	2.7087244	5.2649540	1.4708629	C	0.3843413	4.4222743	-0.2661458
H	2.1197923	5.9153789	2.1091030	C	0.4093620	4.2714145	1.1233440
N	2.0322223	4.3929616	0.7425029	N	1.7019467	4.0803864	1.5353482
N	2.0310245	-0.4651242	3.6729037	C	-0.7739103	4.3315938	1.8566853
N	2.0297349	-4.3567388	-0.7346657	C	-1.9558285	4.4885701	1.1647310
N	2.0437584	0.4080320	-3.6622019	C	-1.9652883	4.6358128	-0.2426959
C	2.5892066	-1.1801862	4.6349234	C	-0.7940273	4.6301000	-0.9701624
H	1.9099264	-1.7218100	5.2852506	O	-3.1698430	4.8232564	-0.8621001
C	2.7010479	-5.2395689	-1.4551806	C	-3.7187426	3.7300421	-1.4926723
H	2.1081227	-5.8929781	-2.0866837	C	-4.8214149	3.0895508	-0.9358237
C	2.8202693	0.2186469	2.8642280	C	-5.3428991	2.0069871	-1.6355207
H	2.3305869	0.7956285	2.0854889	C	-4.8205763	1.5381875	-2.8361972
C	2.5931705	1.0992785	-4.6465571	C	-3.7161312	2.2108174	-3.3515029
H	1.9070956	1.6039685	-5.3190891	C	-3.1916245	3.3124394	-2.7008135

O	-3.1564280	4.5474510	1.8208234	F	3.8202729	2.0174657	1.7249271
C	-3.7093860	3.3522718	2.2176711	F	4.1148412	0.9259194	5.8840170
C	-3.1837221	2.7014592	3.3186561	F	6.7702586	0.9341373	5.6773372
C	-3.7113303	1.4939431	3.7374506	Br	8.5351411	-0.4321826	3.6184135
C	-4.8156081	0.9379810	3.0989642	F	6.4749296	-1.7586372	1.8404375
C	-5.3385206	1.6380976	2.0173458	F	3.8226108	-1.7263902	2.0125322
C	-4.8157312	2.8380894	1.5473150	F	3.8194166	-2.0129473	-1.7352873
C	-5.4276706	3.5716783	0.3685956	F	6.4716441	-1.8418200	-1.7721972
C	-6.9547097	3.5191713	0.3663297	Br	8.5335197	-3.6187635	-0.4469149
C	-5.4310549	0.3582310	-3.5690353	F	6.7702478	-5.6753926	0.9249334
C	-4.8218818	-0.9449600	-3.0872694	F	4.1148669	-5.8814254	0.9212245
C	-3.7183603	-1.4993406	-3.7284196	F	3.8160212	1.7294986	-2.0212268
C	-3.1881092	-2.7061676	-3.3110132	F	6.4688191	1.7643072	-1.8559486
C	-3.7102240	-3.3577794	-2.2088172	Br	8.5257945	0.4427764	-3.6413042
C	-4.8156010	-2.8451341	-1.5357117	F	6.7569864	-0.9224185	-5.6976631
C	-5.3411994	-1.6458505	-2.0044345	F	4.1009375	-0.9172060	-5.8969630
O	-3.1637674	1.8154721	-4.5474874	F	6.4727550	1.8492749	1.7551793
C	-1.9617116	1.1619369	-4.4899122	Br	8.5293701	3.6288593	0.4252990
C	-1.9684001	-0.2456221	-4.6359109	F	6.7604004	5.6838082	-0.9417456
C	-0.7956494	-0.9706645	-4.6303744	F	4.1047994	5.8865931	-0.9317930
C	0.3814013	-0.2640027	-4.4242470	C	-6.9580373	0.3531865	-3.5150715
C	0.4037898	1.1257234	-4.2751942	C	-6.9489756	-0.3630787	3.5319923
C	-0.7810457	1.8565464	-4.3351154	O	2.0819068	4.1449648	-3.3258215
N	1.6958017	1.5405608	-4.0860828	C	3.0483887	4.7926951	-4.1166322
C	2.4161232	0.4450341	-4.1162453	O	2.0876707	3.3236403	4.1407162
N	1.6809578	-0.6670111	-4.3247584	C	3.0491081	4.1170042	4.7928097
O	-3.1718201	-0.8675615	-4.8220944	O	2.0858753	-3.3203293	-4.1462508
C	3.8730936	0.4148995	-3.9751110	C	3.0557834	-4.1064136	-4.7946243
C	4.5183666	1.0926351	-2.9492236	O	2.0950604	-4.1420511	3.3204012
C	5.8958926	1.1057215	-2.8528806	C	3.0616265	-4.7900328	4.1108782
C	6.6750757	0.4311169	-3.7779771	H	-2.3890545	3.8705864	-3.1581994
C	6.0459927	-0.2651841	-4.7962632	H	-6.2026697	1.4979052	-1.2199441
C	4.6672293	-0.2655426	-4.8886376	H	-2.3798122	3.1582739	3.8753332
O	-3.1613407	0.8631057	4.8299532	H	-6.1997307	1.2233833	1.5100015
C	-1.9574423	0.2429103	4.6409910	H	-2.3849181	-3.1618537	-3.8696493
C	-1.9490940	-1.1646046	4.4945666	H	-6.2017697	-1.2323559	-1.4949959
C	-0.7678233	-1.8574614	4.3366639	H	-2.3757747	-3.8738996	3.1637412
C	0.4158112	-1.1249106	4.2740774	H	-6.1978807	-1.5070093	1.2351610
C	0.3918255	0.2647078	4.4238245	H	-5.1569021	-0.4721397	4.6337326
C	-0.7857371	0.9696234	4.6330657	H	-5.1642217	4.6235809	0.4746980
N	1.6905312	0.6696090	4.3209988	H	-5.1688110	0.4646584	-4.6212060
C	2.4267347	-0.4412745	4.1097888	H	-5.1588686	-4.6310510	-0.4621390
N	1.7078638	-1.5378112	4.0812527	H	-7.3474217	4.1119669	-0.4593507
C	-5.4218660	-0.3660383	3.5822112	H	-7.3631600	2.5137925	0.2642832
C	-4.8115136	-1.5450872	2.8478104	H	-7.3404246	0.4628360	4.1252977
C	-3.7047565	-2.2160412	3.3603237	H	-7.3385170	-1.2927092	3.9459189
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C	-4.8148256	-3.0964595	0.9474590	H	-7.3498735	1.2822314	-3.9281486
C	-5.3362198	-2.0147198	1.6484998	H	-7.3653424	0.2506287	-2.5092796
O	-3.1546177	-4.5522034	-1.8133882	H	-7.3589035	-0.2609655	2.5272216
C	-1.9524496	-4.4916464	-1.1603393	H	-7.3405303	-4.1225834	0.4772014
C	-1.9581772	-4.6385714	0.2471410	H	-7.3498248	-0.4733336	-4.1073132
C	-0.7851064	-4.6309999	0.9716575	H	-7.3444589	3.9324185	1.2961768
C	0.3911855	-4.4217199	0.2646134	H	-0.7885723	4.7848918	-2.0392036
C	0.4125526	-4.2712302	-1.1249772	H	-0.7569715	4.2584457	2.9348167
C	-0.7724815	-4.3333027	-1.8553130	H	-0.7792661	2.0387576	4.7871227
N	1.7038740	-4.0786886	-1.5402732	H	-0.7517505	-2.9356668	4.2643414
C	2.4248779	-4.1081369	-0.4451381	H	-0.7767016	-4.7855522	2.0407119
N	1.6907004	-4.3196098	0.6670534	H	-0.7583903	-4.2605987	-2.9335196
C	-5.4235841	-3.5795270	-0.3554466	H	-0.7880316	-2.0398122	-4.7842809
C	-6.9506930	-3.5292554	-0.3494602	H	-0.7663574	2.9348042	-4.2632486
O	-3.1500714	-1.8198626	4.5549462	H	1.9930037	1.6640496	4.2884589
C	3.8832504	-0.4091656	3.9646043	H	1.9953575	-4.2883618	1.6608711
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C	6.0575979	0.2746857	4.7788731	H	1.9852310	4.2911224	-1.6664954
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C	5.9039042	-1.0992503	2.8379430	H	3.0643960	5.8485998	-3.8497617
C	4.5266229	-1.0875543	2.9379063	H	4.0574529	4.3933004	-3.9640584
O	-3.1608996	-4.8277075	0.8695797	H	2.8147987	4.7197701	-5.1825232
C	3.8814921	-3.9634860	-0.4157495	H	2.0067570	-3.6096204	-3.2055388
C	4.5241120	-2.9378256	-1.0964599	H	3.0727978	-3.8363144	-5.8496884
C	5.9014095	-2.8383220	-1.1105967	H	2.8252519	-5.1732207	-4.7253315
C	6.6831402	-3.7597544	-0.4339427	H	2.0135922	-3.2016445	3.6100549
C	6.0567797	-4.7775470	0.2655125	H	3.0838834	-5.8440774	3.8372209
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H	4.0637089	-3.9520281	-4.3930540

Cl-capsule

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C	-12.9976427	3.8076720	-1.3163685
C	-14.6123376	2.0870173	-1.5542607
H	-11.6544934	4.0322868	-2.9621688
H	-15.4735018	1.5551102	-1.1709745
O	-12.4604092	4.8719713	-0.6300989
C	-11.2555507	4.6633400	-0.0175788
C	-11.2476037	4.4511564	1.3808831
C	-11.2018268	1.3772549	-4.4034629
C	-11.2105496	-0.0200934	-4.6246765
O	-12.4128229	-0.6285414	-4.8618897
C	-12.9959360	3.2489249	2.3673678
C	-14.0888116	0.7871245	3.1241027
C	-12.4652127	2.5441911	3.4321233
C	-14.0984182	2.7628166	1.6699482
C	-14.6152926	1.5383308	2.0792465
C	-12.9851482	1.3134642	3.7879589
H	-11.6619644	2.9751060	4.0100760
H	-15.4744786	1.1451110	1.5514977
C	-12.9732969	-1.3148143	-3.8088337
C	-14.0913189	-2.7647298	-1.6936797
C	-12.4532302	-2.5449644	-3.4511978
C	-14.0791780	-0.7892177	-3.1480834
C	-14.6080829	-1.5407666	-2.1046835
C	-12.9861957	-3.2498348	-2.3876562
H	-11.6481362	-2.9755378	-4.0268402
H	-15.4692319	-1.1482997	-1.5795854
O	-12.4267756	0.6273695	4.8422224
O	-12.4408554	-4.4673812	-2.0540734
C	-11.2234582	0.0197701	4.6080708
C	-11.2132668	-1.3776484	4.3873329
C	-11.2398680	-4.4504958	-1.3951987
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C	-12.9783682	-2.3788663	3.2232250
C	-14.1003033	-3.1376162	0.7743215
C	-14.0854047	-1.6813392	2.7482812
C	-12.4636573	-3.4515467	2.5191568
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C	-14.6156579	-2.0897177	1.5290169
H	-11.6608886	-4.0332335	2.9457465
H	-15.4760822	-1.5583940	1.1432735
O	-12.4124149	-2.0395942	4.4298720
C	-14.6910325	-0.5402804	3.5434018
H	-14.4201143	-0.6990406	4.5867289
C	-14.7126423	3.5492090	0.5267145
H	-14.4559975	4.5962506	0.6848111
C	-14.6811456	0.5377869	-3.5690457
H	-14.4074347	0.6968113	-4.6115965
C	-14.7086184	-3.5517201	-0.5524871
H	-14.4509149	-4.5985876	-0.7100069
C	-8.8779485	0.0614414	4.3560454
C	-8.8513330	-1.3179440	4.1314762
C	-8.8657734	-0.0605270	-4.3656416
C	-8.8406711	1.3187979	-4.1404923
O	-12.4011866	2.0385638	-4.4490361
O	-12.4508859	4.4671494	2.0356165
O	-12.4593626	-4.8734565	0.6112849
C	-16.2392083	3.4875209	0.5179070
H	-16.6337297	4.1180800	-0.2784351
H	-16.6410037	2.4859054	0.3649488
C	-16.2184572	-0.5357345	3.5021054

H	-16.6067324	0.2588902	4.1386684
H	-16.6053624	-1.4854346	3.8704961
C	-16.2352401	-3.4907886	-0.5484405
H	-16.6266591	-3.8547792	-1.4979807
H	-16.6380105	-2.4894310	-0.3963428
C	-16.2086845	0.5321898	-3.5319960
H	-16.5952290	1.4816765	-3.9013139
H	-16.6268370	0.3790025	-2.5371331
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H	-16.6319077	-4.1218495	0.2464341
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H	-16.6337592	3.8516840	1.4660873
C	-8.8718203	-4.2652974	-1.3431771
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C	12.3389783	3.7381724	-1.4900749
C	13.4230251	1.5405188	-2.8374856
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H	10.9863933	3.8721999	-3.1374509
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O	11.7545172	1.8195956	-4.5370755
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C	10.5576572	-0.2423271	-4.5899733
C	10.6086809	4.7137257	-0.2367276
C	10.6034965	4.5849953	1.1716176
O	11.8101354	4.5883458	1.8177774
C	12.3156871	-1.5034793	-3.7068481
C	13.4475890	-2.8480630	-1.5320596
C	11.7983304	-2.7157603	-3.2875467
C	13.4248796	-0.9449067	-3.0794004
C	13.9589412	-1.6433668	-2.0025530
C	12.3418339	-3.3705453	-2.1973984
H	10.9918847	-3.1758861	-3.8381990
H	14.8216798	-1.2249802	-1.5009912
C	12.3363916	3.3765858	2.1997685
C	13.4224379	0.9522263	3.0814308
C	11.7931148	2.7206041	3.2893284
C	13.4430088	2.8557728	1.5346594
C	13.9560309	1.6517438	2.0050924
C	12.3117992	1.5087573	3.7081484
H	10.9860951	3.1795706	3.8401065
H	14.8196074	1.2347734	1.5037948
O	11.8166852	-4.5826724	-1.8150450
O	11.7512372	0.8747105	4.7928831
C	10.6104297	-4.5805299	-1.1680757
C	10.6166481	-4.7109935	0.2400756
C	10.5553024	0.2442474	4.5897578
C	10.5535102	-1.1634305	4.4664213
C	12.3454066	-3.7334355	1.4929320
C	13.4245393	-1.5333738	2.8402642
C	13.4513573	-3.0904146	0.9454628
C	11.8007969	-3.3120295	2.6917629
C	12.3177328	-2.2087159	3.3466407
C	13.9602597	-2.0027595	1.6455789
H	10.9928437	-3.8700529	3.1401982
H	14.8217250	-1.4909880	1.2369012
O	11.8232930	-4.8412493	0.8677090
C	14.0690572	-3.5730407	-0.3533035
H	13.8181738	-4.6282716	-0.4562626
C	14.0259525	0.3581341	-3.5723709
H	13.7516549	0.4599972	-4.6218717
C	14.0633196	3.5816464	0.3558756
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C	15.5950789	-3.5023873	-0.3480724	C	-6.8353138	0.6175242	-3.9654138
H	15.9915967	-3.9134014	-1.2760280	C	6.1873202	4.6142267	0.5050873
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C	3.4315508	1.0662506	-14.5485010	C	1.9603649	-3.0112035	13.9026494
H	4.4409996	1.3794461	-14.2842134	H	2.5345870	-3.8986516	13.6381178
C	1.0662506	-3.4315508	-14.5485010	C	3.0112035	1.9603649	13.9026494
H	1.3794461	-4.4409996	-14.2842134	H	3.8986516	2.5345870	13.6381178
C	-4.3859086	-0.6386489	-8.7332425	C	-1.9603649	3.0112035	13.9026494
C	-3.9699851	-1.9732281	-8.7182600	H	-2.5345870	3.8986516	13.6381178
C	4.3859086	0.6386489	-8.7332425	C	-3.0112035	-1.9603649	13.9026494
C	3.9699851	1.9732281	-8.7182600	H	-3.8986516	-2.5345870	13.6381178
O	4.1014001	2.6898633	-12.2870169	C	3.0776113	-3.3783517	8.0634694
O	-2.6898633	4.1014001	-12.2870169	C	1.8808856	-4.0994793	8.0787292
O	0.1118334	-4.8991237	-12.2861704	C	-3.0776113	3.3783517	8.0634694
C	-1.0507009	3.3823959	-16.0753340	C	-1.8808856	4.0994793	8.0787292
H	-0.3579601	4.1272593	-16.4661009	O	-1.4466960	4.6655041	11.6338036
H	-0.7509392	2.4174696	-16.4839173	O	4.6655041	1.4466960	11.6338036
C	-3.3823959	-1.0507009	-16.0753340	O	-3.2146089	-3.7180230	11.6459180
H	-4.1272593	0.3579601	-16.4661009	C	2.9690897	1.9313925	15.4294389
H	-3.6041073	-2.0432334	-16.4667401	H	2.9141132	2.9468783	15.8210388
C	1.0507009	-3.3823959	-16.0753340	H	2.1219715	1.3815558	15.8387485
H	2.0432334	-3.6041073	-16.4667401	C	1.9313925	-2.9690897	15.4294389
H	0.7509392	-2.4174696	-16.4839173	H	2.9468783	-2.9141132	15.8210388
C	3.3823959	1.0507009	-16.0753340	H	1.4665732	-3.8741246	15.8196359
H	3.6041073	2.0432334	-16.4667401	C	-2.9690897	-1.9313925	15.4294389
H	2.4174696	0.7509392	-16.4839173	H	-3.8741246	-1.4665732	15.8196359
H	-2.4174696	-0.7509392	-16.4839173	H	-2.1219715	-1.3815558	15.8387485
H	0.3579601	-4.1272593	-16.4661009	C	-1.9313925	2.9690897	15.4294389
H	4.1272593	0.3579601	-16.4661009	H	-2.9468783	2.9141132	15.8210388
H	-2.0432334	3.6041073	-16.4667401	H	-1.4665732	3.8741246	15.8196359
C	1.9732281	-3.9699851	-8.7182600	H	1.3815558	-2.1219715	15.8387485
C	0.6386489	-4.3859086	-8.7332425	H	-2.9141132	-2.9468783	15.8210388
C	-1.9732281	3.9699851	-8.7182600	H	-1.3815558	2.1219715	15.8387485
C	-0.6386489	4.3859086	-8.7332425	H	3.8741246	1.4665732	15.8196359
C	-0.3833824	3.9863305	12.1795150	C	-4.0994793	-1.8808856	8.0787292
C	1.8197406	2.6738394	13.2928508	C	-3.3783517	-3.0776113	8.0634694
C	-0.5811483	3.1737298	13.2917487	C	4.0994793	1.8808856	8.0787292
C	0.8804587	4.1700553	11.6500186	C	3.3783517	3.0776113	8.0634694
C	1.9680120	3.5046516	12.1858740	C	-1.3152317	3.5515568	-2.4624291
C	0.5382739	2.5380365	13.8160096	C	-1.7301254	2.5011764	-3.2610722
H	1.0266130	4.8677402	10.8393201	C	-1.6857962	2.6194716	-4.6354266
H	0.4049240	1.8996156	14.6794944	C	-1.2457407	3.7861724	-5.2469808
O	3.2146089	3.7180230	11.6459180	C	-0.8220639	4.8215556	-4.4244853
C	3.4790543	3.1319122	10.4372036	C	-0.8514647	4.7161905	-3.0467272
C	4.2260300	1.9319706	10.4339146	F	-2.1567374	1.3769637	-2.6989766
C	-1.9319706	4.2260300	10.4339146	F	-2.0607112	1.5799803	-5.3677509
C	-3.1319122	3.4790543	10.4372036	F	-0.3992659	5.9591399	-4.9608371
O	-3.7180230	3.2146089	11.6459180	F	-0.4539139	5.7259648	-2.2875691
C	3.9863305	0.3833824	12.1795150	C	1.3152317	-3.5515568	-2.4624291
C	2.6738394	-1.8197406	13.2928508	C	1.7301254	-2.5011764	-3.2610722
C	4.1700553	-0.8804587	11.6500186	C	1.6857962	-2.6194716	-4.6354266
C	3.1737298	0.5811483	13.2917487	C	1.2457407	-3.7861724	-5.2469808
C	2.5380365	-0.5382739	13.8160096	C	0.8220639	-4.8215556	-4.4244853
C	3.5046516	-1.9680120	12.1858740	C	0.8514647	-4.7161905	-3.0467272

F	2.1567374	-1.3769637	-2.6989766	N	4.3605968	0.2303352	-7.4305199
F	2.0607112	-1.5799803	-5.3677509	H	4.5244744	-0.7475000	-7.1175032
F	0.3992659	-5.9591399	-4.9608371	N	-0.2303352	4.3605968	-7.4305199
F	0.4539139	-5.7259648	-2.2875691	H	0.7475000	4.5244744	-7.1175032
C	3.5515568	1.3152317	-2.4624291	N	-1.5261144	4.2438140	6.7668894
C	2.5011764	1.7301254	-3.2610722	H	-0.6389633	4.6619804	6.4548087
C	2.6194716	1.6857962	-4.6354266	N	4.2438140	1.5261144	6.7668894
C	3.7861724	1.2457407	-5.2469808	H	4.6619804	0.6389633	6.4548087
C	4.8215556	0.8220639	-4.4244853	N	1.5261144	-4.2438140	6.7668894
C	4.7161905	0.8514647	-3.0467272	H	0.6389633	-4.6619804	6.4548087
F	1.3769637	2.1567374	-2.6989766	N	-4.2438140	-1.5261144	6.7668894
F	1.5799803	2.0607112	-5.3677509	H	-4.6619804	-0.6389633	6.4548087
F	5.9591399	0.3992659	-4.9608371	F	-3.4368318	-1.3571077	-1.1506224
F	5.7259648	0.4539139	-2.2875691	F	1.3571077	-3.4368318	-1.1506224
C	-3.5515568	-1.3152317	-2.4624291	F	3.4368318	1.3571077	-1.1506224
C	-4.7161905	-0.8514647	-3.0467272	F	-1.3571077	3.4368318	-1.1506224
C	-4.8215556	-0.8220639	-4.4244853	C	-2.4635688	3.6299430	4.5541054
C	-3.7861724	-1.2457407	-5.2469808	C	-1.3825196	3.0960311	3.8497115
C	-2.6194716	-1.6857962	-4.6354266	C	-3.5443366	4.1723308	3.8507179
C	-2.5011764	-1.7301254	-3.2610722	C	-1.4584961	3.1137866	2.4599859
F	-5.7259648	-0.4539139	-2.2875691	H	-0.6434171	2.6941249	1.8773410
F	-5.9591399	-0.3992659	-4.9608371	C	3.6299430	2.4635688	4.5541054
F	-1.5799803	-2.0607112	-5.3677509	C	3.0960311	1.3825196	3.8497115
F	-1.3769637	-2.1567374	-2.6989766	C	4.1723308	3.5443366	3.8507179
C	0.0187576	4.7269392	-9.9079336	C	3.1137866	1.4584961	2.4599859
H	1.0376295	5.0856642	-9.8968063	H	2.6941249	0.6434171	1.8773410
C	-2.6968065	3.8884323	-9.9053828	C	-3.6299430	-2.4635688	4.5541054
H	-3.7406952	3.6090502	-9.8951487	C	-3.0960311	-1.3825196	3.8497115
C	-4.7269392	0.0187576	-9.9079336	C	-4.1723308	-3.5443366	3.8507179
H	-5.0856642	1.0376295	-9.8968063	C	2.4635688	-3.6299430	4.5541054
C	-3.8884323	-2.6968065	-9.9053828	C	1.3825196	-3.0960311	3.8497115
H	-3.6090502	-3.7406952	-9.8951487	C	3.5443366	-4.1723308	3.8507179
C	-0.0187576	-4.7269392	-9.9079336	C	1.4584961	-3.1137866	2.4599859
H	-1.0376295	-5.0856642	-9.8968063	H	0.6434171	-2.6941249	1.8773410
C	2.6968065	-3.8884323	-9.9053828	C	2.4992298	0.1810232	4.5160824
H	3.7406952	-3.6090502	-9.8951487	H	3.2622083	-0.5267607	4.8405039
C	4.7269392	-0.0187576	-9.9079336	H	1.9058337	0.4444179	5.3919327
H	5.0856642	-1.0376295	-9.8968063	H	1.8537636	-0.3532737	3.8215465
C	3.8884323	2.6968065	-9.9053828	C	4.8160725	4.7201887	4.5223504
H	3.6090502	3.7406952	-9.8951487	H	5.3513881	5.3282191	3.7941521
C	-1.2845572	3.9372823	-6.7029931	H	4.0862489	5.3586516	5.0175212
C	-3.9372823	-1.2845572	-6.7029931	H	5.5299465	4.4091654	5.2850545
C	1.2845572	-3.9372823	-6.7029931	C	-0.1810232	2.4992298	4.5160824
C	3.9372823	1.2845572	-6.7029931	H	0.5267607	3.2622083	4.8405039
C	-2.4805565	3.6349227	6.0254761	H	-0.4444179	1.9058337	5.3919327
C	3.6349227	2.4805565	6.0254761	H	0.3532737	1.8537636	3.8215465
C	-3.6349227	-2.4805565	6.0254761	C	-4.7201887	4.8160725	4.5223504
C	2.4805565	-3.6349227	6.0254761	H	-5.3586516	4.0862489	5.0175212
C	-1.2991415	4.5554820	9.2528222	H	-4.4091654	5.5299465	5.2850545
H	-0.4006661	5.1551795	9.2366946	H	-5.3282191	5.3513881	3.7941521
C	-3.7228775	3.0715675	9.2588956	C	4.7201887	-4.8160725	4.5223504
H	-4.6651734	2.5415432	9.2577042	H	5.3282191	-5.3513881	3.7941521
C	3.0715675	3.7228775	9.2588956	H	5.3586516	-4.0862489	5.0175212
H	2.5415432	4.6651734	9.2577042	H	4.4091654	-5.5299465	5.2850545
C	4.5554820	1.2991415	9.2528222	C	0.1810232	-2.4992298	4.5160824
H	5.1551795	0.4006661	9.2366946	H	-0.5267607	-3.2622083	4.8405039
C	-4.5554820	-1.2991415	9.2528222	H	0.4444179	-1.9058337	5.3919327
H	-5.1551795	-0.4006661	9.2366946	H	-0.3532737	-1.8537636	3.8215465
C	-3.0715675	-3.7228775	9.2588956	C	-4.8160725	-4.7201887	4.5223504
H	-2.5415432	-4.6651734	9.2577042	H	-5.3513881	-5.3282191	3.7941521
C	1.2991415	-4.5554820	9.2528222	H	-4.0862489	-5.3586516	5.0175212
H	0.4006661	-5.1551795	9.2366946	H	-5.5299465	-4.4091654	5.2850545
C	3.7228775	-3.0715675	9.2588956	C	-2.4992298	-0.1810232	4.5160824
H	4.6651734	-2.5415432	9.2577042	H	-1.9058337	-0.4444179	5.3919327
N	3.4270664	-3.1026959	6.7643074	H	-1.8537636	0.3532737	3.8215465
N	-3.1026959	-3.4270664	6.7643074	H	-3.2622083	0.5267607	4.8405039
N	3.1026959	3.4270664	6.7643074	C	-3.4802371	4.1259514	2.4622575
N	-3.4270664	3.1026959	6.7643074	H	-4.2956527	4.5404976	1.8772648
N	-2.3499099	3.6995348	-7.4294093	N	-2.4751235	3.6085345	1.7779382
N	3.6995348	2.3499099	-7.4294093	N	-3.6085345	-2.4751235	1.7779382
N	-3.6995348	-2.3499099	-7.4294093	N	2.4751235	-3.6085345	1.7779382
N	2.3499099	-3.6995348	-7.4294093	N	3.6085345	2.4751235	1.7779382
N	-4.3605968	-0.2303352	-7.4305199	C	-4.1259514	-3.4802371	2.4622575
H	-4.5244744	0.7475000	-7.1175032	H	-4.5404976	-4.2956527	1.8772648
N	0.2303352	-4.3605968	-7.4305199	C	3.4802371	-4.1259514	2.4622575
H	-0.7475000	-4.5244744	-7.1175032	H	4.2956527	-4.5404976	1.8772648

C	-3.1137866	-1.4584961	2.4599859	C	-5.3295075	2.0092792	-1.6324126
H	-2.6941249	-0.6434171	1.8773410	C	-4.8068242	1.5423289	-2.8336520
C	4.1259514	3.4802371	2.4622575	C	-3.7021692	2.2157146	-3.3476268
H	4.5404976	4.2956527	1.8772648	C	-3.1782272	3.3166498	-2.6954016
O	5.2599841	-1.0318393	6.4514838	O	-3.1414312	4.5433990	1.8278113
H	4.6147085	-1.7753430	6.5053263	C	-3.6951537	3.3479216	2.2226491
O	1.0318393	5.2599841	6.4514838	C	-3.1701700	2.6956580	3.3230596
H	1.7753430	4.6147085	6.5053263	C	-3.6985190	1.4879126	3.7402540
O	-5.2599841	1.0318393	6.4514838	C	-4.8023873	0.9328378	3.1004679
H	-4.6147085	1.7753430	6.5053263	C	-5.3248187	1.6344942	2.0196489
O	-1.0318393	-5.2599841	6.4514838	C	-4.8017305	2.8351060	1.5515403
H	-1.7753430	-4.6147085	6.5053263	C	-5.4141015	3.5708062	0.3743518
C	6.3686221	-1.4349264	5.6852646	C	-6.9411196	3.5184585	0.3725893
H	7.0872727	-0.6159827	5.6608156	C	-5.4176630	0.3638223	-3.5685182
H	6.8731368	-2.3043535	6.1185009	C	-4.8086364	-0.9401951	-3.0889007
H	6.1018445	-1.6748613	4.6504865	C	-3.7055899	-1.4936412	-3.7314944
C	1.4349264	6.3686221	5.6852646	C	-3.1745297	-2.7006909	-3.3157671
H	1.6748613	6.1018445	4.6504865	C	-3.6957995	-3.3537873	-2.2140862
H	0.6159827	7.0872727	5.6608156	C	-4.8013525	-2.8425556	-1.5400976
H	2.3043535	6.8731368	6.1185009	C	-5.3273334	-1.6426634	-2.0068315
C	-6.3686221	1.4349264	5.6852646	O	-3.1492382	1.8225764	-4.5440848
H	-6.1018445	1.6748613	4.6504865	C	-1.9478592	1.1675892	-4.4877710
H	-7.0872727	0.6159827	5.6608156	C	-1.9562542	-0.2393540	-4.6377941
H	-6.8731368	2.3043535	6.1185009	C	-0.7843303	-0.9656782	-4.6349944
C	-1.4349264	-6.3686221	5.6852646	C	0.3933315	-0.2609502	-4.4275950
H	-1.6748613	-6.1018445	4.6504865	C	0.4180737	1.1282787	-4.2754093
H	-0.6159827	-7.0872727	5.6608156	C	-0.7660787	1.8604867	-4.3317610
H	-2.3043535	-6.8731368	6.1185009	N	1.7117542	1.5408648	-4.0895079
O	2.4018334	4.7256339	-6.9898443	C	2.4301029	0.4442426	-4.1230738
H	2.8898920	3.8745386	-7.1028124	N	1.6923949	-0.6661751	-4.3308079
C	3.0165160	5.4832666	-5.9772551	O	-3.1601458	-0.8600747	-4.8246606
H	2.5038008	6.4414954	-5.9014341	C	3.8876851	0.4077754	-3.9897524
H	2.9664018	4.9987553	-4.9952524	C	4.5419463	1.0806672	-2.9656635
H	4.0685429	5.6830137	-6.2005917	C	5.9198772	1.0869219	-2.8748838
O	4.7256339	-2.4018334	-6.9898443	C	6.6771280	0.4045871	-3.8093698
H	3.8745386	-2.8898920	-7.1028124	C	6.0507989	-0.2879556	-4.8288843
C	5.4832666	-3.0165160	-5.9772551	C	4.6714809	-0.2763788	-4.9104823
H	6.4414954	-2.5038008	-5.9014341	O	-3.1495291	0.8553295	4.8322144
H	4.9987553	-2.9664018	-4.9952524	C	-1.9450893	0.2364895	4.6426901
H	5.6830137	-4.0685429	-6.2005917	C	-1.9348982	-1.1704084	4.4922441
O	-2.4018334	-4.7256339	-6.9898443	C	-0.7524205	-1.8614565	4.3333794
H	-2.8898920	-3.8745386	-7.1028124	C	0.4304746	-1.1273997	4.2745318
C	-3.0165160	-5.4832666	-5.9772551	C	0.4040073	0.2617098	4.4274747
H	-2.5038008	-6.4414954	-5.9014341	C	-0.7742694	0.9645843	4.6377327
H	-2.9664018	-4.9987553	-4.9952524	N	1.7022536	0.6689020	4.3279810
H	-4.0685429	-5.6830137	-6.2005917	C	2.4411489	-0.4403070	4.1178417
O	-4.7256339	2.4018334	-6.9898443	N	1.7243225	-1.5379669	4.0854287
H	-3.8745386	2.8898920	-7.1028124	C	-5.4082958	-0.3720827	3.5815945
C	-5.4832666	3.0165160	-5.9772551	C	-4.7975889	-1.5496792	2.8451710
H	-6.4414954	2.5038008	-5.9014341	C	-3.6904590	-2.2212300	3.3562151
H	-4.9987553	2.9664018	-4.9952524	C	-3.1663788	-3.3212656	2.7025831
H	-5.6830137	4.0685429	-6.2005917	C	-3.6966981	-3.7380907	1.4955819
				C	-4.8014971	-3.0981597	0.9425351
				C	-5.3226706	-2.0174746	1.6453011
				O	-3.1393275	-4.5485384	-1.8208667
				C	-1.9379039	-4.4889758	-1.1662600
				C	-1.9454454	-4.6398026	0.2406155
				C	-0.7732768	-4.6346196	0.9665305
				C	0.4036503	-4.4240736	0.2614839
				C	0.4275014	-4.2705902	-1.1276155
				C	-0.7567845	-4.3292974	-1.8594440
				N	1.7205667	-4.0812160	-1.5405129
				C	2.4394648	-4.1140101	-0.4442064
				N	1.7026369	-4.3246076	0.6662884
				C	-5.4097338	-3.5790817	-0.3613652
				C	-6.9368271	-3.5290152	-0.3558886
				O	-3.1351497	-1.8271835	4.5512500
				C	3.8983040	-0.4016420	3.9806596
				C	4.6835615	0.2850070	4.8983062
				C	6.0626373	0.2986150	4.8129544
				C	6.6873053	-0.3943184	3.7926988
				C	5.9285915	-1.0789835	2.8611139
				C	4.5508977	-1.0746944	2.9555586
				O	-3.1486641	-4.8297746	0.8616909
				C	3.8967260	-3.9772486	-0.4082250
				C	4.5484769	-2.9526761	-1.0829021

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Energy = -6708.190736897

C	4.6754721	4.9015610	-0.2891394
C	3.8917904	3.9826820	0.3976680
C	4.5461882	2.9588511	1.0709294
C	5.9240326	2.8665450	1.0748226
C	6.6811322	3.7992842	0.3899460
C	6.0546789	4.8184328	-0.3029959
C	2.4344546	4.1175598	0.4368838
N	1.6946312	4.3276465	-0.6717281
C	0.3964601	4.4248549	-0.2636779
C	0.4239507	4.2706325	1.1252780
N	1.7182835	4.0830514	1.5349042
C	-0.7585287	4.3271559	1.8601610
C	-1.9416309	4.4855944	1.1701027
C	-1.9529544	4.6369772	-0.2366784
C	-0.7826162	4.6339299	-0.9655881
O	-3.1580428	4.8252816	-0.8546987
C	-3.7060250	3.7326186	-1.4869964
C	-4.8082961	3.0908523	-0.9310333

C	5.9261957	-2.8585680	-1.0895027	H	2.8027299	-5.1833529	-4.7306695
C	6.6858256	-3.7901749	-0.4058853	H	2.0291275	-3.2000587	3.6109274
C	6.0620541	-4.8099896	0.2885001	H	3.0611324	-5.8569276	3.8506442
C	4.6829392	-4.8949619	0.2772697	H	4.0674064	-4.4126020	3.9855455
F	3.8547069	2.0282340	1.7136112	H	2.8045002	-4.7316667	5.1849583
F	4.1107848	0.9302916	5.9055650	H	2.0247171	3.6125550	3.1976629
F	6.7850271	0.9546361	5.7081202	H	3.0588486	3.8485789	5.8545679
F	8.0045803	-0.3992976	3.7043855	H	4.0558771	4.0073870	4.4063621
F	6.5315159	-1.7267622	1.8721935	H	2.7818460	5.1901974	4.7428783
F	3.8577323	-1.7170278	2.0259356	H	4.0605550	-3.9757008	-4.4227916
F	3.8544841	-2.0231853	-1.7245549				
F	6.5283254	-1.8700553	-1.7386545				
F	8.0031136	-3.7022403	-0.4131874				
F	6.7853026	-5.7051679	0.9435555				
F	4.1110288	-5.9019124	0.9238098				
F	3.8502181	1.7209083	-2.0335357				
F	6.5244541	1.7344220	-1.8867950				
F	7.9946260	0.4114862	-3.7245823				
F	6.7717660	-0.9416125	-5.7269179				
F	4.0969046	-0.9213215	-5.9169150				
F	6.5286467	1.8786519	1.7225977				
F	7.9985506	3.7130786	0.3946821				
F	6.7754803	5.7147579	-0.9591845				
F	4.1010018	5.9078651	-0.9343925				
C	-6.9446101	0.3589777	-3.5145681				
C	-6.9353880	-0.3694604	3.5314334				
O	2.0927932	4.1442242	-3.3265503				
C	3.0432377	4.8030460	-4.1272100				
O	2.0984130	3.3234681	4.1390795				
C	3.0412964	4.1294290	4.8022809				
O	2.0946545	-3.3202252	-4.1452712				
C	3.0442781	-4.1194667	-4.8070190				
O	2.1039079	-4.1409904	3.3206135				
C	3.0521353	-4.8020538	4.1220604				
H	-2.3757951	3.8755523	-3.1521191				
H	-6.1892931	1.4994622	-1.2177728				
H	-2.3662693	3.1517403	3.8803647				
H	-6.1859852	1.2206747	1.5115002				
H	-2.3714603	-3.1556585	-3.8751810				
H	-6.1878393	-1.2301178	-1.4965161				
H	-2.3617929	-3.8788078	3.1571649				
H	-6.1843859	-1.5090686	1.2329324				
H	-5.1432595	-0.4799263	4.6329161				
H	-5.1505020	4.6224833	0.4822516				
H	-5.1553971	0.4720309	-4.6204959				
H	-5.1448358	-4.6303727	-0.4698349				
H	-7.3340491	4.1130651	-0.4516771				
H	-7.3497046	2.5133438	0.2685321				
H	-7.3270023	0.4550510	4.1265679				
H	-7.3246737	-1.3000912	3.9433395				
H	-7.3278388	-3.9409803	-1.2857698				
H	-7.3466610	-2.5245028	-0.2509100				
H	-7.3362736	1.2889718	-3.9256602				
H	-7.3519456	0.2542916	-2.5090105				
H	-7.3453672	-0.2652191	2.5269047				
H	-7.3268546	-4.1241410	0.4693830				
H	-7.3364974	-0.4661989	-4.1086038				
H	-7.3304707	3.9297669	1.3034579				
H	-0.7785183	4.7918972	-2.0341548				
H	-0.7403521	4.2507903	2.9380653				
H	-0.7691369	2.0332683	4.7948255				
H	-0.7351549	-2.9394519	4.2579977				
H	-0.7660827	-4.7920047	2.0351607				
H	-0.7415470	-4.2535341	-2.9374423				
H	-0.7779114	-2.0343941	-4.7917985				
H	-0.7503157	2.9385384	-4.2568448				
H	2.0033905	1.6633535	4.2950711				
H	2.0056844	-4.2933635	1.6602280				
H	1.9952781	-1.6602035	-4.2992145				
H	1.9954473	4.2965283	-1.6664196				
H	2.0167619	3.2032639	-3.6164988				
H	3.0480608	5.8595999	-3.8622809				
H	4.0588981	4.4171789	-3.9833788				
H	2.8010215	4.7254531	-5.1908465				
H	2.0226639	-3.6093602	-3.2037300				
H	3.0470406	-3.8528769	-5.8631672				

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194							
Energy = -7807.618976761							
C	-3.6531587	2.2152177	-3.3147447				
C	-4.8319628	3.1280564	-0.9477101				
C	-4.7614354	1.5372887	-2.8138857				
C	-3.1647180	3.3421367	-2.6778846				
C	-3.7323229	3.7812090	-1.4956807				
C	-5.3174671	2.0207061	-1.6344449				
H	-2.3636976	3.9039745	-3.1337445				
H	-6.1776173	1.5055288	-1.2273132				
O	-3.2318436	4.9080051	-0.8830326				
C	-2.0268159	4.7878937	-0.2503189				
C	-2.0229322	4.6622997	1.1595588				
C	-1.8681186	1.1421083	-4.3726830				
C	-1.8758985	-0.2638533	-4.5188917				
O	-3.0736115	-0.8825654	-4.7561491				
C	-3.7267538	3.4333803	2.1840399				
C	-4.7366838	0.9644485	3.0306511				
C	-3.1511924	2.7698707	3.2525789				
C	-4.8239498	2.8937993	1.5196093				
C	-5.3013275	1.6692329	1.9745107				
C	-3.6285443	1.5344758	3.6497162				
H	-2.3471949	3.2331992	3.8038144				
H	-6.1598041	1.2390914	1.4755376				
C	-3.6546953	-1.5224660	-3.6871642				
C	-4.8241617	-2.8837796	-1.5431205				
C	-3.1576171	-2.7482774	-3.2817261				
C	-4.7626884	-0.9587537	-3.0617565				
C	-5.3159133	-1.6659538	-2.0003500				
C	-3.7199504	-3.4119386	-2.2063870				
H	-2.3519471	-3.2077910	-3.8337838				
H	-6.1776716	-1.2438751	-1.5002228				
O	-3.0292859	0.8941013	4.7081180				
O	-3.2128102	-4.6350893	-1.8309985				
C	-1.8302178	0.2842974	4.4576554				
C	-1.8191168	-1.1212798	4.3012928				
C	-2.0089470	-4.6471016	-1.1808121				
C	-2.0196444	-4.8001440	0.2264767				
C	-3.6160503	-2.2057654	3.2685098				
C	-4.8207601	-3.1304446	0.9216900				
C	-4.7316812	-1.5327247	2.7792699				
C	-3.1394680	-3.3399065	2.6378841				
C	-3.7203038	-3.7848966	1.4646542				
C	-5.3004769	-2.0209122	1.6089591				
H	-2.3341685	-3.8991971	3.0894339				
H	-6.1643569	-1.5069456	1.2080216				
O	-3.0108559	-1.7848805	4.4272173				
C	-5.3167264	-0.3475605	3.5235970				
H	-5.0204211	-0.4521701	4.5670132				
C	-5.4610573	3.6108312	0.3449609				
H	-5.2259083	4.6698894	0.4443712				
C	-5.3522568	0.3504790	-3.5523501				
H	-5.0659473	0.4545596	-4.5985470				
C	-5.4545363	-3.6092798	-0.3697948				
H	-5.2163800	-4.6669487	-0.4766739				
C	0.5037671	0.3218394	4.1444295				
C	0.5307420	-1.0645625	3.9757685				
C	0.4585938	-0.2947647	-4.1994991				
C	0.4839367	1.0941586	-4.0490397				
O	-3.0637089	1.8037675	-4.4851520				
O	-3.2286117	4.6610840	1.8070832				
O	-3.2274222	-4.9167968	0.8531997				

C	-6.9854767	3.5157744	0.3405405	C	2.3668298	4.4114683	0.4700235
H	-7.3935580	4.0906036	-0.4904111	C	2.5364613	-0.3689980	3.7749526
H	-7.3658082	2.4986980	0.2468202	C	2.3813667	-4.4552080	-0.4691253
C	-6.8452835	-0.3493770	3.5210343	C	2.4792944	0.3982355	-3.7926894
H	-7.2206182	0.4753027	4.1263830	N	1.6432544	4.3854674	1.5631181
H	-7.2190230	-1.2802946	3.9465638	N	1.7674327	1.4994191	-3.7986650
C	-6.9791511	-3.5195181	-0.3582992	N	1.8192416	-1.4681211	3.7424524
H	-7.3847760	-3.9226538	-1.2858214	N	1.6633560	-4.4147084	-1.5656558
H	-7.3629039	-2.5048966	-0.2525763	N	1.7975141	0.7341868	4.0166349
C	-6.8805176	0.3493824	-3.5343927	H	2.0877212	1.7290627	4.0524908
H	-7.2602632	1.2788944	-3.9576037	N	1.6410557	-4.6382246	0.6448746
H	-7.3115691	0.2488913	-2.5383223	H	1.9552734	-4.5309366	1.6320047
H	-7.2864487	-0.2483739	2.5294265	N	1.7473270	-0.7061497	-4.0425277
H	-7.3807910	-4.1034375	0.4693942	H	2.0383564	-1.6997183	-4.0468781
H	-7.2600632	-0.4769291	-4.1348169	N	1.6349438	4.5940826	-0.6487965
H	-7.3878317	3.9258635	1.2663742	H	1.9520856	4.4952660	-1.6370970
C	0.3655238	-4.5608291	-1.1490354	I	8.8544645	-0.3165124	3.1600605
C	0.3387992	-4.7048162	0.2414978	I	8.7171622	-4.0928184	-0.3995916
C	0.3500674	4.5431561	1.1391323	I	8.7742578	0.3297583	-2.9865627
C	0.3316364	4.6733858	-0.2529398	I	8.7021950	4.0665788	0.5313328
C	6.6313775	4.1733828	0.4986951	O	2.1556655	4.1445241	-3.2351338
C	5.8667537	3.2267290	1.1568310	H	2.0763907	3.1767142	-3.4268977
C	4.4876429	3.2833070	1.1224512	C	3.1734238	4.6934712	-4.0361609
C	3.8266855	4.3010803	0.4491445	H	3.2075786	5.7690414	-3.8659253
C	4.6041562	5.2407578	-0.2142478	H	4.1630112	4.2855518	-3.8006865
C	5.9852043	5.1807655	-0.1956092	H	2.9850353	4.5280798	-5.1006704
F	6.4512787	2.2375206	1.8178070	O	2.0245465	-3.4045571	-4.0982257
F	3.7996260	2.3270943	1.7328449	H	1.9597676	-3.8005634	-3.1991073
F	4.0190352	6.2392667	-0.8643821	C	2.9215835	-4.1600346	-4.8752279
F	6.6782039	6.1069127	-0.8393724	H	2.9274332	-3.7568040	-5.8870255
C	6.6462931	-4.2040269	-0.4104177	H	3.9480098	-4.1221705	-4.4941014
C	5.8931053	-3.2618728	-1.0880162	H	2.6224398	-5.2104771	-4.9350502
C	4.5135689	-3.3270478	-1.0898621	O	2.1654266	-4.1398754	3.2263066
C	3.8410257	-4.3455650	-0.4285914	H	2.1098765	-3.1678718	3.3968009
C	4.6076493	-5.2802156	0.2551641	C	3.1453837	-4.7026811	4.0643798
C	5.9883387	-5.2139117	0.2690682	H	3.1509672	-5.7818432	3.9151709
F	6.4884012	-2.2723382	-1.7378507	H	4.1523065	-4.3292642	3.8465424
F	3.8369295	-2.3775780	-1.7223548	H	2.9347520	-4.5107998	5.1201721
F	4.0127700	-6.2790884	0.8957422	O	2.0550980	3.4251580	4.1022391
F	6.6701104	-6.1362577	0.9300739	H	1.9582836	3.8074946	3.1988635
C	6.7163748	0.3380842	-3.2443006	C	2.9729983	4.1970562	4.8375320
C	5.8985276	1.0207734	-2.3619800	H	3.0145224	3.8101727	5.8548607
C	4.5262417	1.0297789	-2.5265169	H	3.9866904	4.1588010	4.4232424
C	3.9270176	0.3564599	-3.5829176	H	2.6702215	5.2467642	4.8906307
C	4.7585535	-0.3355021	-4.4538875	C	0.6400354	-0.9945879	-0.1137386
C	6.1308324	-0.3500168	-4.2915272	C	-0.7461573	-1.2528132	0.4471428
F	6.4278607	1.6750423	-1.3365437	C	-1.2946580	0.9725889	0.1425576
F	3.7867076	1.6871615	-1.6439425	C	0.0871755	1.2381366	-0.4277708
F	4.2359095	-0.9830301	-5.4893767	H	-1.4131349	-1.5986509	-0.3579815
F	6.8754233	-1.0183935	-5.1585792	H	-0.7090586	-2.0342177	1.2074417
C	6.7904403	-0.3275724	3.3590834	H	1.3398388	-0.7965298	0.7121707
C	6.1744148	0.3633142	4.3869208	H	1.0016519	-1.8677107	-0.6586618
C	4.7975492	0.3565557	4.5055733	H	-2.0001287	0.7626060	-0.6759931
C	3.9903120	-0.3322800	3.6094580	H	-1.6582563	1.8511401	0.6781442
C	4.6221153	-1.0132281	2.5770378	H	0.0329526	2.0032546	-1.2036573
C	5.9982954	-1.0094602	2.4527756	H	0.7511551	1.6052250	0.3712059
F	6.8936179	1.0289816	5.2768398	O	-1.2600975	-0.0959860	1.0592538
F	4.2459815	1.0076728	5.5234071	O	0.6270071	0.0812974	-1.0217824
F	3.9073999	-1.6704807	1.6717347				
F	6.5546409	-1.6657499	1.4438098				
C	-0.8490962	4.8235009	-0.9679755	dithiane@I-RA4			
H	-0.8435568	4.9618547	-2.0394900				
C	-0.8401295	4.5693938	1.8624631	194			
C	-0.8300671	4.5104792	2.9415750	Energy = -8453.027063292			
H	-0.6668180	1.0190452	4.4083123	C	-3.6503209	2.2564341	-3.3776099
H	-0.6584000	2.0865704	4.5736991	C	-4.7554230	3.1479145	-0.9639346
C	-0.6442052	-1.8060426	4.0826257	C	-4.7458521	1.5770979	-2.8502779
H	-0.6239641	-2.8841622	4.0055584	C	-3.1373902	3.3725485	-2.7387419
C	-0.8461204	-4.8600544	0.9483264	C	-3.6649468	3.8015296	-1.5326514
H	-0.8478499	-5.0181092	2.0171557	C	-5.2641544	2.0510082	-1.6504804
C	-0.8226018	-4.5572386	-1.8777430	H	-2.3402487	3.9334002	-3.2043774
H	-0.8068150	-4.4809095	-2.9558421	H	-6.1136418	1.5339396	-1.2238219
C	-0.7086635	-0.9950995	-4.4612211	O	-3.1288308	4.9135642	-0.9222635
H	-0.6976461	-2.0643621	-4.6136315	C	-1.9226279	4.7432586	-0.2949556
C	-0.6916170	1.8312911	-4.1638066	C	-1.9175119	4.5570411	1.1074231
H	-0.6743200	2.9099161	-4.0941161	C	-1.8922117	1.1947472	-4.4897367

C	-1.8987493	-0.2177126	-4.5767114	F	4.2937373	5.8475859	-0.8300422
D	-3.0978446	-0.8471410	-4.7652940	F	6.9345469	5.5142602	-0.6745506
C	-3.6442449	3.3901081	2.1693891	C	6.6033791	-3.5817259	-0.5493236
C	-4.7363980	0.9735400	3.0560145	C	5.7209110	-2.6436202	-1.0551995
C	-3.0982307	2.7338203	3.2577385	C	4.3569163	-2.8440088	-0.9770740
C	-4.7565228	2.8758469	1.5106028	C	3.8331550	-3.9892877	-0.3924614
C	-5.2750980	1.6747269	1.9828124	C	4.7254237	-4.9087061	0.1377637
C	-3.6193219	1.5234547	3.6759938	C	6.0925442	-4.7135042	0.0612777
H	-2.2899853	3.1878637	3.8100597	F	6.1755333	-1.5317990	-1.6178692
H	-6.1472574	1.2644648	1.4905861	F	3.5472464	-1.9067311	-1.4522376
C	-3.6577275	-1.4765582	-3.6780191	F	4.2640640	-6.0157069	0.7064827
C	-4.8031307	-2.8134979	-1.5065510	F	6.9046162	-5.6293895	0.5652022
C	-3.1455911	-2.6904796	-3.2558442	C	6.7510672	0.5180774	-3.7804685
C	-4.7674904	-0.9137276	-3.0560099	C	5.9779501	1.2976183	-2.9398457
C	-5.3103324	-1.6081088	-1.9797950	C	4.5987326	1.2630157	-3.0084145
C	-3.6959365	-3.3393182	-2.1651531	C	3.9421842	0.4681134	-3.9392357
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214

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C	-3.6816696	-3.3404090	-4.2996823				
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H	-3.8369614	-4.3449517	-4.7041015				
H	-4.3342592	-3.2183854	-3.4297239				
C	-1.7734140	5.1888721	-4.4294621				
H	-2.8421000	5.1767227	-4.6709109				
H	-1.4762690	6.2296068	-4.3029844				
H	-1.2289741	4.7880430	-5.2897676				

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214

Energy = -6057.604907236

C	3.9357309	3.8120482	-1.3251695
C	5.0013634	1.6619258	-2.7622905
C	5.0345814	3.1373132	-0.8042035
C	3.3890339	3.4420740	-2.5404736
C	3.8976354	2.3617279	-3.2392233
C	5.5378375	2.0797940	-1.5510345
H	2.5840100	4.0229102	-2.9662113
H	6.3904295	1.5406406	-1.1589600
O	3.3234663	2.0153454	-4.4411487
C	2.1130647	1.3770792	-4.3847590
C	2.0974899	-0.0286213	-4.5294199
C	2.2044911	4.7603397	-0.0486905
C	2.1868330	4.5310915	1.3466702
O	3.3878978	4.4698110	1.9970793
C	3.8564731	-1.3434048	-3.7003502
C	5.0211671	-2.7998809	-1.6183982
C	3.3463053	-2.5765432	-3.3407928
C	4.9797346	-0.8207338	-3.0674530
C	5.5263520	-1.5704647	-2.0315997
C	3.9109564	-3.2902667	-2.2998466
H	2.5332820	-3.0050750	-3.9068669
H	6.3985130	-1.1792969	-1.5238865
C	3.8868332	3.2308397	2.3196829
C	4.9491225	0.7643087	3.1027522
C	3.3146851	2.5220204	3.3598800
C	5.0034949	2.7398840	1.6498291
C	5.5041270	1.5117777	2.0691647
C	3.8242176	1.2906843	3.7300326
H	2.4990244	2.9546574	3.9189575
H	6.3783283	1.1186293	1.5667055
O	3.4102279	-4.5311355	-1.9834356
O	3.2460642	0.6099198	4.7746192
C	2.2030003	-4.5843136	-1.3430475
C	2.2043734	-4.8131376	0.0515103
C	2.0545659	-0.0161184	4.5301133
C	2.0603478	-1.4205954	4.3777180
C	3.9219911	-3.8785282	1.3474861
C	4.9655790	-1.7176558	2.7916942
C	5.0259818	-3.2002787	0.8359171
C	3.3601791	-3.5031108	2.5553155
C	3.8554135	-2.4179700	3.2576242
C	5.5192508	-2.1394447	1.5877606
H	2.5499386	-4.0822403	2.9734025
H	6.3775898	-1.6018762	1.2063617
O	3.4121797	-4.9654446	0.6773099
C	5.6508903	-3.5953843	-0.4887402
H	5.4086513	-4.6437343	-0.6596843
C	5.5870669	0.4920080	-3.5286604

H	5.3069898	0.6209535	-4.5737191	C	-4.5632660	-1.4527138	4.8035852
C	5.6446325	3.5332777	0.5262886	C	-3.6846834	-4.6222253	-0.7090291
H	5.4015452	4.5819339	0.6946163	C	-4.4313598	-3.7545504	0.0904852
C	5.5476574	-0.5513849	3.5671708	C	-4.3455073	-5.5260266	-1.5506533
H	5.2558245	-0.6832812	4.6086020	C	-5.8175038	-3.8144461	-0.0330141
C	-0.1736662	-4.5471373	-1.3360531	H	-6.4324694	-3.1440398	0.5608953
C	-0.1566962	-4.7636000	0.0449713	C	-3.6587563	-0.8771157	-1.9053353
C	-0.1895413	4.5425227	1.3208677	H	-3.3517945	-1.8476349	-2.2957136
C	-0.1579785	4.7615396	-0.0589155	H	-2.7624051	-0.3815139	-1.5366472
O	3.4181045	4.9011001	-0.6600629	H	-4.3017387	-1.0711740	-1.0490179
O	3.2878515	-0.6624807	-4.7495770	C	-3.9439003	2.2908450	-5.8967706
O	3.2664866	-2.0709642	4.4500577	H	-4.7179562	2.5879305	-6.6030767
C	7.1148833	0.4753718	-3.5030336	H	-3.4761252	3.1979909	-5.5171144
H	7.5051310	1.4094595	-3.9060648	H	-3.1775543	1.7483913	-6.4499103
H	7.5396775	0.3527369	-2.5067046	C	-3.8950261	2.8788781	-1.0854351
C	7.1758407	-3.5116295	-0.4762092	H	-3.5856470	3.3480977	-2.0196205
H	7.5764641	-3.8619476	-1.4269897	H	-3.0252260	2.3634304	-0.6787418
H	7.5785729	-4.1435682	0.3148619	H	-4.6352001	2.1249184	-1.3459077
C	7.0756564	-0.5404380	3.5568866	C	-3.5854507	6.6220880	2.3673595
H	7.4469035	0.2721600	4.1807157	H	-3.0969221	6.1503899	3.2180574
H	7.5110381	-0.4108607	2.5660973	H	-2.8071200	7.1344668	1.8020632
C	7.1697766	3.4497747	0.5324054	H	-4.2683087	7.3784084	2.7524566
H	7.5601349	3.7994642	1.4878070	C	-3.6321218	-6.5488299	-2.3839924
H	7.5810799	4.0822872	-0.2537409	H	-4.3405184	-7.2754650	-2.7799830
H	7.5634916	-2.5058645	-0.3145007	H	-3.1070515	-6.1022202	-3.2262738
H	7.4592758	-1.4783266	3.9574637	H	-2.8878791	-7.0937515	-1.8031565
H	7.5594716	2.4443618	0.3733337	C	-3.8227122	-2.7862133	1.0548613
H	7.4908759	-0.3426374	-4.1170907	H	-3.5922886	-3.2653478	2.0070058
C	-0.2893919	-0.0121874	4.2603502	H	-2.9007124	-2.3324392	0.6890757
C	-0.3061742	-1.4041435	4.1361110	H	-4.5244921	-1.9850283	1.2792229
C	-0.2507152	-0.0096601	-4.3022111	C	-3.9607934	-2.2966991	5.8861334
C	-0.2555863	1.3818414	-4.1752589	H	-4.7219392	-2.5864373	6.6094332
C	-2.2246662	4.6447044	0.6673964	H	-3.5171178	-3.2084422	5.4893746
C	-2.2897207	0.7356295	-4.0157815	H	-3.1725027	-1.7701981	6.4234177
C	-2.3334506	-0.7400059	3.9830459	C	-3.7410843	0.9111877	1.9205233
C	-2.2130211	-4.6025915	-0.6940127	H	-2.8733745	0.3900082	1.5180008
C	1.0312418	4.8989510	-0.7634835	H	-4.4114684	1.1412644	1.0936533
H	1.0364126	5.1051158	-1.8243521	H	-3.3936829	1.8638486	2.3213859
C	0.9981975	4.4416594	2.0412314	C	-5.7193787	5.6338472	1.5238506
H	0.9826764	4.3159982	3.1148807	H	-6.2493671	6.3369319	2.1590968
C	0.9425537	2.0914574	-4.2322717	N	-6.4697955	4.8294597	0.7914076
H	0.9499517	3.1702172	-4.1590542	N	-6.5813031	-0.6466255	3.7852262
C	0.9139878	-0.7358590	-4.5065753	N	-6.4589634	-4.6421746	-0.8364147
H	0.8885688	-1.8066721	-4.6472093	N	-6.5298011	0.6865010	-3.7165093
C	0.8769670	0.7020572	4.4855516	C	-5.9471770	-1.3781168	4.6844241
H	0.8570301	1.7716310	4.6351128	H	-6.5717603	-1.9448961	5.3681796
C	0.8847464	-2.1242458	4.2058724	C	-5.7348628	-5.4771330	-1.5620587
H	0.8830230	-3.2032179	4.1325906	H	-6.2872068	-6.1632196	-2.1969281
C	1.0232007	-4.9275855	0.7577753	C	-5.8475484	0.0655685	2.9497267
H	1.0143918	-5.1341138	1.8185368	H	-6.3893328	0.6595196	2.2193592
C	1.0208119	-4.4745457	-2.0470025	C	-5.9119981	1.4041175	-4.6385738
H	1.0169223	-4.3511292	-3.1209068	H	-6.5485370	1.9714156	-5.3107394
N	-1.4722131	-4.4520951	-1.7675192	O	-1.9906763	-3.1073566	-4.1521665
N	-1.6001536	-1.8309230	3.9689096	H	-1.8387602	-3.6089469	-3.3173655
N	-1.5458608	1.8198559	-4.0006462	O	-1.5631575	4.4961335	-3.2176511
N	-1.4928871	4.4747935	1.7437071	H	-1.6595386	3.5530694	-3.4859961
N	-1.4696748	4.8177169	-0.4450420	O	-1.9824378	3.1195653	4.1327819
H	-1.7694832	4.8506279	-1.4239179	H	-1.8476596	3.6192275	3.2953659
N	-1.5590575	-0.3892194	-4.1956099	O	-1.5920816	-4.5034391	3.1869906
H	-1.8788499	-1.3705482	-4.1884660	H	-1.7034369	-3.5600764	3.4502320
N	-1.4705429	-4.7939872	0.4218425	C	-2.9926283	-3.7479240	-4.9050571
H	-1.7772085	-4.8131515	1.4001952	H	-3.1877979	-3.1516110	-5.7963210
N	-1.5916342	0.3781044	4.1563665	H	-2.6836275	-4.7444997	-5.2361799
H	-1.9021302	1.3600644	4.1512585	H	-3.9346763	-3.8456104	-4.3555365
C	-3.6958751	4.7101547	0.6775046	C	-1.9256614	5.3274759	-4.2930009
C	-4.4717697	3.8714845	-0.1259650	H	-3.0011987	5.3077301	-4.4999580
C	-4.3286320	5.6323576	1.5204120	H	-1.6566853	6.3535373	-4.0430010
C	-5.8549034	3.9800013	-0.0102656	H	-1.3989129	5.0606891	-5.2142867
H	-6.4906493	3.3326888	-0.6076643	C	-2.9376545	3.7882055	4.9206991
C	-3.7571366	0.7101327	-3.9039332	H	-3.8980186	3.9070707	4.4080557
C	-4.3911759	-0.0614745	-2.9257101	H	-3.1127115	3.2007494	5.8218259
C	-4.5311804	1.4629816	-4.7938181	H	-2.5915505	4.7783966	5.2342865
C	-5.7827892	-0.0249744	-2.8923359	C	-2.0309977	-5.3360879	4.2320599
H	-6.3117386	-0.6072474	-2.1433964	H	-3.1167997	-5.3022563	4.3733782
C	-3.8031066	-0.6998310	3.9015403	H	-1.7615279	-6.3643109	3.9914524
C	-4.4557678	0.0901208	2.9495439	H	-1.5574529	-5.0827167	5.1855998

C	2.2707150	-0.5693442	0.6202124
C	1.0558817	-1.4686126	0.5440698
C	-0.3584741	0.5867263	-0.6616858
C	0.8694599	1.4666281	-0.5744075
H	1.0568187	-2.0353146	-0.3884466
H	1.0672498	-2.1794979	1.3708910
H	2.2766566	-0.0014321	1.5522225
H	3.1771678	-1.1752525	0.5943682
H	-0.3647385	0.0418645	-1.6064506
H	-1.2582492	1.2056507	-0.6240851
H	0.8510511	2.1976115	-1.3835932
H	0.8847564	2.0133880	0.3706015
S	-0.5088671	-0.5766521	0.7181688
S	2.4141216	0.5570597	-0.7857658

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Energy = -13219.87149054

C	-13.1467744	2.4098662	-3.2404167
C	-14.3189899	3.1808765	-0.8212052
C	-14.2556350	1.7051751	-2.7797214
C	-12.6530213	3.4933537	-2.5361471
C	-13.2147954	3.8594329	-1.3272221
C	-14.8098961	2.1196062	-1.5735058
H	-11.8486507	4.0782701	-2.9555474
H	-15.6713718	1.5835689	-1.1967241
O	-12.7033946	4.9398934	-0.6450836
C	-11.4997588	4.7701497	-0.0187551
C	-11.5001160	4.5594981	1.3805013
C	-11.3625790	1.3941150	-4.3443800
C	-11.3717986	-0.0003438	-4.5686592
O	-12.5682660	-0.6034249	-4.8528150
C	-13.2231992	3.2883395	2.3272062
C	-14.2661930	0.7875891	3.0300030
C	-12.6642785	2.5616647	3.3622612
C	-14.3232435	2.7991337	1.6291213
C	-14.8168860	1.5565372	2.0120343
C	-13.1584437	1.3121740	3.6881363
H	-11.8588913	2.9858862	3.9421450
H	-15.6762475	1.1640014	1.4840091
C	-13.1525764	-1.3023171	-3.8234042
C	-14.3265051	-2.7809524	-1.7617060
C	-12.6543642	-2.5475892	-3.4834598
C	-14.2615404	-0.7737376	-3.1698263
C	-14.8175617	-1.5397373	-2.1516764
C	-13.2171908	-3.2695105	-2.4468863
H	-11.8460863	-2.9761393	-4.0563332
H	-15.6808965	-1.1465006	-1.6308847
O	-12.5728066	0.6065984	4.7117021
O	-12.7077283	-4.5098205	-2.1385512
C	-11.3762961	0.0055243	4.4265802
C	-11.3702756	-1.3888822	4.1968965
C	-11.5093087	-4.5603685	-1.4777373
C	-11.5348365	-4.7981923	-0.0830480
C	-13.1644716	-2.4008416	3.0988302
C	-14.3438459	-3.1742967	0.6857603
C	-14.2703424	-1.6924509	2.6379298
C	-12.6840310	-3.4953190	2.4043730
C	-13.2504986	-3.8637607	1.1986163
C	-14.8277252	-2.1069159	1.4339558
H	-11.8846320	-4.0836819	2.8285308
H	-15.6842484	-1.5648666	1.0543191
O	-12.5660931	-2.0539575	4.2853070
C	-14.8566356	-0.5475840	3.4425388
H	-14.5702685	-0.7124469	4.4809097
C	-14.9476280	3.5902131	0.4964038
H	-14.7025297	4.6390376	0.6599243
C	-14.8472880	0.5631608	-3.5855277
H	-14.5588632	0.7261207	-4.6235627
C	-14.9651656	-3.5739620	-0.6379122
H	-14.7252040	-4.6233003	-0.8057381
C	-9.0464315	0.0539630	4.0944832
C	-9.0219084	-1.3227765	3.8595571
C	-9.0448677	-0.0590486	-4.2029199
C	-9.0178761	1.3193754	-3.9747485

O	-12.5555897	2.0658931	-4.4315686
O	-12.7087826	4.5289958	2.0235366
O	-12.7501451	-4.9540564	0.5225783
C	-16.4729069	3.5112662	0.4805705
H	-16.8714026	4.1399687	-0.3153211
H	-16.8629679	2.5057754	0.3231394
C	-16.3850364	-0.5421133	3.4259888
H	-16.7627323	0.2492360	4.0729933
H	-16.7667522	-1.4937175	3.7950158
C	-16.4899804	-3.4857636	-0.6338260
H	-16.8876832	-3.8315598	-1.5876074
H	-16.8752283	-2.4795571	-0.4693357
C	-16.3755799	0.5646748	-3.5699188
H	-16.7524995	1.5175165	-3.9405925
H	-16.8080827	0.4095708	-2.5814705
H	-16.8160713	-0.3835947	2.4374023
H	-16.8978022	-4.1192124	0.1534735
H	-16.7563505	-0.2257730	-4.2161723
H	-16.8751442	3.8680230	1.4283437
C	-9.1330479	-4.4985541	-1.4193444
C	-9.1752278	-4.7220941	-0.0396062
C	-9.1249318	4.4491898	1.3616948
C	-9.1398132	4.6607617	-0.0204576
C	12.5223771	3.7977548	-1.5826506
C	13.5249009	1.5259885	-2.8768487
C	13.6182156	3.1403477	-1.0331664
C	11.9530514	3.3551918	-2.7631066
C	12.4274602	2.2140174	-3.3855918
C	14.0887072	2.0188979	-1.7067006
H	11.1535306	3.9198315	-3.2196715
H	14.9423592	1.4979959	-1.2933059
O	11.8256501	1.7905915	-4.5469929
C	10.6286867	1.1406100	-4.4033232
C	10.6222430	-0.2686167	-4.4983904
C	10.8242778	4.8294058	-0.3285989
C	10.8335792	4.6905324	1.0802614
O	12.0440980	4.6574106	1.7148492
C	12.3998753	-1.5447891	-3.6871802
C	13.6034958	-2.9024286	-1.5650008
C	11.9100595	-2.7709961	-3.2760444
C	13.5184674	-0.9797866	-3.0837013
C	14.0885736	-1.6849273	-2.0314822
C	12.4894953	-3.4329664	-2.2086441
H	11.0979739	-3.2335475	-3.8164328
H	14.9595701	-1.2637517	-1.5470084
C	12.5421993	3.4317264	2.0921323
C	13.5931864	0.9843938	2.9556374
C	11.9814411	2.7713020	3.1702869
C	13.6443579	2.9016511	1.4284605
C	14.1405799	1.6867189	1.8881915
C	12.4841936	1.5487383	3.5796005
H	11.1780740	3.2325497	3.7246533
H	15.0032156	1.2660594	1.3885952
O	11.9864097	-4.6552990	-1.8208452
O	11.9150307	0.9162860	4.6585069
C	10.7918702	-4.6721141	-1.1540815
C	10.8200334	-4.8036009	0.2551783
C	10.7250910	0.2765583	4.4471826
C	10.7341047	-1.1332476	4.3586821
C	12.5457674	-3.7721773	1.4671603
C	13.5965206	-1.5165797	2.7489790
C	13.6384951	-3.1256635	0.8983527
C	11.9995894	-3.3255845	2.6563759
C	12.5031406	-2.1963720	3.2784794
C	14.1323203	-2.0097560	1.5643129
H	11.2033733	-3.8833215	3.1258272
H	14.9826033	-1.4957046	1.1357791
O	12.0355198	-4.9030921	0.8707959
C	14.2499867	-3.6208359	-0.3973695
H	14.0056269	-4.6783952	-0.4895027
C	14.1037911	0.3226372	-3.5979215
H	13.8100753	0.4093646	-4.6436790
C	14.2636412	3.6253199	0.2496866
H	14.0252909	4.6829675	0.3552179
C	14.1933042	-0.3156841	3.4597933
H	13.9218772	-0.4025633	4.5114712

C	8.4112563	-4.6728110	-1.1033800	H	-10.3814649	-5.1284255	1.7030122
C	8.4582638	-4.8025450	0.2874081	C	-10.3148474	-4.4369302	-2.1566025
C	8.4556291	4.7161488	1.0989030	H	-10.2881333	-4.2965309	-3.2281787
C	8.4605249	4.8404842	-0.2928702	C	-10.2074911	-0.7380724	-4.5298293
O	12.0236568	4.9301180	-0.9761776	H	-10.1951774	-1.7972909	-4.7404495
O	11.8051973	-0.9047634	-4.7481201	C	-10.1877610	2.0660788	-4.0746424
O	11.9388346	-1.7780542	4.4597386	H	-10.1684786	3.1388686	-3.9440437
C	15.6324891	0.3193222	-3.5933384	C	-7.0998455	4.3987553	0.6979047
H	16.0096767	1.2402554	-4.0369643	C	-7.0164823	-0.6188356	3.6766124
H	16.0721993	0.2370527	-2.5993920	C	-7.1192046	-4.4789440	-0.7189935
C	15.7749542	-3.5375833	-0.4096393	C	-7.0323942	0.5994260	-3.7083097
H	16.1640237	-3.9520151	-1.3391513	C	6.4069428	4.7790006	0.4784377
H	16.1870240	-4.1150550	0.4173970	C	6.2764028	0.4652865	-3.7274646
C	15.7211871	-0.3114840	3.4207900	C	6.3536616	-0.4842526	3.8630534
H	16.1075196	0.5272689	3.9991820	C	6.3832598	-4.7376200	-0.4164227
H	16.1385621	-0.2310130	2.4171325	C	9.6367741	4.9190602	-1.0283283
C	15.7882056	3.5374307	0.2230617	H	9.6220578	5.0539955	-2.1001710
H	16.2023655	3.9450850	1.1447849	C	9.6576034	4.6538906	1.8004754
H	16.1806498	4.1188260	-0.6106856	H	9.6641279	4.5986601	2.8801270
H	16.1648125	-2.5237162	-0.3207307	C	9.4626758	1.8478933	-4.2014950
H	16.1084148	-1.2314561	3.8576591	H	9.4613093	2.9280445	-4.1611183
H	16.1726680	2.5231046	0.1173235	C	9.4517425	-0.9864949	-4.3822102
H	16.0061208	-0.5182092	-4.1818172	H	9.4332914	-2.0607971	-4.4911340
C	8.3856162	0.2611468	4.1604946	C	9.5465207	0.9889262	4.3681331
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C	-4.9158661	3.3658472	1.3354898	C	9.5944229	-4.6236039	-1.8393731
C	-5.6353534	4.3553925	0.6784943	H	9.5720271	-4.5729331	-2.9190537
C	-4.9068474	5.3515032	0.0404954	N	7.1013248	-4.6322277	-1.5113184
C	-3.5261821	5.3708232	0.0731708	N	7.0870565	-1.5734226	3.9129341
F	-2.9002219	2.4302690	2.0376889	N	6.9994078	1.5596178	-3.8039214
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F	-2.8899942	6.3570101	-0.5458020	N	-7.7388335	1.7036322	-3.6724957
C	-2.8373516	-4.4505574	-0.6453146	N	-7.7348371	-1.7153855	3.5991515
C	-3.5420081	-3.4496559	-1.2902369	N	-7.8282667	-4.3584256	-1.8166848
C	-4.9244064	-3.4358394	-1.2926009	N	-7.7549220	0.4715892	3.9731410
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C	-4.9401274	-5.4256691	-0.0034757	N	-7.8757325	-4.7058598	0.3765732
C	-3.5588498	-5.4333978	0.0082543	H	-7.5706771	-4.6602392	1.3712160
F	-2.8956834	-2.4799990	-1.9233266	N	-7.7622730	-0.4842684	-4.0392066
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F	-5.5866615	-6.4129058	0.6092109	N	-7.8332757	4.6286524	-0.4123700
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C	-2.8092846	0.4246022	-3.0692077	N	7.1415167	4.8802167	-0.6566369
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C	-5.0035393	1.1211773	-2.3568555	N	7.0043952	-0.6571184	-3.9162738
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C	-4.7563717	-0.1259161	-4.3613838	N	7.1529009	-4.8423420	0.6938941
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C	-5.5640948	-0.5630748	3.5138345	C	4.1752736	3.9174301	-0.2551735
C	-4.9132081	-1.2104608	2.4712109	C	4.2820557	5.6648885	1.4082431
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F	-5.6123496	-1.8661716	1.5510868	C	4.3519288	-0.2864571	-2.3495613
F	-2.9629463	-1.8146157	1.3428050	C	3.9384141	1.0788053	-4.3026868
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H	-10.3107554	5.0513751	-1.7903985	H	2.5552510	-0.8033350	-1.2883999
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C	-10.1979017	-2.0653792	3.9372355	C	4.1686407	-3.9053094	0.4048877
H	-10.1810515	-3.1382312	3.8057384	C	4.2385200	-5.6238855	-1.2923786
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H	2.1746265	-3.2465174	0.8538155	H	-6.3216911	4.6951294	-4.8159156
C	5.2447458	-0.9664988	-1.3592682	O	-7.4926974	-3.1804406	-4.2742436
H	5.5861979	-1.9403408	-1.7090595	H	-7.5395148	-3.6330473	-3.4008622
H	6.1304007	-0.3741649	-1.1299960	C	-6.5699135	-3.8554517	-5.0934266
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C	4.3734419	1.8430172	-5.5152159	H	-5.5473825	-3.8140075	-4.7030672
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C	4.7527810	2.9895220	-1.2743148	C	-6.3631542	-4.9378654	3.7614627
H	4.9507624	3.5040573	-2.2145195	H	-6.3456534	-6.0111591	3.5753784
H	5.6859207	2.5245663	-0.9555898	H	-5.3760713	-4.5371224	3.5050610
H	4.0441571	2.1964957	-1.4964216	H	-6.5218868	-4.7851393	4.8328988
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H	4.9628737	-3.5444109	2.3642808	C	-9.1818005	1.2443670	-0.3605993
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C	4.5827905	-2.0007755	5.6824926	H	-8.1256588	-0.9239214	0.7217674
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Energy = -14510.68453508

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H	-14.6336186	-0.6205870	4.5976431	H	11.1907610	-3.9836289	3.1297626
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O	-12.6935942	4.4881297	1.9352192	C	8.4260157	-4.7236123	0.2251593
O	-12.7155277	-4.9095645	0.7141713	C	8.3881018	4.5338695	1.1960639
C	-16.4858515	3.5062328	0.4749358	C	8.4113543	4.7207415	-0.1878877
H	-16.8830933	4.1369956	-0.3198535	O	11.9814489	4.8587781	-0.8137646
H	-16.8859541	2.5039901	0.3215027	O	11.8779804	-0.8217852	-4.7573094
C	-16.4372269	-0.4956307	3.5168646	O	11.9467917	-1.9368432	4.5418941
H	-16.8270331	0.3150741	4.1320961	C	15.6935627	0.3671353	-3.5341976
H	-16.8175691	-1.4363903	3.9138211	H	16.0821928	1.2908490	-3.9618213
C	-16.4748367	-3.4997900	-0.4678754	H	16.1186056	0.2713912	-2.5350783
H	-16.8727067	-3.8584023	-1.4169667	C	15.7582247	-3.5340223	-0.4008174
H	-16.8802581	-2.5012560	-0.3042008	H	16.1466846	-3.9202494	-1.3426208
C	-16.4780813	0.5077667	-3.5003409	H	16.1646312	-4.1409938	0.4076664
H	-16.8669509	1.4461534	-3.8946449	C	15.7366307	-0.4323138	3.5210934
H	-16.8856867	0.3867570	-2.4967107	H	16.1213975	0.3978332	4.1127151
H	-16.8578277	-0.3744860	2.5185812	H	16.1494190	-0.3311956	2.5174135
H	-16.8626213	-4.1380140	0.3255734	C	15.7536759	3.4783793	0.3914908
H	-16.8722444	-0.3056669	-4.1090279	H	16.1485333	3.8588072	1.3331611
H	-16.8791331	3.8684897	1.4244236	H	16.1511532	4.0931928	-0.4154552
C	-9.1153492	-4.2881498	-1.2101874	H	16.1545971	-2.5261253	-0.2785352
C	-9.1493249	-4.5595134	0.1606170	H	16.1300243	-1.3580431	3.9399096
C	-9.1356955	4.2729920	1.1837186	H	16.1532250	2.4732331	0.2569743
C	-9.1680487	4.5483138	-0.1867639	H	16.0711196	-0.4659450	-4.1265401
C	12.5051476	3.7558492	-1.4511875	C	8.3973368	0.1281466	4.3610597
C	13.5756710	1.5680643	-2.8262879	C	8.3734923	-1.2654207	4.2622637
C	13.6111887	3.1050017	-0.9163468	C	8.3333380	-0.1804359	-4.3692347
C	11.9543752	3.3461235	-2.6519948	C	8.3192916	1.2116404	-4.2557960
C	12.4664138	2.2476683	-3.3194251	C	-2.8478444	4.1120752	0.5467290
C	14.1160583	2.0264449	-1.6314691	C	-3.5854787	3.1175705	1.1640659
H	11.1442929	3.9095723	-3.0914221	C	-4.9668775	3.1171497	1.1126828
H	14.9751258	1.5062181	-1.2283906	C	-5.6661295	4.1191572	0.4509390
O	11.8947354	1.8634009	-4.5112332	C	-4.9149915	5.0998821	-0.1841215
C	10.6893302	1.2197601	-4.4470184	C	-3.5346270	5.0950931	-0.1418432
C	10.6830180	-0.1893978	-4.5689495	F	-2.9729617	2.1416297	1.8233539
C	10.7737059	4.7260589	-0.1911160	F	-5.6205395	2.1264831	1.7106384
C	10.7654166	4.5304054	1.2106747	F	-5.5252982	6.0960880	-0.8192210
O	11.9701519	4.4987708	1.8550301	F	-2.8778773	6.0718589	-0.7547959
C	12.4387779	-1.4639018	-3.6785831	C	-2.8252527	-4.1051224	-0.5407216
C	13.5979199	-2.8467103	-1.5452988	C	-3.5636930	-3.1063584	-1.1509984
C	11.9220965	-2.6803002	-3.2729215	C	-4.9459475	-3.1160755	-1.1125883
C	13.5596847	-0.9189828	-3.0610530	C	-5.6420341	-4.1346533	-0.4730987
C	14.1050495	-1.6332854	-2.0000287	C	-4.8911889	-5.1195621	0.1551977

C	-3.5109168	-5.1036910	0.1269057	H	-7.5436542	-4.5244715	1.5681691
F	-2.9516535	-2.1175454	-1.7902837	N	-7.8589648	-0.4141405	-4.2095641
F	-5.6053042	-2.1214472	-1.6960234	H	-7.5556919	-1.4061439	-4.1773783
F	-5.5029227	-6.1269605	0.7713744	N	-7.8704676	4.5100494	-0.5997641
F	-2.8528756	-6.0837895	0.7330389	H	-7.5744509	4.5142441	-1.5958169
C	-2.8654381	0.5756410	-3.6374127	N	7.0979179	4.7430900	-0.5711892
C	-3.6392739	1.2460055	-2.7071909	H	6.7979289	4.7546723	-1.5488757
C	-5.0175272	1.2807580	-2.8160830	N	7.0279535	-0.5677094	-4.2586375
C	-5.6695107	0.6483724	-3.8653893	H	6.7301112	-1.5521265	-4.2389269
C	-4.8856621	-0.0327189	-4.7868860	N	7.1146086	-4.7317574	0.6118449
C	-3.5101624	-0.0731609	-4.6749972	H	6.8198849	-4.7315215	1.5927123
F	-3.0632245	1.8735745	-1.6889454	N	7.0974555	0.5233281	4.2497951
F	-5.7163335	1.9203265	-1.8861014	H	6.8003003	1.5076450	4.2277719
F	-5.4617745	-0.6416933	-5.8192977	I	-0.7106503	-0.4812921	3.5371070
F	-2.8146611	-0.7280028	-5.5960750	I	-0.7352399	-4.1572277	-0.6312379
C	-2.8001165	-0.4938562	3.6396206	I	-0.7777211	0.5554562	-3.5158970
C	-3.4521689	0.1677191	4.6642831	I	-0.7599502	4.1734273	0.6565671
C	-4.8288129	0.1346800	4.7655146	C	4.8757141	4.5453979	0.5529905
C	-5.6084959	-0.5527927	3.8446071	C	4.1680095	3.6650777	-0.2708652
C	-4.9474530	-1.1982146	2.8082356	C	4.1704071	5.3844932	1.4252979
C	-3.5688794	-1.1695532	2.7088542	C	2.7839920	3.6401522	-0.1433409
F	-2.7626651	0.8281177	5.5854302	H	2.1985940	2.9582365	-0.7528687
F	-5.4089112	0.7552908	5.7884156	C	4.8280208	0.5282158	-3.9236627
F	-5.6411382	-1.8449153	1.8759364	C	4.2232757	-0.2892109	-2.9619322
F	-2.9881059	-1.8083576	1.7007625	C	4.0294056	1.3489770	-4.7295776
C	-10.3551059	4.7956019	-0.8627810	C	2.8379881	-0.2257724	-2.8513619
H	-10.3627621	5.0308994	-1.9175858	H	2.3265522	-0.8382307	-2.1154339
C	-10.3116463	4.2681866	1.9276439	C	4.8896069	-0.5436431	3.9372910
H	-10.2827134	4.1116113	2.9963999	C	4.2986606	0.2704605	2.9648566
C	-10.2730643	0.7863456	4.5615470	C	4.0772909	-1.3259191	4.7666882
H	-10.2626392	1.8534112	4.7283740	C	4.8916716	-4.5370430	-0.5067636
C	-10.2572149	-2.0366135	4.2351692	C	4.1871260	-3.6523210	0.3143578
H	-10.2446554	-3.1138369	4.1450060	C	4.1843147	-5.3839791	-1.3703412
C	-10.3364502	-4.7999916	0.8385119	C	2.8023679	-3.6289854	0.1887041
H	-10.3463420	-5.0370681	1.8926676	H	2.2186451	-2.9434346	0.7957584
C	-10.2943952	-4.2570921	-1.9504167	C	4.9720232	-1.1896858	-2.0285987
H	-10.2670353	-4.0940634	-3.0184568	H	5.1529730	-2.1694122	-2.4707313
C	-10.3189987	-0.7275144	-4.5614509	H	5.9363326	-0.7879780	-1.7265107
H	-10.2988811	-1.7982070	-4.7003333	H	4.3894324	-1.3570725	-1.1252859
C	-10.3202613	2.1023974	-4.3158379	C	4.5749227	2.2333343	-5.8092266
H	-10.3157094	3.1822165	-4.2584011	H	3.7791968	2.5428585	-6.4851728
C	-7.1272753	4.1971647	0.4813971	H	5.0281855	3.1343308	-5.3986951
C	-7.0636130	-0.6091063	3.9934202	H	5.3412957	1.7335713	-6.3999154
C	-7.1026615	-4.2193262	-0.5112905	C	4.8114639	2.7435806	-1.2568533
C	-7.1244839	0.7016613	-4.0239484	H	5.0231874	3.2458227	-2.2007039
C	6.3483226	4.5760110	0.5462029	H	5.7495357	2.3279282	-0.8921542
C	6.2901257	0.5532150	-4.0815553	H	4.1466785	1.9136192	-1.4864272
C	6.3516590	-0.5931517	4.0868819	C	4.8284918	6.4121418	2.2959429
C	6.3640631	-4.5676393	-0.5034460	H	5.3195557	5.9628126	3.1570036
C	9.5966316	4.8435068	-0.9023854	H	5.5896326	6.9734671	1.7553773
H	9.5965995	5.0206356	-1.9683198	H	4.0915087	7.1225704	2.6677855
C	9.5809744	4.4515052	1.9128147	C	4.8394948	-6.4225543	-2.2304397
H	9.5714458	4.3415302	2.9882432	H	4.0998882	-7.1328384	-2.5974015
C	9.5137389	1.9285111	-4.3136869	H	5.3355475	-5.9843555	-3.0941747
H	9.5155248	3.0078966	-4.2518053	H	5.5961671	-6.9826516	-1.6822797
C	9.5039253	-0.9035205	-4.5504810	C	4.8347675	-2.7220506	1.2882104
H	9.4855454	-1.9768398	-4.6700826	H	5.0522101	-3.2201879	2.2333654
C	9.5673690	0.8436235	4.5606748	H	5.7681666	-2.2962505	0.9196011
H	9.5514839	1.9163194	4.6841264	H	4.1611298	-1.9002401	1.5203429
C	9.5626300	-1.9884074	4.3370079	C	4.6117542	-2.2009934	5.8592829
H	9.5574107	-3.0683997	4.2840320	H	3.8126821	-2.4917157	6.5396005
C	9.6113930	-4.8713675	0.9339942	H	5.0561326	-3.1124479	5.4626202
H	9.6105028	-5.0399757	2.0014304	H	5.3833841	-1.7003347	6.4426195
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H	9.5771270	-4.4103298	-2.9603039	H	6.0389559	0.6933708	1.7515839
N	7.0990184	-4.4616164	-1.5868526	H	4.5046017	1.2421802	1.0802413
N	7.0779469	-1.6885036	4.0993158	H	5.2437707	2.1211634	2.4001366
N	7.0273396	1.6423921	-4.0808851	C	2.7859681	5.2589387	1.4467753
N	7.0869400	4.4530129	1.6247980	H	2.1971829	5.8876495	2.1060029
N	-7.8420487	4.0588106	1.5736666	N	2.1102447	4.4042741	0.6968651
N	-7.8400915	1.7995286	-4.0457434	N	2.1365775	-0.5026012	3.6340477
N	-7.7797662	-1.7091935	3.9589964	N	2.1264175	-4.3960679	-0.6470270
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H	-7.5082359	1.4921317	4.2100805	H	2.0349491	-1.8472910	5.1756927
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C	2.9112894	0.2446752	2.8688479
H	2.4097932	0.8557498	2.1248824
C	2.6582614	1.3155863	-4.5088188
H	1.9982946	1.9320328	-5.1101470
O	6.8775626	-3.3207516	-4.1170782
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O	7.0586661	4.3533579	-3.3541105
H	6.9395701	3.4121065	-3.6124350
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H	6.8768731	3.7157296	3.2652721
O	7.0871136	-4.3887686	3.3813840
H	6.9735568	-3.4429464	3.6294078
C	6.3337373	-4.2028566	-5.0695134
H	6.4648357	-3.7652481	-6.0588610
H	6.8406548	-5.1725714	-5.0669847
H	5.2624046	-4.3762386	-4.9219713
C	6.8746981	5.1811975	-4.4780775
H	5.8302623	5.2270614	-4.8044331
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H	6.4246337	3.6606870	6.0880008
H	6.7680936	5.1054768	5.1393166
C	6.7678120	-5.2090808	4.4794936
H	5.6939479	-5.2308947	4.6945612
H	7.0785524	-6.2283080	4.2513972
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C	-6.4040923	4.9864740	-3.9923207
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O	-7.4818007	-3.0889438	-4.1305753
H	-7.5338369	-3.4495461	-3.2133251
C	-6.5238659	-3.8194321	-4.8566905
H	-6.5277656	-3.4680340	-5.8877297
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O	-7.3568683	-4.3326094	3.2312280
H	-7.4527003	-3.3888686	3.5026602
C	-6.2902668	-4.9084982	3.9449190
H	-6.2314994	-5.9652527	3.6875481
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H	-6.4386935	-4.8341863	5.0261622
O	-7.4546283	3.1606357	4.1236421
C	-6.4844298	3.9245179	4.7971133
H	-6.4582493	3.6118922	5.8403015
H	-5.4788999	3.7920117	4.3825732
H	-6.7212479	4.9921422	4.7724769
C	-8.3554215	0.1956553	0.5625097
C	-8.9904850	-1.1795619	0.5464643
C	-11.2711406	-0.1460562	-0.6215764
C	-10.6318003	1.2273380	-0.6185362
H	-8.7579730	-1.6827396	-0.3939530
H	-8.5885528	-1.7845459	1.3600310
H	-8.5994619	0.7276248	1.4836691
H	-7.2691462	0.1070269	0.5021646
H	-11.0444893	-0.6774173	-1.5481607
H	-12.3574633	-0.0509403	-0.5529751
H	-11.0250872	1.8206312	-1.4441856
H	-10.8645789	1.7542969	0.3091222
C	10.8536948	-0.4084445	0.7504501
C	9.7485026	-1.4371891	0.6497517
C	8.2213586	0.3737251	-0.7816082
C	9.3346081	1.3916974	-0.6561889
H	9.8767565	-2.0492583	-0.2443274
H	9.7735633	-2.0965842	1.5173479
H	10.7352001	0.2059621	1.6448806
H	11.8169862	-0.9152023	0.8214614
H	8.3562869	-0.2216901	-1.6855730
H	7.2580429	0.8832501	-0.8547845
H	9.2972636	2.0807122	-1.5012043
H	9.2194289	1.9774504	0.2580760

S	-10.7823254	-1.1495336	0.8037619
S	-8.8381441	1.1918250	-0.8680423
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H	-7.5338187	3.4875238	3.1937014

dioxane@I-capsule in N-hemisphere

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Energy = -12912.85137082

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C	-14.6476539	3.1222886	-0.8508738
C	-14.6364417	1.6461736	-2.8099896
C	-13.0064191	3.4109683	-2.5951053
C	-13.5400639	3.7815781	-1.3749849
C	-15.1670974	2.0695042	-1.5959657
H	-12.1996107	3.9848163	-3.0245739
H	-16.0305961	1.5461682	-1.2061870
O	-12.9931224	4.8467682	-0.6985355
C	-11.7906493	4.6355472	-0.0806675
C	-11.7879436	4.4424562	1.3203313
C	-11.7632102	1.3192818	-4.4379050
C	-11.7730065	-0.0799627	-4.6417029
O	-12.9759630	-0.6901250	-4.8741560
C	-13.5496941	3.2657549	2.3170444
C	-14.6629346	0.8206635	3.1000801
C	-13.0304433	2.5721028	3.3944822
C	-14.6530665	2.7784049	1.6218023
C	-15.1793655	1.5621045	2.0432824
C	-13.5609766	1.3500206	3.7646072
H	-12.2266852	3.0054236	3.9698856
H	-16.0377631	1.1673532	1.5153490
C	-13.5367724	-1.3616194	-3.8119907
C	-14.6558246	-2.7844816	-1.6793490
C	-13.0160765	-2.5865420	-3.4372531
C	-14.6421161	-0.8266398	-3.1575330
C	-15.1719488	-1.5654245	-2.1054472
C	-13.5488869	-3.2776436	-2.3647588
H	-12.2096806	-3.0240671	-4.0057375
H	-16.0330427	-1.1662791	-1.5853353
O	-13.0130432	0.6752796	4.8314225
O	-13.0029586	-4.4899629	-2.0146007
C	-11.8108298	0.0601334	4.6082357
C	-11.8052530	-1.3386728	4.4012192
C	-11.8030695	-4.4651724	-1.3527510
C	-11.8189804	-4.6617646	0.0476591
C	-13.5653117	-2.3475366	3.2408423
C	-14.6724915	-3.1295358	0.7929927
C	-14.6675178	-1.6523341	2.7514202
C	-13.0463258	-3.4267919	2.5498772
C	-13.5733271	-3.7955732	1.3262490
C	-15.1913638	-2.0732639	1.5336440
H	-12.2461939	-4.0049415	2.9860156
H	-16.0489032	-1.5452076	1.1371611
O	-13.0070076	-1.9964892	4.4473610
C	-15.2734826	-0.4997770	3.5300624
H	-15.0095817	-0.6481350	4.5767236
C	-15.2588153	3.5556431	0.4682037
H	-14.9943715	4.6024718	0.6145533
C	-15.2423386	0.4967425	-3.5931985
H	-14.9693779	0.6431417	-4.6378072
C	-15.2756367	-3.5587702	-0.5311613
H	-15.0160297	-4.6070290	-0.6759796
C	-9.4659477	0.0927554	4.3514897
C	-9.4444798	-1.2887092	4.1386126
C	-9.4302886	-0.1216411	-4.3655510
C	-9.4049414	1.2602921	-4.1560348
O	-12.9617795	1.9820297	-4.4936073
O	-12.9934821	4.4748390	1.9716423
O	-13.0280841	-4.8652019	0.6551755
C	-16.7858724	3.5054553	0.4574492
H	-17.1742829	4.1293191	-0.3471778
H	-17.1949056	2.5050844	0.3158601
C	-16.8005836	-0.4894025	3.4791652
H	-17.1895881	0.3139123	4.1043322

H	-17.1938275	-1.4334038	3.8555129	H	15.7297076	1.2833288	-3.9364244
C	-16.8024052	-3.4999036	-0.5328671	H	15.7739663	0.2613777	-2.5114085
H	-17.1901756	-3.8743654	-1.4798641	C	15.4454759	-3.5396639	-0.3721648
H	-17.2068738	-2.4974788	-0.3927673	H	15.8473317	-3.9418394	-1.3016255
C	-16.7698375	0.4944613	-3.5542211	H	15.8461255	-4.1281366	0.4527351
H	-17.1550607	1.4401792	-3.9345129	C	15.3391650	-0.3680109	3.5019244
H	-17.1868815	0.3543035	-2.5569618	H	15.7179602	0.4621982	4.0973667
H	-17.2090359	-0.3460054	2.4788128	H	15.7716301	-0.2746740	2.5058115
H	-17.2009348	-4.1229498	0.2674233	C	15.4579185	3.5222356	0.3544236
H	-17.1582068	-0.3073840	-4.1816592	H	15.8605932	3.9173362	1.2866339
H	-17.1792141	3.8838347	1.4005842	H	15.8626050	4.1132122	-0.4666301
C	-9.4338086	-4.2885510	-1.2989386	H	15.8341146	-2.5271419	-0.2644248
C	-9.4660684	-4.4824109	0.0852867	H	15.7184465	-1.2944548	3.9320242
C	-9.4189492	4.2555992	1.2880197	H	15.8416755	2.5084697	0.2410679
C	-9.4383997	4.4442969	-0.0971604	H	15.7258465	-0.4731073	-4.1042150
C	12.2141945	3.8102756	-1.4886012	C	7.9898966	0.2027639	4.1625830
C	13.2312214	1.5564969	-2.8017554	C	7.9781102	-1.1916240	4.0786721
C	13.3037247	3.1455873	-0.9353211	C	8.0093852	-0.2060158	-4.1624142
C	11.6572049	3.3830721	-2.6803952	C	7.9956939	1.1881218	-4.0722364
C	12.1391238	2.2510061	-3.3132281	C	-3.1168682	4.2037761	0.6710281
C	13.7818170	2.0333299	-1.6185900	C	-3.8262180	3.2004181	1.3070844
H	10.8629733	3.9536646	-3.1387106	C	-5.2080325	3.1657122	1.2649629
H	14.6308003	1.5067585	-1.2027652	C	-5.9331924	4.1415319	0.5939129
O	11.5521495	1.8458036	-4.4885433	C	-5.2112872	5.1344548	-0.0561027
C	10.3510729	1.1980129	-4.3733684	C	-3.8311789	5.1637817	-0.0228650
C	10.3436903	-0.2102133	-4.4831087	F	-3.1856709	2.2502670	1.9757957
C	10.5025943	4.8275212	-0.2444557	F	-5.8389774	2.1713948	1.8789568
C	10.4933849	4.6721014	1.1624935	F	-5.8519973	6.1062882	-0.6989124
O	11.6956575	4.6306345	1.8119221	F	-3.2013318	6.1489365	-0.6500110
C	12.1112416	-1.4996419	-3.6641873	C	-3.1378994	-4.2203145	-0.6334011
C	13.2897316	-2.8885856	-1.5483772	C	-3.8491053	-3.2203080	-1.2722703
C	11.6162096	-2.7312594	-3.2767636	C	-5.2308837	-3.1924914	-1.2384498
C	13.2244699	-0.9452027	-3.0413218	C	-5.9549256	-4.1733839	-0.5737548
C	13.7813455	-1.6652139	-1.9921791	C	-5.2317284	-5.1625806	0.0803832
C	12.1839586	-3.4096288	-2.2134565	C	-3.8510749	-5.1845943	0.0555074
H	10.8099385	-3.1847559	-3.8332842	F	-3.2097626	-2.2657698	-1.9360718
H	14.6469461	-1.2515919	-1.4917095	F	-5.8626888	-2.1993823	-1.8536675
C	12.1863327	3.3985632	2.1782804	F	-5.8715839	-6.1377415	0.7190155
C	13.2202714	0.9373753	3.0223067	F	-3.2195592	-6.1667673	0.6855976
C	11.6080402	2.7235525	3.2379746	C	-3.1578808	0.4489459	-3.4408321
C	13.2967779	2.8755262	1.5228487	C	-3.9657389	1.0899781	-2.5188446
C	13.7844433	1.6534952	1.9730004	C	-5.3399836	1.1160393	-2.6704645
C	12.1023178	1.4942631	3.6367368	C	-5.9539878	0.5032885	-3.7551220
H	10.7972939	3.1779992	3.7872066	C	-5.1356040	-0.1466469	-4.6688618
H	14.6536305	1.2382357	1.4802915	C	-3.7641730	-0.1779813	-4.5144046
O	11.6776685	-4.6385674	-1.8513937	F	-3.4278134	1.6946472	-1.4662110
O	11.5160104	0.8476897	4.6977070	F	-6.0729097	1.7259957	-1.7464505
C	10.4737338	-4.6637520	-1.2022441	F	-5.6731049	-0.7330936	-5.7347806
C	10.4819659	-4.8110932	0.2055469	F	-3.0345929	-0.8047757	-5.4287118
C	10.3279536	0.2128877	4.4630840	C	-3.1853715	-0.5073044	3.4942756
C	10.3364811	-1.1959236	4.3577556	C	-3.8031337	0.1414643	4.5480814
C	12.1897222	-3.7977169	1.4557327	C	-5.1764790	0.1176273	4.6859035
C	13.2228276	-1.5601766	2.7823244	C	-5.9865380	-0.5451450	3.7736227
C	13.2909754	-3.1446053	0.9114647	C	-5.3608207	-1.1776114	2.7068927
C	11.6258124	-3.3659479	2.6421698	C	-3.9846746	-1.1600791	2.5731147
C	12.1207217	-2.2453357	3.2861229	F	-3.0830037	0.7803356	5.4614071
C	13.7757480	-2.0381649	1.5993717	F	-5.7240023	0.7230561	5.7361038
H	10.8221005	-3.9285052	3.0927908	F	-6.0835666	-1.7997717	1.7828100
H	14.6327736	-1.5193450	1.1903534	F	-3.4361703	-1.7860609	1.5384104
O	11.6883059	-4.9205483	0.8369227	C	-10.6151831	4.6588640	-0.8014529
C	13.9205186	-3.6228563	-0.3819924	H	-10.6049511	4.8507925	-1.8644574
H	13.6774633	-4.6790461	-0.4915404	C	-10.6080331	4.2753952	2.0144620
C	13.8177396	0.3625851	-3.5320434	H	-10.5970681	4.1710810	3.0902689
H	13.5363739	0.4633112	-4.5799362	C	-10.6386297	0.7864658	4.6147735
C	13.9333603	3.6131145	0.3619198	H	-10.6280890	1.8481425	4.8134036
H	13.6956421	4.6698493	0.4777385	C	-10.6265283	-2.0235242	4.1926558
C	13.8108633	-0.3701780	3.5180781	H	-10.6114035	-3.0972810	4.0715986
H	13.5236000	-0.4705712	4.5643455	C	-10.6499068	-4.6941809	0.7784784
C	8.0929988	-4.6507330	-1.1851800	H	-10.6500291	-4.8886296	1.8410802
C	8.1207353	-4.7947483	0.2048160	C	-10.6163691	-4.3015564	-2.0359604
C	8.1158595	4.6880550	1.1490012	H	-10.5953746	-4.1939631	-3.1112701
C	8.1393162	4.8278495	-0.2411835	C	-10.6037297	-0.8111204	-4.6369214
O	11.7104865	4.9358780	-0.8740307	H	-10.5961193	-1.8733451	-4.8327963
O	11.5295243	-0.8445295	-4.7227691	C	-10.5833516	1.9997930	-4.2218961
O	11.5394984	-1.8427559	4.4646121	H	-10.5648455	3.0738014	-4.1036568
C	15.3462008	0.3571881	-3.5093662	C	-7.3973128	4.1800180	0.6157975

C	-7.4376798	-0.5944864	3.9567299	H	4.9449882	1.3494151	-6.2762919
C	-7.4184128	-4.2176188	-0.6079753	C	4.4796917	2.9253727	-1.2710344
C	-7.4031234	0.5582625	-3.9537025	H	4.6976259	3.4382229	-2.2074661
C	6.0765017	4.7409910	0.4998374	H	5.4075259	2.4685262	-0.9259755
C	5.9777895	0.5288189	-3.8370903	H	3.7832863	2.1261129	-1.5099306
C	5.9555135	-0.5389136	3.8679870	C	4.6125872	6.6524671	2.2156561
C	6.0568379	-4.6941368	-0.5239529	H	5.1521456	6.2325912	3.0621484
C	9.3247490	4.9217330	-0.9594418	H	5.3388424	7.2097697	1.6247873
H	9.3236984	5.0694401	-2.0297265	H	3.8847534	7.3634833	2.6040038
C	9.3081422	4.6238022	1.8664700	C	4.5778007	-6.5911470	-2.2385468
H	9.3000002	4.5557119	2.9453502	H	3.8459460	-7.2935576	-2.6348139
C	9.1824273	1.9065457	-4.1916623	H	5.1191464	-6.1633288	-3.0802108
H	9.1823063	2.9864633	-4.1442670	H	5.3025763	-7.1596506	-1.6564603
C	9.1696443	-0.9265233	-4.3987398	C	4.4762938	-2.8996676	1.2891480
H	9.1511286	-1.9996048	-4.5196807	H	4.6759363	-3.4272554	2.2217172
C	9.1506881	0.9273908	4.3830918	H	5.4145587	-2.4521470	0.9611597
H	9.1275286	2.0010725	4.4992263	H	3.7901054	-2.0924868	1.5324161
C	9.1667390	-1.9070740	4.1887692	C	4.2159982	-2.0752652	5.7002554
H	9.1690069	-2.9871404	4.1463828	H	3.4175145	-2.3336263	6.3941491
C	9.3051687	-4.8951861	0.9217698	H	4.6601015	-3.0048582	5.3462145
H	9.3028046	-5.0408894	1.9921591	H	4.9884049	-1.5477108	6.2581765
C	9.2864166	-4.6028564	-1.9040748	C	4.6998104	1.0385794	1.6898834
H	9.2796002	-4.5398602	-2.9832931	H	5.6169495	0.5295774	1.3947214
N	6.7886544	-4.5894289	-1.6094835	H	4.1037648	1.2066702	0.7951312
N	6.6894361	-1.6284321	3.9011954	H	4.9769501	2.0201132	2.0757953
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N	-8.1236744	4.0942076	1.7051575	N	1.8432415	4.6126210	0.7471709
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N	-8.1709416	0.5037482	4.2356959	C	2.3117605	-1.2117096	4.3388370
H	-7.8690057	1.4978750	4.2613264	H	1.6387349	-1.7732191	4.9784322
N	-8.1658589	-4.4339054	0.4946470	C	2.5141583	-5.4316823	-1.4469684
H	-7.8622177	-4.4312608	1.4894505	H	1.9392386	-6.0759811	-2.1033871
N	-8.1379147	-0.5376812	-4.2369005	C	2.5242682	0.2067483	2.5763682
H	-7.8391616	-1.5331101	-4.2570233	C	2.0249274	0.7742363	1.7973386
N	-8.1346989	4.3918105	-0.4945194	C	2.3111995	1.0640344	-4.2986983
H	-7.8211486	4.3885843	-1.4862364	H	1.6120602	1.5606672	-4.9635065
N	6.8255298	4.8606433	-0.6236127	O	5.9834845	-3.2321103	-3.9447739
H	6.5243108	4.8487568	-1.6019313	H	6.2393523	-3.7784130	-3.1684294
N	6.7101319	-0.5942310	-4.0051770	O	6.7457389	4.3749510	-3.3832346
H	6.3764136	-1.5741422	-3.9853033	H	6.6309224	3.4111051	-3.5459460
N	6.8103132	-4.8213056	0.5945088	O	6.2771521	3.3068974	3.9820479
H	6.5139254	-4.8189885	1.5739181	H	6.4268849	3.8182479	3.1553657
N	6.6883025	0.5856620	4.0256551	O	6.7599328	-4.3689870	3.3620122
H	6.3743883	1.5671017	3.9989520	H	6.6260459	-3.4118915	3.5509366
I	-1.1005524	-0.5004745	3.3300224	C	4.6806115	-3.5610113	-4.3712284
I	-1.0495600	-4.3175536	-0.7182225	H	4.3970197	-2.8701395	-5.1650150
I	-1.0770570	0.4161363	-3.2436013	H	4.6264658	-4.5739315	-4.7808394
I	-1.0298335	4.3199938	0.7649450	H	3.9381344	-3.4727905	-3.5716251
C	4.6043033	4.7347462	0.5265827	C	6.4600568	5.0850487	-4.5647739
C	3.8705179	3.8504582	-0.2680528	H	5.4026845	5.0309973	-4.8458308
C	3.9269904	5.5989942	1.3976703	H	6.7050287	6.1344556	-4.4047219
C	2.4903381	3.8340546	-0.1003517	H	7.0535550	4.7286651	-5.4119014
H	1.8854794	3.1460729	-0.6835873	C	5.3128587	3.9556547	4.7764032
C	4.5205922	0.4769213	-3.6501571	H	4.3530365	4.0731126	4.2625360
C	3.9761679	-0.2255194	-2.5711462	H	5.1405646	3.3524393	5.6674613
C	3.6769711	1.1394676	-4.5449925	H	5.6494185	4.9430933	5.1074320
C	2.5913168	-0.2271332	-2.4479133	C	6.5634115	-5.1149390	4.5395294
H	2.1194238	-0.7561076	-1.6258245	H	5.5186573	-5.1203288	4.8683706
C	4.4944838	-0.5073273	3.7074675	H	6.8531244	-6.1474041	4.3466661
C	3.9096354	0.2496156	2.6868936	H	7.1754083	-4.7450692	5.3675883
C	3.6819841	-1.2545527	4.5661979	O	-7.6744163	4.2480748	-3.1430510
C	4.5848556	-4.6849852	-0.5366524	H	-7.7831523	3.3063258	-3.4225030
C	3.8597888	-3.8075620	0.2742747	C	-6.6205225	4.8260123	-3.8729414
C	3.8988840	-5.5462122	-1.4041026	H	-6.5497361	5.8795848	-3.6055609
C	2.4774427	-3.7921222	0.1217614	H	-5.6516503	4.3605115	-3.6587455
H	1.8777983	-3.1099682	0.7172127	H	-6.7924798	4.7642519	-4.9515319
C	4.8121902	-0.8972488	-1.5266457	O	-7.7615944	-3.2072935	-4.2524687
H	5.1896534	-1.8652484	-1.8556474	H	-7.8309962	-3.5608544	-3.3329041
H	5.6734517	-0.2933179	-1.2396887	C	-6.7742124	-3.9258456	-4.9503011
H	4.2218393	-1.0688421	-0.6297465	H	-6.7493515	-3.5710590	-5.9798999
C	4.1816682	1.9033187	-5.7308315	H	-5.7731322	-3.7915909	-4.5259087
H	3.3689205	2.1228978	-6.4213442	H	-6.9914298	-4.9977937	-4.9700682
H	4.6299006	2.8510551	-5.4337381	O	-7.7373758	-4.2886261	3.1475366

H	-7.8339842	-3.3443326	3.4227161	C	-14.4931201	-0.5062488	3.4546991
C	-6.7044542	-4.8827419	3.8943200	H	-14.1986287	-0.6594518	4.4926053
H	-6.6403397	-5.9354178	3.6217377	C	-14.6149999	3.5974123	0.4635075
H	-5.7265546	-4.4270160	3.7017121	H	-14.3753646	4.6495841	0.6129398
H	-6.8967317	-4.8255314	4.9697268	C	-14.5019572	0.5191199	-3.5801075
O	-7.7913275	3.1731857	4.2578685	H	-14.2098643	0.6696165	-4.6190256
H	-7.8436007	3.5256692	3.3368329	C	-14.6328719	-3.5845154	-0.5854895
C	-6.8227367	3.8983945	4.9749925	H	-14.3978817	-4.6367687	-0.7416014
H	-6.8216925	3.5498921	6.0070114	C	-8.6799956	0.1216410	4.0687275
H	-5.8115106	3.7643436	4.5755049	C	-8.6524545	-1.2561388	3.8400355
H	-7.0432734	4.9698120	4.9830176	C	-8.6956049	-0.1151701	-4.1835708
C	10.0270512	-1.0223415	-0.0297887	C	-8.6664502	1.2657368	-3.9714074
C	8.5494029	-1.2195616	0.2559150	O	-12.2047730	2.0094966	-4.4356395
C	8.2051583	1.0640476	-0.0778863	O	-12.3804121	4.5685944	1.9791994
C	9.6859437	1.2332133	-0.3595435	O	-12.4202622	-4.9611876	0.5857200
H	8.0383495	-1.5371643	-0.6671661	C	-16.1397656	3.5095944	0.4512142
H	8.4087298	-1.9990598	1.0070831	H	-16.5431237	4.1253549	-0.3523167
H	10.5722127	-0.8644268	0.9135115	H	-16.5242854	2.4998706	0.3078987
H	10.4380100	-1.9124531	-0.5064892	C	-16.0216948	-0.5034799	3.4498339
H	7.6673906	0.9510772	-1.0331450	H	-16.3956855	0.2936511	4.0918679
H	7.8121350	1.9492087	0.4275609	H	-16.3989497	-1.4520130	3.8311566
H	9.8377271	2.0344582	-1.0829803	C	-16.1571698	-3.4896777	-0.5768202
H	10.2120453	1.5084239	0.5678625	H	-16.5598406	-3.8455383	-1.5247993
O	7.9607043	-0.0406722	0.7648289	H	-16.5375518	-2.4798775	-0.4234144
O	10.2241022	0.0576605	-0.9093592	C	-16.0303449	0.5222869	-3.5697648

dioxane@I-capsule in I-hemisphere

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Energy = -12912.84808044

C	-12.8020567	2.3694009	-3.2524849	C	-8.8093142	-4.5327410	-1.3721956
C	-13.9852032	3.1734337	-0.8490528	C	-8.8471043	-4.7419021	0.0100181
C	-13.9123783	1.6704375	-2.7863767	C	-8.7978539	4.4840440	1.3140995
C	-12.3143659	3.4651235	-2.5632767	C	-8.8144209	4.6744430	-0.0711795
C	-12.8825081	3.8486508	-1.3627177	C	12.8350485	3.7464421	-1.5187263
C	-14.4714954	2.1005916	-1.5878401	C	13.9054620	1.5524770	-2.8838234
H	-11.5100038	4.0451199	-2.9894076	C	13.9477755	3.1039374	-0.9846478
H	-15.3331582	1.5681091	-1.2065170	C	12.2810166	3.3293831	-2.7147147
O	-12.3782021	4.9415368	-0.6953687	C	12.7940429	2.2290962	-3.3780225
C	-11.1738047	4.7857259	-0.0674022	C	14.4517476	2.0192175	-1.6929339
C	-11.1724563	4.5961728	1.3346135	H	11.4695348	3.8893787	-3.1543307
C	-11.0125096	1.3376680	-4.3363759	H	15.3183505	1.5081956	-1.2943178
C	-11.0232574	-0.0592932	-4.5447675	O	12.2220856	1.8383478	-4.5669833
O	-12.2200214	-0.6634691	-4.8261144	C	11.0227192	1.1838309	-4.4829892
C	-12.8860077	3.3273866	2.2960817	C	11.0243549	-0.2230801	-4.6173529
C	-13.9093265	0.8260132	3.0244542	C	11.1179026	4.7235802	-0.2439571
C	-12.3176241	2.6128537	3.3347379	C	11.1280330	4.5904077	1.1648680
C	-13.9839949	2.8238942	1.6048954	O	12.3411371	4.5849401	1.7972078
C	-14.4683308	1.5817862	2.0012476	C	12.7860997	-1.4879473	-3.7558056
C	-12.8012458	1.3624039	3.6724942	C	13.9319630	-2.8402185	-1.5937408
H	-11.5125661	3.0466254	3.9079985	C	12.2675478	-2.6989593	-3.3337735
H	-15.3269593	1.1788010	1.4800073	C	13.9006710	-0.9324553	-3.1354027
C	-12.8101451	-1.3514358	-3.7928930	C	14.4425557	-1.6358027	-2.0656438
C	-13.9941173	-2.8069771	-1.7202330	C	12.8169128	-3.3564693	-2.2483755
C	-12.3185697	-2.5962152	-3.4419937	H	11.4563823	-3.1571349	-3.8791356
C	-13.9195970	-0.8137403	-3.1475119	H	15.3115977	-1.2219417	-1.5713603
C	-14.4801436	-1.5677695	-2.1228767	C	12.8699128	3.3706254	2.1685614
C	-12.8873423	-3.3071839	-2.4010140	C	13.9668138	0.9436333	3.0296923
H	-11.5109816	-3.0323107	-4.0100718	C	12.3380348	2.7102993	3.2611553
H	-15.3427573	-1.1662634	-1.6072675	C	13.9701309	2.8532757	1.4904767
O	-12.2052639	0.6686565	4.6980729	C	14.4885290	1.6476248	1.9505557
O	-12.3852160	-4.5476424	-2.0811842	C	12.8629283	1.4976932	3.6704000
C	-11.0086724	0.0687991	4.4095278	H	11.5366118	3.1667612	3.8222592
C	-10.9994379	-1.3270590	4.1892079	H	15.3476399	1.2337208	1.4391788
C	-11.1851288	-4.5965945	-1.4237374	O	12.2895139	-4.5668367	-1.8627737
C	-11.2067803	-4.8193777	-0.0267750	O	12.3163912	0.8601242	4.7604927
C	-12.8017650	-2.3612114	3.1205779	C	11.0925005	-4.5656908	-1.1998719
C	-14.0037306	-3.1705897	0.7302589	C	11.1180595	-4.7063405	0.2078665
C	-13.9116799	-1.6595063	2.6590093	C	11.1195759	0.2283248	4.5719158
C	-12.3315900	-3.4693748	2.4412190	C	11.1192242	-1.1801659	4.4493002
C	-12.9102400	-3.8568570	1.2470061	C	12.8655497	-3.7354305	1.4418475
C	-14.4792744	-2.0906927	1.4658923	C	13.9659339	-1.5413820	2.7822786
H	-11.5304017	-4.0525123	2.8692832	C	13.9649178	-3.0919860	0.8820596
H	-15.3377390	-1.5526355	1.0850074	C	12.3393381	-3.3193248	2.6506399
O	-12.1918220	-1.9958694	4.2951998	C	12.8672144	-2.2192283	3.3024471

C	14.4844356	-2.0070083	1.5785790	F	-4.9870088	0.7828059	5.4720866
H	11.5378995	-3.8792433	3.1082770	F	-5.2276040	-1.7683970	1.5264685
H	15.3406922	-1.4948038	1.1597226	F	-2.5750852	-1.7162968	1.3395494
O	12.3325171	-4.8394958	0.8184451	C	-9.9944594	4.8523540	-0.7807658
C	14.5651331	-3.5717838	-0.4256211	H	-9.9873041	5.0416513	-1.8444796
H	14.3095749	-4.6257935	-0.5296137	C	-9.9901539	4.4729277	2.0348985
C	14.5000943	0.3715995	-3.6283628	H	-9.9819517	4.3661513	3.1104858
H	14.2175282	0.4781106	-4.6751980	C	-9.8459145	0.8054330	4.3789192
C	14.5783061	3.5841222	0.3086842	H	-9.8331075	1.8639971	4.5934257
H	14.3262510	4.6384292	0.4177789	C	-9.8263869	-2.0013501	3.9269321
C	14.5764972	-0.3595329	3.5120362	H	-9.8075480	-3.0751444	3.8029619
H	14.3162793	-0.4640995	4.5648383	C	-10.0384657	-4.9219309	0.6995378
C	8.7134931	-4.5492394	-1.1538182	H	-10.0498933	-5.1338423	1.7589850
C	8.7589888	-4.6809741	0.2367333	C	-9.9925252	-4.4816706	-2.1072060
C	8.7499706	4.5842143	1.1798423	H	-9.9683087	-4.3527540	-3.1802393
C	8.7585100	4.7048465	-0.2120230	C	-9.8596757	-0.7975512	-4.4983829
O	12.3172066	4.8516565	-0.8847026	H	-9.8483859	-1.8590287	-4.6976327
O	12.2180293	-0.8515177	-4.8358459	C	-9.8367569	2.0117846	-4.0755163
O	12.3228958	-1.8298623	4.5049279	H	-9.8169966	3.0861386	-3.9577890
C	16.0279459	0.3655469	-3.6046321	C	-6.7756170	4.4108232	0.6464961
H	16.4119756	1.2945254	-4.0249892	C	-6.6479688	-0.5486748	3.6569951
H	16.4553294	0.2622088	-2.6073033	C	-6.7952450	-4.4902179	-0.6763475
C	16.0913653	-3.5063957	-0.4384504	C	-6.6783456	0.5482421	-3.7133777
H	16.4752655	-3.9145009	-1.3729302	C	6.7036992	4.6505381	0.5500711
H	16.4969759	-4.0980553	0.3817156	C	6.6620317	0.4750485	-3.9011372
C	16.1034689	-0.3541946	3.4557080	C	6.7375623	-0.4923616	4.0051643
H	16.4961478	0.4736491	4.0454325	C	6.6854942	-4.6243198	-0.4692048
H	16.5094713	-0.2542529	2.4491460	C	9.9329908	4.7938184	-0.9468891
C	16.1043139	3.5171087	0.2873063	H	9.9155647	4.9288942	-2.0184663
H	16.5094173	3.9260104	1.2124487	C	9.9521170	4.5387664	1.8842773
H	16.4921170	4.1073729	-0.5424436	H	9.9591741	4.4888509	2.9643116
H	16.4930724	-2.4982030	-0.3378732	C	9.8469818	1.8811486	-4.2979184
H	16.4959135	-1.2821174	3.8705926	H	9.8391607	2.9594724	-4.2261078
H	16.5027526	2.5084007	0.1790645	C	9.8516244	-0.9468361	-4.5566965
H	16.4073533	-0.4606976	-4.2051602	H	9.8419773	-2.0178904	-4.6952489
C	8.7737287	0.2312370	4.3291913	C	9.9431133	0.9474148	4.5365771
C	8.7537922	-1.1619819	4.2248926	H	9.9296629	2.0199512	4.6636387
C	8.6859584	-0.2389815	-4.3058656	C	9.9417507	-1.8840090	4.3049135
C	8.6653668	1.1534383	-4.1872347	H	9.9373806	-2.9630067	4.2432384
C	-2.4966439	4.3653495	0.7033314	C	9.9515098	-4.7777005	0.9403249
C	-3.2233635	3.3633965	1.3214844	H	9.9612183	-4.9201087	2.0110280
C	-4.6047520	3.3509143	1.2756889	C	9.8980979	-4.5041448	-1.8881083
C	-5.3122312	4.3524683	0.6248336	H	9.8785055	-4.4506201	-2.9677630
C	-4.5744659	5.3444244	-0.0081450	N	7.4036274	-4.5133751	-1.5637740
C	-3.1936933	5.3497011	0.0258655	N	7.4617413	-1.5876239	4.0319848
F	-2.5994343	2.3907944	1.9731576	N	7.3795348	1.5733912	-3.9444370
F	-5.2523227	2.3515164	1.8632703	N	7.4521420	4.5509930	1.6254206
F	-5.2005047	6.3347762	-0.6365156	N	-7.5031932	4.3266502	1.7347624
F	-2.5464547	6.3328864	-0.5865102	N	-7.3846074	1.6528136	-3.6836847
C	-2.5160868	-4.4170238	-0.6177477	N	-7.3639912	-1.6469961	3.5822643
C	-3.2331751	-3.4199113	-1.2545201	N	-7.5066147	-4.3878212	-1.7739643
C	-4.6153905	-3.4205579	-1.2520760	N	-7.3891136	0.5414878	3.9467578
C	-5.3330064	-4.4293678	-0.6235500	H	-7.0993989	1.5321002	4.0361904
C	-4.6053237	-5.4171716	0.0278560	N	-7.5469015	-4.7115799	0.4234200
C	-3.2241521	-5.4103831	0.0346262	H	-7.2325320	-4.6506112	1.4149917
F	-2.5992070	-2.4408889	-1.8859241	N	-7.4121869	-0.5392367	-4.0233194
F	-5.2532674	-2.4256231	-1.8567284	H	-7.1248906	-1.5316634	-4.0746196
F	-5.2406956	-6.4136773	0.6369353	N	-7.5091017	4.6285623	-0.4655937
F	-2.5863794	-6.3902646	0.6620895	H	-7.1855649	4.5723065	-1.4553696
C	-2.4424972	0.3817646	-3.1492872	N	7.4423703	4.7456812	-0.5815770
C	-3.2513776	1.0321163	-2.2348862	H	7.1333172	4.7398300	-1.5572296
C	-4.6240882	1.0813804	-2.4017482	N	7.3934491	-0.6396485	-4.1216456
C	-5.2335618	0.4788467	-3.4945127	H	7.0622636	-1.6202023	-4.0817247
C	-4.4133996	-0.1797105	-4.4009528	N	7.4536503	-4.7262776	0.6416245
C	-3.0449146	-0.2316814	-4.2324984	H	7.1707850	-4.7304046	1.6252162
F	-2.7135574	1.6247073	-1.1750628	N	7.4744208	0.6261311	4.1875674
F	-5.3559182	1.7114969	-1.4919246	H	7.1586787	1.6100738	4.1524536
F	-4.9450260	-0.7538576	-5.4769035	I	-0.2990827	-0.3905054	3.1837759
F	-2.3143350	-0.8639037	-5.1423756	I	-0.4240817	-4.4559274	-0.6526524
C	-2.3858275	-0.4296545	3.2961443	I	-0.3646159	0.3195645	-2.9410507
C	-3.0353489	0.2134285	4.3338546	I	-0.4071076	4.4267621	0.7981727
C	-4.4110567	0.1794388	4.4358976	C	5.2321094	4.6676847	0.5841126
C	-5.1937639	-0.4915876	3.5052605	C	4.4770858	3.8110443	-0.2226172
C	-4.5345317	-1.1256218	2.4600009	C	4.5731572	5.5378600	1.4641395
C	-3.1556033	-1.0934732	2.3579720	C	3.0970765	3.8205311	-0.0508118
F	-2.3444751	0.8584706	5.2650016	H	2.4764429	3.1529650	-0.6412938

C	5.2191719	0.4056777	-3.6250290	O	7.3557979	4.3044399	-3.3527531
C	4.7596175	-0.2847988	-2.5004564	H	7.2703068	3.3410748	-3.5355399
C	4.3087403	1.0405652	-4.4721644	O	6.9247943	3.3097637	4.0840046
C	3.3855495	-0.3117287	-2.2891760	H	7.0749493	3.8048663	3.2466539
H	2.9780094	-0.8362498	-1.4303944	O	7.4376213	-4.3160904	3.4157593
C	5.2843831	-0.4382236	3.7876162	H	7.3467954	-3.3575560	3.6191503
C	4.7649049	0.2896029	2.7130699	C	5.2479453	-3.5148045	-4.2946288
C	4.4196577	-1.1300833	4.6396474	H	4.9592411	-2.8373600	-5.0981657
C	5.2139323	-4.6502952	-0.4667809	H	5.0982828	-4.5366930	-4.6547562
C	4.4719617	-3.8041447	0.3629773	H	4.5677401	-3.3438912	-3.4543070
C	4.5420075	-5.5200079	-1.3375574	C	6.9963290	5.0264185	-4.5063698
C	3.0884464	-3.8210200	0.2203692	H	5.9267127	4.9562003	-4.7335377
H	2.4759832	-3.1608702	0.8274714	H	7.2302747	6.0779332	-4.3434612
C	5.6784074	-0.9162599	-1.5009784	H	7.5512742	4.6938146	-5.3885508
H	6.0502040	-1.8857061	-1.8303367	C	5.8146715	3.8426187	4.7683303
H	6.5469962	-0.2888863	-1.2973487	H	4.9080218	3.8565036	4.1548340
H	5.1556048	-1.0733401	-0.5603095	H	5.6172600	3.2178033	5.6392294
C	4.7291237	1.7940395	-5.6965818	H	6.0033931	4.8584630	5.1285105
H	3.8673614	2.0359920	-6.3165295	C	7.1518977	-5.0676983	4.5709203
H	5.2276214	2.7282363	-5.4393860	H	6.0930883	-5.0299243	4.8499848
H	5.4281049	1.2193990	-6.3040278	H	7.4042026	-6.1096318	4.3766438
C	5.0581972	2.8990962	-1.2554697	H	7.7397631	-4.7370187	5.4322802
H	5.2525159	3.4278136	-2.1887266	O	-6.9419925	4.2732215	-3.0608648
H	5.9951055	2.4366344	-0.9462339	H	-7.0482612	3.3112789	-3.2722057
H	4.3531454	2.1057535	-1.4893361	C	-5.8321112	4.7766908	-3.7627001
C	5.2790785	6.5763096	2.2843256	H	-5.7613828	5.8483332	-3.5792199
H	5.8260789	6.1456854	3.1200974	H	-4.8878100	4.3193870	-3.4454955
H	6.0030173	7.1316965	1.6887572	H	-5.9333508	4.6268149	-4.8415400
H	4.5626606	7.2907173	2.6874633	O	-7.1574526	-3.2388318	-4.2437489
C	5.2375231	-6.5437803	-2.1848836	H	-7.2128456	-3.6825113	-3.3662594
H	4.5165812	-7.2543626	-2.5866923	C	-6.2331939	-3.9273335	-5.0498877
H	5.7709520	-6.0997752	-3.0228559	H	-6.2250558	-3.4673868	-6.0372855
H	5.9724277	-7.1058207	-1.6091912	H	-5.2127319	-3.8867881	-4.6537546
C	5.0697188	-2.9014915	1.3950205	H	-6.5059638	-4.9798140	-5.1728841
H	5.2659659	-3.4381703	2.3235671	O	-6.9547801	-4.2978900	3.0100217
H	6.0089995	-2.4468859	1.0823013	H	-7.0430153	-3.3306492	3.1959321
H	4.3744530	-2.1021423	1.6389024	C	-5.8478416	-4.8010213	3.7172139
C	4.8958679	-1.9218350	5.8188120	H	-5.8018658	-5.8794148	3.5691596
H	4.0634191	-2.1768019	6.4727145	H	-4.8978795	-4.3748124	3.3747106
H	5.3728143	-2.8514632	5.5100216	H	-5.9343015	-4.6131636	4.7913433
H	5.6285736	-1.3710175	6.4077742	O	-7.1507542	3.2284394	4.2190911
C	5.6223717	1.0014098	1.7128835	H	-7.2151430	3.6608663	3.3353987
H	6.5183585	0.4321336	1.4635962	C	-6.2355719	3.9403170	5.0151694
H	5.0652748	1.1630236	0.7927582	H	-6.2231507	3.4968736	6.0099986
H	5.9454210	1.9792683	2.0681198	H	-5.2141796	3.9057870	4.6206980
C	3.1871643	5.4489049	1.5260167	H	-6.5210375	4.9912722	5.1205090
H	2.6341121	6.1020286	2.1924137	C	-8.4948363	-1.0460046	-0.1867169
N	2.4678174	4.6038283	0.8058760	C	-9.9165644	-1.2644487	0.2963256
N	2.5565353	-0.3721573	3.3431184	C	-10.3250300	1.0066355	0.1502416
N	2.4463178	-4.6041091	-0.6269575	C	-8.9072288	1.2340785	-0.3423692
N	2.5131708	0.2912494	-3.0785718	H	-10.5664350	-1.5056567	-0.5595485
C	3.0610605	-1.0569433	4.3562358	H	-9.9579002	-2.1034875	0.9919667
H	2.3468001	-1.5760793	4.9868675	H	-7.8216696	-0.9555044	0.6785068
C	3.1546946	-5.4410361	-1.3673119	H	-8.1582584	-1.8926886	-0.7866022
H	2.5909746	-6.0933917	-2.0255114	H	-11.0040429	0.9027623	-0.7102767
C	3.3840302	0.2870622	2.5509466	H	-10.6624465	1.8607483	0.7398919
H	2.9324060	0.8372329	1.7312504	H	-8.8844616	2.0574532	-1.0570605
C	2.9633202	0.9462099	-4.1362903	H	-8.2585815	1.5003317	0.5075269
H	2.2138264	1.4218062	-4.7604134	O	-10.3906677	-0.1298493	0.9788261
O	6.5962869	-3.2621054	-3.9666039	O	-8.4080870	0.0968912	-1.0047248
H	6.8534281	-3.7725666	-3.1665412				

Cartesian coordinates (in Å) and SCF energies (in a.u.) of the modified iodine capsules and the modified hemispheres on the PBEh-3c level of theory.

I-capsule with H instead of F				H	-16.8753304	2.4335075	0.5867542
380				C	-16.4629935	-0.8982783	3.4024806
Energy = -11021.08731644				H	-16.8481460	-0.1724912	4.1183183
C	-13.1884228	2.7112964	-2.9915500	H	-16.8520921	-1.8799338	3.6716290
C	-14.3374639	3.2159800	-0.4907857	C	-16.4962639	-3.3955198	-0.9470941
C	-14.2967774	1.9651973	-2.6005469	H	-16.8852125	-3.6429538	-1.9345402
C	-12.6951525	3.7189369	-2.1840566	H	-16.8895451	-2.4142531	-0.6817049
C	-13.2463550	3.9537931	-0.9377680	C	-16.4224035	0.9135709	-3.4937828
C	-14.8374740	2.2437882	-1.3503450	H	-16.8009130	1.8981728	-3.7671820
H	-11.8928704	4.3442088	-2.5450927	H	-16.8501990	0.6618602	-2.5233790
H	-15.6933119	1.6663308	-1.0246584	H	-16.8792325	-0.6425723	2.4281179
O	-12.7235257	4.9539851	-0.1497020	H	-16.9046892	-4.1099345	-0.2327664
C	-11.5088608	4.6883344	0.4232301	H	-16.8064015	0.1904998	-4.2129851
C	-11.4794504	4.2691360	1.7711309	H	-16.8726121	3.6620154	1.8397927
C	-11.4073314	1.8107504	-4.2156300	C	-9.1317816	-4.1201358	-1.6780705
C	-11.4217797	0.4511856	-4.5975067	C	-9.1907881	-4.5634859	-0.3530149
O	-12.6244569	-0.1245915	-4.9100478	C	-9.1121932	4.0787092	1.6568822
C	-13.2225894	2.9681674	2.6549511	C	-9.1563219	4.5216588	0.3311290
C	-14.3303873	0.4507261	3.1615200	C	12.5376594	3.6421009	-1.7491889
C	-12.6968903	2.1575618	3.6439591	C	13.5992849	1.3492965	-2.9485963
C	-14.3334502	2.5652085	1.9184690	C	13.6403627	3.0290651	-1.1617306
C	-14.8559827	1.3083507	2.2011520	C	11.9853106	3.1428527	-2.9144248
C	-13.2254098	0.9009387	3.8764618	C	12.4937161	1.9946588	-3.4952956
H	-11.8908879	2.5244074	4.2611090	C	14.1401272	1.8934792	-1.7885795
H	-15.7197437	0.9764210	1.6394612	H	11.1790990	3.6743495	-3.3969876
C	-13.1941128	-0.9113069	-3.9349089	H	14.9994769	1.4046813	-1.3487755
C	-14.3363341	-2.5670276	-1.9891767	O	11.9246482	1.5241116	-4.6564688
C	-12.6790567	-2.1727077	-3.6980356	C	10.7236115	0.8778280	-4.5317313
C	-14.3029842	-0.4523312	-3.2315168	C	10.7236745	-0.5350036	-4.5648913
C	-14.8455011	-1.3057846	-2.2768247	C	10.8213274	4.7275027	-0.5653028
C	-13.2218175	-2.9792943	-2.7148756	C	10.8177812	4.6871498	0.8488775
H	-11.8701988	-2.5460220	-4.3075140	O	12.0246256	4.7080343	1.4924843
H	-15.7121936	-0.9668032	-1.7239535	C	12.4824293	-1.7439446	-3.6159566
O	-12.6726288	0.1098771	4.8577309	C	13.6221641	-2.9493022	-1.3648200
O	-12.6836437	-4.2249776	-2.4999153	C	11.9668532	-2.9279238	-3.1198224
C	-11.4707813	-0.4738635	4.5571190	C	13.5942145	-1.1477639	-3.0291226
C	-11.4616317	-1.8324245	4.1717337	C	14.1322168	-1.7771078	-1.9122573
C	-11.4987301	-4.2949693	-1.8149080	C	12.5141824	-3.5126776	-1.9922472
C	-11.5435854	-4.7139826	-0.4674291	H	11.1596293	-3.4223466	-3.6386587
C	-13.2377895	-2.7207146	2.9305099	H	14.9969921	-1.3285473	-1.4414079
C	-14.3683483	-3.2177766	0.4197598	C	12.5317250	3.5141186	1.9496135
C	-14.3371258	-1.9665384	2.5295049	C	13.5948584	1.1415686	2.9851156
C	-12.7451973	-3.7325590	2.1279021	C	11.9738109	2.9279480	3.0715603
C	-13.2872771	-3.9641153	0.8769640	C	13.6372289	2.9448981	1.3235882
C	-14.8686520	-2.2415330	1.2745984	C	14.1393925	1.7692051	1.8705746
H	-11.9511134	-4.3638339	2.4965355	C	12.4817572	1.7404452	3.5672248
H	-15.7171555	-1.6577612	0.9410805	H	11.1648877	3.4227645	3.5875504
O	-12.6587989	-2.5020115	4.1579423	H	15.0034765	1.3169806	1.4019968
C	-14.9355287	-0.9110698	3.4399698	O	11.9930051	-4.6995267	-1.5329451
H	-14.6629665	-1.1792644	4.4601214	O	11.9122373	1.1784984	4.6864549
C	-14.9501473	3.4753132	0.8721922	C	10.7886184	-4.6654243	-0.8843309
H	-14.6954364	4.4977886	1.1490874	C	10.7990901	-4.7160603	0.5292185
C	-14.8945629	0.9141240	-3.5163985	C	10.7171406	0.5353556	4.5221465
H	-14.6099611	1.1796044	-4.5339458	C	10.7168153	-0.8782711	4.4967500
C	-14.9705061	-3.4720944	-0.9488823	C	12.5223922	-3.6439149	1.7097340
H	-14.7217015	-4.4966511	-1.2234801	C	13.5922257	-1.3550043	2.9081343
C	-9.1256982	-0.3967046	4.2944336	C	13.6264363	-3.0345759	1.1213737
C	-9.1016126	-1.7347890	3.8891993	C	11.9722193	-3.1429785	2.8752572
C	-9.0797583	0.3594080	-4.3114314	C	12.4847578	-1.9964141	3.4554641
C	-9.0508842	1.6985849	-3.9102476	C	14.1309040	-1.9009289	1.7479502
O	-12.6000394	2.4883479	-4.2138189	H	11.1638001	-3.6710026	3.3578211
O	-12.6712467	4.2089730	2.4451630	H	14.9914699	-1.4148392	1.3074698
O	-12.7655823	-4.9694056	0.0945420	O	12.0076614	-4.7953077	1.1610811
C	-16.4764202	3.4114479	0.8560139	C	14.2462471	-3.5977189	-0.1435401
H	-16.8721075	4.1292925	0.1379715	H	13.9981301	-4.6579581	-0.1797424
				C	14.1955174	0.1195610	-3.6072369
				H	13.9171758	0.1540675	-4.6600428

C	14.2647100	3.5898197	0.1022308	H	-10.2940001	1.2757441	4.9905225
H	14.0225707	4.6514349	0.1378715	C	-10.2803808	-2.4755063	3.8576032
C	14.1914931	-0.1265869	3.5660118	H	-10.2633754	-3.5225356	3.5902594
H	13.9115467	-0.1585627	4.6184682	C	-10.3875471	-4.8852425	0.2677653
C	8.4100402	-4.6556803	-0.8649997	H	-10.4153092	-5.2551933	1.2825613
C	8.4400324	-4.7022814	0.5313710	C	-10.2964374	-4.0146069	-2.4332681
C	8.4412819	4.6994140	0.8410964	H	-10.2514477	-3.7231955	-3.4729515
C	8.4616872	4.7298675	-0.5553031	C	-10.2533693	-0.2799624	-4.6803119
O	12.0279825	4.7964546	-1.2020733	H	-10.2522846	-1.3075207	-5.0138210
O	11.9171993	-1.1793490	-4.7363468	C	-10.2249789	2.4470490	-3.8922454
O	11.9187235	-1.5236223	4.6170642	H	-10.2037138	3.4947305	-3.6277844
C	15.7233586	0.1149530	-3.5768553	C	-7.0984260	4.0951561	0.9355074
H	16.1094614	1.0127914	-4.0586092	C	-7.0910367	-1.0099773	3.7743462
H	16.1463928	0.0805906	-2.5729454	C	-7.1255683	-4.1443697	-0.9368555
C	15.7720189	-3.5225344	-0.1425803	C	-7.0463858	0.9610268	-3.7725004
H	16.1700801	-3.9896208	-1.0429574	C	6.4000000	4.7192517	0.1923245
H	16.1713476	-4.0548203	0.7202874	C	6.3586306	0.2181636	-3.9131264
C	15.7193729	-0.1272516	3.5377955	C	6.3401853	-0.2224877	3.9442562
H	16.1034551	0.7384418	4.0767036	C	6.3744902	-4.6793336	-0.1997692
H	16.1439976	-0.0969171	2.5344356	C	9.6434026	4.7631761	-1.2829994
C	15.7899805	3.5060168	0.1003470	H	9.6374779	4.8255873	-2.3613634
H	16.1911000	3.9720927	0.9998928	C	9.6355297	4.6924125	1.5588599
H	16.1919168	4.0348732	-0.7634217	H	9.6309082	4.7095048	2.6398438
H	16.1660033	-2.5069967	-0.1050776	C	9.5479808	1.5882944	-4.4031884
H	16.1015254	-1.0253534	4.0222049	H	9.5428794	2.6690766	-4.4067109
H	16.1782643	2.4882457	0.0641301	C	9.5492025	-1.2505419	-4.4563380
H	16.1050689	-0.7508533	-4.1172578	H	9.5380198	-2.3289392	-4.5154896
C	8.3739908	0.5210048	4.2508183	C	9.5415684	1.2502225	4.4219075
C	8.3537722	-0.8759077	4.2403866	H	9.5261625	2.3292111	4.4712982
C	8.3834146	-0.5248607	-4.2625621	C	9.5407573	-1.5903909	4.3839448
C	8.3638455	0.8725529	-4.2461705	H	9.5373236	-2.6711505	4.3929069
C	-2.8594018	3.9675731	0.7195712	C	9.6248484	-4.7496646	1.2522668
C	-3.5343751	3.0582628	1.5257214	H	9.6238365	-4.8224840	2.3299562
C	-4.9191517	3.0837009	1.5858348	C	9.6018510	-4.6534105	-1.5879525
C	-5.6446977	4.0089360	0.8375707	H	9.5931614	-4.6665328	-2.6689237
C	-4.9559391	4.8904835	0.0060681	N	7.1053653	-4.6391822	-1.2906905
C	-3.5745927	4.8734117	-0.0534859	N	7.0641822	-1.3134137	4.0564486
H	-2.9901803	2.3282352	2.1100746	N	7.0776734	1.3101876	-4.0368686
H	-5.4357387	2.3724882	2.2180025	N	7.1408758	4.6923619	1.2771756
H	-5.4940536	5.6322475	-0.5693006	N	-7.8105711	3.8206875	2.0043221
H	-3.0599808	5.5850808	-0.6846413	N	-7.7644288	2.0450696	-3.5836890
C	-2.8893519	-4.0085221	-0.6830912	N	-7.8141101	-2.0886544	3.5744914
C	-3.5600868	-3.0993349	-1.4927985	N	-7.8260312	-3.8671843	-2.0126230
C	-4.9438701	-3.1285675	-1.5650279	N	-7.8306490	0.0307192	4.2241571
C	-5.6730724	-4.0575352	-0.8250751	H	-7.5289990	1.0143807	4.3342945
C	-4.9892718	-4.9391891	0.0102839	N	-7.8974002	-4.5797777	0.0860421
C	-3.6083304	-4.9184543	0.0815586	H	-7.6042854	-4.6891515	1.0741000
H	-3.0130580	-2.3661717	-2.0703865	N	-7.7882139	-0.0762398	-4.2266303
H	-5.4569938	-2.4171625	-2.1997051	H	-7.4924261	-1.0621391	-4.3330632
H	-5.5305673	-5.6833747	0.5795665	N	-7.8588570	4.5321240	-0.0953260
H	-3.0969021	-5.6300032	0.7154479	H	-7.5565168	4.6411097	-1.0805232
C	-2.8709301	0.5815313	-3.0757362	N	7.1480960	4.7461880	-0.9372102
C	-3.6133611	1.4985492	-2.3414390	H	6.8477372	4.6675788	-1.9117721
C	-4.9744188	1.6255728	-2.5729401	N	7.0903618	-0.9097161	-4.0519179
C	-5.6114137	0.8383711	-3.5310835	H	6.7601169	-1.8861379	-3.9440259
C	-4.8539497	-0.0806113	-4.2554113	N	7.1299860	-4.7200639	0.9237174
C	-3.4944108	-0.2085024	-4.0336581	H	6.8366583	-4.6514465	1.9011781
H	-3.1453320	2.1123514	-1.5832071	N	7.0769318	0.9049199	4.0650475
H	-5.5459534	2.3345458	-1.9879747	H	6.7714781	1.8859744	3.9638348
H	-5.3149810	-0.6853845	-5.0253415	I	-0.8266541	-0.4580752	2.8898382
H	-2.9242493	-0.9162382	-4.6204109	I	-0.7917768	-4.1030412	-0.6468843
C	-2.9052724	-0.6520451	3.1317219	I	-0.7974998	0.3747227	-2.8020192
C	-3.5362580	0.1360439	4.0863044	I	-0.7618879	4.0749031	0.6977411
C	-4.8991689	0.0150970	4.2897886	C	4.9290676	4.7087939	0.2257276
C	-5.6527057	-0.8950012	3.5502622	C	4.1927992	3.7908084	-0.5286008
C	-5.0084857	-1.6801640	2.5953510	C	4.2524224	5.5978379	1.0727284
C	-3.6438149	-1.5596801	2.3819777	C	2.8175756	3.7523456	-0.3245326
H	-2.9692931	0.8363335	4.6849656	H	2.2134152	3.0321618	-0.8690390
H	-5.3664188	0.6175232	5.0577609	C	4.9179672	0.1671973	-3.6169582
H	-5.5768149	-2.3822075	1.9989408	C	4.4751432	-0.4455555	-2.4415110
H	-3.1696181	-2.1716380	1.6261182	C	3.9926068	0.7484482	-4.4863403
C	-10.3449205	4.8508942	-0.3012130	C	3.1043795	-0.4485467	-2.2026775
H	-10.3603415	5.2209911	-1.3162050	H	2.7133450	-0.9098396	-1.3008828
C	-10.2848961	3.9804949	2.4008359	C	4.8933621	-0.1851824	3.6790498
H	-10.2518944	3.6891781	3.4410146	C	4.4079270	0.4809514	2.5496042
C	-10.2985083	0.2492455	4.6537976	C	4.0000921	-0.8439112	4.5282888

C	4.9035911	-4.6738920	-0.2213619	H	-7.4244010	3.6420719	-3.0526012
C	4.1703674	-3.7595735	0.5402614	C	-6.2980642	5.1849475	-3.5197172
C	4.2252381	-5.5666316	-1.0629644	H	-6.2413245	6.2407249	-3.2520228
C	2.7929307	-3.7289596	0.3492424	H	-5.3091223	4.7409782	-3.3580990
H	2.1893830	-3.0118473	0.8984784	H	-6.5213808	5.1264225	-4.5890403
C	5.4080733	-1.0145719	-1.4177474	O	-7.3180598	-2.7447237	-4.4150564
H	5.7386259	-2.0219033	-1.6695513	H	-7.4588513	-3.1679135	-3.5282867
H	6.3017032	-0.4016993	-1.2958052	C	-6.4190238	-3.5278982	-5.1585223
H	4.9116342	-1.0703302	-0.4518144	H	-6.3830066	-3.1464063	-6.1796675
C	4.3934748	1.4225224	-5.7626331	H	-5.4013079	-3.5050482	-4.7516226
H	3.5215929	1.6272801	-6.3820409	H	-6.7345009	-4.5742133	-5.2067436
H	4.8970151	2.3702059	-5.5727105	O	-7.3561047	-4.6224139	2.7374675
H	5.0821109	0.8101754	-6.3446165	H	-7.4783080	-3.6870511	3.0453368
C	4.7868844	2.8546199	-1.5308086	C	-6.3637107	-5.2357184	3.5212284
H	4.9654839	3.3526762	-2.4837889	H	-6.3096426	-6.2915939	3.2533410
H	5.7332664	2.4189478	-1.2113112	H	-5.3715619	-4.7961064	3.3675796
H	4.0946583	2.0417473	-1.7313277	H	-6.5950535	-5.1768239	4.5888309
C	4.9307982	6.7068654	1.8209031	O	-7.3384201	2.6957173	4.4134280
H	5.5060871	6.3467821	2.6706616	H	-7.4646768	3.1183764	3.5243522
H	5.6240998	7.2538936	1.1824297	C	-6.4430697	3.4732582	5.1671067
H	4.1931875	7.4160598	2.1941379	H	-6.4249358	3.0947979	6.1898445
C	4.9068511	-6.6605569	-1.8304358	H	-5.4198820	3.4399338	4.7749264
H	4.1707714	-7.3597973	-2.2247726	H	-6.7497576	4.5225034	5.2075056
H	5.4914477	-6.2837406	-2.6672535				
H	5.5936481	-7.2231120	-1.1981559				
C	4.7688687	-2.8289900	1.5451779				
H	4.9361753	-3.3315640	2.4980170				
H	5.7221763	-2.4042780	1.2331037				
H	4.0848160	-2.0084568	1.7429231				
C	4.4352912	-1.5712832	5.7635091				
H	3.5782953	-1.8088388	6.3919819				
H	4.9381283	-2.5068854	5.5204077				
H	5.1339355	-0.9821920	6.3569216				
C	5.2932738	1.1646675	1.5541791				
H	6.2198499	0.6169517	1.3809932				
H	4.7790153	1.2551322	0.6002867				
H	5.5623130	2.1728687	1.8685526				
C	2.8732152	5.4541478	1.1707697				
H	2.3073861	6.1148620	1.8192158				
N	2.1752172	4.5430655	0.5139849				
N	2.1805413	-0.1894932	3.1127848				
N	2.1474223	-4.5274768	-0.4795161				
N	2.2171098	0.1055702	-3.0110816				
C	2.6535307	-0.8064957	4.1832419				
H	1.9208571	-1.3058118	4.8091965				
C	2.8438871	-5.4348572	-1.1432146				
H	2.2751275	-6.0997295	-1.7848167				
C	3.0348198	0.4431807	2.3275633				
H	2.6139658	0.9415012	1.4595883				
C	2.6527554	0.6826666	-4.1191925				
H	1.8940670	1.1226435	-4.7585397				
O	6.3078215	-3.5167181	-3.7549806				
H	6.5542175	-3.9823322	-2.9243152				
O	7.1031456	4.0846192	-3.6726882				
H	6.9956159	3.1112469	-3.7702480				
O	6.6755393	3.6037946	3.8078010				
H	6.7888650	4.0377726	2.9310643				
O	7.1010052	-4.0875216	3.6640058				
H	6.9833216	-3.1178684	3.7824336				
C	4.9555977	-3.7613507	-4.0738841				
H	4.6791656	-3.1141590	-4.9064198				
H	4.7897109	-4.7953721	-4.3897729				
H	4.2772340	-3.5427692	-3.2434723				
C	6.7630598	4.7078443	-4.8877999				
H	5.6968175	4.6201821	-5.1249726				
H	6.9971204	5.7690244	-4.8094746				
C	7.3301792	4.3020823	-5.7309806				
H	5.7163203	4.2974408	4.5697349				
H	4.7322930	4.3203123	4.0898616				
H	5.6082054	3.7897631	5.5280741				
H	6.0227176	5.3275222	4.7767248				
C	6.8209856	-4.7423928	4.8777188				
H	5.7597792	-4.7006415	5.1471620				
H	7.0936011	-5.7922538	4.7747198				
H	7.3964870	4.3281509	5.7110409				
O	-7.2992834	4.5765821	-2.7433354				

I-RA4 with H instead of F

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Energy = -5915.874749621

C	4.6214335	4.5371653	-0.5866697
C	3.8662333	3.8745390	0.3793715
C	4.5140066	3.0227473	1.2722590
C	5.8846483	2.8382792	1.2062878
C	6.6213116	3.5169336	0.2451608
C	5.9938448	4.3655795	-0.6560261
C	2.4219306	4.0717809	0.4596007
N	1.6720664	4.3825149	-0.6230284
C	0.3749157	4.4641294	-0.2010630
C	0.4112595	4.2137231	1.1740257
N	1.7059920	3.9745114	1.5563226
C	-0.7632022	4.2365509	1.9213838
C	-1.9532879	4.4439907	1.2538250
C	-1.9763800	4.6681908	-0.1409858
C	-0.8096362	4.7139043	-0.8775814
O	-3.1869868	4.8666084	-0.7471945
C	-3.7273776	3.7801675	-1.3981328
C	-4.8240770	3.1187173	-0.8544997
C	-5.3422764	2.0510817	-1.5797725
C	-4.8181359	1.6119511	-2.7903758
C	-3.7108721	2.2954985	-3.2853770
C	-3.1942269	3.3872233	-2.6123224
O	-3.1456535	4.4846608	1.9271014
C	-3.7032830	3.2850300	2.3003374
C	-3.1842359	2.6116551	3.3907306
C	-3.7177641	1.3982294	3.7856236
C	-4.8170583	0.8557951	3.1274850
C	-5.3374382	1.5813478	2.0610981
C	-4.8131421	2.7911932	1.6201188
C	-5.4277248	3.5599909	0.4650736
C	-6.9547584	3.5067468	0.4649107
C	-5.4300530	0.4550403	-3.5584670
C	-4.8231227	-0.8627569	-3.1164383
C	-3.7245921	-1.4036120	-3.7771505
C	-3.1884170	-2.6162748	-3.3835235
C	-3.7039404	-3.2903796	-2.2919176
C	-4.8129057	-2.7981545	-1.6091086
C	-5.3399685	-1.5890650	-2.0488552
O	-3.1528238	1.9235541	-4.4852778
C	-1.9584007	1.2538943	-4.4435919
C	-1.9770502	-0.1413960	-4.6651077
C	-0.8080346	-0.8746302	-4.7074638
C	0.3740150	-0.1942660	-4.4563507
C	0.4058766	1.1814561	-4.2088831
C	-0.7705834	1.9253961	-4.2359630
N	1.6986277	1.5676200	-3.9654293
C	2.4176779	0.4724686	-4.0570557

C	1.6719456	-0.6126794	-4.3688846	C	3.0902199	4.1532578	4.7359092
D	-3.1856324	-0.7516046	-4.8636564	D	2.1768382	-3.2652408	-4.1342010
C	3.8605222	0.3955521	-3.8485783	C	3.0879550	-4.1470709	-4.7415018
C	4.4985168	1.2898821	-2.9909905	D	2.1844478	-4.1423939	3.2705357
C	5.8669725	1.2246996	-2.7909968	C	3.1033965	-4.7396962	4.1510902
C	6.6113090	0.2629302	-3.4602284	H	-2.3924778	3.9567890	-3.0570284
C	5.9939315	-0.6383799	-4.3161478	H	-6.2009400	1.5301851	-1.1765089
C	4.6234314	-0.5700365	-4.5028793	H	-2.3804840	3.0557689	3.9579437
D	-3.1754062	0.7470526	4.8709493	H	-6.1981933	1.1790634	1.5429329
C	-1.9664091	0.1385286	4.6697135	H	-2.3853835	-3.0592493	-3.9526454
C	-1.9462795	-1.2567130	4.4480202	H	-6.2001051	-1.1880174	-1.5286871
C	-0.7579676	-1.9265206	4.2377290	H	-2.3796871	-3.9602763	3.0624146
C	0.4173866	-1.1809162	4.2081706	H	-6.1959980	-1.5391689	1.1907307
C	0.3841180	0.1947210	4.4559157	H	-5.1554633	-0.6008558	4.6185613
C	-0.7983327	0.8733773	4.7097061	H	-5.1645328	4.6081908	0.6034267
N	1.6812437	0.6149970	4.3656379	H	-5.1673480	0.5933832	-4.6067864
C	2.4278255	-0.4690110	4.0518969	H	-5.1592175	-4.6156560	-0.5916244
N	1.7101645	-1.5652168	3.9618868	H	-7.3495932	4.1250175	-0.3408374
C	-5.4210594	-0.4628899	3.5709235	H	-7.3629395	2.5048409	0.3321091
C	-4.8093482	-1.6189545	2.8013915	H	-7.3408735	0.3451201	4.1400888
C	-3.6999212	-2.3008662	3.2937856	H	-7.3359142	-1.4041191	3.9067445
C	-3.1832653	-3.3918535	2.6195454	H	-7.3402494	-3.9010357	-1.3913573
C	-3.7186837	-3.7855788	1.4066016	H	-7.3601893	-2.5156707	-0.3152057
C	-4.8176267	-3.1257354	0.8655444	H	-7.3471565	1.3934475	-3.8892574
C	-5.3356779	-2.0588519	1.5920209	H	-7.3647592	0.3186774	-2.5028184
D	-3.1437141	-4.4892022	-1.9199861	H	-7.3588135	-0.3292102	2.5205052
C	-1.9498319	-4.4468227	-1.2495023	H	-7.3428015	-4.1358324	0.3576912
C	-1.9693422	-4.6710908	0.1453556	H	-7.3502153	-0.3558254	-4.1223683
C	-0.8008015	-4.7152179	0.8792026	H	-7.3426478	3.8902460	1.4082029
C	0.3817871	-4.4635940	0.1999384	H	-0.8193357	4.9318396	-1.9357999
C	0.4145365	-4.2130510	-1.1752109	H	-0.7352360	4.0933662	2.9922066
C	-0.7616063	-4.2377056	-1.9198381	H	-0.8054903	1.9320521	4.9254382
N	1.7079892	-3.9717344	-1.5605017	H	-0.7321293	-2.9976467	4.0964833
C	2.4266464	-4.0680262	-0.4654790	H	-0.8076857	-4.9333566	1.9373994
N	1.6797925	-4.3799800	0.6188846	H	-0.7363084	-4.0946538	-2.9907434
C	-5.4236637	-3.5678572	-0.4526461	H	-0.8141553	-1.9333583	-4.9229712
C	-6.9507737	-3.5169481	-0.4489577	H	-0.7459405	2.9965719	-4.0948939
D	-3.1396490	-1.9280805	4.4923883	H	1.9794565	1.6063046	4.3422196
C	3.8700252	-0.3899161	3.8398443	H	1.9792096	-4.3588252	1.6099992
C	4.6330370	0.5771649	4.4918097	H	1.9717046	-1.6035742	-4.3463426
C	6.0029954	0.6474080	4.3018740	H	1.9691717	4.3618303	-1.6148575
C	6.6197072	-0.2534649	3.4450280	H	2.0388734	3.1980	

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C	2.9627963	1.0322485	-5.2038181
C	4.3490118	1.0712059	-5.2958946
C	5.0715718	0.3679915	-4.3255072
C	4.3878523	-0.3438048	-3.3361372
C	2.9984790	-0.2970248	-3.3630939
N	2.3039901	0.3736424	-4.2651010
C	6.5425005	0.3853994	-4.3604201
N	7.2780551	1.4732032	-4.3582586
C	8.5781478	1.0370866	-4.4370026
C	8.5963914	-0.3587352	-4.4901215
N	7.2858073	-0.7425048	-4.4375512
C	9.7721993	1.7533649	-4.4817875
C	10.9515282	1.0417237	-4.5548293

C	10.9508317	-0.3708556	-4.6277145	C	4.3884248	0.3406717	3.3366990
C	9.7718135	-1.0864831	-4.6093827	C	2.9989862	0.2931701	3.3604847
O	12.1583653	1.6839732	-4.6095729	N	2.3028100	-0.3756738	4.2625403
C	12.7000112	2.1054977	-3.4171880	C	2.9597905	-1.0315532	5.2044642
C	13.8075691	1.4522078	-2.8842933	C	4.3458176	-1.0697177	5.2996582
C	14.3313250	1.9579420	-1.6991932	C	5.0764855	-4.3648042	-0.3636963
C	13.8074794	3.0583087	-1.0305720	C	4.3873072	-3.3802695	0.3493228
C	12.6960530	3.6725469	-1.5994305	C	2.9980888	-3.4131827	0.3002733
C	12.1653003	3.2173774	-2.7922448	N	2.3086330	-4.3172062	-0.3727475
O	12.1520812	4.7853058	-1.0015943	C	2.9726094	-5.2520571	-1.0317745
C	10.9511335	4.6407488	-0.3675245	C	4.3592740	-5.3376499	-1.0691734
C	10.9508287	4.5659804	1.0449700	C	5.0618642	2.2973973	-1.1288116
C	9.7708979	4.4952151	1.7558396	C	5.0060077	6.4519970	1.8287962
C	8.5770875	4.4555329	1.0388219	C	5.0746109	-1.1177222	-2.2530901
C	8.5962289	4.5115711	-0.3568914	C	4.9965485	1.8214098	-6.4202333
C	9.7724782	4.6273684	-1.0838577	C	5.0777459	1.1134721	2.2544853
N	7.2855306	4.4655825	-0.7413669	C	4.9917192	-1.8173576	6.4266272
C	6.5413183	4.3891145	0.3859919	C	5.0677001	-2.2982584	1.1301323
N	7.2764787	4.3808771	1.4740020	C	5.0131084	-6.4588296	-1.8186995
C	14.4186623	0.2497246	-3.5783454	O	7.0370570	-3.4766499	-4.0874850
C	15.9455689	0.2456324	-3.5255623	C	6.4538435	-4.4441869	-4.9268819
C	14.4183139	3.5868111	0.2538371	O	7.0347539	3.4758881	4.0960466
C	15.9451855	3.5335476	0.2502073	C	6.4541525	4.4448525	4.9355883
O	12.1510199	-1.0058374	-4.7749265	O	7.0575930	4.1053953	-3.4780363
C	12.6966531	-1.6040731	-3.6631994	C	6.5035713	4.9423122	-4.4647316
C	12.1678169	-2.7980350	-3.2087899	O	7.0570892	-4.1053372	3.4842257
C	12.7039247	-3.4232394	-2.0976745	C	6.4949084	-4.9400926	4.4681445
C	13.8107216	-2.8890970	-1.4441077	I	-0.5943856	-4.3287503	-0.4974789
C	14.3325437	-1.7028291	-1.9491159	C	-2.6922308	-4.3767090	-0.6175701
C	13.8079300	-1.0344937	-3.0492426	C	-3.3781341	-3.3785059	-1.2912512
O	12.1574467	4.6179657	1.6878302	C	-4.7675455	-3.4017786	-1.3485760
C	12.6983438	3.4249827	2.1085675	C	-5.5091844	-4.4246097	-0.7530302
C	12.1628818	2.7994302	3.2197652	C	-4.7968484	-5.4240420	-0.0841436
C	12.6934811	1.6064653	3.6748009	C	-3.4041977	-5.3979526	-0.0128586
C	13.8055456	1.0381347	3.0611875	C	-6.9693467	-4.4264579	-0.8118671
C	14.3298139	1.7071391	1.9612778	N	-7.6713346	-4.2062221	-1.8985001
C	13.8063254	2.8924090	1.4556972	C	-8.9797891	-4.3392351	-1.5087496
C	14.4230411	-3.5825828	-0.2418746	C	-9.0289770	-4.6442141	-0.1446722
C	15.9498324	-3.5272464	-0.2373580	N	-7.7326239	-4.7022854	0.2691766
O	12.1647403	-4.6173053	-1.6776481	C	-10.2213209	-4.8423938	0.5359968
C	10.9576718	-4.5668039	-1.0355327	C	-11.3827997	-4.7000538	-0.1900964
C	10.9569958	-4.6406932	0.3770003	C	-11.3549147	-4.4018175	-1.5742196
C	9.7778261	-4.6276145	1.0924492	C	-10.1613609	-4.2355893	-2.2441469
C	8.6020741	-4.5131372	0.3645316	O	-12.5530409	-4.3530894	-2.2358861
C	8.5838340	-4.4585874	-1.0312414	C	-13.0988776	-3.1214748	-2.5080494
C	9.7781809	-4.4978376	-1.7473420	C	-14.2166654	-2.6829436	-1.8025849
N	7.2911272	-4.4673486	0.7480825	C	-14.7466504	-1.4482268	-2.1596246
C	6.5476379	-4.3926524	-0.3798860	C	-14.2275638	-0.6489763	-3.1711358
N	7.2834920	-4.3852690	-1.4674118	C	-13.1184676	-1.1351422	-3.8550540
C	14.4171859	-0.2456037	3.5903596	C	-12.5707959	-2.3649906	-3.5383997
C	15.9441274	-0.2401549	3.5387268	O	-12.5962179	-0.4083776	-4.8990735
O	12.1484666	1.0077549	4.7866085	C	-11.3829429	0.1877302	-4.7011305
C	10.9487077	0.3720870	4.6389114	C	-11.3588232	1.5722187	-4.4044521
C	10.9501478	-1.0403860	4.5642876	C	-10.1671812	2.2450226	-4.2360550
C	9.7712105	-1.7524763	4.4890638	C	-8.9839257	1.5119408	-4.3353952
C	8.5768574	-1.0366927	4.4444126	C	-9.0294302	0.1474843	-4.6388709
C	8.5944239	0.3590351	4.4999253	C	-10.2195933	-0.5360058	-4.8398509
C	9.7693772	1.0871612	4.6208854	N	-7.6766406	1.9041448	-4.1978261
N	7.2769603	-1.4732098	4.3637424	C	-6.9718179	0.8185117	-4.4137517
C	6.5410745	-0.3856661	4.3667436	N	-7.7320418	-0.2641185	-4.6911193
N	7.2837440	0.7424023	4.4466443	O	-12.5587491	2.2307768	-4.3577613
O	12.1575815	-4.7837965	1.0120620	C	-13.1051874	2.5026545	-3.1263568
C	12.6997463	-3.6704394	1.6103397	C	-14.2209252	1.7944977	-2.6869197
C	13.8106650	-3.0546716	1.0420576	C	-14.7508192	2.1506142	-1.4518740
C	14.3325527	-1.9535073	1.7108251	C	-14.2333031	3.1633408	-0.6530828
C	13.8075395	-1.4484981	2.8956986	C	-13.1260385	3.8495599	-1.1400176
C	12.7003894	-2.1030721	3.4278332	C	-12.5790270	3.5344008	-2.3704978
C	12.1677296	-3.2159447	2.8028422	C	-14.8400434	3.5213610	0.6898124
O	12.1572455	-1.6820924	4.6197274	C	-16.3667659	3.4682732	0.6846678
C	5.0702028	4.3609224	0.3692910	C	-14.8351385	0.6932238	-3.5305641
C	4.3812304	3.3775216	-0.3455829	C	-16.3619451	0.6866535	-3.4797391
C	2.9920559	3.4096546	-0.2959651	O	-12.6046827	4.8940144	-0.4132892
N	2.3024360	4.3122207	0.3788239	C	-11.3902196	4.6983494	0.1812441
C	2.9661258	5.2462581	1.0392115	C	-11.3638750	4.4007521	1.5655363
C	4.3527851	5.3322545	1.0766066	C	-10.1709882	4.2358125	2.2370043
C	5.0701337	-0.3685906	4.3291345	C	-8.9886067	4.3397737	1.5030005

C	-9.0363204	4.6435781	0.1386462	H	-16.7750593	2.4777852	0.4839011
C	-10.2279312	4.8408705	-0.5435282	H	-16.7592932	0.0679231	4.1347000
N	-7.7394742	4.7016392	-0.2738297	H	-16.7533079	-1.6617886	3.7842341
C	-6.9773985	4.4270229	0.8082858	H	-16.7474607	-3.7961027	-1.6676098
N	-7.6804710	4.2076095	1.8943270	H	-16.7703711	-2.4868173	-0.4998528
O	-12.5628744	4.3508726	2.2255393	H	-16.7513012	1.6526223	-3.8002846
C	-13.1074743	3.1185593	2.4971112	H	-16.7715389	0.4863115	-2.4897002
C	-12.5794575	2.3628293	3.5280445	H	-16.7737289	-0.4956729	2.4734771
C	-13.1251933	1.1318793	3.8437722	H	-16.7540107	-4.1486919	0.0616709
C	-14.2326321	0.6439655	3.1584146	H	-16.7539886	-0.0770581	-4.1509595
C	-14.7518382	1.4425013	2.1463646	H	-16.7557191	3.7875177	1.6512299
C	-14.2234383	2.6780608	1.7899311	H	11.3558745	3.7565626	-3.2605965
C	-14.8383804	-0.6992953	3.5169018	H	15.1958263	1.4662740	-1.2729468
C	-16.3651194	-0.6952224	3.4640836	H	11.3589697	-3.2672246	-3.7481582
O	-12.6027251	0.4058444	4.8882362	H	15.1964670	-1.2756026	-1.4572925
C	-11.3885085	-0.1887337	4.6910559	H	11.3531664	3.2676485	3.7586548
C	-11.3624444	-1.5732795	4.3948082	H	15.1947154	1.2812313	1.4700239
C	-10.1698648	-2.2444554	4.2268607	H	11.3588387	-3.7561384	3.2709794
C	-8.9877343	-1.5097881	4.3261654	H	15.1964889	-1.4605468	1.2849276
C	-9.0348863	-0.1454145	4.6297226	H	14.1617284	-4.6379820	-0.3120148
C	-10.2260793	0.5365260	4.8300755	H	14.1555485	0.3194461	-4.6333232
N	-7.6800809	-1.9003379	4.1883091	H	14.1555386	4.6418536	0.3239929
C	-6.9765774	-0.8138303	4.4040499	H	14.1533899	-0.3158411	4.6451321
N	-7.7379514	0.2677903	4.6819102	H	16.3373274	1.1595970	-3.9709711
C	-14.8334854	-3.5274016	-0.7034999	H	16.3542750	0.1776237	-2.5174507
C	-16.3602876	-3.4766100	-0.7004158	H	16.3426173	-3.9715042	-1.1514404
O	-12.5613224	-2.2335994	4.3472612	H	16.3414177	-4.0910513	0.6088490
C	-13.1056168	-2.5064197	3.1150981	H	16.3338605	0.6063530	4.1033606
C	-14.2214313	-1.7995632	2.6739583	H	16.3535351	-0.1712920	2.5309604
C	-14.7491165	-2.1564574	1.4381694	H	16.3368388	3.9781306	1.1646166
C	-14.2291069	-3.1685481	0.6402134	H	16.3365069	4.0980524	-0.5956524
C	-13.1215758	-3.8533240	1.1287410	H	16.3568872	-2.5185221	-0.1686090
C	-12.5768565	-3.5374419	2.3600281	H	16.3364042	-1.1539556	3.9840123
O	-12.5977795	-4.8971363	0.4028778	H	16.3536411	2.5253861	0.1814886
C	-5.5170477	4.4253137	0.7517538	H	16.3365003	-0.6007721	-4.0895170
C	-4.7769712	3.3984750	1.3421701	H	-2.8577471	2.5528370	1.7492837
C	-3.3875181	3.3749549	1.2866643	C	-5.4257028	2.2745183	1.9314951
C	-2.7003648	4.3769800	0.6198710	C	-5.4648770	6.5314779	-0.5349771
C	-3.4109744	5.4022230	0.0202779	H	-2.8992321	6.1981904	-0.5033438
C	-4.8037046	5.4283033	0.0896075	H	-2.8474183	-2.5594941	-1.7582826
I	-0.6027047	4.3276383	0.5010107	C	-5.4134145	-2.2813752	-1.9476893
C	-5.5162616	-0.7576372	4.3949418	C	-5.4581274	-6.5240675	0.5455884
C	-4.7979159	-0.1027961	5.3988867	H	-2.8936234	-6.1912236	0.5159757
C	-3.4054263	-0.0333495	5.3660081	H	-2.8617423	1.7485237	-2.5134948
C	-2.7004723	-0.6256771	4.3326396	C	-5.4319458	1.9297065	-2.2474846
C	-3.3928513	-1.2849489	3.3291976	C	-5.4504597	-0.5161321	-6.5156010
C	-4.7822372	-1.3402149	3.3594902	H	-2.8859112	-0.4878094	-6.1691278
I	-0.6030016	-0.5045321	4.2744199	H	-2.8894200	0.4848394	6.1627706
C	-5.5115197	0.7628053	-4.4053388	C	-5.4539318	0.5159942	6.5083023
C	-4.7768778	1.3478038	-3.3716928	C	-5.4378170	-1.9182251	2.2333084
C	-3.3875860	1.2905910	-3.3407348	H	-2.8673732	-1.7413411	2.5008793
C	-2.6958785	0.6274391	-4.3419720	H	-10.2370456	5.1094054	-1.5897307
C	-3.4014446	0.0333068	-5.3739526	H	-10.1447648	4.0387688	3.2996654
C	-4.7937864	0.1045741	-5.4075678	H	-10.2347216	1.5830530	5.0973248
I	-0.5985626	0.5035657	-4.2821764	H	-10.1435687	-3.3071404	4.0301032
O	-7.6004706	-3.0304459	-4.5053645	H	-10.2316426	-5.1116968	1.5819992
C	-6.9306053	-3.9235746	-5.3640164	H	-10.1339162	-4.0376594	-3.3066168
O	-7.5987716	3.0314315	4.4973275	H	-10.2266894	-1.5824984	-5.1072732
C	-6.9341975	3.9267762	5.3576698	H	-10.1424431	3.3077481	-4.0392787
O	-7.5812551	-4.5035685	3.0268256	H	9.7594197	4.7171140	-2.1602136
C	-6.9312942	-5.3562527	3.9399966	H	9.7673100	4.4827904	2.8368013
O	-7.5893945	4.5069630	-3.0334632	H	9.7692921	2.8343312	-4.4705420
C	-6.9323489	5.3648762	-3.9366126	H	9.7578632	-2.1629418	-4.6978953
H	-11.7628531	4.1209813	-2.7647844	H	9.7548163	2.1635284	4.7103476
H	-15.6146657	1.6073495	-1.0911123	H	9.7687160	-2.8334216	4.4758710
H	-11.7628685	2.7577169	4.1136811	H	9.7639643	-4.7165459	2.1688612
H	-15.6162556	1.0813315	1.6042863	H	9.7754708	-4.4866743	-2.8283181
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H	-15.6121854	-1.0883998	-1.6184460	H	-7.4593796	-4.6929545	1.2637435
H	-11.7604755	-4.1229611	2.7554563	H	-7.4577499	-1.2578920	-4.6808824
H	-15.6132012	-1.6143778	1.0761910	H	-7.4649205	4.6922231	-1.2679314
H	-14.5750652	-0.9044208	4.5539222	H	6.9803306	4.4098661	-1.7216565
H	-14.5770155	4.5583314	0.8955420	H	6.9797185	-1.7228604	-4.3813673
H	-14.5708271	0.8987047	-4.5672588	H	6.9851323	-4.4111998	1.7281562
H	-14.5685952	-4.5639296	-0.9090305	H	6.9773555	1.7226886	4.3898416
H	-16.7604916	4.1394968	-0.0781744	H	2.4149716	2.6614223	-0.8306127

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H	2.4208793	-2.6638690	0.8332713
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H	5.9689260	-0.6142170	-1.8862834
H	4.4017831	-1.2631695	-1.4101754
H	4.2591168	2.0884671	-7.1755890
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H	5.7731914	1.2311977	-6.9058657
H	5.3550344	2.6396634	-2.1213751
H	5.9590890	1.9267273	-0.6335392
H	4.3870678	1.4561747	-1.2748972
H	5.4797825	6.1033646	2.7448882
H	5.7819652	6.9374770	1.2375100
H	4.2715493	7.2085469	2.1006610
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H	5.4927669	-6.1112106	-2.7320718
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H	5.3605524	-2.6379593	2.1236505
H	5.9650527	-1.9289183	0.6341143
H	4.3929041	-1.4566355	1.2737030
H	4.2525925	-2.0863646	7.1796219
H	5.4675726	-2.7348160	6.0843168
H	5.7646807	-1.2241679	6.9145914
H	5.9749774	0.6114778	1.8928274
H	4.4082216	1.2549777	1.4082992
H	5.3730092	2.1075064	2.5906186
H	2.3653193	5.9780004	1.5690509
H	2.3537380	-1.5568678	5.9351689
H	2.3720254	-5.9848031	-1.5604713
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H	7.0549306	-3.8127032	-3.1616575
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H	5.4255425	-4.7558999	4.6177394
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H	6.9984493	-4.8322738	5.4336840
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H	-5.8644213	-5.1284339	4.0398355
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I-RA4 with 2 CN and 2 H instead of 4 F

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C	0.2917072	-4.6299721	0.2740282
N	1.5882991	-4.6554933	0.6899606
C	-0.8433394	-4.4111902	-1.8524490
C	-2.0354269	-4.5205749	-1.1690913
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C	-0.8994939	-4.7682254	0.9714707
O	-3.2342391	-4.5348190	-1.8291594
C	-3.7827503	-3.3333915	-2.2104029
C	-3.2559492	-2.6722329	-3.3048067
C	-3.8031631	-1.4748657	-3.7283983
C	-4.9117930	-0.9294474	-3.0897527
C	-5.4304588	-1.6359912	-2.0109758
C	-4.8999313	-2.8340009	-1.5454855
C	-5.5202494	0.3754707	-3.5665968
C	-7.0470158	0.3733406	-3.5127293
O	-3.2788778	-0.8431914	-4.8321355
C	-2.0661697	-0.2335736	-4.6846275
C	-2.0424313	1.1724023	-4.5120040
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C	0.3317764	1.1178135	-4.4318414
C	0.2868525	-0.2680616	-4.6143511
C	-0.9031553	-0.9670328	-4.7553965
N	1.6386558	1.5214736	-4.3329930
C	2.3437858	0.4215987	-4.4571904
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C	-5.5156940	-3.5769013	-0.3745143
C	-7.0425008	-3.5246268	-0.3733478
O	-3.2419636	1.8310786	-4.5279985
C	-3.7895736	2.2134912	-3.3265034
C	-4.9048959	1.5473685	-2.8247392
C	-5.4338820	2.0129156	-1.6260207
C	-4.9149489	3.0926159	-0.9210072
C	-3.8081505	3.7323145	-1.4688121
C	-3.2629918	3.3090917	-2.6671818
O	-3.2837457	4.8365344	-0.8381935
C	-2.0686738	4.6915152	-0.2327288
C	-2.0396386	4.5177935	1.1730415
C	-0.8460462	4.4103637	1.8540846
C	0.3351352	4.4479210	1.1111158
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N	1.6441042	4.3562455	1.5104352
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C	3.8040411	4.5062681	0.3545049
C	4.4974002	5.4612222	-0.3957005
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C	6.6135148	4.5246674	0.2520173
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I	8.7027546	4.5237635	0.1626376
O	-3.2371623	4.5302468	1.8355282
C	-3.7830706	3.3279579	2.2178559
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C	-5.4286600	1.6280878	2.0217976
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C	-5.5201303	3.5689714	0.3855739
C	-7.0468654	3.5146448	0.3875457
O	-3.2700123	0.8383546	4.8383976
C	-2.0567062	0.2305741	4.6882544
C	-2.0312137	-1.1753872	4.5157857
C	-0.8395037	-1.8584382	4.4015467
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C	-0.8946512	0.9657754	4.7564539	H	-7.4345624	3.9179999	1.3225942
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N	1.6500600	-1.5188803	4.3289171	H	-0.9027762	2.0314875	4.9318794
C	-5.5122359	-0.3834746	3.5777142	H	-0.8134501	-2.9344875	4.3012040
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C	3.8037969	0.3780068	-4.4695236	H	-0.8175410	-4.3100377	-2.9284571
C	4.5509824	1.0655848	-3.5102785	H	-0.9100919	-2.0327400	-4.9309407
C	5.9413606	1.0395556	-3.5113861	H	-0.8268206	2.9332807	-4.2994111
C	6.6132235	0.3043988	-4.4732010	H	1.8665905	1.6752265	4.5397477
C	5.9029495	-0.3967247	-5.4302210	H	1.8630583	-4.5638357	1.6805509
C	4.5092315	-0.3555871	-5.4279785	H	1.8597423	-1.6722760	-4.5446692
I	8.7033986	0.2385670	-4.4634130	H	1.8530915	4.5660629	-1.6843374
O	-3.2297282	-1.8359015	4.5343901	H	1.7928396	3.2804143	-3.6780417
C	-3.7793956	-2.2190048	3.3340178	H	2.2524943	6.0517593	-4.1341933
C	-4.8967834	-1.5545470	2.8346556	H	3.4178184	4.7843163	-4.5202579
C	-5.4275074	-2.0207501	1.6369569	H	1.8771052	4.8645751	-5.3899261
C	-4.9085388	-3.0997019	0.9308488	H	1.7893123	-3.6817555	-3.2770513
C	-3.7997206	-3.7378592	1.4763586	H	2.2475933	-4.1054594	-6.0531475
C	-3.2526865	-3.3138997	2.6736123	H	1.8746385	-5.3786224	-4.8838147
C	3.8137111	-0.3719894	4.4607790	H	1.8052625	-3.2777422	3.6744845
C	4.5201041	0.3629595	5.4174982	H	2.2677879	-6.0492469	4.1277520
C	5.9137654	0.4058938	5.4169015	H	3.4258205	-4.7786820	4.5254442
C	6.6229807	-0.2946441	4.4586588	H	1.8797770	-4.8675333	5.3847374
C	5.9501280	-1.0310901	3.4985132	H	1.7915177	3.6859431	3.2734285
C	4.5597845	-1.0590207	3.5002956	H	2.2411680	4.1081553	6.0514145
O	-3.2750515	-4.8412955	0.8446012	H	3.4026629	4.5182614	4.7883568
I	8.7130354	-0.2259713	4.4444876	H	1.8587983	5.3809667	4.8846896
I	8.7089514	-4.5139041	-0.1812054	H	3.4109499	-4.5025680	-4.7875089
O	1.7491178	-4.2185909	3.4115605	N	3.3675638	1.7050813	7.2946857
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C	2.3499764	5.0040256	-4.4134439	N	3.3389346	-7.3196406	1.7343668
O	1.7222361	-3.4134119	-4.2151751	N	3.4852445	-2.2599512	1.4941496
C	2.3432920	-4.3981449	-5.0089016	N	3.5222523	-1.5617451	-2.3035740
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C	3.8494544	1.0928940	6.4475814				
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H	6.4879239	-1.5691706	2.7301101				
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C	3.9445819	-2.4769210	-1.7509169				
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C	3.9150681	1.7361063	-2.4246214				
H	6.4800236	1.5780265	-2.7438618				
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C	3.8374310	-1.0860034	-6.4569596				
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H	6.3877236	6.2277710	-1.0413693				
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H	-2.4485985	3.8590523	-3.1140431				
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H	-5.2471522	-0.4955193	4.6285065				
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H	-7.4421967	4.1155632	-0.4309958				
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H	-7.4267850	-1.3178985	3.9328018				
H	-7.4315706	-3.9284610	-1.3076190				
H	-7.4516953	-2.5206653	-0.2608740				
H	-7.4370578	1.3069822	-3.9170823				
H	-7.4550517	0.2617098	-2.5082013				
H	-7.4497537	-0.2726777	2.5239659				
H	-7.4353338	-4.1261216	0.4459737				
H	-7.4400272	-0.4468153	-4.1129718				

I-capsules with 4 CN instead of F

396

Energy = -12493.54012231

C	-2.1305943	1.8409160	-6.6497024
C	-0.7397368	1.8959234	-6.7352360
C	-0.0040302	1.1392286	-5.8241964
C	-0.6380039	0.3266458	-4.8797998
C	-2.0288775	0.2319200	-4.8249233
C	-2.7677299	1.0143364	-5.7093023
C	-0.0590307	2.6938142	-7.7547997
N	0.8688184	2.2125097	-8.5470936
C	1.1919114	3.2503294	-9.3829174
C	0.4224295	4.3699675	-9.0509955
N	-0.3716632	3.9813181	-8.0133948
C	0.5226583	5.5744935	-9.7324766
C	1.4445842	5.6360925	-10.7538343
C	2.2241934	4.5087742	-11.1128937
C	2.0945607	3.3103509	-10.4450818
O	1.5930716	6.7790555	-11.4856625
C	2.3721645	7.7756202	-10.9453314
C	3.6138318	8.0553811	-11.5058454
C	4.3361260	9.1045655	-10.9492205
C	3.8882718	9.8669717	-9.8765461
C	2.6439713	9.5409955	-9.3433681
C	1.8844103	8.5223556	-9.8888050
O	2.1237537	10.2806582	-8.3079363
C	2.0897492	9.7139147	-7.0631620
C	3.0853610	10.1102691	-6.1362823
C	3.0823629	9.6480285	-4.8389482
C	2.0823410	8.7489027	-4.4968766
C	1.0984533	8.3364273	-5.4011849
C	1.0858604	8.8417911	-6.7016573
N	1.7989176	8.1149047	-3.3237992
C	0.7035370	7.3600299	-3.5529209
N	0.2475295	7.4597883	-4.7786925
C	0.0508340	6.5644249	-2.5137637

C	-0.3050453	5.2389426	-2.7591568	C	7.8142315	3.3405102	0.0151140
C	-0.9815300	4.4815652	-1.7986178	N	8.9633678	3.2956211	-0.0198945
C	-1.3357898	5.0283222	-0.5649820	I	3.4036899	1.5529218	2.7424655
C	-0.9490020	6.3402487	-0.3018963	C	3.4385496	4.7102505	-1.7058280
C	-0.2600486	7.0980504	-1.2633851	N	2.7171918	5.1976546	-2.4560505
I	-2.3815210	3.8842502	0.8425791	C	1.4180084	1.2270526	-5.7898400
C	0.0717741	4.6000526	-3.9759995	N	2.5627616	1.2597421	-5.6941296
N	0.3551008	4.0162648	-4.9244726	I	-2.9530091	-1.0225178	-3.4262364
C	0.0964500	8.4417321	-0.9384088	C	-2.9429402	2.6119748	-7.5350181
N	0.3822920	9.5164079	-0.6433149	N	-3.6225161	3.2330862	-8.2250203
O	4.0251571	11.0102382	-6.5493808	C	9.2987583	6.2205124	-12.3332981
C	5.2596772	10.5143220	-6.8990011	O	3.9407425	8.1146673	-1.6040528
C	5.6459730	10.5157030	-8.2350046	C	3.9843740	8.5218372	-0.2551516
C	6.9228985	10.0484022	-8.5238271	O	2.7602744	0.0865578	-8.7468420
C	7.8106620	9.5820880	-7.5606311	C	2.0877327	-1.0930856	-9.1258023
C	7.3730299	9.5897287	-6.2387694	O	8.1383261	2.0764376	-3.6903589
C	6.1204026	10.0742296	-5.9101597	C	8.8650504	1.0531168	-3.0487355
C	4.7065618	11.0148199	-9.3161843	O	-1.4300921	6.1300848	-6.6658502
C	5.4219957	11.8200711	-10.3994792	C	-2.7783800	6.3702896	-6.3314503
C	4.1391029	7.2472629	-12.6767226	N	-4.0928171	-2.6458170	-1.4594482
C	4.8691160	8.1039808	-13.7093492	C	-4.7295754	-3.7671218	-1.7526299
O	3.0612133	4.6351263	-12.1877929	C	-5.3333078	-4.5815970	-0.8028328
C	4.3999958	4.8336660	-11.9461997	C	-5.2514012	-4.1707158	0.5326078
C	4.9730058	6.0806583	-12.1814784	C	-4.5897810	-2.9825548	0.8537148
C	6.3395232	6.2016224	-11.9557063	C	-4.0250647	-2.2658993	-0.1950882
C	7.1452021	5.1569480	-11.5180847	C	-6.0614203	-5.8161001	-1.2408989
C	6.5282595	3.9284741	-11.3076410	C	-5.8891861	-4.9909506	1.5748572
C	5.1748221	3.7636767	-11.5378634	N	-5.6356436	-6.2614219	1.7864620
C	8.6335357	5.3310498	-11.2843939	C	-6.5018389	-6.6468006	2.7802506
C	8.8953357	5.7960056	-9.8642663	C	-7.2880399	-5.5556496	3.1590067
C	9.1296599	4.8834671	-8.8391839	N	-6.8695027	-4.5157220	2.3770018
C	9.4122038	5.3159803	-7.5564595	C	-8.2915125	-5.6535594	4.1125705
C	9.4171524	6.6665625	-7.2594288	C	-8.4607650	-6.8814995	4.7179703
C	9.1785237	7.6167433	-8.2465336	C	-7.6593707	-7.9909738	4.3608769
C	8.9266135	7.1450702	-9.5296803	C	-6.6939353	-7.8887308	3.3810789
O	7.2843852	2.8470391	-10.9196039	C	-4.4611667	-2.4667263	2.2548036
C	7.1270567	2.4019192	-9.6385303	O	-7.9078257	-9.1841223	4.9821265
C	8.1025729	2.7724280	-8.6800738	C	-7.0779237	-9.5338188	6.0219251
C	8.0305543	2.3237499	-7.3791136	C	-7.5466965	-9.4987509	7.3319179
C	6.9482600	1.5167320	-7.0269928	C	-6.6680003	-9.9071374	8.3297343
C	6.0018361	1.1515045	-7.9897966	C	-5.3666169	-10.3308436	8.0868946
C	6.0772795	1.5731759	-9.3097111	C	-4.9428193	-10.3400662	6.7618043
N	5.1106457	0.3440741	-7.3476872	C	-5.7974546	-9.9724205	5.7395349
C	5.5246208	0.2621200	-6.0654107	O	-9.4501082	-7.0770793	5.6388190
N	6.6186241	0.9446660	-5.8252671	C	-9.2235409	-6.6354596	6.9210445
O	9.1530816	3.5359700	-9.1103200	C	-9.2938412	-5.2816739	7.1916085
C	4.8552767	-0.5632883	-5.0604091	C	-9.0738816	-4.8119602	8.4734574
C	4.5569707	-0.0394725	-3.8032133	C	-8.8246978	-5.6922857	9.5221260
C	3.9710419	-0.8299703	-2.8103113	C	-8.7935692	-7.0486352	9.2158485
C	3.6762005	-2.1746515	-3.0368057	C	-8.9866717	-7.5565422	7.9364676
C	3.9386418	-2.6916430	-4.3032225	C	-8.9595147	-9.0457471	7.6475015
C	4.5165672	-1.8938658	-5.3048653	C	-9.6177829	-9.8754433	8.7484652
O	9.7183220	7.0765067	-5.9814101	C	-4.4430912	-10.7809058	9.2035115
C	8.7695085	6.8735986	-5.0209498	C	-3.6750569	-9.5994034	9.7643058
C	7.9679100	7.9756223	-4.6328675	C	-2.4223848	-9.2527559	9.2665221
C	7.0205844	7.8533191	-3.6395163	C	-1.7174010	-8.1900937	9.8011923
C	6.8543634	6.6007153	-3.0480516	C	-2.2674997	-7.4230582	10.8109718
C	7.6631759	5.5277619	-3.4359707	C	-3.5124891	-7.7340423	11.3484395
C	8.6396248	5.6436017	-4.4151132	C	-4.1809311	-8.8231958	10.8014173
N	7.2835047	4.4752467	-2.6572332	O	-3.6758079	-10.7768070	6.4542741
C	6.2883006	4.9261326	-1.8645172	C	-2.7579580	-9.8394551	6.0746566
N	5.9969030	6.1899872	-2.0600433	C	-1.7856665	-9.4426803	7.0221652
C	9.2022791	9.0983874	-7.9233542	C	-0.7798062	-8.5604298	6.6866425
C	9.8549164	9.9355133	-9.0220073	C	-0.7736373	-8.0367967	5.3957128
O	8.2156683	9.1796909	-5.2331211	C	-1.7536851	-8.4233565	4.4779865
C	5.6472142	4.1020072	-0.8402921	C	-2.7458226	-9.3428529	4.7877077
C	6.3880781	3.3589558	0.0784475	N	-1.4537983	-7.7582414	3.3221613
C	5.7564554	2.6292364	1.0992832	C	-0.3418579	-7.0259247	3.5620501
C	4.3688707	2.6171370	1.2192718	N	0.0959556	-7.1614250	4.7921099
C	3.6285491	3.3216814	0.2695059	O	-1.8435541	-10.0028418	8.2690058
C	4.2573810	4.0572981	-0.7391862	C	0.3267950	-6.2362474	2.5153759
C	4.7819660	1.3388996	-3.5194066	C	-0.3508062	-5.2218519	1.8336756
N	4.9197709	2.4411592	-3.2249655	C	0.3541194	-4.5349492	0.8518751
I	2.8305613	-3.3458016	-1.5211064	N	1.6098377	-4.7991341	0.5339180
C	4.7704797	-2.4848370	-6.5792981	C	2.2382542	-5.7670164	1.1798607
N	4.9500354	-2.9836318	-7.6004105	C	1.6552821	-6.5278235	2.1855357

O	-9.1600012	-3.4598714	8.7126320	H	6.1628569	11.2496005	-10.9590427
C	-8.1232342	-2.6830062	8.2730375	H	5.1760539	7.4895415	-14.5553179
C	-7.1498057	-2.2845097	9.2186169	H	5.7633368	8.5946541	-13.3255640
C	-6.0922649	-1.4756182	8.8575007	H	9.3324953	9.8970839	-9.9775307
C	-6.0185951	-1.0943333	7.5252924	H	5.9387591	12.6690561	-9.9528217
C	-6.9830375	-1.4620654	6.5834977	H	4.2070138	8.8857990	-14.0808518
C	-8.0599997	-2.2605908	6.9615013	H	10.3729751	6.2676210	-12.1567027
N	-6.6736351	-0.8975743	5.3701149	H	-5.4788107	-10.0671342	4.7125251
C	-5.5689736	-0.2180651	5.5721356	H	-7.0174145	-9.8931518	9.3539113
N	-5.1294420	-0.3072062	6.8485271	H	-9.5626117	-4.5903611	6.4072765
C	-8.6101117	-5.1875195	10.9361278	H	-8.6072640	-7.7487294	10.0197988
C	-7.1332924	-4.9606284	11.1997732	H	-0.7151967	-7.9849938	9.4561206
C	-6.5491173	-3.7186103	10.9725801	H	-5.1512923	-9.0817285	11.2047677
C	-5.2140225	-3.4986281	11.2547188	H	-4.7994888	-2.5071400	11.1523356
C	-4.4177642	-4.5297239	11.7181114	H	-6.7423262	-6.9396077	11.8725718
C	-4.9529291	-5.7925939	11.9543907	H	-9.1016932	-4.2179580	11.0090239
C	-6.3071146	-5.9657814	11.6887894	H	-9.5569943	-9.2095468	6.7512391
O	-1.5444693	-6.3741945	11.3284664	H	-3.7125412	-11.4581911	8.7617844
C	-1.4458377	-5.2403789	10.5735165	H	-3.2561507	-6.4649346	13.0174572
C	-2.2487138	-4.1327455	10.9330160	H	-9.6272686	-10.9281552	8.4675962
C	-2.1458387	-2.9298071	10.2658897	H	-9.1198358	-9.8037400	9.7150434
C	-1.2552878	-2.8490432	9.1976713	H	-10.3391136	-6.1565568	11.7929414
C	-0.4844587	-3.9588848	8.8423854	H	-9.1422491	-5.6367600	12.9801253
C	-0.5459763	-5.1620579	9.5308758	H	-4.1419956	-8.5374280	13.9218709
N	0.2853407	-3.5470376	7.7907981	H	-5.6889994	-8.3082579	13.1271810
C	-0.0228234	-2.2507002	7.5563758	H	-4.4506392	-11.9390256	11.0257518
N	-0.9431595	-1.7951050	8.3739566	H	-5.6469065	-12.4575868	9.8372693
C	-4.0933129	-6.9214477	12.4903345	H	-8.8709404	-7.0870068	12.0310595
C	-4.8192841	-7.7833393	13.5216866	H	-5.1639986	-7.1643946	14.3495187
O	-7.3201023	-2.6757564	10.5159574	H	-5.9348016	-11.0280910	10.8126094
C	-4.9049416	0.6236120	4.5639546	H	-10.6489365	-9.5540437	8.8923512
C	-3.5652555	0.4198812	4.2231406	H	5.3564429	1.2474486	-10.0453371
C	-3.0156012	1.2696087	3.2702279	H	8.7900942	2.5752074	-6.6522731
N	-3.6880584	2.2488562	2.6901646	H	9.2788369	4.8116587	-4.6718162
C	-4.9528082	2.4378428	3.0267483	H	6.4297578	8.6986429	-3.3155021
C	-5.6266273	1.6590820	3.9591107	H	3.8089860	9.9823795	-4.1130112
O	-3.0948503	-4.2765891	11.9984580	H	0.3040141	8.5624843	-7.3939028
C	0.6737181	-1.4429631	6.5423483	H	-0.1089794	6.4146700	-9.4834195
C	0.6757176	-1.8196386	5.1967855	H	2.6625763	2.4377987	-10.7356905
C	1.3696004	-1.0049550	4.3095854	H	-3.4610495	-9.6665117	4.0457669
N	2.0233785	0.0839350	4.6762930	H	-0.0079520	-8.2938838	7.3949909
C	2.0219458	0.4259790	5.9535979	H	-6.1137402	-8.7473719	3.0731439
C	1.3646068	-0.2938331	6.9433899	H	-8.9217308	-4.8095499	4.3517022
C	-1.7738101	-4.8491925	2.1194928	H	0.0975659	-5.9899458	9.2710986
C	2.4419781	-7.6268314	2.8334702	H	-2.7241096	-2.0684592	10.5696326
C	-0.0322696	-3.0362732	4.6835942	H	-5.3637724	-1.1354379	9.5789629
C	1.4508761	0.1588167	8.3696345	H	-8.8292840	-2.5244089	6.2493576
C	-2.7197303	-0.6603986	4.8256846	H	7.5542143	3.4974027	-2.8552266
C	-7.0520841	1.9754583	4.2974982	H	2.4647393	8.0580163	-2.5348930
C	-5.1648514	-11.5873720	10.2817885	H	-0.8961620	4.6468191	-7.4210067
C	-9.2707250	-6.0741321	11.9903933	H	4.1905179	0.0881448	-7.7435663
O	1.6142358	-5.6307411	6.5527690	H	-2.0439295	-7.7766806	2.4787360
C	2.9932884	-5.8330343	6.3544244	H	-7.2086793	-3.5487818	2.4764129
O	-7.9140681	-2.0862275	3.1799232	H	-4.2569547	0.0568177	7.2565073
C	-8.7138126	-1.1630815	2.4796161	H	0.9068371	-4.1688994	7.2548587
O	-3.4541121	-7.9539670	1.4247217	H	-0.1252655	-3.7339345	0.2979092
C	-3.4050287	-8.4588979	0.1113611	H	-3.4945423	-1.3396625	0.0022941
O	-2.8470739	0.2342384	8.3090363	H	-1.9807813	1.1488970	2.9656763
C	-2.2997899	1.4689191	8.7065291	H	-5.3593633	-1.9375573	2.5746466
H	4.7261749	2.7866188	-11.4396101	H	-4.2813250	-3.2659776	2.9736061
H	6.8022233	7.1644581	-12.1298525	H	-3.6366954	-1.7587954	2.3250502
H	9.6709138	4.5954192	-6.7953420	H	-6.1923696	-5.8187209	-2.3218452
H	8.7433968	7.8692299	-10.3127521	H	-5.5231873	-6.7222515	-0.9680295
H	0.8888553	8.3391912	-9.5133129	H	-7.0487846	-5.8856783	-0.7853117
H	5.3028073	9.3411184	-11.3746123	H	-2.4750831	-5.5190622	1.6210137
H	5.8321146	10.1469787	-4.8723656	H	-2.0005170	-4.8753632	3.1851476
H	7.2440208	10.0465047	-9.5573087	H	-1.9846759	-3.8449843	1.7547530
H	9.8262884	9.2252144	-7.0394037	H	2.7242037	-7.3752651	3.8543843
H	9.0928839	4.3486970	-11.3895723	H	1.8743264	-8.5557315	2.8820708
H	3.2754422	6.8281448	-13.1919045	H	3.3551849	-7.8237164	2.2737905
H	4.0085745	11.7045594	-8.8423166	H	-7.3377949	2.9408113	3.8826424
H	9.1367526	5.8082370	-13.3288878	H	-7.7376751	1.2270097	3.9037449
H	8.9281271	7.2451472	-12.3446477	H	-7.2122189	2.0150722	5.3746086
H	10.8737758	9.5912668	-9.1977422	H	-2.3244887	-0.3686312	5.7991553
H	9.8980038	10.9814254	-8.7193201	H	-3.2742908	-1.5885678	4.9648388
H	4.6990457	12.2036395	-11.1189737	H	-1.8627643	-0.8727151	4.1882512

H	2.2136870	0.9279705	8.4805554	C	-1.1169552	4.7246641	-1.1834274
H	0.5069890	0.5718836	8.7211365	C	-2.3276338	4.6794425	-0.5292846
H	1.7054284	-0.6619917	9.0395654	C	-2.4011566	4.5432878	0.8799386
H	-0.9950443	-3.1894176	5.1714567	C	-1.2611691	4.4389097	1.6463458
H	-0.2072460	-2.9512665	3.6122630	D	-3.4949641	4.8175373	-1.2216769
H	0.5571484	-3.9410304	4.8357214	C	-3.9841778	3.6983873	-1.8559388
H	3.2622322	-5.9605117	0.8794294	C	-3.3601416	3.2399371	-3.0014912
H	2.5811554	1.3181212	6.2138332	C	-3.8443796	2.1263946	-3.6625947
H	-5.4636150	3.2599321	2.5373472	C	-4.9952106	1.4785885	-3.2216376
H	1.3958772	-1.2500838	3.2524986	C	-5.6040136	1.9808944	-2.0769331
H	-4.7740904	-4.0351338	-2.8026555	C	-5.1294491	3.0784074	-1.3680137
H	-7.4526185	-1.6232327	3.9169227	D	-3.2138321	1.7044241	-4.8092491
H	-4.2069611	-7.3234037	1.5028151	C	-2.0226700	1.0448902	-4.6857534
H	1.1097774	-6.1480603	5.8830715	C	-2.0394304	-0.3659514	-4.8238008
H	-2.1364572	-0.4478362	8.2961539	C	-0.8774795	-1.1039098	-4.7923219
H	-9.2946034	-1.7049560	1.7340047	C	0.3025150	-0.4046178	-4.5806396
H	-9.4197401	-0.6495420	3.1394020	C	0.3373936	0.9851644	-4.4269904
H	-8.1222876	-0.4054755	1.9549854	C	-0.8411416	1.7289139	-4.5017709
H	-3.1464874	-7.6918505	-0.6261557	N	1.5978532	-0.8211094	-4.4994768
H	-2.6397822	-9.2332364	0.0671325	C	2.3419527	0.2860565	-4.2937457
H	-4.3538108	-8.9147664	-0.1874860	N	1.6340393	1.3895601	-4.2439314
H	3.3495466	-5.4120018	5.4082405	D	-3.2408633	-0.9740597	-5.0425823
H	3.5344595	-5.3398699	7.1612340	C	-3.8476115	-1.5721473	-3.9618638
H	3.2590116	-6.8941684	6.3783918	C	-4.9948000	-1.0045883	-3.4175294
H	-1.6006878	1.8776025	7.9690406	C	-5.5909173	-1.6785572	-2.3576498
H	-3.1122097	2.1850499	8.8257859	C	-5.0995415	-2.8638805	-1.8219827
H	-1.7801184	1.3961686	9.6668030	C	-3.9417829	-3.3851859	-2.3935819
H	2.0991927	0.7922895	-8.5956124	C	-3.3382602	-2.7593186	-3.4687265
H	2.8329658	-1.8576305	-9.3389846	D	-3.4237397	-4.5739823	-1.9363239
H	1.4332084	-1.4752114	-8.3350090	C	-2.2733592	-4.5347132	-1.1987715
H	1.4827120	-0.9460454	-10.0248418	C	-2.3933496	-4.6697497	0.2073359
H	-0.8593928	6.5130812	-5.9691406	C	-1.2833227	-4.7186524	1.0206253
H	-3.4034902	5.9889825	-7.1373817	C	-0.0476617	-4.5912812	0.4016484
H	-3.0781968	5.8637527	-5.4074358	C	0.0900101	-4.4420855	-0.9822070
H	-2.9851742	7.4377917	-6.2150539	C	-1.0390823	-4.4351217	-1.8024828
H	4.5882594	7.3929200	-1.7369429	N	1.2197636	-4.6001751	0.9033930
H	3.2983821	9.3578112	-0.1283329	C	2.0481713	-4.4478333	-0.1513221
H	3.6748756	7.7277281	0.4330400	N	1.4202921	-4.3502003	-1.2991611
H	4.9843140	8.8535484	0.0380001	D	-3.6449403	-4.8035000	0.7336066
H	7.5534245	1.6742550	-4.3640245	C	-4.2133438	-3.6829214	1.2949565
H	9.5444006	1.5139075	-2.3331676	C	-3.7517118	-3.2269009	2.5160447
H	8.2185378	0.3613786	-2.4981419	C	-4.3188989	-2.1118674	3.1051546
H	9.4601591	0.4701344	-3.7571010	C	-5.3954681	-1.4596441	2.5098089
C	-4.1939715	0.9850704	-5.6763980	C	-5.8423406	-1.9593539	1.2916474
N	-5.3444501	0.9780167	-5.6636626	C	-5.2787431	-3.0590395	0.6544572
C	0.1777676	-0.3762324	-3.9456850	D	-3.8510916	-1.6925574	4.3283883
N	0.8861841	-0.9126185	-3.2159124	C	-2.6517891	-1.0375021	4.3697060
C	3.6262429	-4.0510136	-4.6040490	C	-1.4590599	-1.7265739	4.3504479
N	3.3788436	-5.1433190	-4.8674975	C	-0.2781351	-0.9877935	4.4365607
C	3.6459797	-0.2124334	-1.5673792	C	-0.3280888	0.4023574	4.5820925
N	3.4009426	0.3404362	-0.5894234	C	-1.5229499	1.1067151	4.6294943
C	6.5644290	1.8980639	2.0205886	C	-2.6815846	0.3736214	4.5026755
N	7.2331799	1.3120632	2.7507691	N	0.9679234	0.8138669	4.6776238
C	2.2037447	3.2791350	0.2779388	C	1.7286749	-0.2965098	4.5769112
N	1.0549370	3.2767719	0.2295885	N	1.0298172	-1.3974264	4.4322832
C	-1.2524676	6.9411025	0.9562927	C	3.1854742	-0.2857245	4.6954886
N	-1.4838797	7.4426397	1.9656116	C	3.8369458	0.3883921	5.7286832
C	-1.2676510	3.1181255	-2.1004481	C	5.2311481	0.3168890	5.8785535
N	-1.4659147	2.0251976	-2.3975121	C	6.0009176	-0.4310154	4.9909798
				C	5.3613524	-1.0611686	3.9245198
				C	3.9718954	-0.9883943	3.7831628
				C	3.0955538	1.1512250	6.6804090
				N	2.5260301	1.7846290	7.4536432
				C	3.3842446	-1.5966087	2.6365042
				N	2.9883919	-2.0889429	1.6766437
				I	8.0502480	-0.5996138	5.2409772
				D	-3.8990513	0.9871243	4.5546964
				C	-4.3497554	1.5870328	3.4009998
				C	-5.4134536	1.0235874	2.7043625
				C	-5.8560142	1.6993653	1.5730650
				C	-5.2916797	2.8826766	1.1098057
				C	-4.2216254	3.3998493	1.8350469
				C	-3.7733084	2.7721057	2.9824522
				C	-5.7970531	-3.5720064	-0.6755864
				C	-7.3201380	-3.5163195	-0.7807108
				C	-6.0569650	-0.2667052	3.1748082

I-RA4 with 4 CN instead of F

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Energy = -7388.297401641

C	4.1547627	3.4966774	1.2702127
C	3.4812908	4.4584682	0.5177944
C	4.2457273	5.4421277	-0.1102547
C	5.6390267	5.4964013	0.0544960
C	6.2945129	4.5610798	0.8514323
C	5.5426988	3.5431833	1.4363541
C	2.0224149	4.4410475	0.4315660
N	1.3459838	4.5959964	-0.7261535
C	0.0221428	4.5920808	-0.4017985
C	-0.0307646	4.4421007	0.9877852
N	1.2435233	4.3454603	1.4831192

C	-7.5764106	-0.2650566	3.0168888	H	1.8675884	-1.8114887	-4.3710685
C	3.5053060	-4.4688575	-0.0386622	H	1.7409774	-3.7655527	-3.0563897
C	4.2765211	-3.5063836	-0.6895504	H	2.4713369	-4.2469558	-5.7682779
C	5.6739908	-3.5560749	-0.6662649	H	3.5229017	-4.6103410	-4.3989075
C	6.3373969	-4.5779453	0.0113292	H	1.9980663	-5.4889164	-4.6033659
C	5.5780766	-5.5147983	0.7079950	H	1.2626622	-3.1727658	3.8602040
C	4.1754215	-5.4572127	0.6827094	H	1.7677863	-5.9314340	4.3655608
C	-5.5629791	0.2881081	-3.9716338	H	1.2986530	-4.7411636	5.5847448
C	-7.0898850	0.2911459	-4.0235937	H	1.3154502	3.7585793	3.2675136
C	3.8012292	0.2702942	-4.2145804	H	1.6754633	4.2285650	6.0548956
C	4.5835323	-0.4089477	-5.1489325	H	2.8966373	4.6011206	4.8369596
C	5.9854314	-0.3409407	-5.1108642	H	1.3568733	5.4772692	4.8455307
C	6.6313211	0.4083441	-4.1305629	H	1.7897594	3.1648223	-3.6461634
C	5.8563464	1.0445182	-3.1619563	H	2.3661663	5.9206058	-4.0851888
C	4.4602688	0.9747860	-3.2074956	H	3.5272948	4.6238106	-4.3736270
C	3.9747251	-1.1736286	-6.1890913	H	2.0557857	4.7304089	-5.3543403
N	3.5127102	-1.8087996	-7.0296407	H	2.8870097	-4.6406453	4.8062844
I	8.6963218	0.5689694	-4.1026302	C	6.3680669	6.5315259	-0.6004850
C	3.7261344	1.5891720	-2.1522263	N	6.9371770	7.3713322	-1.1429404
N	3.2068106	2.0865174	-1.2559073	C	6.1639912	2.5066662	2.1916307
C	-5.8228257	3.5932156	-0.1212241	N	6.6054063	1.6423138	2.8084947
C	-7.3461727	3.5436833	-0.2253155	C	5.8430918	1.0150967	6.9602728
O	-3.6414521	4.5866771	1.4535357	N	6.3182712	1.5905918	7.8357512
C	3.6582133	-2.4009670	-1.3421550	C	6.1012789	-1.7683097	2.9329618
N	3.2354687	-1.4691573	-1.8651027	N	6.6412560	-2.3495361	2.1004707
I	8.4056267	-4.6908178	-0.0128439	C	6.2100941	-6.5546734	1.4504980
C	3.4475210	-6.4565793	1.3959283	N	6.7005261	-7.3979477	2.0602756
N	2.8877645	-7.2665184	1.9909786	C	6.3943260	-2.5187017	-1.3263437
C	3.6246863	6.4394466	-0.9207687	N	6.9179239	-1.6538827	-1.8743882
N	3.1543072	7.2473753	-1.5911526	C	6.7340993	-1.0437551	-6.0996256
I	8.3403085	4.6711926	1.1568609	N	7.3185505	-1.6227918	-6.9037242
C	3.4507850	2.3945894	1.8357511	C	6.4586010	1.7560636	-2.0840100
N	2.9580408	1.4653839	2.2985907	N	6.8831955	2.3423242	-1.1904113
O	1.2348752	3.4996170	4.2076417				
C	1.8199548	4.5006263	5.0107570				
O	1.7921482	-3.5078004	-3.9989256	I-capsule without methyl groups			
C	2.4781161	-4.5125778	-4.7126236				
O	1.7554740	4.1087110	-3.3906440	356			
C	2.4600778	4.8683426	-4.3478268	Energy = -12291.96639186			
O	1.2621351	-4.1159472	3.5997338	C	3.1272659	1.5507689	-4.0784938
C	1.8312106	-4.8798856	4.6399411	C	4.4866855	1.5423492	-4.3280467
H	-2.4912185	-3.2241975	-3.9500720	C	5.2406724	0.4491702	-3.9084632
H	-6.4881587	-1.2564801	-1.9247456	C	4.5782626	-0.5864833	-3.2547873
H	-2.5164143	3.7767110	-3.4082694	C	3.2133278	-0.4743618	-3.0423979
H	-6.4982445	1.4891366	-1.7169531	N	2.4998869	0.5690908	-3.4428056
H	-2.9737798	-3.7667441	3.0344037	C	6.6824956	0.4312602	-4.1349298
H	-6.6759321	-1.4638219	0.8119329	N	7.4204730	1.5151398	-4.2286863
H	-2.9982731	3.2341535	3.5751008	C	8.7070008	1.0709374	-4.3784457
H	-6.6870686	1.2800510	1.0212016	C	8.7135572	-0.3272308	-4.3889703
H	-5.5638622	4.6466509	-0.0203096	N	7.4098748	-0.7016923	-4.2343883
H	-5.2281079	0.3702905	-5.0051889	C	9.9040177	1.7764801	-4.4816590
H	-5.5307876	-4.6265397	-0.7400859	C	11.0757359	1.0545731	-4.5602054
H	-5.8673069	-0.3499384	4.2444814	C	11.0633507	-0.3603258	-4.6048058
H	-7.4437687	-0.5441477	-4.6271580	C	9.8779687	-1.0654799	-4.5367036
H	-7.5671298	0.2084802	-3.0473006	O	12.2863805	1.6893914	-4.6251763
H	-7.6800155	4.1216851	-1.0866031	C	12.8247106	2.1102532	-3.4296430
H	-7.7964589	3.9758011	0.6678475	C	13.9240000	1.4503081	-2.8885480
H	-7.9955265	-1.1860397	3.4211005	C	14.4435159	1.9537307	-1.7002961
H	-7.9146323	-0.1826470	1.9841456	C	13.9194590	3.0544495	-1.0326788
H	-7.6458078	-3.9472252	-1.7270011	C	12.8097872	3.6699157	-1.6043635
H	-7.7317865	-2.5086217	-0.7266685	C	12.2894242	3.2225189	-2.8048202
H	-7.7507788	2.5376702	-0.3360040	O	12.2567127	4.7752066	-1.0001770
H	-8.0074424	0.5723255	3.5649012	C	11.0632575	4.6148458	-0.3551623
H	-7.7708917	-4.0922323	0.0269747	C	11.0746266	4.5690147	1.0597030
H	-7.4467406	1.2140678	-4.4797329	C	9.9024086	4.4893565	1.7806981
H	-0.8771446	-2.1730090	-4.9461660	C	8.7059645	4.3856591	1.0742029
H	-0.8182275	2.8071633	-4.4293433	C	8.7137944	4.3974506	-0.3239353
H	-1.0511996	4.8774952	-2.2506425	C	9.8805207	4.5470440	-1.0612618
H	-1.3097406	4.3687017	2.7239220	N	7.4108492	4.2408603	-0.6998749
H	-1.5390391	2.1760682	4.7806500	C	6.6825414	4.1391436	0.4322121
H	-1.4311160	-2.8050464	4.2832270	N	7.4192090	4.2338063	1.5169682
H	-1.3645767	-4.8703098	2.0870083	C	14.5322924	0.2434824	-3.5770968
H	-0.9398323	-4.3657096	-2.8766175	C	16.0592692	0.2366486	-3.5234765
H	1.6921485	4.4847105	-1.6945916	C	14.5316094	3.5861031	0.2501392
H	1.2564365	1.8029841	4.5859040	C	16.0585745	3.5323229	0.2436022
H	1.4309831	-4.4898010	1.9100532	O	12.2563213	-1.0062209	-4.7652511

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Energy = -12291.96639186

C	3.1272659	1.5507689	-4.0784938
C	4.4866855	1.5423492	-4.3280467
C	5.2406724	0.4491702	-3.9084632
C	4.5782626	-0.5864833	-3.2547873
C	3.2133278	-0.4743618	-3.0423979
N	2.4998869	0.5690908	-3.4428056
C	6.6824956	0.4312602	-4.1349298
N	7.4204730	1.5151398	-4.2286863
C	8.7070008	1.0709374	-4.3784457
C	8.7135572	-0.3272308	-4.3889703
N	7.4098748	-0.7016923	-4.2343883
C	9.9040177	1.7764801	-4.4816590
C	11.0757359	1.0545731	-4.5602054
C	11.0633507	-0.3603258	-4.6048058
C	9.8799687	-1.0654799	-4.5367036
O	12.2863805	1.6893914	-4.6251763
C	12.8247106	2.1102532	-3.4296430
C	13.9240000	1.4503081	-2.8885480
C	14.4435159	1.9537307	-1.7002961
C	13.9194590	1.03544495	-1.0326788
C	12.8097872	3.6699157	-1.6043635
O	12.2894242	3.2225189	-2.8048202
O	12.567127	4.7752066	-1.0001770
C	11.0632575	4.6148458	-0.3551623
C	11.0746266	4.5690147	1.0597030
C	9.9024086	4.4893565	1.7806981
C	8.7059645	4.3856591	1.0742029
C	8.7137944	4.3974506	-0.3239353
C	9.8805027	4.5470460	-1.0612618
N	7.4108492	4.2408603	-0.6998749
C	6.6825414	4.1391436	0.4322121
N	7.4192090	4.2338063	1.5169682
C	14.5322924	0.2434824	-3.5770968
C	16.0592692	0.2366486	-3.5234765
C	14.5316094	3.5861031	0.2501392
C	16.0585745	3.5323229	0.2436022
O	12.2563213	-1.0062209	-4.7652512

C	12.8100919	-1.6107151	-3.6604818	C	-4.6297843	-1.2398898	2.8859002
C	12.2905675	-2.8117703	-3.2137777	C	-3.2520598	-1.2422585	2.7845542
C	12.8266555	-3.4372867	-2.1022572	F	-2.3854571	0.6888871	5.6881155
C	13.9256134	-2.8958735	-1.4420143	F	-5.0351984	0.6653410	5.9051104
C	14.4445458	-1.7071734	-1.9450150	C	-6.7272825	-0.6373818	4.0845594
C	13.9200348	-1.0392131	-3.0453068	N	-7.4489722	-1.7303332	4.0099550
D	12.2848450	4.6336932	1.6953934	C	-8.7404598	-1.3237105	4.2180386
C	12.8229648	3.4379758	2.1159890	C	-8.7625793	0.0585417	4.4260503
C	12.2869104	2.8125012	3.2275253	N	-7.4630467	0.4647400	4.3412478
C	12.8070985	1.6119356	3.6748035	C	-9.9251749	-2.0559028	4.2472934
C	13.9175727	1.0409031	3.0601806	C	-11.1060957	-1.3685333	4.4322208
C	14.4422395	1.7090066	1.9600406	C	-11.1127134	0.0306209	4.6390765
C	13.9228323	2.8973150	1.4566175	C	-9.9395063	0.7552744	4.6635225
C	14.5339544	-3.5842468	-0.2350627	D	-12.3166496	0.6444861	4.8541881
C	16.0608832	-3.5296675	-0.2274379	C	-12.8647359	1.3240789	3.7909415
D	12.2893324	-4.6336213	-1.6823507	C	-13.9684651	0.7982154	3.1263720
C	11.0784428	-4.5697764	-1.0478803	C	-14.4896188	1.5466580	2.0768749
C	11.0655672	-4.6146503	0.3669789	C	-13.9662479	2.7668199	1.6628827
C	9.8819936	-4.5465797	1.0716983	C	-12.8614165	3.2505402	2.3579287
C	8.7160851	-4.3976598	0.3329561	C	-12.3368867	2.5494868	3.4282273
C	8.7097487	-4.3871304	-1.0652103	D	-12.3092965	4.4630813	2.0177664
C	9.9070012	-4.4912372	-1.7702218	C	-11.1063940	4.4344147	1.3618208
N	7.4127351	-4.2406805	0.7073110	C	-11.1119502	4.6414255	-0.0373216
C	6.6857091	-4.1395577	-0.4256623	C	-9.9382153	4.6656001	-0.7611228
N	7.4235706	-4.2353797	-1.5095312	C	-8.7618448	4.4277963	-0.0635502
C	14.5299886	-0.2416222	3.5922391	C	-8.7407753	4.2194461	1.3186619
C	16.0570088	-0.2341336	3.5398571	C	-9.9260238	4.2489585	2.0500016
D	12.2531347	1.0071836	4.7793375	N	-7.4620496	4.3427181	-0.4688397
C	11.0603266	0.3612815	4.6177336	C	-6.7271132	4.0855665	0.6337429
C	11.0727742	-1.0535812	4.5721103	N	-7.4496139	4.0110131	1.7261708
C	9.9011604	-1.7754487	4.4914320	D	-12.3153728	4.8570547	-0.6520250
C	8.7043026	-1.0697775	4.3869625	C	-12.8634138	3.7940922	-1.3321041
C	8.7109729	0.3283719	4.3985922	C	-13.9675874	3.1297035	-0.8069477
C	9.8770995	1.0665237	4.5487442	C	-14.4885425	2.0803917	-1.5557876
N	7.4179105	-1.5136775	4.2348863	C	-13.9646879	1.6665287	-2.7757846
C	6.6803538	-0.4295711	4.1403319	C	-12.8596170	2.3615860	-3.2589448
N	7.4076590	0.7031724	4.2420420	C	-12.3351249	3.4315719	-2.5573791
D	12.2584160	-4.7742552	1.0132762	D	-12.3071608	2.0216641	-4.4713990
C	12.8104633	-3.6686888	1.6179022	C	-11.1041828	1.3658818	-4.4425135
C	13.9204940	-3.0528733	1.0472742	C	-11.1095066	-0.0332526	-4.6495245
C	14.4434650	-1.9518967	1.7153295	C	-9.9356864	-0.7569309	-4.6732456
C	13.9226727	-1.4486403	2.9031066	C	-8.7595035	-0.0592663	-4.4348591
C	12.8230569	-2.1089422	3.4431400	C	-8.7386622	1.3229765	-4.2266457
C	12.2888080	-3.2214389	2.8178428	C	-9.9239562	2.0542020	-4.2566685
D	12.2834131	-1.6883307	4.6381497	N	-7.4476371	1.7306401	-4.0176647
C	5.2412597	3.9093509	0.4479755	C	-6.7250188	0.6382786	-4.0918874
C	4.5818912	3.2559542	-0.5898363	N	-7.4597009	-0.4644027	-4.3492452
C	3.2171736	3.0407027	-0.4805943	C	-14.5753918	3.5527511	0.5170398
N	2.5011111	3.4378630	0.5623052	C	-16.1024671	3.5019298	0.5100879
C	3.1256847	4.0726185	1.5463644	C	-14.5734415	0.5206752	-3.5620206
C	4.4845976	4.3250390	1.5407505	C	-16.1005318	0.5135324	-3.5118105
C	5.2389174	-0.4467356	3.9115515	D	-12.3127893	-0.6481238	-4.8654475
C	4.5784777	0.5888220	3.2557327	C	-12.8609957	-1.3281637	-3.8025399
C	3.2137115	0.4779448	3.0416727	C	-12.3323363	-2.5531091	-3.4394357
N	2.4986626	-0.5643141	3.4423237	C	-12.8569934	-3.2546077	-2.3694921
C	3.1242212	-1.5460837	4.0796554	C	-13.9626938	-2.7718056	-1.6751836
C	4.4833170	-1.5387890	4.3310904	C	-14.4867827	-1.5520634	-2.0895035
C	5.2446245	-3.9085912	-0.4432139	C	-13.9655919	-0.8032126	-3.1386893
C	4.5845346	-3.2551810	0.5941507	C	-14.5754717	-0.5261817	3.5493120
C	3.2202215	-3.0383252	0.4832138	C	-16.1025305	-0.5203543	3.4980149
N	2.5051296	-3.4339417	-0.5609340	C	-14.5719956	-3.5582345	-0.5297683
C	3.1303769	-4.0686350	-1.5446050	C	-16.0991179	-3.5086687	-0.5238998
C	4.4889942	-4.3225646	-1.5373410	D	-12.3040412	-4.4666663	-2.0289514
D	7.0010190	-3.3501940	-4.0426676	C	-11.1016396	-4.4369552	-1.3721255
C	6.4657088	-4.3162310	-4.9122497	C	-11.1080483	-4.6439336	0.0270196
D	7.0092357	3.3532897	4.0538038	C	-9.9348411	-4.6669805	0.7516990
C	6.4423826	4.3095721	4.9143136	C	-8.7581830	-4.4280541	0.0550008
D	7.0252358	4.0558634	-3.3521703	C	-8.7362379	-4.2198040	-1.3272155
C	6.4257144	4.9065203	-4.2975189	C	-9.9209272	-4.2503941	-2.0594319
D	7.0241447	-4.0547337	3.3591387	N	-7.4587537	-4.3420464	0.4612361
C	6.4199227	-4.9037822	4.3029666	C	-6.7231800	-4.0844138	-0.6408009
I	-0.3807569	-0.5791856	3.5385223	N	-7.4449351	-4.0102652	-1.7337519
C	-2.4630038	-0.5995481	3.7208228	D	-12.3085543	-2.0253097	4.4603054
C	-3.0943214	0.0545311	4.7629630	C	-12.8598892	-2.3656697	3.2474522
C	-4.4719734	0.0497654	4.8694330	C	-13.9651917	-1.6715197	2.7635108
C	-5.2711517	-0.6003113	3.9383059	C	-14.4878510	-2.0858058	1.5431396

C	-13.9654943	-3.1346739	0.7946564	H	15.3036306	1.2794299	1.4657976
C	-12.8611489	-3.7981612	1.3205929	H	11.4859443	-3.7670347	3.2898937
C	-12.3340350	-3.4352348	2.5462532	H	15.3045431	-1.4567779	1.2861288
O	-12.3117242	-4.8606174	0.6408500	H	14.2724798	-4.6398332	-0.3015490
F	-5.3378106	-1.8471569	1.9407036	H	14.2701029	0.3097178	-4.6325270
F	-2.6912311	-1.8694534	1.7582511	H	14.2694987	4.6415413	0.3165041
C	-5.2709999	3.9387018	0.5975459	H	14.2670124	-0.3081205	4.6474556
C	-4.6303838	2.8861606	1.2376814	H	16.4528072	1.1478403	-3.9729640
C	-3.2526932	2.7840179	1.2404720	H	16.4671683	0.1727371	-2.5147726
C	-2.4629328	3.7196294	0.5976472	H	16.4552035	-3.9787041	-1.1385153
C	-3.0934721	4.7620452	-0.0567583	H	16.4505242	-4.0893673	0.6223869
C	-4.4710599	4.8693193	-0.0523404	H	16.4459223	0.6156183	4.1001739
I	-0.3809252	3.5356637	0.5769972	H	16.4657021	-0.1697226	2.5315064
F	-2.6926049	1.7575635	1.8680646	H	16.4520081	3.9814270	1.1550291
F	-5.3391088	1.9415184	1.8449799	H	16.4485260	4.0923517	-0.6058625
F	-5.0334914	5.9052690	-0.6681887	H	16.4681258	-2.5207289	-0.1630551
F	-2.3839089	5.6866229	-0.6911498	H	16.4505914	-1.1452828	3.9893930
C	-5.2671682	-3.9367802	-0.6034753	H	16.4663853	2.5236039	0.1793572
C	-4.6265680	-2.8837400	-1.2428063	H	16.4490177	-0.6130967	-4.0832236
C	-3.2489187	-2.7808827	-1.2444449	H	-9.9294475	4.8643356	-1.8228917
C	-2.4592183	-3.7162886	-0.6012364	H	-9.9121898	4.1298953	3.1241272
C	-3.0897663	-4.7591826	0.0524012	H	-9.9315751	1.8170510	4.8622485
C	-4.4672907	-4.8671348	0.0468629	H	-9.9105274	-3.1300280	4.1283355
I	-0.3773071	-3.5315141	-0.5787358	H	-9.9266542	-4.8657932	1.8134590
F	-2.6888411	-1.7539185	-1.8712020	H	-9.9064170	-4.1313864	-3.1335556
F	-5.3352940	-1.9394025	-1.8505772	H	-9.9267450	-1.8186650	-4.8721487
F	-5.0296803	-5.9035665	0.6619381	H	-9.9102688	3.1283337	-4.1376419
F	-2.3802643	-5.6834790	0.6872702	H	9.8571027	4.6053544	-2.1394710
C	-5.2689629	0.6022372	-3.9446461	H	9.9080348	4.5013287	2.8615048
C	-4.6287640	1.2417708	-2.8915087	H	9.9101892	2.8572777	-4.4946347
C	-3.2511125	1.2448883	-2.7891463	H	9.8562063	-2.1437384	-4.5939326
C	-2.4609841	0.6030692	-3.7251233	H	9.8530661	2.1447268	4.6068768
C	-3.0911445	-0.0508507	-4.7680636	H	9.9072866	-2.8562555	4.5035201
C	-4.4687195	-0.0468829	-4.8755283	H	9.8573672	-4.6040913	2.1499224
I	-0.3788119	0.5838331	-3.5413792	H	9.9140901	-4.5043172	-2.8510071
F	-2.6913959	1.8720202	-1.7621951	H	-7.1590642	1.4586409	4.3533724
F	-5.3378843	1.8481942	-1.9465789	H	-7.1549800	-4.3545557	1.4551628
F	-5.0308343	-0.6623500	-5.9118750	H	-7.1548038	-1.4580251	-4.3611669
F	-2.3812179	-0.6842351	-5.6930701	H	-7.1575521	4.3552510	-1.4625632
O	-7.0644993	-4.2957841	3.1286013	H	7.0952543	4.2046143	-1.6856316
C	-6.0619973	-4.9562988	3.8611602	H	7.0918187	-1.6864193	-4.1983914
O	-7.0654034	4.2962112	-3.1358162	H	7.0960164	-4.2038310	1.6927044
C	-6.0625018	4.9571895	-3.8674156	H	7.0904017	1.6882922	4.2060660
O	-7.0662988	3.1315769	4.2924852	H	2.6790462	2.5196554	-1.2637126
C	-6.0635717	3.8644122	4.9523408	H	2.6727959	-1.2556341	-2.5210544
O	-7.0599010	-3.1307473	-4.2998651	H	2.6816009	-2.5173259	1.2660251
C	-6.0556630	-3.8626552	-4.9584463	H	2.5088606	4.4004909	2.3751962
H	-11.5303580	4.0085276	-2.9867639	H	2.5081002	-2.3743163	4.4103577
H	-15.3486591	1.5526978	-1.1644511	H	2.5144029	-4.3950100	-2.3746533
H	-11.5324714	2.9794131	4.0052656	H	2.6746728	1.2591685	2.5187159
H	-15.3495185	1.1548818	1.5491547	H	2.5124105	2.3798610	-4.4093966
H	-11.5271333	-2.9823461	-4.0158878	H	7.1052421	-3.7191856	-3.1301244
H	-15.3472945	-1.1609540	-1.5622858	H	7.1133396	3.1389194	-3.7142244
H	-11.5291173	-4.0115550	2.9762032	H	7.1054092	3.7190391	3.1390916
H	-15.3481465	-1.5588415	1.1512206	H	7.1115281	-3.1374198	3.7205024
H	-14.3113445	-0.6796473	4.5951635	H	6.5303914	-3.9399984	-5.9327822
H	-14.3110700	4.5985236	0.6707068	H	7.0192451	-5.2585307	-4.8686984
H	-14.3087148	0.6743874	-4.6076828	H	5.4110432	-4.5318668	-4.7069142
H	-14.3067041	-4.6037902	-0.6832374	H	5.3519181	4.7204255	-4.4129566
H	-16.4934096	4.1313971	-0.2889125	H	6.5465405	5.9373971	-3.9659083
H	-16.5114915	2.5024256	0.3624836	H	6.8938572	4.8167005	-5.2818789
H	-16.4942586	0.2783604	4.1273557	H	5.3777342	4.4781773	4.7165366
H	-16.4927829	-1.4675734	3.8693238	H	6.5328225	3.9527898	5.9398668
H	-16.4889735	-3.8803987	-1.4711167	H	6.9562782	5.2729168	4.8503517
H	-16.5090700	-2.5095034	-0.3765731	H	5.3455148	-4.7176776	4.4125476
H	-16.4913372	1.4604288	-3.8833621	H	6.5426736	-5.9352712	3.9739690
H	-16.5099431	0.3658418	-2.5124771	H	6.8830178	-4.8119764	5.2895288
H	-16.5113531	-0.3730576	2.4983833	H	-7.1466270	3.3684272	-3.4647087
H	-16.4901044	-4.1384702	0.2748147	H	-6.0270552	5.9974829	-3.5463671
H	-16.4911198	-0.2854954	-4.1414625	H	-5.0682101	4.5243195	-3.7099404
H	-16.4933018	3.8733551	1.4570218	H	-6.2692958	4.9442881	-4.9415045
H	11.4866010	3.7676651	-3.2774587	H	-7.1424089	-3.4586152	-3.3718383
H	15.3045271	1.4590755	-1.2704263	H	-6.0181291	-3.5421147	-5.9988235
H	11.4878729	-3.2843551	-3.7591612	H	-5.0622508	-3.7048964	-4.5236581
H	15.3055229	-1.2772277	-1.4503748	H	-6.2624270	-4.9367485	-4.9454235
H	11.4837351	3.2848139	3.7724309	H	-7.1465304	-3.3680625	3.4574469

H	-6.0249665	-5.9962838	3.5392903	C	1.0233851	-4.5541005	0.5431610
H	-5.0679317	-4.5222477	3.7055189	C	1.6207839	-4.0954450	-0.6226382
H	-6.2703918	-4.9445222	4.9349547	C	2.8747214	-3.4769673	-0.6300671
H	-7.1480974	3.4595252	3.3644205	C	3.5562391	-3.2652100	0.5662679
H	-6.0272535	3.5441155	5.9928364	N	1.2118292	-4.1112987	-1.9253038
H	-5.0694197	3.7073718	4.5189870	C	2.1849668	-3.5230814	-2.6529265
H	-6.2711818	4.9383359	4.9388083	N	3.2049369	-3.1414924	-1.9164464
H	4.9416140	-2.3537933	4.8724262	C	-3.1196710	-1.7823278	5.1924933
H	5.1045079	1.4646020	2.8983699	C	-3.0767867	-1.7540953	6.7193650
H	4.9418712	4.8639348	2.3579151	O	-4.7344297	-1.1756625	2.9181679
H	5.1088647	2.9008327	-1.4659989	C	-4.3062572	-1.6864510	1.7243732
H	4.9464842	2.3574432	-4.8679574	C	-3.6487074	-2.9390124	1.7358922
H	5.1026371	-1.4635970	-2.8983372	C	-3.2597411	-3.5522057	0.5633909
H	4.9467617	-4.8609346	-2.3545581	C	-3.4701456	-2.8695586	-0.6325170
H	5.1106841	-2.9011964	1.4712700	C	-4.0888724	-1.6157901	-0.6245811

N-RA4 without Methyl groups

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Energy = -4791.315601055

C	2.9469456	3.1273470	-6.2159644	C	0.1512843	-4.0052726	3.4724317
C	3.2146605	3.2423209	-4.8631533	C	0.3962682	-3.2017588	4.5821927
C	3.2847352	2.0840584	-4.0939300	C	-0.6848383	-2.5023270	5.1055058
C	3.0905832	0.8647257	-4.7362365	C	-1.9732729	-2.5678797	4.5852701
C	2.8154863	0.8669969	-6.0966700	C	-2.1720005	-3.3977140	3.4856508
N	2.7394037	1.9694665	-6.8284677	C	-1.1238465	-4.1257798	2.9512556
C	3.5141400	2.1778656	-2.6548237	O	-3.4305268	-3.5406352	2.9467480
N	3.1330285	3.1983723	-1.9188397	C	-2.0922278	3.2941798	-4.0921631
C	3.4701456	2.8695586	-0.6325170	C	-0.8735495	3.0970252	-4.7348273
C	4.0888724	1.6157901	-0.6245811	C	-0.8770223	2.8217712	-6.0951943
N	4.1034833	1.2056512	-1.9268895	N	-1.9799313	2.7484579	-6.8266474
C	3.2597411	3.5522057	0.5633909	C	-3.1371148	2.9589791	-6.2137994
C	3.6487074	2.9390124	1.7358922	C	-3.2509140	3.2271107	-4.8609875
C	4.3062572	1.6864510	1.7243732	C	-3.2847352	-2.0840584	-4.0939300
C	4.5493207	1.0196852	0.5411820	C	-3.0905832	-0.8647257	-4.7362365
O	3.4305268	3.5406352	2.9467480	C	-2.8154863	-0.8669969	-6.0966700
C	2.1720005	3.3977140	3.4856508	N	-2.7394037	-1.9694665	-6.8284677
C	1.9732729	2.5678797	4.5852701	C	-2.9469456	-3.1273470	-6.2159644
C	0.6848383	2.5023270	5.1055058	C	-3.2146605	-3.2423209	-4.8631533
C	-0.3962682	3.2017588	4.5821927	C	2.0922278	-3.2941798	-4.0921631
C	-0.1512843	4.0052726	3.4724317	C	0.8735495	-3.0970252	-4.7348273
C	1.1238465	4.1257798	2.9512556	C	0.8770223	-2.8217712	-6.0951943
O	-1.1769008	4.7362844	2.9205117	N	1.9799313	-2.7484579	-6.8266474
C	-1.6889847	4.3096395	1.7267067	C	3.1371148	-2.9589791	-6.2137994
C	-2.9417057	3.6524458	1.7386465	C	3.2509140	-3.2271107	-4.8609875
C	-3.5562391	3.2652100	0.5662679	O	-5.1197321	1.2568009	-2.2858840
C	-2.8747214	3.4769673	-0.6300671	C	-6.2386067	1.6998695	-3.0108765
C	-1.6207839	4.0954450	-0.6226382	O	5.1197321	-1.2568009	-2.2858840
C	-1.0233851	4.5541005	0.5431610	C	6.2386067	-1.6998695	-3.0108765
N	-1.2118292	4.1112987	-1.9253038	O	1.2534757	5.1173965	-2.2884063
C	-2.1849668	3.5230814	-2.6529265	C	1.7068456	6.2406601	-3.0001616
N	-3.2049369	3.1414924	-1.9164464	O	-1.2534757	-5.1173965	-2.2884063
C	3.1196710	1.7823278	5.1924933	C	-1.7068456	-6.2406601	-3.0001616
C	3.0767867	1.7540953	6.7193650	H	1.3103450	4.8210838	2.1469503
C	-1.7824682	3.1200221	5.1942856	H	0.5142442	1.8684785	5.9658808
C	-1.7533628	3.0760307	6.7211124	H	4.8211018	-1.3125229	2.1475929
O	4.7344297	1.1756625	2.9181679	H	1.8678986	-0.5138934	5.9655413
C	4.0044089	0.1500708	3.4714551	H	-4.8211018	1.3125229	2.1475929
C	4.1256066	-1.1255017	2.9516106	H	-1.8678986	0.5138934	5.9655413
C	3.3982739	-2.1735509	3.4872054	H	-1.3103450	-4.8210838	2.1469503
C	2.5681740	-1.9740191	4.5864983	H	-0.5142442	-1.8684785	5.9658808
C	2.5021803	-0.6851600	5.1056185	H	2.3028497	-4.0405340	4.9310225
C	3.2011595	0.3957382	4.5812457	H	4.0399957	2.3025580	4.9283110
O	-3.5419647	3.4326669	2.9498891	H	-2.3028497	4.0405340	4.9310225
C	-3.3982739	2.1735509	3.4872054	H	-4.0399957	-2.3025580	4.9283110
C	-4.1256066	1.1255017	2.9516106	H	3.0834706	2.7705969	7.1120363
C	-4.0044089	-0.1500708	3.4714551	H	2.1981213	1.2560595	7.1284396
C	-3.2011595	-0.3957382	4.5812457	H	2.7696713	-3.0823699	7.1143062
C	-2.5021803	0.6851600	5.1056185	H	1.2340079	-3.9512527	7.1105823
C	-2.5681740	1.9740191	4.5864983	H	-3.9522560	-1.2348775	7.1084791
C	1.7824682	-3.1200221	5.1942856	H	-2.1981213	-1.2560595	7.1284396
C	1.7533628	-3.0760307	6.7211124	H	-2.7696713	3.0823699	7.1143062
O	3.5419647	-3.4326669	2.9498891	H	-1.2340079	3.9512527	7.1105823
C	2.9417057	-3.6524458	1.7386465	H	1.2550772	-2.1970967	7.1293041
C	1.6889847	-4.3096395	1.7267067	H	-3.0834706	-2.7705969	7.1120363
				H	-1.2550772	2.1970967	7.1293041

H	3.9522560	1.2348775	7.1084791	C	-14.2507847	-1.1284882	-2.9610247
H	-0.0776583	5.0752784	0.5186691	C	-14.7601936	-1.7947456	-1.8516990
H	-4.5336320	2.8035712	0.5714970	C	-13.1180456	-3.5014942	-2.0037796
H	2.7977296	4.5294247	0.5682008	H	-11.8030643	-3.3548646	-3.6776670
H	5.0708763	0.0741601	0.5168561	H	-15.6209882	-1.3693686	-1.3525275
H	-5.0708763	-0.0741601	0.5168561	O	-12.5500441	0.9664027	4.8766994
H	-2.7977296	-4.5294247	0.5682008	O	-12.5482433	-4.6742472	-1.5672189
H	0.0776583	-5.0752784	0.5186691	C	-11.3446506	0.3441334	4.6944957
H	4.5336320	-2.8035712	0.5714970	C	-11.3333996	-1.0669476	4.6030268
H	-0.3077941	4.5065656	-2.2410638	C	-11.3429322	-4.5711706	-0.9232812
H	4.4980128	0.3011217	-2.2419824	C	-11.3385744	-4.6688060	0.4873941
H	0.3077941	-4.5065656	-2.2410638	C	-13.0921946	-2.1668397	3.5256541
H	-4.4980128	-0.3011217	-2.2419824	C	-14.2065030	-3.1371326	1.1489234
H	0.0567279	2.6373543	-6.6138614	C	-14.2047896	-1.5205076	2.9944079
H	2.6337667	-0.0674234	-6.6150794	C	-12.5645933	-3.2869428	2.9100920
H	-0.0567279	-2.6373543	-6.6138614	C	-13.0947433	-3.7494329	1.7198743
H	-4.0251725	2.9086109	-6.8340671	C	-14.7318446	-2.0349197	1.8146337
H	-2.8945961	-4.0151286	-6.8364722	H	-11.7540964	-3.8225131	3.3800395
H	4.0251725	-2.9086109	-6.8340671	H	-15.5978042	-1.5464033	1.3873338
H	-2.6337667	0.0674234	-6.6150794	O	-12.5320652	-1.7239119	4.7007270
H	2.8945961	4.0151286	-6.8364722	C	-14.8171063	-0.3189289	3.6894702
H	4.4431564	-1.9771709	-2.2166149	H	-14.5461043	-0.3862551	4.7426911
H	1.9709462	4.4376437	-2.2187888	C	-14.8631060	3.5031315	0.3386309
H	-4.4431564	1.9771709	-2.2166149	H	-14.6044435	4.5594790	0.4054445
H	-1.9709462	-4.4376437	-2.2187888	C	-14.8715213	0.1531387	-3.4843561
H	7.0461701	-0.9793740	-2.8819776	H	-14.6161045	0.2239805	-4.5412463
H	6.5983512	-2.6690099	-2.6529166	C	-14.8187007	-3.6688748	-0.1334624
H	6.0403425	-1.7860179	-4.0854806	H	-14.5471078	-4.7216321	-0.2048667
H	1.8062982	6.0496214	-4.0749156	C	-8.9959473	0.3644924	4.4523809
H	0.9854342	7.0480074	-2.8751313	C	-8.9708660	-1.0300170	4.3573902
H	2.6717087	6.5971136	-2.6277146	C	-9.0561918	-0.4525413	-4.3169036
H	-6.0403425	1.7860179	-4.0854806	C	-9.0463699	0.9422215	-4.2229458
H	-7.0461701	0.9793740	-2.8819776	O	-12.6198293	1.5899210	-4.5280090
H	-6.5983512	2.6690099	-2.6529166	O	-12.5934642	4.5443498	1.7454087
H	-1.8062982	-6.0496214	-4.0749156	O	-12.5362133	-4.8561507	1.1228567
H	-0.9854342	-7.0480074	-2.8751313	C	-16.3899277	3.4434234	0.3448047
H	-2.6717087	-6.5971136	-2.6277146	H	-16.7890965	4.0020067	-0.5014893
H	4.2200178	-3.4032175	-4.4162343	H	-16.7935695	2.4327993	0.2836421
H	-0.0657836	-3.1262368	-4.1970544	C	-16.3445689	-0.3254311	3.6474715
H	3.3884720	4.2121282	-4.4190405	H	-16.7372916	0.5189791	4.2134043
H	3.1221661	-0.0745531	-4.1984373	H	-16.7269801	-1.2420022	4.0958473
H	-3.3884720	-4.2121282	-4.4190405	C	-16.3462187	-3.6293432	-0.1198322
H	-3.1221661	0.0745531	-4.1984373	H	-16.7400435	-4.0785965	-1.0311601
H	-4.2200178	3.4032175	-4.4162343	H	-16.7623172	-2.6243182	-0.0505321
H	0.0657836	3.1262368	-4.1970544	C	-16.3981590	0.1396780	-3.4208926

I-capsule with piperidyl groups

380

Energy = -12306.45518351

C	-13.1690357	2.0242363	-3.3444950
C	-14.2606866	2.9783535	-0.9511850
C	-14.2650764	1.3627552	-2.7977335
C	-12.6462086	3.1499585	-2.7352062
C	-13.1643294	3.6047213	-1.5367374
C	-14.7813597	1.8698156	-1.6098945
H	-11.8492445	3.6958044	-3.2163404
H	-15.6346532	1.3701044	-1.1702133
O	-12.6109969	4.7178067	-0.9467917
C	-11.4051610	4.5455667	-0.3224475
C	-11.3939865	4.4557036	1.0885869
C	-11.4114318	0.9487632	-4.4456499
C	-11.4060069	-0.4622304	-4.5368526
O	-12.6052407	-1.1003550	-4.7031801
C	-13.1388604	3.3624104	2.1887892
C	-14.2210170	0.9709100	3.1577179
C	-12.6028795	2.7534673	3.3084549
C	-14.2432469	2.8162766	1.5410865
C	-14.7548647	1.6295012	2.0553805
C	-13.1163478	1.5556814	3.7699880
H	-11.7989513	3.2336812	3.8448285
H	-15.6148531	1.1907810	1.5665852
C	-13.1462173	-1.6974175	-3.5879668
C	-14.2234605	-2.9727569	-1.3431852
C	-12.6071644	-2.8859376	-3.1316423

C	-14.2507847	-1.1284882	-2.9610247
C	-14.7601936	-1.7947456	-1.8516990
C	-13.1180456	-3.5014942	-2.0037796
H	-11.8030643	-3.3548646	-3.6776670
H	-15.6209882	-1.3693686	-1.3525275
O	-12.5500441	0.9664027	4.8766994
O	-12.5482433	-4.6742472	-1.5672189
C	-11.3446506	0.3441334	4.6944957
C	-11.3333996	-1.0669476	4.6030268
C	-11.3429322	-4.5711706	-0.9232812
C	-11.3385744	-4.6688060	0.4873941
C	-13.0921946	-2.1668397	3.5256541
C	-14.2065030	-3.1371326	1.1489234
C	-14.2047896	-1.5205076	2.9944079
C	-12.5645933	-3.2869428	2.9100920
C	-13.0947433	-3.7494329	1.7198743
C	-14.7318446	-2.0349197	1.8146337
H	-11.7540964	-3.8225131	3.3800395
H	-15.5978042	-1.5464033	1.3873338
O	-12.5320652	-1.7239119	4.7007270
C	-14.8171063	-0.3189289	3.6894702
H	-14.5461043	-0.3862551	4.7426911
C	-14.8631060	3.5031315	0.3386309
H	-14.6044435	4.5594790	0.4054445
C	-14.8715213	0.1531387	-3.4843561
H	-14.6161045	0.2239805	-4.5412463
C	-14.8187007	-3.6688748	-0.1334624
H	-14.5471078	-4.7216321	-0.2048667
C	-8.9959473	0.3644924	4.4523809
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C	-9.0561918	-0.4525413	-4.3169036
C	-9.0463699	0.9422215	-4.2229458
O	-12.6198293	1.5899210	-4.5280090
O	-12.5934642	4.5443498	1.7454087
O	-12.5362133	-4.8561507	1.1228567
C	-16.3899277	3.4434234	0.3448047
H	-16.7890965	4.0020067	-0.5014893
H	-16.7935695	2.4327993	0.2836421
C	-16.3445689	-0.3254311	3.6474715
H	-16.7372916	0.5189791	4.2134043
H	-16.7269801	-1.2420022	4.0958473
C	-16.3462187	-3.6293432	-0.1198322
H	-16.7400435	-4.0785965	-1.0311601
H	-16.7623172	-2.6243182	-0.0505321
C	-16.3981590	0.1396780	-3.4208926
H	-16.7988575	1.0507769	-3.8644077
H	-16.7985542	0.0707839	-2.4094442
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H	-16.7270154	-4.1954048	0.7300027
H	-16.7879257	-0.7102101	-3.9807188
H	-16.7777587	3.8902531	1.2598660
C	-8.9826784	-4.3034677	-0.9099366
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C	-9.0314620	4.2134081	1.0536751
C	-9.0565965	4.3080126	-0.3409403
C	-2.7533816	3.7878304	0.4773112
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C	-4.9073054	2.8854769	1.0639176
C	-5.5631266	3.8862306	0.3592535
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F	-2.9492250	1.8746124	1.8289869
F	-5.6054391	1.9470809	1.6927324
F	-5.3590698	5.8005241	-0.9885344
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C	-2.7022602	-3.8117359	-0.3921541
C	-3.4930571	-2.8933509	-1.0584482
C	-4.8724095	-2.9519647	-0.9834365
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F	-2.9343219	-1.9410152	-1.7969040
F	-5.5858776	-2.0377665	-1.6304959
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C	-2.7551456	0.4271267	-3.8962728

C	-3.5167073	1.0686418	-2.9364387	H	-6.1125691	3.9176882	5.6921485
C	-4.8972627	0.9963433	-2.9558915	H	-5.2332062	3.9228179	4.1615339
C	-5.5654661	0.2844482	-3.9431347	H	-6.3673182	5.2292046	4.5392143
C	-4.7921633	-0.3815609	-4.8838104	C	2.7322745	4.4698227	-0.3363272
C	-3.4129772	-0.3146957	-4.8599879	C	4.2204020	4.7930867	-0.2558376
F	-2.9282472	1.7783955	-1.9801954	C	4.9732162	3.6891736	0.4981055
F	-5.5837365	1.6206059	-2.0057551	C	4.3191230	3.4344968	1.8538309
F	-5.3835766	-1.0684053	-5.8567818	C	2.8281816	3.1569177	1.6862318
F	-2.7289014	-0.9515536	-5.8031149	N	2.1237746	4.1981690	0.9559071
C	-2.6859829	-0.4564871	3.9856066	C	6.4337174	3.9879350	0.6105618
C	-3.3431537	0.2790893	4.9546890	N	7.1557410	3.9144129	1.7025404
C	-4.7229491	0.3339699	4.9891499	C	8.4481887	4.1894017	1.3149298
C	-5.4984580	-0.3373298	4.0538568	C	8.4684625	4.4477676	-0.0566383
C	-4.8311890	-1.0455867	3.0630945	N	7.1711506	4.3254544	-0.4704974
C	-3.4500614	-1.1058428	3.0328137	C	9.6363668	4.7380401	-0.7427930
F	-2.6574696	0.9214655	5.8929209	C	10.8134071	4.7077680	-0.0219214
F	-5.3124718	1.0141138	5.9680022	C	10.8123222	4.4505569	1.3660811
F	-5.5188386	-1.6787229	2.1198247	C	9.6320397	4.2155890	2.0460435
F	-2.8633757	-1.8115674	2.0727034	D	12.0097154	4.9498179	-0.6403236
C	-10.2344134	4.4993026	-1.0506176	C	12.5545973	3.9041215	-1.3504096
H	-10.2290359	4.6116450	-2.1249234	C	13.6654658	3.2332684	-0.8495808
C	-10.2121187	4.3165493	1.7845475	C	14.1865380	2.2055168	-1.6274669
H	-10.1935163	4.2895296	2.8647051	C	13.6551642	1.8165489	-2.8522354
C	-10.1745104	1.0731847	4.6444738	C	12.5384604	2.5123619	-3.3078863
H	-10.1703173	2.1475242	4.7578311	C	12.0154595	3.5643313	-2.5781289
C	-10.1514082	-1.7620662	4.4596243	C	14.2717603	0.6988038	-3.6722676
H	-10.1321187	-2.8422181	4.4314532	C	15.7991324	0.7061174	-3.6320750
C	-10.1615462	-4.6131736	1.2044159	C	14.2809648	3.6282030	0.4793313
H	-10.1440626	-4.7297243	2.2781600	C	15.8083588	3.5897231	0.4581667
C	-10.1696908	-4.4142906	-1.6302004	D	11.9774543	2.1985099	-4.5237439
H	-10.1619112	-4.3789415	-2.7102753	C	10.7897826	1.5146100	-4.5130388
C	-10.2266315	-1.1763885	-4.4985861	C	10.8224513	0.1285560	-4.7792132
H	-10.2086558	-2.2505667	-4.6111291	C	9.6607225	-0.6153730	-4.8328411
C	-10.2369711	1.6591198	-4.3147057	C	8.4751004	0.0449504	-4.5546584
H	-10.2315268	2.7394416	-4.2862949	C	8.4235861	1.4136675	-4.2852072
C	-7.0218647	4.0127016	0.3753620	C	9.5927507	2.1686856	-4.2897134
C	-6.9591837	-0.3526082	4.1658946	N	7.1200032	1.7725102	-4.0230399
C	-6.9679592	-4.0849554	-0.2497996	C	6.4218163	0.6666356	-4.1153405
C	-7.0263651	0.2869820	-4.0450533	N	7.1850537	-0.3959792	-4.4536596
N	-7.7402389	4.0310682	1.4725546	D	12.0336715	-0.4650988	-5.0079595
N	-7.7577431	1.3758712	-4.0554935	C	12.5824824	-1.1631548	-3.9560774
N	-7.6789031	-1.4490606	4.1803063	C	12.0610065	-2.3979231	-3.6143849
N	-7.6975554	-4.1057536	-1.3400556	C	12.5899782	-3.1156469	-2.5570496
N	-7.6966736	0.7649951	4.3312759	C	13.6973039	-2.6413240	-1.8587415
H	-7.3885847	1.7570498	4.2726852	C	14.2099475	-1.4085288	-2.2479468
N	-7.6926128	-4.2677008	0.8734059	C	13.6803500	-0.6415911	-3.2797067
H	-7.3790833	-4.2167885	1.8637468	D	12.0141372	4.4765403	2.0247974
N	-7.7523544	-0.8385183	-4.2046443	C	12.5882699	3.2648035	2.3311958
H	-7.4353702	-1.8275962	-4.1480532	C	12.0917452	2.5385077	3.3981836
N	-7.7583553	4.1818294	-0.7419227	C	12.6404081	1.3129910	3.7296411
H	-7.4515247	4.1330793	-1.7348147	C	13.7334650	0.8098055	3.0320543
I	-0.5935040	-0.6343370	4.0329322	C	14.2299659	1.5851215	1.9902960
I	-0.6129374	-3.8296701	-0.6001279	C	13.6891902	2.8088761	1.6110259
I	-0.6656522	0.6253006	-3.9663190	C	14.3255574	-3.4509669	-0.7396891
I	-0.6617969	3.8190220	0.6588690	C	15.8522443	-3.3879545	-0.7494052
O	-7.3421508	3.9909933	-3.3912515	D	12.0422877	-4.3367072	-2.2387519
H	-7.4383209	3.0440892	-3.6584621	C	10.8539318	-4.3315090	-1.5555094
C	-6.3142590	4.5853338	-4.1443026	C	10.8872879	-4.5889097	-0.1678760
H	-6.2549283	5.6400401	-3.8785028	C	9.7258967	-4.6389297	0.5771341
H	-5.3331978	4.1364053	-3.9516578	C	8.5396029	-4.3672375	-0.0848213
H	-6.5089441	4.5206417	-5.2188383	C	8.4875078	-4.1098792	-1.4556601
O	-7.3129400	-3.4792235	-3.9692796	C	9.6563051	-4.1170703	-2.2110870
H	-7.3937824	-3.7257951	-3.0152992	N	7.2494072	-4.2623631	0.3557491
C	-6.2923385	-4.2424458	-4.5631221	C	6.4853216	-3.9343500	-0.7099593
H	-6.2498418	-3.9986138	-5.6239786	N	7.1839647	-3.8531278	-1.8165716
H	-5.3050753	-4.0382350	-4.1333944	C	14.3533188	-0.5213281	3.4115739
H	-6.4834249	-5.3157988	-4.4728984	C	15.8794427	-0.5061121	3.3393885
O	-7.2723384	-4.0629352	3.5202657	D	12.1235043	0.6064093	4.7917859
H	-7.3611000	-3.1132130	3.7803096	C	10.9162266	-0.0037031	4.5872094
C	-6.2655371	-4.6641043	4.2959815	C	10.8985246	-1.3896065	4.3190736
H	-6.2210016	-5.7235065	4.0465728	C	9.7068569	-2.0610926	4.1198148
H	-5.2743321	-4.2349326	4.1108902	C	8.5266793	-1.3234503	4.1428669
H	-6.4742720	-4.5800037	5.3665229	C	8.5635857	0.0453991	4.4137425
O	-7.2586297	3.4074631	4.0905799	C	9.7451191	0.7230717	4.6665886
H	-7.3829815	3.6556966	3.1418259	N	7.2226785	-1.7016204	3.9114884
C	-6.1962678	4.1527334	4.6317739	C	6.5096917	-0.6069039	4.0229280

N	7.2649308	0.4666332	4.3442675	H	5.3637600	-4.5174805	-4.9368927
O	12.0999452	-4.8099945	0.4259499	H	5.2724552	4.9406209	-4.5203320
C	12.6410593	-3.7543580	1.1241074	H	6.3033428	6.1826312	-3.8074557
C	13.7309164	-3.0659787	0.6013972	H	6.9527872	5.1118446	-5.0493963
C	14.2508112	-2.0295495	1.3686676	H	5.4350799	4.5896928	4.8880234
C	13.7371633	-1.6479266	2.6032392	H	6.4668466	3.8817404	6.1327074
C	12.6399226	-2.3603689	3.0801756	H	7.1396131	5.0527882	4.9980729
C	12.1198168	-3.4210723	2.3611669	H	5.5058845	-4.9004011	4.5077656
O	12.0964327	-2.0553804	4.3061136	H	6.5147117	-6.1227714	3.7318020
C	5.0385864	-0.4809758	3.7869319	H	7.2190516	-5.0353781	4.9294340
C	4.3329162	0.2261111	4.9516716	H	4.3854841	0.3840295	-5.9207861
C	2.8333119	0.3273397	4.6909436	H	4.8636609	-0.1244592	-2.9555581
N	2.2052124	-0.9474337	4.3830851	H	4.7440082	2.3198572	-2.6548287
C	2.8690531	-1.6371125	3.2887937	H	4.4237069	2.5414864	-4.3626091
C	4.3686824	-1.8224865	3.5026582	H	2.6430562	1.0510683	-2.3679806
C	5.0251430	-3.6436739	-0.5701164	H	2.2938646	2.6001233	-3.1038041
C	4.3003333	-4.7164360	0.2525656	H	2.0971094	1.5597251	-5.1833054
C	2.8116404	-4.4007338	0.3539799	H	2.5879923	-0.9844503	-3.8553829
N	2.1690349	-4.1963669	-0.9340568	H	2.2143925	-0.7439219	-5.5475917
C	2.8452116	-3.1837360	-1.7282642	H	6.9019963	-1.3857338	-4.5070319
C	4.3343411	-3.4549641	-1.9189736	H	4.5153739	-0.3295605	5.8772366
C	4.9595515	0.5196204	-3.8426248	H	4.8132292	-2.2970302	2.6252278
C	4.2328223	-0.1834259	-4.9969728	H	4.5394848	-2.5024212	4.3430533
C	2.7416488	-0.3043275	-4.6998786	H	2.6910933	-1.0593178	2.3755050
N	2.1099596	0.9616638	-4.3644136	H	2.3796598	-2.6014330	3.1415064
C	2.7914443	1.6442503	-3.2766814	H	2.2151218	-1.5365817	5.2083654
C	4.2824165	1.8501153	-3.5259941	H	2.6525711	0.9978193	3.8443304
O	6.7096349	4.3000185	-3.1494176	H	2.3231780	0.7700397	5.5475001
C	6.2910320	5.1580591	-4.1791025	H	4.9120202	0.1521124	2.8957747
O	6.8385977	-4.2331959	3.0476944	H	4.7212590	-4.7857934	1.2583579
C	6.5047408	-5.0978931	4.1025905	H	4.7919304	-2.6347258	-2.4754427
O	6.7959922	3.1353507	4.2681282	H	4.4690187	-4.3546418	-2.5274337
C	6.4435191	4.2140052	5.0948332	H	2.7013690	-2.2193529	-1.2291672
O	6.7613432	-3.0749286	-4.3730504	H	2.3409725	-3.1083253	-2.6933048
C	6.3634297	-4.1460588	-5.1890429	H	2.1551318	-5.0716063	-1.4462403
H	11.2055363	4.1473931	-2.9896503	H	4.9422288	-2.6963627	-0.0159687
H	15.0549829	1.6764712	-1.2571239	H	2.6679645	-3.4882678	0.9416689
H	11.2589663	-2.8239419	-4.1978063	H	2.2853224	-5.1946772	0.8856033
H	15.0693569	-1.0226235	-1.7152623	H	4.3684009	5.7494139	0.2563476
H	11.2943102	2.9513739	3.9970211	H	4.7987409	2.5952399	2.3615268
H	15.0855769	1.2133687	1.4413710	H	4.4605489	4.3077595	2.4982476
H	11.3259092	-4.0144826	2.7883663	H	2.6812185	2.2148244	1.1470157
H	15.1036796	-1.4873233	0.9814015	H	2.3479413	3.0324390	2.6584974
H	14.0677891	-4.4946911	-0.9167850	H	2.1122111	5.0484058	1.5084997
H	13.9989683	0.8773155	-4.7118077	H	2.5814372	3.5854905	-0.9640637
H	14.0103405	4.6677221	0.6616374	H	2.1866107	5.2838180	-0.8157759
H	14.1046606	-0.7047672	4.4563406	H	4.8821969	2.7674136	-0.0960943
H	16.1782427	1.6669527	-3.9789067	H	4.6169493	4.9130922	-1.2668096
H	16.2172391	0.5334922	-2.6403717	H	4.6479317	-1.1796527	-5.1670249
H	16.2351601	-3.7306527	-1.7102191	H	4.4433870	-5.6949694	-0.2175075
H	16.2573099	-4.0355949	0.0276105	H	4.7398574	1.2291069	5.1005890
H	16.2759295	0.2748960	3.9875521	N-RA4 with piperidyl groups			
H	16.2739354	-0.3258911	2.3394372				
H	16.2048415	3.9403735	1.4106231	200			
H	16.1874560	4.2418786	-0.3281778				
H	16.2554013	-2.3897089	-0.5791059	Energy = -4805.793990390			
H	16.2798674	-1.4618098	3.6764178				
H	16.2236749	2.5975260	0.2820754	C	-5.7210559	4.5028046	-0.2687023
H	16.1927579	-0.0703040	-4.2875332	C	-4.2264759	4.8164866	-0.2071602
H	9.6255199	4.9679419	-1.7981343	C	-3.4832074	3.7301260	0.5815972
H	9.6258433	4.0437291	3.1131823	C	-4.1363231	3.5319310	1.9474923
H	9.5623903	3.2344457	-4.1120136	C	-5.6336593	3.2701181	1.7894305
H	9.6757339	-1.6687391	-5.0717512	N	-6.3377827	4.2741475	1.0201184
H	9.7494318	1.7761972	4.9069579	C	-2.0179595	4.0108413	0.6789300
H	9.6889023	-3.1268760	3.9401843	N	-1.2894870	3.9459000	1.7676877
H	9.7408723	-4.8678765	1.6326824	C	0.0033825	4.1989815	1.3687481
H	9.6254780	-3.9454774	-3.2778317	C	0.0193662	4.4359220	-0.0068945
H	6.8674177	4.3827773	-1.4536064	N	-1.2816054	4.3224452	-0.4112451
H	6.9680955	-4.3229183	1.3449341	C	1.1871008	4.7053616	-0.7020651
H	6.9688624	1.4521009	4.4056575	C	2.3671794	4.6767617	0.0147188
H	6.8587296	-3.3810750	-3.4336164	C	2.3700825	4.4367896	1.4053932
H	6.7974744	3.3728516	-3.4929239	C	1.1907693	4.2231701	2.0938186
H	6.8657350	3.4384009	3.3253130	O	3.5633082	4.9085913	-0.6100881
H	6.9175668	-3.3029774	3.3854649	C	4.1046723	3.8575535	-1.3137280
H	6.3391721	-3.8066890	-6.2245826	C	5.2159623	3.1887113	-0.8107064
H	7.0583973	-4.9894532	-5.1315936	C	5.7340723	2.1544993	-1.5819129

C	5.2001264	1.7583239	-2.8032452	C	-4.2384606	-0.2891241	-4.8046131
C	4.0846381	2.4535679	-3.2627971	C	-5.7286680	-0.3842469	-4.4781649
C	3.5637007	3.5104841	-2.5384830	N	-6.3701713	0.8900020	-4.2359763
C	5.8114903	0.6323864	-3.6156484	C	-5.6736010	1.6671790	-3.2326525
C	7.3390812	0.6385219	-3.5801468	C	-4.1821117	1.8580326	-3.5054846
C	5.8327271	3.5925866	0.5147991	O	-1.6668445	4.2863399	-3.1050231
C	7.3601235	3.5543446	0.4924998	C	-2.2106381	5.1169074	-4.0967455
O	3.5207889	2.1319869	-4.4750683	O	-1.5071484	-4.3212060	3.1475289
C	2.3288957	1.4535179	-4.4512590	C	-2.0468484	-5.1528077	4.1408605
C	2.3531926	0.0635424	-4.6937490	O	-1.5621807	3.1074673	4.3204488
C	1.1877165	-0.6767069	-4.7212313	C	-2.0794835	4.1025967	5.1639097
C	0.0071829	-0.0055744	-4.4467537	O	-1.6328196	-3.1336775	-4.2785538
C	-0.0358685	1.3688555	-4.2058351	C	-2.1352317	-4.1497192	-5.1058472
C	1.1366297	2.1177375	-4.2323243	H	2.7514343	4.0893178	-2.9510191
N	-1.3354130	1.7402286	-3.9450990	H	6.6009816	1.6249667	-1.2082707
C	-2.0416626	0.6369060	-4.0098457	H	2.7953695	-2.8923604	-4.1040322
N	-1.2846438	-0.4368513	-4.3287840	H	6.6162733	-1.0746165	-1.6495947
O	3.5610223	-0.5374762	-4.9277457	H	2.8420731	2.9363034	4.0333821
C	4.1176709	-1.2293744	-3.8767860	H	6.6343793	1.1818997	1.4892620
C	3.6006385	-2.4638003	-3.5270615	H	2.8875800	-4.0463723	2.8811514
C	4.1374252	-3.1772101	-2.4706698	H	6.6522354	-1.5170463	1.0482910
C	5.2461690	-2.6963543	-1.7790205	H	5.6202879	-4.5425501	-0.8258674
C	5.7552605	-1.4648932	-2.1766639	H	5.5350729	0.8024838	-4.6556839
C	5.2202348	-0.7043919	-3.2102922	H	5.5615287	4.6330790	0.6901595
O	3.5751142	4.4579754	2.0604448	H	5.6539449	-0.7118731	4.5198711
C	4.1418989	3.2439222	2.3702624	H	7.7178867	1.5960152	-3.9366911
C	3.6415286	2.5215966	3.4384260	H	7.7594905	0.4750198	-2.5878681
C	4.1864986	1.2955898	3.7745760	H	7.7853266	-3.7826642	-1.6289241
C	5.2815749	0.7888985	3.0821194	H	7.8115743	-4.0758116	0.1112870
C	5.7797798	1.5581154	2.0367578	H	7.8233084	0.2702097	4.0430431
C	5.2413905	2.7811897	1.6520850	H	7.8246841	-0.3491355	2.4016635
C	5.8778029	-3.4976172	-0.6561683	H	7.7572951	3.9099109	1.4429078
C	7.4044540	-3.4337692	-0.6694374	H	7.7383126	4.2027689	-0.2974378
O	3.5975202	-4.3997192	-2.1469256	H	7.8071983	-2.4340257	-0.5070480
C	2.4083708	-4.3984344	-1.4631391	H	7.8320373	-1.4703630	3.7511346
C	2.4435689	-4.6409856	-0.0734063	H	7.7755870	2.5613371	0.3208967
C	1.2819287	-4.6906118	0.6717537	H	7.7306671	-0.1444633	-4.2290329
C	0.0932984	-4.4382256	0.0059688	H	1.1727281	4.9188558	-1.7608393
C	0.0394741	-4.1984666	-1.3682740	H	1.1867897	4.0666691	3.1633987
C	1.2092861	-4.2023099	-2.1221090	H	1.1117874	3.1864975	-4.0724987
N	-1.1986220	-4.3450760	0.4429241	H	1.1943458	-1.7353574	-4.9358961
C	-1.9665941	-4.0415272	-0.6274741	H	1.2794588	1.7526063	4.8987355
N	-1.2666505	-3.9630273	-1.7340045	H	1.2591972	-3.1719897	4.0472455
C	5.9035179	-0.5378098	3.4737190	H	1.2965533	-4.9058328	1.7301963
C	7.4297495	-0.5192705	3.4032363	H	1.1771859	-4.0431028	-3.1908060
O	3.6659413	0.5937334	4.8372761	H	-1.5865114	4.3682536	-1.3944284
C	2.4628505	-0.0270355	4.6312131	H	-1.4777982	-4.3957466	1.4335207
C	2.4559156	-1.4176613	4.3913023	H	-1.4894137	1.3967974	4.3996947
C	1.2701439	-2.1023693	4.2029136	H	-1.5701959	-3.4586757	-3.3418885
C	0.0851300	-1.3730330	4.2025882	H	-1.6195506	3.3502402	-3.4342322
C	0.1109906	0.0026347	4.4385607	H	-1.5374411	3.4360906	3.3832708
C	1.2862031	0.6938649	4.6846843	H	-1.4754764	-3.3828214	3.4721586
N	-1.2138712	-1.7668223	3.9738641	H	-2.0979870	-3.8085823	-6.1406584
C	-1.9367425	-0.6751843	4.0519356	H	-1.5423658	-5.0670800	-5.0369814
N	-1.1902329	0.4120789	4.3492708	H	-3.1761432	-4.4054906	-4.8765619
O	3.6583751	-4.8526729	0.5217381	H	-3.2658321	4.8993936	-4.2991203
C	4.1981404	-3.7924669	1.2127620	H	-2.1440386	6.1521292	-3.7613318
C	5.2855140	-3.1046941	0.6836002	H	-1.6657022	5.0386886	-5.0426108
C	5.8037419	-2.0613962	1.4423366	H	-3.1374567	4.3139196	4.9698210
C	5.2918226	-1.6739894	2.6759025	H	-1.9929606	3.7651415	6.1969915
C	4.1997141	-2.3881908	3.1617694	H	-1.5284788	5.0439806	5.0748796
C	3.6800225	-3.4540298	2.4497226	H	-3.1119730	-4.9638326	4.3188658
O	3.6591579	-2.0762494	4.3871448	H	-1.9426014	-6.1906353	3.8235717
C	-3.4058085	-0.5710815	3.7947126	H	-1.5237543	-5.0435885	5.0959041
C	-4.1281092	0.2268327	4.8883292	H	-4.0982990	0.2033711	-5.7727385
C	-5.6266851	0.2967586	4.5955523	H	-3.5886891	-0.0625403	-2.7816046
N	-6.2551453	-0.9891347	4.3822335	H	-3.7153653	2.3966031	-2.6774262
C	-5.5697960	-1.7685754	3.3729044	H	-4.0466944	2.4779901	-4.3974596
C	-4.0697648	-1.9341290	3.6136816	H	-5.8029382	1.1633634	-2.2673873
C	-3.4324091	-3.7808909	-0.4915361	H	-6.1666278	2.6367248	-3.1359775
C	-4.1413218	-4.8796896	0.3114609	H	-6.4288357	1.4157550	-5.0988457
C	-5.6371203	-4.5831146	0.4152508	H	-5.8592084	-1.0010297	-3.5813207
N	-6.2913660	-4.3560798	-0.8551880	H	-6.2584765	-0.8996256	-5.2813630
C	-5.6192433	-3.3418300	-1.6395305	H	-1.5693402	-1.4261725	-4.3743522
C	-4.1238000	-3.5860065	-1.8388339	H	-3.9579068	-0.2525602	5.8581707
C	-3.5024732	0.5075938	-3.7190718	H	-3.6142029	-2.4759163	2.7813842

H	-3.9040369	-2.5407068	4.5097576	C	-14.7604449	-1.9773901	1.8585012
H	-5.7282759	-1.2787888	2.4047114	H	-11.7835073	-3.8147954	3.3679935
H	-6.0505342	-2.7462402	3.2994700	H	-15.6255745	-1.4744454	1.4464636
H	-6.2879096	-1.5053401	5.2522146	O	-12.5290746	-1.7281634	4.7254442
H	-5.7865929	0.9015127	3.6952800	C	-14.7983050	-0.2746680	3.7464053
H	-6.1452499	0.8135764	5.4051390	H	-14.5192947	-0.3552429	4.7965738
H	-3.5232613	-0.0137261	2.8528542	C	-14.7988171	3.5747756	0.4263843
H	-3.7162529	-4.9639274	1.3151377	H	-14.5097454	4.6230712	0.4954345
H	-3.6769203	-2.7506744	-2.3829924	C	-14.9666188	0.2532036	-3.4167950
H	-3.9740569	-4.4774192	-2.4562861	H	-14.7377840	0.3278110	-4.4794583
H	-5.7638656	-2.3776716	-1.1376538	C	-14.8957751	-3.5964327	-0.0987341
H	-6.1199531	-3.2574880	-2.6062341	H	-14.6353714	-4.6511188	-0.1823357
H	-6.3388183	-5.2211473	-1.3783811	C	-8.9595599	0.3046199	4.5256285
H	-3.5355837	-2.8439095	0.0765462	C	-8.9539768	-1.0892665	4.4208946
H	-5.7815541	-3.6879437	1.0313500	C	-9.1870533	-0.4503946	-4.4621643
H	-6.1476174	-5.3956725	0.9354424	C	-9.1502995	0.9433501	-4.3617150
H	-4.0670428	5.7867428	0.2751833	O	-12.7196854	1.6558571	-4.5093970
H	-3.6652615	2.7037047	2.4820989	O	-12.4809366	4.5462065	1.8037446
H	-3.9805003	4.4270654	2.5580645	O	-12.6092853	-4.8176741	1.1096367
H	-5.7812240	2.3027498	1.2946510	C	-16.3265004	3.5569391	0.4585388
H	-6.1071220	3.1836864	2.7696165	H	-16.7245828	4.1327418	-0.3765947
H	-6.3794657	5.1408300	1.5411451	H	-16.7587453	2.5582680	0.3969051
H	-5.8723701	3.6034741	-0.8770758	C	-16.3257981	-0.2542942	3.7172731
H	-6.2546455	5.3074420	-0.7779179	H	-16.6990241	0.5918085	4.2937386
H	-3.5889109	2.7894871	0.0199933	H	-16.7206208	-1.1679627	4.1608192
H	-3.8298599	4.8999704	-1.2224485	C	-16.4223988	-3.5421340	-0.0600542
H	-3.8211780	-1.2951001	-4.8987404	H	-16.8353705	-3.9800490	-0.9684151
H	-3.9840994	-5.8457850	-0.1798348	H	-16.8273171	-2.5336756	0.0244478
H	-3.7240700	1.2399280	4.9620555	C	-16.4908104	0.2670944	-3.3126119

I-capsule with quinuclidyl groups

396

Energy = -12615.45496830

C	-13.2210157	2.0862697	-3.3035216	C	-16.6861156	4.0069692	1.3835123
C	-14.2336391	3.0427406	-0.8769323	C	-9.0855227	-4.2666677	-0.9768581
C	-14.3188544	1.4450226	-2.7365154	C	-9.0762876	-4.3793013	0.4163906
C	-12.6524999	3.1893241	-2.6929004	C	-8.9412303	4.1160412	1.0520002
C	-13.1316574	3.6438882	-1.4780815	C	-8.9865248	4.2178341	-0.3413790
C	-14.7962632	1.9535427	-1.5333793	C	12.2776293	3.9250308	-1.3209838
H	-11.8518723	3.7199849	-3.1850112	C	13.3716036	1.8488640	-2.8416611
H	-15.6524303	1.4717169	-1.0797804	C	13.3929283	3.2534625	-0.8308052
O	-12.5364601	4.7351625	-0.8879799	C	11.7350814	3.5961868	-2.5501399
C	-11.3261468	4.5255760	-0.2839456	C	12.2590200	2.5539811	-3.2927679
C	-11.2949629	4.4285068	1.1269206	C	13.9076308	2.2284524	-1.6160176
C	-11.5213661	0.9926506	-4.4801900	H	10.9208486	4.1799294	-2.9523968
C	-11.5441130	-0.4176245	-4.5810337	H	14.7750936	1.6937718	-1.2512619
O	-12.7595981	-1.0331465	-4.7062875	O	11.7048959	2.2626085	-4.5175530
C	-13.0524889	3.3774433	2.2496325	C	10.4997459	1.6115614	-4.5325834
C	-14.1833385	1.0081027	3.2187282	C	10.5036741	0.2174320	-4.7557919
C	-12.5209276	2.7509643	3.3617868	C	10.5460647	4.6979150	0.0340375
C	-14.1789420	2.8633228	1.6139263	C	10.5665608	4.4435617	1.4220353
C	-14.7132987	1.6858367	2.1263557	O	11.7763274	4.4842156	2.0648409
C	-13.0610416	1.5653073	3.8243025	C	12.2499851	-1.1060558	-3.9168120
H	-11.6996689	3.2091276	3.8911487	C	13.3706470	-2.6071195	-1.8417083
H	-15.5886163	1.2706735	1.6440807	C	11.7132987	-2.3325182	-3.5726891
C	-13.2752308	-1.6250237	-3.5766548	C	13.3689522	-0.6057424	-3.2586856
C	-14.3146054	-2.8976950	-1.3133778	C	13.8985669	-1.3816696	-2.2346012
C	-12.7389505	-2.8214368	-3.1376657	C	12.2509505	-3.0648393	-2.5298500
C	-14.3546473	-1.0429246	-2.9186870	H	10.8936035	-2.7405556	-4.1444018
C	-14.8464688	-1.7088480	-1.8014749	H	14.7701399	-1.0102409	-1.7113413
C	-13.2300525	-3.4357351	-2.0004134	C	12.3596118	3.2759687	2.3662221
H	-11.9540744	-3.2981345	-3.7046410	C	13.5292010	0.8299883	3.0568711
H	-15.6888695	-1.2746618	-1.2789841	C	11.8798362	2.5484683	3.4399730
O	-12.5047357	0.9592163	4.9265602	C	13.4525665	2.8247854	1.6317466
O	-12.6632035	-4.6166366	-1.5816495	C	14.0062082	1.6051934	2.0060626
C	-11.3092527	0.3197577	4.7431507	C	12.4414207	1.3282654	3.7670668
C	-11.3195745	-1.0905412	4.6379536	H	11.0873549	2.9560713	4.0492279
C	-11.4471522	-4.5274989	-0.9553808	H	14.8561874	1.2373915	1.4458691
C	-11.4213540	-4.6357183	0.4546331	O	11.6943976	-4.2827817	-2.2141142
C	-13.1022162	-2.1469460	3.5480083	O	11.9523856	0.6294192	4.8454213
C	-14.2582112	-3.0806288	1.1772748	C	10.5018327	-4.2557346	-1.5400658
C	-14.2118328	-1.4801797	3.0357265	C	10.5239808	-4.4488482	-0.1420577
C	-12.5941499	-3.2657796	2.9138682	C	10.7421199	0.0091944	4.7040159
C	-13.1455333	-3.7105541	1.7263357	C	10.7310753	-1.3840294	4.4756727
				C	12.3173186	-3.6674081	1.1546613

C	13.5142936	-1.6203727	2.6360528	C	-5.4644623	-0.4427823	4.2188549
C	13.4250746	-3.0158223	0.6211540	C	-4.7640490	-1.1776974	3.2711577
C	11.8382795	-3.3407693	2.4099529	C	-3.3832386	-1.2448591	3.2945761
C	12.4170873	-2.3158036	3.1363453	F	-2.6855455	0.8496845	6.1299916
C	13.9899807	-2.0020619	1.3861017	F	-5.3391212	0.9509862	6.1101549
H	11.0352975	-3.9172983	2.8438725	F	-5.4180690	-1.8267458	2.3146855
H	14.8491988	-1.4798274	0.9859304	F	-2.7640012	-1.9711798	2.3713975
O	11.7287164	-4.6949801	0.4564540	C	-10.1693367	4.4483963	-1.0313204
C	13.9933337	-3.4230217	-0.7252353	H	-10.1772392	4.5603687	-2.1056848
H	13.7087606	-4.4616290	-0.8907533	C	-10.1065591	4.2517317	1.8029555
C	13.9760372	0.7246941	-3.6610914	H	-10.0714167	4.2147361	2.8824588
H	13.7022329	0.9017391	-4.7006272	C	-10.1281545	1.0309873	4.7095319
C	14.0227052	3.6475611	0.4918019	H	-10.1076694	2.1038143	4.8344345
H	13.7481462	4.6850574	0.6794615	C	-10.1476103	-1.8035083	4.4997870
C	14.1597585	-0.4990265	3.4282849	H	-10.1455875	-2.8836854	4.4616855
H	13.9378297	-0.6782797	4.4797851	C	-10.2333042	-4.5907767	1.1533222
C	8.1333223	-4.0531441	-1.4781006	H	-10.1983265	-4.7118817	2.2260689
C	8.1742584	-4.2252155	-0.0933339	C	-10.2841378	-4.3705282	-1.6794162
C	8.2078133	4.1469970	1.4032286	H	-10.2936374	-4.3249212	-2.7591573
C	8.2065062	4.4001362	0.0307354	C	-10.3769344	-1.1527091	-4.5967072
O	11.7305084	4.9607786	-0.5988733	H	-10.3841380	-2.2261397	-4.7177632
O	11.7051815	-0.4002047	-4.9629619	C	-10.3305109	1.6817151	-4.3959845
O	11.9354531	-2.0295790	4.3920417	H	-10.3045378	2.7616172	-4.3617866
C	15.5032618	0.7159344	-3.6243389	C	-6.9523322	3.8338172	0.3387231
H	15.8913390	1.6714487	-3.9759486	C	-6.9279825	-0.4419111	4.2778738
H	15.9218928	0.5432141	-2.6329012	C	-7.0634774	-4.0338815	-0.3421443
C	15.5208429	-3.3966270	-0.7549387	C	-7.1351788	0.2562323	-4.2802828
H	15.8819345	-3.7594018	-1.7168099	C	6.1825141	3.9425025	0.7346823
H	15.9210731	-4.0448420	0.0241590	C	6.0807700	0.9327136	-4.4947372
C	15.6829396	-0.4878571	3.3155411	C	6.3153741	-0.7162397	4.6053264
H	16.0983383	0.2954310	3.9489631	C	6.1092049	-3.9493110	-0.7804102
H	16.0514362	-0.3137620	2.3046932	C	9.3600685	4.7049548	-0.6725440
C	15.5499244	3.6189444	0.4485794	H	9.3312583	4.9292346	-1.7286788
H	15.9576883	3.9690639	1.3964657	C	9.4000161	4.1918688	2.1183791
H	15.9133608	4.2765320	-0.3406213	H	9.4090218	4.0239228	3.1860297
H	15.9498601	-2.4062973	-0.6027004	C	9.3138963	2.3082514	-4.3984653
H	16.0895525	-1.4429111	3.6469973	H	9.3107133	3.3822543	-4.2734023
H	15.9691937	2.6301284	0.2626624	C	9.3246607	-0.4973605	-4.8293507
H	15.8877082	-0.0671753	-4.2772479	H	9.3187883	-1.5577616	-5.0356462
C	8.3822391	0.0067474	4.7125343	C	9.5652382	0.7182500	4.8411169
C	8.3532485	-1.3722778	4.4968022	H	9.5641181	1.7779260	5.0516129
C	8.1458997	0.2102352	-4.6544252	C	9.5441970	-2.0852320	4.3944401
C	8.1217844	1.5909950	-4.4507244	H	9.5401603	-3.1590200	4.2684032
C	-2.7136215	3.2385013	0.3011078	C	9.3563603	-4.4481903	0.5956088
C	-3.5394828	2.4295569	1.0589916	H	9.3619611	-4.6230910	1.6615926
C	-4.9114167	2.5999196	1.0500858	C	9.3109701	-4.0826291	-2.2180057
C	-5.5078328	3.6011754	0.2928670	H	9.2922424	-3.9768473	-3.2937416
C	-4.6704314	4.3983778	-0.4765816	N	6.8278365	-3.8836661	-1.8761749
C	-3.3013275	4.2174023	-0.4787586	N	7.0464338	-1.7932524	4.4340368
F	-3.0213262	1.4691417	1.8165453	N	6.8134644	2.0109419	-4.3545037
F	-5.6573634	1.7745206	1.7744999	N	6.9237305	3.8689110	1.8137683
F	-5.1851251	5.3826572	-1.2085602	N	-7.6520392	3.8792412	1.4480507
F	-2.5533726	5.0216558	-1.2242050	N	-7.8491915	1.3558755	-4.2512923
C	-2.8136236	-3.5227451	-0.4168769	N	-7.6649196	-1.5271166	4.2677478
C	-3.6416395	-2.7055877	-1.1636407	N	-7.8079526	-4.0548457	-1.4229543
C	-5.0160143	-2.8502599	-1.1227369	N	-7.6529373	0.6859860	4.4330938
C	-5.6138698	-3.8337946	-0.3435926	H	-7.3363305	1.6730497	4.3615466
C	-4.7734409	-4.6419178	0.4116016	N	-7.7727014	-4.2342182	0.7894203
C	-3.4020667	-4.4848417	0.3828821	H	-7.4537845	-4.2003434	1.7770202
F	-3.1237421	-1.7608647	-1.9413737	N	-7.8851566	-0.8575559	-4.4119366
F	-5.7628832	-2.0161829	-1.8367866	H	-7.5834411	-1.8502859	-4.3458110
F	-5.2876910	-5.6128311	1.1616925	N	-7.7016608	4.0417471	-0.7652585
F	-2.6531363	-5.2970883	1.1187581	H	-7.4225253	4.0002232	-1.7646686
C	-2.8622776	0.3765625	-4.3443078	N	6.9038216	4.2707461	-0.3620200
C	-3.5738339	1.0110800	-3.3427192	H	6.5882113	4.3408707	-1.3385732
C	-4.9528118	0.9410425	-3.2920224	N	6.8341677	-0.1779925	-4.6766853
C	-5.6711436	0.2388090	-4.2502294	H	6.5283453	-1.1587135	-4.6849250
C	-4.9479131	-0.4196611	-5.2354354	N	6.8714026	-4.1548232	0.3195788
C	-3.5686909	-0.3533576	-5.2818002	H	6.5813711	-4.1681218	1.3046871
F	-2.9359737	1.7065420	-2.4082338	N	7.0696946	0.3914833	4.7820292
F	-5.5878941	1.5565192	-2.3013108	H	6.7681080	1.3736502	4.7913782
F	-5.5893212	-1.0984805	-6.1818352	I	-0.5548141	-0.6878341	4.3343947
F	-2.9321113	-0.9842143	-6.2613595	I	-0.7218789	-3.3604831	-0.5098361
C	-2.6512737	-0.5708945	4.2550814	I	-0.7716270	0.5406820	-4.4659811
C	-3.3402941	0.1848508	5.1852143	I	-0.6257134	3.0381198	0.3561844
C	-4.7199210	0.2450386	5.1684707	O	6.4127514	-2.8988048	-4.4086725

H	6.5206364	-3.2536443	-3.4905640	H	2.3781057	2.2657497	2.3354189
O	6.4270644	4.3844982	-3.0679580	C	2.5852459	3.2380416	1.8825720
H	6.5082273	3.5382683	-3.5751122	N	2.1963012	3.1671182	0.4792997
O	6.7444343	3.1067316	4.4349812	H	4.1788413	4.5984440	2.5238139
H	6.7432841	3.3609570	3.4780290	C	3.9987378	4.7396473	-0.1812739
O	6.4325593	-4.0841159	3.0740299	H	4.3769404	4.7373617	-1.2058082
H	6.6301333	-3.2581601	3.5842563	H	1.9338180	3.9553911	2.3844727
C	6.1371175	-3.9629341	-5.2857553	C	2.4837048	4.4427919	-0.1678660
H	6.1469797	-3.5837322	-6.3076968	H	2.0784688	4.4144109	-1.1812925
H	6.8853298	-4.7584578	-5.2188243	H	4.2073094	5.7297871	0.2293593
H	5.1545323	-4.4119661	-5.1047566	H	1.9320925	5.2212513	0.3619162
C	6.1031518	5.4355053	-3.9429764	H	4.5251114	-0.6558126	-6.0548881
H	5.0843989	5.3542839	-4.3378809	C	4.0987804	0.3331237	-5.8728716
H	6.1739668	6.3770924	-3.3984200	H	2.2038576	-0.7608230	-5.9990039
H	6.7895280	5.4902998	-4.7933791	H	4.4575730	0.9803140	-6.6760334
C	6.2910447	4.1952637	5.2002965	H	4.4534125	-1.0544092	-3.5358453
H	5.2318916	4.4188826	5.0292570	C	2.5539959	0.2632280	-5.8572773
H	6.4132236	3.9542361	6.2561922	H	2.1231155	0.8536520	-6.6672425
H	6.8628667	5.1056796	4.9980504	C	4.0478359	-0.0473698	-3.4136418
C	6.3715519	-5.1734235	3.9613937	C	4.5855937	0.8805453	-4.5158952
H	5.4698554	-5.1576324	4.5831440	H	2.1303859	-1.0815068	-3.6462590
H	6.3581488	-6.0967269	3.3817856	C	2.5039916	-0.0655490	-3.4995930
H	7.2368203	-5.2127695	4.6304128	N	2.0155281	0.7568818	-4.5960886
O	-7.4331333	3.39314443	-3.44777160	H	4.3853725	0.3116105	-2.4379454
H	-7.5256023	2.9999887	-3.7631584	C	3.9678453	2.2675231	-4.3123550
C	-6.5036601	4.6024418	-4.2622446	H	4.3443603	2.9555348	-5.0712207
H	-6.4607083	5.6462101	-3.9535046	H	2.0480757	0.2997445	-2.5770192
H	-5.4927023	4.1878712	-4.1819891	C	2.4288140	2.1403522	-4.3964678
H	-6.7958396	4.5764993	-5.3161391	H	2.0273075	2.7347671	-5.2187471
O	-7.4771732	-3.4999279	-4.0913752	H	4.2722830	2.6736175	-3.3452272
H	-7.5408271	-3.7058316	-3.1273052	H	1.9488322	2.5113122	-3.4878728
C	-6.4604005	-4.2840653	-4.6648372	H	4.7119447	-1.8294167	2.7518144
H	-6.4211960	-4.0726584	-5.7329102	C	4.3115757	-0.8952697	3.1490176
H	-5.4715392	-4.0682287	-4.2448391	H	2.3792821	-1.8547660	2.7680336
H	-6.6532493	-5.3538107	-4.5413083	H	4.6904892	-0.0896941	2.5131620
O	-7.3934305	-4.1198680	3.4586377	H	4.6665026	-2.8118311	5.0659827
H	-7.4217762	-3.1833130	3.7705547	C	2.7661894	-0.9149958	3.1680159
C	-6.4753065	-4.8389068	4.2448380	H	2.3493248	-0.1194881	2.5454221
H	-6.5010315	-5.8844295	3.9402009	C	4.2669570	-1.8671639	5.4348941
H	-5.4465411	-4.4814436	4.1278661	C	4.8178200	-0.7068261	4.5888515
H	-6.7298640	-4.7932502	5.3077767	H	2.3383617	-2.7872075	4.9451456
O	-7.2239669	3.3262740	4.1026468	C	2.7223050	-1.8515990	5.3558218
H	-7.3230504	3.5301397	3.1412311	N	2.2443289	-0.7579617	4.5172600
C	-6.1855553	4.1101812	4.6359082	H	4.6100472	-1.7641380	6.4663647
H	-6.1114831	3.9068281	5.7036269	C	4.2306720	0.6013377	5.1350007
H	-5.2120131	3.8870076	4.1848294	H	4.5809129	1.4535754	4.5484019
H	-6.3778540	5.1798142	4.5104553	H	2.2756565	-1.7408690	6.3452272
C	2.4407257	-4.0093575	-1.9151748	C	2.6877247	0.5122729	5.0764337
C	3.9730088	-4.1396656	-2.0585385	H	2.2690284	1.3173453	4.4694352
C	4.6237584	-3.7820435	-0.7156720	H	4.5709278	0.7647703	6.1601499
C	3.9951756	-4.6693913	0.3714644	H	2.2482173	0.6174202	6.0695409
C	2.4804577	-4.3700092	0.4362785	N-RA4 with quinuclidyl groups			
N	2.0720491	-3.4513146	-0.6193787	216			
H	2.0233692	-3.3699462	-2.6958454	Energy = -5114.791893487			
H	1.9483086	-4.9782077	-2.0162256	C	4.4590392	3.7867734	-1.3876557
H	4.2567149	-5.1519606	-2.3521166	C	5.5410284	1.6488544	-2.8314373
H	4.3453894	-3.4733591	-2.8372987	C	5.5648034	3.1200544	-0.8688537
H	4.1786981	-5.7206643	0.1374862	C	3.9226010	3.4236168	-2.6099092
H	4.4503861	-4.4782527	1.3448639	C	4.4411518	2.3525755	-3.3147518
H	2.2075683	-3.9238414	1.3951690	C	6.0732117	2.0633783	-1.6154319
H	1.8921485	-5.2842322	0.3452240	H	3.1161873	4.0014350	-3.0355600
C	2.7317765	-2.1663428	-0.4334710	H	6.9312704	1.5309636	-1.2259442
H	2.4200859	-1.5105868	-1.2469878	O	3.8951025	2.0270646	-4.5340663
C	4.2702402	-2.3181807	-0.3948729	C	2.6795875	1.3936847	-4.5350291
H	2.3521902	-1.7157020	0.4851920	C	2.6625054	-0.0066261	-4.7084968
H	4.6697068	-2.0498472	0.5851538	C	2.7268001	4.6214868	-0.0664139
H	4.7517576	-1.6576217	-1.1182703	C	2.7398595	4.4188041	1.3296205
H	4.9109698	1.5083107	0.5865099	O	3.9484651	4.4666779	1.9768100
C	4.4692556	2.3012474	-0.0229058	C	4.3863870	-1.3267748	-3.8182742
H	2.6208641	1.1459379	0.2303348	C	5.4775638	-2.7777744	-1.6926699
H	4.9714543	2.2639291	-0.9925233	C	3.8322864	-2.5352500	-3.4391020
H	4.5938030	2.9048491	2.6748072	C	5.5081145	-0.8200998	-3.1691183
C	2.9425943	2.1055005	-0.1815606	C	6.0227627	-1.5713170	-2.1192239
H	2.6557711	2.1031295	-1.2352682				
C	4.0729118	3.6241351	2.0417640				
C	4.7166872	3.6639833	0.6526179				

C	4.3550340	-3.2423378	-2.3715602	H	1.5997463	-3.0934285	4.4020299
H	3.0097384	-2.9490675	-4.0023754	C	1.4281514	-4.5052048	0.7805912
H	6.8957544	-1.1946218	-1.6021195	H	1.4278970	-4.6530648	1.8507336
C	4.5116854	3.2596903	2.3180562	C	1.4012334	-4.2057242	-2.0397842
C	5.6402820	0.8167532	3.0870123	H	1.3879811	-4.1223287	-3.1175774
C	4.0127826	2.5689877	3.4074676	N	-1.0772253	-3.9437440	-1.7147514
C	5.6031649	2.7711192	1.6055398	N	-0.8821389	-1.7026115	4.5193893
C	6.1365513	1.5547775	2.0185283	N	-0.9974107	1.8586028	-4.3892276
C	4.5531601	1.3500613	3.7729963	N	-0.9028587	3.8555223	1.7249570
H	3.2203856	3.0031861	3.9979860	N	-0.9143320	4.1790683	-0.4633662
H	6.9846958	1.1587169	1.4751234	H	-1.2222071	4.2235826	-1.4431139
O	3.7825927	-4.4426881	-2.0207424	N	-1.0144590	-0.3401471	-4.6306019
O	4.0443753	0.6893957	4.8653784	H	-1.3360718	-1.3147512	-4.6112705
C	2.5867953	-4.3815149	-1.3526605	N	-1.0500194	-4.1657923	0.4865572
C	2.5997714	-4.5399204	0.0490056	H	-1.3468692	-4.1490668	1.4695829
C	2.8283960	0.0770386	4.7293214	N	-0.8405886	0.4924059	4.7866392
C	2.8055087	-1.3226119	4.5516235	H	-1.1336181	1.4768964	4.7708017
C	4.3942092	-3.7369461	1.3283853	O	-1.4390206	-3.0551857	-4.2858743
C	5.5996568	-1.6488689	2.7464208	H	-1.3532294	-3.3684656	-3.3498436
C	5.5108594	-3.1126684	0.7806001	O	-1.2799547	4.2815752	-3.1863048
C	3.9104445	-3.3621411	2.5683131	H	-1.2510903	3.4179714	-3.6706035
C	4.4931321	-2.3174694	3.2629229	O	-1.0866019	3.2043824	4.3735710
C	6.0797562	-2.0777256	1.5136323	H	-1.0897824	3.4123031	3.4047997
H	3.0979325	-3.9144629	3.0156001	O	-1.5412570	-4.0217232	3.2380324
H	6.9450692	-1.5761140	1.1004718	H	-1.3219302	-3.1831594	3.7190569
O	3.7994549	-4.7821064	0.6622721	C	-1.7065243	-4.1564363	-5.1162717
C	6.0830332	-3.5675011	-0.5485277	H	-1.7533177	-3.8103093	-6.1489852
H	5.7863847	-4.6069911	-0.6848292	H	-0.9254193	-4.9210772	-5.0569401
C	6.1352768	0.4894507	-3.6086992	H	-2.6623214	-4.6365873	-4.8804270
H	5.8710492	0.6361399	-4.6554701	C	-1.6811991	5.3066130	-4.0579008
C	6.1903360	3.5505995	0.4442264	H	-2.7172440	5.1916375	-4.3960011
H	5.9258013	4.5965392	0.5961217	H	-1.6076999	6.2588896	-3.5323388
C	6.2511040	-0.5078669	3.5050726	H	-1.0436170	5.3664295	-4.9455091
H	6.0193087	-0.6495992	4.5601968	C	-1.6090748	4.3012376	5.0783785
C	0.2212859	-4.1372602	-1.3067057	H	-2.6781135	4.4541758	4.8903644
C	0.2523957	-4.2781487	0.0822152	H	-1.4821316	4.1225791	6.1462867
C	0.3799524	4.1316633	1.3119941	H	-1.0898651	5.2324862	4.8324686
C	0.3851625	4.3344378	-0.0690499	C	-1.5375985	-5.0897583	4.1505001
O	3.9174702	4.8508188	-0.7039165	H	-2.2763837	-4.9585489	4.9481188
O	3.8565249	-0.6489200	-4.8895969	H	-1.7876030	-6.0059228	3.6150635
O	4.0046607	-1.9835203	4.5035688	H	-0.5604041	-5.2364694	4.6232667
C	7.6620043	0.4618505	-3.5603461	C	-5.4697397	-3.8169053	-1.7650493
H	8.0652574	1.3998081	-3.9411390	C	-3.9508312	-4.0868544	-1.8941900
H	8.0710149	0.3177679	-2.5603153	C	-3.2792172	-3.7287420	-0.5614478
C	7.6109577	-3.5606600	-0.5682465	C	-3.9483783	-4.5575129	0.5484112
H	7.9740540	-3.9555031	-1.5167266	C	-5.4595774	-4.2155307	0.5682293
H	7.9978671	-4.1906090	0.2323497	N	-5.8144574	-3.2640054	-0.4680005
C	7.7752893	-0.5181857	3.4036691	H	-5.8070411	-3.1200572	-2.5358321
H	8.1955007	0.2813306	4.0133124	H	-6.0431652	-4.7354262	-1.9076583
H	8.1527723	-0.3827306	2.3901875	H	-3.7503074	-5.1323974	-2.1385430
C	7.7174488	3.5039172	0.4130185	H	-3.5189258	-3.4901197	-2.6979932
H	8.1224929	3.8807975	1.3518257	H	-3.7860189	-5.6217636	0.3598757
H	8.0938788	4.1305550	-0.3951358	H	-3.5030482	-4.3375135	1.5206363
H	8.0509898	-2.5715320	-0.4417831	H	-5.7468066	-3.7921460	1.5337877
H	8.1682202	-1.4663171	3.7698332	H	-6.0642884	-5.1146093	0.4335730
H	8.1266835	2.5047531	0.2634442	C	-5.0878818	-2.0254134	-0.2590270
H	8.0408238	-0.3482053	-4.1831021	H	-5.3901153	-1.3180154	-1.0340032
C	0.4684376	0.0964661	4.7214443	C	-3.5543088	-2.2395646	-0.2761956
C	0.4274653	-1.2895139	4.5563056	H	-5.4106141	-1.5951189	0.6914637
C	0.3040621	0.0252702	-4.6162040	H	-3.1025816	-1.9558877	0.6772068
C	0.3025359	1.4128739	-4.4628825	H	-3.0729940	-1.6285150	-1.0428003
C	-1.6389098	3.8781195	0.6390248	H	-2.6778231	1.3974474	0.6265228
C	-1.7498669	0.7896008	-4.4940000	C	-3.2382067	2.0964469	0.0002889
C	-1.6055570	-0.6152559	4.6615080	H	-4.9576032	0.8831161	0.6058894
C	-1.8027626	-3.9622696	-0.6211484	H	-2.7948518	2.0412498	-0.9980297
C	1.5430591	4.6101615	-0.7776882	H	-3.2406257	2.8661290	2.6119090
H	1.5186349	4.7915730	-1.8421540	C	-4.7457659	1.7442663	-0.0323653
C	1.5688277	4.2014854	2.0301076	H	-5.0578805	1.4635000	-1.0419804
H	1.5716825	4.0713269	3.1030659	C	-3.7491089	3.5627561	1.9432521
C	1.5046458	2.1130218	-4.4305086	C	-3.0889382	3.5255959	0.5607104
H	1.5162380	3.1905352	-4.3419680	H	-5.4980887	2.3332795	2.4146216
C	1.4725758	-0.7059905	-4.7604107	C	-5.2421079	3.1869959	1.7816947
H	1.4505622	-1.7731723	-4.9267502	N	-5.5727209	2.8516540	0.4083892
C	1.6570563	0.8016818	4.8294157	H	-3.6339068	4.5564867	2.3820613
H	1.6633844	1.8682880	5.0014613	C	-3.8597968	4.4805352	-0.3671308
C	1.6126407	-2.0155391	4.4858756	H	-3.4154294	4.4899893	-1.3648551

H	-5.8886181	4.0085855	2.0973495	O	-12.3724539	4.4627959	1.9129175
C	-5.3327983	4.0049341	-0.4395815	C	-11.1760532	4.4484901	1.2494835
H	-5.6029654	3.7372093	-1.4643327	C	-11.2055555	4.6159535	-0.1571024
H	-3.7900817	5.5009368	0.0173785	C	-10.0451012	4.6879652	-0.8952310
H	-6.0152924	4.8026104	-0.1397606	C	-8.8515709	4.5513879	-0.2006600
H	-3.3319534	-0.7242439	-6.1258559	C	-8.8028541	4.3729776	1.1855417
C	-3.6905094	0.2937191	-5.9533743	C	-9.9824671	4.3419881	1.9299036
H	-5.6501163	-0.6113850	-6.3144757	N	-7.5541560	4.5760497	-0.6182543
H	-3.2322698	0.9205407	-6.7217829	C	-6.7943715	4.4056907	0.4842921
H	-3.4373550	-1.1785873	-3.6144999	N	-7.4949112	4.2810846	1.5863420
C	-5.2360235	0.3554733	-6.0216670	O	-12.4215154	4.7589890	-0.7611056
H	-5.5635585	1.0747361	-6.7750510	C	-12.9468459	3.6520689	-1.3868658
C	-3.8550775	-0.1740818	-3.5136547	C	-14.0481908	3.0079278	-0.8328803
C	-3.2438876	0.7759461	-4.5571712	C	-14.5646588	1.9241000	-1.5336397
H	-5.7288845	-1.1943371	-4.0074260	C	-14.0385665	1.4586025	-2.7336230
C	-5.3914738	-0.1954655	-3.7211595	C	-12.9300795	2.1305227	-3.2421784
N	-5.8155269	0.7379454	-4.7465355	C	-12.4064753	3.2303850	-2.5878407
H	-3.5919720	0.1736922	-2.5107081	O	-12.3849915	1.7468535	-4.4445473
C	-3.8283258	2.1737120	-4.3277481	C	-11.1807062	1.0979194	-4.4275569
H	-3.4450002	2.8597443	-5.0858657	C	-11.1927706	-0.3088262	-4.5959501
H	-5.9143482	0.0516159	-2.7937595	C	-10.0233348	-1.0329118	-4.6651766
C	-5.3721047	2.0743072	-4.3944231	C	-8.8386270	-0.3241898	-4.5244607
H	-5.7757135	2.7773640	-5.1259315	C	-8.8072541	1.0624198	-4.3451759
H	-3.5011655	2.5627590	-3.3604899	C	-9.9957403	1.7925829	-4.3173814
H	-5.8214433	2.3385197	-3.4334194	N	-7.5046942	1.4788782	-4.2482851
H	-3.3318357	-1.8492587	2.9637221	C	-6.7904666	0.3853126	-4.3706706
C	-3.6963717	-0.8837938	3.3197851	N	-7.5361922	-0.7261945	-4.5444593
H	-5.6607658	-1.8277112	3.1028847	C	-14.6522617	3.4835587	0.4745773
H	-3.3487582	-0.1295445	2.6069569	C	-16.1786523	3.4201662	0.4813508
H	-3.2120693	-2.6642294	5.3498852	C	-14.6490613	0.2809475	-3.4704002
C	-5.2421359	-0.8765479	3.4403843	C	-16.1755410	0.2686873	-3.4100915
H	-5.6803086	-0.1036196	2.8035235	O	-12.4009989	-0.9274432	-4.7419428
C	-3.6012307	-1.6966933	5.6686881	C	-12.9207707	-1.5596326	-3.6360164
C	-3.1024990	-0.5996411	4.7108762	C	-12.3664550	-2.7538645	-3.2133341
H	-5.5428093	-2.6469605	5.3243170	C	-12.8839519	-3.4146253	-2.1144504
C	-5.1488141	-1.6871462	5.6655124	C	-14.0000111	-2.9198771	-1.4447982
N	-5.6804400	-0.6461179	4.8034145	C	-14.5397142	-1.7262493	-1.9110312
H	-3.2031847	-1.5150791	6.6699843	C	-14.0298204	-1.0190415	-2.9937569
C	-3.6570776	0.7467135	5.1978117	C	-14.6071970	-0.4618766	3.6763327
H	-3.3529831	1.5499121	4.5215866	C	-16.1342536	-0.4716719	3.6315315
H	-5.5403907	-1.5322600	6.6731099	C	-14.6040143	-3.6642876	-0.2686647
C	-5.2023948	0.6463131	5.2562415	C	-16.1311722	-3.6228883	-0.2599109
H	-5.6642048	1.4204271	4.6391707	O	-12.3245274	-4.6099995	-1.7296365
H	-3.2445797	0.9895615	6.1803690	C	-11.1220828	-4.5776533	-1.0778063
H	-5.5629845	0.8076945	6.2741725	C	-11.1353485	-4.7460825	0.3289021

I-capsule with 4 CN and piperidyl groups

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Energy = -12194.16942130

I	-0.3408457	-0.6712575	4.7021448
C	-2.4375262	-0.5280177	4.5941889
C	-3.1604496	0.1726364	5.5565297
C	-4.5630114	0.2246682	5.5145716
C	-5.2764777	-0.4259273	4.5083371
C	-4.5472787	-1.0854564	3.5195470
C	-3.1501620	-1.1342132	3.5602250
C	-2.4802665	0.8480966	6.6141055
C	-5.2453546	0.9396837	6.5447594
C	-6.7388266	-0.4528938	4.4955511
N	-7.4381664	-1.5567659	4.3807946
C	-8.7457902	-1.1592022	4.4898033
C	-8.7955600	0.2269428	4.6683705
N	-7.4990409	0.6478018	4.6751980
C	-9.9238509	-1.9064774	4.4747981
C	-11.1175596	-1.2289522	4.5973372
C	-11.1482219	0.1775406	4.7651759
C	-9.9887812	0.9185596	4.8212995
O	-12.3636625	0.7786067	4.9241934
C	-12.9041293	1.4035215	3.8241422
C	-14.0117777	0.8468610	3.1932090
C	-14.5430403	1.5465877	2.1158604
C	-14.0256475	2.7480906	1.6445161
C	-12.9102557	3.2591908	2.3029604
C	-12.3719445	2.6059959	3.3963800

C	-2.4347921	-4.5538398	-0.4954984	H	-6.6738059	4.0308337	6.0848539
C	-3.1435507	-5.5152442	0.2206447	H	-5.5319613	4.3556249	4.7793046
C	-4.5453464	-5.4765145	0.2952909	H	-7.0163012	5.3127770	4.9169540
I	-0.3419210	-4.6610483	-0.6886621	N	-1.9818443	-1.3951817	-7.3695612
C	-2.4902869	-2.4601879	-1.7676223	N	-5.7991446	-1.5989400	-7.2558118
C	-5.2303791	-2.3708503	-1.5980392	N	-2.0301120	2.3617970	-1.5313679
C	-5.2134659	-6.5064829	1.0239018	N	-5.7329875	2.1012684	-1.3490585
C	-2.4498038	-6.5693885	0.8875798	N	-1.9931087	1.5847571	2.3878915
C	-5.3281555	0.3815434	-4.3938307	N	-5.6997158	1.3900768	2.1853835
C	-4.6046906	1.0567335	-3.4113980	N	-2.0290854	7.4323235	-1.3595676
C	-3.2094811	1.1328985	-3.4633392	N	-5.8465667	7.3018226	-1.5028755
C	-2.4924692	0.5390790	-4.5013295	N	-1.9643022	-2.3446349	1.6200833
C	-3.2080094	-0.1808500	-5.4546533	N	-5.6767245	-2.1502953	1.4681701
C	-4.6091870	-0.2596126	-5.4023216	N	-1.9475721	1.4036701	7.4693339
I	-0.4013863	0.7378366	-4.6245370	N	-5.7648033	1.5339731	7.3818538
C	-2.5311767	1.8095144	-2.4069530	N	-1.9054487	-7.4216474	1.4363332
C	-5.2688113	1.6330579	-2.2902937	N	-5.7213931	-7.3431939	1.6286048
C	-5.2849858	-0.9915880	-6.4248411	N	-1.9972194	-1.5810711	-2.3216028
C	-2.5214546	-0.8471009	-6.5138410	N	-5.7051842	-1.4354031	-2.0671607
O	-7.2871329	-3.4286803	-4.1367700	C	2.9168363	4.8870601	-0.4424830
C	-6.5831683	-4.3770381	-4.9064446	C	4.4333370	5.0392702	-0.4369163
O	-7.2951180	3.3548398	4.2698415	C	5.0900158	3.9883768	0.4687779
C	-6.5960749	4.3101132	5.0354154	C	4.4450373	4.0034299	1.8543743
O	-7.3384425	4.1672689	-3.3245570	C	2.9280107	3.8906440	1.7542957
C	-6.6448886	4.9381692	-4.2795162	N	2.3319196	4.9016457	0.8913333
O	-7.2400510	-4.2398126	3.4573073	C	6.5728354	4.1753608	0.5407584
C	-6.5227967	-4.9989893	4.4041814	N	7.3011091	4.1117581	1.6294030
H	-11.5985759	3.7854086	-3.0401378	C	8.6009470	4.3097842	1.2217591
H	-15.4244642	1.4128833	-1.1208993	C	8.6223438	4.5055789	-0.1599429
H	-11.5585571	3.0601960	3.9417298	N	7.3173944	4.4219200	-0.5605100
H	-15.4079624	1.1319324	1.6149818	C	9.7942989	4.7374511	-0.8618292
H	-11.5519798	-3.1962229	-3.7667756	C	10.9722536	4.7169369	-0.1421124
H	-15.4054939	-1.3241475	-1.4013770	C	10.9703203	4.5131711	1.2547878
H	-11.5120287	-3.9229992	3.2159503	C	9.7882512	4.3334477	1.9472723
H	-15.3896202	-1.6047020	1.3347230	O	12.1705321	4.9313641	-0.7653983
H	-14.3376914	-0.5698520	4.7264573	C	12.7153852	3.8672558	-1.4462097
H	-14.3957818	4.5368516	0.5833561	C	13.8265910	3.2109012	-0.9269026
H	-14.3918311	0.3930333	-4.5231605	C	14.3483437	2.1629341	-1.6766999
H	-14.3335091	-4.7137714	-0.3801917	C	13.8186436	1.7424934	-2.8920463
H	-16.5801947	4.0153516	-0.3383324	C	12.7042269	2.4279270	-3.3682926
H	-16.5810640	2.4127719	0.3753733	C	12.1786444	3.4967059	-2.6655396
H	-16.5300937	0.3472612	4.2315411	C	14.4347689	0.6013475	-3.6794932
H	-16.5145526	-1.4070003	4.0411793	C	15.9620903	0.6083184	-3.6370090
H	-16.5219003	-4.0330079	-1.1907274	C	14.4395469	3.6418990	0.3921124
H	-16.5469700	-2.6214370	-0.1492844	C	15.9667922	3.6002696	0.3769349
H	-16.5734738	1.1984624	-3.8156344	O	12.1450097	2.0861433	-4.5776457
H	-16.5786282	0.1574073	-2.4035322	C	10.9527454	1.4114305	-4.5479665
H	-16.5491104	-0.3665334	2.6291090	C	10.9780571	0.0156880	-4.7565867
H	-16.5157058	-4.2241229	0.5635047	C	9.8125647	-0.7238069	-4.7776810
H	-16.5656332	-0.5558031	-4.0062626	C	8.6293870	-0.0436452	-4.5402060
H	-16.5657452	3.8251343	1.4159330	C	8.5839441	1.3369854	-4.3389510
H	-10.0574109	4.8632804	-1.9609919	C	9.7588622	2.0826053	-4.3626433
H	-9.9525782	4.2489903	3.0064703	N	7.2770839	1.7201249	-4.1337199
H	-10.0012383	1.9842851	4.9967763	C	6.5698868	0.6178719	-4.1975908
H	-9.8925382	-2.9829925	4.3816907	N	7.3329844	-0.4685487	-4.4517760
H	-9.9661576	-4.9758447	2.1215654	O	12.1859579	-0.5881907	-4.9724143
H	-9.9188263	-4.3585210	-2.8463862	C	12.7388243	-1.2620553	-3.9079144
H	-10.0223433	-2.0986410	-4.8410614	C	12.2183301	-2.4885724	-3.5376563
H	-9.9789785	2.8693643	-4.2236320	C	12.7516439	-3.1834216	-2.4675944
H	-7.2250572	1.6409428	4.5872056	C	13.8587797	-2.6917586	-1.7810742
H	-7.1947083	-4.5594396	1.7448720	C	14.3718852	-1.4690334	-2.2007572
H	-7.2468250	-1.7151960	-4.4586266	C	13.8410527	-0.7267164	-3.2495244
H	-7.2765302	4.4904046	-1.6105036	O	12.1738144	4.5408929	1.9090527
H	-7.3199358	3.2290414	-3.6033980	C	12.7350004	3.3300918	2.2421617
H	-6.7349382	5.9873481	-4.0029161	C	12.2211509	2.6253649	3.3153932
H	-5.5779017	4.6935811	-4.3212243	C	12.7623272	1.4055476	3.6774648
H	-7.0607159	4.8128328	-5.2831695	C	13.8664150	0.8878653	3.0080344
H	-7.2670429	-3.7071250	-3.1983759	C	14.3754787	1.6387090	1.9546508
H	-6.6707713	-4.0992165	-5.9554818	C	13.8402488	2.8542770	1.5419832
H	-5.5169785	-4.4111437	-4.6573554	C	14.4854049	-3.4709467	-0.6399940
H	-6.9919981	-5.3839949	-4.7845938	C	16.0119283	-3.4065819	-0.6457514
H	-7.2330408	-3.3011768	3.7357966	O	12.2086227	-4.4004622	-2.1267936
H	-6.6037356	-6.0501126	4.1322915	C	11.0159388	-4.3897857	-1.4522777
H	-5.4584660	-4.7409454	4.4292771	C	11.0445585	-4.6008420	-0.0569486
H	-6.9253182	-4.8753494	5.4134380	C	9.8792946	-4.6442641	0.6818925
H	-7.2874257	3.6357943	3.3320274	C	8.6920902	-4.4264491	0.0020735

C	8.6431532	-4.2226517	-1.3780186	H	9.7827154	4.2117444	3.0213533
C	9.8189063	-4.2238022	-2.1231660	H	9.7357900	3.1559226	-4.2361662
N	7.3940553	-4.3649637	0.4268984	H	9.8213675	-1.7863049	-4.9718194
C	6.6256214	-4.1231148	-0.6590353	H	9.8421400	1.8795081	4.7726866
N	7.3325679	-4.0423721	-1.7607385	H	9.8399822	-3.0679374	4.0662296
C	14.4852422	-0.4304945	3.4319868	H	9.8922583	-4.8414567	1.7438126
C	16.0118878	-0.4143141	3.3721329	H	9.7943846	-4.0962900	-3.1963621
O	12.2305290	0.7226834	4.7467946	H	7.0149515	4.4375417	-1.5445224
C	11.0303873	0.0981638	4.5476856	H	7.1063873	-4.3858494	1.4155259
C	11.0273339	-1.2990717	4.3456090	H	7.0705888	1.4942554	4.3387827
C	9.8433850	-1.9934022	4.1847340	H	6.9868514	-3.4953549	-3.3650404
C	8.6537679	-1.2705960	4.1795918	H	6.9598581	3.3306312	-3.5885222
C	8.6774385	0.1113586	4.3734562	H	7.0318081	3.5587673	3.2443501
C	9.8517182	0.8158471	4.5848442	H	7.0218061	-3.2855028	3.4599338
N	7.3504920	-1.6796871	4.0082212	H	6.6277809	-3.8356082	-6.1890267
C	6.6217261	-0.5916621	4.0861091	H	7.4067462	-4.9878025	-5.1041933
N	7.3706413	0.5103695	4.3154594	H	5.6643109	-4.7010180	-4.9900144
O	12.2555587	-4.7977207	0.5470290	H	5.5770895	4.9626107	-4.7282007
C	12.7917280	-3.7251354	1.2217183	H	6.6244940	6.1534008	-3.9540198
C	13.8845388	-3.0503059	0.6876964	H	7.2977290	5.0304845	-5.1359155
C	14.3987409	-1.9936585	1.4304909	H	5.5899252	4.5938791	4.9148414
C	13.8779754	-1.5817598	2.6526222	H	6.7435070	3.9226030	6.0703257
C	12.7812009	-2.2851940	3.1432314	H	7.2734823	5.1391910	4.9087057
C	12.2645958	-3.3629984	2.4477307	H	5.9070715	-4.9572261	4.7863325
O	12.2318051	-1.9521980	4.3595971	H	6.7831543	-6.1233865	3.7926035
C	5.1349116	-0.5222901	3.9239529	H	7.6729618	-5.0375151	4.8610789
C	4.5023033	0.4704721	4.9081867	H	4.7019535	0.2421477	-6.1245386
C	2.9837430	0.4792260	4.7774505	H	4.9139891	-0.0799010	-3.1020320
N	2.3871476	-0.8422960	4.9107431	H	4.8132774	2.3748871	-2.9484775
C	2.9620683	-1.7928754	3.9683920	H	4.6685600	2.5108678	-4.6878735
C	4.4798031	-1.8965053	4.0649572	H	2.6473437	1.1844035	-2.8096685
C	5.1422726	-3.9591774	-0.5511648	H	2.4350696	2.7046367	-3.6503319
C	4.5175692	-5.0628675	0.3139348	H	2.4351910	1.5491895	-5.6933884
C	3.0008174	-4.9231459	0.3669671	H	2.6626763	-0.9173525	-4.1579150
N	2.3799007	-4.8698347	-0.9497982	H	2.4703208	-0.7874427	-5.8928145
C	2.9502429	-3.8134820	-1.7752184	H	7.0435039	-1.4573283	-4.4653863
C	4.4648884	-3.9128867	-1.9200117	H	4.7825014	0.1978635	5.9307824
C	5.0898209	0.5073910	-4.0151137	H	4.8475771	-2.5804034	3.2988085
C	4.4429979	-0.2520164	-5.1824407	H	4.7586691	-2.3339291	5.0290909
C	2.9277432	-0.3064670	-5.0271590	H	2.6678221	-1.4779210	2.9620676
N	2.3197775	1.0048450	-4.8447460	H	2.5014120	-2.7683891	4.1317865
C	2.9103684	1.7249733	-3.7245622	H	2.5273420	-1.1796927	5.8575944
C	4.4243681	1.8700495	-3.8349785	H	2.6937259	0.8762249	3.7989330
O	6.8719945	4.2588914	-3.2506834	H	2.5394603	1.1406457	5.5224823
C	6.5792002	5.1263816	-4.3162238	H	4.9323637	-0.1541289	2.9071234
O	6.8991353	-4.2073283	3.1134045	H	4.9130472	-5.0299858	1.3313229
C	6.8121908	-5.1084966	4.1887961	H	4.8335826	-3.0693517	-2.5061790
O	6.9732805	3.2169743	4.1735638	H	4.7212106	-4.8157664	-2.4833855
C	6.6278356	4.2661995	5.0424118	H	2.6758670	-2.8560132	-1.3209237
O	6.8684303	-3.1497660	-4.2872848	H	2.4692437	-3.8379847	-2.7543174
C	6.6313822	-4.2182009	-5.1684093	H	2.5024230	-5.7636330	-1.4147804
H	11.3682109	4.0677582	-3.0923914	H	4.9544950	-2.9994013	-0.0473249
H	15.2157045	1.6429691	-1.2912712	H	2.7281506	-4.0054810	0.8986557
H	11.4150041	-2.9273427	-4.1096464	H	2.5595541	-5.7473440	0.9290160
H	15.2329807	-1.0714228	-1.6796009	H	4.7028432	6.0406890	-0.0863662
H	11.4171966	3.0507613	3.8965961	H	4.8345242	3.1889328	2.4678119
H	15.2366496	1.2540648	1.4238613	H	4.7113294	4.9324230	2.3686013
H	11.4691841	-3.9467842	2.8853281	H	2.6461665	2.9104254	1.3567062
H	15.2520557	-1.4592457	1.0335898	H	2.4726317	3.9633313	2.7432473
H	14.2292994	-4.5192742	-0.7900721	H	2.4640549	5.8187768	1.3055860
H	14.1635414	0.7505263	-4.7241271	H	2.6366898	3.9399461	-0.9158667
H	14.1698893	4.6864273	0.5447409	H	2.4547895	5.6769504	-1.0361673
H	14.2282570	-0.5828122	4.4797708	H	4.9033101	3.0015479	0.0189614
H	16.3424534	1.5586852	-4.0103043	H	4.8034934	4.9559166	-1.4613871
H	16.3782767	0.4637787	-2.6400567	H	4.8332319	-1.2703020	-5.2445155
H	16.3983933	-3.7737288	-1.5960554	H	4.7852329	-6.0416876	-0.0970107
H	16.4147245	-4.0336277	0.1491600	H	4.8782667	1.4823560	4.7402675
H	16.4013945	0.3877945	3.9984220				
H	16.4144593	-0.2653256	2.3702582				
H	16.3606330	3.9747816	1.3213289				
H	16.3493524	4.2318758	-0.4243410				
H	16.4136539	-2.4038947	-0.5000451				
H	16.4108810	-1.3580945	3.7427263				
H	16.3814816	2.6034168	0.2273982				
H	16.3565335	-0.1867205	-4.2691798				
H	9.7846138	4.9267264	-1.9252144				
				I-capsule with 4 CN and quinuclidyl groups			
				412			
				Energy = -12503.16823762			
C	5.6768782	-1.5637887	-1.1346040				
N	5.3182213	-0.9925004	0.1594355				
C	4.1532757	-1.6857731	0.6981724				

C	4.4160176	-3.2026745	0.8504607	C	5.4173305	-12.8117425	3.5960939
C	5.8735267	-3.4912627	0.4513618	C	6.4126788	-12.1219951	2.9120855
C	6.0626384	-3.0554532	-1.0076801	C	6.6954555	-10.8280351	3.3402384
C	6.7814692	-2.6160610	1.3333265	C	6.0104238	-10.2693376	4.4036359
C	6.4416187	-1.1307789	1.0829807	D	7.7069823	-10.1119298	2.7454524
C	6.2121634	-4.9360496	0.6634567	C	1.3735573	-5.1545143	-2.9285664
N	6.3874686	-5.4844073	1.8437338	C	0.7947951	-4.8409142	-1.5351201
C	6.7217150	-6.7955098	1.6017702	C	0.2797832	-3.3813828	-1.5374637
C	6.7341915	-7.0196413	0.2239167	N	0.6484273	-2.6900102	-2.7671348
N	6.4081142	-5.8165156	-0.3431998	C	2.0939243	-2.7653809	-2.9529403
C	7.0525887	-7.8265804	2.4764686	C	2.5617925	-4.2193311	-3.1673869
C	7.3523964	-9.0634646	1.9405005	C	0.2861853	-4.8308081	-3.9684810
C	7.3646462	-9.2711471	0.5439460	C	-0.0225820	-3.3200743	-3.9034351
C	7.0696016	-8.2451382	-0.3315506	C	-3.3164391	-5.8535998	0.7333300
D	7.7381289	-10.5015557	0.0797297	C	-4.6338639	-5.6811724	1.5167794
C	6.7409601	-11.3591663	-0.3215448	C	-5.1629573	-4.2472106	1.2945443
C	6.4370205	-12.4761587	0.4502831	N	-4.2091591	-3.4459534	0.5335749
C	5.4479516	-13.3261711	-0.0312538	C	-2.9218309	-3.4296694	1.2185138
C	4.7543713	-13.1113935	-1.2173802	C	-2.3019258	-4.8452117	1.2983046
C	5.0877749	-11.9753412	-1.9489602	C	-3.5813256	-5.4897955	-0.7308619
C	6.0915613	-11.1267429	-1.5194561	C	-4.0433887	-4.0175780	-0.8001376
D	4.4522509	-11.7082638	-3.1391397	C	1.1402755	-4.1048479	4.3668012
C	3.5246746	-10.6996125	-3.1226146	C	-0.2644843	-3.7525411	4.8723549
C	2.1595079	-11.0551780	-3.0836242	C	-0.5856718	-2.2984437	4.4692048
C	1.1706203	-10.0912729	-3.0857680	N	0.4713466	-1.7277469	3.6393487
C	1.5802506	-8.7679854	-3.0752740	C	1.7106987	-1.6661490	4.4090386
C	2.9257734	-8.3994530	-3.1170523	C	2.1221436	-3.0624951	4.9268306
C	3.9153929	-9.3753596	-3.1663164	C	0.6713656	-2.5540632	2.4554421
N	0.8827488	-7.5932654	-3.0225555	C	1.1376781	-3.9801039	2.8316930
C	1.7880043	-6.5872568	-3.0208450	D	-1.8463411	-7.7307029	-2.6924008
N	3.0211396	-7.0271286	-3.0868575	C	-2.8752852	-7.9515864	-3.6252801
D	1.8330765	-12.3838387	-3.0656306	D	5.2439865	-4.7236505	4.2081080
C	1.4582826	-12.9033321	-1.8479448	C	6.2377792	-4.4028577	5.1514271
C	2.3323056	-13.7296753	-1.1489797	D	5.5936908	-6.0939407	-2.9539523
C	1.8872194	-14.2325046	0.0682174	C	6.0042901	-5.6684651	-4.2296700
C	0.6369252	-13.9550858	0.6098926	D	-2.0315807	-6.8176512	4.5852188
C	-0.2060505	-13.1311376	-0.1312293	C	-2.7235579	-6.6485425	5.7984594
C	0.1938565	-12.6320691	-1.3573703	I	-0.2462281	0.8733685	3.2018343
C	0.2016802	-14.5326972	1.9433723	C	-0.7649087	2.9104114	3.1336524
C	0.6597701	-15.9758105	2.1457105	C	-1.5801388	3.4252640	2.1303797
C	3.6964391	-14.0788180	-1.7133282	C	-1.9721305	4.7735323	2.1304170
C	4.0755903	-15.5399841	-1.4767241	C	-1.5299943	5.6444332	3.1212460
D	-1.4759621	-12.8539351	0.3191534	C	-0.6894523	5.1335422	4.1134178
C	-1.7215853	-11.5938487	0.7953945	C	-0.3182803	3.7853541	4.1266943
C	-1.7146902	-11.4037168	2.1943172	C	-1.9229732	7.0552225	3.1038038
C	-2.0014924	-10.1723485	2.7489709	N	-3.1674018	7.4603293	3.0281383
C	-2.2764663	-9.1342036	1.8728898	C	-3.1006115	8.8294749	3.0400425
C	-2.3057430	-9.3073079	0.4879765	C	-1.7634163	9.2269140	3.1236445
C	-2.0338454	-10.5569352	-0.0630235	N	-1.0392335	8.0741813	3.1763167
N	-2.6576303	-8.1167751	-0.1090444	C	-1.3755584	10.5592151	3.1248467
C	-2.8364490	-7.2647254	0.8716094	C	-2.3785546	11.4950072	3.0120230
N	-2.6153127	-7.8256743	2.0843484	C	-3.7423518	11.1135707	2.9607580
D	-1.4829188	-12.4892277	2.9909518	C	-4.1132574	9.7868498	2.9889101
C	-0.2312142	-12.6221231	3.5423731	D	-4.6766685	12.1123834	2.9244651
C	0.1382961	-11.8025914	4.5920224	C	-5.2758105	12.3745128	1.7155169
C	1.3903712	-11.9221151	5.1667394	C	-4.9326019	13.5186445	1.0012416
C	2.2792913	-12.9032965	4.7382082	C	-5.5909610	13.7315153	-0.2051916
C	1.8607851	-13.7271103	3.6986231	C	-6.5558570	12.8723845	-0.7187516
C	0.6230250	-13.6160292	3.0762179	C	-6.8751248	11.7528270	0.0413303
C	3.6358219	-13.0727660	5.3944795	C	-6.2593805	11.5187689	1.2560300
C	4.0222733	-14.5389705	5.5825543	D	-7.8575031	10.8966693	-0.3963346
D	1.7283221	-11.0869754	6.2067667	C	-7.4777990	9.6569168	-0.8208027
C	2.0383132	-9.7944753	5.8756324	C	-7.4067263	9.4270087	-2.2185330
C	3.4014646	-9.4383245	5.7948284	C	-7.1145458	8.1786576	-2.7219294
C	3.7835186	-8.1490703	5.4787553	C	-6.8474570	7.1515853	-1.8113725
C	2.7736278	-7.2359916	5.2177119	C	-6.9070758	7.4035096	-0.4358820
C	1.4209841	-7.5681170	5.3126289	C	-7.2390925	8.6475424	0.0841446
C	1.0436999	-8.8606139	5.6618803	N	-6.5336316	5.8344795	-2.0198463
N	2.7989064	-5.9120639	4.8705727	C	-6.4104893	5.3213440	-0.8167554
C	1.5138419	-5.4972333	4.7686595	N	-6.6281436	6.2185051	0.1721361
N	0.6599376	-6.4593194	5.0264382	D	-7.7160729	10.4710237	-3.0469366
C	7.1664842	-12.7460669	1.7528502	C	-6.6904271	11.1978033	-3.6057333
C	7.4718110	-14.2271035	1.9676265	C	-6.4402293	12.4978055	-3.1721539
D	4.3359732	-10.3924644	6.0888352	C	-5.4289893	13.1979631	-3.8198259
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C	4.6954548	-12.2764089	4.6566298	C	-4.9598293	11.3754452	-5.2613916

C	-5.9696464	10.6509916	-4.6523546	H	-2.5683614	14.9303735	-3.4741231
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C	-3.9810639	14.9497245	-5.7457545	H	-5.3352045	14.6134398	-0.7781728
C	-7.2419986	13.1249313	-2.0471665	H	0.2843280	12.4590836	1.9160519
C	-7.5528748	14.6010962	-2.2855810	H	-2.6742541	15.3012566	-0.7518616
D	-4.2671577	10.8194630	-6.3138478	H	0.8083693	15.0077967	-1.9394893
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C	-1.4394892	7.9778682	-5.3346640	H	-4.9058157	15.0145721	-6.3183358
C	-2.7918645	7.6383301	-5.4272677	H	-4.1386849	15.4945722	-4.8152341
C	-3.7739589	8.5559254	-5.7720482	H	-0.3131424	16.8106662	-3.1120249
N	-2.8632986	6.3176734	-5.1006099	H	-0.3994378	17.0397613	-1.3647477
C	-1.6056102	5.9194747	-4.8102840	H	-5.2548457	16.1678556	1.7223686
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D	-1.6589116	11.4945709	-6.2617581	H	-8.0880499	14.7239063	-3.2268178
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C	2.8494639	7.7523796	-0.8995368	H	8.1323239	-12.2459165	1.6906891
N	2.6773439	8.3238838	-2.1138063	H	0.2849624	-16.6040583	1.3380903
C	-3.9020440	14.4942293	1.5383891	H	1.7423986	-16.0973901	2.1730822
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D	1.3427720	13.2826723	-0.3095242	H	4.9709328	-14.6105124	6.1138433
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C	-2.5150854	14.1510123	1.0285630	H	3.3208112	-16.1966434	-1.9086261
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C	4.6206880	4.4441588	-1.4575645	H	0.1236208	-10.3560338	-3.0869961
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I	-5.0526886	-0.8650046	0.2293669	H	-3.7424583	5.8202155	-4.9473698
D	-5.7389824	6.4367294	2.7169669	H	-0.1408939	-7.5324763	-2.9370080
C	-6.2065177	6.0868487	4.0003018	H	-2.5560074	-7.3593089	2.9983227
D	1.9922912	7.3513013	-4.5422698	H	3.6560534	-5.3882523	4.6514114
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D	-5.7157003	5.8812874	-4.8710237	H	-1.0655713	-6.6602637	4.7371637
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H	6.8768977	-3.5800595	4.8158539	H	-2.6802544	-5.6379621	-1.3273482
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H	-6.0402491	5.0474984	-6.6956996	H	3.7380038	-3.7872811	0.2211882
H	-6.0792313	3.8854109	-5.3727404	H	6.6329586	-2.8787615	2.3809960
H	-7.4442477	4.9905105	-5.6232651	H	3.3052210	-1.4918698	0.0370650
H	-4.8005773	6.7175903	2.7833890	H	6.1834979	-0.6222083	2.0137690
H	-7.2749117	5.8910672	3.9360240	H	7.8285664	-2.8231136	1.1043692
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