

## Supporting Information For

### **Borane carbene or not? A theoretical verification of Lewis acid-catalyzed transformation of diazos**

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## Part 1: ELF analysis for key intermediates

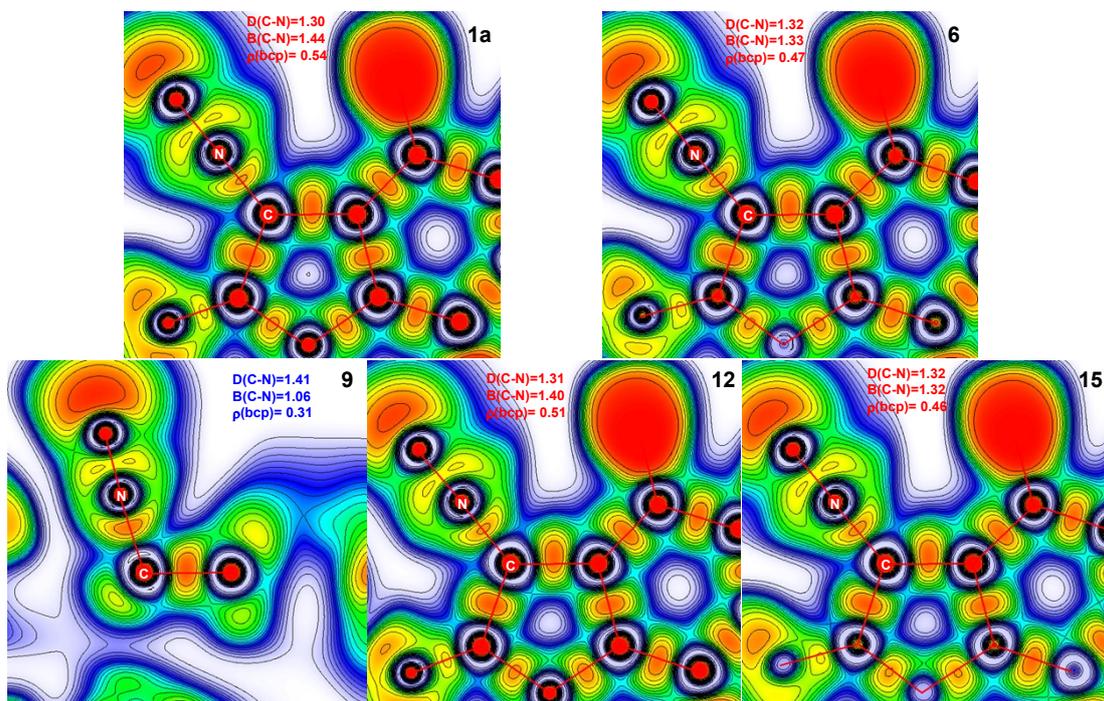
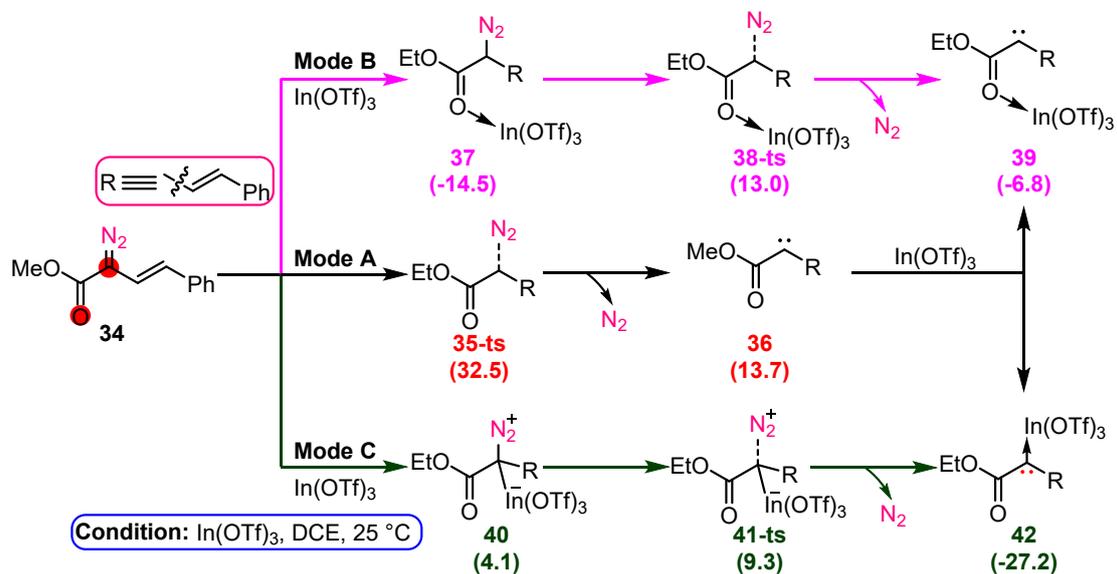


Fig. S1 ELF analysis for the key intermediates involved in the formation of carbene species

## Part 2: Computational model for $\text{In}(\text{OTf})_3$ -catalyzed activation of vinyl diazo compound



**Scheme S1.** Computational model for  $\text{In}(\text{OTf})_3$ -catalyzed activation of vinyl diazo compound

(Values in brackets are relative Gibbs free energies obtained at M06-2X/6-31G(d, p) (sdd for

$\text{In}$ )/IEF-PCM(DCE)//M06-2X(D3)/Def2-TZVP/IEF-PCM(DCE) level)

## Part 3: Energy Information of All the Stationary Points

Table S1. Energy Information of All the Stationary Points

	Gibbs Free Energy (a.u.)	Thermal Correction to Free Energy (a.u.)	Imaginary frequency (cm <sup>-1</sup> )
<b>1a</b>	-586.286923	0.113921	/
<b>2a</b>	-991.554297	0.181642	/
<b>3a</b>	-959.50991	0.206264	/
<b>4-ts</b>	-586.224175	0.107685	324.71 <i>i</i>
<b>N<sub>2</sub>(HFIP)</b>	-109.500404	-0.012636	/
<b>5</b>	-476.747026	0.104326	/
<b>B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub></b>	-2207.408936	0.096441	690.44 <i>i</i>
<b>6</b>	-2793.717942	0.237581	/
<b>7-ts</b>	-2793.650028	0.231243	184.02 <i>i</i>
<b>8</b>	-2684.176023	0.224775	/
<b>9</b>	-2793.691993	0.237693	/
<b>10-ts</b>	-2793.681885	0.235724	386.45 <i>i</i>
<b>11</b>	-2684.240671	0.228356	/
<b>HFIP</b>	-789.515069	0.028338	/
<b>12</b>	-1375.802528	0.163625	/
<b>13-ts</b>	-1375.736943	0.156585	291.33 <i>i</i>
<b>14</b>	-1266.274894	0.151648	/
<b>B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>/HFIP</b>	-2996.920442	0.15286	/
<b>15</b>	-3583.229064	0.332669	/
<b>16-ts</b>	-3583.157287	0.285362	200.85 <i>i</i>
<b>17</b>	-3473.674444	0.280321	/
<b>18-ts</b>	-3675.76492	0.440113	295.37 <i>i</i>
<b>19</b>	-3675.813375	0.440312	/
<b>20-ts</b>	-3675.796512	0.440096	67.67 <i>i</i>

<b>21</b>	-3675.804454	0.436109	/
<b>22-ts-Z</b>	-3675.785294	0.43573	412.40 <i>i</i>
<b>22-ts-E</b>	-3675.789796	0.437017	426.82 <i>i</i>
<b>B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>-F</b>	-2307.42958	0.094139	/
<b>23</b>	-1368.427627	0.312188	/
<b>24-ts</b>	-3675.842732	0.439168	138.12 <i>i</i>
<b>M06-2X/6-31G(d, p)/IEF-PCM(DCE)</b>			
<b>25</b>	-607.328099	0.123523	/
<b>26-ts</b>	-607.276309	0.116335	337.92 <i>i</i>
<b>27</b>	-497.784298	0.114985	/
<b>N<sub>2</sub></b>	-109.494500	-0.012662	/
<b>28</b>	-2715.546394	0.255246	/
<b>29-ts</b>	-2715.503342	0.249451	327.04 <i>i</i>
<b>30</b>	-2606.047109	0.244832	/
<b>31</b>	-2715.518158	0.255727	/
<b>32-ts</b>	-2715.508497	0.25366	288.48 <i>i</i>
<b>33</b>	-2606.053817	0.247675	/
<b>M06-2X/6-31G(d, p)(SDD for In atom)/IEF-PCM(DCE)</b>			
<b>In(OTf)<sub>3</sub></b>	-2885.566058	0.029434	/
<b>34</b>	-684.665973	0.152311	/
<b>35-ts</b>	-684.614171	0.145956	357.92 <i>i</i>
<b>36</b>	-575.143764	0.1419	/
<b>37</b>	-3570.255124	0.2052	/
<b>38-ts</b>	-3570.21125	0.201659	389.4 <i>i</i>
<b>39</b>	-3460.74253	0.196589	/
<b>40</b>	-3570.225457	0.204586	/
<b>41-ts</b>	-3570.21714	0.206461	416.64 <i>i</i>
<b>42</b>	-3460.775023	0.196252	/



## Part 4: Cartesian Coordinates of All the Stationary Points

### 1a

C	-0.80374500	0.58940200	-0.00008200
C	-0.36793800	-0.75235600	0.00009500
C	-1.28837300	-1.79060800	0.00018800
C	-2.64852200	-1.47056600	0.00015900
C	-3.07113300	-0.14131900	-0.00002100
C	-2.15206800	0.91160700	-0.00019700
C	1.49047600	0.75172600	0.00017500
C	1.07935500	-0.66301800	-0.00024000
H	-0.96001900	-2.82482600	0.00026300
H	-3.38278900	-2.26879400	0.00024800
H	-4.13230900	0.08383100	-0.00004300
H	-2.48127200	1.94533100	-0.00032600
N	1.95398600	-1.63114500	0.00116200
N	2.70984700	-2.46610900	-0.00129200
O	2.61236500	1.23413100	0.00050300
N	0.29476200	1.44839000	-0.00021300
C	0.21625600	2.89232900	-0.00022400
H	-0.30617600	3.24782800	0.89208700
H	1.23643600	3.27499800	-0.00183400
H	-0.30880200	3.24745000	-0.89113000

### 2a

C	-0.18977400	1.85119300	-0.11560800
F	-1.43652300	2.28761100	-0.24543500
F	0.60037400	2.81711000	0.32102500
C	3.92495500	0.26597800	0.04370400
C	2.67170300	0.84736000	-0.11308900
C	1.52732200	0.04239700	-0.20944300
C	1.67366900	-1.34933100	-0.16473900
C	2.93085100	-1.92444300	-0.00730800
C	4.06178600	-1.11986000	0.10086700
H	4.80157700	0.90205100	0.11295300
H	2.58919000	1.92553800	-0.17071100
H	0.79405100	-1.97620400	-0.26250600
H	3.02512600	-3.00506000	0.02837600
H	5.04271800	-1.56756600	0.22205200
C	0.16389800	0.58983700	-0.36672900
O	-0.79578300	-0.27887100	-0.79788500
Si	-2.18883000	-0.73064300	0.07068500
C	-2.02790600	-0.11957100	1.83103300
H	-1.06990200	-0.42354100	2.26462100

H	-2.10802700	0.96855700	1.89803200
H	-2.82603700	-0.55525700	2.44018500
C	-3.68029100	-0.01452500	-0.79692900
H	-3.65751700	1.07779000	-0.79013800
H	-3.72054400	-0.35146400	-1.83684300
H	-4.59966700	-0.34207600	-0.30161300
C	-2.22612100	-2.59788400	-0.00559400
H	-2.14612600	-2.94469500	-1.04007400
H	-1.40426000	-3.03836800	0.56645600
H	-3.16590000	-2.97912900	0.40539600

**3a**

C	0.40236600	0.30452800	-0.66240700
F	0.60413300	1.60897500	-0.90703400
C	4.06283300	1.32415200	1.40882300
C	2.87697800	0.94612600	0.78735700
C	2.89449300	-0.04984300	-0.19448900
C	4.10058100	-0.66523500	-0.54778300
C	5.28247200	-0.28040400	0.06985600
C	5.26290800	0.71447400	1.04888400
H	4.05047000	2.09355100	2.17296300
H	1.94540700	1.42605100	1.06922800
H	4.08895300	-1.44026900	-1.30674000
H	6.21866800	-0.75304300	-0.20684700
H	6.18673400	1.01406500	1.53296600
C	1.65136500	-0.52066400	-0.85933200
O	1.61112200	-1.50224600	-1.57038300
C	-3.05221000	-0.18514200	0.22519100
C	-2.03800300	0.69583300	-0.19341300
C	-2.32704600	2.03608200	-0.41350000
C	-3.63619900	2.47948000	-0.20598300
C	-4.62921800	1.59369300	0.20945800
C	-4.35373600	0.24034700	0.43208200
C	-1.18285500	-1.51184900	0.09249900
C	-0.82073800	-0.10533000	-0.31773500
H	-1.55318100	2.72147600	-0.73778500
H	-3.88054000	3.52287700	-0.37062300
H	-5.63960700	1.95741100	0.36451800
H	-5.12906200	-0.44630600	0.75361400
O	-0.46960900	-2.49081500	0.19634200
N	-2.53065400	-1.47192400	0.38162400
C	-3.28461500	-2.61595700	0.84316700
H	-4.10383800	-2.83751900	0.15414100
H	-2.60232500	-3.46418300	0.88259800

H	-3.69265700	-2.42868100	1.84018200
<b>4-ts</b>			
C	-0.83486500	0.58061800	-0.00275500
C	-0.36056100	-0.71261300	-0.34286100
C	-1.25536700	-1.78718700	-0.38690600
C	-2.58889300	-1.57067100	-0.06088700
C	-3.03227200	-0.28008800	0.25664000
C	-2.17210100	0.82045600	0.27763500
C	1.38566400	0.82207400	-0.37370700
C	0.99600800	-0.59952700	-0.82074000
H	-0.89495000	-2.77582500	-0.65396600
H	-3.29394100	-2.39367500	-0.06586600
H	-4.08181500	-0.12494500	0.48592400
H	-2.53691300	1.81396900	0.51337100
N	2.18067900	-1.57991100	0.49447700
N	2.85565500	-2.43210800	0.67193100
O	2.49521400	1.31641400	-0.36254800
N	0.21519400	1.49082500	-0.04605500
C	0.14195100	2.87824000	0.35559300
H	-0.21095100	2.96374700	1.38725000
H	1.14799600	3.29058100	0.28190400
H	-0.52922200	3.43537900	-0.30277600
<b>N2</b>			
N	0.00000000	0.00000000	0.54924100
N	0.00000000	0.00000000	-0.54924100
<b>5</b>			
C	0.16280300	0.42267100	-0.00072500
C	0.51230200	-0.97508900	-0.00022600
C	1.88490400	-1.33745100	0.00024300
C	2.84765100	-0.35451400	0.00045500
C	2.45778300	1.00589700	0.00026800
C	1.13219400	1.42397500	-0.00031500
C	-1.74533800	-0.75370900	-0.00029100
C	-0.60776700	-1.82159900	-0.00028700
H	2.14481000	-2.39147500	0.00052500
H	3.90173700	-0.60385300	0.00092600
H	3.23538800	1.76428600	0.00062000
H	0.87435500	2.47668800	-0.00040700
O	-2.93522700	-0.95843900	0.00081200
N	-1.19391100	0.54737200	-0.00162400
C	-1.95251400	1.77974600	0.00075100

H	-1.73066400	2.37247100	-0.89037700
H	-3.00820500	1.50895600	0.00041700
H	-1.73033400	2.36926700	0.89393800

**B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>**

B	0.05362700	0.00000800	0.00007100
C	2.70408400	2.72009600	-0.79357700
C	2.04784500	1.50594600	-0.68632200
C	0.80577400	1.36449000	-0.05565400
C	0.25890700	2.53804600	0.47562800
C	0.89782700	3.76618900	0.40170300
C	2.12351500	3.85576400	-0.24253500
F	0.34942300	4.85157000	0.94028800
F	2.74282400	5.02247900	-0.32716200
F	3.87715000	2.80937300	-1.41323700
F	2.64554400	0.45108400	-1.24125400
F	-0.90778800	2.51280700	1.11981400
C	0.25801100	-2.53808500	-0.47548800
C	0.80531900	-1.36472500	0.05577900
C	2.04737100	-1.50664300	0.68637500
C	2.70319200	-2.72102800	0.79355900
C	2.12219400	-3.85647800	0.24252900
C	0.89649000	-3.76645500	-0.40161500
F	-0.90871200	-2.51247200	-1.11961000
F	0.34767800	-4.85163100	-0.94018500
F	2.74115200	-5.02338900	0.32701600
F	3.87626300	-2.81073600	1.41314800
F	2.64552200	-0.45198000	1.24119000
C	-3.63840500	-0.02322700	1.20275600
C	-2.25171600	-0.02596000	1.18069900
C	-1.52732000	0.00029800	0.00009500
C	-2.25154100	0.02676600	-1.18062000
C	-3.63822200	0.02441100	-1.20288700
C	-4.33167500	0.00066900	-0.00011400
F	-4.30509900	-0.03987900	2.35519000
F	-1.59473900	-0.03191000	2.34775000
F	-5.66099600	0.00086100	-0.00020900
F	-4.30474900	0.04125900	-2.35541700
F	-1.59436500	0.03250700	-2.34756600

**6**

C	-3.78546100	1.01380300	-1.25821500
C	-3.94592400	-0.18415100	-1.97517300
C	-5.20196200	-0.56976000	-2.43223600

C	-6.27836000	0.26863800	-2.15719800
C	-6.10690400	1.46290100	-1.44855500
C	-4.85330700	1.85732400	-0.98709000
C	-1.70475700	0.15073100	-1.37095300
C	-2.61026300	-0.73293400	-2.03800600
H	-5.33767000	-1.49278300	-2.98476700
H	-7.26819500	-0.00969000	-2.50135300
H	-6.96458000	2.09688800	-1.25339300
H	-4.72046300	2.78571900	-0.44319500
N	-2.19364500	-1.89155900	-2.51494200
N	-1.83134700	-2.87030100	-2.91285100
O	-0.44486100	-0.05054900	-1.29366700
N	-2.43226200	1.18142200	-0.90317000
C	-1.95946200	2.36199400	-0.19325300
H	-2.59037600	2.51628000	0.68440400
H	-0.93520300	2.21512500	0.13581600
H	-2.01439400	3.23189700	-0.85070800
B	0.48476600	0.01166600	-0.06304400
C	2.17560700	3.46462000	-1.07562800
C	1.31332200	2.37251900	-1.05940700
C	1.35794800	1.38802500	-0.08147700
C	2.34243700	1.55897900	0.88731700
C	3.22195200	2.62818200	0.91054900
C	3.13859700	3.58963900	-0.08886600
F	4.14260700	2.74449400	1.86918700
F	3.97324700	4.62752400	-0.09018000
F	2.08236700	4.38854500	-2.03413800
F	0.39543700	2.33712200	-2.04009100
F	2.44941000	0.64900400	1.86940100
C	2.19048400	-1.28059700	-1.55297000
C	1.55015300	-1.20232700	-0.31850000
C	1.94825300	-2.15527500	0.61058800
C	2.88856900	-3.14153400	0.33442500
C	3.48325100	-3.19032900	-0.91572700
C	3.13293900	-2.24792300	-1.87085500
F	1.91963800	-0.37493400	-2.50591700
F	3.71038800	-2.27169500	-3.07399900
F	4.38735900	-4.12764600	-1.19500600
F	3.22541600	-4.03834400	1.26390100
F	1.43669300	-2.17011600	1.85033600
C	-1.49059400	0.36982700	3.38419500
C	-0.63330900	0.63610600	2.32112300
C	-0.47176900	-0.21961800	1.23924000
C	-1.24832000	-1.37624200	1.28943800

C	-2.11546300	-1.68383400	2.32424500
C	-2.23200000	-0.79945600	3.38822100
F	-1.61087100	1.23581900	4.39098100
F	0.00897200	1.81370100	2.37448500
F	-3.06006900	-1.06804400	4.39407400
F	-2.82838200	-2.81044800	2.31346400
F	-1.17301500	-2.26499900	0.28051100
<b>7-ts</b>			
C	-3.89383300	1.01879700	-1.00001700
C	-3.94456800	0.14588400	-2.11083400
C	-5.16754600	-0.09126300	-2.74784500
C	-6.31039100	0.51435600	-2.23815300
C	-6.22001000	1.40316100	-1.16234900
C	-5.00131100	1.69675200	-0.53673100
C	-1.78875600	0.36692300	-1.33512900
C	-2.58976100	-0.02085300	-2.54315100
H	-5.21276500	-0.75589200	-3.60392400
H	-7.27567500	0.32056700	-2.69073300
H	-7.11919000	1.89360700	-0.80460900
H	-4.94670600	2.41383500	0.27438700
N	-2.07502300	-2.14756300	-2.43335100
N	-1.72189400	-3.08246300	-2.89030900
O	-0.57436800	0.04397200	-1.22219000
N	-2.54937000	1.13018200	-0.54084300
C	-2.20018200	2.04073900	0.54132800
H	-2.76585900	1.76503000	1.43438800
H	-1.13877200	1.98497000	0.75800600
H	-2.45366700	3.05953400	0.23916000
B	0.43153700	0.02767500	-0.04685500
C	1.65322100	3.77328700	-0.60732900
C	0.90494500	2.60366700	-0.69095300
C	1.17289400	1.47433900	0.06999200
C	2.25795400	1.58706700	0.93459000
C	3.02974000	2.73006100	1.05319900
C	2.72555600	3.83401500	0.26624400
F	4.05320200	2.78515000	1.90635100
F	3.45242700	4.94485200	0.36283800
F	1.34457800	4.83196200	-1.35792800
F	-0.14058800	2.63428600	-1.53848400
F	2.57421000	0.54491600	1.71963400
C	2.10426900	-0.87470200	-1.83455500
C	1.56011000	-1.03736500	-0.56208700
C	2.09527500	-2.08639000	0.17558500
C	3.07640000	-2.93981200	-0.31578100

C	3.57046700	-2.75064500	-1.59595200
C	3.08166500	-1.70499700	-2.36444200
F	1.69700400	0.14049000	-2.61213600
F	3.55992600	-1.50210800	-3.59374200
F	4.51279600	-3.55729900	-2.08053400
F	3.54793900	-3.93543900	0.43785800
F	1.69088100	-2.33040900	1.43093400
C	-1.09909500	-0.36163200	3.61458600
C	-0.42690800	0.15724800	2.51344100
C	-0.37091900	-0.48054600	1.27989200
C	-1.04831700	-1.69611100	1.22465100
C	-1.73416600	-2.25210500	2.29220500
C	-1.75486000	-1.57652400	3.50415000
F	-1.12076800	0.30281300	4.77048600
F	0.14353700	1.35868100	2.69689300
F	-2.40317400	-2.08786200	4.54665700
F	-2.35766000	-3.42440700	2.17239400
F	-1.03401500	-2.40707100	0.08425400

**8**

C	-3.91459300	-0.46285500	-1.96953900
C	-3.96874700	-0.30256400	-0.55285500
C	-5.21878700	-0.34340300	0.09569000
C	-6.36406600	-0.53873600	-0.66491700
C	-6.25862700	-0.68840500	-2.05195600
C	-5.02960800	-0.65258800	-2.74274300
C	-1.82958200	-0.18429800	-1.26674100
C	-2.69542700	-0.10527400	0.03005600
H	-5.26143800	-0.22283000	1.17321000
H	-7.33952600	-0.57568100	-0.19633300
H	-7.16478800	-0.83837300	-2.63046200
H	-4.98968100	-0.76892300	-3.81923200
O	-0.58251500	-0.08687600	-1.34361500
N	-2.56408600	-0.38860800	-2.36558700
C	-2.06420500	-0.56690100	-3.72026900
H	-2.32478700	0.29662300	-4.33466100
H	-0.98204600	-0.67428500	-3.66465900
H	-2.50019400	-1.47190000	-4.14637400
B	0.38251100	0.08545600	-0.12470200
C	-0.78870600	3.07997400	2.21438900
C	-0.46926600	1.80164800	1.76892800
C	0.03285100	1.54535800	0.49812900
C	0.18367100	2.66883700	-0.31063700
C	-0.12398600	3.95918700	0.09111100

C	-0.61685400	4.16521200	1.37133600
F	0.04750100	4.99541700	-0.73273400
F	-0.92306200	5.39366200	1.78397100
F	-1.26965000	3.26744400	3.44584400
F	-0.68316700	0.81550400	2.64770000
F	0.66271000	2.52561000	-1.55702200
C	1.12534800	-1.17741600	1.99588000
C	0.26588500	-1.17302800	0.90092100
C	-0.51258500	-2.31285100	0.76933700
C	-0.46656100	-3.37880000	1.66125700
C	0.40120400	-3.32996300	2.73903000
C	1.20648300	-2.21206400	2.91246700
F	1.91818700	-0.11259400	2.20088800
F	2.04484900	-2.14998900	3.94828200
F	0.46033500	-4.34179800	3.60295000
F	-1.24702700	-4.44640500	1.48278200
F	-1.38748500	-2.45102400	-0.25063100
C	3.33791100	-1.29720100	-2.30118900
C	2.11088300	-1.08358400	-1.68981000
C	1.85476400	-0.02610900	-0.82053700
C	2.93985200	0.80485600	-0.56899800
C	4.18693200	0.62507100	-1.15621900
C	4.38678400	-0.43118600	-2.03050600
F	3.52086000	-2.32582600	-3.13177300
F	1.14241400	-1.97427200	-1.96511800
F	5.57553800	-0.61616200	-2.60177400
F	5.19270800	1.45937900	-0.88402500
F	2.83337800	1.84392800	0.27070200

**9**

C	2.88300100	0.31492400	1.82937500
C	1.69058900	1.04277100	1.83114200
C	1.69410500	2.42484400	1.80451300
C	2.92860800	3.07494500	1.73575400
C	4.11310500	2.34171000	1.68542500
C	4.11366300	0.94502700	1.73511300
C	1.28853300	-1.32749300	2.00902800
C	0.55449500	0.04630100	1.79984200
H	0.76879800	2.99050900	1.83574500
H	2.96282400	4.15791400	1.71276000
H	5.06123700	2.86403900	1.61680600
H	5.03900600	0.38046400	1.71390700
N	-0.21187100	0.26426400	2.97907100
N	-0.76355400	0.46605100	3.90895700

O	0.75605900	-2.40152800	2.15421800
N	2.62136400	-1.05781800	1.92271300
C	3.63747600	-2.09298400	1.89561600
H	4.29526000	-2.00239500	2.76281100
H	3.12939600	-3.05603200	1.91931200
H	4.22660600	-2.00883100	0.97882900
B	-0.26531500	-0.02622100	0.22812000
C	2.09629100	-2.61764900	-1.64867200
C	1.03018400	-2.03724500	-0.96961800
C	0.94419200	-0.67301200	-0.68186500
C	2.03261400	0.07418700	-1.13993000
C	3.11857400	-0.46782900	-1.81250700
C	3.15138400	-1.82875200	-2.07393000
F	4.12649800	0.31062700	-2.20837200
F	4.18066600	-2.36753200	-2.72080300
F	2.10855800	-3.92955800	-1.88863700
F	0.07798100	-2.89561800	-0.58262400
F	2.09321000	1.39733300	-0.93773000
C	-2.20568200	-1.13764300	-1.05462900
C	-1.61416300	-0.95679500	0.19768800
C	-2.29134900	-1.58445600	1.23309000
C	-3.45556400	-2.32728100	1.06225200
C	-3.99950400	-2.46968500	-0.20091700
C	-3.36240000	-1.86631400	-1.27557500
F	-1.62852700	-0.60092800	-2.14126600
F	-3.86338800	-1.99517600	-2.50496500
F	-5.11321500	-3.17476200	-0.38481800
F	-4.04741100	-2.89967400	2.11187500
F	-1.84740400	-1.51748600	2.50028700
C	-2.05672600	3.49479900	0.22713100
C	-1.51933500	2.26495600	0.57467000
C	-0.74107000	1.46757800	-0.25810300
C	-0.58157800	1.98971100	-1.54294500
C	-1.10195600	3.21615500	-1.94085300
C	-1.84161100	3.97926900	-1.05279900
F	-2.77579000	4.19854500	1.10142400
F	-1.78357400	1.84483700	1.82961700
F	-2.34341600	5.15337100	-1.42498400
F	-0.90289000	3.65777900	-3.18366200
F	0.07849400	1.32601100	-2.49861600
<b>10-ts</b>			
C	2.99996700	0.22779100	2.00497700
C	1.85176700	0.96438000	1.66938600

C	1.91281600	2.34413200	1.52196400
C	3.14173800	2.97539200	1.70277500
C	4.27851700	2.22682400	2.01457400
C	4.23205200	0.83841900	2.16872200
C	1.36608600	-1.36608000	1.88730700
C	0.72679200	0.01665000	1.51158900
H	1.02462500	2.91120000	1.26276400
H	3.21782700	4.05078400	1.59410600
H	5.22917200	2.73391900	2.14270400
H	5.12165500	0.26836800	2.41077900
N	-0.05771600	0.28363400	3.09973600
N	-0.38157000	0.58024100	4.10486200
O	0.78700400	-2.42333900	1.94658700
N	2.69493600	-1.13146400	2.11714500
C	3.64844400	-2.17277100	2.44609500
H	4.10721700	-1.97245600	3.41720800
H	3.10348000	-3.11498300	2.48707100
H	4.42384000	-2.23054700	1.67840300
B	-0.25235700	-0.00408600	0.17207700
C	2.22056200	-2.31367900	-1.94801900
C	1.16929200	-1.86185300	-1.15896400
C	0.97264100	-0.51777700	-0.82807800
C	1.93317500	0.34855600	-1.35932300
C	2.99647200	-0.06416700	-2.14811300
C	3.14437600	-1.40999100	-2.44506900
F	3.87225600	0.82192200	-2.62336300
F	4.15615800	-1.82589300	-3.19969600
F	2.34385800	-3.61151900	-2.22762900
F	0.33848800	-2.81556500	-0.72619600
F	1.86673900	1.66677700	-1.13414400
C	-2.09988100	-1.34042900	-1.05176400
C	-1.51213800	-1.04582900	0.17833500
C	-2.14682800	-1.62668800	1.26642500
C	-3.26020000	-2.45357700	1.15814100
C	-3.79653000	-2.72211100	-0.08837900
C	-3.20718300	-2.15692600	-1.21027600
F	-1.57053400	-0.82631200	-2.17366700
F	-3.70797700	-2.40457100	-2.42204900
F	-4.86346100	-3.50922900	-0.21070100
F	-3.81601100	-2.98342800	2.25009800
F	-1.71176600	-1.41940400	2.52028100
C	-2.33506000	3.32715800	0.42160400
C	-1.67245400	2.13720000	0.68282600
C	-0.89047900	1.44737400	-0.23934600

C	-0.87957200	2.01510000	-1.51321300
C	-1.52660400	3.20626100	-1.82194700
C	-2.25410400	3.87271300	-0.84963100
F	-3.05594500	3.93169500	1.36632600
F	-1.83536800	1.62994000	1.92102200
F	-2.87780300	5.01261000	-1.13600300
F	-1.46172300	3.70783300	-3.05624400
F	-0.24731100	1.43153900	-2.53846800

**11**

C	-2.25036500	-0.78948200	2.99722300
C	-1.50280400	-1.23490700	1.84039100
C	-1.55125900	-2.61352800	1.46398100
C	-2.29767800	-3.47535500	2.21754900
C	-3.00851000	-3.00075500	3.35576300
C	-3.00423400	-1.67716700	3.76328800
C	-1.25151900	1.04065100	2.17259300
C	-0.81711000	-0.16385500	1.30789300
H	-1.01871600	-2.94688300	0.58141900
H	-2.36059300	-4.52480500	1.95879100
H	-3.58750700	-3.71534900	3.93269600
H	-3.56104600	-1.35070500	4.63295600
O	-0.95832400	2.19633200	2.02798500
N	-2.08796700	0.54531100	3.18188800
C	-2.69826400	1.36108300	4.21609500
H	-2.35808200	1.03892300	5.20203800
H	-2.38587600	2.38978900	4.04147300
H	-3.78624600	1.29492600	4.15678800
B	0.07329100	0.06853100	-0.00288800
C	-2.36119000	2.61660300	-1.87728300
C	-1.29384200	2.10288400	-1.15111200
C	-1.13050600	0.74032500	-0.90600500
C	-2.14677100	-0.07302600	-1.40795000
C	-3.22689800	0.39935600	-2.13683700
C	-3.33486500	1.76176400	-2.37160300
F	-4.15829300	-0.43436500	-2.60144400
F	-4.36184500	2.24443000	-3.06496400
F	-2.45988100	3.92769800	-2.10069000
F	-0.41092800	3.00039200	-0.70312000
F	-2.09733700	-1.39864800	-1.20299800
C	2.02068900	1.64802500	-0.76122900
C	1.34688300	1.03907300	0.29056700
C	1.93263300	1.19276200	1.53889100
C	3.09314800	1.92758200	1.75023700

C	3.71962000	2.53201800	0.67213100
C	3.17890800	2.39195100	-0.59909100
F	1.53821900	1.52402800	-2.00762300
F	3.77977700	2.96740100	-1.64276900
F	4.83376900	3.24011100	0.85270200
F	3.61108400	2.04978700	2.97437900
F	1.38468400	0.62006200	2.62804200
C	2.10420000	-3.27858200	-0.24378100
C	1.44321800	-2.14196100	0.19754600
C	0.70976600	-1.29720000	-0.63128200
C	0.70660100	-1.65468900	-1.97477400
C	1.35638900	-2.78321300	-2.46271700
C	2.05931800	-3.60100600	-1.59257200
F	2.78077700	-4.05393200	0.60521900
F	1.52159600	-1.86742600	1.51153400
F	2.68730700	-4.68411100	-2.04583200
F	1.31306000	-3.08240000	-3.76236100
F	0.06030200	-0.91219400	-2.88410800

**HFIP**

C	-0.00159800	0.55787300	-0.51779500
H	-0.00178600	0.52351700	-1.61338700
C	-1.26918200	-0.13848200	-0.04108300
C	1.25989900	-0.15426100	-0.03543500
F	-1.41343900	-0.04696600	1.28202200
F	-1.25265800	-1.43470400	-0.36980200
F	1.25794300	-0.33354600	1.28771100
F	1.40767500	-1.34792800	-0.61618200
F	-2.33944400	0.42151100	-0.60933600
F	2.32673600	0.59312000	-0.34553500
O	-0.04541400	1.85091000	0.00330500
H	0.54905000	2.41503200	-0.50708000

**12**

C	3.52366500	0.60197800	0.09866000
C	3.02766700	-0.65201700	-0.30833200
C	3.85004100	-1.77078300	-0.29813700
C	5.17107500	-1.61282300	0.12449200
C	5.65403100	-0.36581400	0.52603900
C	4.83441800	0.76522100	0.51923900
C	1.34368500	1.01720000	-0.45687900
C	1.64486100	-0.39745900	-0.66245800
H	3.47665700	-2.74036200	-0.61013400
H	5.83043900	-2.47357300	0.13996900

H	6.68452400	-0.26952400	0.85012300
H	5.20879300	1.73419900	0.83119400
N	0.74678100	-1.25213500	-1.08436400
N	-0.03753400	-1.97363400	-1.43858700
O	0.29274500	1.64607400	-0.64514000
N	2.51290100	1.56332000	0.00122500
C	2.67003900	2.96473800	0.33368700
H	3.43736000	3.41906900	-0.29752600
H	1.71438400	3.45611800	0.15803300
H	2.95086400	3.07413800	1.38375600
C	-2.53983300	0.44674500	0.04549700
H	-2.32732300	1.39975100	0.54594000
C	-2.09722000	-0.66450700	0.99303200
C	-4.03641800	0.39836800	-0.22767000
F	-2.38794700	-1.87622000	0.51029700
F	-2.65545800	-0.55540500	2.20207500
F	-4.38104800	-0.71631100	-0.87981300
F	-4.74458000	0.44557100	0.90729600
F	-0.76454800	-0.60353200	1.15149800
F	-4.39778800	1.43938900	-0.98241900
O	-1.88872600	0.30517400	-1.17219600
H	-1.05661200	0.84084700	-1.11401900

**13-ts**

C	2.79836800	-0.72439600	0.38885200
C	2.96242500	0.67192100	0.20614000
C	3.99092000	1.14471100	-0.61597600
C	4.80429400	0.22774700	-1.27126200
C	4.62605800	-1.14531700	-1.06236300
C	3.63279600	-1.64828200	-0.21670300
C	1.16309700	0.24661100	1.59572200
C	2.12445000	1.35411400	1.16002900
H	4.12313700	2.21336500	-0.75263600
H	5.58915700	0.57106000	-1.93493300
H	5.28601700	-1.84544500	-1.56443000
H	3.52035800	-2.71442300	-0.05495500
N	0.74907400	2.42471700	0.05545200
N	0.41809700	3.40026700	-0.33185100
O	0.09219700	0.36572800	2.18076500
N	1.73986700	-0.95767900	1.27320700
C	1.10557300	-2.24226500	1.48426500
H	1.82998900	-2.96467300	1.86453800
H	0.31549600	-2.10242000	2.22178600
H	0.67274400	-2.61343900	0.54939700

C	-2.18318800	-0.06814100	0.25556100
H	-1.88952500	-0.78328800	1.03240900
C	-1.41419200	-0.43977300	-1.00999800
C	-3.68853100	-0.18935500	0.05747600
F	-1.81632700	0.26461800	-2.06957600
F	-1.53972700	-1.73929900	-1.30077500
F	-4.14516300	0.72106600	-0.80609500
F	-4.02353300	-1.40043200	-0.40399200
F	-0.10540600	-0.19228100	-0.83292000
F	-4.31788900	-0.00046500	1.21997000
O	-1.91155200	1.25171400	0.60183600
H	-1.24181100	1.22427900	1.31038500

**14**

C	3.36154400	0.27519400	-0.16479800
C	2.45668700	-0.85175600	-0.04506300
C	2.99566100	-2.14471500	0.23817600
C	4.34801100	-2.28681700	0.38810100
C	5.19803600	-1.15155600	0.26166200
C	4.74084300	0.12771300	-0.01112900
C	1.28725600	1.04195700	-0.49535400
C	1.14041600	-0.47544500	-0.23488200
H	2.31700300	-2.98673000	0.32760700
H	4.78952200	-3.25202600	0.60271600
H	6.26681800	-1.29792000	0.38658200
H	5.42242000	0.96516900	-0.09904500
O	0.40839500	1.83500700	-0.72608200
N	2.65313000	1.39876900	-0.43116800
C	3.17802500	2.73578700	-0.62970300
H	3.85647700	2.75663800	-1.48527200
H	2.32918600	3.39052500	-0.82384800
H	3.70267100	3.07639200	0.26546300
C	-2.05322200	-0.25499100	-0.18881500
H	-1.53130100	0.38792600	-0.91266900
C	-2.20435700	0.58188600	1.07911900
C	-3.40245000	-0.61270800	-0.78956000
F	-3.01240100	0.00057100	1.97716000
F	-2.69550800	1.80261500	0.82482900
F	-4.08656200	-1.46398000	-0.01714500
F	-4.16821400	0.47380900	-0.97175100
F	-1.00840400	0.73904100	1.66119400
F	-3.23616700	-1.19750400	-1.98138400
O	-1.37800500	-1.42676300	0.09052300
H	-0.38121000	-1.19556900	-0.04153000

**Borane/HFIP**

C	1.18490400	-1.93826000	-1.28848900
H	0.95792200	-2.58397000	-0.43774700
C	2.67532500	-1.54896800	-1.26737200
C	0.88610500	-2.69771400	-2.59717000
F	2.88554700	-0.43596200	-1.96244700
F	3.38507300	-2.54012600	-1.81274000
F	1.52096800	-2.14959300	-3.63109400
F	1.24529300	-3.96648200	-2.48610800
F	3.12905100	-1.37567400	-0.02832000
F	-0.42725300	-2.64073600	-2.85947500
O	0.35612700	-0.76976300	-1.28552700
H	-0.45529900	-0.95430800	-1.80978500
B	-0.13498800	0.12047000	0.04886600
C	-2.63439200	-2.63713100	1.46393300
C	-1.69907800	-2.00218200	0.65420800
C	-1.11921200	-0.78296800	0.96526800
C	-1.57788700	-0.19870200	2.14456000
C	-2.50652100	-0.78936500	2.98320500
C	-3.04060600	-2.02503900	2.63722900
F	-2.89870800	-0.18713200	4.10405400
F	-3.93608500	-2.61063100	3.42552500
F	-3.14411800	-3.81589200	1.11223400
F	-1.37113700	-2.64585500	-0.48581100
F	-1.10032200	1.00311200	2.49960700
C	-1.02558500	2.61543300	-0.31582700
C	-1.04787300	1.26604600	-0.65432700
C	-2.03495300	0.91248400	-1.56669000
C	-2.92589900	1.79842500	-2.14713700
C	-2.85687200	3.13600700	-1.78338200
C	-1.90277600	3.54431300	-0.86372300
F	-0.14574000	3.08845200	0.57176700
F	-1.83611100	4.82506100	-0.50733000
F	-3.69714300	4.01739300	-2.31337100
F	-3.83556700	1.38519300	-3.02497800
F	-2.14641700	-0.39254600	-1.93575800
C	2.96542200	0.63432700	2.43942400
C	1.73940300	0.20955700	1.94235500
C	1.24157500	0.61418700	0.70694400
C	2.06627000	1.48049700	-0.00962100
C	3.29925500	1.91793100	0.44402000
C	3.75117600	1.48945000	1.68430700
F	3.39627500	0.21215100	3.62769500

F	1.06558400	-0.64699000	2.71826800
F	4.92988000	1.89524700	2.14243000
F	4.04736800	2.74009800	-0.29006900
F	1.67762900	1.91914200	-1.21328600

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C	1.31899200	-1.26385100	2.09505900
H	2.31830200	-0.82750000	2.14622200
C	1.46390600	-2.75546900	1.75545500
C	0.71248900	-1.14361700	3.50485400
F	0.27846900	-3.34774900	1.57815900
F	2.09275500	-3.39268400	2.75251500
F	-0.31976500	-1.98630900	3.67679400
F	1.62814500	-1.42865100	4.43162900
F	2.17458800	-2.94325100	0.64361000
F	0.25131900	0.08293400	3.73924600
O	0.49234000	-0.62188700	1.17100900
H	-0.71621200	0.11755500	1.60519500
B	0.89772600	0.05388100	-0.17097700
C	2.07469600	3.58637800	1.26194700
C	1.66447900	2.25896800	1.19130500
C	1.28651600	1.63588000	0.01285700
C	1.40194300	2.42912700	-1.12551600
C	1.80260000	3.75457200	-1.10832100
C	2.13935100	4.34188800	0.10400100
F	1.87441700	4.46664000	-2.23557700
F	2.53140200	5.61441000	0.14860200
F	2.42192400	4.12889800	2.43170400
F	1.68783400	1.57715700	2.34779800
F	1.10324100	1.90207000	-2.32556700
C	-0.90938200	-1.47806700	-1.26599600
C	-0.49659700	-0.16966200	-1.01631400
C	-1.42609100	0.79426200	-1.39068500
C	-2.64211600	0.50273200	-2.00283900
C	-2.99923200	-0.81400700	-2.23072600
C	-2.11711800	-1.81870100	-1.85558800
F	-0.11860600	-2.49729300	-0.90283200
F	-2.46469200	-3.09936600	-2.00577500
F	-4.18398900	-1.11385900	-2.75277900
F	-3.50275800	1.48742300	-2.27333600
F	-1.25763000	2.09480900	-1.09328400
C	4.67699500	-0.90415100	-0.80791400
C	3.48215200	-0.44148900	-0.27957400
C	2.23223200	-0.60242400	-0.87868400

C	2.28660000	-1.22209400	-2.12559000
C	3.46118600	-1.69800000	-2.69921300
C	4.66645900	-1.54478800	-2.03669400
F	5.82693000	-0.72417900	-0.15696800
F	3.58774100	0.19765200	0.90481100
F	5.79671800	-1.99648500	-2.57411100
F	3.43369200	-2.29113200	-3.89404200
F	1.19135300	-1.39058600	-2.87997600
C	-4.47805400	-0.63588700	0.56626000
C	-4.79610800	0.71934500	0.37606700
C	-6.00876800	1.08472600	-0.19877900
C	-6.88749000	0.06719300	-0.55764300
C	-6.56515400	-1.27958900	-0.35289300
C	-5.35015800	-1.65605300	0.21337600
C	-2.65640200	0.47727400	1.27846700
C	-3.62366300	1.42784200	0.84319000
H	-6.25856600	2.12676700	-0.36333900
H	-7.83988600	0.32420400	-1.00734900
H	-7.27270900	-2.04805600	-0.64275900
H	-5.09950100	-2.69935600	0.36879400
N	-3.35016400	2.72044200	0.77929600
N	-3.12417300	3.81129600	0.71935400
O	-1.49406300	0.78797800	1.75042200
N	-3.18273500	-0.74424200	1.11153500
C	-2.56219300	-2.01432700	1.46789700
H	-2.74990500	-2.73286900	0.66796000
H	-1.48815500	-1.88082000	1.55835600
H	-2.97892300	-2.38264000	2.40684500

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C	1.30547400	-0.26944700	2.11858400
H	2.33821600	-0.44164600	1.81316800
C	0.90249200	-1.47691400	2.96859400
C	1.27960800	0.99729500	2.99929800
F	-0.42004000	-1.52070000	3.18200200
F	1.51539800	-1.42678600	4.15555200
F	1.07729200	2.08883400	2.26164700
F	0.29451900	0.95131500	3.90902600
F	1.24847000	-2.62391000	2.38130800
F	2.43131000	1.13403900	3.65852200
O	0.45689600	-0.13263700	1.01441100
H	-0.84355600	0.23022100	1.49267000
B	1.00916200	0.00594900	-0.46697300
C	3.22030600	3.29318000	-0.14261400

C	2.66688400	2.03461400	0.01406800
C	1.61336400	1.51942100	-0.73948500
C	1.17906600	2.39282000	-1.73655700
C	1.70200700	3.66757700	-1.93789800
C	2.72720600	4.12810900	-1.13355500
F	1.21989100	4.44370600	-2.91073100
F	3.23859500	5.34318400	-1.31164700
F	4.22625600	3.69846300	0.63433700
F	3.24471200	1.27612900	0.96701600
F	0.21307000	2.05829100	-2.60642400
C	-0.55444200	-1.26937600	-2.30117800
C	-0.34509900	-0.26625600	-1.35824600
C	-1.44626700	0.56187400	-1.16465900
C	-2.68529800	0.38388900	-1.75786700
C	-2.85940600	-0.66463900	-2.64931100
C	-1.77501200	-1.47915800	-2.93990700
F	0.42383600	-2.10733900	-2.66643300
F	-1.91013500	-2.46655200	-3.82482400
F	-4.03721900	-0.87065400	-3.22977800
F	-3.70288000	1.19663800	-1.45860800
F	-1.32888900	1.63653400	-0.36170700
C	4.35802000	-2.11091100	-1.03901200
C	3.46258200	-1.04527500	-0.99583200
C	2.12570300	-1.18164900	-0.63013200
C	1.74434000	-2.49349300	-0.34690500
C	2.59919400	-3.58138900	-0.36788100
C	3.92794400	-3.38561100	-0.71648000
F	5.62841400	-1.90850900	-1.39199000
F	3.98083700	0.13774100	-1.35292900
F	4.77302300	-4.41210900	-0.75031800
F	2.15877800	-4.80511000	-0.07307500
F	0.45932200	-2.76261300	-0.05761200
C	-4.54728800	-0.83369100	0.67824100
C	-5.07464300	0.39622400	1.13510100
C	-6.41772100	0.69698200	0.89815900
C	-7.18426400	-0.21410400	0.17476300
C	-6.63693500	-1.42985200	-0.23975200
C	-5.30321800	-1.78032800	0.02802400
C	-2.85579700	0.22380600	1.66852600
C	-4.10712300	0.97052700	2.02836900
H	-6.83445600	1.63618600	1.24548900
H	-8.21906300	0.01070000	-0.05413300
H	-7.26138400	-2.13630800	-0.77583500
H	-4.90323000	-2.74273800	-0.27077200

N	-3.43614300	2.80482400	1.04494000
N	-3.37852200	3.89221000	0.89950800
O	-1.69197000	0.62153800	1.99569000
N	-3.17381400	-0.91014000	1.05037700
C	-2.32139400	-2.04598700	0.73535100
H	-1.30128000	-1.83077400	1.03916500
H	-2.68841700	-2.92759000	1.26416700
H	-2.34541300	-2.22202500	-0.34246900

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C	0.95555700	-1.67430700	1.84513500
H	2.02264400	-1.48551100	1.94212200
C	0.74208800	-3.05539100	1.21886600
C	0.33073900	-1.62221400	3.25060000
F	-0.53234800	-3.24044700	0.86730700
F	1.08075800	-4.00120400	2.09766000
F	-0.84668400	-2.26559000	3.28369900
F	1.14315800	-2.20986200	4.12432000
F	1.48849800	-3.20814000	0.12705800
F	0.11226600	-0.37091700	3.63327800
O	0.37442100	-0.67804400	1.02666000
H	-0.60222900	-0.45189000	1.27657500
B	0.96225800	0.25428000	-0.19805500
C	3.11714100	2.75905000	2.01911500
C	2.33350200	1.67148400	1.64858200
C	1.78960200	1.52128400	0.38321100
C	2.13136300	2.52054500	-0.52499600
C	2.90550800	3.62211500	-0.20358500
C	3.40098600	3.74361600	1.08820000
F	3.18402000	4.55508500	-1.11433500
F	4.15089300	4.79056100	1.42274300
F	3.60836000	2.84903600	3.25557900
F	2.15297500	0.73185600	2.59187100
F	1.68684000	2.43060900	-1.78875600
C	-1.24511500	-0.45148800	-1.36546600
C	-0.47060800	0.60683800	-0.88329800
C	-1.10492600	1.84424800	-0.88814900
C	-2.40523900	2.03123800	-1.35464300
C	-3.12253400	0.94872200	-1.83929800
C	-2.53851900	-0.31136600	-1.83718200
F	-0.74722000	-1.69688900	-1.34279300
F	-3.25022500	-1.37126500	-2.22582400
F	-4.37490100	1.10111600	-2.25236500
F	-2.96732300	3.23604500	-1.32983400

F	-0.52031500	2.93880300	-0.39427800
C	4.21187800	-1.67312500	-1.28690600
C	3.22768400	-1.00759900	-0.57508600
C	2.00008900	-0.61166400	-1.10530400
C	1.85127500	-0.88547600	-2.46355000
C	2.81362000	-1.54530000	-3.22017900
C	4.00021100	-1.94617700	-2.62994900
F	5.35142000	-2.03733400	-0.70129800
F	3.51040300	-0.75796000	0.71996100
F	4.92705000	-2.57807700	-3.34196100
F	2.60477000	-1.78217200	-4.51469600
F	0.76111900	-0.50505600	-3.14022900
C	-5.02243700	-0.39185700	0.44050700
C	-5.04587400	1.02666600	0.62394900
C	-6.17047900	1.75799200	0.18906500
C	-7.22516200	1.08380000	-0.40508200
C	-7.15674100	-0.30771100	-0.56614700
C	-6.05818800	-1.07854200	-0.15305900
C	-3.05407600	0.18985300	1.31849900
C	-3.85756000	1.52431800	1.20743500
H	-6.18047500	2.83547100	0.31938600
H	-8.09993300	1.61889200	-0.75341300
H	-7.99057200	-0.81789600	-1.03854300
H	-6.03822800	-2.15068100	-0.30928400
O	-1.88447000	0.11425200	1.69272800
N	-3.80723700	-0.87931800	0.92084100
C	-3.36051900	-2.25893200	0.88448800
H	-2.98719400	-2.52526900	-0.10818400
H	-2.56544000	-2.37214400	1.61871900
H	-4.19003600	-2.91432000	1.15330400

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C	1.85931500	-1.63493700	-1.81789700
C	0.87881800	-1.67809600	-0.77348400
C	0.45763000	-2.94756000	-0.30409000
C	1.00877500	-4.08572400	-0.84741500
C	1.99025800	-4.00095000	-1.86247400
C	2.42486500	-2.78689800	-2.36522300
C	1.26071500	0.51401500	-1.44047800
C	0.43238300	-0.36188600	-0.49788700
H	-0.29989100	-3.02437200	0.46154900
H	0.69342400	-5.06114400	-0.49602600
H	2.40802600	-4.91751500	-2.26694400
H	3.16857200	-2.73012300	-3.15170200

O	1.30037500	1.71762900	-1.53042400
N	2.08838000	-0.34183800	-2.17914900
C	3.05638500	0.12200400	-3.14991300
H	2.74302800	-0.14274700	-4.16266700
H	3.11822600	1.20571300	-3.05360200
H	4.03422800	-0.31904400	-2.94142800
B	-1.10331300	-0.01866500	0.08801700
C	-1.90998600	3.53968300	-1.45366100
C	-1.50679700	2.23129900	-1.23511700
C	-1.56897300	1.57149200	-0.00271500
C	-2.24898200	2.30624600	0.97076200
C	-2.67441700	3.62068500	0.79682100
C	-2.49146700	4.25327900	-0.41852700
F	-3.29122900	4.26304500	1.79332800
F	-2.89900100	5.50852700	-0.60202400
F	-1.78514100	4.09727200	-2.66136600
F	-1.09470400	1.57821800	-2.33351600
F	-2.59474200	1.77901000	2.15481800
C	-3.52491800	-0.77579200	-0.60543000
C	-2.18283300	-0.70329700	-0.98242300
C	-1.94929000	-1.07164800	-2.30291500
C	-2.93891100	-1.54208300	-3.16161900
C	-4.24585500	-1.63267500	-2.71943900
C	-4.54290600	-1.23819700	-1.42282200
F	-3.89164200	-0.38178200	0.62541400
F	-5.80181500	-1.29774900	-0.98122100
F	-5.20736100	-2.07663200	-3.52820200
F	-2.63531800	-1.88495400	-4.41644700
F	-0.73043200	-0.95855800	-2.86307100
C	-0.92946500	-0.49558000	4.04362100
C	-0.81907900	-0.01020500	2.74943800
C	-1.26974700	-0.67308900	1.60770100
C	-1.87780900	-1.89387500	1.89865500
C	-2.01053500	-2.42749700	3.17572500
C	-1.53466500	-1.72133800	4.26510900
F	-0.46342300	0.21355900	5.07516300
F	-0.23495300	1.19066500	2.64681400
F	-1.65030200	-2.21061700	5.49805900
F	-2.59783200	-3.61385700	3.35266400
F	-2.36986200	-2.68358500	0.92419800
C	2.10893400	0.41248000	1.06492100
F	1.70190500	1.66338900	1.19075300
F	1.72888700	-0.34386100	2.08082900
C	4.03044300	-3.50875300	0.67258300

C	3.42500800	-2.27952700	0.89734200
C	3.92265100	-1.12481900	0.26241800
C	5.05358300	-1.23555700	-0.57533500
C	5.64405600	-2.46766100	-0.79613200
C	5.12584100	-3.61109000	-0.18078200
H	3.63203600	-4.39387400	1.15625700
H	2.57004700	-2.22862800	1.55579400
H	5.45183300	-0.34088100	-1.04079500
H	6.50795700	-2.54287100	-1.44717200
H	5.58608300	-4.57732800	-0.35910000
C	3.30719700	0.18445500	0.38837300
O	3.81950400	1.17747000	-0.31893800
Si	4.25973500	2.78370500	0.17147100
C	2.98417200	4.00176300	-0.42186500
H	3.30302800	5.01377900	-0.15234600
H	2.88709200	3.94666100	-1.50900600
H	2.00137200	3.80997500	0.01141400
C	4.47947600	2.74764300	2.02543500
H	3.52850700	2.64072200	2.55257200
H	5.14045500	1.92833200	2.32423500
H	4.94137300	3.68414900	2.35262600
C	5.87727100	3.01077100	-0.72775700
H	5.73848000	2.86618500	-1.80346600
H	6.26791900	4.02026100	-0.57010700
H	6.62664200	2.29499100	-0.37857700

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C	0.36533500	3.09521400	0.26778400
C	0.19403300	2.23116000	-0.82538700
C	-0.18783500	2.76892900	-2.04584900
C	-0.43202000	4.14245200	-2.14050800
C	-0.30247200	4.97048700	-1.02716000
C	0.10666900	4.45523400	0.20478100
C	1.26205700	1.13735900	0.94079100
C	0.56007600	0.83206600	-0.37566100
H	-0.30679400	2.13016000	-2.91149800
H	-0.72979700	4.56559500	-3.09369800
H	-0.50578900	6.03239900	-1.11808800
H	0.24661700	5.09679600	1.06806900
O	2.07691600	0.39614200	1.48754300
N	0.93321400	2.39416000	1.34021500
C	1.47245200	3.01093000	2.53250100
H	0.67557700	3.50462600	3.09245800
H	1.91212800	2.22216600	3.14129800

H	2.24156800	3.74401600	2.26711600
B	-0.84465300	-0.22477600	0.08191500
C	0.36077600	-1.77410100	3.55734600
C	-0.04881200	-0.90831100	2.55777100
C	-0.29944800	-1.27849200	1.23369200
C	-0.04764400	-2.62641800	0.99187400
C	0.35491800	-3.53812400	1.96257400
C	0.56333600	-3.11319700	3.26013600
F	0.60423700	-4.80741200	1.62434600
F	0.96972900	-3.96412200	4.20162900
F	0.57230800	-1.32866900	4.79963000
F	-0.18809600	0.37282100	2.94151700
F	-0.13838300	-3.15274800	-0.24366800
C	-2.79469600	0.67644300	1.81940200
C	-2.11011500	0.72774700	0.60142400
C	-2.73934300	1.56901000	-0.32632200
C	-3.78802100	2.43016900	-0.03870500
C	-4.34596800	2.41857900	1.22850800
C	-3.85489300	1.51595100	2.15294200
F	-2.52873200	-0.24267200	2.75809200
F	-4.42762900	1.42304400	3.35675100
F	-5.36274500	3.22294900	1.53406400
F	-4.29516200	3.22307900	-0.98651100
F	-2.39191800	1.53060100	-1.62240500
C	-2.15835100	-1.71476300	-3.41982400
C	-1.42227000	-0.98867000	-2.48913800
C	-1.58439100	-1.08580800	-1.11762300
C	-2.60823800	-1.95661600	-0.73622900
C	-3.36870900	-2.70442200	-1.62089000
C	-3.13896900	-2.58689200	-2.98386000
F	-1.93326300	-1.56205000	-4.72813300
F	-0.53010700	-0.13095600	-3.00775900
F	-3.85860400	-3.29359000	-3.85565300
F	-4.32062200	-3.52927000	-1.17549000
F	-2.90443100	-2.11414100	0.56612300
C	1.65285900	0.16437700	-1.23312400
F	1.48681100	-1.18224500	-1.29018000
F	1.70250400	0.61838500	-2.51693300
C	3.71543800	4.12297600	-1.01053700
C	3.17394600	2.86952200	-1.27347800
C	3.65551800	1.75399200	-0.57329300
C	4.68734800	1.89773800	0.37154400
C	5.20493900	3.15410100	0.63643100
C	4.71634900	4.26744500	-0.05328100

H	3.35085100	4.98516300	-1.55733500
H	2.41197200	2.76128800	-2.03308200
H	5.03805000	1.02504500	0.91173100
H	5.98385000	3.27204900	1.38100500
H	5.12386200	5.25092600	0.15607800
C	3.12219000	0.40888000	-0.77274000
O	3.92013000	-0.54664000	-0.67292300
Si	4.12510600	-2.31777100	-0.94665400
C	3.04613000	-3.15390100	0.30592700
H	2.75357700	-2.42857800	1.07232400
H	2.14166200	-3.55574100	-0.15296500
H	3.59182700	-3.96775200	0.79025500
C	3.74133700	-2.58066000	-2.74432600
H	2.67550000	-2.48928600	-2.95669000
H	4.29105300	-1.86513000	-3.36192500
H	4.06810600	-3.58604300	-3.02743300
C	5.93677000	-2.44305200	-0.56312100
H	6.52759800	-1.81243300	-1.23217300
H	6.13597000	-2.14105000	0.46869700
H	6.27074600	-3.47771400	-0.68400400

**20-ts**

C	-0.01096800	3.08955100	0.05398900
C	0.04908100	2.19659100	-1.04698200
C	-0.52421200	2.59316200	-2.25507800
C	-1.19049000	3.81825400	-2.32460800
C	-1.29005900	4.65253700	-1.20852400
C	-0.69129300	4.29845100	0.00273400
C	1.27787700	1.34743200	0.72328500
C	0.76548800	1.02012300	-0.58478300
H	-0.48511000	1.93682300	-3.11691900
H	-1.65281700	4.11896000	-3.25927700
H	-1.82917200	5.59137900	-1.28358000
H	-0.73923400	4.95204900	0.86816300
O	2.12466100	0.70906600	1.38199500
N	0.73151300	2.56119500	1.09950900
C	0.96096900	3.19894200	2.37224600
H	0.01686400	3.35467600	2.90280700
H	1.59669100	2.53628800	2.95934800
H	1.46028200	4.16307500	2.23660400
B	-1.35737800	-0.63631700	0.35606100
C	0.60495000	-1.06487300	3.73169200
C	-0.09307200	-0.52679800	2.66236200
C	-0.51636000	-1.25809800	1.54475600

C	-0.15199800	-2.61122700	1.59684300
C	0.51677400	-3.19379900	2.66184200
C	0.90787200	-2.41547100	3.73857100
F	0.85495600	-4.48313800	2.61530200
F	1.58286900	-2.95280100	4.74755700
F	0.98676400	-0.28638400	4.74371200
F	-0.34656100	0.77750200	2.75994300
F	-0.39575400	-3.44544900	0.57810900
C	-2.90554200	0.94700500	1.80254800
C	-2.35960100	0.57312800	0.56926600
C	-2.85981600	1.29407800	-0.52394300
C	-3.69246500	2.39618400	-0.40303100
C	-4.11787900	2.78759600	0.85632700
C	-3.73903100	2.04431900	1.96412800
F	-2.70552400	0.21064900	2.90045800
F	-4.21501200	2.36152900	3.16889200
F	-4.92503000	3.83280900	0.99718500
F	-4.11841300	3.05179100	-1.48106400
F	-2.57401800	0.91984800	-1.77195500
C	-1.91549800	-2.36381200	-3.17973200
C	-1.42184200	-1.48945100	-2.21721100
C	-1.75495600	-1.58516300	-0.87375700
C	-2.65459000	-2.60119700	-0.55915500
C	-3.17261700	-3.49072500	-1.48474300
C	-2.79350500	-3.37029700	-2.81411400
F	-1.56008600	-2.22623000	-4.45824200
F	-0.62376800	-0.51919000	-2.66950800
F	-3.27449100	-4.20885200	-3.72843300
F	-4.02121800	-4.45012300	-1.11415800
F	-3.03569900	-2.75481700	0.72016700
C	1.71652400	0.22940200	-1.39268800
F	1.54081000	-1.13099100	-1.29894100
F	1.66770000	0.52996200	-2.72344300
C	3.69696000	4.16405200	-1.56282100
C	3.11830400	2.90348800	-1.61580600
C	3.76741400	1.81996600	-1.00020500
C	4.99510100	2.01208800	-0.34128700
C	5.55508200	3.27723000	-0.28317600
C	4.90524900	4.35263900	-0.89324800
H	3.20320500	5.00038100	-2.04434700
H	2.18779500	2.76167600	-2.15039300
H	5.47974800	1.16823200	0.13726200
H	6.49292600	3.43113800	0.23806300
H	5.34562900	5.34321200	-0.84679100

C	3.20761400	0.47841000	-1.01527600
O	3.99230800	-0.47711000	-0.80803500
Si	4.05932100	-2.26497800	-0.68398000
C	2.86483400	-2.72549000	0.65759500
H	2.51584900	-1.80753700	1.14565900
H	1.99891800	-3.24740500	0.24503200
H	3.34219000	-3.36609000	1.40392000
C	3.73372200	-2.90424000	-2.39771800
H	2.69390300	-2.76214500	-2.69470400
H	4.38298400	-2.40524000	-3.12219600
H	3.96259400	-3.97407100	-2.42415800
C	5.83975800	-2.43962900	-0.18218500
H	6.50730700	-2.01613700	-0.93702800
H	6.02533800	-1.93556600	0.77030100
H	6.08976500	-3.49761800	-0.05948700

**21**

C	-3.84185100	2.92054100	0.64632900
C	-3.54730100	1.52658300	0.58851100
C	-4.53074100	0.63813800	1.04187700
C	-5.73581200	1.13309400	1.55002800
C	-5.98866100	2.50250000	1.61060900
C	-5.03480400	3.41569000	1.15078400
C	-1.76109500	2.75037500	-0.30335600
C	-2.23402000	1.42729800	0.00186700
H	-4.38714300	-0.43832600	1.00886000
H	-6.48622100	0.43140600	1.90046900
H	-6.93051800	2.86437400	2.00939100
H	-5.22087200	4.48501900	1.18170600
O	-0.70502200	3.13975200	-0.82303100
N	-2.77370800	3.62295200	0.12270400
C	-2.69415100	5.05637800	0.00023100
H	-2.74813600	5.53991100	0.98090600
H	-1.73497700	5.28621700	-0.46420800
H	-3.50347300	5.44343100	-0.62739900
B	2.22076800	-0.13407300	-0.11004100
C	2.34308700	-1.80870500	-3.62975500
C	2.56879500	-0.95089700	-2.56108100
C	1.94462200	-1.09799900	-1.32338200
C	1.04913700	-2.16267000	-1.23021500
C	0.80392400	-3.04471200	-2.26644800
C	1.44979100	-2.85915200	-3.48130700
F	-0.07153400	-4.04075100	-2.12292200
F	1.20094200	-3.67784900	-4.49410700

F	2.96717000	-1.62616000	-4.79054400
F	3.43765700	0.04100300	-2.76497500
F	0.35700700	-2.36619300	-0.09905500
C	1.91779500	2.08325800	-1.39823100
C	2.52384600	1.37964200	-0.35542400
C	3.35074900	2.13241500	0.48428700
C	3.57233900	3.48568800	0.30573800
C	2.93334400	4.14481300	-0.73829500
C	2.09950100	3.44416700	-1.59318200
F	1.12223700	1.45753800	-2.25949100
F	1.48215900	4.07739700	-2.58532400
F	3.12636100	5.44684700	-0.91271400
F	4.38119200	4.16238200	1.12133700
F	3.98220200	1.54977800	1.50946300
C	1.74402800	-0.50460900	3.73216800
C	1.80646100	0.01265000	2.44900000
C	2.24376100	-0.72815400	1.34842000
C	2.62416900	-2.04160800	1.62675000
C	2.57910900	-2.59238900	2.89933900
C	2.12510400	-1.81934100	3.95758700
F	1.27407500	0.23218600	4.73930400
F	1.37608100	1.26719600	2.29621800
F	2.04562500	-2.33475600	5.17663200
F	2.95299700	-3.85260300	3.10845200
F	3.05886200	-2.84226800	0.64947700
C	-1.42614800	0.28015000	-0.31773700
F	-1.13267500	0.11046500	-1.66449900
F	-0.14243100	0.32548600	0.24151000
C	-1.40977600	-1.19548600	3.80957400
C	-1.44869100	-0.70587900	2.51186400
C	-1.95294400	-1.52519300	1.48310600
C	-2.40526200	-2.82948300	1.76665800
C	-2.34272800	-3.31034000	3.06179700
C	-1.84569800	-2.49247400	4.08118800
H	-1.02510900	-0.57149800	4.60822500
H	-1.11119000	0.30167900	2.29509100
H	-2.78965500	-3.44620100	0.96178300
H	-2.67849400	-4.31621800	3.28504900
H	-1.79966600	-2.87078900	5.09712400
C	-2.04409500	-1.04706200	0.12548400
O	-2.66776900	-1.73172200	-0.72792100
Si	-3.33985500	-1.54422700	-2.40076500
C	-2.01258800	-1.98912900	-3.62110700
H	-1.18427000	-1.27877600	-3.60205900

H	-1.63614000	-3.00003800	-3.45248200
H	-2.46630300	-1.96342100	-4.61761100
C	-4.65596000	-2.84924000	-2.27079100
H	-4.21742500	-3.82551700	-2.04776600
H	-5.37423500	-2.60205800	-1.48433800
H	-5.20017000	-2.92723400	-3.21638600
C	-4.03771100	0.16572400	-2.57271200
H	-4.66861000	0.42561300	-1.71796100
H	-3.25970500	0.92272900	-2.67702300
H	-4.66373900	0.16958200	-3.47165000

**22-ts-Z**

C	-3.87295900	0.38067500	-1.22691900
C	-2.75944500	1.08255700	-0.70437300
C	-2.87890500	1.67236300	0.55503400
C	-4.09248500	1.59308300	1.23862300
C	-5.17729100	0.89803500	0.70200800
C	-5.07564100	0.27104500	-0.54232000
C	-2.21958300	0.16091900	-2.80355500
C	-1.70266900	0.96307400	-1.69084000
H	-2.03808700	2.18487900	1.01050300
H	-4.18101500	2.05388000	2.21662000
H	-6.10596300	0.83220900	1.25946500
H	-5.90947200	-0.28149700	-0.96376500
O	-1.70311200	-0.18108100	-3.86483500
N	-3.54011600	-0.14233400	-2.46514200
C	-4.41780400	-0.92518900	-3.29919700
H	-5.31619100	-0.35850100	-3.56244200
H	-3.86665500	-1.17360300	-4.20596900
H	-4.71709700	-1.84762500	-2.79088800
B	0.54970000	-1.32695500	0.82723600
C	1.82933500	-0.38998400	4.40796400
C	1.11771100	-0.95591600	3.35904700
C	1.35496800	-0.65026600	2.02049900
C	2.39005100	0.25493400	1.80006500
C	3.11480600	0.85417400	2.81762500
C	2.83228100	0.52769500	4.13578100
F	4.08507800	1.72625900	2.53790900
F	3.52020500	1.08353800	5.12630400
F	1.55682800	-0.72113000	5.66918100
F	0.17183200	-1.83960900	3.69650100
F	2.75058200	0.58377100	0.55098200
C	-1.79047700	-0.94912300	1.89497300
C	-0.97085700	-1.69870000	1.04479700

C	-1.60135400	-2.78887600	0.43799700
C	-2.94460100	-3.08771300	0.61770300
C	-3.70929500	-2.31259500	1.47580900
C	-3.11603100	-1.25944900	2.15338700
F	-1.30161300	0.11292800	2.54383400
F	-3.82057400	-0.56389600	3.04336600
F	-4.98986100	-2.59978300	1.67580900
F	-3.49635500	-4.12972500	-0.00550700
F	-0.92073000	-3.64320300	-0.33312900
C	1.63958900	-2.57469400	-2.69360300
C	0.89940600	-2.09340800	-1.62653100
C	1.39972000	-1.99850000	-0.32699900
C	2.71167900	-2.43835700	-0.15727300
C	3.48099400	-2.94019500	-1.19971600
C	2.94253100	-3.00259400	-2.47522600
F	1.12253800	-2.62408000	-3.91973700
F	-0.34682100	-1.70186200	-1.88630300
F	3.66845300	-3.47051700	-3.48405700
F	4.72894800	-3.35447600	-0.98363400
F	3.29839300	-2.40850400	1.04490300
C	-0.32825400	1.22233600	-1.52485200
F	0.25832000	0.46525500	-0.24488100
F	0.45501400	0.75353300	-2.51111000
C	-2.46428300	5.13633000	-0.60688600
C	-1.79717300	4.03596100	-1.12587300
C	-0.54223400	3.68521500	-0.60172500
C	0.04777600	4.45855900	0.41478000
C	-0.64630800	5.53272000	0.94808000
C	-1.90090700	5.87047000	0.43629900
H	-3.42611500	5.42244200	-1.01671700
H	-2.22020800	3.46297300	-1.94121700
H	1.02497100	4.18098400	0.79633000
H	-0.21177500	6.11126400	1.75514800
H	-2.43748600	6.71903900	0.84751500
C	0.23051500	2.57185800	-1.12613400
O	1.46862600	2.76134700	-1.26372600
Si	2.98964500	2.32155900	-2.09325400
C	3.22361800	0.50308300	-2.39223800
H	2.79024700	0.20371500	-3.34893800
H	4.29878100	0.29699900	-2.41051400
H	2.77145800	-0.09100200	-1.59839600
C	2.79585900	3.29376800	-3.66614800
H	3.70259800	3.18715200	-4.26926900
H	1.95380500	2.91641900	-4.25298900

H	2.63753600	4.35547800	-3.46380900
C	4.20625900	3.04763500	-0.89255500
H	4.00363600	4.10967300	-0.73245500
H	4.16732100	2.53217100	0.06962400
H	5.21948800	2.94807400	-1.29289500

**22-ts-E**

C	-4.18330700	-0.36766700	-0.82243200
C	-3.00695400	-0.60126000	-1.57547000
C	-2.97774400	-1.68930100	-2.44922000
C	-4.10368000	-2.50791400	-2.55562100
C	-5.25429700	-2.25475700	-1.80726500
C	-5.30792700	-1.17284500	-0.92429200
C	-2.72117200	1.28476000	-0.20392400
C	-2.08855900	0.46862700	-1.23588900
H	-2.08419700	-1.91375000	-3.01923500
H	-4.07961100	-3.35795300	-3.22978900
H	-6.11740900	-2.90476200	-1.90680400
H	-6.19709000	-0.96911300	-0.33629600
O	-2.28546600	2.23794300	0.44360400
N	-3.99260200	0.74770200	-0.01868800
C	-4.96011200	1.28699800	0.90642200
H	-5.29020100	0.52028100	1.61342500
H	-4.47196600	2.09338700	1.45412000
H	-5.83382500	1.67860600	0.37618500
B	0.82313100	-0.84194800	1.28202500
C	3.01565300	1.41912400	3.60569900
C	2.03273100	0.55910600	3.13547300
C	1.94904300	0.14850200	1.80644400
C	2.94550000	0.64879900	0.97289500
C	3.93415200	1.52155800	1.39683900
C	3.97014200	1.90998300	2.72801300
F	4.84948200	1.97905800	0.54078900
F	4.91343800	2.73929100	3.15874300
F	3.04654700	1.77794700	4.88827900
F	1.14755000	0.12364900	4.03829700
F	2.99410000	0.28482000	-0.31638500
C	-1.14281700	0.42245700	2.40142200
C	-0.60577400	-0.78804700	1.95437500
C	-1.42871200	-1.90354300	2.12007800
C	-2.70672600	-1.82941000	2.65399100
C	-3.19951500	-0.60079300	3.06693600
C	-2.41292000	0.53436500	2.94547500
F	-0.42501100	1.54286600	2.33612200

F	-2.88498500	1.71335600	3.34655200
F	-4.42380200	-0.51473500	3.58187000
F	-3.45207400	-2.92571500	2.79369500
F	-1.00245900	-3.12787600	1.79176400
C	0.81900600	-3.65296300	-1.40341200
C	0.42993700	-2.65670300	-0.52427700
C	1.28268900	-2.09144300	0.42473300
C	2.57491900	-2.61321900	0.44904400
C	2.99915200	-3.62304700	-0.40572000
C	2.11759700	-4.14029600	-1.34215100
F	-0.02934900	-4.12742200	-2.31526400
F	-0.82435700	-2.22014900	-0.63395400
F	2.51233100	-5.09659900	-2.17439700
F	4.24502800	-4.09048200	-0.33721400
F	3.48400500	-2.15891800	1.31861600
C	-0.74161100	0.58324800	-1.61694100
F	0.30857000	0.26234500	-0.44014000
F	-0.35996400	-0.33858200	-2.53080100
C	-2.51947900	4.75657900	-2.19272300
C	-2.04175200	3.45459500	-2.20219300
C	-0.68452600	3.21624100	-1.92630600
C	0.18541400	4.29329100	-1.67290900
C	-0.31163800	5.58532000	-1.63261800
C	-1.66356500	5.81636500	-1.89488600
H	-3.56142100	4.94680500	-2.42337100
H	-2.69394700	2.62990700	-2.45995300
H	1.23354100	4.09461100	-1.47600200
H	0.34998400	6.41329400	-1.40529700
H	-2.04880000	6.83055200	-1.87829400
C	-0.09387200	1.89347300	-2.01066700
O	1.06587400	1.83260600	-2.50751600
Si	2.27200500	0.86913300	-3.39855200
C	2.35572800	-0.92059200	-2.90562200
H	1.70333100	-1.53152600	-3.53365400
H	3.38791700	-1.26579000	-3.02198400
H	2.06208800	-1.04646800	-1.86422000
C	1.66315400	1.11250400	-5.13983100
H	2.35251500	0.62401200	-5.83520600
H	0.67542500	0.66177900	-5.27105600
H	1.60370500	2.17219900	-5.39845200
C	3.80320100	1.84012600	-2.99494500
H	3.67429300	2.89170100	-3.26401600
H	4.04950700	1.77447400	-1.93304500
H	4.64778000	1.44230200	-3.56563900

**(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>B-F**

B	-0.08295300	-0.05794400	-0.95376600
C	-3.41086000	-1.92367800	0.27381200
C	-2.07110100	-1.64444100	0.01630600
C	-1.62670900	-0.44771800	-0.52854300
C	-2.64033300	0.46065000	-0.82177500
C	-3.98623100	0.23033300	-0.58469000
C	-4.37640400	-0.98082300	-0.03094200
F	-4.90785900	1.15275300	-0.88054800
F	-5.66568400	-1.23056900	0.20398300
F	-3.77207600	-3.09806800	0.80164900
F	-1.21528800	-2.63290200	0.32956800
F	-2.32896800	1.65887900	-1.34565600
C	1.16362100	-1.34203800	0.96838800
C	1.04123100	-1.12018700	-0.39903700
C	1.99179600	-1.75825000	-1.18300100
C	2.98817300	-2.57520900	-0.65213100
C	3.06037400	-2.77070500	0.71596400
C	2.13353200	-2.14710100	1.54125000
F	0.28495600	-0.75880300	1.80473100
F	2.19254100	-2.32986200	2.86480200
F	4.00871100	-3.55141800	1.23870300
F	3.87864800	-3.17113100	-1.45324500
F	2.00306300	-1.62738700	-2.51777600
C	2.06387500	3.19821000	-0.43402300
C	1.53604800	1.99220300	-0.87564300
C	0.39324000	1.40313400	-0.34239700
C	-0.18199300	2.10417700	0.70988800
C	0.31053000	3.31404400	1.18639800
C	1.44132200	3.86741400	0.60834800
F	3.16557600	3.71311400	-0.99027900
F	2.21177200	1.37710100	-1.86075700
F	1.92910500	5.02713800	1.05326900
F	-0.29358400	3.94740400	2.19769800
F	-1.27520900	1.63999600	1.33823200
F	-0.05635900	0.00926900	-2.36662000

**23**

C	-3.10525400	-0.60490400	0.32808000
C	-1.86959100	0.07621000	0.37025500
C	-1.77084000	1.25933000	1.10425800
C	-2.90475500	1.75899400	1.73845000
C	-4.12483100	1.08561300	1.65117200

C	-4.24245900	-0.11432400	0.94981900
C	-1.69905100	-2.00537200	-0.79583100
C	-0.92543400	-0.75449300	-0.37418600
H	-0.83190800	1.79056900	1.19854500
H	-2.83548500	2.67881500	2.30701200
H	-4.99824100	1.49460700	2.14769200
H	-5.18489900	-0.64748900	0.90011300
O	-1.27986800	-2.97463600	-1.39035900
N	-2.98768800	-1.80173700	-0.37725000
C	-4.05560700	-2.76159800	-0.56773100
H	-4.87694900	-2.30752100	-1.12654300
H	-3.64739500	-3.59723700	-1.13435800
H	-4.42340100	-3.11870700	0.39746900
C	0.37293400	-0.63475200	-0.70748100
F	1.01195100	-1.65074600	-1.30371800
C	-0.36294600	3.56964700	-1.57634500
C	-0.06818000	2.22553900	-1.42525700
C	0.98706400	1.84226600	-0.57367400
C	1.75021000	2.81278000	0.10650200
C	1.43201900	4.15133000	-0.03932300
C	0.37769300	4.52626800	-0.87783000
H	-1.16524300	3.87727200	-2.23622300
H	-0.63121600	1.47651100	-1.97121200
H	2.55801300	2.49598900	0.75714100
H	1.99734100	4.90574500	0.49486600
H	0.13411400	5.57736800	-0.99125500
C	1.31504100	0.45315100	-0.39638600
O	2.47932400	0.14079300	-0.00055500
Si	3.24386500	-1.36703200	0.63028700
C	1.89971400	-2.36979400	1.43590200
H	1.24950600	-1.74000200	2.05030900
H	1.28968100	-2.92139500	0.71813900
H	2.37882900	-3.09285100	2.10356200
C	4.07641300	-2.12757000	-0.84252500
H	3.35473800	-2.49227100	-1.57507800
H	4.73859300	-1.40391500	-1.32450000
H	4.68594400	-2.97191100	-0.50686000
C	4.41936500	-0.61160700	1.85103300
H	5.10707800	0.07693200	1.35358300
H	3.87900400	-0.06612500	2.62901100
H	5.00935500	-1.39661600	2.33268200
<b>24-ts</b>			
C	-2.48007400	3.36832000	-0.22571000

C	-2.07749200	2.74889300	0.97233200
C	-1.50520700	3.50539300	1.98932100
C	-1.32380400	4.87321900	1.77855100
C	-1.69502700	5.46355100	0.57122100
C	-2.28685800	4.71950700	-0.45459700
C	-3.10927500	1.18642000	-0.50041900
C	-2.40699200	1.33105900	0.83628400
H	-1.19990100	3.04267400	2.91903800
H	-0.87175800	5.47804200	2.55584800
H	-1.53116000	6.52582500	0.42334900
H	-2.59172000	5.18495900	-1.38520100
O	-3.57711200	0.18754800	-1.01051200
N	-3.08352800	2.43325200	-1.06898000
C	-3.47717200	2.67962400	-2.43931400
H	-2.64320000	3.12797600	-2.98580100
H	-3.72498000	1.71707500	-2.88537200
H	-4.34274100	3.34494500	-2.48432500
B	1.15158300	-0.29227000	-0.12293300
C	-1.80369800	-1.21077400	-2.63267500
C	-0.88006800	-0.48407300	-1.88508500
C	-0.01742500	-1.05402700	-0.95584100
C	-0.18159200	-2.43076000	-0.80078900
C	-1.10231200	-3.18919900	-1.49835100
C	-1.93335100	-2.56902400	-2.42269200
F	-1.23149800	-4.49758000	-1.25897000
F	-2.84506400	-3.27679000	-3.08317200
F	-2.59853200	-0.59064400	-3.50358300
F	-0.90555800	0.84054700	-2.10250600
F	0.60167400	-3.09103000	0.06406000
C	1.23826200	2.30938500	0.57625500
C	1.27137800	1.30487600	-0.38195600
C	1.58164400	1.73032300	-1.67068200
C	1.78657600	3.05431300	-2.01913600
C	1.72798600	4.02630700	-1.02896000
C	1.47052400	3.64930700	0.27772900
F	1.00245300	2.03367600	1.86574600
F	1.48007000	4.56806400	1.24525300
F	1.94087100	5.30583400	-1.33129900
F	2.05504600	3.40163400	-3.27966100
F	1.67824400	0.81661600	-2.65152200
C	4.97128700	-0.91050900	0.49409000
C	3.66418600	-0.44904100	0.52575200
C	2.63703800	-0.94532000	-0.27589000
C	3.03594000	-1.92410200	-1.18250600

C	4.33613900	-2.41232400	-1.25415500
C	5.30995700	-1.90719600	-0.40862600
F	5.89887100	-0.39714500	1.30240700
F	3.40670700	0.54092300	1.39563400
F	6.55667300	-2.36648700	-0.46749000
F	4.65362600	-3.35887100	-2.13832300
F	2.17766100	-2.45743600	-2.06152000
C	-2.01723100	0.33592200	1.64668200
F	0.78281100	-0.44314600	1.40079200
F	-1.25867200	0.66700300	2.70908700
C	-5.79906800	-1.84636300	0.94040600
C	-4.63393600	-1.16083000	1.25536000
C	-3.39979900	-1.81524700	1.16296000
C	-3.34042200	-3.16139500	0.77490700
C	-4.50542600	-3.83175600	0.43207900
C	-5.73356400	-3.17337900	0.51610800
H	-6.75782200	-1.34652300	1.01927100
H	-4.68067600	-0.12722000	1.58132000
H	-2.37996800	-3.66369200	0.73832400
H	-4.45996500	-4.86568600	0.10858100
H	-6.64574200	-3.70048800	0.25620300
C	-2.14844500	-1.15414900	1.54687500
O	-1.16421800	-1.82675200	1.86859800
Si	0.66279500	-1.33462400	3.06259400
C	1.62938100	0.03373700	3.89782700
H	2.49201100	0.37983700	3.33445200
H	0.97887100	0.89023500	4.09405200
H	1.96030400	-0.35892100	4.86545600
C	-0.59583500	-1.77184800	4.40137800
H	-1.30854400	-0.96159300	4.57390300
H	-1.14975100	-2.68582400	4.18080300
H	-0.02902900	-1.91916600	5.32786400
C	1.66077400	-2.85128400	2.66411700
H	1.02062200	-3.68161000	2.36209100
H	2.40731800	-2.68279900	1.88580100
H	2.17568700	-3.13292300	3.58935600

**25**

C	-1.62168000	-0.54851800	0.00005000
O	-1.52016800	-1.75690700	0.00007500
O	-2.80035000	0.09593400	-0.00003800
C	-3.95607800	-0.74973500	-0.00007000
H	-4.81185100	-0.07691100	-0.00014400
H	-3.96914700	-1.37891100	-0.89219000

H	-3.96924600	-1.37884300	0.89209600
C	-0.49723400	0.39091300	0.00002900
C	0.94268000	0.07547200	0.00000900
C	1.39085400	-1.25354100	0.00000600
C	1.89410000	1.10772900	-0.00000600
C	2.75508300	-1.53053800	-0.00001300
H	0.67327200	-2.06274900	0.00001700
C	3.25325600	0.81796600	-0.00002500
H	1.58026800	2.14775200	-0.00000400
C	3.69434800	-0.50346200	-0.00002900
H	3.08149100	-2.56614600	-0.00001600
H	3.96933900	1.63398800	-0.00003600
H	4.75600500	-0.72804500	-0.00004400
N	-0.84806300	1.66013400	0.00002500
N	-1.13450400	2.74842700	0.00002100

**26-ts**

C	1.56285700	-0.52901500	-0.41477300
O	1.56721700	-1.64849900	-0.90362200
O	2.59486400	-0.01596800	0.26881600
C	3.73376400	-0.87774300	0.37347200
H	4.48791600	-0.30522900	0.91135800
H	3.48058100	-1.78273500	0.93006100
H	4.10145700	-1.15192400	-0.61728600
C	0.45983900	0.36408000	-0.73291100
C	-0.88885300	0.01982700	-0.30815500
C	-1.18743200	-1.11257300	0.47534000
C	-1.94462100	0.84576400	-0.73725100
C	-2.50283100	-1.41532000	0.79836400
H	-0.38254600	-1.76401400	0.80192600
C	-3.25612600	0.56384800	-0.38036400
H	-1.70765800	1.71215100	-1.34817100
C	-3.53424300	-0.57236800	0.38037900
H	-2.72903000	-2.29830900	1.38718800
H	-4.06258900	1.21296700	-0.70521400
H	-4.56097200	-0.80524900	0.64620900
N	0.89575100	1.94028500	0.39625600
N	1.02168700	3.02815500	0.51056800

**27**

C	-1.74302600	-0.00263600	-0.00253000
O	-1.77083800	1.21326200	-0.01031200
O	-2.87327400	-0.72191700	0.00461200
C	-4.08558500	0.03423500	0.00352800

H	-4.89359900	-0.69592100	0.00947800
H	-4.14047100	0.67058700	0.89024600
H	-4.14478200	0.66090700	-0.88978500
C	-0.56283200	-0.97097400	-0.00101100
C	0.73850500	-0.38824200	0.00023800
C	1.10172500	0.99265600	0.00326400
C	1.79190400	-1.34567200	-0.00198000
C	2.43177700	1.36717800	0.00373500
H	0.32365500	1.74454100	0.00515200
C	3.12357000	-0.96681700	-0.00150900
H	1.50895900	-2.39337400	-0.00420200
C	3.43818500	0.39259000	0.00132000
H	2.70202900	2.41799500	0.00597600
H	3.91224400	-1.71151000	-0.00331800
H	4.47952000	0.70210200	0.00172000

**28**

B	0.41154700	-0.07055400	0.16263500
C	-0.90619600	-0.45059800	-0.70941800
C	-1.41764400	-1.74026400	-0.59728600
C	-1.63038300	0.38986500	-1.54748900
C	-2.56070600	-2.18485700	-1.23838500
C	-2.77819100	-0.01490000	-2.21909300
C	-3.24863500	-1.30674900	-2.06336800
C	0.92909300	1.46583100	0.06325600
C	1.34846800	1.92233800	-1.18339900
C	1.14676400	2.34883400	1.11195100
C	1.88592200	3.17820700	-1.40560300
C	1.68027700	3.62174600	0.93574100
C	2.05372000	4.03874200	-0.32968500
C	1.71100400	-1.01613300	-0.15439900
C	1.87910400	-1.84969300	-1.25315000
C	2.80288400	-0.96046600	0.71015300
C	3.02889000	-2.60046100	-1.47101700
C	3.96327600	-1.69836800	0.53635700
C	4.07655900	-2.52808800	-0.56903900
F	-4.36189000	-1.69753700	-2.68031200
F	-3.00087000	-3.43398500	-1.07369100
F	-0.78366000	-2.63220300	0.19442700
F	-1.27704500	1.66762400	-1.73823000
F	-3.45346600	0.84912900	-2.97896200
F	0.83853800	2.02172700	2.37925700
F	1.85098100	4.43389800	1.98166200
F	2.57132600	5.25210300	-0.51510700

F	2.25206200	3.56392900	-2.62986600
F	2.76744300	-0.15102600	1.78381200
F	4.97029900	-1.60719700	1.40799500
F	5.18367100	-3.24208400	-0.76263800
F	3.13024600	-3.38821300	-2.54380200
F	0.92197900	-1.97371300	-2.18479200
C	-0.81326400	-0.93160700	2.33773800
O	0.10381700	-0.38977500	1.66491500
O	-0.49851700	-1.84989500	3.21964300
C	0.84677400	-2.37849800	3.17720600
H	0.87767400	-3.12477100	3.96769100
H	1.02231100	-2.83906800	2.20317000
H	1.56492600	-1.58018800	3.36280400
C	-2.19608500	-0.60011800	2.28426900
C	-2.85665400	0.48566500	1.52984700
C	-4.07154800	0.25193700	0.87952200
C	-2.24628200	1.74054700	1.44803200
C	-4.65644600	1.26524500	0.12586700
H	-4.54881700	-0.72275800	0.94481500
C	-2.82381600	2.73771900	0.66976500
H	-1.32533400	1.92689200	1.98908800
C	-4.02495800	2.50147200	0.00253000
H	-5.59443600	1.07790900	-0.38764800
H	-2.33345700	3.70277600	0.58757600
H	-4.47205500	3.28109200	-0.60582200
N	-2.97124000	-1.41608500	3.00212300
N	-3.64699100	-2.08962200	3.58282600
F	1.22429000	1.11133900	-2.24768400

**29-ts**

B	0.52339700	-0.05268900	0.18973300
C	-0.59852600	-0.94854100	-0.59122300
C	-1.34247700	-1.90862600	0.08929300
C	-0.80740700	-0.92412000	-1.96700800
C	-2.29916200	-2.71348700	-0.51241300
C	-1.74662800	-1.71696900	-2.61231800
C	-2.50760000	-2.61236600	-1.87829800
C	0.81913400	1.43689900	-0.42844100
C	2.01026900	2.09887300	-0.13513200
C	-0.09017700	2.19855400	-1.15676600
C	2.30973400	3.38451400	-0.56389400
C	0.16570200	3.48646700	-1.60729500
C	1.37922300	4.08442400	-1.31368600
C	1.86030300	-0.98961900	0.29722500

C	2.70355800	-1.12008400	-0.80248300
C	2.21378000	-1.76791100	1.39555200
C	3.82567400	-1.93308400	-0.82740500
C	3.33287200	-2.59472400	1.41270300
C	4.14567800	-2.67915600	0.29651300
F	-3.42010300	-3.37452400	-2.47935500
F	-3.01153200	-3.58333000	0.20903000
F	-1.16556100	-2.08917700	1.40901300
F	-0.09731100	-0.10578600	-2.75720200
F	-1.91894700	-1.62602700	-3.93346800
F	-1.30738600	1.72052600	-1.46205600
F	-0.75229200	4.15491200	-2.30989400
F	1.64241300	5.32015500	-1.73332100
F	3.47677200	3.95266000	-0.25260400
F	1.48615300	-1.77351200	2.52476700
F	3.62361000	-3.31137100	2.50223700
F	5.21818800	-3.47077900	0.29856900
F	4.59507300	-2.00552100	-1.91641100
F	2.44481300	-0.42703600	-1.92464300
C	-0.72641800	1.03958000	2.15700500
O	0.12480100	0.22533700	1.65240200
O	-0.39484500	1.65100600	3.27226400
C	0.97824600	1.51138400	3.70424100
H	1.04459900	2.10735500	4.61175200
H	1.19913200	0.46392400	3.90942700
H	1.65639500	1.89413300	2.93964100
C	-1.90388600	1.34691600	1.47784100
C	-3.05238300	0.55739000	1.17980900
C	-3.44438100	-0.51672500	2.01165800
C	-3.77146400	0.82296500	-0.00536500
C	-4.50597000	-1.32540800	1.64227300
H	-2.89294500	-0.70541300	2.92797800
C	-4.82873800	0.00512700	-0.37149000
H	-3.46570000	1.65661900	-0.62697900
C	-5.18844800	-1.06690200	0.44928600
H	-4.80033100	-2.16137600	2.26711300
H	-5.37224900	0.19352500	-1.29091000
H	-6.01345900	-1.70967500	0.15679600
N	-2.56387300	2.83849800	2.59440200
N	-3.04441000	3.81259500	2.76334100
F	2.94865100	1.51033600	0.62688200
<b>30</b>			
B	0.51754900	-0.11496900	0.20487000

C	1.69701200	-1.23358900	0.09968100
C	2.75653100	-1.16834100	1.00039800
C	1.79004800	-2.24545500	-0.84663000
C	3.82483000	-2.05246400	0.99386000
C	2.84342500	-3.15059700	-0.89136300
C	3.86703100	-3.05461200	0.03706200
C	-0.84547700	-0.44982600	-0.62639700
C	-1.52932200	0.41066000	-1.48343500
C	-1.51318500	-1.64035700	-0.33150600
C	-2.80726200	0.14605300	-1.96081800
C	-2.78975000	-1.93537600	-0.77128200
C	-3.45145700	-1.01846800	-1.58069900
C	1.18523500	1.33172700	-0.14284200
C	1.69309900	1.51682200	-1.42469100
C	1.39365200	2.39078000	0.72779300
C	2.35333000	2.66058600	-1.83760800
C	2.05381300	3.55851300	0.35983800
C	2.53839700	3.69403600	-0.92909400
F	4.88256700	-3.91656800	0.01040600
F	4.80970300	-1.94447200	1.88912900
F	2.78653400	-0.20324500	1.93515800
F	0.84022400	-2.40124200	-1.78182200
F	2.87666500	-4.10998000	-1.81913700
F	-0.93962600	-2.52984700	0.49234900
F	-3.41588000	-3.04626100	-0.38386900
F	-4.70640400	-1.24408500	-1.95161200
F	-3.45185500	1.04379900	-2.70743000
F	0.94861100	2.35462400	1.99923400
F	2.21982400	4.54801300	1.24094300
F	3.16866600	4.80837500	-1.29838300
F	2.80644100	2.78352600	-3.08738100
F	1.51501000	0.54532000	-2.33716500
C	-0.91506700	0.42629000	2.16392700
O	0.12535000	-0.14569300	1.69192300
O	-0.98329600	0.60406600	3.46273800
C	0.21130300	0.32500200	4.23194200
H	-0.01390400	0.68267300	5.23414600
H	0.40009400	-0.74914300	4.23955600
H	1.06222500	0.85546500	3.80620400
C	-1.92905900	1.05583800	1.42223600
C	-3.26931200	0.70285000	1.27595900
C	-3.80852300	-0.52270400	1.77202300
C	-4.11581800	1.57131300	0.52665900
C	-5.13016100	-0.84836000	1.53914100

H	-3.15986600	-1.19888000	2.32422400
C	-5.43366800	1.23253400	0.28863700
H	-3.68835600	2.48969200	0.13493400
C	-5.93332700	0.02638000	0.79520600
H	-5.54105700	-1.77959300	1.91246900
H	-6.07573500	1.88570100	-0.29125300
H	-6.96805700	-0.24091400	0.60134300
F	-1.02464000	1.59953700	-1.83055600

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B	0.12494300	0.06999300	-0.08776300
C	-1.21869600	-0.31396000	-0.93024800
C	-1.60978100	-1.64669000	-1.08761700
C	-2.09239500	0.59161500	-1.53403100
C	-2.75465800	-2.06105700	-1.74626800
C	-3.25338200	0.21995700	-2.20484400
C	-3.59378000	-1.11477900	-2.31133200
C	0.62475900	1.62373100	-0.29509500
C	1.75585600	1.99601400	-1.02581000
C	-0.08631000	2.71110100	0.20924900
C	2.15646700	3.31769500	-1.20065500
C	0.27045300	4.03931400	0.06503000
C	1.41632100	4.34793300	-0.65198000
C	1.40179200	-0.91381000	-0.34864100
C	1.59953400	-1.70300400	-1.47718800
C	2.49116200	-0.88779000	0.51398500
C	2.75139500	-2.44764400	-1.69880200
C	3.65323700	-1.62068300	0.34877500
C	3.78584200	-2.41394400	-0.77930100
F	-4.70173600	-1.48417300	-2.94734000
F	-3.05447200	-3.35846400	-1.83312700
F	-0.87023300	-2.63210700	-0.55907400
F	-1.87062600	1.91360500	-1.52831500
F	-4.03462300	1.15199500	-2.75432200
F	-1.21706100	2.47395500	0.90143500
F	-0.47453200	5.01009100	0.59345300
F	1.79096700	5.61276400	-0.81528900
F	3.25353900	3.59391700	-1.90681100
F	2.44158500	-0.09682800	1.61204500
F	4.63500700	-1.55779000	1.24999300
F	4.89260600	-3.12524700	-0.97899700
F	2.87391700	-3.18410800	-2.80446600
F	0.68683700	-1.76147800	-2.45740800
C	0.29527500	-1.42647400	2.38814200

O	0.26695800	-2.51520600	1.88626500
O	0.83456600	-1.13441100	3.56489700
C	1.55019500	-2.21158500	4.19851100
H	1.91319800	-1.80476600	5.13970900
H	0.87969000	-3.05368800	4.37376200
H	2.38497000	-2.51811500	3.56447500
C	-0.37061900	-0.18915800	1.73570800
C	-1.87409900	-0.24631400	2.05438800
C	-2.55925700	-1.43023900	1.76206200
C	-2.56184800	0.81035800	2.65565300
C	-3.92127700	-1.53228800	2.02697700
H	-2.03220900	-2.27642400	1.33791300
C	-3.92334600	0.69652000	2.92300900
H	-2.06026800	1.73279800	2.92539100
C	-4.61103900	-0.46929300	2.60283100
H	-4.43867200	-2.45531600	1.78579600
H	-4.44031200	1.52879900	3.38914400
H	-5.67287100	-0.55258800	2.81009100
N	0.18743700	0.91804400	2.43310900
N	0.68210200	1.79416200	2.87900500
F	2.53904600	1.10027600	-1.64251500

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B	0.11342400	-0.00013000	0.01075800
C	-1.02380300	-0.93652400	-0.75789200
C	-1.54036900	-2.13485500	-0.27702900
C	-1.51137000	-0.60361600	-2.02631100
C	-2.48210900	-2.91427300	-0.94232500
C	-2.44201800	-1.34765600	-2.72978300
C	-2.94114000	-2.51945700	-2.18237900
C	-0.13986300	1.61730600	-0.29241600
C	0.89260200	2.55534000	-0.25666700
C	-1.37554200	2.17957800	-0.62859800
C	0.74523300	3.90476700	-0.55360600
C	-1.57144400	3.51869500	-0.93314800
C	-0.49900700	4.39434000	-0.90399600
C	1.63695900	-0.46402700	-0.48699800
C	1.90924600	-0.97565500	-1.75696200
C	2.78387500	-0.38394600	0.30603100
C	3.16417500	-1.40728300	-2.17953700
C	4.04852900	-0.80806300	-0.06038000
C	4.24750600	-1.32982900	-1.32770000
F	-3.83578800	-3.25018300	-2.84365700
F	-2.93035600	-4.04299900	-0.38722500

F	-1.14731300	-2.63369800	0.90544300
F	-1.06990300	0.49074800	-2.66261500
F	-2.85403700	-0.94990100	-3.93652200
F	-2.49142900	1.43392800	-0.65400100
F	-2.78822800	3.96740700	-1.24504400
F	-0.66702100	5.68284100	-1.18558300
F	1.79308500	4.72683500	-0.48603700
F	2.71705300	0.13377200	1.55347900
F	5.07036500	-0.70463400	0.79236200
F	5.45356400	-1.73912100	-1.71325100
F	3.32077600	-1.89098300	-3.41369700
F	0.96103600	-1.09105300	-2.69786300
C	0.86457500	-1.27763000	2.38707200
O	1.24241900	-2.28075200	1.84538100
O	1.17039500	-0.91090100	3.62462100
C	2.12441500	-1.75863500	4.29018400
H	2.29450600	-1.29936800	5.26144500
H	1.71562600	-2.76382300	4.40500100
H	3.04922800	-1.79389500	3.71066600
C	-0.08274600	-0.27046500	1.70185900
C	-1.41661300	-0.21541800	2.37599800
C	-1.82575100	-1.28306100	3.19117900
C	-2.27362000	0.88149000	2.21214200
C	-3.08713200	-1.27726800	3.77260800
H	-1.18054000	-2.14120400	3.35023000
C	-3.52079900	0.89593600	2.82072700
H	-1.94225100	1.75336500	1.66177200
C	-3.93743600	-0.19020200	3.58851500
H	-3.39703900	-2.11999300	4.38098400
H	-4.16583200	1.75939200	2.69797100
H	-4.91695700	-0.18123400	4.05581800
N	0.64955600	1.24869600	2.42741400
N	0.95863800	2.20403000	2.86786400
F	2.12799100	2.20637800	0.13997100

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B	0.09470200	0.01919300	0.08559800
C	-1.06480700	-1.06780300	-0.39354000
C	-1.55824600	-2.03609300	0.47513800
C	-1.58538100	-1.15156800	-1.68565300
C	-2.53639500	-2.96451500	0.13963700
C	-2.56493000	-2.05456400	-2.06468500
C	-3.05298800	-2.96839500	-1.14234000
C	-0.06176300	1.51504000	-0.66378200

C	1.01121000	2.41158900	-0.70833600
C	-1.19286600	2.01940900	-1.32039900
C	0.99542300	3.64684100	-1.34435100
C	-1.25625600	3.24833200	-1.96329500
C	-0.15052300	4.07810500	-1.98249100
C	1.60144600	-0.65599900	-0.23312800
C	1.80664300	-1.55770100	-1.28629900
C	2.78935200	-0.40982800	0.46642600
C	3.01623100	-2.17857700	-1.58159500
C	4.01539800	-1.00672000	0.21329400
C	4.13899400	-1.90923700	-0.82568700
F	-3.98911300	-3.84705000	-1.49368400
F	-2.96309000	-3.85428500	1.03873700
F	-1.08527000	-2.12377400	1.73153800
F	-1.11690000	-0.36478600	-2.66333900
F	-3.02872800	-2.06689300	-3.31693600
F	-2.35674900	1.34240900	-1.38126000
F	-2.38539500	3.63033100	-2.56236000
F	-0.19335300	5.25909600	-2.59139300
F	2.08267700	4.42007400	-1.32937900
F	2.83473400	0.46567500	1.48446500
F	5.07538100	-0.70114400	0.96609600
F	5.30407900	-2.49199200	-1.09511900
F	3.09242800	-3.03135000	-2.60630500
F	0.82897700	-1.90364700	-2.13593300
C	0.86293000	-0.09975300	2.75031700
O	1.22645600	-1.23570300	2.91944300
O	1.27853400	0.96332300	3.42625400
C	2.34446900	0.71191300	4.35985800
H	2.65325800	1.69041700	4.72164600
H	1.98224700	0.09466100	5.18467800
H	3.16904000	0.20856000	3.85337700
C	-0.19805500	0.25020700	1.73421600
C	-1.41543700	0.64712100	2.33992700
C	-1.56173600	0.67429200	3.76489900
C	-2.56125300	0.96295600	1.55602000
C	-2.76171700	1.02065500	4.34737000
H	-0.73352900	0.41076600	4.41054500
C	-3.75412400	1.32169500	2.14663200
H	-2.50556200	0.90539300	0.48249000
C	-3.85481600	1.35473800	3.54107500
H	-2.85829900	1.03052700	5.42674700
H	-4.61272700	1.56655200	1.53203200
H	-4.79692500	1.63132600	4.00523400

F	2.17635000	2.12644900	-0.11687400
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**In(OTf)<sub>3</sub>**

In	0.00532900	-0.03010000	-0.29489900
S	-2.33047800	-1.50238500	-0.25321200
O	-2.76614400	-2.81167400	-0.65295900
O	-1.81028100	-0.56350600	-1.32717700
S	2.47305400	-1.27119200	-0.32743900
O	1.87170600	-0.36665200	0.73316200
O	3.79723200	-0.97037700	-0.79676700
S	-0.16138000	2.72801400	-0.26516800
O	-1.11421800	3.72076000	-0.67957500
O	0.42525500	1.81749400	-1.32862000
C	1.30210600	3.58247900	0.45645100
C	-3.76102900	-0.59449400	0.47062500
C	2.48359200	-2.94079200	0.45202700
F	-4.20275600	-1.26313200	1.51601000
F	-3.34175500	0.60418900	0.83285200
F	-4.70192800	-0.49580400	-0.44665200
F	1.82713500	4.36278100	-0.46633000
F	0.90576700	4.29232700	1.49338800
F	2.17154400	2.66286100	0.83180400
F	2.84413100	-3.82582500	-0.45444000
F	1.26262600	-3.19593500	0.88516300
F	3.33583100	-2.93194000	1.45658400
O	-1.24349700	-1.40750100	0.80208300
O	-0.58899200	1.73547000	0.79962600
O	1.35369200	-1.34373900	-1.35028300

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C	-0.76059600	0.74563700	0.00031000
C	1.72336300	0.58687300	0.00033300
H	-0.70679100	1.83409900	0.00022100
C	-2.12264200	0.19678300	0.00027800
C	-3.20413900	1.08869000	-0.00252900
C	-2.39976600	-1.17964700	0.00296800
C	-4.51693400	0.62792100	-0.00287500
H	-3.00734900	2.15749500	-0.00452100
C	-3.71016200	-1.63983200	0.00259100
H	-1.58722700	-1.89959200	0.00560700
C	-4.77648600	-0.73983200	-0.00036100
H	-5.33709200	1.33886500	-0.00514300
H	-3.90214000	-2.70817100	0.00472000
H	-5.79859900	-1.10389300	-0.00060400

C	2.98198400	-0.16038100	-0.00029100
O	4.08454800	0.34812400	-0.00000900
O	2.76000100	-1.48021700	-0.00119700
C	3.94087600	-2.29042800	-0.00171100
H	4.53749500	-2.08667900	-0.89235100
H	4.53867000	-2.08612400	0.88799900
H	3.59110700	-3.32019200	-0.00119300
N	1.89389300	1.89460200	0.00119200
N	2.01155000	3.01343700	0.00193600
C	0.37861700	0.03500000	0.00015800
H	0.37275000	-1.05004700	-0.00020400

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C	0.73336800	0.44226000	-0.56552200
C	-1.66832000	0.44950000	-0.48703600
H	0.61417200	1.20136300	-1.33799400
C	2.10513700	0.08429300	-0.22203000
C	3.14479300	0.56265000	-1.03334400
C	2.42198000	-0.72748500	0.88012700
C	4.46603300	0.22309700	-0.76725400
H	2.90494100	1.19768400	-1.88150100
C	3.74192600	-1.06317000	1.14609600
H	1.63580300	-1.08222800	1.53831500
C	4.76568900	-0.59180300	0.32244300
H	5.26031300	0.59502500	-1.40557800
H	3.97833800	-1.68711600	2.00146600
H	5.79673500	-0.85401100	0.53661800
C	-2.89870300	-0.20834300	-0.03804700
O	-3.88609300	0.27510200	0.48059300
O	-2.83638500	-1.49796500	-0.44306100
C	-4.04940400	-2.23893000	-0.28874200
H	-4.31800000	-2.31382600	0.76675100
H	-4.86443100	-1.75516800	-0.83034700
H	-3.84958900	-3.22556700	-0.70218800
N	-1.94253900	2.11887000	0.47214600
N	-1.93923600	3.22044000	0.50098900
C	-0.40456100	-0.06626400	-0.03163700
H	-0.35365400	-0.86326400	0.71193000

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C	-0.53728300	-0.86103200	0.05467800
C	1.81462400	-0.96063400	0.16557400
H	-0.44043400	-1.92446800	-0.15998700
C	-1.87219100	-0.31184600	-0.00487100

C	-2.93862900	-1.19045200	-0.26660000
C	-2.14218700	1.05507900	0.20063900
C	-4.24411100	-0.72141400	-0.31071400
H	-2.72942300	-2.24357500	-0.43071800
C	-3.44668600	1.51942800	0.15530800
H	-1.33033600	1.74912600	0.38917100
C	-4.49689700	0.63306000	-0.09903000
H	-5.06176300	-1.40496900	-0.51053600
H	-3.65226000	2.57224300	0.31412000
H	-5.51613300	1.00385200	-0.13548600
C	3.07107500	-0.24543800	0.30115900
O	3.63086400	-0.09117600	1.37450200
O	3.60519800	0.12222400	-0.87804100
C	4.90499300	0.71473300	-0.79729300
H	4.87722700	1.62442500	-0.19453300
H	5.61703700	0.01508500	-0.35560500
H	5.18798900	0.94802900	-1.82186400
C	0.64255900	-0.20545400	0.32626700
H	0.62800200	0.85569700	0.58303800

### 37

In	-0.79963100	-0.10921700	-0.22225600
S	-0.34206600	2.61308100	0.54031900
O	0.52019900	3.68508000	0.09712000
O	0.32471500	1.33954800	1.00277900
S	0.14970600	-2.73184900	0.18796200
O	-0.87635200	-2.26687600	-0.80693100
O	-0.20967800	-3.79851700	1.08727700
S	-3.54658300	-0.24441400	0.26833600
O	-4.55880400	0.73907200	0.55943000
O	-2.37707100	-0.33329300	1.23358300
C	-4.34642800	-1.89988300	0.36541900
C	-1.26831600	3.23122800	2.00185200
C	1.57607200	-3.31336100	-0.81239400
F	-1.98376300	4.27844800	1.63250300
F	-2.05985300	2.27151800	2.44318400
F	-0.40506600	3.57720900	2.93899100
F	-5.02168900	-1.97920600	1.49758000
F	-5.16604400	-2.02697800	-0.66314600
F	-3.41832100	-2.83633500	0.32387400
F	1.96496400	-2.32771700	-1.60914100
F	1.21107700	-4.35704500	-1.53093300
F	2.56071400	-3.64038100	0.00636700
O	-1.39170900	2.12066000	-0.41436400

O	-2.88148100	-0.20873800	-1.07739900
O	0.64265700	-1.43717400	0.79328800
C	3.97807300	1.15850600	-0.28982000
C	2.03908100	1.68610600	-1.77582900
H	4.42897800	2.13627700	-0.45492400
C	4.73054800	0.24176300	0.57834900
C	6.07878900	0.50916100	0.84638200
C	4.14708800	-0.90403500	1.14011800
C	6.83427500	-0.35776200	1.63027300
H	6.53735700	1.40036700	0.42670000
C	4.90380100	-1.77174000	1.91723800
H	3.08993200	-1.10529900	0.99096200
C	6.25128100	-1.50469600	2.16307200
H	7.87893300	-0.13693600	1.82438200
H	4.43728600	-2.65514400	2.34185600
H	6.83885700	-2.18136100	2.77478300
C	0.78239700	1.31169500	-2.31869200
O	0.22775000	0.21862600	-1.98930200
O	0.22972800	2.13401500	-3.16820800
C	-1.08905200	1.80144900	-3.65824700
H	-1.06367900	0.82592800	-4.14273800
H	-1.79482000	1.80262100	-2.82698800
H	-1.32661700	2.58655600	-4.37025900
N	2.43917800	2.92917700	-2.05577700
N	2.78788500	3.97159500	-2.24670400
C	2.82571000	0.83793900	-0.89164800
H	2.39161400	-0.14894700	-0.76984700

**38-ts**

In	0.67902200	-0.10849400	0.25903800
S	-0.12083000	2.61403700	0.56422600
O	-1.20189100	3.31921500	1.21306700
O	-0.49683600	1.61794900	-0.50265700
S	-0.01378500	-2.42624300	-1.22888300
O	1.15422300	-2.26684200	-0.30798000
O	0.21535200	-2.96717600	-2.54538500
S	3.40468300	0.38403600	-0.19043800
O	4.22871000	1.55302400	-0.00203400
O	2.22239300	0.52174300	-1.13040600
C	4.46952200	-0.88562500	-0.98681600
C	0.88409500	3.88734900	-0.29787800
C	-1.15694600	-3.58017300	-0.36969500
F	1.28565600	4.77868100	0.59217800
F	1.92853200	3.31644100	-0.86777900

F	0.13132600	4.47252900	-1.21438100
F	4.88665100	-0.41030000	-2.14841900
F	5.50345100	-1.12107500	-0.19681600
F	3.78120700	-1.99385500	-1.17376000
F	-1.31554400	-3.18626500	0.88713200
F	-0.65818000	-4.80075600	-0.39705600
F	-2.33220700	-3.55623600	-0.98432100
O	0.85313100	1.85634200	1.41791600
O	2.81033300	-0.26865900	1.02072000
O	-0.72448000	-1.09742700	-1.13328400
C	-3.23410300	0.78730200	0.16124600
C	-2.14669700	-0.02453800	2.11684900
H	-3.08398500	1.77107900	0.60449300
C	-3.80995100	0.76254800	-1.16553100
C	-4.22354900	1.98191700	-1.72720000
C	-3.94653200	-0.42219700	-1.91218000
C	-4.78236700	2.01844700	-2.99758900
H	-4.10275300	2.89734100	-1.15487200
C	-4.49958900	-0.38073600	-3.18213600
H	-3.59954000	-1.36662800	-1.50768300
C	-4.92168600	0.83667200	-3.72322100
H	-5.10449500	2.96212000	-3.42375100
H	-4.59866900	-1.29401600	-3.75847100
H	-5.35379000	0.86238500	-4.71841500
C	-1.08807800	-0.73475000	2.69150100
O	-0.01828600	-0.91114500	2.01400400
O	-1.11211200	-1.11147000	3.94984900
C	0.13316200	-1.55862300	4.52007500
H	0.47211000	-2.46041900	4.01037300
H	0.88668900	-0.77540700	4.43450500
H	-0.09443000	-1.76620400	5.56238500
N	-3.41538100	-0.03021000	3.54827100
N	-4.22846600	0.42398500	4.13421500
C	-2.82474500	-0.28356700	0.90527600
H	-2.96489400	-1.30080700	0.54501600

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In	0.82760400	-0.14326500	0.16903500
S	-0.83898200	2.18719400	-0.09239800
O	-2.15864300	2.64153500	0.28890300
O	-0.75829400	0.94027800	-0.93856200
S	1.46018700	-2.59166300	-1.09747400
O	2.08700300	-2.02232100	0.13992900
O	2.32859200	-3.04830700	-2.15529500

S	3.26516800	1.25652100	0.17417700
O	3.59692900	2.65424600	0.30838800
O	2.35646400	0.87555500	-0.97883600
C	4.83771200	0.37424200	-0.18613800
C	-0.15917000	3.53568200	-1.14017100
C	0.50545900	-4.04691400	-0.51358100
F	-0.14909200	4.65111200	-0.42859500
F	1.06678400	3.23786600	-1.52628300
F	-0.94090400	3.68432600	-2.19751800
F	5.41881400	0.95791700	-1.22107300
F	5.61888800	0.45950000	0.87770400
F	4.58894100	-0.89075000	-0.46492900
F	-0.29958000	-3.67014600	0.46507100
F	1.34511900	-4.97006700	-0.07660800
F	-0.20616400	-4.52486400	-1.52105500
O	0.18940000	1.96195500	0.97304900
O	2.65882300	0.55391700	1.34942400
O	0.40148100	-1.57841300	-1.45547800
C	-4.33086200	0.18043600	0.52958800
C	-2.36790600	-0.24977900	1.75037200
H	-3.80425200	1.07726700	0.20297300
C	-5.63679500	-0.03344800	0.01628300
C	-6.15037700	0.91733300	-0.89632100
C	-6.42445100	-1.15411500	0.37458200
C	-7.41291300	0.75214400	-1.43869300
H	-5.54026500	1.77397700	-1.16597800
C	-7.68420000	-1.31011900	-0.16977200
H	-6.04408900	-1.88937800	1.07457100
C	-8.17487100	-0.36017900	-1.07466600
H	-7.80751400	1.47753700	-2.14029400
H	-8.29204000	-2.16569400	0.10007000
H	-9.16445300	-0.49167900	-1.50031900
C	-1.17198100	-0.43237000	2.34729400
O	-0.17772400	-0.98378600	1.70813000
O	-0.98206200	0.05086700	3.57291700
C	0.37921800	0.32958100	3.94413700
H	0.97649200	-0.58234700	3.92746100
H	0.81219000	1.07325000	3.27083100
H	0.31908000	0.72693900	4.95488100
C	-3.61785000	-0.64123800	1.41955600
H	-4.05677600	-1.55848500	1.80841300
<b>40</b>			
In	0.46476500	0.14047800	0.07884600

S	0.29987700	3.00320000	0.13201600
O	-0.62735200	3.96728100	0.67279200
O	-0.25474200	2.01348000	-0.86718900
S	-0.17385400	-2.11533100	-1.50723400
O	0.54277500	-2.10877800	-0.18558500
O	0.50586700	-2.70841300	-2.63258100
S	3.27241900	0.01819000	0.01975300
O	4.30186200	1.00195300	0.24858000
O	2.28457300	0.30263700	-1.09496100
C	4.11755300	-1.52537200	-0.51370400
C	1.58720100	3.93755100	-0.79244300
C	-1.70741300	-3.10234200	-1.22742800
F	2.10318100	4.85087700	0.01022700
F	2.52662700	3.10432900	-1.19524000
F	1.01575500	4.51784500	-1.83299000
F	4.86671800	-1.25251600	-1.56804300
F	4.87602400	-1.95336800	0.48208200
F	3.22018400	-2.44113300	-0.82224300
F	-2.55721000	-2.40528700	-0.49636400
F	-1.37727200	-4.21911900	-0.60405100
F	-2.24791500	-3.38207400	-2.40021500
O	1.04778000	2.13378600	1.10114500
O	2.39774300	-0.37695200	1.17269800
O	-0.63963000	-0.68600300	-1.65125000
C	-2.98001200	0.69163300	0.50812500
C	-1.05683300	-0.27631500	1.78791400
H	-2.29354400	1.35900100	-0.01097500
C	-4.38386900	0.80959300	0.09423900
C	-4.66872200	1.50875400	-1.08533100
C	-5.43992100	0.24163400	0.82044300
C	-5.97700200	1.61977800	-1.54464000
H	-3.85405300	1.95955400	-1.64569700
C	-6.74599600	0.35559200	0.36212300
H	-5.24429200	-0.27590400	1.75425900
C	-7.01770100	1.04105300	-0.82271900
H	-6.18351400	2.15896900	-2.46303500
H	-7.55669900	-0.08589700	0.93225200
H	-8.03964300	1.12886500	-1.17667200
C	-0.65635700	-1.67542100	2.26332200
O	-1.32706800	-2.64307400	2.02942000
O	0.51588700	-1.64526100	2.87262000
C	1.09446100	-2.92817900	3.17607800
H	0.43942100	-3.48188400	3.84892200
H	1.23543700	-3.48062900	2.24575000

H	2.04854100	-2.71051000	3.64829600
N	-0.72811700	0.64300400	2.81806900
N	-0.45880100	1.41395000	3.56010200
C	-2.50862000	-0.17084800	1.41533600
H	-3.14876300	-0.89451000	1.91185800

**41-ts**

In	0.39536200	0.10890600	-0.10123000
S	-0.86760200	2.70005500	-0.20696300
O	-2.19564200	3.18969900	0.08569600
O	-0.78399200	1.59113000	-1.23276300
S	0.97185500	-2.16018300	-1.72664300
O	1.37616100	-1.97013700	-0.29500100
O	1.98829400	-2.54057300	-2.67648000
S	2.95267900	1.11907800	0.51772800
O	3.41591500	2.42422100	0.92182100
O	2.22300700	1.03122900	-0.80838400
C	4.44655000	0.07783600	0.27293500
C	0.07946100	4.09325500	-0.94250100
C	-0.28575000	-3.50502500	-1.68521700
F	0.08904900	5.09567100	-0.08113100
F	1.31282200	3.69859400	-1.19337200
F	-0.51600900	4.46354200	-2.06276000
F	5.23581000	0.67266800	-0.60508700
F	5.07044400	-0.04207000	1.43332800
F	4.09088700	-1.11192300	-0.17347200
F	-1.39500000	-3.02988100	-1.14198600
F	0.18184200	-4.50657600	-0.96182700
F	-0.52906100	-3.91027800	-2.91868900
O	-0.03249000	2.20158700	0.92905900
O	2.07616300	0.34858900	1.45600800
O	0.16178200	-0.92211200	-2.03270000
C	-3.08568100	-0.14992500	0.51820700
C	-0.93918900	-0.88975100	1.43099000
H	-2.53563200	0.47890700	-0.17903000
C	-4.53111400	-0.09161000	0.35604000
C	-5.04380900	0.82797400	-0.57170500
C	-5.41778300	-0.90201500	1.08384000
C	-6.41484400	0.94089700	-0.76753200
H	-4.35639100	1.45809700	-1.12973800
C	-6.78522500	-0.78990200	0.88232900
H	-5.03974900	-1.62458900	1.79940100
C	-7.28528500	0.13111700	-0.04186400
H	-6.80349300	1.65587700	-1.48420900

H	-7.46632800	-1.42022300	1.44367900
H	-8.35638400	0.21394800	-0.19482700
C	-0.31404400	-2.20869300	1.85583300
O	-0.81645900	-3.25307000	1.52631900
O	0.83034600	-2.05954400	2.49771400
C	1.58747000	-3.26753200	2.68512600
H	1.04212800	-3.95135800	3.33642600
H	1.76121000	-3.73046300	1.71244700
H	2.52232400	-2.95538800	3.14337900
N	-0.49109900	0.10584600	2.81153300
N	-0.32088900	0.89894300	3.55115000
C	-2.39138400	-0.89610700	1.40621000
H	-2.89539200	-1.55689700	2.10655100

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In	0.48694600	0.01725000	0.34077800
S	0.25572600	2.87685400	0.01147600
O	-0.65020300	3.88147900	0.52347400
O	-0.32511900	1.81730000	-0.87492500
S	-0.16171900	-2.35971500	-1.14331500
O	0.57452100	-2.24254000	0.16042300
O	0.46561800	-3.11751300	-2.20016700
S	3.27098100	-0.04759300	-0.11753200
O	4.30091100	0.96408200	-0.10524900
O	2.13877500	0.12768600	-1.10280000
C	4.08432100	-1.61191800	-0.63753800
C	1.47434900	3.76639900	-1.03446400
C	-1.70389900	-3.25228700	-0.70864000
F	2.04466600	4.71416400	-0.30712700
F	2.39290600	2.92345700	-1.46961600
F	0.84098600	4.31056300	-2.06241100
F	4.76489600	-1.38661200	-1.74963600
F	4.90857900	-1.99940100	0.32308800
F	3.17298900	-2.54266000	-0.85015700
F	-2.36273800	-2.56219200	0.21607400
F	-1.40061100	-4.44843500	-0.23520700
F	-2.45836300	-3.37225700	-1.78841200
O	1.08807800	2.12764600	1.01201700
O	2.57325100	-0.36249900	1.17054200
O	-0.61309600	-0.96482100	-1.45117900
C	-3.03981900	0.44674700	0.19146600
C	-1.21632700	0.01149400	1.69386000
H	-2.29935700	0.49840100	-0.60630900
C	-4.38439800	0.58794800	-0.18835400

C	-4.66106700	0.76905100	-1.57080300
C	-5.45810700	0.54636400	0.74358300
C	-5.96410700	0.90395000	-2.00607700
H	-3.83357400	0.79708100	-2.27326600
C	-6.75445300	0.68305500	0.29717800
H	-5.26112400	0.40930600	1.80034100
C	-7.00416000	0.86039900	-1.07198800
H	-6.18142300	1.04179200	-3.05832500
H	-7.58041000	0.65329300	0.99765800
H	-8.02908700	0.96562000	-1.41345700
C	-0.79312500	-0.27250600	3.10855700
O	-1.49921100	-0.31192200	4.08630100
O	0.52718900	-0.48121300	3.10955700
C	1.13923000	-0.77134800	4.37302700
H	0.96203900	0.05272600	5.06546500
H	0.72070300	-1.69307200	4.78003500
H	2.19981100	-0.88379200	4.16304900
C	-2.54421600	0.22860800	1.50440700
H	-3.21858100	0.19380600	2.35802200
N <sub>2</sub> (DCE)			
N	0.00000000	0.00000000	0.54929200
N	0.00000000	0.00000000	-0.54929200