Supplementary Material for

Mechanism and Reactivity in the Morita-Baylis-Hillman Reaction: The Challenge of Accurate Computations

Zhen Liu,[ac] Chandan Patel,[b] Jeremy N. Harvey,*[a] and Raghavan B. Sunoj*[b]

[a] Department of Chemistry, KU Leuven, Celestijnenlaan 200F, Leuven B-3001, Belgium

[b] Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai, 400076, India

[c] State Key Laboratory of Chemical Engineering, East China University of Science and Technology, Meilong Road 130, Shanghai 200237, China

Contents

In this supplementary material, we provide additional detailed information concerning the evaluation of the relative free energy using the following equation (equation 1 in the main text).

$$\Delta G_A = \Delta E^{elec} + \Delta E^{thermal} - T\Delta S + \Delta G^{solv}$$

where ΔG is the free energy change relative to the separated reactants for species A; ΔE^{elec} is the total electronic energy change in vacuum; $\Delta E^{thermal}$ is the total internal thermal energy change including the contributions due to translation, rotational, and vibrational motions; ΔS is the total solute entropy change; and ΔG^{solv} is the solvation free energy change in a specific solvent.

All possible diastereomers have been considered. The centers are referred to using the S or R terminology for the chiral centers positioned adjacent to the ester group, on the carbon atom corresponding to the first aldehyde carbonyl carbon, and the C atom of the second aldehyde, in that order. Stereocenters of species 6 are graphically shown in Figure S1 as an example. In all cases the first chiral center was chosen to have S stereochemistry, so we have carried out calculations on species with *S* configurations (**3**, **11**, **TS1**), *SS* or *SR* (**5**, **10**, **TS2**, **TS7**, **TS8**), or *SSS*, *SSR*, *SRS* or *SRR* configurations (**6**, **7**, **TS3**, **TS4**).

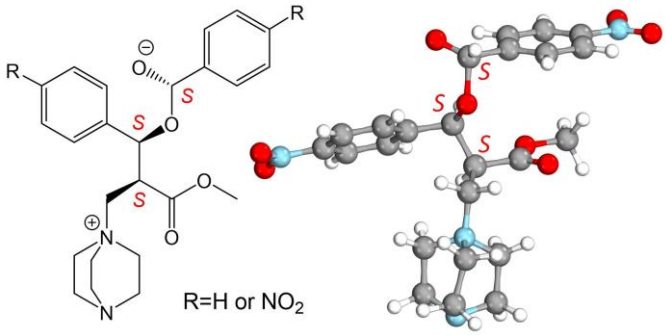

Figure S1. Stereocenters of species **6** as an example.

Efforts have been made to achieve 1) a good accuracy of the electronic energies for the structures being selected; 2) an analysis of the thermal energy contributions; 3) the evaluation of the solvation free energies using the SMD solvation model and the COSMO-RS model, as well as the computationally expensive free energy perturbation (FEP) method. At the end of this Supporting Material, the Cartesian coordinates for all the complexes are included.

S1. Computational Details

For all systems considered here, the different stationary points have initially been subjected to an exhaustive conformational search using the Tinker program[1] package together with the MMFF forcefield. The structure of *all* resulting conformers was then re-optimized with the Gaussian 09 program[2] using the B3LYP functional together with the def2-SVP basis set, the –D3 dispersion correction with Becke-Johnson damping, and the SMD continuum solvent model with parameters for THF or methanol as appropriate, followed by frequency calculations at the same level of theory. Gas-phase single-point energy calculations at these optimized structures were performed using B3LYP-D3(BJ) and the larger def2-TVZP basis set. Combining the gas-phase def2-SVP and def2-TZVP electronic energies, the SMD-corrected def2-SVP energy, and the free-energy correction yields an estimate of the solution-phase free energies that was used to rank the conformers and to select low-lying structures (within 3 kcal/mol of the lowest-free-energy structure) for

more refined calculations. At least one member of each diastereoisomeric variant was retained for all species, even if the lowest free-energy structure for a given diastereoisomer lay higher than the cut-off of 3 kcal/mol.

The selected structures were re-optimized using B3LYP-D3, SMD, and the 6-31+G(d,p) basis set including diffuse functions, thereby giving a somewhat better description of species with partial negative charges. The –D3 dispersion correction rather than the more sophisticated D3(BJ) correction was chosen for backwards compatibility with the work in ref. 3; results from the two D3 variants are however in any case rather close to one another. Frequencies were computed at the optimized structures at the same level of theory. Free energy corrections were obtained using the quasi-harmonic approximation[4-5] with a frequency magnitude cut-off of 20 cm^{-1}. Tests were performed using raw frequencies (with any spurious imaginary frequencies converted to real frequencies of same magnitude), quasi-harmonic frequency analysis[4] with a cut-off of 50 cm^{-1} or 100 cm^{-1}, or Grimme's quasi-harmonic approach.[5] The values obtained from the raw frequencies or with the 20 cm^{-1} cut-off are very similar, while values with the larger cut-offs, or the Grimme approach, yielded lower vibrational partition functions hence higher relative free energies (by up to 4 kcal/mol) for the larger species. The translational part of the partition functions was modified with respect to the standard Gaussian 09 output to reflect the correct standard state, of 1 M for all solutes or 24.9 M for methanol solvent. Gas-phase single-point energies were also obtained using the B3LYP-D3, M06-D3, and M06-2X-D3 functionals with the large triple-*zeta* basis set 6-311++G(3df,3pd).

Local correlation methods were employed to calculate CCSD(T) *ab initio* energies for all the molecular systems studied here, some of which contain as many as 64 atoms. For a set of small molecules, canonical CCSD(T)-F12 energies were computed as a reference to benchmark the accuracy of the local coupled cluster methods. Two local methods were used: the domain-based explicitly correlated local coupled-cluster method (LCCSD(T)-F12) developed by Werner and co-workers[6-8], and the domain-based local pair natural orbital correlation methods (DLPNO-CCSD(T)) by Neese and co-workers.[9-12] The computations using the explicitly correlated DF-LMP2-F12, DF-MP2-F12, DF-LCCSD(T)-F12 and CCSD(T)-F12 methods were performed with the Molpro program[13] and a combination of the cc-pVDZ-F12 basis set for the orbitals, the def2-QZVPP basis set for the density fitting, and the def2-TZVPP basis set as the complementary auxiliary basis set. Pipek-Mezey localization and the default criteria were adopted for the local coupled-cluster calculations. Tests show that almost no change in the results was observed upon increase the default weak and distant pair selection criteria (RCLOSE=3; RWEAK=5; RDIST=8; RVDIST=15). For the DLPNO-MP2 and DLPNO-CCSD(T) calculations, the default settings in ORCA program[14] were employed with TCutPNO=3.33×10^{-7}, TCutPairs=1×10^{-4}, and TCutMKN=1×10^{-3}, which set the cutoff for PNO occupation numbers, the cut-off for pair correlation energies, and controls the domain size for the local fit to the PNOs, respectively. The complete basis set extrapolation of the DLPNO-MP2 and DLPNO-CCSD(T) calculations was evaluated on the basis of the correlation-consistent polarized double- and triple-*zeta* basis sets cc-pVDZ/cc-pVTZ basis sets using the parameters determined by Truhlar[15], and we refer to the basis set extrapolation at this level as DLPNO-CCSD(T)/CBS1. Where computationally feasible, extrapolation using the augmented basis sets aug-cc-pVDZ/aug-cc-pVTZ was also performed, and the basis set extrapolation at this level was referred to as DLPNO-CCSD(T)/CBS2. Unless we specify otherwise, references simply to 'CCSD(T)' should be taken as referring to the DLPNO-CCSD(T) level of theory. We note that the extrapolated energies with or without augmentation are in good agreement for all neutral and zwitterionic molecular systems, while the augmented basis sets are – unsurprisingly – required to obtain accurate results for the negatively charged methoxide ion. As will be seen in this Supplementary Information, extensive additional calculations at e.g.

the CCSD(T)-F12/AVDZ, LCCSD(T0)-F12/cc-pVDZ-F12, DLPNO-CCSD(T)/CBS, MP2-F12/cc-pVDZ-F12, LMP2-F12/cc-pVDZ-F12, and DLPNO-MP2/CBS levels of theory, indicate that both the CCSD(T)/CBS1 and the CCSD(T)/CBS2 results should be highly accurate.

As mentioned above, the free energies of solvation were first calculated using the SMD continuum solvent model. Additional calculations of this quantity used the conductor-like screening model for realistic solvents (COSMO-RS) as implemented in ADF.[16-18] Moreover, the relative solvation free energies along the reaction pathway leading from a given species, over a transition state, to another local minimum or two separated fragments were also computed using free-energy perturbation methods (FEP).[19-21] The approach used here involved selection of a starting structure, a final structure, and in most cases an intermediate TS structure, which were aligned with one another using the Pymol software.[22] The structures were taken from B3LYP-D3/6-31+G(d,p)(SMD) geometry optimization. In cases where the end-point of a path represented two separate molecular fragments, a 'structure' for this product or reactant pair was obtained by combining the fully optimized B3LYP-D3 structures of the separate species, and placing them with a relative orientation similar to that in the corresponding TS, but with a separation defined by a reaction coordinate for the breaking bond of 10 Å. Additional structures were then generated by linear interpolation using either Cartesian or Z-matrix coordinates so as to obtain a smoothly varying set of structures. The B3LYP-D3/6-31+G(d,p)(SMD) electronic energies were computed for these structures, and it was checked that they also vary smoothly. At each structure, partial charges were computed using the ESP method in Gaussian 09, together with the B3LYP-D3/6-31+G(d,p)(SMD) method. About 1400 structures in total were generated in order to map the whole reactions of MA and *p*NBA in methanol solvents, catalyzed by DABCO. For each structure, a box was then constructed by soaking the solute (structure A) into a rectangular box (x=30 Å, y=35 Å, z=30 Å) filled with 460~480 methanol molecules to reach the density of 0.792 kg dm^{-3} at 298 K. The standard OPLS-AA forcefield was chosen for the molecular dynamics simulation in the framework of periodic boundary conditions. For the solute (structure A), an appropriate atom type from the OPLS-AA forcefield was chosen for each atom, and the corresponding van der Waals radii were then used to describe interactions with solvent. The charges were replaced by the ESP partial charges as computed individually with Gaussian 09 at the B3LYP-D3/6-31+G(d,p)(SMD) level of theory – these were found to be very similar to OPLS-AA partial charges for appropriate similar atom types. For the solvent molecules, both the default charges and van der Waals radii were adopted. Benchmark tests described below show that the interaction energy between the solvents in the first solvent layer and the solute obtained in this way is in good agreement with values obtained with B3LYP-D3. All molecular dynamics (MD) simulations were carried out with the RESPA integrator,[23] Bussi thermostat,[24] and 2 fs time step using the Tinker program.[1] After 100 ps NVT equilibration, 5000 snapshots were selected from a 500 ps production run (i.e. the snapshots had a time interval of 100 fs). At each of these snapshots, the solute structure A was replaced by a perturbed structure B and the potential energy change with appropriate modified parameters was computed. After applying the standard free energy perturbation expression, this yields a solvation free energy change from structure A to structure B. The total free energy change from the reactant to the product can then be obtained by summing up all the energy changes of every sub-step. Numerous tests were performed to ensure accuracy of the obtained values. In particular we will note that both forward and reverse free energies for each reaction were obtained, and agree to within better than 1 kcal/mol in all cases.

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S2. Benchmarks on *ab initio* methods and DFT methods

The MBH reaction proceeds on a single potential energy surface with all species having a closed-shell electronic structure; there is no participation of any transition metal, and no unusual bonding patterns are present in the species involved (bond making and breaking never leads to unpaired electrons). For reactions of this type, it is relatively easy to compute benchmark electronic energies, e.g. based on coupled cluster theory. The CCSD(T) method is widely considered to be highly accurate, and to yield results close to the full CI limit for many systems with straightforward electronic structures. Since no unusual bonding patterns are present in the intermediates and TSs, this should also be true here. To obtain accurate energies, it is however also crucial to use large one-particle basis sets, and indeed to estimate the energies that would be obtained at the infinite basis set limit. Here, we report and discuss the calibration of the local correlated methods against canonical CCSD(T)/cc-pVDZ-F12 energies, together with a comparison of energies obtained with various DFT functionals.

Figure S2 compares relative energies obtained at four levels of theory, in each case based on structures optimized with B3LYP-D3/6-31+G(d,p) including the SMD solvation model with parameters for methanol. The first level of theory is local coupled-cluster CCSD with explicit treatment of correlation with the –F12a ansatz, with approximate perturbative triples (T0 correction), and the cc-pVDZ-F12 basis set. These calculations were performed using MOLPRO 2012. For these calculations, the default procedure was used to select orbital domains for local correlation, and to select strong, close, and weak pairs for correlation. The second method is DLPNO-CCSD(T) with basis set extrapolation using the formula proposed by Truhlar, together with the cc-pVDZ and cc-pVTZ basis sets. This combination is referred to as CBS1. The third method is also DLPNO-CCSD(T), also with Truhlar basis set extrapolation, but with the augmented aug-cc-pVDZ and aug-cc-pVTZ basis sets (CBS2). Finally, the fourth method is standard canonical (i.e. not local) CCSD(T) with –F12a explicit correlation and a combination of the AVDZ basis set for the orbitals, the def2-QZVPP basis set for the density fitting, and the def2-TZVPP basis set as the complementary auxiliary basis set. Due to the high scaling of canonical CCSD(T) with system size, this fourth type of calculation was performed only for a restricted set of smaller molecules.

Figure S3 also compares relative energies at four levels of theory, using the same structures as in Figure S2. Here however, MP2 and LMP2 results are shown. For DLPNO-MP2 results, extrapolation to the infinite basis set limits (CBS1 and CBS2) is also performed using the approach suggested by Truhlar, in this case using the extrapolation coefficients for MP2.

From Figure S2, it can be seen that for the species where canonical CCSD(T)-F12 is available, DLPNO-CCSD(T) agrees very well with it – with roughly similar accuracy for CBS1 and CBS2. For species **3**, it appears that LCCSD(T0)-F12 agrees less well than the DLPNO-CCSD(T) values – the error with respect to canonical CCSD(T)-F12 is 3.1 kcal/mol compared to 1.5 or 1.6 kcal/mol. For larger molecules, where the CCSD(T)-F12 method cannot be applied, we note that large differences exist between DLPNO-CCSD(T)/CBS1 energies and LCCSD(T0)-F12 energies - up to *ca.* 7 kcal/mol in the cases of **5'**, **TS7**, and **10'**. Figure S3 suggests that in these cases, the DLPNO-CCSD(T) results are likely more accurate. With MP2, it is possible to obtain the canonical MP2-F12 results for all species, not just the smaller ones, and this serves as a useful benchmark. The DLPNO-MP2/CBS energies (with both CBS1 and CBS2) are in very good agreement with the MP2-F12 energies in general, with a slightly larger difference in the case of the product species **11**. On the other hand, significant differences are found between LMP2-F12 energies and MP2-F12 energies – the pattern of these errors matches the differences between LCCSD(T0)-F12 and DLPNO-CCSD(T) in Figure S2. Taken together, the benchmark results in Figure S2 and Figure S3 suggest that the DLPNO method is more robust for these

particular systems. No significant improvement was achieved by playing with the pair selection criteria as well as the Pipek-Mezey and the natural orbitals localization methods of LCCSD(T0) as implemented in the Molpro package. It is possible that manual definition of the orbital domains would improve the results, but this was not attempted here.

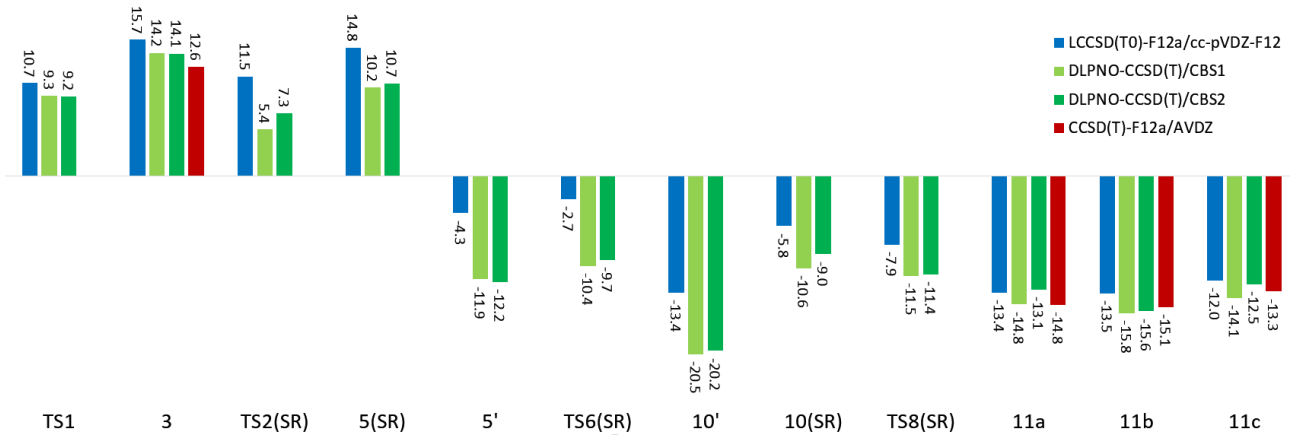

Figure S2. Relative coupled cluster energies (kcal/mol) for various complexes in the MBH reaction of MA with *p*NBA in methanol.

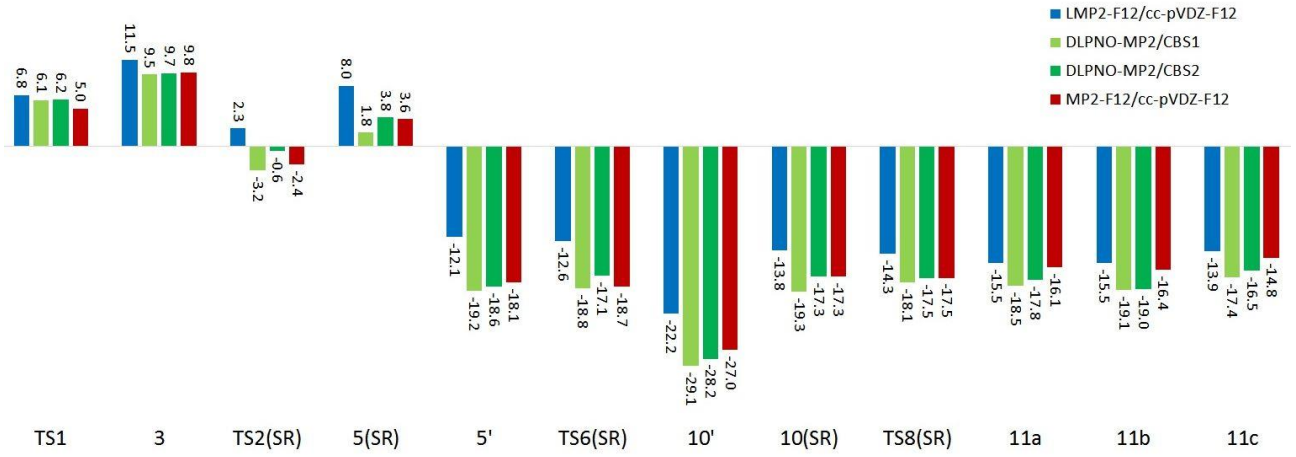

Figure S3. Relative MP2 energies (kcal/mol) for various complexes in the MBH reaction of MA with *p*NBA in methanol.

Three popular DFT functionals including B3LYP, M06, and M06-2X were tested with/without dispersion corrections against DLPNO-CCSD(T)/CBS energies. Figure S4 shows that B3LYP is in very poor agreement with CCSD(T) due to the important effect of dispersion, while M06 and M06-2X show a pretty good performance with a largest energy discrepancy of *ca.* 4 kcal/mol to the reference energies. Without dispersion correction, M06 slightly underestimates the relative energies for most of the intermediates, where M06-2X does the opposite. As shown in Figure S5, upon inclusion of Grimme's empirical dispersion corrections, B3LYP energies are dramatically improved with B3LYP-D3 now lying close to the other DFT methods, whereas no marked improvement is noted between M06 and M06-D3 energies. For M06-2X, the inclusion of Grimme's empirical dispersion correction (-D3) also does not lead to improvement – in this case, the results seem to even deteriorate, perhaps due to error cancellation or over-correction for dispersion effects.

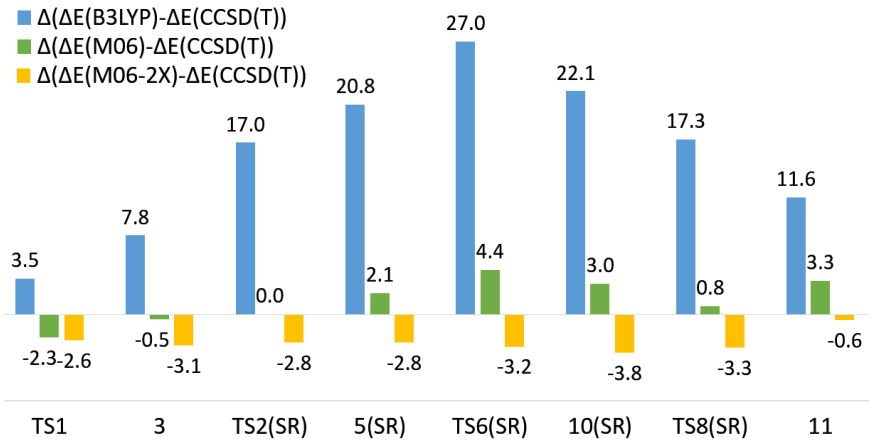

Figure S4. Differences in the relative electronic energy (in vacuum, computed at the B3LYP/6-31+G(d,p)(SMD) structures, kcal/mol) between DFT and CCSD(T) for various complexes in the MBH reaction of MA with *p*NBA in methanol.

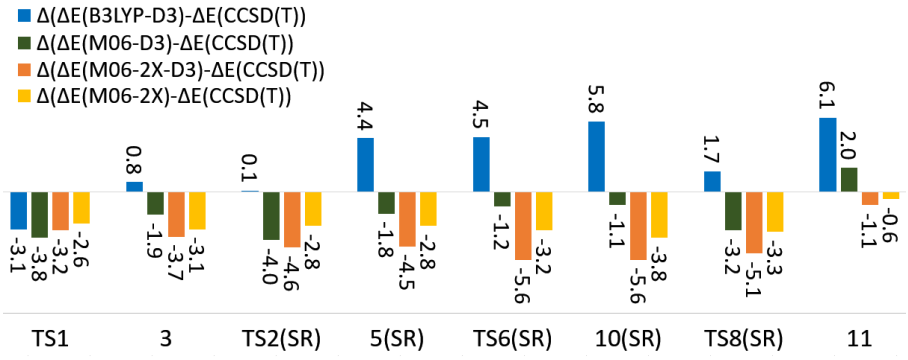

Figure S5. Differences in the relative electronic energy (in vacuum, computed at the B3LYP/6-31+G(d,p)(SMD) structures, kcal/mol) between DFT-D3 and CCSD(T) for various complexes in the MBH reaction of MA with *p*NBA in methanol. M06-2X energies are also included to facilitate comparison with the M06-2X-D3 energies.

Figure S6 summarizes all dispersion-corrected (B3LYP-D3, M06-D3 and M06-2X-D3) functionals together with the original M06-2X functional with a comparison to DLPNO-CCSD(T). It should be noted that in the main paper, none of the energies is obtained based purely on DFT, so the detail of which functional performs best is to some extent irrelevant, but it is included here for reference. Also, we do use structures, vibrational frequencies, and solvation properties derived using DFT.

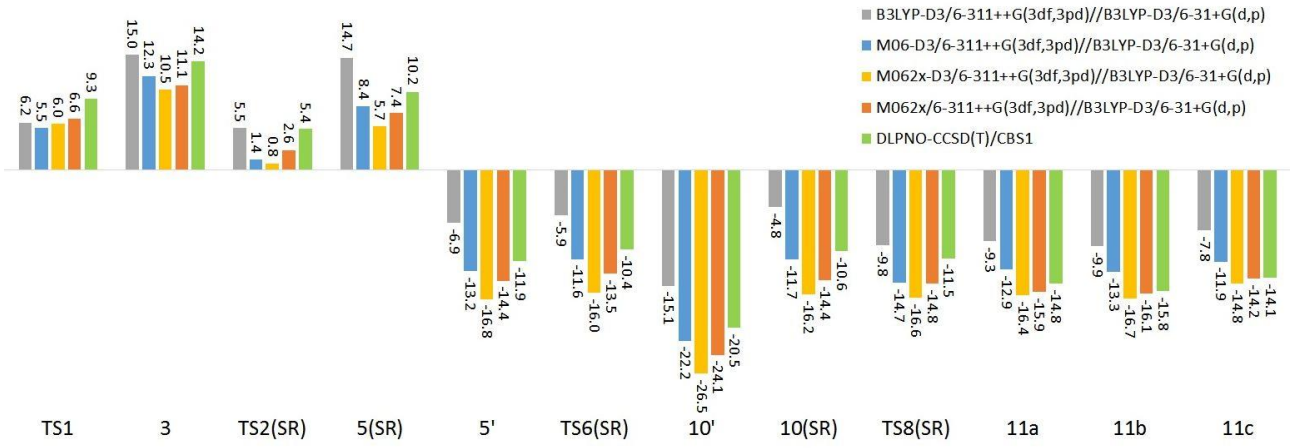

Figure S6. Benchmarks on DFT energies (kcal/mol) for various complexes in the MBH reaction of MA with *p*NBA in methanol.

S3. Thermal energy contributions

The raw frequencies were computed at the same level, after the geometry optimization at B3LYP-D3/6-31+G(d,p)(SMD) level of theory, and used to obtain enthalpic and entropic energy corrections. One problematic aspect here is that for large conformationally flexible species such as those studied here, geometry optimization and frequency analysis typically returns multiple vibrational frequencies with small magnitudes, and in a very limited number of cases, spurious additional imaginary frequencies are obtained. Both of these factors affect the raw entropy as output by the quantum chemistry code quite significantly, and various tests have been performed to check the reliability of the results.

Five procedures have been used. In the first, we use the 'raw' analysis performed by Gaussian (with the exception that if spurious imaginary frequencies are obtained, the analysis is repeated using our own statistical mechanics code, after changing the sign of these frequencies – i.e. we do not discard such frequencies as is the default in Gaussian. Note that very few spurious imaginary frequencies were obtained, and none for any of the compounds reported in the main text). The second, third and fourth analysis use the quasi-harmonic frequency analysis method, together with a frequency cut-off of 20 cm^{-1}, 50 cm^{-1}, or 100 cm^{-1}. In this analysis, standard harmonic oscillator statistical mechanics are used, but frequencies smaller than the threshold are set equal to the threshold value for calculating the zero-point energy and the partition function. The fifth method is Grimme's quasi-harmonic approach. This method in practice is somewhat similar to the method using a 100 cm^{-1} cutoff, since here too, for frequencies smaller in magnitude than 100 cm^{-1}, an adjusted partition function is used.

Figure S7 clearly shows that the values obtained from the raw frequencies or with the 20 cm^{-1} cut-off are very similar, while values with the larger cut-offs, or the Grimme approach, yielded lower vibrational partition functions hence higher relative free energies (by up to 4 kcal/mol) for the larger species (TS4 in Figure S7 as an example). The method with the 100 cm^{-1} cutoff yields slightly different results to the Grimme analysis, in part due to the use of modified frequencies also for calculating the zero-point energy (e.g. for TS4(SSR) in Figure S6, if the original frequencies are used to compute the ZPE, instead of applying the threshold, the free energy becomes 45.6 kcal/mol instead of 46.2 – much closer to the value of 45.2 obtained using the Grimme approach). Note that for all free energy calculations, the translational part of the partition functions was modified with respect to the standard Gaussian 09 output to reflect the correct standard state, of 1 M for all solutes or 24.9 M for methanol solvent.

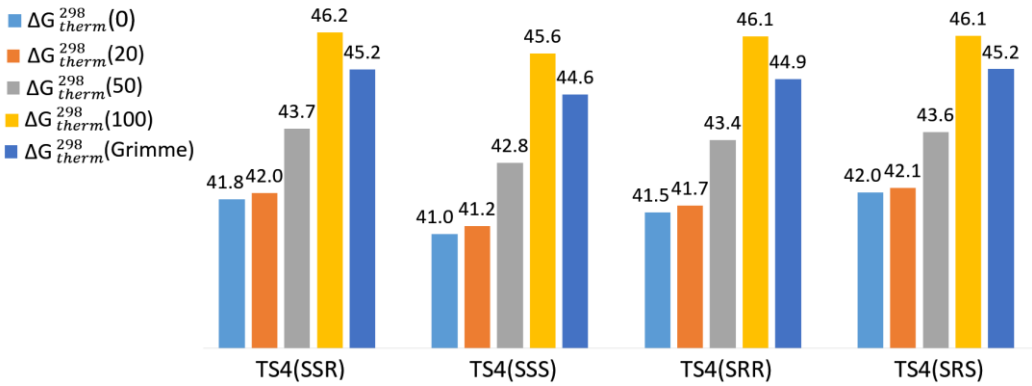

Figure S7. Thermal contributions to the free energies (298 K, 1 M) of TS4 in the MBH reaction of the methyl acrylate with *p*NBA in methanol. $\Delta G_{therm}(0)$, $\Delta G_{therm}(20)$, $\Delta G_{therm}(50)$, and $\Delta G_{therm}(100)$ are the free energy corrections computed by a modified quasi-harmonic method using raw frequencies, frequencies with a cut-off of 20 cm^{-1}, 50 cm^{-1}, and 100 cm^{-1}, in which vibrational frequencies smaller in magnitude than the cut-off value were replaced by frequencies of the cut-off value; ΔG_{therm}(Grimme) is computed, in which the low frequencies below 100 cm^{-1} are modified by Grimme's quasi-harmonic approach.

S4. Solvation free energy

Solvation free energy is of great importance to understand the reactions in condensed phase, especially where the solute interacts with the solvents strongly. The MBH reaction is 'simple' in electronic structure terms as only atoms in the first and second row are present in the molecule, and the bonding in the molecule is straightforward. However, there are several intermediates with zwitterionic character. The separated partial charges may make the computation of the solvation free energies more difficult due to the inaccurate solvent field constructed by the solvation models. To test for errors due to such effects, we performed several tests. First, we studied the neutral complexes **3**, **5** and the separate ionic systems with the positive ions **4**, and **9** together with negative methoxide (Scheme 2 in the main text) through microsolvation with explicit solvents in combination with the SMD solvation model. Second, a complete reaction pathway to the product was explored using the FEP method, and the accuracy and the convergence of the FEP method were tested. The solvation energies obtained with SMD model, COSMO-RS model, and FEP method were also compared.

S4.1 Microsolvation of **3**, **4 + methoxide**, **5**, and **9 + methoxide.**

Figure S8 explains why **3** and **4** have such different solvation free energies. It also explains why the species **3** has a free energy that is slightly modified by explicit solvation, given the presence of a center of very negative electrostatic potential (shown in red) at the position of the formal negative charge on oxygen. The 'solvated' structure of **3** is graphically shown in Figure S9.

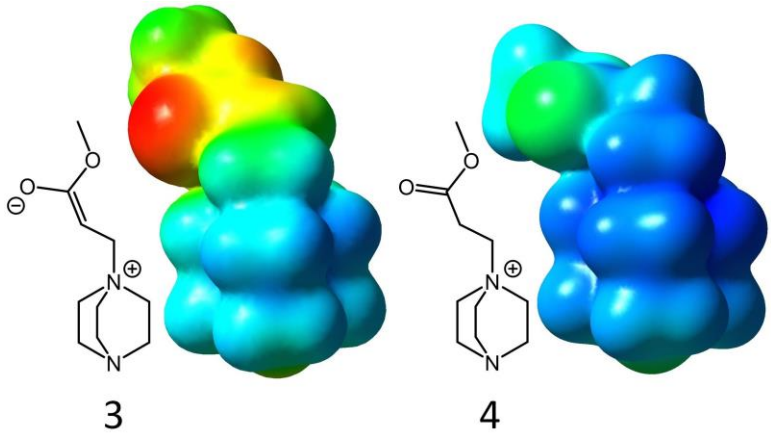

Figure S8. Electron density from total SCF density mapped with ESP (isoval=0.004) for complexes **3** and **4**.

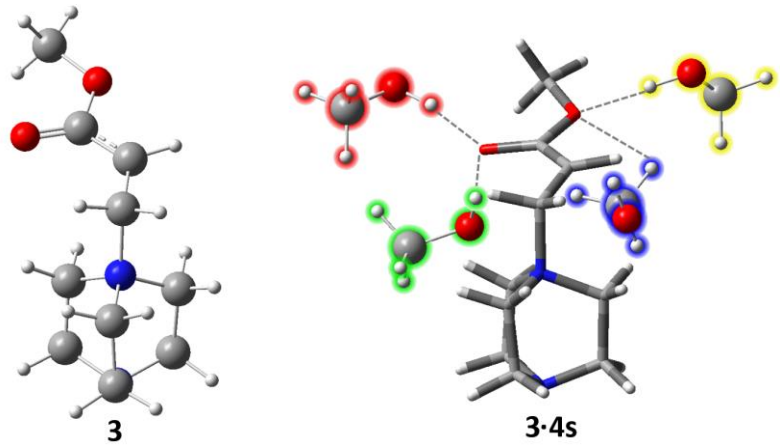

Figure S9. The structure **3** and the solvated complexes **3•4s** (with four explicit methanol molecules as an example).

The electronic energies for the micro-solvated species were computed with the DLPNO-CCSD(T) method with extrapolation to the basis set limit, on the basis of the geometries optimized at B3LYP-D3/6-31+G(d,p)(SMD) level. Table S1 shows the relative free energies obtained for a number of reaction intermediate points **3**, **4 + methoxide**, **5**, and **9 + methoxide**, as well as their micro-solvated variants. As explained in the main text, we use a quasi-variational argument to select free energies for a given species based on computed free energies for different micro-solvated forms: the lowest free energy obtained is used.(Pliego, J. R.; Riveros, J. M., *J. Phys. Chem. A* **2001**, 105, 7241.) For the zwitterionic intermediate **3**, the lowest computed free energy is that of the form without microsolvation, so the predicted relative free energy with respect to reactants remains 12.2 kcal/mol. In contrast, for the zwitterionic intermediate **5**, which has a larger spatial separation between the charged sites, the lowest free energy is obtained with two explicit solvents. For positively charged species **4** and **9**, the lowest free energy occurs when methoxide is surrounded by three explicit solvent molecules (but with no explicit solvent around the cationic species – test calculations, not shown here, indicate no stabilization by such solvation). It should be noted that for the isolated methoxide anion, with its high charge density, it appears that the extrapolation with the un-augmented basis sets (CBS1) is less accurate. For other species, CCSD(T)/CBS1 energies and CCSD(T)/CBS2 match well.

Table S1: Relative free energies (kcal/mol) for various intermediates with explicit solvents, at 298 K.

	$\Delta G_{solv,1}$ (SMD)	$\Delta G_{solv,2}$ (COSMO-RS)	ΔG_{therm}	ΔG_1 CCSD(T) /CBS1	ΔG_2 CCSD(T) /CBS2	Expt.
DABCO+MA	0.0	0.0	0.0	0.0	0.0	
DABCO+MA•1s	1.9	1.8	7.0	2.8	3.2	
DABCO+MA•2s	5.5	4.6	13.4	5.9	6.4	
3	-16.4	-13.7	14.4	12.2	12.1	8.6
3•1s	-7.8	-5.2	21.9	13.3	14.1	
3•2s	-3.2	-0.6	29.6	13.5	14.9	
4+MeO^-	-125.3	-126.9	14.4	22.4	15.8	
4+(MeO^-•1s)	-106.5	-106.6	19.2	14.1	11.5	
4+(MeO^-•2s)	-92.9	-91.8	27.0	11.2	10.8	
4+(MeO^-•3s)	-82.4	-80.5	33.1	8.5	9.0	7.3
4+(MeO^-•4s)	-76.8	-74.7	42.3	8.7	10.2	
5	-32.0	-30.8	30.0	8.7	9.2	
5•1s	-19.6	-17.0	37.4	5.1	6.1	
5•2s	-14.2	-10.2	44.5	3.5	4.2	6.1
5•3s	-14.6	-11.1	52.1	5.8	-	
5•4s	-9.2	-3.3	62.0	11.0	-	
9+MeO^-	-126.0	-129.4	28.9	21.2	15.9	
9+(MeO^-•1s)	-107.1	-109.1	33.7	12.8	11.6	
9+(MeO^-•2s)	-93.6	-94.3	41.5	10.0	10.9	
9+(MeO^-•3s)	-83.1	-83.0	47.6	7.3	9.1	6.8
9+(MeO^-•4s)	-77.5	-77.2	56.8	7.5	10.3	

ΔG_1, and ΔG_2 are the free energies including the electronic energy obtained at CCSD(T)/CBS1 level and CCSD(T)/CBS2 level, respectively, the thermal correction to the Gibbs free energy at B3LYP-D3/6-31+G(d,p) level, and the solvation free energy obtained using the SMD model; All the energies relative to DABCO, MA, and the corresponding number of *p*NBA and methanol. Experimental value as reported in ref (*Plata, R. E.; Singleton, D. A. J. Am. Chem. Soc.* ***2015****, 137, 3811*).

S4.2 The transition state **TS7**

We obtained 87 distinct structures for the 'proton-shuttle' (**TS6**, Scheme 2 in the main text) or 'stepwise proton transfer' transition state (**TS7**, Scheme 2 in the main text) for the MBH reaction in a protic solvent. Computationally, it can be difficult in some cases to decide whether a given structure corresponds to **TS6** or **TS7** since they all involve deprotonation of the position adjacent to the carboxylate, and many of them include quite strong hydrogen bonding with the adjacent OH group. Accordingly, all results for these two TSs are shown in Tables as corresponding to **TS7**. Figure S10 shows the relative solvation free energies (SMD model, left-hand y axis) and the dipole moment (Debye, right-hand y axis) of 87 **TS7** transition states, in the order of relative free energies (23~45 kcal/mol, in green). In general, an inverse correlation between the dipole moment and the relative solvation free energies is observed, as shown in Figure S10.

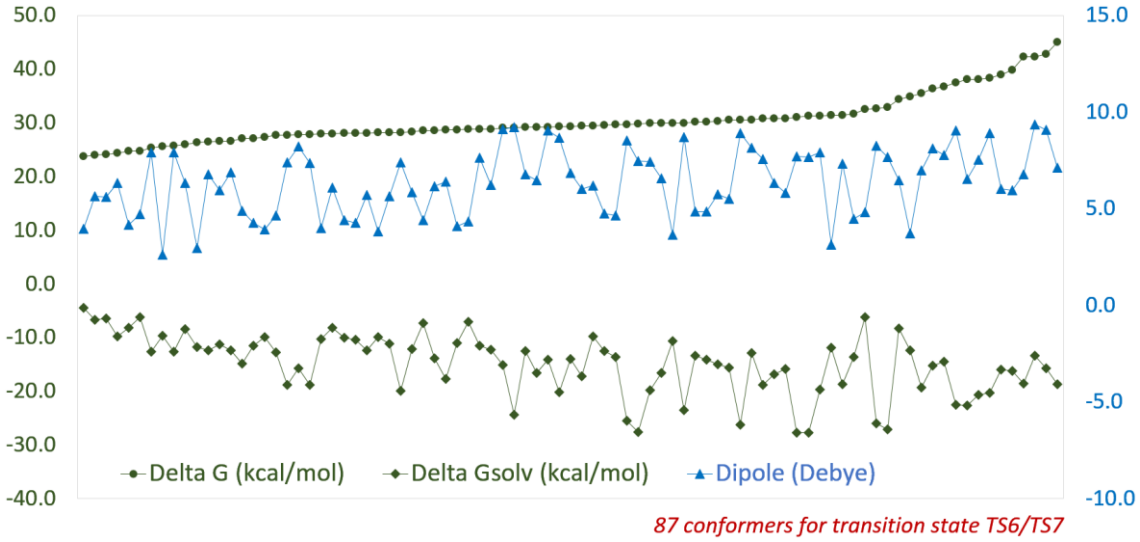

Figure S10. Relative solvation free energies (SMD model, left-hand y axis) and the dipole moment (Debye, right-hand y axis) of 87 **TS7** structures in the MBH reaction of MA with *p*NBA in methanol, shown in the order of relative free energies (23~45 kcal/mol, in green). The lines are a guide to the eye.

For each structure of the 87 transition states, Figure S11 shows the calculated free energy as well as the key O1-H1 and O1-H2 distances found. In all cases, the O1-H1 distance is near 1.3 Å, as befits a proton-transfer step. The O1-H2 distance is very large for some conformers, indicating pure **TS7** character – but is much smaller in others, which indicates some 'shuttle' or **TS6** character, and would likely lead to different isotope effects. Indeed, even within the sets of **TS6**-like and **TS7**-like the structural changes are large enough that the predicted behaviour would differ somewhat. Figure S11 suggests that the lowest-energy **TS7** structures should all be **TS6**-like, but this is only true when using B3LYP-D3 electronic energies and the SMD solvation model. If we assume a maximum 5 kcal/mol error for the relative solvation free energies computed with SMD model, then the structures within 5 kcal/mol among the 87 structures should be treated more carefully, especially for those with a large dipole moment where the solvation free energy may be underestimated by the continuum solvation model. When switching to FEP solvation, we find that of the five structures **TS7**s, three are '**TS6**-like' and two are '**TS7**-like', and they lie so close to one another that we cannot conclude which of them is lowest nor what the thermally-averaged mean TS properties are likely to be. Below, we show a test study on five low-lying TS7 transition state structures using the free energy perturbation method.

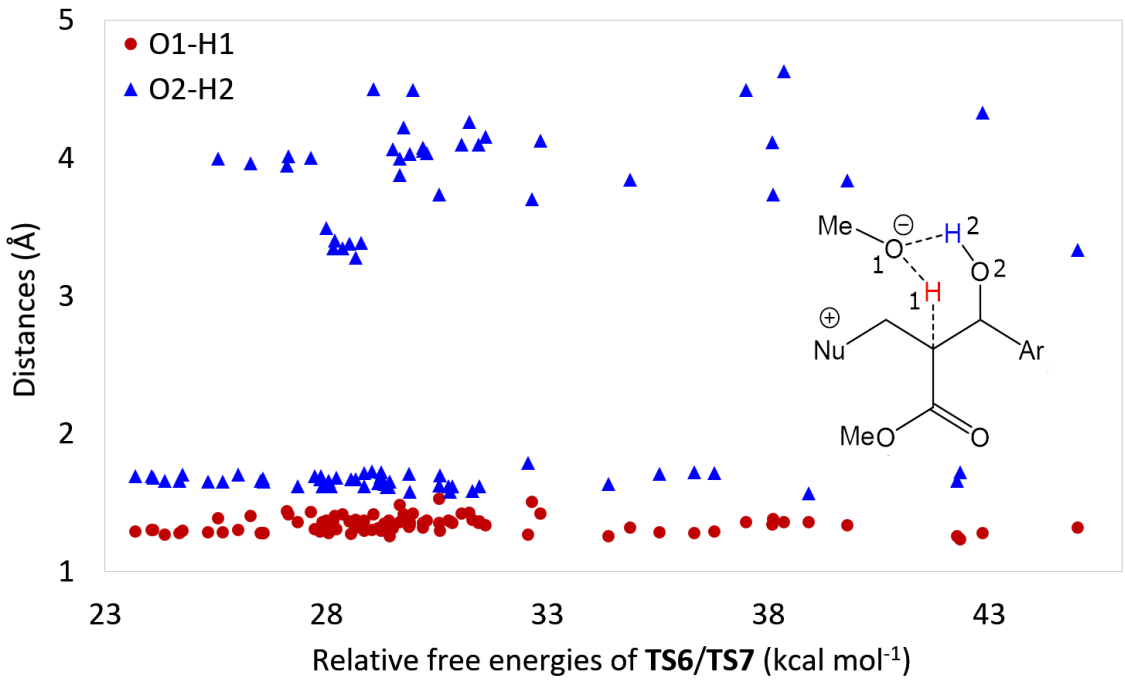

Figure S11. Structural diversity in the conformer space of **TS6/TS7**: key distances as a function of calculated relative free energy based on B3LYP-D3 electronic structure theory (the relative ordering of the different TS structures is slightly different with CCSD(T)).

S4.3 Free energy perturbation

The difference in the solvation free energy between reactants and products of a given step can be obtained using the free energy perturbation method. (W. L. Jorgensen, *Acc. Chem. Res.* **1989**, 22, 184) This approach involved selection of a starting structure (X) and a final structure (Y), and a large number of intermediate structures by linear interpolation of X and Y. The geometric change of a distance or an angle or a dihedral angle must be small to ensure a quick convergence of the perturbation.

For the reaction of MA and *p*NBA in methanol solvents catalyzed by DABCO (reaction I), a total of 1400 structures were generated. For each structure, a box was then constructed by soaking the solute (structure A) into a rectangular box (x=30 Å, y=35 Å, z=30 Å) filled with between 460 and 480 methanol molecules to reach the density of 0.792 kg dm^{-3} at 298 K. An appropriate atom type from the OPLS-AA forcefield was chosen for each atom in the solute (structure A), and the corresponding van der Waals radii were then used to describe interactions with solvent. The charges were replaced by the ESP partial charges as computed individually with Gaussian 09 at the B3LYP-D3/6-31+G(d,p)(SMD) level of theory. Both the default charges and van der Waals radii were adopted for the solvent molecules. The solute was kept fixed during the molecular dynamic simulation, so that no intramolecular MM terms are used. After 100 ps equilibration, at least 5000 snapshots were generated in the following NVT simulation (i.e. the snapshots has a time interval of 100 fs). The same method was applied for the reaction of MA and *p*NBA in THF (reaction II), and for the reaction of MA and BA in THF (reaction III), respectively. In total, 809 structures were used to evaluate the relative solvation free energies of the key intermediates in reaction II and reaction III. The same size of the solvent box (x=30 Å, y=35 Å, z=30 Å) was used with a fixed solute in the center of the box, which is filled by 210~230 THF molecules to reach the density of 0.889 kg dm^{-3} at 298 K.

In order to validate the approach adopted here, numerous tests were performed to ensure accuracy of the obtained values. We first validated the Tinker MM Hamiltonian through a comparison of the interaction energy between the solute and a small number of solvent molecules, computed using the force field potential and the B3LYP-D3 method. The intermediate **3** and a structure containing separated DABCO and MA with the orientation needed to react to form **3** (denoted as *pre*-**3**) were selected for the validation. In the molecular dynamic simulations on **3** and *pre*-**3**, 15 snapshots were randomly chosen, respectively. Since a full DFT calculation on the full solvent box is not possible, a stripped-down supramolecular system was generated to test the MM treatment. This system includes the solute and the explicit solvent molecules having the strongest interaction with the solute according to the forcefield. The interaction energy between each solvent and the solute was calculated individually by removing the periodic condition and only keeping the solute and the selected solvent. All solvent molecules with an interaction energy larger than 5 kcal/mol with the solute were retained in the supramolecular system. For example, Figure S12 shows four stripped-down structures with their associated strongly interacting solvent molecules from the snapshots of the molecular dynamic simulations on **3** and *pre*-**3** as the fixed solute inside the solvent box, respectively.

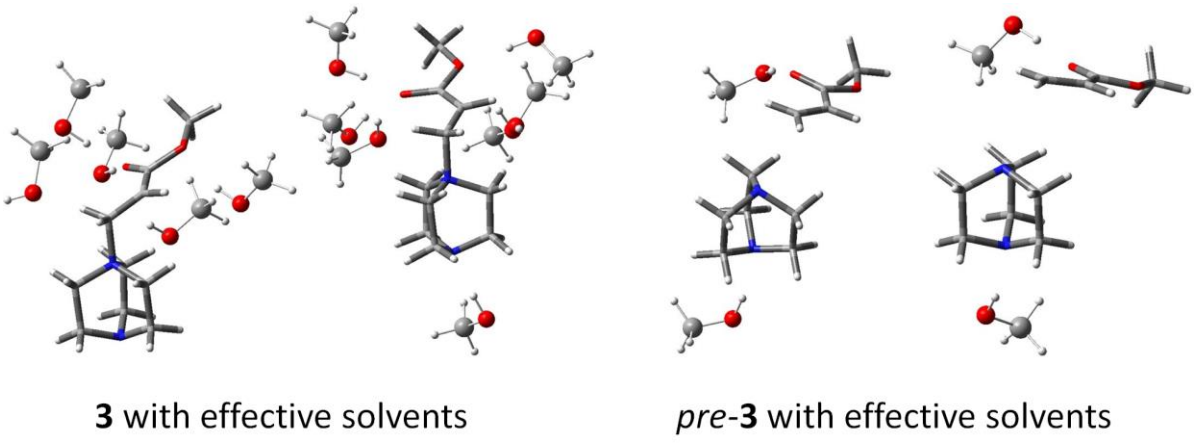

Figure S12. Stripped-down structures from the MD simulations, showing the solute structure with the effective solvents. The solvent molecules shown are those with a strong interaction with the solute (cut-off of the interaction energy: 5 kcal/mol).

Figure S13 shows the difference of the interaction energy (ΔΔE) between the solute and the group of selected solvent molecules in each of the stripped-down structures, calculated using the force field potential and the B3LYP-D3 method, respectively. Here, the interaction energy (ΔE(MM)) at MM level is calculated using the "group-interaction" keyword as implemented in TINKER program. One group is the cluster of strongly interacting solvent molecules and the other is the solute molecule. The interaction energy (ΔE(DFT)) at DFT level is calculated by subtracting the total energy of the solute and the solvent clusters from the total energy of the whole stripped-down structure, without carrying out any geometry optimization. As shown in Figure S13, the average of the energy difference between MM and DFT levels is 2.9 kcal/mol and 0.0 kcal/mol for **3** and *pre*-**3**, respectively. This level of agreement is fairly good, certainly adequate for the purposes of our FEP solvation free energy tests. Obviously though the agreement is far from perfect, perhaps not surprisingly given the simple MM parameter fitting procedure used.

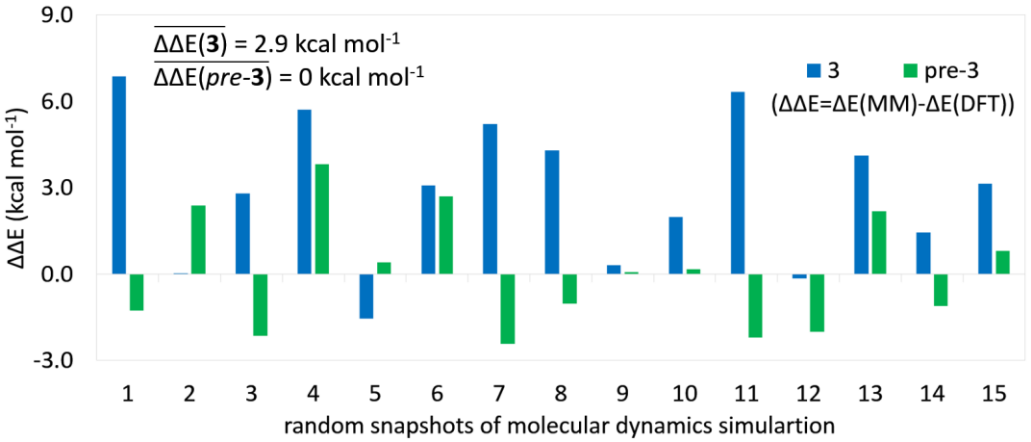

Figure S13. The difference in interaction energy between solute and strongly interacting solvent molecules for each of the stripped-down structures, calculated using the force field potential and the B3LYP-D3 method, respectively.

For each of the interpolated structures between a given reactant structure and product structure, more than 5000 snapshots were generated from the MD simulation. The solute structure *i* in each of the snapshots was then replaced by a perturbed structure *j* (or *i*+1). Then, the potential energy change for that snapshot can be computed. After applying the standard free energy perturbation expression to take the Boltzmann average of the resulting 5000 values, this yields a solvation free energy change from structure *i* to structure *j* within the fluctuating solvent cavity. The total change in the free energy of solvation from the reactant to the product is the sum of all the energy changes *i* → *j* along the interpolated pathway. The same procedure was also used in reverse, i.e. the energy obtained by replacing structure *i* with structure *j'*=*i*-1 was computed at snapshots during the molecular dynamics simulation for structure *i*. For example, as shown in Figure S14, the blue line shows the cumulative sum of the forward FEP energies for the formation of **3** from the 'reactant' *pre*-**3** structure (DABCO and MA separated by 10 Å in the reaction coordinate), while the red line shows the cumulative sum of the backward FEP energies for the dissociation of **3** back to the separated DABCO and MA. The total 'forward' solvation free energy change of 19.9 kcal/mol obtained by summing up the forward FEP energies is in very good agreement with the 'reverse' solvation free energy change of 20.4 kcal/mol obtained using the backward FEP procedure. The agreement found here is typical: forward and reverse free energy changes for each reaction agree to within better than 1 kcal/mol in all cases.

It should also be noted that the solvation free energy plateaus near the structure *pre*-**3** on the left-hand side of Figure S14. In each case where the reactant or product state was a separated pair of molecules, this plateau behavior was observed upon approaching this asymptote. This is expected given that the computed charges no longer change in this regime, and the large 10 Å separation means that there is space for more than one solvent shell between the two fragments.

In the example in Figure S14, the solvation free energy is lowered by *ca*. 20 kcal/mol in the formation of species **3** from the separated DABCO and MA, which differs noticeably from 16.4 kcal/mol obtained by using the SMD model. As reported in the original paper(Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, 113, 6378.), the continuum solvation model SMD was parameterized to reach a mean unsigned errors of 0.6-1.0 kcal/mol in the solvation free energies of neutral systems. However, the mean unsigned errors are still as large as 4 kcal/mol on average for ions. Species **3** is a structure with a zwitterionic character, which may account for a larger error for this species (though we note that the FEP value obtained here is not exact either!).

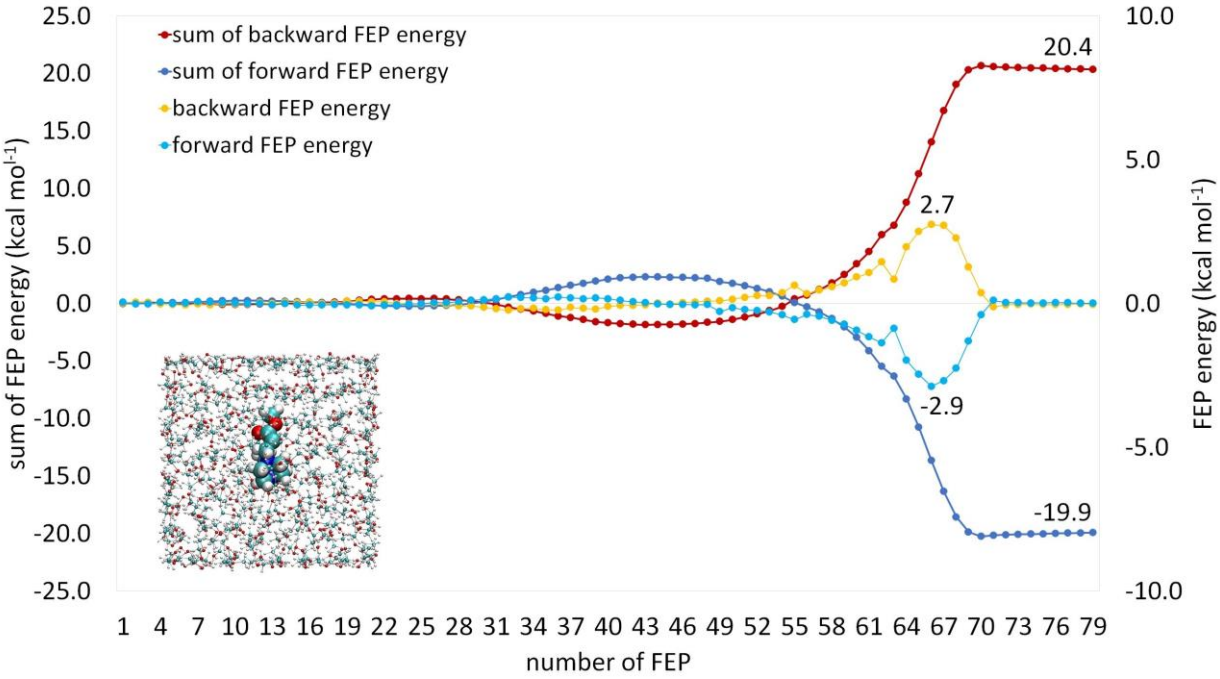

Figure S14. Statistical convergence of FEP procedure for **3**. The solvent box in the left-bottom corner shows the structure of **3** in the solvent box.

To explore the possible origin of the discrepancy between FEP and SMD solvation free energies, we performed a further analysis: the electrostatic potential created by the PCM (Polarized Continuum Model with SMD parameters) at the nuclei of solute **3** was compared to the explicit solvent 'reaction potential' computed by averaging over the Coulombic potential created by the point charges of the MM solvent at the positions of the solute nuclei, using a cut-off of 12 Å. The results are graphically shown in Figure S15. Positive values of the reaction potential indicate that for that nucleus, the solvent field would stabilize a negatively-charged solute atom at that position and destabilize a positively-charged solute atom, and vice-versa for negative values. As can be seen, and as expected, the reaction potential is positive near the negatively charged carboxylate enolate end of the molecule, and negative near the positively charged DABCO moiety. Although the MD and SMD profiles have a similar shape, there are noticeable differences, e.g. in the region of the DABCO moiety, the SMD reaction potential is much larger in magnitude than the MD reaction potential. This may account for the difference of the solvation free energies calculated by the SMD model and the FEP method.

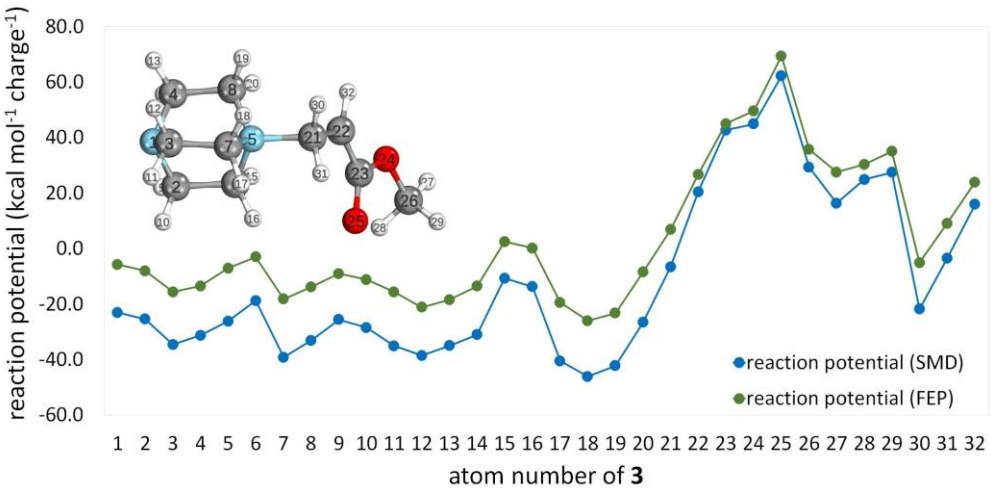

Figure S15. The reaction potential at the nuclei of 3 (the SMD model vs. the FEP method).

Free energy is a state quantity, so the change in free energy between two particular states of the system only depends on the initial and the final structures, not the path followed between them. This also applies to components of the free energy, e.g. the solvation free energy. Unlike SMD, the FEP procedure used here does not guarantee that path invariance will result when considering three (or more) connected states A, B and C, when taking the difference in solvation free energy between A and C along a path connecting them, compared to that following paths from A to B then B to C. Accordingly, we made additional tests to explore whether large discrepancies were found in such cases. Figure S16 shows three pathways leading to the formation of the product **11a**. The first pathway in orange follows the proposed mechanism for MBH reaction that goes through the zwitterionic intermediates **3** and **5**, an ensuing H-shift, and an elimination step. The second route in gray is an arbitrarily designed (not experimentally possible) pathway that brings the reactants directly together with appropriate H abstraction/transfers. The third route in green is similar to the second route, but it visits the minima corresponding to four additional conformational isomers before reaching **11a**. The FEP-predicted solvation free energies for the three routes should all be equal in case the FEP approach as implemented here truly is path-invariant. In practice, the relative solvation free energy obtained for **11a** compared to reactants is 0.7 kcal/mol, 0.5 kcal/mol, and 1.3 kcal/mol via the first route, the second route, and the third route, respectively. These small discrepancies are certainly acceptable given the other inaccuracies in the FEP procedure. In a similar test, we computed the solvation free energy change from the separated DABCO and MA to reach a transition state **TS7b**(SR) via two different routes. A free energy change of 20.4 kcal/mol was computed by summing FEP contributions along an extended reaction pathway leading first to **TS7**(SR) then through internal rotation. This agrees very nicely with a value of 21.4 kcal/mol obtained by following a much more 'direct' reaction pathway shown here in blue. The agreement in the FEP relative solvation free energy of **11a** and **TS7b**(SR) shows the validity and the accuracy of the approach adopted here.

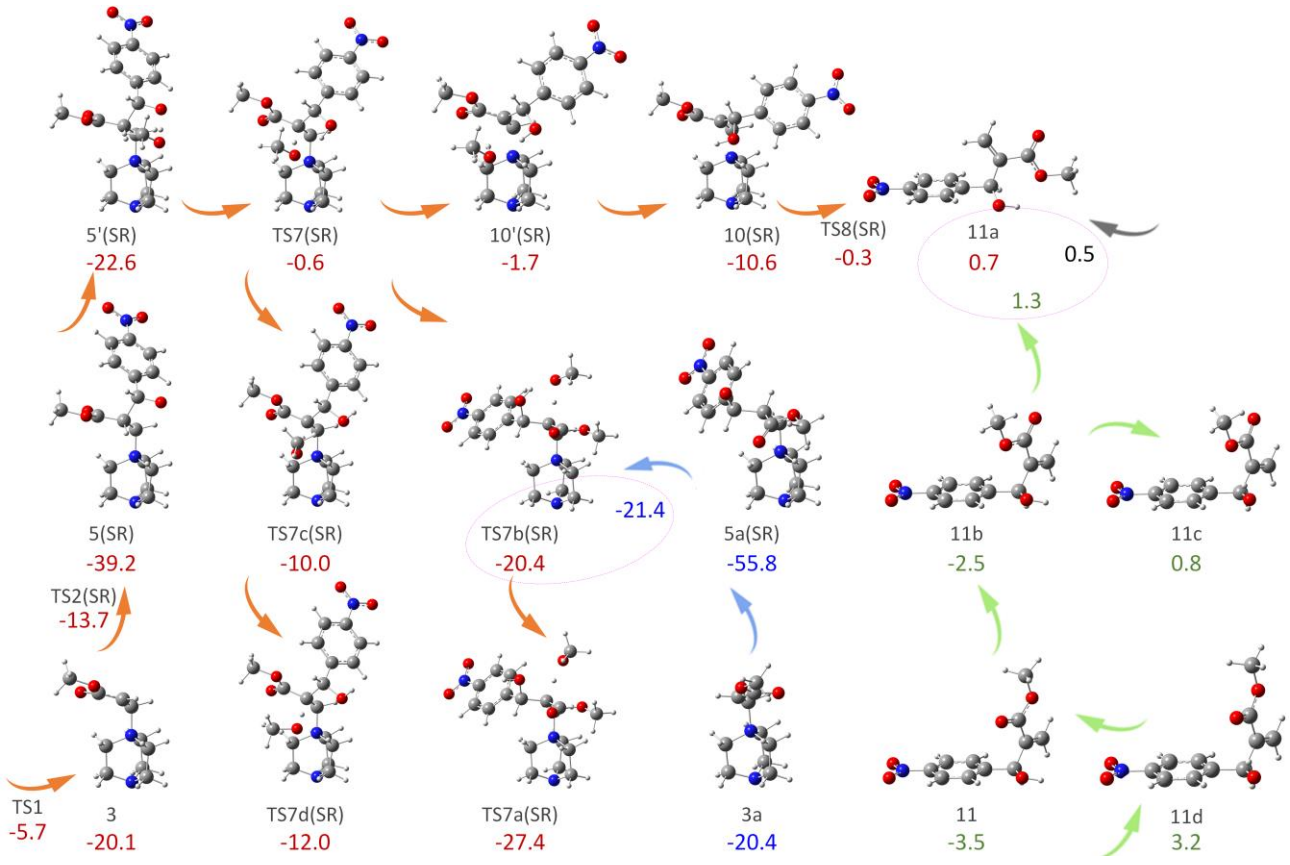

Figure S16. Triangulation of the FEP relative free energies of the product 11a.

S4.4 A comparison of the solvation free energies

We studied three reactions in this work. The first reaction is the addition of MA and *p*NBA catalyzed by DABCO in methanol (reaction I), the second reaction is in tetrahydrofuran for the addition of MA and *p*NBA (reaction II), and the third reaction is also in tetrahydrofuran for the addition of MA and BA (reaction III). Figure S17 shows a comparison of the differences of the relative solvation free energies using the SMD model and the COSMO-RS model to that obtained using the FEP method for the key transition states TS7 in reaction I, and the transition states TS4 in reaction I, reaction II, and reaction III. In general, the ΔΔG is large for the structure with a large dipole moment in reaction I. In the polar methanol solvent, of the continuum model-derived values, the relative solvation free energies obtained using the SMD model are slightly more close to that obtained using the FEP method than are the COSMO-RS values. However, in nonpolar THF solvent, the agreement between the COSMO-RS and the FEP method is better than that between the SMD model and the FEP method. This test clearly shows the challenge in computation of the solvation free energies for the MBH reaction in both polar and non-polar mediums. The FEP method may generate more reliable relative solvation free energies for the species involved in a chemical reaction. However, the nature of the method itself is extremely computational extensive (and subject to accuracy of the solvent-solvent and solvent-solute potential), which limits a general application of the FEP method in many circumstances.

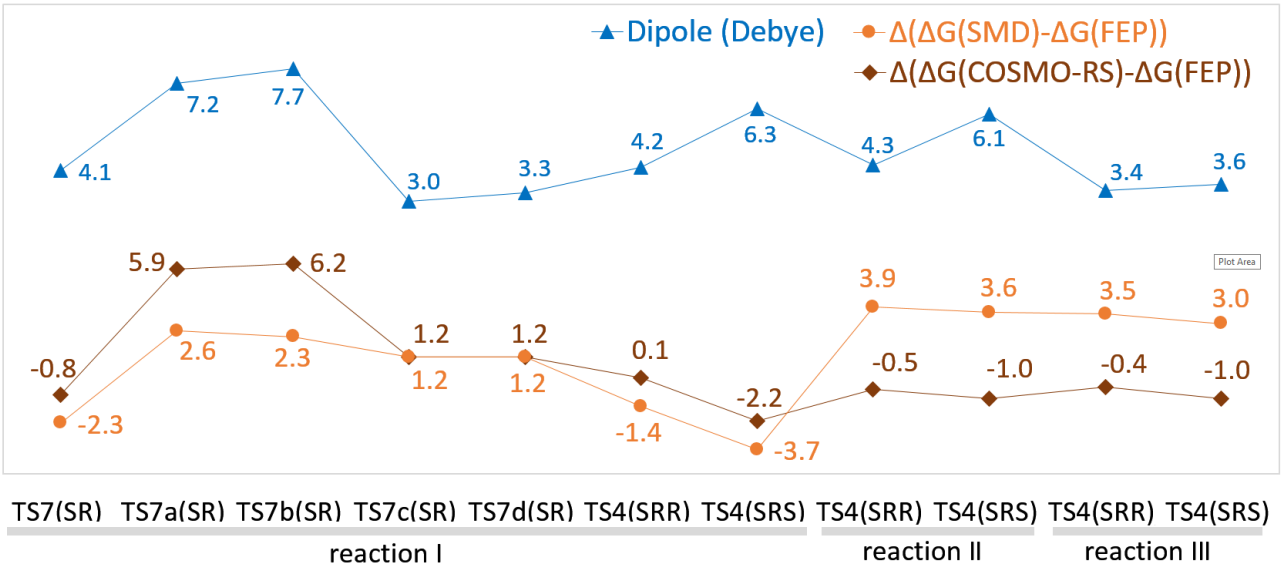

Figure S17. Differences of solvation free energies (kcal/mol) and the dipole moments for the key transition states of the MBH reactions (reaction I: MA with *p*NBA in methanol; reaction II: MA with *p*NBA in THF; reaction III: MA with BA in THF).

S5. Full tables for the MBH reactions of MA with *p*NBA in methanol (reaction I), MA with *p*NBA in THF (reaction II), MA with BA in THF (reaction III)

Table S2: Relative energies (kcal/mol) of various species involved in the MBH reaction (I) of MA with *p*NBA in methanol, catalyzed by DABCO at 298 K.

	Dipole	ΔG_{therm}	$\Delta G_{solv,1}$ (SMD)	$\Delta G_{solv,2}$ (COSMO)	$\Delta G_{solv,3}$ (FEP)	ΔG_1 (B3LYP-D3)	ΔG_2 (M06-D3)	ΔG_3 (M06-2X)	ΔG_4 CCSD(T)/CBS1	ΔG_5 CCSD(T)/CBS2
Reactants	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS1	2.6	12.2	-4.0	-3.8	-5.7	14.6	13.9	15.1	17.7	17.6
3	4.6	14.4	-16.4	-13.7	-20.1	15.6	12.9	11.7	14.8	14.8
4	1.8	33.1	-82.4	-80.5	-	10.1	9.6	7.4	10.4	10.9
TS2(*SS*)	7.3	27.7	-15.7	-11.7	-	21.6	17.1	18.9	21.8	24.0
TS2(*SR*)	6.5	27.9	-16.2	-12.4	-13.7	21.0	16.9	18.1	20.9	22.8
5(*SS*)	8.9	30.0	-32.0	-30.8	-	14.3	7.6	7.4	10.0	10.5
5(*SR*)	7.9	30.4	-30.8	-29.5	-39.2	15.6	9.3	8.4	11.2	11.7
TS3(*SSR*)	11.2	44.5	-26.6	-21.5	-	22.2	12.6	12.8	13.7	-
TS3(*SSS*)	9.4	44.4	-27.7	-22.1	-	24.0	14.1	15.5	17.3	-
TS3(*SRR*)	8.7	44.4	-26.1	-19.2	-	24.6	15.0	16.5	18.5	-
TS3(*SRS*)	11.8	43.7	-30.8	-25.1	-	22.1	12.3	12.3	13.7	-
6(*SSR*)	11.7	45.1	-32.0	-27.9	-	20.2	9.2	7.9	9.6	-
6(*SSS*)	10.4	45.5	-34.5	-30.4	-	21.7	10.3	10.2	12.8	-
6(*SRR*)	7.1	45.6	-26.7	-22.4	-	21.4	11.6	11.5	14.2	-
6(*SRS*)	12.0	44.1	-34.4	-30.7	-	19.7	8.8	8.0	9.8	-
TS4(*SSR*)	5.1	42.0	-9.6	-6.4	-	34.9	25.6	21.6	24.3	-
TS4(*SSS*)	8.5	41.2	-10.6	-7.6	-	33.8	24.2	20.2	23.5	-
TS4(*SRR*)	4.2	41.7	-4.8	-3.4	-3.5	31.2	21.7	17.9	21.3	-
TS4(*SRS*)	6.3	42.1	-4.4	-2.9	-0.7	32.3	23.1	19.0	22.8	-
7(*SSR*)	8.9	44.5	-5.2	-4.4	-	24.8	15.6	9.9	14.8	-
7(*SSS*)	9.4	44.7	-8.0	-6.3	-	22.8	13.1	8.3	13.8	-
7(*SRR*)	5.8	43.3	-4.0	-2.9	-3.5	19.2	9.8	5.5	9.8	-
7(*SRS*)	7.9	44.5	-4.7	-3.8	-2.8	20.5	11.0	6.5	11.4	-
9	7.4	47.6	-83.1	-83.0	-	13.0	8.3	3.8	7.4	9.2
TS7(*SS*)	6.4	36.7	-8.6	-5.2	-	31.4	25.0	23.4	26.3	26.5
TS7(*SR*)	4.1	36.8	-2.9	-1.4	-0.6	29.5	23.8	21.9	25.1	25.8
10(*SS*)	6.9	28.9	-11.9	-10.0	-	16.9	10.4	7.3	11.1	12.2
10(*SR*)	4.0	29.2	-9.3	-8.2	-10.6	16.2	9.3	6.6	10.4	12.0
TS8(*SS*)	4.7	25.8	-1.6	-1.8	-	15.7	11.3	10.7	13.5	14.6
TS8(*SR*)	2.8	26.5	0.1	-0.8	-0.3	15.9	11.0	10.9	14.2	14.3
11	4.7	13.5	-2.5	-3.8	-3.5	2.6	-1.5	-4.0	-3.5	-2.8

ΔG_{therm}, the relative Gibbs free energy correction at the standard state of 1 M, computed at the B3LYP-D3/6-31+G(d,p)(SMD) level of theory; $\Delta G_{solv,1}$, $\Delta G_{solv,2}$, $\Delta G_{solv,3}$ are the relative solvation energies calculated with SMD model, COSMO-RS model, and FEP method, respectively; ΔG_1, ΔG_2, ΔG_3, ΔG_4, ΔG_5, are the relative Gibbs free energies calculated at B3LYP-D3/6-311++G(3df,3pd), M06-D3/6-311++G(3df,3pd), M06-2X/6-311++G(3df,3pd), DLPNO-CCSD(T)/CBS1, DLPNO-CCSD(T)/CBS2, respectively, including the solvation free energy calculated with COSMO-RS model and the free energy correction at B3LYP-D3/6-31+G(d,p)(SMD) level of theory.

Table S3: Relative energies (kcal/mol) of various species involved in the MBH reaction (II) of MA with *p*NBA in THF, catalyzed by DABCO at 298 K.

	Dipole	ΔG_{therm}	$\Delta G_{solv,1}$ (SMD)	$\Delta G_{solv,2}$ (COSMO)	$\Delta G_{solv,3}$ (FEP)	ΔG_1 (B3LYP-D3)	ΔG_2 (M06-D3)	ΔG_3 (M06-2X)	ΔG_4 CCSD(T)/CBS1	ΔG_5 CCSD(T)/CBS2
Reactants	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS1	3.0	12.5	-4.4	-4.9	-4.9	17.2	15.7	15.9	19.1	18.9
3	4.0	13.5	-8.2	-8.1	-7.8	18.3	15.6	14.6	17.8	17.7
TS2(*SS*)	7.4	28.1	-10.1	-10.6	-	26.3	20.7	21.9	24.1	26.3
TS2(*SR*)	6.7	27.8	-9.9	-10.6	-9.2	25.7	20.1	20.9	24.2	25.3
5(*SS*)	8.2	27.6	-14.6	-14.4	-	25.1	18.1	18.3	20.3	21.4
5(*SR*)	7.3	29.2	-13.6	-13.6	-11.5	26.9	20.2	19.8	22.2	22.7
TS3(*SSR*)	10.5	42.9	-9.0	-11.5	-	25.5	16.1	16.7	18.2	-
TS3(*SSS*)	6.2	43.9	-5.8	-7.7	-	27.1	17.4	17.5	19.8	-
TS3(*SRR*)	7.1	43.3	-8.5	-11.0	-	27.4	19.4	19.0	21.4	-
TS3(*SRS*)	8.3	43.1	-4.1	-7.8	-4.9	25.4	18.1	17.6	19.5	-
6(*SSR*)	10.3	42.7	-8.2	-10.7	-	25.5	14.5	14.5	15.8	-
6(*SSS*)	5.9	43.5	-4.5	-6.4	-	25.5	16.8	19.6	21.6	-
6(*SRR*)	6.2	43.7	-3.9	-7.0	-6.2	25.9	16.1	14.2	16.6	-
6(*SRS*)	7.9	44.0	-3.9	-7.7	-5.2	26.0	16.7	14.8	16.7	-
TS4(*SSR*)	5.2	41.7	0.5	-3.8	-	35.8	26.7	22.5	25.4	-
TS4(*SSS*)	7.8	41.4	-0.6	-5.5	-	34.8	25.4	21.3	24.5	-
TS4(*SRR*)	4.3	41.9	2.7	-1.6	-1.2	32.2	22.9	18.9	22.0	-
TS4(*SRS*)	6.1	41.6	3.0	-1.7	-0.6	32.4	23.4	19.2	22.4	-
7(*SSR*)	7.6	44.3	2.9	-2.6	-	24.1	15.2	9.8	14.3	-
7(*SSS*)	8.4	44.5	-0.6	-6.1	-	21.8	12.1	7.4	13.5	-
7(*SRR*)	5.1	43.9	3.2	-1.4	-1.1	19.4	9.7	5.6	10.4	-
7(*SRS*)	7.3	44.9	1.9	-2.9	-1.9	21.0	11.5	7.0	11.8	-
11	3.2	13.7	2.5	0.2	-	2.5	-1.1	-4.0	-3.4	-2.8

ΔG_{therm}, the relative Gibbs free energy correction at the standard state of 1 M, computed at the B3LYP-D3/6-31+G(d,p)(SMD) level of theory; $\Delta G_{solv,1}$, $\Delta G_{solv,2}$, $\Delta G_{solv,3}$ are the relative solvation energies calculated with SMD model, COSMO-RS model, and FEP method, respectively; ΔG_1, ΔG_2, ΔG_3, ΔG_4, ΔG_5, are the relative Gibbs free energies calculated at B3LYP-D3/6-311++G(3df,3pd), M06-D3/6-311++G(3df,3pd), M06-2X/6-311++G(3df,3pd), DLPNO-CCSD(T)/CBS1, DLPNO-CCSD(T)/CBS2, respectively, including the solvation free energy calculated with COSMO-RS model and the free energy correction at B3LYP-D3/6-31+G(d,p)(SMD) level of theory.

Table S4: Relative energies (kcal/mol) of various species involved in the MBH reaction (III) of MA with BA in THF, catalyzed by DABCO at 298 K.

	Dipole	ΔG_{therm}	$\Delta G_{solv,1}$ (SMD)	$\Delta G_{solv,2}$ (COSMO)	$\Delta G_{solv,3}$ (FEP)	ΔG_1 (B3LYP-D3)	ΔG_2 (M06-D3)	ΔG_3 (M06-2X)	ΔG_4 CCSD(T)/CBS1	ΔG_5 CCSD(T)/CBS2
Reactants	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS1	3.0	12.5	-4.4	-4.9	-4.9	17.2	15.7	15.9	19.1	18.9
3	4.0	13.5	-8.2	-8.1	-7.8	18.3	15.6	14.6	17.8	17.7
TS2(*SS*)	5.4	27.5	-11.2	-11.1	-	31.8	26.0	26.4	28.9	30.4
TS2(*SR*)	5.1	27.5	-10.9	-10.8	-8.6	31.5	25.8	25.9	28.8	29.7
5(*SS*)	6.2	28.2	-15.7	-15.0	-	31.9	24.9	24.4	25.8	26.6
5(*SR*)	5.7	28.6	-14.6	-14.0	-11.2	32.5	25.9	24.8	26.7	27.3
TS3(*SSR*)	5.8	41.4	-7.1	-8.4	-	35.4	25.8	26.0	26.5	-
TS3(*SSS*)	6.5	42.0	-6.8	-9.0	-	33.9	24.3	23.2	25.0	-
TS3(*SRR*)	4.7	42.1	-3.9	-6.4	-4.9	34.9	27.2	25.5	27.1	-
TS3(*SRS*)	4.8	42.2	-4.6	-7.5	-4.6	34.3	27.0	25.8	26.6	-
6(*SSR*)	6.2	42.1	-7.9	-9.3	-	35.7	24.4	23.3	23.5	-
6(*SSS*)	5.8	41.9	-6.6	-8.2	-	35.2	25.1	23.0	24.1	-
6(*SRR*)	4.9	43.2	-4.7	-6.9	-5.9	34.7	24.9	21.9	23.7	-
6(*SRS*)	5.1	42.5	-4.9	-7.8	-5.2	34.1	25.0	21.9	23.1	-
TS4(*SSR*)	4.3	41.6	0.4	-3.4	-	44.3	35.4	30.1	33.5	-
TS4(*SSS*)	4.6	40.2	-1.5	-5.3	-	43.0	33.6	28.6	30.3	-
TS4(*SRR*)	3.4	40.4	2.4	-1.4	-1.0	38.9	29.8	24.7	26.6	-
TS4(*SRS*)	3.6	40.4	2.6	-1.4	-0.4	40.0	31.2	25.8	28.1	-
7(*SSR*)	4.5	43.3	1.6	-2.6	-	31.6	22.0	17.3	20.1	-
7(*SSS*)	6.0	43.3	-0.9	-5.5	-	30.1	20.3	14.9	18.8	-
7(*SRR*)	4.3	42.2	3.1	-1.0	-1.4	25.5	15.8	11.2	14.4	-
7(*SRS*)	4.4	43.1	3.4	-1.4	-0.7	27.3	18.1	12.3	15.7	-
11	1.7	13.1	2.6	0.6	-	5.3	1.9	-1.6	-1.3	-0.8

ΔG_{therm}, the relative Gibbs free energy correction at the standard state of 1 M, computed at the B3LYP-D3/6-31+G(d,p)(SMD) level of theory; $\Delta G_{solv,1}$, $\Delta G_{solv,2}$, $\Delta G_{solv,3}$ are the relative solvation energies calculated with SMD model, COSMO-RS model, and FEP method, respectively; ΔG_1, ΔG_2, ΔG_3, ΔG_4, ΔG_5, are the relative Gibbs free energies calculated at B3LYP-D3/6-311++G(3df,3pd), M06-D3/6-311++G(3df,3pd), M06-2X/6-311++G(3df,3pd), DLPNO-CCSD(T)/CBS1, DLPNO-CCSD(T)/CBS2, respectively, including the solvation free energy calculated with COSMO-RS model and the free energy correction at B3LYP-D3/6-31+G(d,p)(SMD) level of theory.

Table S5. Relative free energies (kcal/mol) at 298 K of the key diastereomeric transition states for the MBH reactions of MA with *p*NBA in methanol (reaction I), MA with *p*NBA in THF (reaction II), MA with BA in THF (reaction III), catalyzed by DABCO.

	$\Delta G_{reaction\ I}$	$\Delta G_{reaction\ II}$	$\Delta G_{reaction\ III}$
Reactants	0.0	0.0	0.0
TS2(*SS*)	17.8/21.8/-	24.6/24.1/-	28.7/28.9/-
TS2(*SR*)	17.1/20.9/19.6	24.8/24.2/25.6	28.8/28.8/31.1
TS3(*SSR*)	8.6/13.7/-	20.8/18.2/-	27.7/26.5/-
TS3(*SSS*)	11.7/17.3/-	21.7/19.8/-	27.2/25.0/-
TS3(*SRR*)	11.6/18.5/-	24.0/21.4/-	29.6/27.1/28.6
TS3(*SRS*)	8.0/13.7/-	23.2/19.5/22.4	29.5/26.6/29.5
TS4(*SSR*)	21.1/24.3/-	29.7/25.4/-	37.3/33.5/-
TS4(*SSS*)	20.6/23.5/-	29.3/24.5/-	34.1/30.3/-
TS4(*SRR*)	19.9/21.3/21.3	26.4/22.0/22.5	30.5/26.6/27.0
TS4(*SRS*)	21.3/22.8/25.1	27.1/22.4/23.4	32.1/28.1/29.1
TS7(*SS*)	22.9/26.3/-	-	-
TS7(*SR*)	23.5/25.1/24.3	-	-
11	-2.2/-3.5/-3.2	-1.1/-3.4/-	0.8/-1.3/-

The relative free energies include the electronic energy at DLPNO-CCSD(T)/CBS1 level, and the solvation free energy obtained using the SMD/COSMO-RS/FEP method. All the energies relative to DBACO, MA, and the corresponding number of *p*NBA (or BA) and methanol.

Table S6. The mean unsigned error of 10 structures: calculated energy vs. expt. (kcal/mol)

Structures in the reaction	unsigned error with respect to expt.
3 in reaction I	0.1
TS2 in reaction I	0.6
5 in reaction I	4.7
9 in reaction I	0.5
TS7 in reaction I	3.1
10 in reaction I	0.1
11 in reaction I	0.7
TS4 in reaction I	1.2
TS4 in reaction II	3.7
TS4 in reaction III	3.9
Average:	1.86

S6. Lists of Cartesian coordinates.

The geometries optimized at B3LYP-D3/6-31+G(d,p)(SMD) level of theory (reaction I: MA with *p*NBA in methanol; reaction II: MA with *p*NBA in THF; reaction III: MA with BA in THF).

(a) Structures in reaction I.

r1_DABCO
Final geometry with 20 atoms:

N	-1.2960	0.0022	-0.0002
C	-0.7812	-0.3075	1.3530
C	-0.7781	1.3276	-0.4092
C	-0.7820	-1.0162	-0.9441
N	1.2960	-0.0023	0.0002
C	0.7797	-0.3024	1.3550
C	0.7828	1.3226	-0.4165
C	0.7788	-1.0241	-0.9382
H	-1.1743	-1.2858	1.6509
H	-1.1804	0.4386	2.0488
H	-1.1683	2.0760	0.2894
H	-1.1778	1.5583	-1.4029
H	-1.1730	-0.7842	-1.9409
H	-1.1840	-1.9908	-0.6464
H	1.1784	-1.2748	1.6645
H	1.1723	0.4536	2.0439
H	1.1844	2.0756	0.2705
H	1.1746	1.5402	-1.4162
H	1.1797	-0.8064	-1.9343
H	1.1684	-1.9997	-0.6272

r1_MA
Final geometry with 12 atoms:

C	2.5029	-0.0195	0.0001
C	1.3190	-0.6426	-0.0001
C	0.0473	0.1144	-0.0001
O	-1.0128	-0.7128	0.0000
O	-0.0599	1.3373	-0.0001
C	-2.3238	-0.0961	0.0001
H	-3.0309	-0.9252	-0.0004
H	-2.4509	0.5175	-0.8955
H	-2.4512	0.5168	0.8961
H	3.4313	-0.5831	0.0002
H	2.5722	1.0655	0.0005
H	1.2383	-1.7256	-0.0003

r1_*p*NBA
Final geometry with 16 atoms:

C	3.1793	0.3453	0.0006
H	3.5605	1.3822	0.0020
C	1.7052	0.2076	0.0004
C	0.9216	1.3714	0.0006
C	-0.4680	1.2810	0.0002
C	-1.0441	0.0097	-0.0001
C	-0.2870	-1.1672	-0.0003
C	1.0978	-1.0599	-0.0002
H	1.3989	2.3470	0.0009
H	-1.0873	2.1692	0.0003
H	-0.7733	-2.1347	-0.0007
H	1.7146	-1.9524	-0.0007
N	-2.5091	-0.0972	-0.0002
O	-3.1748	0.9430	-0.0014
O	-3.0172	-1.2226	0.0014
O	3.9573	-0.6027	-0.0009

r1_CH3O
Final geometry with 5 atoms:

C	0.0000	0.0000	-0.5821
H	0.0000	1.0228	-1.0230
H	0.8858	-0.5114	-1.0230
H	-0.8858	-0.5114	-1.0230
O	0.0000	0.0000	0.8202

r1_CH3OH
Final geometry with 6 atoms:

C	0.6750	-0.0199	0.0000
H	1.0959	0.9889	-0.0012
H	1.0243	-0.5502	0.8952
H	1.0241	-0.5523	-0.8940
O	-0.7552	0.1240	0.0000
H	-1.1531	-0.7588	0.0000

r1_TS1a
Final geometry with 32 atoms:

N	-3.0743	-0.9578	0.1283
C	-2.7036	-0.4243	1.4558
C	-3.3453	0.1767	-0.7800
C	-1.9297	-1.7297	-0.4011
N	-1.0078	0.5392	-0.0663
C	-1.4270	0.4683	1.3493
C	-2.0970	1.1130	-0.8834
C	-0.6742	-0.8155	-0.5561
H	-2.5326	-1.2672	2.1323
H	-3.5479	0.1543	1.8428
H	-4.2101	0.7272	-0.3973
H	-3.6079	-0.2255	-1.7631
H	-2.2156	-2.1556	-1.3676
H	-1.7275	-2.5566	0.2864
H	-0.5901	0.0582	1.9224
H	-1.6153	1.4886	1.6966
H	-2.3090	2.1176	-0.5046
H	-1.7381	1.2003	-1.9133
H	-0.3627	-0.7248	-1.5999
H	0.1767	-1.1803	0.0266
C	0.6637	1.7107	-0.1888
C	1.7468	1.1825	0.4979
C	2.6608	0.2826	-0.1332
O	3.6446	-0.1500	0.7247
O	2.6495	-0.1037	-1.3183
C	4.6343	-1.0433	0.1802
H	5.3092	-1.2694	1.0072
H	5.1873	-0.5638	-0.6332
H	4.1696	-1.9639	-0.1855
H	0.6499	1.6584	-1.2745
H	0.1248	2.5501	0.2409
H	1.8891	1.3850	1.5544

r1_3a
Final geometry with 32 atoms:

N	3.0125	0.9168	0.2205
C	2.6178	0.2835	1.4922
C	3.2813	-0.1411	-0.7709
C	1.8895	1.7425	-0.2610
N	0.9091	-0.5411	-0.1200
C	1.2933	-0.5142	1.3381
C	2.0657	-1.0992	-0.9120
C	0.6457	0.8702	-0.5826
H	2.4977	1.0615	2.2508
H	3.4258	-0.3800	1.8115
H	4.1643	-0.7041	-0.4574
H	3.5037	0.3347	-1.7297
H	2.2056	2.2829	-1.1572
H	1.6496	2.4774	0.5119
H	0.4620	-0.0533	1.8724
H	1.3926	-1.5516	1.6646
H	2.2724	-2.0934	-0.5104
H	1.7325	-1.1967	-1.9472
H	0.4400	0.8132	-1.6529
H	-0.2502	1.2144	-0.0664
C	-0.3720	-1.4524	-0.3392
C	-1.5673	-1.0615	0.4173
C	-2.5431	-0.2434	-0.1370
O	-3.6182	-0.0020	0.7336
O	-2.5749	0.2813	-1.2910
C	-4.6884	0.8085	0.2312
H	-5.4089	0.8853	1.0488
H	-5.1699	0.3451	-0.6371
H	-4.3399	1.8099	-0.0439
H	-0.5209	-1.4046	-1.4213
H	0.0011	-2.4439	-0.0687
H	-1.6985	-1.4194	1.4326

r1_TS2a_SR
Final geometry with 48 atoms:

N	3.7598	-2.6329	0.4602
C	3.0419	-1.9800	1.5711
C	2.7876	-3.4075	-0.3330
C	4.3353	-1.5836	-0.4028
N	1.8982	-1.0784	-0.4489
C	2.0597	-0.8991	1.0483
C	1.5564	-2.5413	-0.6973
C	3.2231	-0.8016	-1.1431
H	3.7677	-1.5151	2.2432
H	2.5045	-2.7502	2.1305
H	2.4614	-4.2777	0.2423
H	3.2879	-3.7651	-1.2366
H	5.0065	-2.0417	-1.1341
H	4.9243	-0.9095	0.2247
H	2.4278	0.1121	1.2033
H	1.0694	-0.9998	1.4879
H	0.6904	-2.7650	-0.0721
H	1.2762	-2.6376	-1.7477
H	3.0961	-1.1360	-2.1744
H	3.3901	0.2718	-1.1226
C	0.7779	-0.2355	-1.0331
C	0.6213	1.2271	-0.6813
C	1.6540	2.1855	-0.4603
O	1.2377	3.4485	-0.8052
O	2.7732	2.0264	0.0711
C	2.0935	4.5411	-0.4206
H	1.5684	5.4449	-0.7334
H	3.0602	4.4757	-0.9291
H	2.2482	4.5538	0.6621
H	0.8917	-0.3571	-2.1166
H	-0.1429	-0.7558	-0.7529
H	-0.1909	1.6260	-1.2840
C	-0.4843	1.6898	1.2616
H	0.2413	1.1038	1.8417
C	-1.6871	0.9272	0.8220
C	-1.8304	-0.4333	1.1502
C	-2.9562	-1.1473	0.7579
C	-3.9512	-0.4850	0.0292
C	-3.8404	0.8742	-0.3046
C	-2.7122	1.5701	0.1001
H	-1.0628	-0.9333	1.7310
H	-3.0685	-2.1932	1.0161
H	-4.6254	1.3652	-0.8666
H	-2.6068	2.6216	-0.1457
N	-5.1286	-1.2198	-0.3836
O	-5.2170	-2.4244	-0.0950
O	-6.0162	-0.6246	-1.0159
O	-0.5344	2.9460	1.4141

r1_5a_SR
Final geometry with 48 atoms:

N	-2.9502	3.1173	0.4003
C	-2.0070	2.6276	1.4217
C	-2.1910	3.4474	-0.8187
C	-3.8975	2.0351	0.0803
N	-1.6828	1.0256	-0.4587
C	-1.3908	1.2635	1.0110
C	-1.2618	2.2769	-1.2244
C	-3.1838	0.8642	-0.6416
H	-2.5319	2.5140	2.3733
H	-1.2222	3.3768	1.5522
H	-1.5895	4.3425	-0.6411
H	-2.9023	3.6677	-1.6185
H	-4.6921	2.4247	-0.5610
H	-4.3499	1.6876	1.0123
H	-1.8340	0.4327	1.5573
H	-0.3086	1.2476	1.1305
H	-0.2192	2.4592	-0.9579
H	-1.3275	2.0425	-2.2882
H	-3.3619	0.8610	-1.7182
H	-3.4811	-0.0946	-0.2252
C	-0.9084	-0.1459	-1.0480
C	-0.8036	-1.4978	-0.3004
C	-2.1485	-2.0696	0.1122
O	-2.7861	-2.6377	-0.9230
O	-2.6357	-1.9989	1.2318
C	-4.1209	-3.1461	-0.6696
H	-4.4596	-3.5499	-1.6232
H	-4.7749	-2.3339	-0.3417
H	-4.0860	-3.9307	0.0899
H	-1.3633	-0.3117	-2.0264
H	0.1061	0.2234	-1.2032
H	-0.4327	-2.1581	-1.0929
C	0.2127	-1.6707	0.8785

```
 H  -0.1834  -1.1195   1.7492
 C   1.5654  -1.0438   0.5379
 C   2.1326  -0.0634   1.3681
 C   3.3882   0.4744   1.0998
 C   4.0840   0.0192  -0.0247
 C   3.5522  -0.9652  -0.8705
 C   2.3023  -1.4914  -0.5755
 H   1.5848   0.2818   2.2403
 H   3.8196   1.2311   1.7440
 H   4.1089  -1.3042  -1.7357
 H   1.8905  -2.2636  -1.2177
 N   5.3873   0.5802  -0.3245
 O   5.8523   1.4533   0.4249
 O   5.9996   0.1726  -1.3237
 O   0.3681  -3.0235   1.1482

r1_TS1
Final geometry with  32 atoms:
 N   3.0746  -0.9578   0.1284
 C   1.9304  -1.7294  -0.4023
 C   3.3460   0.1775  -0.7789
 C   2.7031  -0.4253   1.4560
 N   1.0080   0.5392  -0.0663
 C   0.6744  -0.8155  -0.5560
 C   2.0972   1.1130  -0.8834
 C   1.4272   0.4683   1.3493
 H   1.7284  -2.5574   0.2839
 H   2.2166  -2.1537  -1.3694
 H   3.6102  -0.2239  -1.7619
 H   4.2099   0.7282  -0.3946
 H   3.5474   0.1523   1.8445
 H   2.5308  -1.2688   2.1315
 H  -0.1759  -1.1807   0.0273
 H   0.3620  -0.7249  -1.5996
 H   1.7386   1.1993  -1.9135
 H   2.3086   2.1180  -0.5054
 H   1.6164   1.4886   1.6963
 H   0.5900   0.0592   1.9226
 C  -0.6643   1.7110  -0.1890
 C  -1.7472   1.1828   0.4978
 C  -2.6611   0.2825  -0.1332
 O  -3.6449  -0.1499   0.7247
 O  -2.6495  -0.1041  -1.3182
 C  -4.6346  -1.0434   0.1802
 H  -5.3095  -1.2693   1.0073
 H  -4.1698  -1.9641  -0.1852
 H  -5.1874  -0.5641  -0.6333
 H  -0.1253   2.5503   0.2406
 H  -0.6502   1.6582  -1.2747
 H  -1.8897   1.3855   1.5542

r1_3
Final geometry with  32 atoms:
 C  -4.6967   0.7956   0.2348
 O  -3.6179  -0.0047   0.7350
 C  -2.5425  -0.2367  -0.1378
 O  -2.5725   0.3030  -1.2847
 C  -1.5696  -1.0645   0.4070
 C  -0.3727  -1.4483  -0.3503
 N   0.9089  -0.5383  -0.1246
 C   1.3349  -0.5807   1.3208
 C   0.6261   0.8926  -0.5100
 C   2.0437  -1.0487  -0.9781
 H  -1.7076  -1.4399   1.4151
 H  -5.4181   0.8618   1.0526
 H  -4.3595   1.8016  -0.0372
 H  -5.1729   0.3292  -0.6348
 H  -0.0002  -2.4412  -0.0845
 H  -0.5186  -1.3941  -1.4325
 H   0.2407   0.8793  -1.5301
 H  -0.1585   1.2470   0.1587
 C   1.9400   1.7123  -0.3831
 H   1.7287  -0.9396  -2.0179
 C   3.3225  -0.2264  -0.6579
 H   2.1674  -2.1102  -0.7536
 C   2.5339   0.3866   1.5199
 H   0.4681  -0.2966   1.9185
 H   1.5953  -1.6187   1.5401
 H   2.2392   1.2341   2.1445
 H   3.3536  -0.1356   2.0201
 H   4.0655  -0.8569  -0.1626
 H   3.7619   0.1538  -1.5838
 N   3.0162   0.9107   0.2288
 H   2.2763   2.0434  -1.3692
 H   1.7679   2.5994   0.2321

r1_TS2_SS
Final geometry with  48 atoms:
 H   0.3500   1.7749  -1.9652
 C   4.3268   0.1971   0.2388
 C   3.8334  -0.0263  -1.0525
 C   2.6441   0.5853  -1.4243
 C   1.9494   1.4109  -0.5229
 C   2.4787   1.6371   0.7604
 C   3.6615   1.0281   1.1524
 H   4.3678  -0.6692  -1.7408
 H   2.2373   0.4094  -2.4158
 H   1.9442   2.2796   1.4524
 H   4.0664   1.1857   2.1446
 C  -1.8878   0.7873  -0.7288
 H  -1.9790   1.8703  -0.6060
 H  -1.9574   0.5369  -1.7895
 N  -3.2031   0.2376  -0.1123
 C  -4.3755   0.7560  -0.9200
 H  -4.2944   0.3026  -1.9097
 H  -4.2554   1.8370  -1.0113
 C  -3.3694   0.7048   1.3179
 H  -3.4637   1.7918   1.2792
 H  -2.4611   0.4430   1.8601
 C  -3.2410  -1.2750  -0.1356
 H  -2.9852  -1.5911  -1.1472
 H  -2.4678  -1.6192   0.5518
 C  -0.6313   0.2787  -0.1330
 H  -0.4053   0.5398   0.8944
 C  -0.0468  -0.9205  -0.6262
 O   0.8782  -1.4550   0.2377
 O  -0.2501  -1.4540  -1.7379
 C   1.5855  -2.6278  -0.2074
 H   0.8988  -3.4729  -0.3190
 H   2.0985  -2.4447  -1.1544
 H   2.3147  -2.8416   0.5756
 C   0.6674   2.0370  -0.9432
 O   0.2036   3.0643  -0.3850
 C  -5.6907   0.3655  -0.1968
 H  -6.1533   1.2453   0.2578
 H  -6.3955  -0.0554  -0.9185
 C  -4.6248   0.0183   1.9180
 H  -4.3317  -0.7482   2.6401
 H  -5.2347   0.7609   2.4389
 C  -4.6586  -1.7395   0.2925
 H  -5.2073  -2.1319  -0.5677
 H  -4.5745  -2.5371   1.0351
 N  -5.4343  -0.6238   0.8662
 N   5.5580  -0.4516   0.6433
 O   5.9955  -0.2479   1.7870
 O   6.1377  -1.1951  -0.1643

r1_TS2_SR
Final geometry with  48 atoms:
 N  -4.9502  -1.1156  -0.7633
 C  -4.2121  -0.3816  -1.8086
 C  -4.2084  -2.3493  -0.4428
 C  -5.0081  -0.2771   0.4482
 N  -2.5659  -0.5401   0.0491
 C  -2.8477   0.1322  -1.2770
 C  -2.7208  -2.0367  -0.1354
 C  -3.5955  -0.0778   1.0581
 H  -4.8159   0.4647  -2.1460
 H  -4.0627  -1.0531  -2.6581
 H  -4.2709  -3.0382  -1.2890
 H  -4.6862  -2.8232   0.4185
 H  -5.6607  -0.7530   1.1847
 H  -5.4467   0.6867   0.1772
 H  -2.8551   1.2063  -1.0893
 H  -2.0187  -0.1066  -1.9437
 H  -2.0585  -2.3162  -0.9569
 H  -2.3747  -2.5149   0.7827
 H  -3.4376  -0.6767   1.9571
 H  -3.3917   0.9684   1.2843
 C  -1.1321  -0.2452   0.5439
 C  -0.7550   1.1837   0.6379
 C  -0.1407   1.8228  -0.4777
 O  -0.0370   3.1833  -0.3138
 O   0.3453   1.2719  -1.4848
 C   0.6502   3.9074  -1.3526
 H   0.6309   4.9526  -1.0401
 H   0.1351   3.7941  -2.3114
 H   1.6842   3.5647  -1.4502
 H  -1.0867  -0.7287   1.5252
 H  -0.4800  -0.7790  -0.1497
 H  -1.3184   1.8226   1.3077
 C   0.8171   1.0484   2.2699
 H   0.8704   2.1471   2.2571
 C   1.8585   0.3763   1.4435
 C   2.7091   1.1415   0.6248
 C   3.6886   0.5330  -0.1471
 C   3.8147  -0.8617  -0.0934
 C   2.9852  -1.6487   0.7180
 C   2.0153  -1.0218   1.4870
 H   2.5934   2.2209   0.5904
 H   4.3439   1.1197  -0.7791
 H   3.1071  -2.7247   0.7441
 H   1.3677  -1.6101   2.1281
 N   4.8327  -1.5080  -0.8963
 O   5.5682  -0.8075  -1.6102
 O   4.9398  -2.7440  -0.8490
 O   0.2469   0.4525   3.2264

r1_5_SS
Final geometry with  48 atoms:
 H  -0.4109  -1.3736  -2.0624
 C   1.9421  -0.7667  -0.9732
 H   2.0337  -1.8518  -1.0359
 H   2.0365  -0.3384  -1.9730
 N   3.1596  -0.2996  -0.1934
 C   4.3939  -0.5603  -1.0452
 H   4.3239   0.1153  -1.8998
 H   4.3332  -1.5917  -1.3958
 C   3.3171  -1.0698   1.1063
 H   3.4989  -2.1085   0.8254
 H   2.3767  -1.0062   1.6518
 C   3.1141   1.1833   0.1237
 H   2.8581   1.7070  -0.7984
 H   2.3222   1.3271   0.8592
 C   0.5838  -0.4215  -0.3772
 C  -0.4673  -1.5020  -0.9606
 O  -0.1532  -2.7639  -0.5456
 C  -4.4122  -0.2415   0.2540
 C  -3.5788  -0.8804   1.1832
 C  -2.3169  -1.2882   0.7733
 C  -1.8719  -1.0610  -0.5405
 C  -2.7325  -0.4238  -1.4480
 C  -4.0045  -0.0090  -1.0632
 H  -3.9170  -1.0462   2.1989
 H  -1.6601  -1.7888   1.4774
 H  -2.4021  -0.2463  -2.4674
 H  -4.6673   0.4820  -1.7654
 C   0.1260   0.9689  -0.7275
 O  -0.4812   1.5820   0.3000
 O   0.2245   1.4740  -1.8411
 C  -1.0889   2.8688   0.0276
 H  -0.3285   3.5848  -0.2941
 H  -1.8578   2.7640  -0.7419
 H  -1.5338   3.1811   0.9720
 C   4.4938  -0.4496   1.9033
 H   4.1178   0.1394   2.7436
 H   5.1232  -1.2494   2.3016
 C   4.4989   1.6088   0.6802
 H   5.0496   2.1851  -0.0674
 H   4.3570   2.2394   1.5613
 C   5.6551  -0.3004  -0.1834
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 H    6.1271   -1.2445    0.1000
 H    6.3771    0.2823   -0.7611
 N    5.3079    0.4327    1.0477
 H    0.5617   -0.5504    0.7063
 N   -5.7348    0.1883    0.6703
 O   -6.4666    0.7598   -0.1521
 O   -6.0935   -0.0264    1.8381

r1_5_SR
Final geometry with  48 atoms:
 N   -4.9804   -1.1278   -0.6781
 C   -4.4399   -0.0247   -1.4930
 C   -4.1595   -2.3298   -0.9135
 C   -4.8701   -0.7569    0.7447
 N   -2.5124   -0.6649   -0.0517
 C   -3.0332    0.4023   -0.9965
 C   -2.6522   -2.0112   -0.7467
 C   -3.3868   -0.6894    1.1898
 H   -5.1187    0.8301   -1.4396
 H   -4.3914   -0.3574   -2.5329
 H   -4.3431   -2.7011   -1.9249
 H   -4.4689   -3.1017   -0.2045
 H   -5.3980   -1.4950    1.3538
 H   -5.3568    0.2117    0.8852
 H   -3.0668    1.3359   -0.4340
 H   -2.3153    0.4930   -1.8116
 H   -2.1363   -1.9173   -1.7039
 H   -2.1361   -2.7490   -0.1304
 H   -3.0787   -1.5667    1.7615
 H   -3.1751    0.2061    1.7728
 C   -1.0475   -0.4653    0.3078
 C   -0.6688    0.9214    0.8061
 C   -0.3174    1.8729   -0.3072
 O   -0.4239    3.1520    0.0880
 O    0.0758    1.5557   -1.4243
 C   -0.0232    4.1667   -0.8663
 H   -0.1717    5.1169   -0.3537
 H   -0.6500    4.1112   -1.7599
 H    1.0277    4.0367   -1.1365
 H   -0.8447   -1.1966    1.0908
 H   -0.4776   -0.7248   -0.5849
 H   -1.4641    1.3717    1.4023
 C    0.5403    0.8014    1.8901
 H    0.7558    1.8611    2.1341
 C    1.7933    0.2629    1.1864
 C    2.6621    1.1347    0.5067
 C    3.7898    0.6601   -0.1526
 C    4.0506   -0.7151   -0.1245
 C    3.2144   -1.6091    0.5551
 C    2.0961   -1.1080    1.2118
 H    2.4545    2.2013    0.4969
 H    4.4562    1.3358   -0.6750
 H    3.4401   -2.6686    0.5679
 H    1.4469   -1.7830    1.7585
 N    5.2224   -1.2265   -0.8119
 O    5.9632   -0.4299   -1.4078
 O    5.4475   -2.4460   -0.7858
 O    0.1394    0.0690    2.9637

r1_5'_SR
Final geometry with  54 atoms:
 N    4.7202   -1.9717    0.2697
 C    4.1982   -1.4527    1.5466
 C    3.8383   -3.0604   -0.1897
 C    4.6840   -0.8849   -0.7268
 N    2.3033   -1.1010   -0.0309
 C    2.8310   -0.7469    1.3472
 C    2.3542   -2.6142   -0.1758
 C    3.2247   -0.5022   -1.0806
 H    4.9151   -0.7439    1.9682
 H    4.0964   -2.2896    2.2421
 H    3.9638   -3.9277    0.4635
 H    4.1425   -3.3467   -1.1996
 H    5.2047   -1.2055   -1.6327
 H    5.2165   -0.0242   -0.3143
 H    2.9253    0.3389    1.3819
 H    2.0853   -1.0715    2.0729
 H    1.8023   -3.0216    0.6730
 H    1.8330   -2.8691   -1.1003
 H    2.9034   -0.9153   -2.0381
 H    3.0728    0.5761   -1.0944
 C    0.8670   -0.6508   -0.2383
 C    0.5803    0.8076    0.0936
 C    0.1862    1.0262    1.5329
 O    0.3345    2.3127    1.8847
 O   -0.2637    0.1764    2.2923
 C   -0.0994    2.6837    3.2171
 H    0.0922    3.7537    3.2930
 H    0.4776    2.1366    3.9669
 H   -1.1653    2.4749    3.3375
 H    0.6636   -0.8274   -1.2949
 H    0.2484   -1.3169    0.3641
 H    1.4407    1.4463   -0.1117
 C   -0.5395    1.3905   -0.9140
 H   -0.6886    2.4276   -0.5610
 C   -1.8656    0.6595   -0.6972
 C   -2.7394    1.0595    0.3288
 C   -3.9373    0.3923    0.5553
 C   -4.2626   -0.6931   -0.2668
 C   -3.4221   -1.1080   -1.3060
 C   -2.2309   -0.4214   -1.5149
 H   -2.4819    1.9086    0.9559
 H   -4.6086    0.7040    1.3462
 H   -3.6984   -1.9467   -1.9336
 H   -1.5745   -0.7184   -2.3251
 N   -5.5100   -1.4023   -0.0400
 O   -6.2505   -1.0303    0.8823
 O   -5.7959   -2.3602   -0.7735
 O   -0.0838    1.3317   -2.2056
 H    1.2164    2.1666   -2.3133
 O    2.0507    2.7609   -2.3470
 C    1.7348    3.9741   -1.6683
 H    0.8361    4.4524   -2.0854
 H    1.5694    3.8111   -0.5923
 H    2.5749    4.6684   -1.7823

r1_TS3_SSR
Final geometry with  64 atoms:
 H    0.3245   -1.0654   -0.9690
 C    2.8760   -0.6934   -0.4798
 H    2.6954   -1.6657   -0.0204
 H    2.8889   -0.8095   -1.5649
 N    4.2819   -0.2994   -0.0729
 C    5.2539   -1.2603   -0.7440
 H    5.1925   -1.0581   -1.8147
 H    4.8954   -2.2718   -0.5472
 C    4.4803   -0.4101    1.4295
 H    4.3631   -1.4668    1.6755
 H    3.6911    0.1595    1.9181
 C    4.6384    1.1109   -0.5067
 H    4.3585    1.2110   -1.5562
 H    4.0392    1.7897    0.1012
 C    1.7649    0.2713   -0.0686
 C    0.4228   -0.5563    0.0049
 O    0.5179   -1.4738    1.0479
 C   -0.1357   -3.1397    0.6053
 H    0.0128   -3.4750    1.6448
 O    0.5687   -3.6573   -0.3208
 C   -4.0921   -1.7482   -0.2456
 C   -3.3201   -2.2636   -1.2907
 C   -2.0542   -2.7609   -0.9972
 C   -1.5683   -2.7455    0.3170
 C   -2.3966   -2.2913    1.3561
 C   -3.6563   -1.7760    1.0852
 H   -3.6855   -2.2329   -2.3099
 H   -1.4177   -3.1303   -1.7940
 H   -2.0251   -2.2905    2.3763
 H   -4.2821   -1.3806    1.8757
 C   -3.0687    1.9047    0.5275
 C   -2.2229    1.6798    1.6218
 C   -1.0836    0.9098    1.4315
 C   -0.7812    0.3684    0.1715
 C   -1.6230    0.6490   -0.9129
 C   -2.7760    1.4099   -0.7457
 H   -2.4696    2.0803    2.5975
 H   -0.4363    0.6937    2.2748
 H   -1.3962    0.2366   -1.8907
 H   -3.4454    1.5961   -1.5764
 C    1.5836    1.4051   -1.0576
 O    1.3409    2.5708   -0.4485
 O    1.5970    1.2697   -2.2739
 C    1.0205    3.6999   -1.3013
 H    0.8359    4.5293   -0.6194
 H    1.8624    3.9235   -1.9609
 H    0.1267    3.4790   -1.8899
 C    5.8898    0.1342    1.7785
 H    5.8137    1.1182    2.2478
 H    6.3756   -0.5442    2.4842
 C    6.1587    1.3250   -0.2804
 H    6.6898    1.3206   -1.2354
 H    6.3211    2.2947    0.1964
 C    6.6718   -1.0108   -0.1721
 H    6.9571   -1.8167    0.5086
 H    7.3951   -0.9830   -0.9908
 N    6.7237    0.2621    0.5698
 H    1.9251    0.6911    0.9261
 N   -5.3638   -1.1146   -0.5544
 O   -5.9435   -0.4797    0.3377
 O   -5.8174   -1.2110   -1.7040
 N   -4.3028    2.6469    0.7268
 O   -5.0890    2.7649   -0.2234
 O   -4.5335    3.1325    1.8439

r1_TS3_SSS
Final geometry with  64 atoms:
 H    0.8257   -1.1114   -0.5162
 C   -1.0813    1.3561    1.0011
 H   -1.6996    0.5896    1.4673
 H   -0.5036    1.8511    1.7813
 N   -2.0610    2.3869    0.4736
 C   -2.7455    3.0459    1.6626
 H   -1.9766    3.6273    2.1738
 H   -3.0908    2.2465    2.3199
 C   -3.1388    1.7374   -0.3786
 H   -3.7013    1.0833    0.2901
 H   -2.6523    1.1299   -1.1402
 C   -1.3824    3.4769   -0.3363
 H   -0.5279    3.8269    0.2432
 H   -1.0321    3.0188   -1.2616
 C   -0.1504    0.7466   -0.0523
 C    0.1134   -0.7737    0.2549
 O    0.6366   -0.9026    1.5335
 C    1.7318   -2.3812    1.6702
 H    1.7307   -2.2947    2.7692
 O    1.2073   -3.4073    1.1285
 C    5.1660   -0.5560   -0.1283
 C    4.4181   -1.4720   -0.8746
 C    3.3186   -2.0768   -0.2742
 C    2.9559   -1.7557    1.0420
 C    3.7293   -0.8358    1.7686
 C    4.8410   -0.2332    1.1958
 H    4.6929   -1.7011   -1.8969
 H    2.7308   -2.8037   -0.8242
 H    3.4474   -0.5838    2.7869
 H    5.4360    0.4839    1.7478
 C   -3.5773   -2.8891   -0.4401
 C   -3.1071   -2.7628    0.8709
 C   -1.9052   -2.0957    1.0880
 C   -1.1797   -1.5553    0.0183
 C   -1.6718   -1.7098   -1.2895
 C   -2.8671   -2.3735   -1.5317
 H   -3.6705   -3.1767    1.6984
 H   -1.5172   -1.9931    2.0948
 H   -1.1101   -1.3064   -2.1275
 H   -3.2453   -2.4916   -2.5397
 C    1.1801    1.4784   -0.1303
 O    1.8286    1.1806   -1.2626
 O    1.6234    2.2396    0.7172
 C    3.0931    1.8544   -1.4950
 H    3.7397    1.7687   -0.6219
 H    3.5350    1.3534   -2.3553
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 H    2.9043    2.9079   -1.7185
 C   -4.0130    2.8565   -0.9984
 H   -3.7763    2.9842   -2.0576
 H   -5.0672    2.5806   -0.9152
 C   -2.4176    4.6004   -0.6096
 H   -2.2050    5.4742    0.0113
 H   -2.3551    4.9030   -1.6577
 C   -3.9071    3.9269    1.1389
 H   -4.8701    3.4500    1.3382
 H   -3.8913    4.8915    1.6522
 N   -3.7881    4.1435   -0.3145
 H   -0.5859    0.7886   -1.0528
 N    6.2931    0.1109   -0.7583
 O    6.9891    0.8789   -0.0783
 O    6.5170   -0.0991   -1.9593
 N   -4.8354   -3.5765   -0.6779
 O   -5.2453   -3.6864   -1.8428
 O   -5.4623   -4.0291    0.2909

r1_TS3_SRR
Final geometry with  64 atoms:
 H    0.5470   -1.1690    0.7018
 C   -1.0960    0.6116   -0.5416
 H   -1.2525    0.5689   -1.6187
 H   -1.4902   -0.2991   -0.0964
 N   -1.9858    1.7221   -0.0171
 C   -1.4830    3.1070   -0.3806
 H   -1.2491    3.1005   -1.4457
 H   -0.5720    3.2774    0.1938
 C   -2.1367    1.6364    1.4916
 H   -1.1399    1.6069    1.9300
 H   -2.6455    0.6917    1.6929
 C   -3.3667    1.5484   -0.6347
 H   -3.2535    1.7643   -1.6985
 H   -3.6491    0.5033   -0.5095
 C    0.3935    0.7507   -0.2210
 C    1.0211   -0.7037   -0.1797
 O    0.7194   -1.3915   -1.3434
 C    0.3536   -3.1725   -1.0084
 H    0.4572   -3.4086   -2.0796
 O    1.1799   -3.6703   -0.1782
 C   -3.6788   -2.3548    0.1800
 C   -2.7327   -2.6612    1.1636
 C   -1.4361   -2.9721    0.7648
 C   -1.0831   -2.9605   -0.5931
 C   -2.0652   -2.6922   -1.5609
 C   -3.3660   -2.3840   -1.1862
 H   -3.0042   -2.6410    2.2120
 H   -0.6836   -3.2103    1.5085
 H   -1.7958   -2.6922   -2.6130
 H   -4.1220   -2.1544   -1.9268
 C    5.2272   -0.3595    0.6699
 C    4.8230   -0.7029   -0.6244
 C    3.4627   -0.8334   -0.8857
 C    2.5147   -0.6202    0.1239
 C    2.9510   -0.2875    1.4172
 C    4.3034   -0.1537    1.7025
 H    5.5570   -0.8596   -1.4055
 H    3.1260   -1.1014   -1.8807
 H    2.2218   -0.1304    2.2073
 H    4.6411    0.1022    2.6993
 C    1.1323    1.5892   -1.2451
 O    2.1286    2.2868   -0.6850
 O    0.8943    1.6019   -2.4448
 C    2.9972    3.0256   -1.5809
 H    2.4260    3.7912   -2.1118
 H    3.7474    3.4839   -0.9373
 H    3.4671    2.3432   -2.2931
 C   -2.9451    2.8671    1.9742
 H   -3.6936    2.5459    2.7029
 H   -2.2859    3.5918    2.4586
 C   -4.3489    2.5156    0.0694
 H   -4.9740    3.0080   -0.6797
 H   -5.0026    1.9676    0.7527
 C   -2.5895    4.1368   -0.0251
 H   -2.1384    4.9907    0.4860
 H   -3.0773    4.5002   -0.9330
 N   -3.6170    3.5344    0.8441
 H    0.5559    1.1925    0.7636
 N   -5.0174   -1.9620    0.5882
 O   -5.8292   -1.6177   -0.2827
 O   -5.3009   -1.9670    1.7949
 N    6.6454   -0.2142    0.9532
 O    6.9962    0.1034    2.0991
 O    7.4611   -0.4092    0.0405

r1_TS3_SRS
Final geometry with  64 atoms:
 H   -0.6709    1.0919   -1.0054
 C   -3.0037    0.8100    0.2835
 H   -3.1266    1.1466    1.3126
 H   -2.7845    1.6778   -0.3404
 N   -4.3625    0.3141   -0.1713
 C   -5.3976    1.3669    0.2015
 H   -5.0229    2.3292   -0.1503
 H   -5.4446    1.3749    1.2917
 C   -4.7611   -0.9895    0.4980
 H   -4.5846   -0.8725    1.5677
 H   -4.1066   -1.7655    0.0996
 C   -4.4112    0.1237   -1.6779
 H   -4.2709    1.1139   -2.1149
 H   -3.5782   -0.5162   -1.9664
 C   -1.8655   -0.2079    0.1872
 C   -0.5239    0.5911   -0.0328
 O   -0.3527    1.5326    0.9741
 C    0.3010    3.1045    0.3224
 H    0.0961    3.6127    1.2786
 O   -0.3422    3.4653   -0.7199
 C    4.2749    1.5548    0.0136
 C    3.5041    1.6748   -1.1470
 C    2.2454    2.2551   -1.0499
 C    1.7456    2.6748    0.1911
 C    2.5682    2.6060    1.3268
 C    3.8380    2.0485    1.2496
 H    3.8741    1.2969   -2.0921
 H    1.6172    2.3379   -1.9301
 H    2.1891    2.9458    2.2864
 H    4.4621    1.9528    2.1297
 C    2.9570   -1.8816   -0.5673
 C    2.0818   -1.6980   -1.6448
 C    0.9377   -0.9354   -1.4452
 C    0.6674   -0.3529   -0.1970
 C    1.5346   -0.5995    0.8752
 C    2.6864   -1.3565    0.7006
 H    2.3127   -2.1150   -2.6174
 H    0.2685   -0.7502   -2.2809
 H    1.3268   -0.1514    1.8396
 H    3.3769   -1.5159    1.5195
 C   -1.7420   -1.0685    1.4293
 O   -1.2851   -2.2922    1.1346
 O   -1.9755   -0.6951    2.5703
 C   -0.9966   -3.1713    2.2512
 H   -1.9118   -3.3779    2.8116
 H   -0.6067   -4.0842    1.8023
 H   -0.2491   -2.7149    2.9044
 C   -6.2514   -1.2725    0.1720
 H   -6.3667   -2.3208   -0.1142
 H   -6.8750   -1.0870    1.0501
 C   -5.7786   -0.5071   -2.0478
 H   -6.1925    0.0090   -2.9176
 H   -5.6554   -1.5625   -2.3034
 C   -6.7509    0.9838   -0.4482
 H   -7.5525    1.1031    0.2850
 H   -6.9659    1.6347   -1.2992
 N   -6.7283   -0.4111   -0.9247
 H   -1.9784   -0.8673   -0.6757
 N    5.5409    0.8448   -0.0558
 O    6.2840    0.8471    0.9367
 O    5.8269    0.2387   -1.0983
 N    4.2015   -2.5994   -0.7797
 O    5.0070   -2.6886    0.1580
 O    4.4251   -3.0934   -1.8949

r1_6_SSR
Final geometry with  64 atoms:
 H    0.3160   -1.0621   -1.0106
 C    2.8715   -0.7275   -0.5012
 H    2.6780   -1.7001   -0.0480
 H    2.8873   -0.8404   -1.5867
 N    4.2784   -0.3490   -0.0857
 C    5.2429   -1.3203   -0.7537
 H    5.1887   -1.1161   -1.8244
 H    4.8719   -2.3279   -0.5598
 C    4.4673   -0.4652    1.4179
 H    4.3359   -1.5208    1.6609
 H    3.6830    0.1134    1.9036
 C    4.6540    1.0577   -0.5153
 H    4.3836    1.1615   -1.5670
 H    4.0589    1.7432    0.0889
 C    1.7682    0.2506   -0.0927
 C    0.4171   -0.5356   -0.0532
 O    0.4937   -1.4620    1.0157
 C   -0.0932   -2.8720    0.7127
 H   -0.0123   -3.2792    1.7402
 O    0.5875   -3.5180   -0.2128
 C   -4.1532   -1.7822   -0.2073
 C   -3.3756   -2.3757   -1.2061
 C   -2.0841   -2.7849   -0.8858
 C   -1.5751   -2.6055    0.4059
 C   -2.4102   -2.0823    1.4067
 C   -3.6957   -1.6516    1.1101
 H   -3.7578   -2.4693   -2.2155
 H   -1.4431   -3.2094   -1.6511
 H   -2.0251   -1.9575    2.4144
 H   -4.3260   -1.2018    1.8675
 C   -3.0477    1.9435    0.4910
 C   -2.1524    1.7856    1.5566
 C   -1.0186    1.0093    1.3593
 C   -0.7747    0.3972    0.1195
 C   -1.6620    0.6148   -0.9418
 C   -2.8118    1.3787   -0.7641
 H   -2.3565    2.2415    2.5177
 H   -0.3317    0.8460    2.1831
 H   -1.4762    0.1476   -1.9032
 H   -3.5201    1.5146   -1.5720
 C    1.6171    1.3987   -1.0765
 O    1.4289    2.5682   -0.4598
 O    1.6166    1.2649   -2.2920
 C    1.1593    3.7172   -1.3050
 H    1.0237    4.5511   -0.6173
 H    2.0061    3.8996   -1.9709
 H    0.2501    3.5441   -1.8859
 C    5.8817    0.0607    1.7755
 H    5.8153    1.0439    2.2478
 H    6.3555   -0.6261    2.4812
 C    6.1752    1.2542   -0.2784
 H    6.7121    1.2474   -1.2301
 H    6.3451    2.2203    0.2031
 C    6.6606   -1.0878   -0.1743
 H    6.9337   -1.8987    0.5054
 H    7.3881   -1.0657   -0.9896
 N    6.7231    0.1823    0.5714
 H    1.9275    0.6601    0.9066
 N   -5.4525   -1.2341   -0.5557
 O   -6.0305   -0.5076    0.2654
 O   -5.9328   -1.4912   -1.6697
 N   -4.2763    2.6945    0.7044
 O   -5.1056    2.7541   -0.2132
 O   -4.4558    3.2439    1.8004

r1_6_SSS
Final geometry with  64 atoms:
 H    0.7535   -1.1977   -0.6028
 C   -1.0587    1.3227    0.9556
 H   -1.6856    0.5758    1.4415
 H   -0.4448    1.8030    1.7171
 N   -2.0228    2.3792    0.4517
 C   -2.6598    3.0539    1.6589
 H   -1.8631    3.6122    2.1531
 H   -3.0113    2.2623    2.3224
 C   -3.1391    1.7622   -0.3746
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 H  -3.7039   1.1241   0.3075
 H  -2.6904   1.1427  -1.1496
 C  -1.3342   3.4525  -0.3730
 H  -0.4557   3.7765   0.1855
 H  -1.0222   2.9869  -1.3084
 C  -0.1730   0.6853  -0.1219
 C   0.0573  -0.8341   0.1625
 O   0.6075  -0.9599   1.4544
 C   1.6100  -2.1277   1.6204
 H   1.6992  -2.0891   2.7247
 O   1.1831  -3.2716   1.1216
 C   5.2741  -0.5763  -0.0543
 C   4.5408  -1.5160  -0.7868
 C   3.3681  -2.0211  -0.2345
 C   2.9166  -1.5854   1.0192
 C   3.6717  -0.6363   1.7268
 C   4.8548  -0.1282   1.2049
 H   4.8843  -1.8415  -1.7613
 H   2.7927  -2.7665  -0.7731
 H   3.3250  -0.2906   2.6967
 H   5.4380   0.6045   1.7492
 C  -3.7022  -2.8501  -0.3940
 C  -3.1982  -2.7149   0.9031
 C  -1.9710  -2.0832   1.0803
 C  -1.2553  -1.5880  -0.0174
 C  -1.7821  -1.7473  -1.3101
 C  -3.0033  -2.3775  -1.5112
 H  -3.7546  -3.0945   1.7514
 H  -1.5599  -1.9743   2.0769
 H  -1.2288  -1.3756  -2.1680
 H  -3.4090  -2.5019  -2.5077
 C   1.1716   1.3906  -0.2479
 O   1.7792   1.0620  -1.3924
 O   1.6491   2.1585   0.5732
 C   3.0535   1.7007  -1.6689
 H   3.7339   1.5798  -0.8262
 H   3.4411   1.1980  -2.5539
 H   2.8894   2.7626  -1.8703
 C  -3.9954   2.9079  -0.9715
 H  -3.7789   3.0320  -2.0355
 H  -5.0546   2.6610  -0.8649
 C  -2.3437   4.6054  -0.6174
 H  -2.0912   5.4707   0.0004
 H  -2.2983   4.9097  -1.6659
 C  -3.8082   3.9687   1.1654
 H  -4.7791   3.5188   1.3875
 H  -3.7523   4.9311   1.6801
 N  -3.7186   4.1859  -0.2900
 H  -0.6383   0.7359  -1.1086
 N   6.4916  -0.0291  -0.6268
 O   7.1457   0.7932   0.0317
 O   6.8378  -0.3943  -1.7602
 N  -4.9879  -3.5017  -0.5897
 O  -5.4286  -3.6179  -1.7422
 O  -5.6038  -3.9172   0.4019

r1_6_SRR
Final geometry with  64 atoms:
 H   1.2168  -1.9672   0.8982
 C   0.3255   1.1442  -0.3801
 H   1.1555   1.8399  -0.2523
 H   0.3642   0.7243  -1.3852
 N  -0.9434   1.9781  -0.3491
 C  -1.2520   2.5308   1.0303
 H  -0.3397   2.9931   1.4066
 H  -1.5198   1.6830   1.6620
 C  -2.1363   1.1693  -0.8242
 H  -2.1764   0.2660  -0.2246
 H  -1.9356   0.9047  -1.8626
 C  -0.7654   3.1556  -1.2960
 H  -0.0009   3.7935  -0.8493
 H  -0.3956   2.7565  -2.2418
 C   0.3910   0.0194   0.6522
 C   1.2251  -1.2124   0.1035
 O   0.6142  -1.7303  -1.0486
 C  -0.1983  -3.0847  -0.8513
 H  -0.0941  -3.4479  -1.8917
 O   0.2919  -3.8613   0.0827
 C  -4.2001  -1.5872  -0.2797
 C  -3.4499  -1.9619   0.8424
 C  -2.1728  -2.4763   0.6478
 C  -1.6361  -2.5991  -0.6431
 C  -2.4250  -2.2478  -1.7492
 C  -3.7088  -1.7395  -1.5814
 H  -3.8562  -1.8384   1.8390
 H  -1.5718  -2.7700   1.5021
 H  -2.0212  -2.3550  -2.7523
 H  -4.3114  -1.4492  -2.4334
 C   5.3151  -0.0975  -0.6223
 C   4.4088  -0.0604  -1.6867
 C   3.0897  -0.4355  -1.4533
 C   2.6723  -0.8381  -0.1753
 C   3.6096  -0.8754   0.8703
 C   4.9335  -0.5067   0.6592
 H   4.7305   0.2537  -2.6722
 H   2.3787  -0.4220  -2.2715
 H   3.3034  -1.2051   1.8588
 H   5.6557  -0.5407   1.4657
 C   0.9511   0.4719   1.9863
 O   0.6066  -0.3741   2.9645
 O   1.6597   1.4526   2.1633
 C   1.1447  -0.1038   4.2846
 H   0.7946   0.8687   4.6394
 H   0.7627  -0.9040   4.9176
 H   2.2368  -0.1240   4.2554
 C  -3.4176   2.0228  -0.6570
 H  -4.0278   1.9445  -1.5600
 H  -4.0109   1.6586   0.1856
 C  -2.1283   3.8775  -1.4495
 H  -1.9788   4.9570  -1.3679
 H  -2.5651   3.6664  -2.4287
 C  -2.4221   3.5431   0.9022
 H  -3.1554   3.3505   1.6891
 H  -2.0541   4.5652   1.0205
 N  -3.0798   3.4372  -0.4126
 H  -0.5952  -0.4019   0.8449
 N  -5.5081  -0.9855  -0.0856
 O  -6.1422  -0.6014  -1.0790
 O  -5.9430  -0.8591   1.0683
 N   6.6982   0.2936  -0.8570
 O   7.4962   0.2591   0.0896
 O   7.0317   0.6503  -1.9954

r1_6_SRS
Final geometry with  64 atoms:
 H   0.6093  -1.1044  -1.0011
 C   2.9646  -0.8732   0.2675
 H   3.0910  -1.2094   1.2964
 H   2.7201  -1.7379  -0.3509
 N   4.3264  -0.4029  -0.2029
 C   5.3461  -1.4743   0.1600
 H   4.9499  -2.4301  -0.1863
 H   5.4046  -1.4818   1.2497
 C   4.7566   0.8940   0.4605
 H   4.5893   0.7816   1.5323
 H   4.1130   1.6818   0.0674
 C   4.3622  -0.2148  -1.7103
 H   4.1987  -1.2027  -2.1445
 H   3.5385   0.4403  -1.9909
 C   1.8478   0.1710   0.1806
 C   0.4903  -0.5772  -0.0455
 O   0.3105  -1.5114   0.9945
 C  -0.2941  -2.8839   0.5484
 H  -0.1926  -3.4010   1.5218
 O   0.3515  -3.4303  -0.4615
 C  -4.3903  -1.7125  -0.0688
 C  -3.5449  -1.8295  -1.1782
 C  -2.2423  -2.2711  -0.9771
 C  -1.7734  -2.5636   0.3113
 C  -2.6560  -2.4756   1.3987
 C  -3.9675  -2.0516   1.2225
 H  -3.8987  -1.5665  -2.1676
 H  -1.5653  -2.3599  -1.8199
 H  -2.3011  -2.7108   2.3984
 H  -4.6451  -1.9627   2.0630
 C  -2.8066   2.1434  -0.5085
 C  -1.9682   1.8916  -1.6006
 C  -0.9023   1.0172  -1.4281
 C  -0.6697   0.4007  -0.1895
 C  -1.5131   0.6887   0.8915
 C  -2.5897   1.5547   0.7415
 H  -2.1603   2.3555  -2.5603
 H  -0.2557   0.7916  -2.2715
 H  -1.3372   0.2103   1.8477
 H  -3.2530   1.7661   1.5711
 C   1.7552   1.0315   1.4303
 O   1.3437   2.2711   1.1416
 O   1.9814   0.6432   2.5669
 C   1.0946   3.1573   2.2629
 H   2.0205   3.3275   2.8176
 H   0.7361   4.0852   1.8188
 H   0.3349   2.7260   2.9189
 C   6.2482   1.1492   0.1183
 H   6.3794   2.1948  -0.1706
 H   6.8777   0.9532   0.9897
 C   5.7370   0.3904  -2.0955
 H   6.1317  -0.1343  -2.9691
 H   5.6304   1.4476  -2.3511
 C   6.6988  -1.1168  -0.5050
 H   7.5063  -1.2505   0.2192
 H   6.8921  -1.7722  -1.3577
 N   6.6967   0.2779  -0.9826
 H   1.9775   0.8329  -0.6780
 N  -5.7406  -1.2122  -0.2610
 O  -6.4951  -1.1329   0.7197
 O  -6.0958  -0.8713  -1.3991
 N  -3.9425   3.0354  -0.6805
 O  -4.7120   3.2126   0.2743
 O  -4.1056   3.5899  -1.7768

r1_TS4_SSR
Final geometry with  64 atoms:
 H   0.1669   0.6481  -0.2799
 C   0.2436  -1.8591  -0.9146
 H   0.2930  -1.1074  -1.7039
 H   0.8695  -2.7027  -1.2077
 N  -1.1929  -2.3924  -1.0129
 C  -1.3720  -3.0763  -2.3548
 H  -0.7479  -3.9717  -2.3332
 H  -0.9954  -2.3959  -3.1208
 C  -2.1912  -1.2583  -0.9277
 H  -2.0313  -0.6384  -1.8118
 H  -1.9551  -0.6830  -0.0382
 C  -1.5023  -3.4071   0.0703
 H  -0.6905  -4.1348   0.0707
 H  -1.5049  -2.8721   1.0181
 C   0.6557  -1.3037   0.4330
 C   0.8911   0.2407   0.4373
 O   0.6576   0.8392   1.7211
 C  -0.6660   0.6350   2.2704
 H  -0.5693   1.0463   3.2884
 O  -1.0094  -0.7053   2.3109
 C  -3.6020   3.0346   0.2106
 C  -4.0084   1.8714   0.8722
 C  -3.0465   1.1098   1.5273
 C  -1.6975   1.4950   1.5250
 C  -1.3237   2.6797   0.8724
 C  -2.2676   3.4541   0.2051
 H  -5.0483   1.5687   0.8654
 H  -3.3385   0.1944   2.0293
 H  -0.2838   2.9875   0.8722
 H  -1.9782   4.3607  -0.3124
 C   4.8231   1.3423  -0.9147
 C   4.5850   1.2557   0.4608
 C   3.3106   0.9156   0.9005
 C   2.2762   0.6610  -0.0163
 C   2.5432   0.7759  -1.3919
 C   3.8116   1.1095  -1.8523
 H   5.3809   1.4506   1.1693
 H   3.1161   0.8485   1.9627
 H   1.7493   0.6152  -2.1142
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 H    4.0121    1.1991   -2.9130
 C    1.6044   -2.1634    1.1340
 O    2.2028   -1.5603    2.1902
 O    1.8183   -3.3609    0.8848
 C    3.1216   -2.3533    2.9679
 H    3.4947   -1.6830    3.7433
 H    2.6081   -3.2056    3.4217
 H    3.9492   -2.7073    2.3467
 C   -3.6173   -1.8574   -0.8710
 H   -4.0199   -1.7874    0.1429
 H   -4.2775   -1.2978   -1.5384
 C   -2.8820   -4.0464   -0.2383
 H   -2.7580   -5.0711   -0.5982
 H   -3.4814   -4.0768    0.6751
 C   -2.8759   -3.4043   -2.5437
 H   -3.3292   -2.7224   -3.2677
 H   -2.9827   -4.4239   -2.9226
 N   -3.6073   -3.2788   -1.2684
 H   -0.3286   -1.1882    1.3869
 N   -4.5965    3.8305   -0.4954
 O   -4.2306    4.8583   -1.0819
 O   -5.7764    3.4533   -0.4885
 N    6.1533    1.6966   -1.3818
 O    6.3555    1.7805   -2.6019
 O    7.0449    1.9019   -0.5459

r1_TS4_SSS
Final geometry with  64 atoms:
 H    0.7208    0.0967   -1.6628
 C    2.5468   -1.1875   -0.3785
 H    2.6119   -0.9334   -1.4379
 H    3.4960   -0.9290    0.0950
 N    2.5303   -2.7262   -0.3754
 C    3.8617   -3.2194   -0.9112
 H    4.6159   -2.9353   -0.1751
 H    4.0553   -2.6882   -1.8449
 C    1.4359   -3.2681   -1.2727
 H    1.6910   -2.9589   -2.2882
 H    0.4995   -2.8023   -0.9728
 C    2.3524   -3.2934    1.0192
 H    3.0666   -2.7861    1.6662
 H    1.3420   -3.0431    1.3393
 C    1.3747   -0.5017    0.2919
 C    0.5841    0.4728   -0.6383
 O   -0.8225    0.4911   -0.3620
 C   -1.4293   -0.8226   -0.4510
 H   -1.2176   -1.1949   -1.4741
 O   -0.9177   -1.6704    0.5097
 C   -5.6620   -0.1506   -0.1734
 C   -5.0622   -1.0291    0.7325
 C   -3.6884   -1.2438    0.6433
 C   -2.9285   -0.5919   -0.3340
 C   -3.5584    0.2803   -1.2366
 C   -4.9266    0.5118   -1.1637
 H   -5.6552   -1.5287    1.4888
 H   -3.2021   -1.9209    1.3359
 H   -2.9699    0.7827   -1.9980
 H   -5.4167    1.1864   -1.8550
 C    2.1326    4.4846   -0.4864
 C    0.8483    4.2441    0.0103
 C    0.3357    2.9520   -0.0509
 C    1.0913    1.9037   -0.5984
 C    2.3769    2.1793   -1.0974
 C    2.9073    3.4616   -1.0460
 H    0.2656    5.0503    0.4392
 H   -0.6556    2.7563    0.3376
 H    2.9730    1.3840   -1.5327
 H    3.8975    3.6685   -1.4328
 C    1.6774   -0.0257    1.6383
 O    0.7199    0.7968    2.1371
 O    2.6535   -0.3553    2.3290
 C    0.9307    1.3229    3.4624
 H    1.8583    1.9007    3.5054
 H    0.0752    1.9720    3.6536
 H    0.9630    0.5148    4.1986
 C    1.3886   -4.8101   -1.1151
 H    0.5157   -5.1051   -0.5270
 H    1.3090   -5.2765   -2.1005
 C    2.5835   -4.8263    0.9594
 H    3.5397   -5.0861    1.4211
 H    1.7894   -5.3367    1.5101
 C    3.7802   -4.7546   -1.1123
 H    3.7131   -4.9988   -2.1757
 H    4.6819   -5.2243   -0.7111
 N    2.5961   -5.3121   -0.4333
 H    0.2672   -1.3013    0.5099
 N   -7.0980    0.0824   -0.0864
 O   -7.6229    0.8687   -0.8864
 O   -7.7470   -0.5123    0.7846
 N    2.6765    5.8301   -0.4224
 O    3.8200    6.0335   -0.8564
 O    1.9816    6.7335    0.0648

r1_TS4_SRR
Final geometry with  64 atoms:
 N   -1.2190    3.8607   -2.4292
 C   -0.8026    4.5347   -1.1846
 C   -0.0180    3.6237   -3.2525
 C   -1.8072    2.5539   -2.0760
 N    0.4890    2.4097   -1.1372
 C    0.0527    3.5934   -0.2972
 C    1.1006    2.9492   -2.4168
 C   -0.7293    1.5937   -1.5196
 H   -1.6909    4.8485   -0.6303
 H   -0.2356    5.4298   -1.4534
 H    0.3456    4.5762   -3.6463
 H   -0.3004    2.9914   -4.0982
 H   -2.2701    2.1112   -2.9619
 H   -2.5904    2.7205   -1.3316
 H   -0.5172    3.1961    0.5404
 H    0.9565    4.0727    0.0787
 H    1.8785    3.6534   -2.1163
 H    1.5611    2.1089   -2.9394
 H   -0.3891    0.8691   -2.2621
 H   -1.0632    1.0655   -0.6321
 C    1.5370    1.5401   -0.4269
 C    1.2387    1.1337    1.0034
 C    2.0112    1.8806    1.9863
 O    2.0041    1.3313    3.2333
 O    2.5751    2.9674    1.7831
 C    2.6488    2.0872    4.2796
 H    2.5367    1.4835    5.1811
 H    2.1608    3.0569    4.4123
 H    3.7087    2.2338    4.0540
 H    1.6380    0.6740   -1.0832
 H    2.4574    2.1231   -0.4876
 H   -0.0542    1.3667    1.4168
 C    1.0552   -0.3896    1.2450
 H    1.1755   -0.5789    2.3181
 C    2.0661   -1.2459    0.5120
 C    3.4168   -1.1555    0.8939
 C    4.3950   -1.8885    0.2367
 C    4.0097   -2.7200   -0.8229
 C    2.6762   -2.8308   -1.2243
 C    1.7090   -2.0902   -0.5492
 H    3.7023   -0.5036    1.7140
 H    5.4342   -1.8218    0.5343
 H    2.4020   -3.4800   -2.0469
 H    0.6715   -2.1687   -0.8511
 N    5.0256   -3.4892   -1.5229
 O    6.2050   -3.3939   -1.1544
 O    4.6814   -4.2157   -2.4661
 O   -0.2658   -0.8013    0.8614
 C   -1.2816   -0.2404    1.7441
 H   -1.0914   -0.6693    2.7464
 C   -2.5978   -0.7923    1.2134
 C   -3.5166    0.0300    0.5508
 C   -4.7023   -0.4977    0.0457
 C   -4.9546   -1.8615    0.2190
 C   -4.0559   -2.7057    0.8814
 C   -2.8784   -2.1573    1.3768
 H   -3.3022    1.0857    0.4313
 H   -5.4165    0.1320   -0.4707
 H   -4.2782   -3.7585    1.0051
 H   -2.1673   -2.7943    1.8950
 N   -6.1944   -2.4220   -0.3038
 O   -6.9887   -1.6714   -0.8861
 O   -6.4128   -3.6311   -0.1494
 O   -1.2241    1.1388    1.7692

r1_TS4_SRS
Final geometry with  64 atoms:
 N   -4.4905   -3.4604   -0.9795
 C   -3.7317   -3.9661    0.1809
 C   -5.3359   -2.3390   -0.5296
 C   -3.5305   -2.9495   -1.9770
 N   -3.0307   -1.5832    0.0384
 C   -2.7002   -2.9185    0.6750
 C   -4.5046   -1.3077    0.2752
 C   -2.8142   -1.6774   -1.4593
 H   -3.2107   -4.8843   -0.1022
 H   -4.4426   -4.2084    0.9751
 H   -6.1449   -2.7238    0.0966
 H   -5.7813   -1.8699   -1.4108
 H   -4.0602   -2.7187   -2.9051
 H   -2.8032   -3.7381   -2.1873
 H   -1.6859   -3.1721    0.3732
 H   -2.7277   -2.7761    1.7550
 H   -4.6664   -1.3911    1.3516
 H   -4.6989   -0.2805   -0.0380
 H   -3.2296   -0.7615   -1.8843
 H   -1.7424   -1.7039   -1.6390
 C   -2.2201   -0.4303    0.6466
 C   -0.7193   -0.6213    0.7463
 C   -0.2637   -0.9185    2.0982
 O    1.0758   -0.7600    2.2768
 O   -0.9726   -1.3626    3.0151
 C    1.6293   -1.2037    3.5312
 H    2.7007   -1.0138    3.4545
 H    1.4454   -2.2719    3.6779
 H    1.2047   -0.6369    4.3645
 H   -2.4788    0.4249    0.0201
 H   -2.6649   -0.2779    1.6317
 H   -0.2213   -1.7013    0.0523
 C    0.1465    0.3595   -0.0926
 H    1.1414    0.3961    0.3615
 C   -0.3817    1.7783   -0.1101
 C   -0.4016    2.4941    1.1007
 C   -0.8973    3.7891    1.1565
 C   -1.3850    4.3699   -0.0216
 C   -1.3798    3.6831   -1.2380
 C   -0.8748    2.3855   -1.2735
 H   -0.0257    2.0282    2.0069
 H   -0.9070    4.3421    2.0876
 H   -1.7638    4.1529   -2.1352
 H   -0.8663    1.8428   -2.2111
 N   -1.9113    5.7244    0.0234
 O   -1.9112    6.3286    1.1055
 O   -2.3445    6.2326   -1.0207
 O    0.2776   -0.0990   -1.4480
 C    1.0015   -1.3621   -1.5554
 H    0.9495   -1.5785   -2.6337
 C    2.4697   -1.1139   -1.1878
 C    3.1978   -0.1513   -1.9055
 C    4.5220    0.1237   -1.5871
 C    5.1147   -0.5856   -0.5350
 C    4.4168   -1.5541    0.1914
 C    3.0904   -1.8124   -0.1461
 H    2.7184    0.3932   -2.7136
 H    5.0862    0.8681   -2.1355
 H    4.8987   -2.0862    1.0026
 H    2.5253   -2.5515    0.4095
 N    6.5012   -0.3055   -0.1876
 O    7.1102    0.5667   -0.8224
 O    7.0274   -0.9475    0.7318
 O    0.3975   -2.3537   -0.8117

r1_7_SSR
Final geometry with  64 atoms:
 N   -4.5982   -3.1097   -0.9792
 C   -4.5574   -2.6802    0.4318
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C	-5.4563	-2.1748	-1.7301
C	-3.2322	-3.0349	-1.5286
N	-3.6814	-0.6991	-0.7915
C	-3.8616	-1.3008	0.5826
C	-5.0195	-0.7042	-1.4937
C	-2.7246	-1.5689	-1.5734
H	-4.0192	-3.4305	1.0169
H	-5.5841	-2.6310	0.8038
H	-6.4938	-2.3066	-1.4123
H	-5.3911	-2.4269	-2.7918
H	-3.2275	-3.4590	-2.5361
H	-2.5769	-3.6442	-0.9005
H	-2.8661	-1.3790	1.0201
H	-4.4514	-0.5976	1.1699
H	-5.7142	-0.1642	-0.8471
H	-4.9005	-0.1520	-2.4280
H	-2.6965	-1.1677	-2.5886
H	-1.7416	-1.4646	-1.1172
C	-3.1564	0.7846	-0.7070
C	-1.9265	1.0006	0.0901
C	-2.0009	1.3220	1.4432
O	-3.2753	1.5278	1.9458
O	-1.0176	1.4405	2.2448
C	-3.3927	1.7010	3.3665
H	-4.4634	1.7948	3.5593
H	-2.8767	2.6053	3.7031
H	-2.9949	0.8339	3.9036
H	-3.0244	1.0545	-1.7585
H	-4.0151	1.3277	-0.3115
H	-0.3512	-0.1141	2.2179
C	-0.6009	0.9046	-0.6115
O	0.1701	-0.3380	-0.3870
C	0.9016	-0.4984	0.8115
O	0.0995	-0.9336	1.8889
H	-0.8278	0.7922	-1.6775
H	1.3689	0.4567	1.0902
C	0.3262	2.1232	-0.5497
C	-0.1423	3.3843	-0.1500
C	1.6496	2.0148	-1.0169
C	0.6797	4.5058	-0.1956
H	-1.1629	3.4925	0.1978
C	2.4894	3.1202	-1.0699
H	2.0281	1.0519	-1.3408
C	1.9920	4.3597	-0.6538
H	0.3122	5.4742	0.1215
H	3.5067	3.0275	-1.4303
C	2.0023	-1.5171	0.5664
C	2.4314	-1.8345	-0.7305
C	2.6454	-2.1051	1.6677
C	3.4780	-2.7300	-0.9333
H	1.9450	-1.3834	-1.5863
C	3.6947	-2.9993	1.4860
H	2.3219	-1.8607	2.6731
C	4.0970	-3.3014	0.1810
H	3.8073	-2.9795	-1.9345
H	4.1920	-3.4525	2.3348
N	2.8596	5.5252	-0.7045
O	2.4020	6.6256	-0.3643
O	4.0299	5.3824	-1.0864
N	5.1955	-4.2374	-0.0228
O	5.7287	-4.7538	0.9682
O	5.5595	-4.4855	-1.1801

r1_7_SSS
Final geometry with 64 atoms:

H	1.1072	0.5955	-1.8312
C	0.6272	2.8067	-0.6393
H	0.8656	2.8007	-1.7062
H	1.0616	3.7000	-0.1882
N	-0.9135	3.1173	-0.6318
C	-1.1513	4.4719	-1.2576
H	-0.6927	5.2089	-0.5955
H	-0.6316	4.4833	-2.2177
C	-1.6696	2.0875	-1.4355
H	-1.3326	2.1908	-2.4690
H	-1.3772	1.1090	-1.0655
C	-1.4624	3.1449	0.7750
H	-0.8233	3.8072	1.3580
H	-1.3714	2.1327	1.1672
C	1.0632	1.5601	0.0352
C	1.2033	0.3052	-0.7782
O	0.1230	-0.6971	-0.6642
C	-0.4832	-0.8857	0.5989
H	-0.7751	0.0964	1.0003
O	0.3648	-1.5214	1.5290
C	-4.1189	-3.1195	0.1040
C	-3.4145	-3.2185	1.3071
C	-2.2267	-2.5073	1.4450
C	-1.7408	-1.7102	0.3969
C	-2.4701	-1.6304	-0.8005
C	-3.6606	-2.3325	-0.9566
H	-3.7879	-3.8366	2.1144
H	-1.6715	-2.5733	2.3732
H	-2.1040	-1.0228	-1.6188
H	-4.2220	-2.2729	-1.8809
C	5.0882	-1.5727	-0.6444
C	3.9506	-2.3833	-0.5851
C	2.6957	-1.7828	-0.6107
C	2.5636	-0.3880	-0.6815
C	3.7277	0.3988	-0.7557
C	4.9898	-0.1785	-0.7354
H	4.0466	-3.4603	-0.5190
H	1.8095	-2.4011	-0.5595
H	3.6381	1.4789	-0.8124
H	5.8818	0.4339	-0.7840
C	1.5020	1.5763	1.3626
O	1.4813	2.8115	1.9823
O	1.9199	0.5805	2.0339
C	1.8567	2.8511	3.3689
H	1.1992	2.2186	3.9736
H	1.7435	3.8949	3.6685
H	2.8951	2.5360	3.5094
C	-3.1896	2.3488	-1.2789
H	-3.6459	1.5819	-0.6474
H	-3.6730	2.3131	-2.2587
C	-2.9353	3.6321	0.7240
H	-3.0182	4.6385	1.1427
H	-3.5657	2.9641	1.3167
C	-2.6817	4.6860	-1.4116
H	-2.9723	4.6243	-2.4635
H	-2.9537	5.6775	-1.0406
N	-3.4388	3.6651	-0.6622
H	1.0294	-0.8349	1.8021
N	-5.3665	-3.8559	-0.0483
O	-5.9837	-3.7669	-1.1184
O	-5.7701	-4.5460	0.8975
N	6.4014	-2.1892	-0.6142
O	7.4050	-1.4615	-0.6587
O	6.4826	-3.4249	-0.5454

r1_7_SRR
Final geometry with 64 atoms:

N	0.7657	-2.9361	3.3662
C	0.6864	-3.8322	2.1964
C	2.1851	-2.6368	3.6337
C	0.0791	-1.6747	3.0306
N	1.8607	-1.8322	1.2989
C	1.1794	-3.1226	0.9068
C	2.9027	-2.1445	2.3486
C	0.8317	-0.9106	1.9111
H	-0.3494	-4.1560	2.0648
H	1.2953	-4.7168	2.4014
H	2.6783	-3.5378	4.0078
H	2.2325	-1.8736	4.4149
H	0.0158	-1.0499	3.9254
H	-0.9387	-1.9141	2.7108
H	0.3617	-2.8548	0.2373
H	1.9056	-3.7185	0.3549
H	3.5581	-2.9069	1.9227
H	3.4787	-1.2325	2.5180
H	1.3770	-0.0442	2.2899
H	0.1637	-0.5958	1.1126
C	2.5705	-1.1505	0.0663
C	1.7672	-1.0238	-1.1711
C	1.7763	-2.0290	-2.1405
O	2.6743	-3.0592	-1.9296
O	1.0419	-2.0786	-3.1819
C	2.5909	-4.1900	-2.8115
H	3.3326	-4.9009	-2.4419
H	2.8289	-3.9107	-3.8424
H	1.5947	-4.6426	-2.7777
H	2.8853	-0.1864	0.4718
H	3.4545	-1.7705	-0.0826
H	-0.5489	-1.8487	-2.7008
C	0.8847	0.1612	-1.4398
H	0.7975	0.2799	-2.5264
C	1.4463	1.4629	-0.8966
C	2.6237	1.9713	-1.4752
C	3.2037	3.1433	-1.0098
C	2.5943	3.8129	0.0593
C	1.4224	3.3356	0.6519
C	0.8536	2.1620	0.1643
H	3.0896	1.4353	-2.2968
H	4.1069	3.5346	-1.4617
H	0.9664	3.8707	1.4760
H	-0.0576	1.7883	0.6135
N	3.1942	5.0368	0.5619
O	4.2378	5.4501	0.0356
O	2.6456	5.6300	1.5023
O	-0.4890	0.0095	-0.9265
C	-1.4729	-0.3225	-1.8946
H	-1.3233	0.3120	-2.7820
C	-2.8048	0.0020	-1.2490
C	-3.6254	-0.9947	-0.7067
C	-4.8185	-0.6578	-0.0720
C	-5.1770	0.6904	0.0091
C	-4.3766	1.7054	-0.5274
C	-3.1895	1.3481	-1.1551
H	-3.3343	-2.0360	-0.7811
H	-5.4578	-1.4230	0.3510
H	-4.6784	2.7428	-0.4532
H	-2.5521	2.1208	-1.5747
N	-6.4234	1.0513	0.6724
O	-7.1271	0.1508	1.1492
O	-6.7375	2.2473	0.7385
O	-1.4288	-1.6792	-2.2652

r1_7_SRS
Final geometry with 64 atoms:

N	-5.3898	0.1400	-1.7646
C	-5.2335	-1.2047	-1.1782
C	-5.7236	1.0879	-0.6858
C	-4.1002	0.5409	-2.3565
N	-3.5331	0.1452	0.0349
C	-4.0171	-1.2639	-0.2150
C	-4.7096	0.9810	0.4847
C	-3.0140	0.7161	-1.2633
H	-5.1011	-1.9312	-1.9842
H	-6.1542	-1.4543	-0.6442
H	-6.7314	0.8745	-0.3201
H	-5.7206	2.0981	-1.1036
H	-4.2313	1.4799	-2.9009
H	-3.7987	-0.2281	-3.0725
H	-3.1744	-1.8127	-0.6361
H	-4.2708	-1.6965	0.7523
H	-5.1354	0.4805	1.3566
H	-4.3202	1.9549	0.7880
H	-2.7805	1.7645	-1.0699
H	-2.0981	0.1823	-1.5074
C	-2.4257	0.1889	1.1540
C	-1.2977	-0.7600	1.0157
C	-1.3380	-2.0218	1.6130
O	-2.4554	-2.2910	2.3810
O	-0.4467	-2.9292	1.5156
C	-2.5869	-3.6258	2.8953
H	-3.5395	-3.6376	3.4287
H	-1.7741	-3.8698	3.5861
H	-2.6077	-4.3596	2.0833
H	-2.1076	1.2338	1.1354
H	-2.9931	0.0157	2.0688
H	-0.0229	-3.1358	-0.0831

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 C  -0.0503  -0.4322   0.2485
 H   0.7735  -0.9909   0.7037
 C   0.3411   1.0317   0.3107
 C   0.7833   1.5479   1.5420
 C   1.1480   2.8810   1.6720
 C   1.0611   3.7107   0.5467
 C   0.6264   3.2271  -0.6902
 C   0.2716   1.8854  -0.7987
 H   0.8407   0.8925   2.4060
 H   1.4953   3.2731   2.6200
 H   0.5685   3.8859  -1.5481
 H  -0.0573   1.4993  -1.7550
 N   1.4341   5.1098   0.6676
 O   1.8047   5.5360   1.7711
 O   1.3693   5.8348  -0.3360
 O  -0.1118  -0.8385  -1.1714
 C   0.6550  -1.9769  -1.5416
 H   0.5764  -2.0087  -2.6335
 C   2.1270  -1.7949  -1.1655
 C   2.7908  -0.6393  -1.6099
 C   4.1243  -0.4176  -1.2912
 C   4.7931  -1.3750  -0.5194
 C   4.1619  -2.5387  -0.0737
 C   2.8245  -2.7423  -0.4067
 H   2.2530   0.0964  -2.1984
 H   4.6369   0.4749  -1.6283
 H   4.7024  -3.2646   0.5215
 H   2.3207  -3.6399  -0.0671
 N   6.1904  -1.1517  -0.1719
 O   6.7407  -0.1115  -0.5576
 O   6.7821  -2.0088   0.4980
 O   0.1011  -3.1808  -1.0734

r1_TS7_SS
Final geometry with  54 atoms:
 O  -0.5000   1.5084  -2.1065
 C   1.1130  -0.9336   0.2826
 H   0.7706  -1.7399  -0.3669
 H   0.8864  -1.2058   1.3146
 N   2.6416  -1.0189   0.1887
 C   3.1070  -0.9305  -1.2515
 H   2.6544  -0.0464  -1.6957
 C   4.6545  -0.8585  -1.2605
 H   2.7273  -1.8233  -1.7518
 C   3.0856  -2.3610   0.7393
 H   2.4747  -3.1294   0.2620
 C   4.5964  -2.5413   0.4419
 H   2.8702  -2.3442   1.8091
 C   3.3247   0.0656   0.9997
 C   4.8445  -0.2390   1.0446
 H   3.1130   1.0093   0.5018
 H   2.8657   0.0667   1.9883
 C   0.4940   0.3998  -0.0974
 C   0.0285   1.1542   1.0708
 O  -0.7591   2.2042   0.7404
 O   0.3507   0.9449   2.2495
 C  -1.2094   3.0547   1.8123
 H  -1.8347   3.8111   1.3365
 H  -1.7947   2.4851   2.5395
 H  -0.3586   3.5279   2.3110
 C  -0.4691   0.3092  -1.3254
 H  -0.0664  -0.5010  -1.9482
 H   1.1183   4.0373  -0.6561
 C  -4.4522  -0.8332  -0.1505
 C  -4.1944   0.5112  -0.4392
 C  -2.9134   0.8777  -0.8373
 C  -1.8896  -0.0781  -0.9477
 C  -2.1881  -1.4250  -0.6716
 C  -3.4591  -1.8126  -0.2671
 N  -5.7849  -1.2244   0.2712
 H  -4.9798   1.2519  -0.3503
 H  -2.7012   1.9152  -1.0602
 H  -1.4199  -2.1839  -0.7797
 H  -3.6824  -2.8512  -0.0561
 C   1.9998   3.3922  -0.5088
 H   2.0556   3.1553   0.5668
 H   2.8936   3.9840  -0.7581
 O  -6.0025  -2.4160   0.5381
 O  -6.6661  -0.3559   0.3545
 H   5.4053   0.6776   0.8445
 H   5.1337  -0.6067   2.0325
 N   5.2115  -1.2608   0.0454
 H   5.1009  -2.9254   1.3321
 H   4.7439  -3.2587  -0.3695
 H   5.0465  -1.5169  -2.0401
 H   4.9871   0.1605  -1.4751
 H   0.3918   1.9347  -2.0063
 H   1.3696   1.3037  -0.6340
 O   1.9413   2.2181  -1.3050

r1_TS7_SR
Final geometry with  54 atoms:
 N  -4.3763  -2.3368  -0.3014
 C  -4.4547  -1.0974  -1.0968
 C  -3.3645  -3.2203  -0.9087
 C  -3.9355  -1.9884   1.0621
 N  -2.0741  -1.1541  -0.3648
 C  -3.1376  -0.2819  -1.0028
 C  -2.0277  -2.4658  -1.1279
 C  -2.4768  -1.4650   1.0630
 H  -5.2869  -0.4900  -0.7316
 H  -4.6621  -1.3691  -2.1352
 H  -3.7371  -3.5897  -1.8676
 H  -3.2161  -4.0779  -0.2476
 H  -4.0081  -2.8713   1.7025
 H  -4.6125  -1.2255   1.4554
 H  -3.2418   0.5986  -0.3706
 H  -2.7606   0.0193  -1.9788
 H  -1.8632  -2.2085  -2.1759
 H  -1.1680  -3.0276  -0.7580
 H  -1.7658  -2.2098   1.4251
 H  -2.3728  -0.5547   1.6464
 C  -0.6781  -0.5183  -0.4277
 C  -0.5450   0.9166   0.0576
 C  -0.5186   1.8876  -1.0394
 O  -0.0780   3.1202  -0.6733
 O  -0.9162   1.6783  -2.1933
 C  -0.1617   4.1638  -1.6652
 H   0.2269   5.0576  -1.1757
 H  -1.2004   4.3216  -1.9695
 H   0.4473   3.9173  -2.5393
 H  -0.0611  -1.1952   0.1649
 H  -0.3835  -0.6149  -1.4744
 H  -1.5809   1.3405   0.8170
 C   0.5285   1.1056   1.1665
 H   0.7009   2.1808   1.2777
 C   1.8578   0.4649   0.8215
 C   2.6554   1.0529  -0.1785
 C   3.8592   0.4790  -0.5627
 C   4.2708  -0.7026   0.0679
 C   3.5049  -1.3064   1.0688
 C   2.3003  -0.7147   1.4396
 H   2.3281   1.9698  -0.6587
 H   4.4720   0.9346  -1.3309
 H   3.8441  -2.2177   1.5462
 H   1.6986  -1.1729   2.2156
 N   5.5289  -1.3131  -0.3262
 O   6.2010  -0.7738  -1.2174
 O   5.8915  -2.3551   0.2394
 O   0.0555   0.5787   2.4126
 H  -0.8439   0.9722   2.5259
 O  -2.3415   1.7245   1.7853
 C  -2.3382   3.1431   1.8113
 H  -1.3506   3.5544   2.0812
 H  -2.6183   3.5729   0.8348
 H  -3.0620   3.5155   2.5524

r1_TS7a_SR
Final geometry with  54 atoms:
 N  -2.1285   3.8302   0.0547
 C  -1.1767   3.3444   1.0688
 C  -1.4760   3.7696  -1.2652
 C  -3.2967   2.9323   0.0388
 N  -1.3986   1.3980  -0.4732
 C  -0.5942   1.9594   0.6771
 C  -1.1970   2.3025  -1.6797
 C  -2.8651   1.4471  -0.0914
 H  -1.6991   3.2780   2.0265
 H  -0.3625   4.0658   1.1737
 H  -0.5424   4.3357  -1.2139
 H  -2.1217   4.2439  -2.0086
 H  -3.9369   3.2167  -0.8002
 H  -3.8655   3.0659   0.9625
 H  -0.6657   1.2540   1.5021
 H   0.4387   2.0203   0.3344
 H  -0.1712   2.1603  -2.0226
 H  -1.8852   1.9479  -2.4491
 H  -3.4222   0.9170  -0.8626
 H  -2.9626   0.9167   0.8555
 C  -0.9370  -0.0230  -0.8811
 C  -0.9921  -1.1688   0.1117
 C  -2.3371  -1.5080   0.6206
 O  -3.2592  -1.5643  -0.3733
 O  -2.6408  -1.7664   1.7887
 C  -4.6179  -1.8529   0.0134
 H  -5.1953  -1.8189  -0.9110
 H  -4.9858  -1.1009   0.7175
 H  -4.6855  -2.8467   0.4644
 H  -1.5589  -0.2553  -1.7462
 H   0.0863   0.1183  -1.2282
 H  -0.7650  -2.1216  -0.7526
 C   0.0829  -1.2970   1.2015
 H  -0.2058  -0.7662   2.1174
 C   1.4665  -0.8259   0.7842
 C   2.1351   0.1591   1.5239
 C   3.4157   0.5757   1.1701
 C   4.0258  -0.0174   0.0620
 C   3.3913  -1.0152  -0.6878
 C   2.1140  -1.4157  -0.3161
 H   1.6490   0.6114   2.3829
 H   3.9297   1.3403   1.7395
 H   3.8883  -1.4617  -1.5403
 H   1.6055  -2.1877  -0.8851
 N   5.3633   0.4133  -0.3225
 O   5.9179   1.3000   0.3413
 O   5.9020  -0.1198  -1.3019
 O   0.1548  -2.7117   1.5172
 H   0.6703  -2.8107   2.3323
 O  -0.6037  -3.0444  -1.7046
 C  -1.3396  -4.1728  -1.2916
 H  -1.6453  -4.1046  -0.2301
 H  -2.2673  -4.3120  -1.8785
 H  -0.7557  -5.1062  -1.3867

r1_TS7b_SR
Final geometry with  54 atoms:
 N  -1.7073   3.9626   0.1038
 C  -0.7786   3.3502   1.0701
 C  -1.1215   3.8505  -1.2436
 C  -2.9710   3.2044   0.1260
 N  -1.2856   1.4724  -0.4890
 C  -0.3753   1.9162   0.6322
 C  -1.0357   2.3692  -1.6907
 C  -2.7185   1.6820  -0.0414
 H  -1.2676   3.3252   2.0472
 H   0.1168   3.9715   1.1529
 H  -0.1262   4.3018  -1.2245
 H  -1.7362   4.4118  -1.9519
 H  -3.6076   3.5746  -0.6818
 H  -3.4836   3.3861   1.0741
 H  -0.4910   1.2054   1.4479
 H   0.6425   1.8692   0.2457
 H  -0.0505   2.1163  -2.0854
 H  -1.7960   2.1115  -2.4303
 H  -3.3666   1.2337  -0.7929
 H  -2.8367   1.1498   0.9023
 C  -1.0029   0.0083  -0.9338
 C  -1.1200  -1.1203   0.0633
 C  -2.4616  -1.3732   0.6099
 O  -3.4392  -1.2364  -0.3247
 O  -2.7283  -1.7373   1.7598
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 C  -4.7958  -1.4464   0.1144
 H  -5.4160  -1.2568  -0.7624
 H  -5.0536  -0.7498   0.9173
 H  -4.9345  -2.4749   0.4592
 H  -1.6971  -0.1434  -1.7611
 H   0.0061   0.0516  -1.3416
 H  -0.9605  -2.1765  -0.7384
 C  -0.0096  -1.4187   1.0975
 H  -0.2507  -0.9903   2.0752
 C   1.3879  -0.9573   0.7088
 C   2.1160  -0.1212   1.5679
 C   3.4142   0.2741   1.2589
 C   3.9844  -0.1856   0.0689
 C   3.2917  -1.0334  -0.8036
 C   1.9982  -1.4166  -0.4720
 H   1.6604   0.2313   2.4883
 H   3.9719   0.9224   1.9236
 H   3.7579  -1.3822  -1.7169
 H   1.4547  -2.0813  -1.1351
 N   5.3396   0.2246  -0.2697
 O   5.9508   0.9671   0.5113
 O   5.8377  -0.1805  -1.3291
 O   0.0432  -2.8498   1.3286
 H  -0.0748  -3.2801   0.4460
 O  -0.6681  -3.3191  -1.2980
 C  -1.8511  -4.1000  -1.3258
 H  -2.3961  -4.0621  -0.3661
 H  -2.5505  -3.7693  -2.1127
 H  -1.6158  -5.1583  -1.5191

r1_TS7c_SR
Final geometry with  54 atoms:
 N  -4.6874  -1.9402  -0.3233
 C  -4.5380  -0.8227  -1.2746
 C  -3.7621  -3.0174  -0.7189
 C  -4.3022  -1.4626   1.0189
 N  -2.2483  -1.0761  -0.3281
 C  -3.1362  -0.1682  -1.1584
 C  -2.3267  -2.4695  -0.9264
 C  -2.7872  -1.1482   1.0872
 H  -5.3073  -0.0735  -1.0709
 H  -4.6982  -1.2089  -2.2847
 H  -4.1156  -3.4752  -1.6464
 H  -3.7707  -3.7813   0.0629
 H  -4.5513  -2.2266   1.7600
 H  -4.8864  -0.5662   1.2433
 H  -3.1723   0.7927  -0.6490
 H  -2.6489  -0.0446  -2.1250
 H  -2.0678  -2.3693  -1.9821
 H  -1.5732  -3.0829  -0.4292
 H  -2.2182  -1.9331   1.5887
 H  -2.5889  -0.1926   1.5679
 C  -0.7879  -0.6209  -0.3406
 C  -0.5263   0.8159   0.0946
 C  -0.2745   1.7127  -1.0467
 O   0.2166   2.9207  -0.6783
 O  -0.5470   1.4706  -2.2273
 C   0.4295   3.8876  -1.7286
 H   0.8343   4.7689  -1.2301
 H  -0.5148   4.1322  -2.2224
 H   1.1447   3.5056  -2.4623
 H  -0.2881  -1.3293   0.3198
 H  -0.4479  -0.8049  -1.3615
 H  -1.5572   1.4387   0.6290
 C   0.5095   0.9172   1.2392
 H   0.6658   1.9760   1.4633
 C   1.8586   0.3093   0.8710
 C   2.7681   1.0623   0.1045
 C   3.9854   0.5250  -0.2931
 C   4.2973  -0.7857   0.0884
 C   3.4224  -1.5545   0.8612
 C   2.2082  -0.9969   1.2502
 H   2.5177   2.0782  -0.1819
 H   4.6841   1.1072  -0.8813
 H   3.6879  -2.5636   1.1521
 H   1.5272  -1.5808   1.8593
 N   5.5680  -1.3590  -0.3232
 O   6.3422  -0.6688  -1.0016
 O   5.8373  -2.5207   0.0151
 O  -0.0715   0.2699   2.3791
 H   0.5174   0.3931   3.1391
 O  -2.5464   2.1617   1.1628
 C  -2.0137   3.1776   1.9847
 H  -1.3483   2.7787   2.7728
 H  -1.4276   3.9230   1.4160
 H  -2.8168   3.7312   2.5016

r1_TS7d_SR
Final geometry with  54 atoms:
 N  -4.6003  -2.0290  -0.3846
 C  -4.5057  -0.8047  -1.2022
 C  -3.6555  -3.0234  -0.9256
 C  -4.1930  -1.7002   0.9952
 N  -2.1874  -1.0954  -0.3436
 C  -3.1252  -0.1205  -1.0293
 C  -2.2433  -2.4086  -1.1035
 C  -2.6849  -1.3545   1.0653
 H  -5.2952  -0.1107  -0.9024
 H  -4.6719  -1.0776  -2.2477
 H  -4.0213  -3.3825  -1.8910
 H  -3.6196  -3.8725  -0.2382
 H  -4.4035  -2.5515   1.6479
 H  -4.7934  -0.8527   1.3363
 H  -3.1815   0.7557  -0.3877
 H  -2.6677   0.1519  -1.9799
 H  -2.0190  -2.1737  -2.1457
 H  -1.4573  -3.0513  -0.7033
 H  -2.0839  -2.1787   1.4534
 H  -2.4951  -0.4612   1.6550
 C  -0.7419  -0.5970  -0.3412
 C  -0.5063   0.7915   0.2391
 C  -0.2867   1.8100  -0.8029
 O   0.1908   2.9784  -0.3084
 O  -0.5625   1.6899  -2.0020
 C   0.3244   4.0751  -1.2349
 H   0.7168   4.9042  -0.6452
 H  -0.6487   4.3397  -1.6583
 H   1.0208   3.8188  -2.0380
 H  -0.2041  -1.3574   0.2249
 H  -0.4251  -0.6589  -1.3838
 H  -1.5228   1.3255   0.8836
 C   0.5413   0.7949   1.3783
 H   0.6737   1.8282   1.7128
 C   1.8982   0.2569   0.9365
 C   2.7799   1.0925   0.2247
 C   4.0018   0.6180  -0.2343
 C   4.3473  -0.7131   0.0291
 C   3.5008  -1.5641   0.7452
 C   2.2812  -1.0691   1.1965
 H   2.5050   2.1236   0.0299
 H   4.6788   1.2638  -0.7802
 H   3.7917  -2.5883   0.9449
 H   1.6218  -1.7185   1.7615
 N   5.6225  -1.2214  -0.4480
 O   6.3721  -0.4592  -1.0753
 O   5.9203  -2.4019  -0.2149
 O  -0.0133   0.0157   2.4466
 H   0.5692   0.0896   3.2175
 O  -2.4468   1.9679   1.5941
 C  -2.8468   3.1125   0.8750
 H  -2.2839   4.0183   1.1676
 H  -2.7075   2.9971  -0.2166
 H  -3.9178   3.3341   1.0287

r1_10_SS
Final geometry with  48 atoms:
 C  -0.5294   0.2622  -0.2353
 C  -0.3052   1.5641  -0.6937
 O   0.5883   2.2777   0.1064
 O  -0.8175   2.1429  -1.6926
 C   1.0141   3.5619  -0.3704
 H   1.7273   3.9272   0.3715
 H   1.5069   3.4775  -1.3445
 H   0.1725   4.2576  -0.4478
 C  -1.4996  -0.5899  -0.9465
 H  -1.6167  -0.3056  -1.9945
 H  -1.2506  -1.6525  -0.8887
 N  -2.9869  -0.5577  -0.4046
 C  -3.0469  -1.0500   1.0212
 H  -2.6920  -2.0826   1.0109
 H  -2.3570  -0.4386   1.6025
 C  -4.5081  -0.9300   1.5329
 C  -3.8451  -1.4553  -1.2634
 H  -3.3665  -2.4362  -1.2862
 C  -5.2761  -1.5112  -0.6609
 H  -3.8349  -1.0313  -2.2694
 C  -3.5531   0.8408  -0.4608
 C  -5.0481   0.7918  -0.0405
 H  -2.9489   1.4503   0.2115
 H  -3.4186   1.1998  -1.4813
 C   0.2537  -0.3027   0.9284
 H  -0.0910  -1.3286   1.0941
 C   4.4545  -0.6622   0.0008
 C   4.0729   0.1968   1.0362
 C   2.7219   0.3125   1.3499
 C   1.7510  -0.4069   0.6377
 C   2.1685  -1.2684  -0.3946
 C   3.5097  -1.4061  -0.7207
 N   5.8589  -0.7911  -0.3302
 H   4.8182   0.7612   1.5835
 H   2.4227   0.9733   2.1548
 H   1.4257  -1.8312  -0.9525
 H   3.8247  -2.0716  -1.5151
 O   0.0086   0.3573   2.1962
 H   0.0965   1.3114   2.0396
 O   6.1895  -1.5515  -1.2541
 O   6.6923  -0.1388   0.3184
 N  -5.4267  -0.5483   0.4452
 H  -6.0134  -1.2807  -1.4342
 H  -5.4878  -2.5124  -0.2766
 H  -4.8341  -1.8847   1.9539
 H  -4.5734  -0.1720   2.3180
 H  -5.2356   1.5199   0.7529
 H  -5.6881   1.0424  -0.8906

r1_10_SR
Final geometry with  48 atoms:
 N  -2.9353  -3.2424   0.3668
 C  -3.8713  -2.1150   0.1972
 C  -2.2908  -3.5186  -0.9310
 C  -1.8938  -2.8403   1.3310
 N  -1.6827  -1.1457  -0.4801
 C  -3.1191  -0.8059  -0.1644
 C  -1.6707  -2.2285  -1.5330
 C  -1.0251  -1.6860   0.7654
 H  -4.4312  -1.9760   1.1257
 H  -4.5819  -2.3753  -0.5917
 H  -3.0348  -3.9265  -1.6203
 H  -1.5192  -4.2773  -0.7761
 H  -1.2612  -3.7032   1.5559
 H  -2.3862  -2.5298   2.2564
 H  -3.0974  -0.0929   0.6602
 H  -3.5344  -0.3141  -1.0433
 H  -2.2452  -1.8492  -2.3804
 H  -0.6330  -2.3715  -1.8416
 H  -0.0296  -2.0217   0.4702
 H  -0.9282  -0.8566   1.4645
 C  -0.9006   0.1117  -1.0315
 C  -0.9489   1.3472  -0.2211
 C  -1.9653   2.2731  -0.5089
 O  -1.9656   3.3989   0.3139
 O  -2.8528   2.1870  -1.4031
 C  -2.9120   4.4302  -0.0038
 H  -2.7452   5.2167   0.7353
 H  -3.9408   4.0645   0.0733
 H  -2.7440   4.8286  -1.0099
 H   0.1101  -0.2809  -1.1625
 H  -1.3521   0.2614  -2.0144
 H  -1.2525   1.5767   2.3036
 C   0.0668   1.6701   0.8434
 H   0.2090   2.7570   0.8593
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 C   1.4315   1.0674   0.5796
 C   2.1875   1.5743  -0.4936
 C   3.4295   1.0434  -0.8111
 C   3.9234  -0.0146  -0.0359
 C   3.2018  -0.5329   1.0427
 C   1.9579   0.0161   1.3440
 H   1.7875   2.3899  -1.0888
 H   4.0077   1.4365  -1.6383
 H   3.6030  -1.3496   1.6305
 H   1.3913  -0.3804   2.1770
 N   5.2180  -0.5857  -0.3614
 O   5.8483  -0.1265  -1.3255
 O   5.6542  -1.5164   0.3326
 O  -0.3338   1.2869   2.2028

r1_10'_SR
Final geometry with  54 atoms:
 N  -3.5115  -3.1345   0.0773
 C  -4.0733  -1.9904  -0.6622
 C  -2.4806  -3.7753  -0.7584
 C  -2.8746  -2.6297   1.3070
 N  -1.6484  -1.4349  -0.5027
 C  -2.9977  -0.9018  -0.9275
 C  -1.4159  -2.7453  -1.2244
 C  -1.6687  -1.7091   0.9809
 H  -4.8955  -1.5639  -0.0817
 H  -4.4803  -2.3585  -1.6077
 H  -2.9604  -4.2305  -1.6287
 H  -2.0100  -4.5706  -0.1745
 H  -2.5404  -3.4783   1.9096
 H  -3.6256  -2.0800   1.8803
 H  -3.1799   0.0040  -0.3518
 H  -2.9192  -0.6395  -1.9821
 H  -1.4855  -2.5313  -2.2925
 H  -0.3994  -3.0676  -0.9915
 H  -0.7103  -2.1721   1.2242
 H  -1.7319  -0.7489   1.4852
 C  -0.4913  -0.4504  -0.8818
 C  -0.5314   0.9248  -0.3141
 C  -1.1023   1.9232  -1.1305
 O  -0.9613   3.2232  -0.6577
 O  -1.7267   1.7445  -2.2114
 C  -1.6717   4.2480  -1.3676
 H  -1.4845   5.1697  -0.8128
 H  -2.7466   4.0424  -1.3912
 H  -1.3012   4.3537  -2.3922
 H   0.3987  -0.9985  -0.5667
 H  -0.5278  -0.4422  -1.9739
 H  -2.3492   1.5137   0.9072
 C   0.3856   1.3030   0.8385
 H   0.4735   2.3927   0.8472
 C   1.7840   0.7525   0.6320
 C   2.6108   1.3648  -0.3280
 C   3.8765   0.8695  -0.6051
 C   4.3195  -0.2654   0.0897
 C   3.5227  -0.8948   1.0508
 C   2.2582  -0.3772   1.3173
 H   2.2481   2.2363  -0.8657
 H   4.5126   1.3464  -1.3406
 H   3.8854  -1.7695   1.5769
 H   1.6334  -0.8542   2.0630
 N   5.6372  -0.7991  -0.1954
 O   6.3364  -0.2402  -1.0548
 O   6.0274  -1.7997   0.4263
 O  -0.0538   0.8851   2.1594
 H  -0.9661   1.2128   2.2778
 O  -2.7708   1.6879   1.7720
 C  -3.0494   3.0943   1.8807
 H  -2.1258   3.6844   1.8815
 H  -3.6944   3.4342   1.0620
 H  -3.5704   3.2446   2.8297

r1_TS8_SS
Final geometry with  48 atoms:
 C  -0.4086   0.1834  -0.4723
 C  -0.2283   1.6003  -0.6621
 O   0.6314   2.1457   0.2524
 O  -0.7596   2.3135  -1.5300
 C   0.9164   3.5532   0.1314
 H   1.6159   3.7763   0.9380
 H   1.3762   3.7711  -0.8366
 H   0.0035   4.1437   0.2490
 C  -1.3229  -0.4874  -1.2695
 H  -1.6862  -0.0037  -2.1707
 H  -1.3143  -1.5729  -1.2926
 N  -3.2274  -0.5086  -0.4598
 C  -3.2390  -1.4131   0.7115
 H  -2.9034  -2.4006   0.3810
 H  -2.5162  -1.0269   1.4347
 C  -4.6849  -1.4608   1.2981
 C  -4.2011  -0.9806  -1.4657
 H  -3.9230  -2.0001  -1.7498
 C  -5.6331  -0.9196  -0.8420
 H  -4.1165  -0.3406  -2.3491
 C  -3.5740   0.8629  -0.0328
 C  -4.9711   0.8346   0.6636
 H  -2.7852   1.2150   0.6388
 H  -3.5764   1.4979  -0.9224
 C   0.3307  -0.5366   0.6391
 H   0.0105  -1.5836   0.6147
 C   4.5949  -0.6162  -0.0086
 C   4.1139  -0.1336   1.2118
 C   2.7387  -0.1067   1.4268
 C   1.8470  -0.5447   0.4378
 C   2.3622  -1.0311  -0.7771
 C   3.7301  -1.0736  -1.0109
 N   6.0283  -0.6473  -0.2427
 H   4.8003   0.2138   1.9744
 H   2.3583   0.2637   2.3715
 H   1.6804  -1.3727  -1.5497
 H   4.1232  -1.4495  -1.9476
 O  -0.0339  -0.0867   1.9594
 H   0.0979   0.8748   1.9907
 O   6.4470  -1.0756  -1.3282
 O   6.7897  -0.2447   0.6490
 N  -5.5667  -0.5167   0.5794
 H  -6.2550  -0.1934  -1.3739
 H  -6.1234  -1.8958  -0.9045
 H  -5.1087  -2.4653   1.2038
 H  -4.6800  -1.1944   2.3594
 H  -4.8868   1.1050   1.7207
 H  -5.6513   1.5462   0.1858

r1_TS8_SR
Final geometry with  48 atoms:
 N  -2.9504  -3.3238   0.4409
 C  -3.7652  -2.1039   0.6319
 C  -2.6809  -3.4942  -1.0034
 C  -1.6616  -3.1381   1.1407
 N  -1.7236  -1.2756  -0.4867
 C  -3.0631  -0.8691  -0.0152
 C  -1.8559  -2.2868  -1.5556
 C  -0.9507  -1.8415   0.6402
 H  -3.9079  -1.9549   1.7067
 H  -4.7486  -2.2654   0.1797
 H  -3.6409  -3.5757  -1.5221
 H  -2.1367  -4.4325  -1.1483
 H  -1.0404  -4.0192   0.9524
 H  -1.8523  -3.0829   2.2170
 H  -2.9365  -0.0474   0.6966
 H  -3.6194  -0.4922  -0.8771
 H  -2.3498  -1.8186  -2.4125
 H  -0.8482  -2.5862  -1.8593
 H   0.0647  -2.0447   0.2892
 H  -0.8972  -1.0784   1.4196
 C  -0.7469   0.4133  -1.2549
 C  -0.8351   1.5267  -0.4367
 C  -1.9946   2.3810  -0.5779
 O  -2.0461   3.3710   0.3638
 O  -2.8879   2.2833  -1.4352
 C  -3.1651   4.2780   0.2962
 H  -3.0216   4.9761   1.1219
 H  -4.1073   3.7365   0.4192
 H  -3.1694   4.8163  -0.6557
 H   0.1789  -0.1478  -1.3159
 H  -1.3791   0.3651  -2.1349
 H  -1.1773   1.9637   2.1184
 C   0.1504   1.8391   0.6763
 H   0.3305   2.9217   0.6805
 C   1.4962   1.1745   0.4776
 C   2.3309   1.6454  -0.5514
 C   3.5616   1.0546  -0.8025
 C   3.9603  -0.0240  -0.0029
 C   3.1588  -0.5062   1.0345
 C   1.9273   0.1011   1.2685
 H   2.0055   2.4799  -1.1654
 H   4.2018   1.4185  -1.5966
 H   3.4882  -1.3402   1.6420
 H   1.2993  -0.2686   2.0687
 N   5.2446  -0.6569  -0.2586
 O   5.9478  -0.2259  -1.1833
 O   5.5949  -1.6081   0.4543
 O  -0.3497   1.4762   1.9894

r1_11
Final geometry with  28 atoms:
 C  -2.9992  -0.9417   1.7375
 C  -2.3263  -0.6806   0.6083
 C  -2.5599   0.5636  -0.1816
 O  -3.6179   1.2745   0.2364
 O  -1.8562   0.9108  -1.1233
 C  -3.8906   2.5090  -0.4721
 H  -4.7725   2.9268   0.0127
 H  -4.0936   2.3013  -1.5257
 H  -3.0421   3.1916  -0.3803
 H  -2.8028  -1.8496   2.3016
 H  -3.7479  -0.2625   2.1313
 H  -2.4282  -2.6425  -1.1548
 C  -1.2723  -1.6415   0.0733
 H  -1.2284  -2.4881   0.7713
 C   0.1182  -1.0278   0.0361
 C   0.6622  -0.5288   1.2314
 C   1.9370   0.0221   1.2594
 C   2.6708   0.0681   0.0688
 C   2.1560  -0.4242  -1.1335
 C   0.8767  -0.9727  -1.1411
 H   0.0819  -0.5702   2.1482
 H   2.3568   0.4062   2.1808
 H   2.7426  -0.3769  -2.0428
 H   0.4664  -1.3506  -2.0693
 N   4.0080   0.6416   0.0843
 O   4.4540   1.0849   1.1518
 O   4.6581   0.6682  -0.9699
 O  -1.6159  -2.1196  -1.2303

r1_11a
Final geometry with  28 atoms:
 C  -2.9710  -0.6859   1.8796
 C  -2.3353  -0.6109   0.7031
 C  -2.5935   0.4841  -0.2727
 O  -3.3976   1.4505   0.1790
 O  -2.1077   0.4902  -1.4030
 C  -3.7120   2.5232  -0.7458
 H  -4.3770   3.1872  -0.1946
 H  -4.2140   2.1212  -1.6292
 H  -2.7983   3.0474  -1.0360
 H  -2.7676  -1.5007   2.5692
 H  -3.7031   0.0551   2.1834
 H  -1.8181  -1.6645  -1.6210
 C  -1.2964  -1.6386   0.2720
 H  -1.2588  -2.4120   1.0460
 C   0.1019  -1.0270   0.1748
 C   0.6038  -0.2886   1.2602
 C   1.8779   0.2647   1.2181
 C   2.6528   0.0719   0.0694
 C   2.1834  -0.6641  -1.0214
 C   0.9053  -1.2125  -0.9580
 H  -0.0074  -0.1417   2.1452
 H   2.2638   0.8350   2.0541
 H   2.8027  -0.8031  -1.8991
 H   0.5336  -1.7870  -1.7984
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 N   3.9864   0.6532   0.0098
 O   4.3989   1.2984   0.9832
 O   4.6651   0.4842  -1.0124
 O  -1.6914  -2.3241  -0.9174

r1_11b
Final geometry with  28 atoms:
 C   3.1002  -1.9164  -0.8632
 C   2.4750  -0.9228  -0.2187
 C   2.7166   0.4840  -0.6586
 O   2.0746   1.3673   0.1217
 O   3.4133   0.8172  -1.6094
 C   2.2141   2.7717  -0.2085
 H   1.6107   3.2987   0.5297
 H   1.8372   2.9555  -1.2174
 H   3.2625   3.0705  -0.1356
 H   2.9488  -2.9531  -0.5767
 H   3.7739  -1.7147  -1.6906
 H   2.0576   0.3389   2.0599
 C   1.5154  -1.1870   0.9360
 H   1.5119  -2.2679   1.1107
 C   0.0786  -0.7838   0.6011
 C  -0.4915  -1.2173  -0.6078
 C  -1.8024  -0.8927  -0.9354
 C  -2.5457  -0.1225  -0.0347
 C  -2.0070   0.3181   1.1769
 C  -0.6927  -0.0199   1.4873
 H   0.0952  -1.8114  -1.3014
 H  -2.2407  -1.2260  -1.8681
 H  -2.6016   0.9119   1.8602
 H  -0.2686   0.3163   2.4262
 N  -3.9191   0.2279  -0.3679
 O  -4.3926  -0.1735  -1.4397
 O  -4.5694   0.9156   0.4309
 O   1.9844  -0.6246   2.1632

r1_11c
Final geometry with  28 atoms:
 C   3.1709  -1.7104  -1.0899
 C   2.4980  -0.8395  -0.3258
 C   2.7277   0.6231  -0.5381
 O   1.8949   1.3842   0.1789
 O   3.5774   1.0894  -1.2905
 C   2.0172   2.8196   0.0283
 H   1.2518   3.2397   0.6801
 H   1.8370   3.1048  -1.0111
 H   3.0119   3.1461   0.3418
 H   3.0325  -2.7812  -0.9710
 H   3.8661  -1.3734  -1.8526
 H   2.7705  -1.3147   2.2590
 C   1.5229  -1.3157   0.7447
 H   1.5257  -2.4135   0.7085
 C   0.0917  -0.8723   0.4870
 C  -0.4993  -1.1929  -0.7462
 C  -1.8109  -0.8294  -1.0239
 C  -2.5329  -0.1356  -0.0464
 C  -1.9712   0.1925   1.1904
 C  -0.6559  -0.1817   1.4504
 H   0.0737  -1.7290  -1.4966
 H  -2.2665  -1.0761  -1.9749
 H  -2.5496   0.7307   1.9313
 H  -0.2092   0.0730   2.4035
 N  -3.9076   0.2527  -0.3249
 O  -4.3989  -0.0416  -1.4234
 O  -4.5424   0.8648   0.5450
 O   1.9266  -0.8870   2.0491

r1_11d
Final geometry with  28 atoms:
 C   1.3797  -1.4393  -1.2452
 C   1.9536  -0.5397  -0.4350
 C   3.4419  -0.5764  -0.2861
 O   3.8848   0.3423   0.5876
 O   4.1913  -1.3434  -0.8785
 C   5.3166   0.4125   0.8046
 H   5.4557   1.2133   1.5300
 H   5.8249   0.6482  -0.1334
 H   5.6806  -0.5372   1.2035
 H   0.3059  -1.4769  -1.3922
 H   1.9820  -2.1684  -1.7785
 H   2.4851   2.0024   0.1109
 C   1.2022   0.5346   0.3535
 H   1.4916   0.4449   1.4077
 C  -0.3008   0.3840   0.2660
 C  -0.9598  -0.4485   1.1831
 C  -2.3349  -0.6406   1.1100
 C  -3.0469   0.0189   0.1031
 C  -2.4179   0.8568  -0.8219
 C  -1.0399   1.0324  -0.7339
 H  -0.3917  -0.9508   1.9606
 H  -2.8460  -1.2812   1.8181
 H  -2.9925   1.3550  -1.5930
 H  -0.5384   1.6763  -1.4472
 N  -4.4895  -0.1736   0.0165
 O  -5.0400  -0.9196   0.8369
 O  -5.1157   0.4136  -0.8756
 O   1.5553   1.8473  -0.1193

r1-TS7-01
Final geometry with  54 atoms:
 O   0.0028   0.6296   2.3546
 C  -0.6173  -0.4219  -0.6001
 H  -0.4450  -0.3923  -1.6832
 H   0.1323  -1.0859  -0.1528
 N  -1.9275  -1.1942  -0.4466
 C  -2.1321  -1.6398   0.9802
 H  -2.0620  -0.7543   1.6148
 C  -3.5110  -2.3331   1.0870
 H  -1.2988  -2.3142   1.2134
 C  -1.8528  -2.4271  -1.3129
 H  -0.9192  -2.9441  -1.0584
 C  -3.1058  -3.2983  -1.0536
 H  -1.7928  -2.0758  -2.3504
 C  -3.1205  -0.3776  -0.8818
 C  -4.3705  -1.2892  -0.8757
 H  -3.2076   0.4428  -0.1624
 H  -2.8877   0.0287  -1.8718
 C  -0.5642   0.9670  -0.0020
 C  -0.6633   2.0180  -1.0144
 O  -0.2834   3.2428  -0.5735
 O  -1.1152   1.8768  -2.1485
 C  -0.5058   4.3432  -1.4550
 H   0.0499   4.2156  -2.3964
 H  -1.5774   4.4541  -1.6826
 H  -0.1435   5.2343  -0.9265
 C   0.4781   1.1606   1.1289
 H   0.6372   2.2471   1.2278
 H  -1.8478   3.4690   2.1477
 C   4.2492  -0.5998   0.0709
 C   3.5118  -1.1677   1.1112
 C   2.2966  -0.5855   1.4669
 C   1.8191   0.5477   0.7922
 C   2.5883   1.1012  -0.2481
 C   3.8024   0.5356  -0.6154
 N   5.5219  -1.2040  -0.3107
 H   3.8878  -2.0495   1.6288
 H   1.7052  -1.0094   2.2781
 H   2.2285   1.9888  -0.7729
 H   4.4042   0.9595  -1.4184
 C  -2.7098   2.8440   1.8274
 H  -3.0470   3.2477   0.8478
 H  -3.5302   3.0468   2.5472
 O   6.1565  -0.6965  -1.2282
 O   5.9046  -2.1951   0.3004
 H  -5.1848  -0.7895  -0.3323
 H  -4.7146  -1.4764  -1.9027
 N  -4.0824  -2.5755  -0.2389
 H  -3.5651  -3.5771  -2.0123
 H  -2.8271  -4.2238  -0.5301
 H  -3.4043  -3.2881   1.6206
 H  -4.2069  -1.7009   1.6566
 H  -0.9335   0.9630   2.4230
 H  -1.6187   1.2502   0.7754
 O  -2.4114   1.4781   1.7714

r1-TS7-02
Final geometry with  54 atoms:
 O   0.0556   0.5114   2.4592
 C  -0.5970  -0.2840  -0.5789
 H  -0.4761  -0.1603  -1.6607
 H   0.1947  -0.9584  -0.2289
 N  -1.8701  -1.1210  -0.4344
 C  -3.0989  -0.3600  -0.8620
 H  -2.9476  -0.0825  -1.9110
 C  -4.3387  -1.2653  -0.6518
 H  -3.1426   0.5454  -0.2497
 C  -2.0614  -1.5934   0.9874
 H  -2.2384  -0.7013   1.5922
 C  -3.2642  -2.5671   1.0321
 H  -1.1203  -2.0630   1.2961
 C  -1.7277  -2.3349  -1.3219
 C  -3.0333  -3.1642  -1.2594
 H  -1.5117  -1.9695  -2.3329
 H  -0.8562  -2.8890  -0.9517
 C  -0.5502   1.0437   0.1476
 C  -0.6301   2.2418  -0.6901
 O  -1.2419   2.0294  -1.8812
 O  -0.2669   3.3712  -0.3693
 C  -1.4637   3.1722  -2.7084
 H  -2.1090   3.9058  -2.2010
 H  -0.5126   3.6569  -2.9761
 H  -1.9615   2.8008  -3.6133
 C   0.5062   1.1458   1.2756
 H   0.6503   2.2262   1.4528
 H  -1.8138   3.3362   2.4929
 C   4.2830  -0.4735   0.0255
 C   3.5842  -1.1130   1.0505
 C   2.3678  -0.5770   1.4691
 C   1.8500   0.5817   0.8718
 C   2.5820   1.2083  -0.1544
 C   3.7965   0.6893  -0.5838
 N   5.5561  -1.0295  -0.4220
 H   3.9907  -2.0140   1.5086
 H   1.8084  -1.0589   2.2704
 H   2.1923   2.1166  -0.6186
 H   4.3687   1.1695  -1.3766
 C  -2.6862   2.7281   2.1683
 H  -3.0782   3.2071   1.2448
 H  -3.4686   2.8600   2.9448
 O   6.1588  -0.4557  -1.3218
 O   5.9709  -2.0484   0.1183
 H  -3.5332  -3.1573  -2.2380
 H  -2.7987  -4.2075  -1.0063
 N  -3.9493  -2.6199  -0.2592
 H  -2.9276  -3.5804   1.2929
 H  -3.9743  -2.2368   1.8032
 H  -4.9819  -0.8450   0.1339
 H  -4.9247  -1.3124  -1.5804
 H  -0.8859   0.8204   2.5624
 H  -1.5978   1.2406   0.9534
 O  -2.3779   1.3763   1.9827

r1-TS7-03
Final geometry with  54 atoms:
 O  -0.0582   0.5333   2.4633
 C   0.5926  -0.2711  -0.5987
 H  -0.2115  -0.9386  -0.2645
 H   0.4832  -0.1335  -1.6801
 N   1.8526  -1.1254  -0.4479
 C   1.9483  -1.7062   0.9413
 H   1.0622  -2.3401   1.0693
 C   3.2729  -2.4967   1.0575
 H   1.8964  -0.8766   1.6487
 C   3.1110  -0.3457  -0.7450
 H   3.1943   0.4130   0.0398
 C   4.3111  -1.3241  -0.7383
 H   2.9634   0.1433  -1.7135
 C   1.7641  -2.2717  -1.4268
 C   2.9558  -3.2298  -1.1867
 H   0.7935  -2.7578  -1.2675
 H   1.7781  -1.8265  -2.4294
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 C   0.5571   1.0488   0.1443
 C   0.6546   2.2556  -0.6799
 O   1.2719   2.0512  -1.8699
 O   0.2987   3.3846  -0.3502
 C   1.5055   3.2014  -2.6836
 H   2.1538   3.9248  -2.1655
 H   0.5589   3.6959  -2.9497
 H   2.0043   2.8364  -3.5905
 C  -0.5022   1.1568   1.2706
 H  -0.6459   2.2382   1.4394
 H   1.8514   3.3098   2.4699
 C  -4.2784  -0.4635   0.0234
 C  -3.5693  -1.1144   1.0342
 C  -2.3524  -0.5788   1.4517
 C  -1.8449   0.5909   0.8672
 C  -2.5856   1.2276  -0.1461
 C  -3.8009   0.7091  -0.5741
 N  -5.5532  -1.0178  -0.4213
 H  -3.9688  -2.0234   1.4825
 H  -1.7843  -1.0690   2.2419
 H  -2.2018   2.1432  -0.6008
 H  -4.3809   1.1975  -1.3562
 C   2.7166   2.6827   2.1632
 H   3.1290   3.1438   1.2394
 H   3.4914   2.8087   2.9482
 O  -6.1657  -0.4332  -1.3075
 O  -5.9597  -2.0459   0.1078
 H   2.6005  -4.1856  -0.7767
 H   3.4595  -3.4375  -2.1412
 N   3.9140  -2.6449  -0.2495
 H   4.7215  -1.4341  -1.7520
 H   5.1061  -0.9238  -0.0934
 H   3.9662  -1.9720   1.7297
 H   3.0743  -3.4910   1.4820
 H   0.8871   0.8338   2.5662
 H   1.6040   1.2191   0.9567
 O   2.3861   1.3342   1.9880

r1-TS7-04
Final geometry with  54 atoms:
 O  -0.5022   1.6160  -2.0052
 C   1.1644  -1.0044   0.0952
 H   0.9008  -1.7295  -0.6837
 H   0.9049  -1.4345   1.0708
 N   2.6964  -1.0017   0.0801
 C   3.2218  -0.6462  -1.2893
 H   2.8607   0.3621  -1.5142
 C   4.7698  -0.7123  -1.2621
 H   2.7796  -1.3649  -1.9900
 C   3.1714  -2.3896   0.4320
 H   2.7209  -3.0715  -0.2998
 C   4.7198  -2.4181   0.4012
 H   2.7651  -2.6173   1.4251
 C   3.2639  -0.0351   1.0872
 C   4.8105  -0.1266   1.0486
 H   2.9030   0.9594   0.8112
 H   2.8431  -0.3088   2.0606
 C   0.4905   0.3280  -0.1287
 C   0.0066   0.9285   1.1166
 O  -0.8097   1.9859   0.9069
 O   0.3241   0.5958   2.2565
 C  -1.2834   2.6822   2.0578
 H  -1.9446   3.4742   1.6833
 H  -1.8458   2.0107   2.7244
 H  -0.4479   3.1284   2.6193
 C  -0.4792   0.3662  -1.3488
 H  -0.1000  -0.4111  -2.0411
 H   0.8874   3.9499  -0.3752
 C  -4.4614  -0.7878  -0.1903
 C  -4.2285   0.5293  -0.5936
 C  -2.9435   0.8933  -0.9852
 C  -1.8947  -0.0389  -0.9747
 C  -2.1638  -1.3602  -0.5741
 C  -3.4397  -1.7433  -0.1782
 N  -5.8035  -1.1787   0.2243
 H  -5.0448   1.2510  -0.5951
 H  -2.7371   1.9151  -1.3002
 H  -1.3647  -2.1038  -0.5713
 H  -3.6516  -2.7652   0.1336
 C   1.8589   3.4127  -0.3481
 H   2.0549   3.1645   0.7174
 H   2.6402   4.1408  -0.6482
 O  -5.9888  -2.3343   0.5898
 O  -6.6940  -0.3366   0.1926
 H   5.2353   0.8549   0.7962
 H   5.1933  -0.4184   2.0366
 N   5.2605  -1.1041   0.0585
 H   5.1079  -2.7184   1.3844
 H   5.0682  -3.1511  -0.3396
 H   5.1301  -1.4369  -2.0056
 H   5.1883   0.2717  -1.5163
 H   0.4073   2.0085  -1.8874
 H   1.3272   1.3086  -0.5676
 O   1.8761   2.2802  -1.1734

r1-TS7-05
Final geometry with  54 atoms:
 O  -0.5490  -2.6556   1.2968
 C  -0.7188   0.1961  -1.1923
 H   0.3560   0.1409  -1.3882
 H  -1.2353   0.2707  -2.1569
 N  -0.8972   1.5883  -0.5716
 C  -2.3435   1.8814  -0.2651
 H  -2.6714   1.1280   0.4556
 C  -2.4513   3.3178   0.3051
 H  -2.8983   1.7483  -1.1999
 C  -0.4060   2.6082  -1.5685
 H  -1.0019   2.4717  -2.4790
 C  -0.5630   4.0260  -0.9636
 H   0.6391   2.3565  -1.7871
 C  -0.0878   1.7326   0.6931
 C  -0.2634   3.1718   1.2394
 H  -0.4610   0.9814   1.3946
 H   0.9505   1.5060   0.4276
 C  -1.2279  -0.9810  -0.3927
 C  -2.4920  -1.4907  -0.9370
 O  -2.7900  -2.7431  -0.5216
 O  -3.2729  -0.8657  -1.6523
 C  -4.0659  -3.2627  -0.8929
 H  -4.1180  -4.2735  -0.4683
 H  -4.1735  -3.3110  -1.9873
 H  -4.8772  -2.6430  -0.4800
 C  -0.2189  -2.0999   0.0334
 H  -0.2809  -2.9252  -0.6965
 H  -3.9188  -0.4317   1.5814
 C   3.8484  -0.7030  -0.0043
 C   3.3088  -1.2493  -1.1721
 C   1.9970  -1.7124  -1.1436
 C   1.2242  -1.6268   0.0260
 C   1.8018  -1.0899   1.1866
 C   3.1119  -0.6215   1.1808
 N   5.2220  -0.2062  -0.0222
 H   3.9122  -1.3092  -2.0770
 H   1.5597  -2.1434  -2.0477
 H   1.2133  -1.0428   2.1034
 H   3.5650  -0.1954   2.0752
 C  -3.2357  -0.9190   2.3105
 H  -3.4135  -2.0124   2.2294
 H  -3.5818  -0.6099   3.3179
 O   5.6841   0.2672   1.0090
 O   5.8550  -0.2802  -1.0687
 H  -0.6971   3.1370   2.2486
 H   0.7137   3.6701   1.3067
 N  -1.1407   3.9625   0.3773
 H   0.4166   4.5206  -0.9073
 H  -1.2144   4.6362  -1.6046
 H  -3.1118   3.9245  -0.3300
 H  -2.8856   3.2858   1.3140
 H  -1.0107  -1.9412   1.8154
 H  -1.6367  -0.6339   0.8555
 O  -1.8939  -0.5705   2.1047

r1-TS7-06
Final geometry with  54 atoms:
 O   0.0269   0.3902   2.3797
 C  -0.6236  -0.4146  -0.5541
 H  -0.3780  -0.3971  -1.6235
 H   0.0398  -1.1361  -0.0624
 N  -1.9975  -1.0766  -0.4894
 C  -1.9333  -2.3813  -1.2439
 H  -1.1389  -2.9764  -0.7772
 C  -3.3185  -3.0728  -1.1727
 H  -1.6390  -2.1378  -2.2718
 C  -3.0549  -0.2158  -1.1300
 H  -2.7248  -0.0277  -2.1573
 C  -4.4128  -0.9576  -1.0593
 H  -3.0681   0.7337  -0.5886
 C  -2.3860  -1.3740   0.9380
 C  -3.7661  -2.0758   0.9445
 H  -1.5888  -2.0042   1.3492
 H  -2.3874  -0.4185   1.4692
 C  -0.4992   0.9606   0.0639
 C  -0.4598   2.0288  -0.9351
 O  -0.0303   3.2173  -0.4446
 O  -0.8397   1.9346  -2.0998
 C  -0.0714   4.3354  -1.3315
 H   0.5708   4.1669  -2.2095
 H   0.3012   5.1932  -0.7570
 H  -1.1000   4.5317  -1.6714
 C   0.5280   1.0397   1.2242
 H   0.6861   2.1108   1.4325
 H  -3.9171   2.4802   2.7005
 C   4.3087  -0.6548   0.0846
 C   3.8936   0.5513  -0.4918
 C   2.6761   1.0932  -0.1006
 C   1.8704   0.4466   0.8555
 C   2.3182  -0.7565   1.4224
 C   3.5359  -1.3159   1.0405
 N   5.5858  -1.2330  -0.3212
 H   4.5228   1.0482  -1.2293
 H   2.3458   2.0376  -0.5373
 H   1.7041  -1.2527   2.1733
 H   3.8881  -2.2505   1.4758
 C  -3.5248   1.9527   1.8048
 H  -3.7903   2.5892   0.9314
 H  -4.1274   1.0214   1.7066
 O   5.9373  -2.2898   0.1903
 O   6.2553  -0.6387  -1.1583
 H  -3.6859  -3.0577   1.4317
 H  -4.4900  -1.4744   1.5113
 N  -4.2710  -2.2629  -0.4152
 H  -5.1379  -0.3585  -0.4910
 H  -4.8125  -1.1020  -2.0728
 H  -3.7104  -3.2289  -2.1874
 H  -3.2237  -4.0555  -0.6903
 H  -0.8657   0.7921   2.5254
 H  -1.5246   1.3547   0.8385
 O  -2.1561   1.7227   1.9084

r1-TS7-07
Final geometry with  54 atoms:
 O  -0.5080   1.3217  -2.1924
 C   1.0699  -0.8313   0.4514
 H   0.9551  -0.9217   1.5363
 H   0.6470  -1.7323  -0.0082
 N   2.5752  -0.9860   0.2135
 C   2.8866  -1.0400  -1.2624
 H   2.5711  -0.0826  -1.6874
 C   4.4078  -1.2753  -1.4423
 H   2.2800  -1.8517  -1.6821
 C   3.0204  -2.2813   0.8459
 H   2.4317  -3.0792   0.3766
 C   4.5436  -2.4556   0.6233
 H   2.7537  -2.2214   1.9081
 C   3.3560   0.1406   0.8414
 C   4.8650  -0.0942   0.5781
 H   2.9994   1.0667   0.3838
 H   3.1051   0.1414   1.9080
 C   0.4342   0.4292  -0.0882
 C  -0.0487   1.3866   0.9081
 O   0.5377   1.2518   2.1271
```

```
 O  -0.8404   2.2997   0.6974
 C   0.2133   2.2359   3.1090
 H  -0.8666   2.2425   3.3213
 H   0.7696   1.9591   4.0139
 H   0.5180   3.2402   2.7756
 C  -0.5119   0.2192  -1.3088
 H  -0.1201  -0.6779  -1.8265
 H   0.9872   3.8490  -0.9992
 C  -4.5513  -0.7009  -0.1333
 C  -3.5667  -1.6883  -0.0297
 C  -2.2701  -1.3810  -0.4265
 C  -1.9422  -0.1026  -0.9130
 C  -2.9573   0.8624  -1.0154
 C  -4.2620   0.5735  -0.6275
 N  -5.9166  -1.0147   0.2729
 H  -3.8231  -2.6785   0.3448
 H  -1.5044  -2.1567  -0.3675
 H  -2.7102   1.8480  -1.4061
 H  -5.0516   1.3204  -0.7041
 C   1.9592   3.3146  -0.9496
 H   2.2478   3.2823   0.1240
 H   2.7102   3.9565  -1.4549
 O  -6.7752  -0.1477   0.1567
 O  -6.1515  -2.1338   0.7154
 H   5.2739   0.7374  -0.0126
 H   5.4093  -0.1338   1.5319
 N   5.0896  -1.3424  -0.1504
 H   5.0616  -2.5042   1.5912
 H   4.7389  -3.3940   0.0859
 H   4.5838  -2.2140  -1.9858
 H   4.8423  -0.4552  -2.0306
 H   0.4137   1.7027  -2.1536
 H   1.3085   1.2386  -0.7164
 O   1.9067   2.0395  -1.5268

r1-TS7-08
Final geometry with  54 atoms:
 O  -0.0640   0.3021   2.3631
 C  -0.7257  -0.5759  -0.4224
 H  -0.4235  -0.6771  -1.4719
 H  -0.1581  -1.3051   0.1667
 N  -2.1573  -1.0915  -0.3772
 C  -2.6356  -1.2388   1.0481
 H  -2.5670  -0.2444   1.5024
 C  -4.0916  -1.7648   1.0283
 H  -1.9388  -1.9273   1.5406
 C  -2.1898  -2.4484  -1.0370
 H  -1.4499  -3.0721  -0.5204
 C  -3.6241  -3.0237  -0.9401
 H  -1.8656  -2.3003  -2.0746
 C  -3.1058  -0.1762  -1.1178
 C  -4.5141  -0.8223  -1.1209
 H  -3.0987   0.7796  -0.5831
 H  -2.6940  -0.0421  -2.1239
 C  -0.5158   0.8395   0.0836
 C  -0.3299   1.8058  -1.0166
 O   0.1060   3.0135  -0.5979
 O  -0.6087   1.6092  -2.1924
 C   0.2275   4.0373  -1.5884
 H   0.9431   3.7424  -2.3706
 H  -0.7476   4.2504  -2.0520
 H   0.5940   4.9270  -1.0612
 C   0.5040   0.9469   1.2331
 H   0.6482   2.0177   1.4425
 H  -1.6541   2.7041   2.8485
 C   4.2973  -0.7335   0.0843
 C   3.4618  -1.4696   0.9258
 C   2.2442  -0.9142   1.3122
 C   1.8573   0.3584   0.8634
 C   2.7264   1.0788   0.0228
 C   3.9455   0.5413  -0.3719
 N   5.5768  -1.3067  -0.3248
 H   3.7659  -2.4576   1.2693
 H   1.5837  -1.4703   1.9783
 H   2.4446   2.0756  -0.3205
 H   4.6240   1.0951  -1.0197
 C  -2.3420   2.9580   2.0047
 H  -1.8331   3.7811   1.4455
 H  -3.2307   3.4333   2.4847
 O   6.3001  -0.6491  -1.0634
 O   5.8740  -2.4220   0.0863
 H  -5.2430  -0.1169  -0.6977
 H  -4.8241  -1.0541  -2.1496
 N  -4.5362  -2.0558  -0.3350
 H  -3.9886  -3.2831  -1.9439
 H  -3.6244  -3.9394  -0.3324
 H  -4.1694  -2.6785   1.6343
 H  -4.7639  -1.0106   1.4615
 H   0.5255   0.4368   3.1209
 H  -1.5577   1.3215   0.6277
 O  -2.6848   1.8714   1.2183

r1-TS7-09
Final geometry with  54 atoms:
 O   0.5268   1.4573   2.1418
 C  -1.0688  -0.8893  -0.3159
 H  -0.6883  -1.7380   0.2650
 H  -0.9035  -1.1063  -1.3765
 N  -2.5872  -0.9910  -0.1364
 C  -2.9640  -0.9066   1.3225
 H  -2.6316   0.0723   1.6801
 C  -4.4993  -1.0738   1.4518
 H  -2.4077  -1.6999   1.8360
 C  -3.0328  -2.3297  -0.6696
 H  -2.4702  -3.0922  -0.1171
 C  -4.5643  -2.4656  -0.4815
 H  -2.7333  -2.3634  -1.7242
 C  -3.3149   0.0885  -0.8962
 C  -4.8398  -0.1082  -0.7009
 H  -2.9690   1.0450  -0.4957
 H  -3.0050   0.0007  -1.9433
 C  -0.4297   0.4114   0.1140
 C   0.0580   1.2813  -0.9570
 O  -0.5084   1.0354  -2.1674
 O   0.8432   2.2133  -0.8156
 C  -0.1812   1.9365  -3.2251
 H  -0.4970   2.9625  -2.9794
 H   0.9008   1.9345  -3.4266
 H  -0.7260   1.5806  -4.1091
 C   0.5270   0.2953   1.3379
 H   0.1456  -0.5647   1.9225
 H  -0.9600   3.9001   0.8105
 C   4.5516  -0.6822   0.1602
 C   4.2718   0.6104   0.6105
 C   2.9722   0.9178   1.0018
 C   1.9538  -0.0469   0.9462
 C   2.2714  -1.3430   0.5017
 C   3.5625  -1.6693   0.1028
 N   5.9108  -1.0148  -0.2508
 H   5.0643   1.3572   0.6498
 H   2.7315   1.9183   1.3572
 H   1.5010  -2.1158   0.4745
 H   3.8113  -2.6728  -0.2402
 C  -1.9315   3.3633   0.7798
 H  -2.2032   3.2633  -0.2939
 H  -2.6897   4.0356   1.2319
 O   6.1371  -2.1496  -0.6562
 O   6.7734  -0.1471  -0.1759
 H  -5.2728   0.7855  -0.2304
 H  -5.3273  -0.2493  -1.6755
 N  -5.1227  -1.2682   0.1435
 H  -5.0488  -2.6191  -1.4558
 H  -4.7898  -3.3359   0.1503
 H  -4.7328  -1.9373   2.0902
 H  -4.9321  -0.1785   1.9195
 H  -0.3970   1.8314   2.0842
 H  -1.2975   1.2697   0.6862
 O  -1.8882   2.1277   1.4379

r1-TS7-10
Final geometry with  54 atoms:
 O   0.0758   0.1969   2.4916
 C  -0.5776  -0.2647  -0.5377
 H  -0.3753  -0.1096  -1.6034
 H   0.1341  -1.0134  -0.1684
 N  -1.9192  -0.9945  -0.5074
 C  -3.0340  -0.1238  -1.0253
 H  -2.7690   0.1381  -2.0556
 C  -4.3645  -0.9100  -0.9341
 H  -3.0426   0.7894  -0.4252
 C  -2.2517  -1.4674   0.8879
 H  -2.3274  -0.5728   1.5120
 C  -3.5651  -2.2857   0.8385
 H  -1.3963  -2.0623   1.2279
 C  -1.8198  -2.2059  -1.4021
 C  -3.1908  -2.9277  -1.4243
 H  -1.5179  -1.8481  -2.3938
 H  -1.0183  -2.8323  -0.9915
 C  -0.4751   1.0215   0.2551
 C  -0.4280   2.2622  -0.5212
 O  -0.9754   2.1505  -1.7565
 O  -0.0152   3.3471  -0.1187
 C  -1.0717   3.3451  -2.5334
 H  -1.5456   3.0552  -3.4800
 H  -1.6890   4.0991  -2.0214
 H  -0.0755   3.7704  -2.7287
 C   0.5570   0.9781   1.4124
 H   0.6973   2.0250   1.7313
 H  -3.9277   2.1737   3.0156
 C   4.3419  -0.5232   0.0414
 C   3.9235   0.7520  -0.3557
 C   2.7069   1.2311   0.1131
 C   1.9048   0.4529   0.9695
 C   2.3573  -0.8172   1.3588
 C   3.5743  -1.3146   0.8972
 N   5.6157  -1.0379  -0.4508
 H   4.5493   1.3498  -1.0173
 H   2.3721   2.2266  -0.1837
 H   1.7471  -1.4178   2.0326
 H   3.9290  -2.3015   1.1922
 C  -3.5256   1.7135   2.0874
 H  -3.8048   2.4013   1.2579
 H  -4.1116   0.7797   1.9274
 O   6.2797  -0.3311  -1.2003
 O   5.9697  -2.1567  -0.0971
 H  -3.6118  -2.9056  -2.4391
 H  -3.0622  -3.9795  -1.1334
 N  -4.1350  -2.2901  -0.5081
 H  -3.3761  -3.3241   1.1449
 H  -4.2975  -1.8547   1.5350
 H  -5.0387  -0.4274  -0.2131
 H  -4.8610  -0.9120  -1.9145
 H  -0.8281   0.5542   2.6776
 H  -1.5044   1.2823   1.0651
 O  -2.1532   1.5027   2.1745

r1-TS7-11
Final geometry with  54 atoms:
 O  -0.0118   0.0144   2.4274
 C  -0.7172  -0.5912  -0.3675
 H  -0.4126  -0.6264  -1.4206
 H  -0.1555  -1.3592   0.1761
 N  -2.1511  -1.0987  -0.3580
 C  -2.1904  -2.4111  -1.1016
 H  -1.4442  -3.0650  -0.6341
 C  -3.6234  -2.9914  -1.0252
 H  -1.8780  -2.1946  -2.1308
 C  -3.0889  -0.1279  -1.0354
 H  -2.6583   0.1074  -2.0144
 C  -4.4916  -0.7763  -1.1264
 H  -3.0907   0.7642  -0.4020
 C  -2.6432  -1.3276   1.0515
 C  -4.1123  -1.8124   0.9870
 H  -1.9677  -2.0644   1.5019
 H  -2.5568  -0.3712   1.5746
 C  -0.4970   0.7866   0.2300
 C  -0.2977   1.8250  -0.8029
 O   0.1501   2.9916  -0.2934
 O  -0.5696   1.7140  -1.9913
 C   0.2464   4.0986  -1.1914
 H   0.9324   3.8730  -2.0216
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 H    0.6364    4.9362   -0.5997
 H   -0.7432    4.3564   -1.5988
 C    0.5337    0.7959    1.3769
 H    0.6507    1.8416    1.7016
 H   -3.9303    3.3782    1.2697
 C    4.3464   -0.6870    0.0319
 C    3.9808    0.6291   -0.2686
 C    2.7569    1.1036    0.1883
 C    1.8960    0.2794    0.9372
 C    2.2989   -1.0327    1.2333
 C    3.5208   -1.5258    0.7823
 N    5.6295   -1.1948   -0.4461
 H    4.6522    1.2632   -0.8464
 H    2.4649    2.1308   -0.0346
 H    1.6471   -1.6705    1.8312
 H    3.8362   -2.5441    1.0070
 C   -2.9194    3.0201    0.9557
 H   -2.2196    3.8580    1.1994
 H   -2.9653    2.9921   -0.1638
 O    5.9335   -2.3520   -0.1815
 O    6.3487   -0.4435   -1.0936
 H   -4.2243   -2.7435    1.5601
 H   -4.7723   -1.0553    1.4338
 N   -4.5383   -2.0424   -0.3937
 H   -5.2400   -0.0897   -0.7060
 H   -4.7580   -0.9671   -2.1755
 H   -3.9836   -3.2222   -2.0376
 H   -3.6254   -3.9244   -0.4443
 H    0.5730    0.0861    3.1970
 H   -1.5055    1.2452    0.8249
 O   -2.5801    1.8114    1.5333

r1-TS7-12
Final geometry with  54 atoms:
 O   -0.4944    1.9058   -1.7437
 C    1.0686   -0.9359    0.1819
 H    0.7918   -1.3745    1.1482
 H    0.7629   -1.6287   -0.6103
 N    2.5960   -1.0096    0.1525
 C    3.2306   -0.0129    1.0927
 H    2.7780   -0.1770    2.0764
 C    4.7636   -0.2343    1.0873
 H    2.9521    0.9852    0.7408
 C    3.1020   -0.7803   -1.2467
 H    2.6928    0.1708   -1.5941
 C    4.6485   -0.7925   -1.2270
 H    2.6841   -1.5880   -1.8599
 C    3.0212   -2.3931    0.5778
 C    4.5581   -2.5132    0.4210
 H    2.6923   -2.5147    1.6172
 H    2.4757   -3.1052   -0.0535
 C    0.4672    0.4391    0.0057
 C   -0.0148    0.9867    1.2803
 O   -0.7897    2.0817    1.1277
 O    0.2850    0.5815    2.4012
 C   -1.2866    2.6996    2.3137
 H   -1.9002    3.5466    1.9810
 H   -1.9039    1.9980    2.8958
 H   -0.4610    3.0614    2.9457
 C   -0.4724    0.5906   -1.2275
 H   -0.0596   -0.0967   -1.9905
 H    3.6695    2.2492   -1.4164
 C   -4.4519   -0.7629   -0.2792
 C   -3.4453   -1.7055   -0.5111
 C   -2.1729   -1.2540   -0.8425
 C   -1.8894    0.1210   -0.9341
 C   -2.9287    1.0404   -0.7162
 C   -4.2096    0.6091   -0.3855
 N   -5.7898   -1.2241    0.0726
 H   -3.6661   -2.7697   -0.4381
 H   -1.3891   -1.9875   -1.0400
 H   -2.7202    2.1048   -0.8103
 H   -5.0165    1.3200   -0.2108
 C    2.6753    2.6715   -1.6764
 H    2.3259    2.1364   -2.5871
 H    2.8562    3.7215   -1.9873
 O   -6.6649   -0.3874    0.2647
 O   -5.9866   -2.4308    0.1644
 H    4.9982   -2.8769    1.3599
 H    4.8041   -3.2347   -0.3706
 N    5.1511   -1.2205    0.0784
 H    5.0223   -1.4756   -2.0026
 H    5.0402    0.2116   -1.4426
 H    5.2727    0.7162    0.8755
 H    5.1001   -0.5871    2.0722
 H    0.2942    2.3801   -1.3571
 H    1.3312    1.4477   -0.3108
 O    1.7620    2.6123   -0.6196

r1-TS7-13
Final geometry with  54 atoms:
 O   -0.4805   -2.8369    1.2099
 C   -0.8827    0.0769   -1.1979
 H    0.1376   -0.0018   -1.5874
 H   -1.5536    0.2045   -2.0539
 N   -0.8996    1.4521   -0.5128
 C   -2.2671    1.7918    0.0238
 H   -2.4932    1.0469    0.7908
 C   -2.2354    3.2303    0.5989
 H   -2.9712    1.6823   -0.8075
 C   -0.5223    2.4880   -1.5425
 H   -1.2798    2.4322   -2.3340
 C   -0.4723    3.8801   -0.8655
 H    0.4473    2.1870   -1.9576
 C    0.0978    1.5179    0.6152
 C    0.0331    2.9258    1.2585
 H   -0.1737    0.7330    1.3260
 H    1.0782    1.2989    0.1788
 C   -1.2698   -1.1194   -0.3572
 C   -2.5372   -1.7492   -0.7462
 O   -3.4476   -0.8731   -1.2467
 O   -2.8299   -2.9305   -0.5955
 C   -4.7478   -1.3883   -1.5310
 H   -5.3309   -0.5455   -1.9241
 H   -4.7018   -2.1930   -2.2807
 H   -5.2236   -1.7774   -0.6173
 C   -0.1984   -2.2088   -0.0310
 H   -0.2592   -3.0002   -0.7989
 H   -3.2829   -2.1159    2.2851
 C    3.8145   -0.6595   -0.1046
 C    3.1433   -0.7538    1.1175
 C    1.8524   -1.2724    1.1323
 C    1.2268   -1.6840   -0.0540
 C    1.9380   -1.5990   -1.2627
 C    3.2299   -1.0834   -1.3011
 N    5.1667   -0.1075   -0.1318
 H    3.6302   -0.4213    2.0335
 H    1.3147   -1.3587    2.0766
 H    1.4710   -1.9426   -2.1889
 H    3.7841   -1.0118   -2.2361
 C   -3.0354   -1.0547    2.5016
 H   -3.2501   -0.8869    3.5768
 H   -3.7660   -0.4375    1.9345
 O    5.7427   -0.0294   -1.2105
 O    5.6684    0.2578    0.9244
 H   -0.3061    2.8454    2.3006
 H    1.0334    3.3807    1.2606
 N   -0.8894    3.7981    0.5327
 H    0.5490    4.2834   -0.9072
 H   -1.1343    4.5769   -1.3982
 H   -2.9210    3.8780    0.0347
 H   -2.5662    3.2168    1.6467
 H   -0.8857   -2.1401    1.7938
 H   -1.5677   -0.7817    0.9224
 O   -1.7065   -0.7353    2.1922

r1-TS7-14
Final geometry with  54 atoms:
 O   -0.4820    1.9397   -1.6443
 C    1.1312   -0.9820    0.0804
 H    0.8667   -1.5192    0.9997
 H    0.8557   -1.6081   -0.7768
 N    2.6605   -0.9978    0.0588
 C    3.1364   -2.3951    0.3711
 H    2.6078   -3.0747   -0.3087
 C    4.6742   -2.4480    0.1912
 H    2.8238   -2.6074    1.4010
 C    3.2525   -0.0609    1.0840
 H    2.7868   -0.3081    2.0440
 C    4.7899   -0.2457    1.0909
 H    2.9555    0.9535    0.8009
 C    3.1661   -0.6310   -1.3108
 C    4.7103   -0.5624   -1.2693
 H    2.7979   -1.4078   -1.9923
 H    2.7080    0.3219   -1.5846
 C    0.4764    0.3789    0.0244
 C   -0.0291    0.7977    1.3370
 O   -0.8647    1.8562    1.2645
 O    0.2933    0.3234    2.4238
 C   -1.3914    2.3582    2.4918
 H   -0.5846    2.7128    3.1514
 H   -2.0473    3.1955    2.2211
 H   -1.9721    1.5845    3.0174
 C   -0.4768    0.6030   -1.1836
 H   -0.0886   -0.0529   -1.9870
 H    3.6330    2.4162   -1.1763
 C   -4.4907   -0.7150   -0.3217
 C   -3.4517   -1.6514   -0.3421
 C   -2.1652   -1.2148   -0.6355
 C   -1.9016    0.1410   -0.9038
 C   -2.9681    1.0526   -0.8856
 C   -4.2638    0.6361   -0.5938
 N   -5.8435   -1.1615   -0.0113
 H   -3.6581   -2.7002   -0.1320
 H   -1.3551   -1.9456   -0.6544
 H   -2.7661    2.1016   -1.0977
 H   -5.0928    1.3429   -0.5732
 C    2.6282    2.8203   -1.4235
 H    2.3148    2.3457   -2.3795
 H    2.7731    3.8975   -1.6477
 O   -6.7451   -0.3308    0.0011
 O   -6.0265   -2.3504    0.2263
 H    5.1277   -1.1319   -2.1116
 H    5.0483    0.4792   -1.3638
 N    5.2221   -1.1063   -0.0106
 H    5.2781    0.7344    0.9979
 H    5.1155   -0.6977    2.0383
 H    5.1338   -2.8986    1.0820
 H    4.9362   -3.0697   -0.6763
 H    0.2709    2.4100   -1.1868
 H    1.3065    1.4429   -0.1933
 O    1.6987    2.6438   -0.3935

r1-TS7-15
Final geometry with  54 atoms:
 O    0.0593   -0.1913    2.4859
 C   -0.6889   -0.4937   -0.3545
 H   -0.4064   -0.4198   -1.4104
 H   -0.1015   -1.3047    0.0910
 N   -2.1133   -1.0302   -0.3648
 C   -3.0705   -0.0572   -1.0051
 H   -2.7192    0.1039   -2.0302
 C   -4.4978   -0.6551   -0.9450
 H   -2.9924    0.8739   -0.4398
 C   -2.6047   -1.3259    1.0349
 H   -2.6712   -0.3559    1.5417
 C   -3.9834   -2.0230    0.9378
 H   -1.8423   -1.9489    1.5156
 C   -2.1243   -2.3104   -1.1639
 C   -3.5786   -2.8304   -1.2651
 H   -1.6931   -2.0782   -2.1451
 H   -1.4611   -3.0097   -0.6401
 C   -0.4678    0.8128    0.3919
 C   -0.2548    2.0152   -0.4469
 O   -0.6967    1.8826   -1.7118
 O    0.2069    3.0746   -0.0419
 C   -0.6579    3.0490   -2.5387
 H   -1.0558    2.7427   -3.5142
 H   -1.2819    3.8488   -2.1116
 H    0.3734    3.4154   -2.6502
 C    0.5800    0.7044    1.5190
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 H    0.6834    1.7149    1.9457
 H   -3.9998    3.1497    1.5746
 C    4.4082   -0.5604    0.0064
 C    4.0345    0.7815   -0.1178
 C    2.8045    1.1830    0.3906
 C    1.9452    0.2601    1.0157
 C    2.3562   -1.0775    1.1361
 C    3.5843   -1.4978    0.6319
 N    5.6986   -0.9917   -0.5252
 H    4.7047    1.4923   -0.5998
 H    2.5036    2.2278    0.3063
 H    1.7074   -1.7932    1.6421
 H    3.9062   -2.5347    0.7214
 C   -2.9495    2.8914    1.2891
 H   -2.3413    3.7948    1.5485
 H   -2.9648    2.8715    0.1673
 O    6.4109   -0.1590   -1.0731
 O    6.0148   -2.1691   -0.4033
 H   -3.9239   -2.7892   -2.3076
 H   -3.6218   -3.8779   -0.9354
 N   -4.4788   -2.0277   -0.4394
 H   -3.9157   -3.0619    1.2901
 H   -4.7053   -1.4949    1.5768
 H   -5.1316   -0.0473   -0.2841
 H   -4.9462   -0.6452   -1.9483
 H    0.6537   -0.1938    3.2514
 H   -1.4496    1.1871    1.0473
 O   -2.5027    1.7229    1.8697

r1-TS7-16
Final geometry with  54 atoms:
 O   -0.0121    0.2116    2.4448
 C   -0.6638   -0.4473   -0.4343
 H   -0.4034   -0.4372   -1.4985
 H   -0.0336   -1.1981    0.0564
 N   -2.0633   -1.0442   -0.3767
 C   -3.0894   -0.1401   -1.0213
 H   -2.7237    0.0835   -2.0290
 C   -4.4562   -0.8701   -1.0283
 H   -3.1171    0.7777   -0.4240
 C   -2.4780   -1.3156    1.0507
 H   -2.4356   -0.3545    1.5736
 C   -3.9079   -1.9073    1.0460
 H   -1.7319   -2.0039    1.4648
 C   -2.0457   -2.3535   -1.1271
 C   -3.4368   -3.0231   -1.0063
 H   -1.7827   -2.1154   -2.1652
 H   -1.2459   -2.9628   -0.6886
 C   -0.4934    0.9173    0.2142
 C   -0.3299    2.0602   -0.7088
 O   -0.7965    1.8243   -1.9498
 O    0.1003    3.1637   -0.3938
 C   -0.8064    2.9261   -2.8615
 H   -1.4285    3.7470   -2.4741
 H    0.2143    3.2978   -3.0367
 H   -1.2317    2.5417   -3.7970
 C    0.5346    0.9460    1.3605
 H    0.6612    2.0036    1.6402
 H   -1.6774    2.5080    3.1145
 C    4.3376   -0.5906    0.0559
 C    3.5196   -1.3985    0.8472
 C    2.2998   -0.8889    1.2860
 C    1.8931    0.4090    0.9380
 C    2.7459    1.2024    0.1477
 C    3.9671    0.7110   -0.2981
 N    5.6177   -1.1166   -0.4107
 H    3.8383   -2.4062    1.1112
 H    1.6523   -1.5032    1.9126
 H    2.4470    2.2177   -0.1170
 H    4.6325    1.3206   -0.9083
 C   -2.3823    2.8021    2.2977
 H   -1.9006    3.6764    1.7940
 H   -3.2762    3.2199    2.8214
 O    6.3303   -0.3924   -1.0954
 O    5.9257   -2.2611   -0.1002
 H   -3.8242   -3.2560   -2.0081
 H   -3.3560   -3.9658   -0.4472
 N   -4.3817   -2.1466   -0.3176
 H   -3.9240   -2.8539    1.6046
 H   -4.5998   -1.2093    1.5384
 H   -5.2135   -0.2365   -0.5455
 H   -4.7807   -1.0601   -2.0611
 H    0.5864    0.2935    3.2030
 H   -1.5397    1.2941    0.7959
 O   -2.7054    1.7664    1.4388

r1-TS7-17
Final geometry with  54 atoms:
 O   -1.2710   -1.3360   -2.2702
 C   -1.9234    1.0688   -0.5732
 H   -2.0044    1.1400   -1.6642
 H   -2.8049    1.5445   -0.1287
 N   -0.7615    2.0158   -0.2192
 C   -1.2863    3.4326   -0.2328
 H   -2.0264    3.4979    0.5743
 C   -0.1011    4.4094   -0.0271
 H   -1.7930    3.5782   -1.1947
 C    0.3312    1.9267   -1.2547
 H   -0.1222    2.2288   -2.2066
 C    1.5027    2.8445   -0.8363
 H    0.6304    0.8806   -1.3276
 C   -0.1851    1.7488    1.1463
 C    0.8814    2.8276    1.4604
 H   -1.0205    1.7573    1.8526
 H    0.2452    0.7444    1.1190
 C   -1.9274   -0.3797   -0.1506
 C   -2.3271   -0.6183    1.2376
 O   -2.1665   -1.9035    1.6351
 O   -2.8398    0.2088    1.9867
 C   -2.6591   -2.2471    2.9315
 H   -2.4241   -3.3097    3.0729
 H   -2.1675   -1.6472    3.7122
 H   -3.7476   -2.0934    2.9908
 C   -1.0510   -1.4364   -0.8780
 H   -1.4207   -2.4109   -0.5067
 H   -3.8859   -3.2033   -1.8596
 C    3.1780   -1.4628   -0.0636
 C    2.7408   -1.3722   -1.3858
 C    1.3714   -1.3729   -1.6408
 C    0.4399   -1.4510   -0.5928
 C    0.9150   -1.5756    0.7263
 C    2.2776   -1.5753    1.0003
 N    4.6110   -1.4464    0.2164
 H    3.4642   -1.2981   -2.1970
 H    1.0119   -1.2962   -2.6658
 H    0.2085   -1.6748    1.5503
 H    2.6463   -1.6606    2.0216
 C   -4.3740   -2.3086   -1.4098
 H   -4.3227   -2.4555   -0.3069
 H   -5.4519   -2.3751   -1.6780
 O    4.9770   -1.5224    1.3834
 O    5.3885   -1.3547   -0.7261
 H    0.5499    3.4556    2.2993
 H    1.8219    2.3399    1.7531
 N    1.1263    3.6839    0.3005
 H    2.3765    2.2401   -0.5545
 H    1.7916    3.4832   -1.6829
 H    0.0706    4.9985   -0.9388
 H   -0.3382    5.1075    0.7878
 H   -2.2768   -1.3001   -2.3436
 H   -2.9913   -0.6886   -0.8087
 O   -3.7972   -1.1055   -1.8207

r1-TS7-18
Final geometry with  54 atoms:
 O   -0.0412   -0.2395    2.4437
 C    0.6919   -0.4620   -0.4222
 H    0.0693   -1.2782   -0.0379
 H    0.4579   -0.3382   -1.4854
 N    2.1042   -1.0269   -0.3947
 C    2.4931   -1.4663    0.9970
 H    1.7871   -2.2556    1.2810
 C    3.9610   -1.9534    0.9648
 H    2.3631   -0.6039    1.6542
 C    3.1212   -0.0189   -0.8792
 H    3.1316    0.7681   -0.1165
 C    4.4926   -0.7240   -1.0049
 H    2.7553    0.3776   -1.8318
 C    2.1480   -2.2317   -1.3010
 C    3.5393   -2.8993   -1.1810
 H    1.3329   -2.8969   -0.9911
 H    1.9426   -1.8663   -2.3147
 C    0.4701    0.8181    0.3695
 C    0.2574    2.0454   -0.4300
 O    0.7567    1.9734   -1.6792
 O   -0.2463    3.0788   -0.0078
 C    0.7156    3.1697   -2.4625
 H    1.2889    3.9730   -1.9756
 H   -0.3219    3.5044   -2.6104
 H    1.1703    2.9157   -3.4282
 C   -0.5686    0.6785    1.5007
 H   -0.6743    1.6775    1.9531
 H    2.1656    3.6881    1.6429
 C   -4.4109   -0.5630    0.0033
 C   -3.5701   -1.5150    0.5826
 C   -2.3370   -1.1026    1.0808
 C   -1.9371    0.2416    0.9995
 C   -2.8127    1.1783    0.4194
 C   -4.0483    0.7849   -0.0820
 N   -5.7079   -0.9853   -0.5193
 H   -3.8833   -2.5567    0.6420
 H   -1.6753   -1.8299    1.5522
 H   -2.5193    2.2270    0.3646
 H   -4.7314    1.5066   -0.5285
 C    2.9076    2.9039    1.3512
 H    3.0002    2.9914    0.2369
 H    3.8904    3.2641    1.7438
 O   -6.4359   -0.1396   -1.0250
 O   -6.0140   -2.1686   -0.4320
 H    3.4523   -3.8758   -0.6840
 H    3.9555   -3.0662   -2.1845
 N    4.4551   -2.0606   -0.4087
 H    4.7824   -0.8193   -2.0611
 H    5.2595   -0.1224   -0.4965
 H    4.6003   -1.2445    1.5099
 H    4.0382   -2.9323    1.4589
 H   -0.6353   -0.2651    3.2091
 H    1.4795    1.1654    1.0134
 O    2.5904    1.6324    1.7886

r1-TS7-19
Final geometry with  54 atoms:
 O   -0.0145   -2.7750   -1.3931
 C   -1.0167    0.0295    0.9334
 H   -0.0150    0.0751    1.3754
 H   -1.7390   -0.1260    1.7425
 N   -1.2838    1.4897    0.4852
 C   -0.2240    1.9752   -0.4648
 H   -0.2674    1.3266   -1.3439
 C   -0.5057    3.4569   -0.8260
 H    0.7401    1.8412    0.0373
 C   -1.2552    2.3551    1.7217
 H   -0.2825    2.1891    2.2007
 C   -1.4738    3.8337    1.3169
 H   -2.0446    1.9803    2.3847
 C   -2.6244    1.6516   -0.1821
 C   -2.8462    3.1520   -0.5069
 H   -2.6053    1.0411   -1.0913
 H   -3.3763    1.2511    0.5047
 C   -1.1289   -1.0836   -0.0675
 C   -2.4818   -1.3852   -0.5578
 O   -3.4258   -1.2654    0.4116
 O   -2.7827   -1.7697   -1.6810
 C   -4.7730   -1.5504    0.0391
 H   -5.1029   -0.8976   -0.7839
 H   -4.8825   -2.6010   -0.2713
 H   -5.3830   -1.3614    0.9318
 C   -0.0460   -1.3702   -1.1303
 H   -0.2954   -0.8881   -2.0904
 H   -1.4256   -5.1687    1.5444
 C    3.9544   -0.1872   -0.0597
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 C   3.3992   0.2947  -1.2464
 C   2.1004  -0.0858  -1.5745
 C   1.3566  -0.9288  -0.7358
 C   1.9554  -1.4178   0.4406
 C   3.2493  -1.0465   0.7891
 N   5.3130   0.2120   0.3016
 H   3.9770   0.9533  -1.8937
 H   1.6522   0.2854  -2.4988
 H   1.4002  -2.1040   1.0833
 H   3.7155  -1.4137   1.7026
 C  -1.6870  -4.1258   1.2654
 H  -2.3868  -3.7578   2.0479
 H  -2.2766  -4.1977   0.3235
 O   5.7850  -0.2115   1.3497
 O   5.9235   0.9550  -0.4573
 H  -3.0272   3.2758  -1.5836
 H  -3.7294   3.5241   0.0304
 N  -1.6868   3.9547  -0.1241
 H  -2.3483   4.2397   1.8437
 H  -0.5981   4.4348   1.5984
 H   0.3601   4.0771  -0.5558
 H  -0.6679   3.5540  -1.9084
 H  -0.1080  -3.2091  -0.4990
 H  -0.9148  -2.1547   0.6900
 O  -0.5456  -3.3295   1.1343

r1-TS7-20
Final geometry with  54 atoms:
 O  -0.5251   1.7561  -1.9495
 C   0.9594  -0.7457   0.4647
 H   0.8070  -0.9045   1.5366
 H   0.4925  -1.5836  -0.0656
 N   2.4561  -0.9770   0.2535
 C   2.8393  -2.2821   0.9068
 H   2.1702  -3.0515   0.5025
 C   4.3318  -2.5722   0.6061
 H   2.6395  -2.1647   1.9789
 C   3.2855   0.1177   0.8801
 H   2.9831   0.1733   1.9316
 C   4.7842  -0.2347   0.7065
 H   3.0143   1.0567   0.3880
 C   2.7715  -1.0856  -1.2151
 C   4.2983  -1.2643  -1.3874
 H   2.2025  -1.9464  -1.5874
 H   2.3989  -0.1820  -1.7021
 C   0.4169   0.5896   0.0085
 C  -0.0534   1.4746   1.0794
 O   0.5137   1.2173   2.2878
 O  -0.8092   2.4297   0.9418
 C   0.2024   2.1202   3.3487
 H  -0.8787   2.1295   3.5558
 H   0.7473   1.7560   4.2292
 H   0.5278   3.1432   3.1041
 C  -0.5067   0.5329  -1.2426
 H  -0.0789  -0.2624  -1.8828
 H   3.6435   1.8259  -1.8385
 C  -4.5064  -0.6929  -0.2175
 C  -3.5099  -1.6625  -0.3627
 C  -2.2292  -1.2531  -0.7172
 C  -1.9272   0.1072  -0.9125
 C  -2.9577   1.0533  -0.7807
 C  -4.2467   0.6635  -0.4307
 N  -5.8544  -1.1101   0.1515
 H  -3.7452  -2.7153  -0.2116
 H  -1.4544  -2.0092  -0.8581
 H  -2.7365   2.1041  -0.9582
 H  -5.0473   1.3946  -0.3234
 C   2.6840   2.3028  -2.1332
 H   2.2402   1.6652  -2.9297
 H   2.9526   3.2629  -2.6215
 O  -6.7229  -0.2520   0.2597
 O  -6.0654  -2.3030   0.3411
 H   4.4996  -2.1375  -2.0236
 H   4.7297  -0.3805  -1.8775
 N   4.9535  -1.4483  -0.0928
 H   5.3054   0.5961   0.2113
 H   5.2521  -0.3912   1.6885
 H   4.8701  -2.7555   1.5464
 H   4.4247  -3.4719  -0.0182
 H   0.3046   2.2461  -1.6905
 H   1.3257   1.4558  -0.5023
 O   1.8223   2.5122  -1.0527

r1-TS7-21
Final geometry with  54 atoms:
 O   0.0056  -2.7864   1.3963
 C   0.9875   0.0291  -0.9199
 H   1.6808  -0.1288  -1.7541
 H  -0.0280   0.0843  -1.3273
 N   1.2837   1.4856  -0.4788
 C   0.3458   1.9426   0.6036
 H   0.4956   1.2761   1.4581
 C   0.6649   3.4181   0.9605
 H  -0.6703   1.8162   0.2164
 C   1.0875   2.3702  -1.6870
 H   0.0647   2.1949  -2.0418
 C   1.3316   3.8456  -1.2865
 H   1.7928   2.0186  -2.4499
 C   2.6951   1.6555   0.0193
 C   2.9444   3.1557   0.3236
 H   2.7896   1.0413   0.9209
 H   3.3612   1.2635  -0.7558
 C   1.1137  -1.0863   0.0763
 C   2.4692  -1.3878   0.5585
 O   3.4036  -1.2861  -0.4220
 O   2.7784  -1.7607   1.6834
 C   4.7537  -1.5688  -0.0590
 H   4.8637  -2.6144   0.2676
 H   5.0947  -0.9039   0.7497
 H   5.3549  -1.3965  -0.9610
 C   0.0338  -1.3803   1.1411
 H   0.2829  -0.9044   2.1040
 H   2.3687  -3.7662  -2.0545
 C  -3.9573  -0.1729   0.0606
 C  -3.2644  -1.0571  -0.7727
 C  -1.9751  -1.4385  -0.4188
 C  -1.3682  -0.9352   0.7476
 C  -2.0998  -0.0671   1.5712
 C  -3.3945   0.3236   1.2375
 N  -5.3102   0.2386  -0.3080
 H  -3.7362  -1.4344  -1.6793
 H  -1.4280  -2.1407  -1.0511
 H  -1.6450   0.3167   2.4870
 H  -3.9627   1.0019   1.8728
 C   1.6715  -4.1287  -1.2672
 H   1.4055  -5.1719  -1.5404
 H   2.2649  -4.1984  -0.3276
 O  -5.9103   1.0035   0.4374
 O  -5.7880  -0.1966  -1.3487
 H   3.2741   3.2725   1.3652
 H   3.7382   3.5436  -0.3296
 N   1.7334   3.9468   0.1153
 H   2.1202   4.2787  -1.9172
 H   0.4151   4.4329  -1.4365
 H  -0.2350   4.0347   0.8290
 H   0.9760   3.4900   2.0117
 H   0.0986  -3.2161   0.5001
 H   0.9001  -2.1560  -0.6852
 O   0.5328  -3.3286  -1.1343

r1-TS7-22
Final geometry with  54 atoms:
 O   1.2402  -1.4334  -2.2449
 C   1.9167   1.0241  -0.6353
 H   2.8219   1.5034  -0.2452
 H   1.9513   1.0561  -1.7308
 N   0.7847   1.9997  -0.2646
 C   1.3170   3.4074  -0.3976
 H   1.7520   3.4911  -1.4010
 C   0.1573   4.4081  -0.1627
 H   2.1156   3.5117   0.3467
 C   0.2963   1.8176   1.1483
 H   1.1747   1.8614   1.7986
 C  -0.7449   2.9202   1.4656
 H  -0.1364   0.8154   1.2061
 C  -0.3754   1.8599  -1.2174
 C  -1.5070   2.8211  -0.7855
 H   0.0166   2.0908  -2.2152
 H  -0.6900   0.8166  -1.1988
 C   1.9161  -0.4092  -0.1643
 C   2.3374  -0.6086   1.2238
 O   2.1265  -1.8659   1.6823
 O   2.9053   0.2251   1.9238
 C   2.6355  -2.1740   2.9813
 H   3.7318  -2.0771   3.0059
 H   2.3485  -3.2144   3.1801
 H   2.1980  -1.5115   3.7432
 C   1.0220  -1.4789  -0.8488
 H   1.3792  -2.4444  -0.4428
 H   3.8658  -3.3061  -1.7896
 C  -3.2074  -1.4315  -0.0394
 C  -2.3089  -1.4820   1.0309
 C  -0.9459  -1.5061   0.7598
 C  -0.4687  -1.4652  -0.5635
 C  -1.3984  -1.4439  -1.6159
 C  -2.7678  -1.4216  -1.3640
 N  -4.6407  -1.3930   0.2362
 H  -2.6794  -1.5029   2.0549
 H  -0.2408  -1.5587   1.5892
 H  -1.0366  -1.4256  -2.6427
 H  -3.4896  -1.3920  -2.1795
 C   4.3407  -2.3961  -1.3567
 H   5.4253  -2.4681  -1.5951
 H   4.2619  -2.5084  -0.2510
 O  -5.4162  -1.3555  -0.7116
 O  -5.0092  -1.3977   1.4049
 H  -1.8361   3.4166  -1.6487
 H  -2.3707   2.2484  -0.4195
 N  -1.0533   3.7155   0.2780
 H  -1.6693   2.4568   1.8380
 H  -0.3609   3.5886   2.2488
 H   0.4534   5.1406   0.6010
 H  -0.0671   4.9557  -1.0887
 H   2.2460  -1.4111  -2.3226
 H   2.9701  -0.7470  -0.8208
 O   3.7713  -1.2086  -1.8194

r1-TS7-23
Final geometry with  54 atoms:
 O  -0.5840  -3.2534   0.1669
 C  -1.1515   0.2321  -1.2889
 H  -0.2556   0.1345  -1.9123
 H  -1.9903   0.4544  -1.9572
 N  -0.9305   1.5313  -0.5178
 C  -2.1264   1.8778   0.3367
 H  -2.2473   1.0497   1.0438
 C  -1.8464   3.2178   1.0609
 H  -2.9899   1.9301  -0.3352
 C  -0.7147   2.6361  -1.5231
 H  -1.5916   2.6443  -2.1815
 C  -0.5245   3.9764  -0.7710
 H   0.1683   2.3551  -2.1109
 C   0.2909   1.4529   0.3675
 C   0.5048   2.8298   1.0448
 H   0.0951   0.6651   1.1004
 H   1.1284   1.1684  -0.2786
 C  -1.3980  -1.0262  -0.4703
 C  -2.7774  -1.5388  -0.5606
 O  -3.7050  -0.6011  -0.8101
 O  -3.1131  -2.7076  -0.3496
 C  -5.0774  -1.0066  -0.7683
 H  -5.6646  -0.1041  -0.9782
 H  -5.2817  -1.7749  -1.5286
 H  -5.3353  -1.4019   0.2257
 C  -0.3611  -2.1669  -0.7157
 H  -0.4597  -2.5114  -1.7653
 H  -1.0598  -2.5304   2.8669
 C   3.6408  -0.7226  -0.1516
 C   2.8876  -1.0957   0.9655
 C   1.6004  -1.5843   0.7704
 C   1.0646  -1.6970  -0.5229
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 C    1.8555   -1.3405   -1.6247
 C    3.1449   -0.8426   -1.4507
 N    4.9894   -0.1904    0.0460
 H    3.3060   -0.9896    1.9656
 H    0.9867   -1.8474    1.6308
 H    1.4560   -1.4500   -2.6353
 H    3.7610   -0.5566   -2.3021
 C   -1.7574   -1.6593    2.8670
 H   -1.9260   -1.4112    3.9411
 H   -2.7312   -2.0605    2.4977
 O    5.6286    0.1553   -0.9399
 O    5.4212   -0.1102    1.1889
 H    0.5064    2.7072    2.1370
 H    1.4766    3.2494    0.7491
 N   -0.5492    3.7740    0.6758
 H    0.4359    4.4296   -1.0536
 H   -1.3241    4.6784   -1.0453
 H   -2.6332    3.9465    0.8203
 H   -1.8514    3.0597    2.1486
 H   -1.5512   -3.4086    0.1297
 H   -1.3367   -0.8076    0.7974
 O   -1.2961   -0.5676    2.1454

r1-TS7-24
Final geometry with  54 atoms:
 O   -1.0952   -1.4603   -2.2612
 C   -2.0840    0.6510   -0.3910
 H   -2.2323    0.7624   -1.4709
 H   -3.0073    0.9446    0.1205
 N   -1.0854    1.7678   -0.0347
 C   -0.0234    1.8954   -1.0963
 H   -0.5475    2.1497   -2.0257
 C    0.9904    2.9819   -0.6690
 H    0.4439    0.9180   -1.2161
 C   -0.4344    1.5621    1.3070
 H    0.1644    0.6509    1.2306
 C    0.4339    2.8009    1.6376
 H   -1.2384    1.3992    2.0306
 C   -1.8427    3.0743    0.0084
 C   -0.8349    4.2323    0.2168
 H   -2.3927    3.1572   -0.9370
 H   -2.5613    2.9900    0.8327
 C   -1.8109   -0.7941   -0.0564
 C   -2.0836   -1.1768    1.3287
 O   -1.7030   -2.4438    1.6198
 O   -2.6796   -0.4959    2.1593
 C   -2.0453   -2.9426    2.9139
 H   -1.5862   -2.3311    3.7055
 H   -3.1368   -2.9543    3.0556
 H   -1.6522   -3.9663    2.9579
 C   -0.7995   -1.6273   -0.8896
 H   -0.9837   -2.6766   -0.5889
 H   -5.3820   -1.4151   -2.6546
 C    3.4116   -1.0074   -0.2286
 C    2.9097   -0.9446   -1.5294
 C    1.5477   -1.1522   -1.7328
 C    0.6851   -1.4095   -0.6545
 C    1.2289   -1.4971    0.6406
 C    2.5855   -1.2913    0.8631
 N    4.8354   -0.7759   -0.0020
 H    3.5777   -0.7320   -2.3633
 H    1.1361   -1.0982   -2.7396
 H    0.5840   -1.7324    1.4867
 H    3.0057   -1.3487    1.8663
 C   -4.5689   -0.9148   -2.0825
 H   -5.0681   -0.4154   -1.2212
 H   -4.1955   -0.0936   -2.7372
 O    5.2576   -0.8254    1.1472
 O    5.5491   -0.5397   -0.9695
 H   -0.7875    4.8633   -0.6817
 H   -1.1657    4.8610    1.0552
 N    0.5050    3.7165    0.4991
 H    0.0132    3.3400    2.4979
 H    1.4498    2.4773    1.9047
 H    1.9564    2.5212   -0.4186
 H    1.1541    3.6818   -1.5005
 H   -2.0895   -1.6235   -2.3045
 H   -2.8284   -1.2889   -0.6784
 O   -3.5795   -1.8150   -1.6903

r1-TS7-25
Final geometry with  54 atoms:
 O   -0.7438   -2.7432    1.1742
 C   -0.9318    0.1623   -1.2846
 H    0.0871    0.0161   -1.6567
 H   -1.5930    0.2888   -2.1498
 N   -0.8884    1.5566   -0.6505
 C   -2.2292    1.9488   -0.0801
 H   -2.4668    1.2280    0.7080
 C   -2.1388    3.4021    0.4475
 H   -2.9582    1.8337   -0.8893
 C   -0.5224    2.5562   -1.7191
 H   -1.3202    2.5161   -2.4707
 C   -0.3862    3.9563   -1.0699
 H    0.4134    2.2098   -2.1743
 C    0.1606    1.6242    0.4261
 C    0.1332    3.0329    1.0653
 H   -0.0628    0.8360    1.1461
 H    1.1177    1.3971   -0.0580
 C   -1.4092   -0.9716   -0.4058
 C   -2.7506   -1.4110   -0.8180
 O   -3.0600   -2.6678   -0.4324
 O   -3.5785   -0.7156   -1.4039
 C   -4.3871   -3.1188   -0.7022
 H   -4.5956   -3.1163   -1.7831
 H   -4.4446   -4.1439   -0.3139
 H   -5.1292   -2.4846   -0.1930
 C   -0.4251   -2.1391   -0.0687
 H   -0.5252   -2.9209   -0.8437
 H   -1.8175    1.1309    2.9891
 C    3.6764   -0.8426   -0.0990
 C    2.9766   -0.8651    1.1106
 C    1.6571   -1.3046    1.1093
 C    1.0315   -1.7076   -0.0798
 C    1.7712   -1.7012   -1.2738
 C    3.0923   -1.2645   -1.2966
 N    5.0592   -0.3721   -0.1108
 H    3.4644   -0.5393    2.0285
 H    1.0923   -1.3411    2.0404
 H    1.3033   -2.0417   -2.2008
 H    3.6695   -1.2523   -2.2203
 C   -1.5553    0.0539    3.0714
 H   -1.8830   -0.2694    4.0812
 H   -0.4448   -0.0001    3.0764
 O    5.6600   -0.3544   -1.1785
 O    5.5608   -0.0110    0.9471
 H   -0.1996    2.9660    2.1104
 H    1.1445    3.4630    1.0575
 N   -0.7750    3.9207    0.3396
 H    0.6526    4.3075   -1.1410
 H   -1.0247    4.6750   -1.6021
 H   -2.8105    4.0554   -0.1269
 H   -2.4522    3.4351    1.5001
 H   -1.2989   -2.0940    1.6889
 H   -1.7445   -0.6151    0.8743
 O   -2.1540   -0.7256    2.0784

r1-TS7-26
Final geometry with  54 atoms:
 O    0.9946   -2.1144   -1.9426
 C    1.8508    0.5988   -0.8943
 H    2.8295    1.0618   -0.7273
 H    1.7382    0.4119   -1.9693
 N    0.8434    1.7337   -0.5985
 C    1.4708    3.0367   -1.0344
 H    1.7800    2.9071   -2.0788
 C    0.4414    4.1808   -0.8528
 H    2.3636    3.1765   -0.4134
 C    0.5005    1.8467    0.8631
 H    1.4452    1.9432    1.4058
 C   -0.4286    3.0705    1.0689
 H    0.0151    0.9095    1.1507
 C   -0.4226    1.5488   -1.3954
 C   -1.4081    2.6949   -1.0652
 H   -0.1251    1.5396   -2.4507
 H   -0.8269    0.5702   -1.1384
 C    1.8052   -0.7115   -0.1501
 C    2.2490   -0.7482    1.2439
 O    3.1042    0.2553    1.5577
 O    1.9773   -1.6190    2.0658
 C    3.6488    0.2504    2.8782
 H    4.2911    1.1377    2.9448
 H    4.2457   -0.6575    3.0548
 H    2.8502    0.3083    3.6335
 C    0.8167   -1.8310   -0.5695
 H    1.1163   -2.7028    0.0453
 H    5.1085   -3.2665   -1.2324
 C   -3.3624   -1.2244    0.2539
 C   -2.9612   -1.5041   -1.0536
 C   -1.6080   -1.7109   -1.3090
 C   -0.6576   -1.6336   -0.2783
 C   -1.0990   -1.3874    1.0355
 C   -2.4447   -1.1723    1.3082
 N   -4.7759   -0.9846    0.5294
 H   -3.6990   -1.5496   -1.8539
 H   -1.2719   -1.9140   -2.3245
 H   -0.3755   -1.3656    1.8508
 H   -2.7883   -0.9683    2.3215
 C    4.0495   -3.0476   -0.9708
 H    3.4784   -3.9813   -1.1775
 H    4.0282   -2.9153    0.1349
 O   -5.1088   -0.7220    1.6792
 O   -5.5715   -1.0532   -0.4000
 H   -1.7438    3.1751   -1.9950
 H   -2.2932    2.2950   -0.5510
 N   -0.7770    3.6945   -0.2060
 H   -1.3506    2.7529    1.5756
 H    0.0683    3.8166    1.7045
 H    0.8812    4.9785   -0.2383
 H    0.1758    4.6113   -1.8283
 H    1.9964   -2.1560   -2.0523
 H    2.8098   -1.2346   -0.7637
 O    3.5512   -1.9376   -1.6566

r1-TS7-27
Final geometry with  54 atoms:
 O   -0.5771    2.0522   -1.8742
 C    0.8261   -0.7122    0.3336
 H    0.3008   -1.4481   -0.2855
 H    0.5357   -0.8850    1.3770
 N    2.2840   -1.1389    0.2589
 C    2.7731   -1.1408   -1.1703
 H    2.6237   -0.1281   -1.5595
 C    4.2698   -1.5377   -1.1762
 H    2.1409   -1.8560   -1.7115
 C    2.3946   -2.5422    0.8014
 H    1.6779   -3.1593    0.2455
 C    3.8540   -3.0308    0.6346
 H    2.0819   -2.4958    1.8518
 C    3.1725   -0.2346    1.0827
 C    4.6087   -0.8138    1.0712
 H    3.1249    0.7526    0.6083
 H    2.7371   -0.1918    2.0872
 C    0.5190    0.7102   -0.1002
 C    0.2218    1.5765    1.0566
 O   -0.3013    2.7757    0.6935
 O    0.4788    1.3399    2.2278
 C   -0.5811    3.7188    1.7329
 H   -1.0030    4.6003    1.2348
 H   -1.3078    3.3047    2.4473
 H    0.3415    3.9915    2.2660
 C   -0.4770    0.7661   -1.2893
 H   -0.0568    0.1091   -2.0661
 H    1.7691    3.4019   -2.2994
 C   -4.3030   -0.8611   -0.1507
 C   -4.0248    0.4791    0.1357
 C   -2.7986    1.0068   -0.2526
 C   -1.8469    0.2112   -0.9172
 C   -2.1687   -1.1249   -1.2092
 C   -3.3900   -1.6732   -0.8256
 N   -5.5869   -1.4237    0.2592
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H	-4.7634	1.0902	0.6532
H	-2.5793	2.0527	-0.0381
H	-1.4547	-1.7461	-1.7548
H	-3.6406	-2.7092	-1.0504
C	2.4584	3.2581	-1.4346
H	2.0331	3.8790	-0.6094
H	3.4107	3.7618	-1.7230
O	-5.8149	-2.6009	0.0069
O	-6.3828	-0.6958	0.8404
H	5.3161	-0.0334	0.7569
H	4.8965	-1.1464	2.0786
N	4.7149	-1.9508	0.1556
H	4.2342	-3.3972	1.5985
H	3.8966	-3.8615	-0.0838
H	4.4353	-2.3615	-1.8849
H	4.8804	-0.6825	-1.4987
H	-0.5973	2.6966	-1.1453
H	1.5490	1.3171	-0.5852
O	2.6580	1.9295	-1.0898

r1-TS7-28
Final geometry with 54 atoms:

O	-0.6028	2.0761	-1.9650
C	0.7449	-0.5623	0.4278
H	0.5425	-0.5856	1.5039
H	0.1052	-1.3175	-0.0434
N	2.1496	-1.1216	0.2790
C	2.5102	-1.2930	-1.1784
H	2.4533	-0.2999	-1.6368
C	3.9408	-1.8804	-1.2671
H	1.7503	-1.9568	-1.6090
C	2.1901	-2.4769	0.9426
H	1.4073	-3.0842	0.4716
C	3.6032	-3.0839	0.7626
H	1.9298	-2.3181	1.9963
C	3.1758	-0.2323	0.9427
C	4.5656	-0.9050	0.8183
H	3.1394	0.7268	0.4126
H	2.8556	-0.1058	1.9830
C	0.5062	0.8157	-0.1677
C	0.2611	1.8939	0.8071
O	0.7159	1.6484	2.0432
O	-0.2269	2.9906	0.5211
C	0.6516	2.7191	2.9928
H	-0.3909	3.0255	3.1636
H	1.0854	2.3253	3.9201
H	1.2325	3.5845	2.6408
C	-0.5061	0.8073	-1.3450
H	-0.1027	0.1116	-2.0976
H	1.8292	3.1922	-2.6342
C	-4.3501	-0.7116	-0.1246
C	-3.4595	-1.5623	-0.7814
C	-2.2285	-1.0515	-1.1861
C	-1.8771	0.2846	-0.9337
C	-2.8048	1.1184	-0.2828
C	-4.0400	0.6287	0.1267
N	-5.6451	-1.2342	0.3049
H	-3.7347	-2.5980	-0.9766
H	-1.5305	-1.7019	-1.7180
H	-2.5569	2.1630	-0.0946
H	-4.7612	1.2689	0.6335
C	2.5573	3.0854	-1.7957
H	2.2138	3.8058	-1.0139
H	3.5183	3.5038	-2.1798
O	-6.4248	-0.4714	0.8624
O	-5.8972	-2.4140	0.0917
H	5.2596	-0.2239	0.3059
H	4.9748	-1.1204	1.8154
N	4.4869	-2.1548	0.0621
H	4.0363	-3.3191	1.7448
H	3.5414	-4.0180	0.1872
H	3.9299	-2.8124	-1.8495
H	4.6028	-1.1670	-1.7778
H	-0.5701	2.7314	-1.2374
H	1.5447	1.2845	-0.7198
O	2.6996	1.7849	-1.3360

r1-TS7-29
Final geometry with 54 atoms:

O	-0.0775	-2.8070	-1.4725
C	1.0772	-0.1176	0.9095
H	0.0785	-0.0505	1.3544
H	1.7960	-0.3285	1.7094
N	1.3999	1.3501	0.5163
C	0.3608	1.9153	-0.4113
H	-0.6088	1.7892	0.0814
C	0.6902	3.4033	-0.6994
H	0.3868	1.3107	-1.3220
C	2.7455	1.4881	-0.1457
H	2.7060	0.9081	-1.0738
C	3.0186	2.9895	-0.4245
H	3.4834	1.0415	0.5277
C	1.4039	2.1658	1.7868
C	1.6974	3.6473	1.4444
H	0.4199	2.0285	2.2517
H	2.1686	1.7270	2.4390
C	1.1445	-1.1950	-0.1341
C	2.4800	-1.5129	-0.6653
O	3.4457	-1.4637	0.2858
O	2.7416	-1.8641	-1.8086
C	4.7783	-1.7587	-0.1318
H	5.4088	-1.6497	0.7599
H	4.8525	-2.7865	-0.5184
H	5.1119	-1.0575	-0.9128
C	0.0435	-1.4102	-1.1969
H	0.3326	-0.9372	-2.1501
H	0.7187	-4.2669	2.8783
C	-3.8815	0.0242	-0.1639
C	-3.2761	0.4905	-1.3326
C	-2.0015	0.0289	-1.6507
C	-1.3297	-0.8788	-0.8186
C	-1.9796	-1.3495	0.3354
C	-3.2499	-0.8986	0.6759
N	-5.2146	0.5088	0.1872
H	-3.7977	1.1996	-1.9741
H	-1.5154	0.3862	-2.5613
H	-1.4830	-2.0811	0.9701
H	-3.7525	-1.2525	1.5752
C	0.1224	-3.6380	2.1786
H	0.0008	-2.6538	2.6863
H	-0.8934	-4.0927	2.1482
O	-5.7304	0.0977	1.2196
O	-5.7608	1.3079	-0.5637
H	0.8596	4.2809	1.7668
H	2.5997	3.9816	1.9747
N	1.8984	3.8222	0.0075
H	3.9256	3.3083	0.1074
H	3.1838	3.1436	-1.4997
H	0.8392	3.5506	-1.7780
H	-0.1482	4.0390	-0.3826
H	0.0479	-3.2721	-0.5995
H	0.9772	-2.3011	0.5687
O	0.7125	-3.5325	0.9222

r1-TS7-30
Final geometry with 54 atoms:

O	-0.6176	2.1292	-1.9142
C	0.7447	-0.5344	0.4417
H	0.5082	-0.5910	1.5097
H	0.1414	-1.2939	-0.0688
N	2.1673	-1.0530	0.3235
C	2.2195	-2.4279	0.9430
H	1.4718	-3.0385	0.4222
C	3.6541	-2.9924	0.7986
H	1.9148	-2.3120	1.9903
C	3.1521	-0.1615	1.0445
H	2.8021	-0.0770	2.0794
C	4.5620	-0.7944	0.9329
H	3.1109	0.8104	0.5427
C	2.5790	-1.1580	-1.1257
C	4.0162	-1.7319	-1.1918
H	1.8393	-1.8025	-1.6157
H	2.5297	-0.1397	-1.5226
C	0.4868	0.8516	-0.1279
C	0.2011	1.9030	0.8674
O	0.6254	1.6338	2.1092
O	-0.2969	2.9973	0.5936
C	0.5150	2.6791	3.0827
H	-0.5377	2.9607	3.2328
H	0.9320	2.2707	4.0114
H	1.0873	3.5640	2.7674
C	-0.5134	0.8504	-1.3165
H	-0.0939	0.1721	-2.0763
H	2.8561	1.3736	-3.1365
C	-4.3533	-0.7232	-0.1549
C	-3.4414	-1.5613	-0.7988
C	-2.2118	-1.0335	-1.1852
C	-1.8827	0.3073	-0.9271
C	-2.8316	1.1282	-0.2905
C	-4.0656	0.6211	0.1009
N	-5.6474	-1.2634	0.2552
H	-3.6993	-2.6006	-0.9984
H	-1.4974	-1.6740	-1.7072
H	-2.6009	2.1762	-0.1002
H	-4.8031	1.2513	0.5966
C	2.7217	2.2791	-2.4881
H	1.8063	2.7814	-2.8825
H	3.5717	2.9535	-2.7546
O	-6.4443	-0.5122	0.8041
O	-5.8817	-2.4456	0.0350
H	4.0275	-2.6537	-1.7901
H	4.6832	-1.0041	-1.6748
N	4.5333	-2.0261	0.1446
H	5.2469	-0.0824	0.4511
H	4.9564	-1.0229	1.9330
H	4.0623	-3.2333	1.7900
H	3.6368	-3.9172	0.2052
H	-0.5862	2.7721	-1.1749
H	1.5065	1.3590	-0.6482
O	2.6701	1.9960	-1.1370

r1-TS7-31
Final geometry with 54 atoms:

O	-0.8651	-3.0345	0.4013
C	-0.9935	0.3806	-1.3186
H	-0.0432	0.1814	-1.8247
H	-1.7328	0.6384	-2.0858
N	-0.7526	1.6929	-0.5787
C	-1.9898	2.1559	0.1540
H	-2.1793	1.3986	0.9240
C	-1.7075	3.5501	0.7676
H	-2.8076	2.1657	-0.5741
C	-0.3757	2.7361	-1.6022
H	-1.2257	2.8196	-2.2904
C	-0.0636	4.0679	-0.8779
H	0.4888	2.3437	-2.1515
C	0.3745	1.5694	0.4170
C	0.5692	2.9364	1.1196
H	0.0833	0.7907	1.1260
H	1.2585	1.2523	-0.1483
C	-1.4550	-0.8066	-0.4893
C	-2.8890	-1.0687	-0.7312
O	-3.2760	-2.3282	-0.4045
O	-3.7123	-0.2520	-1.1209
C	-4.6726	-2.6317	-0.4802
H	-4.7708	-3.6793	-0.1700
H	-5.0435	-2.5057	-1.5079
H	-5.2473	-1.9820	0.1966
C	-0.5401	-2.0684	-0.5887
H	-0.6556	-2.5166	-1.5951
H	-3.4351	-1.0166	2.2801
C	3.5875	-1.0117	-0.0601
C	3.1004	-1.1978	-1.3550
C	1.7661	-1.5644	-1.5162
C	0.9240	-1.7275	-0.4066
C	1.4486	-1.5480	0.8837
C	2.7796	-1.1897	1.0665
N	4.9859	-0.6225	0.1228
H	3.7580	-1.0633	-2.2127
H	1.3730	-1.7244	-2.5227
H	0.7931	-1.6580	1.7468

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 H    3.1913   -1.0367    2.0633
 C   -2.4163   -1.1062    2.7310
 H   -2.1719   -2.1944    2.7070
 H   -2.5499   -0.8512    3.8080
 O    5.4037   -0.4745    1.2643
 O    5.6794   -0.4586   -0.8732
 H    0.3531    2.8366    2.1926
 H    1.6118    3.2673    1.0125
 N   -0.3169    3.9547    0.5569
 H    0.9892    4.3436   -1.0307
 H   -0.6882    4.8718   -1.2917
 H   -2.3660    4.3053    0.3156
 H   -1.9112    3.5249    1.8475
 H   -1.8278   -3.1616    0.3442
 H   -1.4605   -0.5518    0.7769
 O   -1.4646   -0.3058    2.1177

r1-TS7-32
Final geometry with  54 atoms:
 O    0.5005   -2.9374    1.1343
 C    1.0359    0.0041   -1.2342
 H    1.7767    0.1162   -2.0328
 H    0.0531   -0.0837   -1.7081
 N    0.9943    1.3886   -0.5751
 C    2.2945    1.7141    0.1173
 H    3.0817    1.6123   -0.6372
 C    2.2065    3.1488    0.6945
 H    2.4503    0.9550    0.8894
 C   -0.1447    1.4827    0.4035
 H   -0.0157    0.6803    1.1306
 C   -0.1319    2.8828    1.0610
 H   -1.0598    1.2943   -0.1696
 C    0.7660    2.4222   -1.6491
 C    0.6523    3.8184   -0.9856
 H    1.6153    2.3519   -2.3393
 H   -0.1485    2.1331   -2.1811
 C    1.3560   -1.1718   -0.3379
 C    2.6517   -1.8029   -0.6277
 O    3.5934   -0.9258   -1.0658
 O    2.9382   -2.9811   -0.4486
 C    4.9059   -1.4432   -1.2803
 H    4.9011   -2.2312   -2.0492
 H    5.3238   -1.8558   -0.3490
 H    5.5163   -0.5962   -1.6194
 C    0.2670   -2.2629   -0.0912
 H    0.3419   -3.0221   -0.8921
 H    0.1768   -0.1805    3.0839
 C   -3.7156   -0.6398   -0.2058
 C   -3.1069   -1.0201   -1.4049
 C   -1.8274   -1.5659   -1.3573
 C   -1.1516   -1.7210   -0.1357
 C   -1.8056   -1.3607    1.0519
 C   -3.0837   -0.8129    1.0286
 N   -5.0531   -0.0538   -0.2434
 H   -3.6331   -0.8916   -2.3499
 H   -1.3446   -1.8784   -2.2862
 H   -1.2946   -1.5135    2.0017
 H   -3.5901   -0.5184    1.9471
 C    1.2859   -0.1864    3.1559
 H    1.6108    0.8752    3.1038
 H    1.5247   -0.5340    4.1825
 O   -5.5955    0.0916   -1.3324
 O   -5.5764    0.2722    0.8152
 H    1.3866    4.5029   -1.4325
 H   -0.3494    4.2369   -1.1564
 N    0.8888    3.7371    0.4553
 H   -1.1164    3.3570    0.9440
 H    0.0760    2.7917    2.1361
 H    2.3963    3.1280    1.7764
 H    2.9691    3.7888    0.2291
 H    1.0294   -2.3229    1.7142
 H    1.6147   -0.8446    0.9712
 O    1.9115   -0.9904    2.1994

r1-TS7-33
Final geometry with  54 atoms:
 O    0.1278   -2.8870   -1.1455
 C    1.0610    0.0208    1.0709
 H    0.0400    0.0755    1.4622
 H    1.7489   -0.1061    1.9152
 N    1.3471    1.4675    0.5921
 C    1.1801    2.3757    1.7873
 H    1.9139    2.0474    2.5334
 C    1.3961    3.8443    1.3487
 H    0.1715    2.1980    2.1797
 C    0.3840    1.9040   -0.4764
 H   -0.6232    1.7915   -0.0622
 C    0.7019    3.3678   -0.8790
 H    0.5102    1.2171   -1.3175
 C    2.7452    1.6286    0.0543
 C    2.9906    3.1254   -0.2675
 H    3.4316    1.2370    0.8112
 H    2.8111    1.0052   -0.8439
 C    1.2309   -1.1252    0.1152
 C    2.6368   -1.4225   -0.2092
 O    2.8238   -1.9291   -1.4456
 O    3.5769   -1.2979    0.5702
 C    4.1436   -2.3676   -1.7733
 H    4.8583   -1.5313   -1.7328
 H    4.4768   -3.1583   -1.0839
 H    4.0875   -2.7627   -2.7957
 C    0.2014   -1.4689   -0.9880
 H    0.5264   -1.0699   -1.9624
 H    0.6644   -4.0068    3.3248
 C   -3.8142   -0.0748   -0.2982
 C   -3.2045   -0.8960    0.6556
 C   -1.9057   -1.3350    0.4256
 C   -1.2057   -0.9508   -0.7316
 C   -1.8566   -0.1472   -1.6792
 C   -3.1590    0.3003   -1.4726
 N   -5.1762    0.3985   -0.0622
 H   -3.7457   -1.1813    1.5568
 H   -1.4262   -1.9880    1.1525
 H   -1.3313    0.1418   -2.5922
 H   -3.6643    0.9297   -2.2041
 C    0.1183   -3.4242    2.5485
 H   -0.0443   -2.4137    2.9884
 H   -0.8907   -3.8888    2.4705
 O   -5.6997    1.1136   -0.9081
 O   -5.7380    0.0625    0.9733
 H    3.7876    3.5218    0.3766
 H    3.3144    3.2307   -1.3123
 N    1.7798    3.9177   -0.0599
 H    1.0030    3.4088   -1.9348
 H   -0.1960    3.9892   -0.7570
 H    0.4728    4.4218    1.4948
 H    2.1850    4.3037    1.9602
 H    0.2275   -3.2722   -0.2304
 H    1.0444   -2.1693    0.8926
 O    0.7998   -3.3855    1.3351

r1-TS7-34
Final geometry with  54 atoms:
 O    0.5952    2.1427    1.7855
 C   -0.8168   -0.6736   -0.3501
 H   -0.5008   -0.8810   -1.3797
 H   -0.3154   -1.3948    0.3049
 N   -2.2797   -1.0839   -0.3008
 C   -3.1413   -0.2023   -1.1753
 H   -2.6811   -0.1895   -2.1693
 C   -4.5811   -0.7734   -1.1800
 H   -3.1057    0.7963   -0.7277
 C   -2.8060   -1.0209    1.1124
 H   -2.6644    0.0128    1.4401
 C   -4.3020   -1.4210    1.0988
 H   -2.1872   -1.7035    1.7077
 C   -2.3863   -2.5052   -0.7938
 C   -3.8529   -2.9782   -0.6499
 H   -2.0432   -2.4999   -1.8356
 H   -1.6903   -3.1047   -0.1942
 C   -0.5043    0.7581    0.0478
 C   -0.1799    1.5859   -1.1319
 O    0.3371    2.7944   -0.7957
 O   -0.4090    1.3100   -2.3001
 C    0.6596    3.6969   -1.8590
 H    1.0799    4.5896   -1.3799
 H    1.4002    3.2481   -2.5374
 H   -0.2438    3.9627   -2.4274
 C    0.4839    0.8391    1.2429
 H    0.0504    0.2115    2.0365
 H   -2.8619    1.6158    2.8925
 C    4.3028   -0.8569    0.1875
 C    3.3751   -1.6420    0.8743
 C    2.1556   -1.0720    1.2307
 C    1.8506    0.2589    0.8997
 C    2.8164    1.0279    0.2246
 C    4.0411    0.4779   -0.1371
 N    5.5855   -1.4428   -0.1934
 H    3.6131   -2.6740    1.1291
 H    1.4299   -1.6713    1.7855
 H    2.6090    2.0702   -0.0177
 H    4.7911    1.0679   -0.6626
 C   -2.7134    2.4851    2.2008
 H   -1.8147    3.0169    2.5930
 H   -3.5763    3.1646    2.3988
 O    6.3929   -0.7395   -0.7888
 O    5.8008   -2.6136    0.0964
 H   -4.2114   -3.3727   -1.6109
 H   -3.9205   -3.7846    0.0937
 N   -4.7172   -1.8771   -0.2287
 H   -4.4814   -2.2227    1.8288
 H   -4.9216   -0.5580    1.3809
 H   -5.2905    0.0218   -0.9102
 H   -4.8460   -1.1385   -2.1823
 H    0.5933    2.7649    1.0367
 H   -1.5173    1.3959    0.4955
 O   -2.6195    2.1283    0.8675

r1-TS7-35
Final geometry with  54 atoms:
 O   -0.8718   -3.0262    0.4092
 C   -1.0026    0.3868   -1.3132
 H   -0.0535    0.1865   -1.8212
 H   -1.7425    0.6470   -2.0791
 N   -0.7577    1.6986   -0.5733
 C   -1.9949    2.1682    0.1551
 H   -2.1938    1.4120    0.9236
 C   -1.7072    3.5607    0.7701
 H   -2.8095    2.1832   -0.5767
 C   -0.3741    2.7394   -1.5967
 H   -1.2220    2.8260   -2.2871
 C   -0.0580    4.0705   -0.8726
 H    0.4901    2.3430   -2.1437
 C    0.3669    1.5709    0.4246
 C    0.5661    2.9373    1.1269
 H    0.0709    0.7933    1.1333
 H    1.2506    1.2506   -0.1393
 C   -1.4646   -0.8019   -0.4858
 C   -2.8971   -1.0648   -0.7312
 O   -3.2804   -2.3312   -0.4255
 O   -3.7228   -0.2448   -1.1091
 C   -4.6764   -2.6365   -0.5061
 H   -5.0471   -2.4959   -1.5320
 H   -4.7726   -3.6889   -0.2118
 H   -5.2528   -1.9982    0.1801
 C   -0.5494   -2.0633   -0.5847
 H   -0.6680   -2.5145   -1.5894
 H   -2.5585   -0.8181    3.8138
 C    3.5816   -1.0122   -0.0717
 C    2.7770   -1.1860    1.0578
 C    1.4446   -1.5416    0.8801
 C    0.9153   -1.7229   -0.4081
 C    1.7540   -1.5632   -1.5207
 C    3.0896   -1.1992   -1.3647
 N    4.9818   -0.6270    0.1058
 H    3.1924   -1.0322    2.0530
 H    0.7925   -1.6489    1.7460
 H    1.3571   -1.7243   -2.5256
 H    3.7446   -1.0677   -2.2249
 C   -2.3114   -1.1699    2.7853
 H   -3.2966   -1.3233    2.2818
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 H  -1.8797  -2.1910   2.9114
 O   5.6724  -0.4668  -0.8929
 O   5.4039  -0.4785   1.2455
 H   0.3473   2.8392   2.1995
 H   1.6103   3.2638   1.0218
 N  -0.3145   3.9592   0.5618
 H   0.9962   4.3418  -1.0236
 H  -0.6785   4.8766  -1.2881
 H  -2.3616   4.3191   0.3177
 H  -1.9124   3.5358   1.8497
 H  -1.8347  -3.1530   0.3551
 H  -1.4733  -0.5473   0.7837
 O  -1.4787  -0.2854   2.1161

r1-TS7-36
Final geometry with  54 atoms:
 O   0.0852   1.0271  -1.9830
 C   2.0550   1.1397   0.1486
 H   2.4294   1.6317   1.0522
 H   2.1900   1.8153  -0.7025
 N   3.0618   0.0010  -0.1190
 C   2.7744  -1.2285   0.7032
 H   1.8000  -1.6132   0.3851
 C   3.9140  -2.2554   0.4782
 H   2.7046  -0.9040   1.7462
 C   4.4387   0.4974   0.2551
 H   4.4177   0.6847   1.3356
 C   5.4856  -0.5738  -0.1396
 H   4.5885   1.4494  -0.2688
 C   3.0951  -0.3597  -1.5859
 C   4.0666  -1.5458  -1.7889
 H   2.0771  -0.5916  -1.9052
 H   3.4228   0.5449  -2.1125
 C   0.6002   0.7979   0.3598
 C   0.3090   0.3674   1.7266
 O  -0.8233  -0.3561   1.8575
 O   0.9801   0.6566   2.7179
 C  -1.2426  -0.6913   3.1796
 H  -0.4872  -1.3079   3.6905
 H  -1.4300   0.2146   3.7764
 H  -2.1739  -1.2610   3.0647
 C  -0.1286   0.1790  -0.8545
 H   0.3060  -0.7993  -1.1176
 H   1.1163   4.1554   0.7929
 C  -4.3538  -0.5594  -0.4635
 C  -3.4875  -1.6320  -0.6871
 C  -2.1249  -1.3718  -0.8002
 C  -1.6227  -0.0672  -0.6850
 C  -2.5212   0.9934  -0.4729
 C  -3.8859   0.7548  -0.3585
 N  -5.7848  -0.8177  -0.3388
 H  -3.8804  -2.6447  -0.7701
 H  -1.4338  -2.2005  -0.9712
 H  -2.1389   2.0121  -0.3882
 H  -4.5878   1.5699  -0.1861
 C   0.6323   4.1827  -0.2079
 H   1.4583   4.2069  -0.9535
 H   0.1206   5.1663  -0.2765
 O  -6.5351   0.1319  -0.1452
 O  -6.1798  -1.9745  -0.4313
 H   3.5083  -2.4541  -2.0555
 H   4.7578  -1.3185  -2.6126
 N   4.8305  -1.8090  -0.5699
 H   6.1194  -0.2068  -0.9591
 H   6.1348  -0.7879   0.7209
 H   4.4832  -2.3964   1.4075
 H   3.4851  -3.2262   0.1934
 H  -0.0441   1.9534  -1.6362
 H   0.1303   2.0479   0.2026
 O  -0.2582   3.1244  -0.4035

r1-TS7-37
Final geometry with  54 atoms:
 O   0.8763  -2.1665  -1.9037
 C   1.9791   0.3426  -0.6568
 H   2.9705   0.6956  -0.3561
 H   1.9799   0.1995  -1.7436
 N   1.0591   1.5638  -0.4356
 C   0.5075   1.6420   0.9634
 H   1.3586   1.5832   1.6477
 C  -0.2870   2.9633   1.1171
 H  -0.1265   0.7623   1.1039
 C  -0.0821   1.5548  -1.4216
 H  -0.5999   0.6009  -1.3148
 C  -1.0080   2.7605  -1.1397
 H   0.3725   1.5982  -2.4188
 C   1.8706   2.8131  -0.6875
 C   0.9317   4.0442  -0.6226
 H   2.6495   2.8390   0.0849
 H   2.3451   2.6946  -1.6694
 C   1.7105  -0.9760   0.0232
 C   2.0193  -1.1092   1.4462
 O   2.9046  -0.1834   1.8923
 O   1.6255  -2.0056   2.1867
 C   3.3324  -0.3000   3.2502
 H   4.0232   0.5351   3.4232
 H   3.8514  -1.2557   3.4195
 H   2.4777  -0.2277   3.9400
 C   0.6362  -1.9516  -0.5283
 H   0.8029  -2.8869   0.0422
 H   4.9707  -1.0332  -1.4176
 C  -3.5071  -0.9653   0.0943
 C  -2.6613  -1.0915   1.2009
 C  -1.3281  -1.4226   0.9900
 C  -0.8263  -1.6142  -0.3113
 C  -1.7091  -1.5114  -1.3985
 C  -3.0489  -1.1827  -1.2061
 N  -4.9063  -0.6063   0.3063
 H  -3.0495  -0.9327   2.2062
 H  -0.6618  -1.5368   1.8451
 H  -1.3311  -1.6770  -2.4062
 H  -3.7328  -1.0904  -2.0491
 C   4.3271  -1.6480  -2.0873
 H   5.0239  -2.2891  -2.6720
 H   3.8806  -0.9368  -2.8202
 O  -5.6381  -0.5076  -0.6716
 O  -5.2914  -0.4157   1.4539
 H   1.3533   4.7918   0.0637
 H   0.8422   4.5078  -1.6149
 N  -0.4032   3.6632  -0.1611
 H  -1.1970   3.3071  -2.0743
 H  -1.9749   2.4137  -0.7490
 H  -1.2932   2.7445   1.5013
 H   0.2148   3.6242   1.8376
 H   1.8656  -2.3613  -1.9435
 H   2.6883  -1.6237  -0.5135
 O   3.3866  -2.4060  -1.3918

r1-TS7-38
Final geometry with  54 atoms:
 O  -0.1645   0.5845  -2.2793
 C   1.9192   1.0228  -0.2890
 H   1.9952   1.4114  -1.3104
 H   2.2987   1.7830   0.4008
 N   2.9889  -0.0894  -0.2429
 C   2.7877  -1.1105  -1.3345
 H   2.6286  -0.5633  -2.2707
 C   4.0165  -2.0522  -1.3758
 H   1.8776  -1.6609  -1.0834
 C   3.0172  -0.8173   1.0742
 H   2.0196  -1.2401   1.2346
 C   4.1043  -1.9225   1.0053
 H   3.2195  -0.0693   1.8485
 C   4.3295   0.5786  -0.4512
 C   5.4526  -0.4766  -0.3236
 H   4.2920   1.0426  -1.4447
 H   4.4110   1.3683   0.3051
 C   0.4842   0.7041   0.0390
 C   0.1694   0.4574   1.4432
 O   0.9436   1.1938   2.2874
 O  -0.7143  -0.2665   1.8894
 C   0.7199   1.0164   3.6847
 H   0.8904  -0.0299   3.9834
 H   1.4400   1.6698   4.1942
 H  -0.3057   1.3040   3.9628
 C  -0.3052  -0.0855  -1.0263
 H   0.0989  -1.0970  -1.1771
 H   0.8405   4.2274   0.0320
 C  -4.4940  -0.6587  -0.1950
 C  -3.9996   0.6450  -0.3078
 C  -2.6458   0.8304  -0.5643
 C  -1.7838  -0.2721  -0.7036
 C  -2.3132  -1.5670  -0.5961
 C  -3.6652  -1.7738  -0.3399
 N  -5.9135  -0.8601   0.0784
 H  -4.6725   1.4940  -0.1921
 H  -2.2431   1.8410  -0.6551
 H  -1.6510  -2.4289  -0.7069
 H  -4.0781  -2.7780  -0.2513
 C   0.4790   3.9879  -0.9924
 H   1.3878   3.8277  -1.6147
 H  -0.0001   4.9142  -1.3748
 O  -6.3331  -2.0079   0.1740
 O  -6.6301   0.1265   0.2026
 H   6.1154  -0.4228  -1.1985
 H   6.0570  -0.2805   0.5730
 N   4.8898  -1.8221  -0.2251
 H   4.7755  -1.8323   1.8707
 H   3.6354  -2.9156   1.0425
 H   3.6759  -3.0970  -1.3722
 H   4.5957  -1.8873  -2.2950
 H  -0.2729   1.5526  -2.0706
 H   0.0158   1.9172  -0.2804
 O  -0.4066   2.9088  -1.0123

r1-TS7-39
Final geometry with  54 atoms:
 O   0.0403  -1.3378  -1.7956
 C   1.8827   0.6174  -0.9992
 H   1.8595   0.3145  -2.0515
 H   2.2045   1.6628  -0.9524
 N   3.0460  -0.1827  -0.3906
 C   3.0309  -1.6224  -0.8499
 H   3.0921  -1.5975  -1.9442
 C   4.2236  -2.3703  -0.2041
 H   2.0684  -2.0525  -0.5667
 C   3.0446  -0.1534   1.1167
 H   2.1346  -0.6652   1.4474
 C   4.3269  -0.8583   1.6318
 H   2.9986   0.8980   1.4172
 C   4.3326   0.4474  -0.8756
 C   5.5327  -0.3894  -0.3702
 H   4.2725   0.4857  -1.9700
 H   4.3417   1.4717  -0.4843
 C   0.4998   0.5154  -0.3914
 C   0.3181   1.1761   0.9142
 O   1.0114   2.3338   1.0144
 O  -0.4084   0.7924   1.8215
 C   0.8233   3.0968   2.2065
 H   1.1105   2.5157   3.0961
 H   1.4709   3.9773   2.1096
 H  -0.2264   3.4131   2.3064
 C  -0.2001  -0.8448  -0.4776
 H   0.2233  -1.5446   0.2676
 H  -1.5734   2.8006  -0.3481
 C  -4.4547  -0.7619   0.1153
 C  -3.8859   0.0688  -0.8556
 C  -2.5057   0.0517  -1.0274
 C  -1.6999  -0.7824  -0.2338
 C  -2.2982  -1.6081   0.7283
 C  -3.6780  -1.6044   0.9142
 N  -5.9040  -0.7474   0.3020
 H  -4.5221   0.7172  -1.4572
 H  -2.0273   0.7113  -1.7583
 H  -1.6732  -2.2569   1.3463
 H  -4.1514  -2.2396   1.6618
 C  -1.1596   3.2075  -1.3069
 H  -0.4747   4.0367  -0.9951
 H  -2.0303   3.7114  -1.7951
 O  -6.3908  -1.4842   1.1516
 O  -6.5747   0.0011  -0.3988
```

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 H    6.0617   -0.8465   -1.2178
 H    6.2408    0.2631    0.1593
 N    5.0866   -1.4491    0.5323
 H    4.9674   -0.1360    2.1566
 H    4.0516   -1.6477    2.3447
 H    3.8556   -3.1392    0.4893
 H    4.8122   -2.8716   -0.9851
 H   -0.3312   -2.2307   -1.8560
 H   -0.0532    1.3050   -1.1964
 O   -0.5655    2.2551   -2.1108

r1-TS7-40
Final geometry with  54 atoms:
 O    0.1211    1.1285   -2.1647
 C    2.1649    1.2333    0.0286
 H    2.3715    1.8239   -0.8716
 H    2.5232    1.7918    0.8995
 N    3.1166    0.0264   -0.0916
 C    3.2815   -0.3781   -1.5399
 H    3.7499    0.4785   -2.0399
 C    4.1583   -1.6491   -1.6064
 H    2.2889   -0.5237   -1.9733
 C    2.6629   -1.1579    0.7248
 H    1.7102   -1.4966    0.3057
 C    3.7547   -2.2547    0.6606
 H    2.4896   -0.7921    1.7411
 C    4.4799    0.4392    0.4143
 C    5.4857   -0.7048    0.1338
 H    4.7449    1.3708   -0.1004
 H    4.3619    0.6438    1.4853
 C    0.6806    1.0078    0.1865
 C    0.2700    0.8037    1.5785
 O   -1.0603    0.6521    1.7486
 O    1.0159    0.8613    2.5558
 C   -1.5399    0.4909    3.0817
 H   -2.6187    0.3084    2.9930
 H   -1.0553   -0.3640    3.5773
 H   -1.3623    1.3995    3.6777
 C   -0.0083    0.3066   -1.0164
 H    0.5279   -0.6291   -1.2447
 H   -1.9330    4.0691   -1.0348
 C   -4.0735   -0.9456   -0.3965
 C   -3.8310    0.3047   -0.9712
 C   -2.5133    0.7030   -1.1756
 C   -1.4480   -0.1269   -0.8016
 C   -1.7232   -1.3902   -0.2527
 C   -3.0306   -1.8075   -0.0391
 N   -5.4514   -1.3698   -0.1742
 H   -4.6656    0.9470   -1.2501
 H   -2.3074    1.6676   -1.6379
 H   -0.8960   -2.0487    0.0233
 H   -3.2525   -2.7823    0.3934
 C   -1.1681    3.8692   -0.2529
 H   -1.6562    3.2083    0.4968
 H   -0.9907    4.8411    0.2606
 O   -5.6499   -2.4723    0.3239
 O   -6.3565   -0.6066   -0.4918
 H    6.2017   -0.4026   -0.6430
 H    6.0518   -0.9276    1.0491
 N    4.7909   -1.9125   -0.3136
 H    4.2257   -2.3784    1.6458
 H    3.2971   -3.2143    0.3819
 H    3.5489   -2.5212   -1.8821
 H    4.9327   -1.5206   -2.3759
 H   -0.0117    2.0688   -1.8369
 H    0.3112    2.2424   -0.0951
 O    0.0050    3.3207   -0.7753

r1-TS7-41
Final geometry with  54 atoms:
 O   -0.2365   -2.8211   -1.1114
 C   -0.9750    0.1677    1.0810
 H   -1.6545    0.0941    1.9384
 H    0.0537    0.1893    1.4566
 N   -1.2056    1.6083    0.5613
 C   -0.2097    1.9817   -0.5019
 H   -0.3483    1.2778   -1.3267
 C   -0.4672    3.4447   -0.9478
 H    0.7862    1.8428   -0.0680
 C   -1.0278    2.5414    1.7354
 H   -0.0341    2.3379    2.1524
 C   -1.1828    4.0043    1.2537
 H   -1.7872    2.2593    2.4743
 C   -2.5885    1.8035   -0.0032
 C   -2.7735    3.2980   -0.3722
 H   -2.6647    1.1556   -0.8833
 H   -3.2992    1.4604    0.7546
 C   -1.2083   -0.9969    0.1633
 C   -2.6308   -1.2447   -0.1207
 O   -2.8694   -1.7760   -1.3382
 O   -3.5485   -1.0489    0.6723
 C   -4.2158   -2.1580   -1.6256
 H   -4.5738   -2.9088   -0.9047
 H   -4.2006   -2.5877   -2.6353
 H   -4.8875   -1.2863   -1.5990
 C   -0.2074   -1.4021   -0.9446
 H   -0.4921   -0.9734   -1.9191
 H   -2.4814   -3.5166    2.4240
 C    3.8895   -0.3118   -0.1753
 C    3.2038   -1.0880    0.7645
 C    1.8803   -1.4304    0.5116
 C    1.2325   -0.9936   -0.6595
 C    1.9575   -0.2362   -1.5913
 C    3.2855    0.1137   -1.3596
 N    5.2785    0.0590    0.0860
 H    3.7069   -1.4142    1.6740
 H    1.3396   -2.0527    1.2270
 H    1.4713    0.0934   -2.5122
 H    3.8488    0.7070   -2.0789
 C   -1.8045   -3.9496    1.6551
 H   -1.5705   -4.9835    1.9877
 H   -2.4100   -4.0550    0.7264
 O    5.8706    0.7283   -0.7522
 O    5.7936   -0.3130    1.1335
 H   -3.0739    3.3850   -1.4255
 H   -3.5677    3.7408    0.2447
 N   -1.5394    4.0529   -0.1631
 H   -1.9653    4.5076    1.8384
 H   -0.2422    4.5528    1.4014
 H    0.4500    4.0371   -0.8247
 H   -0.7477    3.4688   -2.0097
 H   -0.2892   -3.1893   -0.1838
 H   -0.9867   -2.0257    0.9673
 O   -0.6426   -3.1968    1.4631

r1-TS7-42
Final geometry with  54 atoms:
 O    0.0914    0.4279   -2.2418
 C   -1.9532    1.0693   -0.2689
 H   -2.3530    1.8061    0.4336
 H   -2.0503    1.4693   -1.2840
 N   -2.9663   -0.0964   -0.2334
 C   -4.3444    0.4849   -0.0217
 H   -4.4816    1.2654   -0.7801
 C   -5.3920   -0.6497   -0.1336
 H   -4.3348    0.9516    0.9710
 C   -2.6927   -1.0666    0.8866
 H   -2.6297   -0.4796    1.8083
 C   -3.8377   -2.1113    0.9307
 H   -1.7191   -1.5272    0.6890
 C   -2.9816   -0.8353   -1.5518
 C   -3.9602   -2.0290   -1.4455
 H   -3.2951   -0.1030   -2.3055
 H   -1.9597   -1.1464   -1.7798
 C   -0.5092    0.7919    0.0645
 C   -0.1797    0.6525    1.4799
 O   -1.0214    1.3507    2.2935
 O    0.7698    0.0417    1.9588
 C   -0.7448    1.3049    3.6923
 H    0.2442    1.7340    3.9156
 H   -1.5274    1.9026    4.1774
 H   -0.7782    0.2708    4.0691
 C    0.2491   -0.1116   -0.9299
 H   -0.1853   -1.1247   -0.9578
 H    0.0190    4.8708   -1.6108
 C    4.4494   -0.6906   -0.1738
 C    3.9758    0.6050   -0.4077
 C    2.6178    0.7924   -0.6367
 C    1.7308   -0.2992   -0.6277
 C    2.2385   -1.5872   -0.4012
 C    3.5951   -1.7958   -0.1704
 N    5.8740   -0.8933    0.0693
 H    4.6683    1.4461   -0.4060
 H    2.2307    1.7963   -0.8202
 H    1.5569   -2.4412   -0.3991
 H    3.9924   -2.7940    0.0098
 C   -0.4967    3.9421   -1.2861
 H   -1.3373    3.7851   -1.9986
 H   -0.9612    4.1748   -0.3026
 O    6.2766   -2.0339    0.2689
 O    6.6121    0.0852    0.0650
 H   -4.6415   -2.0243   -2.3079
 H   -3.4062   -2.9781   -1.4565
 N   -4.7391   -1.9564   -0.2101
 H   -3.4126   -3.1245    0.9208
 H   -4.4177   -1.9966    1.8570
 H   -6.0564   -0.6255    0.7415
 H   -6.0093   -0.5120   -1.0322
 H    0.2075    1.4119   -2.1326
 H   -0.0285    1.9635   -0.3812
 O    0.3839    2.8601   -1.2210

r1-TS7-43
Final geometry with  54 atoms:
 O   -0.3767    1.1812   -2.4777
 C    2.0665    1.0410   -0.5969
 H    2.5564    1.8590   -0.0572
 H    2.1836    1.2186   -1.6736
 N    2.9657   -0.1793   -0.3130
 C    3.0219   -0.5230    1.1537
 H    2.0027   -0.7719    1.4657
 C    3.9853   -1.7224    1.3538
 H    3.3500    0.3785    1.6811
 C    4.3593    0.1854   -0.7745
 H    4.6335    1.1058   -0.2455
 C    5.3252   -0.9846   -0.4703
 H    4.2828    0.4026   -1.8467
 C    2.5195   -1.4101   -1.0589
 C    3.5611   -2.5382   -0.8439
 H    2.4130   -1.1288   -2.1132
 H    1.5408   -1.6843   -0.6539
 C    0.5947    0.9900   -0.2674
 C    0.2199    0.9698    1.1525
 O    1.1013    1.6879    1.9009
 O   -0.7767    0.4862    1.6713
 C    0.8345    1.7763    3.2989
 H   -0.1236    2.2847    3.4878
 H    0.8055    0.7774    3.7616
 H    1.6570    2.3616    3.7297
 C   -0.2799    0.3121   -1.3556
 H    0.2188   -0.5933   -1.7264
 H   -1.5032    3.1414    0.3810
 C   -4.1678   -1.0138   -0.0878
 C   -3.0855   -1.8972   -0.0079
 C   -1.8351   -1.4541   -0.4195
 C   -1.6529   -0.1463   -0.8981
 C   -2.7614    0.7074   -0.9922
 C   -4.0220    0.2856   -0.5817
 N   -5.4849   -1.4654    0.3442
 H   -3.2339   -2.9089    0.3678
 H   -0.9790   -2.1308   -0.3618
 H   -2.6329    1.7106   -1.3977
 H   -4.8865    0.9459   -0.6412
 C   -1.0693    3.8918   -0.3187
 H   -0.7214    4.7374    0.3177
 H   -1.9253    4.2837   -0.9115
 O   -6.4271   -0.6851    0.2617
 O   -5.5991   -2.6076    0.7754
 H    3.0584   -3.4326   -0.4507
 H    4.0304   -2.8057   -1.8008
 N    4.6035   -2.1242    0.0923
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 H    5.8316   -1.2994   -1.3932
 H    6.0933   -0.6625    0.2462
 H    4.7736   -1.4489    2.0686
 H    3.4349   -2.5789    1.7670
 H   -0.3930    2.1175   -2.1127
 H    0.3324    2.2185   -0.5434
 O   -0.0558    3.3708   -1.1220

r1-TS7-44
Final geometry with  54 atoms:
 O    0.0393    1.3801   -2.2060
 C    2.1973    1.2387    0.0209
 H    2.5567    1.7802    0.9025
 H    2.4632    1.8183   -0.8720
 N    3.0967   -0.0151   -0.0694
 C    2.5331   -1.1992    0.6750
 H    1.5997   -1.4788    0.1764
 C    3.5758   -2.3451    0.6502
 H    2.3019   -0.8552    1.6869
 C    4.4397    0.3190    0.5374
 H    4.2581    0.5047    1.6031
 C    5.4090   -0.8647    0.2971
 H    4.7829    1.2482    0.0658
 C    3.3363   -0.3926   -1.5136
 C    4.1690   -1.6947   -1.5608
 H    3.8626    0.4568   -1.9659
 H    2.3643   -0.4963   -2.0040
 C    0.7010    1.0996    0.1206
 C    0.2059    0.9126    1.4871
 O   -1.1353    1.0333    1.5871
 O    0.8959    0.7802    2.4963
 C   -1.7254    0.8112    2.8658
 H   -1.3913    1.5664    3.5936
 H   -2.8097    0.8913    2.7162
 H   -1.4747   -0.1911    3.2460
 C   -0.0038    0.4768   -1.1181
 H    0.5664   -0.4113   -1.4364
 H   -2.0401    3.2339   -0.2405
 C   -3.9454   -1.0707   -0.3745
 C   -2.8313   -1.7775    0.0953
 C   -1.5661   -1.2689   -0.1630
 C   -1.4012   -0.0627   -0.8658
 C   -2.5319    0.6076   -1.3480
 C   -3.8108    0.1141   -1.1017
 N   -5.2806   -1.5906   -0.1040
 H   -2.9672   -2.7055    0.6491
 H   -0.6868   -1.8039    0.2032
 H   -2.4023    1.5252   -1.9213
 H   -4.6967    0.6354   -1.4627
 C   -1.1873    3.9395   -0.1380
 H   -1.5151    4.8916   -0.6088
 H   -1.0910    4.1513    0.9503
 O   -6.2480   -0.9687   -0.5287
 O   -5.3837   -2.6291    0.5398
 H    3.5500   -2.5323   -1.9114
 H    5.0028   -1.5712   -2.2663
 N    4.6938   -2.0245   -0.2362
 H    6.1946   -0.5773   -0.4155
 H    5.8945   -1.1394    1.2440
 H    3.9680   -2.5214    1.6616
 H    3.0959   -3.2724    0.3075
 H   -0.0695    2.2995   -1.8088
 H    0.3621    2.3471   -0.1063
 O    0.0030    3.4743   -0.7029

r1-TS7-45
Final geometry with  54 atoms:
 O   -0.7104   -2.8023   -1.1857
 C   -2.3100    0.4976   -0.3846
 H   -2.5795    0.5654   -1.4465
 H   -3.2187    0.6315    0.2133
 N   -1.5012    1.7857   -0.1296
 C   -0.4621    1.9978   -1.1997
 H   -1.0003    2.0389   -2.1542
 C    0.3197    3.2996   -0.8982
 H    0.1928    1.1251   -1.1979
 C   -0.8259    1.7911    1.2171
 H   -0.0990    0.9737    1.2100
 C   -0.1488    3.1687    1.4316
 H   -1.5968    1.5714    1.9616
 C   -2.4654    2.9478   -0.1791
 C   -1.6743    4.2709   -0.0324
 H   -2.9990    2.8775   -1.1348
 H   -3.1797    2.7950    0.6387
 C   -1.7214   -0.8532   -0.0747
 C   -1.8376   -1.2603    1.3330
 O   -1.2741   -2.4604    1.5933
 O   -2.4760   -0.6677    2.1981
 C   -1.4204   -2.9714    2.9191
 H   -2.4810   -3.1376    3.1621
 H   -0.8792   -3.9259    2.9362
 H   -0.9861   -2.2811    3.6586
 C   -0.6025   -1.4001   -0.9905
 H   -0.7745   -0.8854   -1.9568
 H   -4.2616   -3.0549   -2.9632
 C    3.5670   -0.6374   -0.1838
 C    3.0993   -0.6647   -1.4992
 C    1.7466   -0.9093   -1.7148
 C    0.8576   -1.1215   -0.6460
 C    1.3690   -1.1070    0.6617
 C    2.7184   -0.8596    0.9020
 N    4.9831   -0.3676    0.0629
 H    3.7837   -0.4921   -2.3288
 H    1.3636   -0.9221   -2.7379
 H    0.7166   -1.2912    1.5120
 H    3.1128   -0.8385    1.9171
 C   -3.7042   -2.2514   -2.4327
 H   -4.3899   -1.3743   -2.4029
 H   -2.8654   -1.9671   -3.1101
 O    5.3763   -0.3400    1.2223
 O    5.7157   -0.1799   -0.9003
 H   -1.7518    4.8643   -0.9539
 H   -2.0964    4.8644    0.7905
 N   -0.2616    4.0085    0.2398
 H   -0.6168    3.6907    2.2778
 H    0.9147    3.0241    1.6679
 H    1.3681    3.0634   -0.6688
 H    0.3050    3.9549   -1.7803
 H   -1.7041   -2.9735   -1.2336
 H   -2.6362   -1.6267   -0.5464
 O   -3.2832   -2.6600   -1.1671

r1-TS7-46
Final geometry with  54 atoms:
 O    0.7682    2.2371   -1.7453
 C   -1.1404   -0.7753   -0.6291
 H   -1.1300   -0.9755   -1.7058
 H   -0.6049   -1.5979   -0.1343
 N   -2.6157   -0.9822   -0.2057
 C   -2.6864   -1.8660    1.0206
 H   -2.0637   -1.3877    1.7816
 C   -4.1640   -2.0219    1.4498
 H   -2.2339   -2.8233    0.7336
 C   -3.3380   -1.6926   -1.3267
 H   -2.7369   -2.5719   -1.5878
 C   -4.7634   -2.0732   -0.8556
 H   -3.3456   -1.0004   -2.1778
 C   -3.3526    0.3009    0.0883
 C   -4.8439   -0.0256    0.3498
 H   -2.8688    0.7419    0.9645
 H   -3.2118    0.9699   -0.7650
 C   -0.4998    0.5783   -0.4016
 C   -0.1700    0.8658    0.9903
 O    0.6191    1.9540    1.1407
 O   -0.5876    0.2580    1.9770
 C    0.9717    2.3244    2.4720
 H    1.6372    3.1923    2.3802
 H    1.4963    1.5045    2.9860
 H    0.0782    2.5995    3.0540
 C    0.6248    0.8648   -1.4498
 H    0.3174    0.3151   -2.3615
 H   -0.9850    4.1504    0.0051
 C    4.3714   -0.8163   -0.1669
 C    3.3779   -1.6606   -0.6730
 C    2.1817   -1.0982   -1.1037
 C    1.9633    0.2894   -1.0286
 C    2.9875    1.1117   -0.5310
 C    4.1919    0.5677   -0.0953
 N    5.6310   -1.3943    0.2874
 H    3.5512   -2.7344   -0.7313
 H    1.4082   -1.7496   -1.5150
 H    2.8299    2.1881   -0.4890
 H    4.9882    1.2006    0.2950
 C   -1.9153    3.5915   -0.2324
 H   -2.6959    4.3461   -0.4606
 H   -2.2279    3.0904    0.7090
 O    5.7764   -2.6095    0.2140
 O    6.4943   -0.6428    0.7262
 H   -5.1630    0.4510    1.2874
 H   -5.4672    0.3754   -0.4618
 N   -5.0664   -1.4679    0.4402
 H   -5.4986   -1.7312   -1.5976
 H   -4.8562   -3.1646   -0.7657
 H   -4.3940   -3.0863    1.6001
 H   -4.3423   -1.5008    2.4011
 H   -0.1577    2.6091   -1.7289
 H   -1.2947    1.6246   -0.7991
 O   -1.7516    2.6889   -1.2914

r1-TS7-47
Final geometry with  54 atoms:
 O    0.6618   -3.1093    0.5916
 C    1.0904    0.1665   -1.2364
 H    1.8922    0.3860   -1.9499
 H    0.1699    0.0323   -1.8154
 N    0.8756    1.5024   -0.5169
 C   -0.2896    1.4428    0.4389
 H   -0.0372    0.6938    1.1938
 C   -0.4982    2.8456    1.0631
 H   -1.1554    1.1125   -0.1445
 C    0.5710    2.5438   -1.5653
 H   -0.3305    2.2058   -2.0910
 C    0.3737    3.9168   -0.8761
 H    1.4130    2.5436   -2.2679
 C    2.1080    1.9295    0.2424
 C    1.8341    3.3033    0.9036
 H    2.2933    1.1451    0.9839
 H    2.9282    1.9644   -0.4831
 C    1.4092   -1.0657   -0.3983
 C    2.7664   -1.5831   -0.6742
 O    3.6955   -0.5950   -0.7195
 O    3.0951   -2.7526   -0.8248
 C    5.0497   -0.9904   -0.9357
 H    5.6398   -0.0649   -0.9474
 H    5.1611   -1.5172   -1.8959
 H    5.4014   -1.6470   -0.1248
 C    0.3691   -2.2078   -0.4715
 H    0.4732   -2.7370   -1.4385
 H    2.9033   -0.9350    3.6172
 C   -3.6599   -0.7557   -0.1266
 C   -3.1328   -0.9793   -1.4003
 C   -1.8349   -1.4741   -1.5047
 C   -1.0653   -1.7258   -0.3591
 C   -1.6326   -1.5102    0.9074
 C   -2.9289   -1.0244    1.0341
 N   -5.0182   -0.2278   -0.0037
 H   -3.7334   -0.7728   -2.2852
 H   -1.4124   -1.6660   -2.4937
 H   -1.0342   -1.7046    1.7969
 H   -3.3716   -0.8415    2.0125
 C    2.2410   -1.4028    2.8528
 H    1.6379   -2.1674    3.3973
 H    2.9183   -1.9830    2.1830
 O   -5.4742   -0.0517    1.1191
 O   -5.6419    0.0193   -1.0285
 H    1.9159    3.2121    1.9960
 H    2.5792    4.0380    0.5675
 N    0.4972    3.7987    0.5750
 H    1.1250    4.6314   -1.2402
 H   -0.6205    4.3169   -1.1194
 H   -1.5012    3.2217    0.8171
```

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 H  -0.4196   2.7790   2.1573
 H   0.1228  -3.9044   0.4645
 H   1.4543  -0.7667   0.8938
 O   1.4741  -0.4685   2.1707

r1-TS7-48
Final geometry with  54 atoms:
 O  -0.4727   1.7161  -2.0075
 C   1.1037  -0.9593   0.0356
 H   0.8361  -1.6560  -0.7667
 H   0.7790  -1.3937   0.9892
 N   2.6241  -1.0239   0.0775
 C   3.2147  -0.6633  -1.2654
 H   2.8378   0.3291  -1.5332
 C   4.7570  -0.6684  -1.1378
 H   2.8435  -1.4135  -1.9752
 C   3.0288  -2.4402   0.4048
 H   2.5129  -3.0966  -0.3065
 C   4.5697  -2.5545   0.3078
 H   2.6522  -2.6449   1.4148
 C   3.2001  -0.1080   1.1334
 C   4.7233  -0.3637   1.2269
 H   2.9745   0.9114   0.7973
 H   2.6693  -0.3235   2.0668
 C   0.4954   0.4147  -0.1949
 C  -0.0119   1.0043   1.0626
 O  -0.7256   2.1269   0.8560
 O   0.2292   0.6062   2.1958
 C  -1.2497   2.7899   2.0070
 H  -1.8009   3.6610   1.6309
 H  -1.9301   2.1287   2.5651
 H  -0.4381   3.1190   2.6736
 C  -0.4809   0.4359  -1.3956
 H  -0.0938  -0.3100  -2.1110
 H   1.0382   3.7743  -1.2416
 C  -4.4226  -0.8000  -0.1722
 C  -4.1796   0.5561  -0.4030
 C  -2.9114   0.9476  -0.8212
 C  -1.8890   0.0025  -1.0067
 C  -2.1715  -1.3572  -0.7843
 C  -3.4317  -1.7675  -0.3636
 N  -5.7487  -1.2196   0.2696
 H  -4.9747   1.2859  -0.2540
 H  -2.7032   2.0004  -1.0075
 H  -1.3981  -2.1098  -0.9481
 H  -3.6548  -2.8195  -0.1903
 C   1.9281   3.5344  -0.6151
 H   1.6462   3.8209   0.4273
 H   2.7141   4.2649  -0.9197
 O  -5.9466  -2.4124   0.4700
 O  -6.6108  -0.3624   0.4238
 H   5.2585   0.5948   1.1681
 H   4.9781  -0.8349   2.1870
 N   5.1807  -1.2362   0.1438
 H   4.9626  -3.0278   1.2186
 H   4.8520  -3.1829  -0.5487
 H   5.1970  -1.2513  -1.9594
 H   5.1392   0.3600  -1.2060
 H  -1.0083   1.6685  -2.8143
 H   1.3901   1.3057  -0.4947
 O   2.3631   2.2228  -0.7389

r1-TS7-49
Final geometry with  54 atoms:
 O  -0.2919  -2.3710   1.8088
 C   1.0091  -0.0029  -0.9094
 H   0.0171   0.2358  -1.3115
 H   1.6406  -0.3236  -1.7458
 N   1.5844   1.3517  -0.4853
 C   0.6656   2.0753   0.4667
 H   0.5831   1.4556   1.3622
 C   1.2666   3.4670   0.7933
 H  -0.3122   2.1380  -0.0235
 C   1.7205   2.1861  -1.7409
 H   0.7251   2.2214  -2.1995
 C   2.2578   3.5886  -1.3675
 H   2.3989   1.6382  -2.4054
 C   2.9409   1.2332   0.1608
 C   3.4829   2.6578   0.4516
 H   2.8079   0.6580   1.0835
 H   3.5777   0.6703  -0.5291
 C   0.9080  -1.1444   0.0818
 C   2.1968  -1.7234   0.5370
 O   3.1062  -1.8220  -0.4438
 O   2.4243  -2.1473   1.6673
 C   4.3641  -2.4179  -0.1095
 H   4.8703  -1.8404   0.6785
 H   4.2226  -3.4542   0.2317
 H   4.9600  -2.4022  -1.0301
 C  -0.1114  -1.0738   1.2372
 H   0.2512  -0.3943   2.0292
 H  -0.1225  -5.0176  -1.1859
 C  -4.0454   0.1745   0.0586
 C  -3.4346   0.8061   1.1430
 C  -2.1528   0.4015   1.5096
 C  -1.4869  -0.6088   0.8021
 C  -2.1297  -1.2325  -0.2815
 C  -3.4111  -0.8427  -0.6599
 N  -5.3910   0.5931  -0.3388
 H  -3.9572   1.5931   1.6851
 H  -1.6624   0.8822   2.3587
 H  -1.6021  -2.0113  -0.8425
 H  -3.9183  -1.3123  -1.5020
 C   0.6123  -4.1725  -1.1562
 H   1.5381  -4.5780  -1.6445
 H   0.8795  -4.0781  -0.0720
 O  -5.9201   0.0259  -1.2859
 O  -5.9304   1.4931   0.2926
 H   3.7042   2.7577   1.5231
 H   4.4155   2.8230  -0.1051
 N   2.5157   3.6834   0.0675
 H   3.1903   3.7880  -1.9133
 H   1.5272   4.3593  -1.6492
 H   0.5521   4.2556   0.5204
 H   1.4634   3.5436   1.8714
 H   0.5944  -2.6320   2.1195
 H   0.5224  -1.9916  -0.7027
 O   0.1435  -3.0048  -1.7149

r1-TS7-50
Final geometry with  54 atoms:
 O  -0.1869  -2.6007   1.5896
 C   0.9648  -0.0162  -0.8771
 H  -0.0506   0.1686  -1.2456
 H   1.5867  -0.2925  -1.7363
 N   1.4779   1.3730  -0.4734
 C   0.6296   1.9944   0.6039
 H   0.6791   1.3308   1.4715
 C   1.1804   3.4070   0.9296
 H  -0.3969   2.0195   0.2231
 C   1.4057   2.2478  -1.7049
 H   0.3689   2.2064  -2.0586
 C   1.8527   3.6835  -1.3388
 H   2.0549   1.7808  -2.4553
 C   2.9066   1.3428   0.0083
 C   3.3837   2.7979   0.2549
 H   2.9193   0.7567   0.9328
 H   3.4941   0.8267  -0.7579
 C   0.9638  -1.1566   0.1157
 C   2.3008  -1.5930   0.5887
 O   3.1761  -1.7303  -0.4320
 O   2.6205  -1.8470   1.7407
 C   4.5021  -2.1404  -0.0953
 H   4.9726  -1.4246   0.5962
 H   4.4964  -3.1383   0.3690
 H   5.0607  -2.1708  -1.0392
 C  -0.0860  -1.2179   1.2296
 H   0.2350  -0.6443   2.1173
 H   0.2140  -5.0522  -1.2043
 C  -4.0110   0.0807   0.0631
 C  -3.4132   0.6697   1.1782
 C  -2.1344   0.2531   1.5437
 C  -1.4596  -0.7283   0.8055
 C  -2.0930  -1.3146  -0.3062
 C  -3.3680  -0.9106  -0.6859
 N  -5.3506   0.5140  -0.3341
 H  -3.9431   1.4349   1.7440
 H  -1.6529   0.7016   2.4154
 H  -1.5578  -2.0779  -0.8795
 H  -3.8658  -1.3482  -1.5506
 C   0.9039  -4.1712  -1.2169
 H   1.7913  -4.5032  -1.8164
 H   1.2797  -4.0966  -0.1647
 O  -5.8662  -0.0129  -1.3119
 O  -5.9005   1.3863   0.3270
 H   3.7599   2.8930   1.2828
 H   4.2048   3.0452  -0.4319
 N   2.2963   3.7527   0.0519
 H   2.6769   3.9953  -1.9951
 H   1.0203   4.3863  -1.4811
 H   0.3828   4.1531   0.8090
 H   1.5248   3.4435   1.9722
 H  -0.7071  -2.6583   2.4051
 H   0.6461  -2.0447  -0.6999
 O   0.3153  -3.0126  -1.6771

r1-TS7-51
Final geometry with  54 atoms:
 O  -0.1019  -2.8012  -1.5119
 C   1.0421  -0.1177   0.8771
 H   0.0291  -0.0377   1.2861
 H   1.7253  -0.3468   1.7033
 N   1.4075   1.3400   0.5052
 C   2.8371   1.4709   0.0462
 H   2.9284   0.8922  -0.8788
 C   3.1537   2.9708  -0.1902
 H   3.4672   1.0191   0.8191
 C   1.2203   2.1800   1.7468
 H   1.8893   1.7639   2.5099
 C   1.5387   3.6590   1.4175
 H   0.1818   2.0364   2.0687
 C   0.5161   1.8835  -0.5762
 C   0.9010   3.3593  -0.8580
 H   0.6613   1.2507  -1.4568
 H  -0.5128   1.7806  -0.2178
 C   1.1153  -1.1936  -0.1685
 C   2.4527  -1.5267  -0.6843
 O   3.4009  -1.5126   0.2851
 O   2.7286  -1.8593  -1.8296
 C   4.7380  -1.8107  -0.1147
 H   5.3527  -1.7306   0.7911
 H   4.8096  -2.8294  -0.5254
 H   5.0936  -1.0941  -0.8715
 C   0.0184  -1.4036  -1.2365
 H   0.3084  -0.9345  -2.1908
 H   0.9370  -3.1816   2.9746
 C  -3.8902   0.0432  -0.1620
 C  -3.2798   0.5424  -1.3142
 C  -2.0113   0.0761  -1.6511
 C  -1.3524  -0.8694  -0.8521
 C  -2.0071  -1.3718   0.2860
 C  -3.2707  -0.9174   0.6442
 N  -5.2155   0.5344   0.2094
 H  -3.7928   1.2811  -1.9289
 H  -1.5206   0.4598  -2.5483
 H  -1.5116  -2.1308   0.8904
 H  -3.7766  -1.2954   1.5318
 C   0.1994  -3.6119   2.2586
 H  -0.7698  -3.1060   2.4825
 H   0.0609  -4.6729   2.5634
 O  -5.7357   0.0934   1.2270
 O  -5.7507   1.3689  -0.5103
 H   1.2348   3.4667  -1.8992
 H   0.0244   4.0058  -0.7135
 N   1.9733   3.8036   0.0298
 H   0.6466   4.2804   1.5772
 H   2.3329   4.0272   2.0814
 H   3.9502   3.2972   0.4926
 H   3.5080   3.1163  -1.2201
 H  -0.0262  -3.2638  -0.6365
 H   0.9137  -2.2710   0.5458
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 O   0.6051  -3.5021   0.9330
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r1-TS7-52

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Final geometry with  54 atoms:
 O  -0.2254   2.6986  -1.5964
 C   2.3695   0.5468  -0.1057
 H   2.8723   0.7254  -1.0636
 H   3.0411   0.8735   0.6962
 N   2.3482  -0.9937   0.0220
 C   2.1943  -1.6293  -1.3377
 H   3.0733  -1.3232  -1.9178
 C   2.1029  -3.1637  -1.1731
 H   1.3070  -1.2019  -1.8096
 C   1.2728  -1.4900   0.9537
 H   0.3125  -1.1910   0.5271
 C   1.4023  -3.0268   1.0961
 H   1.4146  -0.9640   1.9016
 C   3.6775  -1.4464   0.5793
 C   3.7261  -2.9960   0.5638
 H   4.4600  -0.9921  -0.0407
 H   3.7430  -1.0351   1.5939
 C   1.1065   1.3644  -0.0043
 C   0.6618   1.6092   1.3740
 O  -0.4496   2.3664   1.4393
 O   1.2618   1.2806   2.3946
 C  -0.9475   2.6901   2.7373
 H  -1.8710   3.2604   2.5751
 H  -1.1675   1.7781   3.3132
 H  -0.2228   3.3023   3.2956
 C   0.0676   1.3802  -1.1721
 H   0.5569   0.8299  -1.9979
 H   3.8761   3.2769  -1.3154
 C  -3.6699  -0.6312  -0.3600
 C  -3.5735   0.7483  -0.1558
 C  -2.3697   1.3856  -0.4343
 C  -1.2531   0.6669  -0.8986
 C  -1.4033  -0.7101  -1.1368
 C  -2.5976  -1.3704  -0.8626
 N  -4.9254  -1.3117  -0.0611
 H  -4.4329   1.3064   0.2144
 H  -2.2847   2.4609  -0.2974
 H  -0.5824  -1.2867  -1.5593
 H  -2.7042  -2.4387  -1.0458
 C   2.9002   3.6482  -1.7012
 H   2.6099   2.9627  -2.5309
 H   3.1128   4.6291  -2.1798
 O  -4.9875  -2.5239  -0.2323
 O  -5.8668  -0.6446   0.3522
 H   4.4778  -3.3472  -0.1567
 H   4.0124  -3.3639   1.5590
 N   2.4260  -3.5584   0.1969
 H   1.6700  -3.2881   2.1294
 H   0.4386  -3.5023   0.8654
 H   1.0885  -3.5148  -1.4094
 H   2.8003  -3.6499  -1.8697
 H   0.5560   3.2779  -1.3235
 H   1.6277   2.5191  -0.2343
 O   1.9265   3.7589  -0.7067
```

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```
Final geometry with  54 atoms:
 O  -0.9114  -2.8765   0.7629
 C  -0.9973   0.3171  -1.2481
 H  -0.0377   0.0993  -1.7280
 H  -1.7206   0.5416  -2.0403
 N  -0.7671   1.6700  -0.5751
 C  -2.0169   2.1829   0.1012
 H  -2.2322   1.4734   0.9087
 C  -1.7397   3.6101   0.6357
 H  -2.8174   2.1530  -0.6453
 C  -0.3656   2.6518  -1.6486
 H  -1.2055   2.7053  -2.3520
 C  -0.0513   4.0191  -0.9938
 H   0.5026   2.2238  -2.1643
 C   0.3422   1.6014   0.4437
 C   0.5212   3.0012   1.0817
 H   0.0464   0.8529   1.1829
 H   1.2367   1.2641  -0.0925
 C  -1.4758  -0.8436  -0.3852
 C  -2.8873  -1.1458  -0.7088
 O  -3.2246  -2.4482  -0.6246
 O  -3.7251  -0.3010  -1.0122
 C  -4.5997  -2.7748  -0.8292
 H  -4.6753  -3.8626  -0.7036
 H  -4.9289  -2.4901  -1.8403
 H  -5.2372  -2.2679  -0.0883
 C  -0.5436  -2.0817  -0.3602
 H  -0.6852  -2.6676  -1.2879
 H  -3.1809  -0.4409   3.4998
 C   3.6047  -0.9988  -0.0674
 C   3.0751  -1.2945  -1.3253
 C   1.7342  -1.6613  -1.4121
 C   0.9282  -1.7207  -0.2655
 C   1.4955  -1.4334   0.9867
 C   2.8329  -1.0699   1.0960
 N   5.0111  -0.6106   0.0360
 H   3.7069  -1.2424  -2.2110
 H   1.3064  -1.9051  -2.3875
 H   0.8662  -1.4783   1.8755
 H   3.2783  -0.8338   2.0617
 C  -2.4781  -0.9926   2.8326
 H  -3.1231  -1.5879   2.1440
 H  -1.9696  -1.7446   3.4818
 O   5.4662  -0.3636   1.1457
 O   5.6743  -0.5465  -0.9918
 H   0.2702   2.9588   2.1509
 H   1.5688   3.3214   0.9914
 N  -0.3408   3.9924   0.4385
 H   1.0087   4.2717  -1.1359
 H  -0.6541   4.8057  -1.4689
 H  -2.3794   4.3411   0.1210
 H  -1.9728   3.6527   1.7091
 H  -0.4366  -3.7185   0.6980
 H  -1.5443  -0.4975   0.8779
 O  -1.6022  -0.1503   2.1634
```

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```
Final geometry with  54 atoms:
 O   0.1608  -0.9117  -1.9925
 C   1.9674   0.8921  -0.8557
 H   2.2755   1.9138  -0.6076
 H   1.9613   0.7860  -1.9455
 N   3.1287   0.0045  -0.3830
 C   3.1141  -0.2237   1.1068
 H   2.2031  -0.7869   1.3367
 C   4.3956  -0.9983   1.5089
 H   3.0567   0.7610   1.5806
 C   4.4173   0.7125  -0.7376
 H   4.4212   1.6509  -0.1703
 C   5.6151  -0.1995  -0.3780
 H   4.3667   0.9446  -1.8082
 C   3.1285  -1.3333  -1.0854
 C   4.3092  -2.1819  -0.5535
 H   2.1616  -1.8065  -0.9047
 H   3.2143  -1.1177  -2.1568
 C   0.5791   0.6795  -0.2893
 C   0.4372   1.1913   1.0884
 O  -0.4509   0.5084   1.8344
 O   1.0254   2.1706   1.5340
 C  -0.7577   1.0279   3.1300
 H   0.1378   1.0420   3.7695
 H  -1.1649   2.0477   3.0546
 H  -1.5122   0.3535   3.5545
 C  -0.1084  -0.6529  -0.6127
 H   0.3119  -1.4667   0.0073
 H  -1.5526   2.8557   0.1060
 C  -4.3762  -0.7567  -0.1338
 C  -3.5997  -1.7231   0.5095
 C  -2.2162  -1.6662   0.3642
 C  -1.6142  -0.6591  -0.4030
 C  -2.4195   0.2971  -1.0444
 C  -3.8035   0.2554  -0.9111
 N  -5.8295  -0.8050   0.0113
 H  -4.0760  -2.4992   1.1074
 H  -1.5917  -2.4116   0.8621
 H  -1.9384   1.0908  -1.6253
 H  -4.4397   0.9957  -1.3952
 C  -1.1157   3.4479  -0.7397
 H  -0.4418   4.1939  -0.2472
 H  -1.9758   4.0409  -1.1386
 O  -6.5001   0.0528  -0.5503
 O  -6.3193  -1.7013   0.6884
 H   3.9293  -3.0494   0.0039
 H   4.9050  -2.5552  -1.3981
 N   5.1657  -1.3963   0.3319
 H   6.1462  -0.5086  -1.2889
 H   6.3221   0.3538   0.2558
 H   5.0289  -0.3694   2.1498
 H   4.1207  -1.8963   2.0794
 H  -0.2122  -1.7786  -2.2134
 H   0.0241   1.5798  -0.9600
 O  -0.4971   2.6760  -1.7030
```

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```
Final geometry with  54 atoms:
 O  -0.6522  -3.1048   0.6017
 C  -1.0783   0.1566  -1.2484
 H  -0.1604   0.0189  -1.8311
 H  -1.8835   0.3727  -1.9595
 N  -0.8602   1.4966  -0.5369
 C  -2.0874   1.9282   0.2286
 H  -2.2545   1.1534   0.9849
 C  -1.8148   3.3140   0.8657
 H  -2.9168   1.9455  -0.4868
 C  -0.5592   2.5302  -1.5941
 H  -1.4072   2.5292  -2.2894
 C  -0.3493   3.9066  -0.9165
 H   0.3361   2.1846  -2.1256
 C   0.3062   1.4426   0.4168
 C   0.5159   2.8491   1.0331
 H   0.0544   0.6992   1.1767
 H   1.1716   1.1073  -0.1641
 C  -1.3920  -1.0707  -0.4026
 C  -2.7491  -1.5932  -0.6731
 O  -3.6852  -0.6119  -0.6631
 O  -3.0711  -2.7599  -0.8537
 C  -5.0411  -1.0083  -0.8699
 H  -5.6364  -0.0867  -0.8392
 H  -5.1658  -1.5022  -1.8457
 H  -5.3737  -1.6943  -0.0757
 C  -0.3518  -2.2104  -0.4661
 H  -0.4491  -2.7461  -1.4300
 H  -2.6464  -2.2422   2.2198
 C   3.6763  -0.7669  -0.0884
 C   2.9303  -1.0219   1.0661
 C   1.6337  -1.5035   0.9281
 C   1.0814  -1.7284  -0.3435
 C   1.8642  -1.4880  -1.4823
 C   3.1631  -0.9979  -1.3664
 N   5.0361  -0.2459   0.0462
 H   3.3619  -0.8317   2.0480
 H   1.0206  -1.6853   1.8106
 H   1.4522  -1.6863  -2.4745
 H   3.7750  -0.8012  -2.2457
 C  -2.5279  -1.2525   2.7174
 H  -2.3587  -1.4784   3.7951
 H  -3.5312  -0.7640   2.6645
 O   5.6729  -0.0100  -0.9732
 O   5.4805  -0.0643   1.1728
 H   0.4333   2.7898   2.1273
 H   1.5207   3.2205   0.7879
 N  -0.4754   3.8013   0.5353
 H   0.6491   4.2953  -1.1614
 H  -1.0932   4.6253  -1.2876
 H  -2.5561   4.0442   0.5116
 H  -1.9034   3.2427   1.9589
 H  -0.1220  -3.9063   0.4779
 H  -1.4532  -0.7632   0.8806
 O  -1.5058  -0.4890   2.1694
```

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Final geometry with 54 atoms:

O	-0.5041	2.0483	-1.7278
C	1.0341	-0.8912	-0.0302
H	0.6554	-1.4270	0.8490
H	0.7779	-1.4738	-0.9216
N	2.5498	-1.0246	0.0590
C	2.8806	-2.4866	0.2275
H	2.3961	-3.0204	-0.5990
C	4.4195	-2.6591	0.2246
H	2.4222	-2.8045	1.1721
C	3.1215	-0.2642	1.2325
H	2.5760	-0.5956	2.1221
C	4.6422	-0.5509	1.3099
H	2.9215	0.7939	1.0385
C	3.2020	-0.5240	-1.2067
C	4.7358	-0.6831	-1.0700
H	2.7845	-1.1166	-2.0301
H	2.9081	0.5267	-1.2961
C	0.4792	0.5210	-0.1132
C	-0.0300	0.9788	1.1982
O	-0.6904	2.1500	1.1206
O	0.1603	0.4308	2.2780
C	-1.2414	2.6675	2.3319
H	-0.4505	2.8623	3.0720
H	-1.7407	3.6068	2.0624
H	-1.9727	1.9653	2.7611
C	-0.4920	0.6941	-1.3069
H	-0.0901	0.0624	-2.1176
H	2.5651	2.5767	-2.4023
C	-4.4078	-0.7643	-0.2564
C	-3.4188	-1.6760	-0.6366
C	-2.1683	-1.1893	-1.0021
C	-1.8928	0.1897	-0.9839
C	-2.9160	1.0807	-0.6179
C	-4.1737	0.6128	-0.2494
N	-5.7229	-1.2640	0.1331
H	-3.6351	-2.7435	-0.6485
H	-1.3969	-1.8962	-1.3128
H	-2.7179	2.1516	-0.6242
H	-4.9682	1.2995	0.0404
C	2.4800	3.1520	-1.4461
H	1.6167	3.8436	-1.5943
H	3.3855	3.8028	-1.4145
O	-6.5805	-0.4535	0.4633
O	-5.9157	-2.4742	0.1158
H	5.1310	-1.2598	-1.9182
H	5.2155	0.3059	-1.0782
N	5.0906	-1.3614	0.1771
H	5.1947	0.3993	1.3094
H	4.8833	-1.0831	2.2408
H	4.7350	-3.1954	1.1304
H	4.7322	-3.2515	-0.6466
H	-1.0364	2.1077	-2.5357
H	1.3966	1.4244	-0.3110
O	2.3758	2.3538	-0.3205

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Final geometry with 54 atoms:

O	-0.5275	1.7472	-2.0624
C	0.9104	-0.7035	0.3800
H	0.7260	-0.8149	1.4534
H	0.3917	-1.5237	-0.1286
N	2.3855	-1.0419	0.2049
C	2.7840	-1.0121	-1.2521
H	2.6560	0.0237	-1.5858
C	4.2565	-1.4780	-1.3727
H	2.0864	-1.6726	-1.7818
C	2.6113	-2.4383	0.7322
H	1.9784	-3.1067	0.1355
C	4.1162	-2.7837	0.6153
H	2.2569	-2.4480	1.7699
C	3.2682	-0.0928	0.9815
C	4.7458	-0.4887	0.7414
H	3.0531	0.9134	0.6055
H	2.9687	-0.1802	2.0322
C	0.4508	0.6511	-0.1422
C	0.0232	1.6011	0.9056
O	0.6273	1.3816	2.0970
O	-0.7164	2.5631	0.7498
C	0.3834	2.3365	3.1314
H	-0.6885	2.3870	3.3758
H	0.9507	1.9905	4.0047
H	0.7304	3.3371	2.8310
C	-0.5116	0.5237	-1.3446
H	-0.0893	-0.2730	-1.9820
H	1.8409	3.3993	-2.5274
C	-4.4530	-0.7261	-0.1363
C	-3.4856	-1.6958	-0.4120
C	-2.2241	-1.2787	-0.8248
C	-1.9145	0.0875	-0.9480
C	-2.9186	1.0362	-0.6859
C	-4.1874	0.6386	-0.2774
N	-5.7820	-1.1513	0.2936
H	-3.7280	-2.7534	-0.3155
H	-1.4720	-2.0313	-1.0699
H	-2.6944	2.0943	-0.8066
H	-4.9679	1.3699	-0.0703
C	2.2010	3.3381	-1.4723
H	1.4030	3.8209	-0.8607
H	3.0781	4.0253	-1.4160
O	-6.6249	-0.2911	0.5192
O	-6.0002	-2.3513	0.4129
H	5.2641	0.3204	0.2075
H	5.2544	-0.6426	1.7036
N	4.8486	-1.7118	-0.0555
H	4.5472	-2.9355	1.6148
H	4.2407	-3.7161	0.0472
H	4.3164	-2.4074	-1.9563
H	4.8433	-0.7101	-1.8961
H	-1.0761	1.6262	-2.8524
H	1.4331	1.3341	-0.6188
O	2.5161	2.0527	-1.0576

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Final geometry with 54 atoms:

O	-1.3742	-2.3986	-1.6206
C	-2.0171	1.1564	-0.5512
H	-2.2249	1.4035	-1.6000
H	-2.8770	1.4695	0.0505
N	-0.8930	2.1457	-0.1463
C	-1.5359	3.4432	0.2828
H	-2.1130	3.2182	1.1882
C	-0.4271	4.4964	0.5301
H	-2.2269	3.7392	-0.5160
C	-0.0032	2.4457	-1.3252
H	-0.6433	2.9082	-2.0863
C	1.1431	3.3790	-0.8724
H	0.3665	1.4940	-1.7091
C	-0.0484	1.6449	0.9986
C	0.9438	2.7599	1.4143
H	-0.7353	1.3702	1.8031
H	0.4665	0.7470	0.6467
C	-1.8420	-0.3286	-0.3787
C	-2.0951	-0.7930	0.9949
O	-1.9838	-2.1293	1.1497
O	-2.4850	-0.0903	1.9252
C	-2.3362	-2.6659	2.4248
H	-3.3969	-2.4762	2.6499
H	-2.1573	-3.7465	2.3575
H	-1.7151	-2.2311	3.2225
C	-0.8852	-1.1004	-1.3326
H	-0.8796	-0.4900	-2.2571
H	-4.3084	-3.1094	-0.3379
C	3.2504	-1.3966	-0.1466
C	2.9205	-0.7181	-1.3201
C	1.5804	-0.6537	-1.6940
C	0.5710	-1.2341	-0.9083
C	0.9460	-1.9460	0.2463
C	2.2783	-2.0247	0.6372
N	4.6508	-1.4629	0.2667
H	3.7001	-0.2584	-1.9264
H	1.3155	-0.1446	-2.6229
H	0.1834	-2.4346	0.8488
H	2.5698	-2.5638	1.5379
C	-4.6547	-2.1105	-0.6864
H	-4.7708	-1.4896	0.2309
H	-5.6837	-2.2568	-1.0833
O	4.9274	-2.0784	1.2888
O	5.4891	-0.8982	-0.4253
H	0.6986	3.1294	2.4198
H	1.9640	2.3522	1.4433
N	0.9004	3.8830	0.4786
H	2.0997	2.8373	-0.8788
H	1.2274	4.2238	-1.5704
H	-0.4781	5.2893	-0.2292
H	-0.5747	4.9608	1.5151
H	-2.3667	-2.2708	-1.7325
H	-2.9185	-0.7734	-0.9451
O	-3.8060	-1.5278	-1.6294

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Final geometry with 54 atoms:

O	-0.2890	-2.3555	-1.9997
C	1.0231	-0.1368	0.8296
H	0.0324	0.0676	1.2524
H	1.6705	-0.4824	1.6417
N	1.5769	1.2467	0.4675
C	0.6517	2.0062	-0.4494
H	-0.3277	2.0337	0.0402
C	1.2351	3.4200	-0.7039
H	0.5797	1.4314	-1.3750
C	2.9358	1.1787	-0.1818
H	2.8118	0.6503	-1.1336
C	3.4606	2.6232	-0.3974
H	3.5792	0.5896	0.4791
C	1.7027	2.0192	1.7637
C	2.2199	3.4461	1.4625
H	0.7082	2.0163	2.2252
H	2.3911	1.4494	2.3988
C	0.9278	-1.2227	-0.2244
C	2.2206	-1.7741	-0.7073
O	3.1517	-1.8663	0.2522
O	2.4250	-2.1967	-1.8407
C	4.4154	-2.4316	-0.1147
H	5.0251	-2.4237	0.7969
H	4.2886	-3.4623	-0.4769
H	4.8974	-1.8264	-0.8971
C	-0.0930	-1.0865	-1.3776
H	0.2763	-0.3757	-2.1387
H	0.3201	-3.8702	3.3089
C	-4.0061	0.1501	-0.1179
C	-3.4034	0.8107	-1.1895
C	-2.1288	0.4090	-1.5831
C	-1.4630	-0.6279	-0.9151
C	-2.0976	-1.2826	0.1554
C	-3.3719	-0.8950	0.5598
N	-5.3439	0.5659	0.3079
H	-3.9265	1.6179	-1.7005
H	-1.6444	0.9139	-2.4216
H	-1.5683	-2.0933	0.6747
H	-3.8744	-1.3891	1.3907
C	0.4665	-3.0139	2.5994
H	1.5659	-2.7960	2.6497
H	-0.0185	-2.1417	3.1157
O	-5.8644	-0.0229	1.2466
O	-5.8861	1.4853	-0.2925
H	1.4772	4.1909	1.7799
H	3.1479	3.6315	2.0207
N	2.4799	3.6162	0.0349
H	4.3894	2.7708	0.1705
H	3.6841	2.7803	-1.4615
H	1.4321	3.5539	-1.7763
H	0.5097	4.1842	-0.3929
H	0.5971	-2.6258	-2.3031
H	0.5247	-2.1455	0.4367
O	-0.0012	-3.2695	1.3308

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Final geometry with 54 atoms:

O	-0.1023	-1.0286	1.8457
C	1.9541	0.7641	0.8875

```
 H    2.3493    1.7782    0.7712
 H    1.9470    0.5197    1.9544
 N    3.0498   -0.1517    0.2979
 C    2.9733   -0.2459   -1.2027
 H    2.9801    0.7793   -1.5872
 C    4.1820   -1.0727   -1.7140
 H    2.0167   -0.7160   -1.4522
 C    2.9768   -1.5378    0.8930
 H    1.9707   -1.9256    0.7231
 C    4.0707   -2.4210    0.2456
 H    3.1214   -1.4134    1.9729
 C    4.3933    0.4354    0.6614
 C    5.5117   -0.5254    0.1867
 H    4.4464    1.4142    0.1696
 H    4.3930    0.5840    1.7481
 C    0.5613    0.7086    0.3076
 C    0.3869    1.3689   -0.9845
 O    1.1449    2.4901   -1.1216
 O   -0.3719    1.0198   -1.8833
 C    1.0315    3.1962   -2.3565
 H    0.0047    3.5627   -2.5098
 H    1.7232    4.0457   -2.2871
 H    1.3119    2.5554   -3.2070
 C   -0.2063   -0.6084    0.4843
 H    0.2290   -1.4201   -0.1233
 H   -2.3707    1.8235    2.9063
 C   -4.4449   -0.6930   -0.2901
 C   -3.8498    0.5414   -0.0159
 C   -2.4759    0.5923    0.1952
 C   -1.6919   -0.5706    0.1334
 C   -2.3227   -1.7946   -0.1457
 C   -3.6950   -1.8696   -0.3614
 N   -5.8860   -0.7541   -0.5137
 H   -4.4592    1.4434    0.0263
 H   -2.0131    1.5565    0.3941
 H   -1.7231   -2.7069   -0.1923
 H   -4.1842   -2.8177   -0.5816
 C   -1.3831    2.3359    2.8764
 H   -1.2625    2.8355    3.8630
 H   -1.4831    3.1557    2.1302
 O   -6.3926   -1.8418   -0.7632
 O   -6.5322    0.2849   -0.4422
 H    6.2385    0.0279   -0.4242
 H    6.0452   -0.9464    1.0502
 N    4.9551   -1.6236   -0.6025
 H    4.6641   -2.9093    1.0313
 H    3.6095   -3.2067   -0.3689
 H    3.8240   -1.8966   -2.3469
 H    4.8413   -0.4389   -2.3233
 H   -0.3082   -0.2038    2.3708
 H    0.0118    1.3624    1.3487
 O   -0.3193    1.4806    2.5983

r1-TS7-61
Final geometry with  54 atoms:
 O   -0.8386   -3.0071   -1.0228
 C   -2.1772    0.4715   -0.5525
 H   -2.3838    0.4913   -1.6293
 H   -3.1092    0.6921   -0.0241
 N   -1.2922    1.7261   -0.3142
 C   -2.1940    2.9000   -0.0182
 H   -2.6890    2.6774    0.9352
 C   -1.3372    4.1897    0.0405
 H   -2.9493    2.9341   -0.8131
 C   -0.5145    2.0548   -1.5638
 H   -1.2582    2.2723   -2.3401
 C    0.4142    3.2577   -1.2826
 H    0.0397    1.1598   -1.8506
 C   -0.3357    1.5716    0.8415
 C    0.3957    2.9190    1.0694
 H   -0.9264    1.2714    1.7109
 H    0.3553    0.7656    0.5806
 C   -1.6896   -0.8897   -0.1367
 C   -1.7691   -1.2261    1.2923
 O   -2.5495   -0.3647    1.9964
 O   -1.3083   -2.2229    1.8334
 C   -2.8016   -0.6925    3.3637
 H   -1.8631   -0.7407    3.9366
 H   -3.4374    0.1116    3.7557
 H   -3.3241   -1.6577    3.4475
 C   -0.6168   -1.6083   -1.0027
 H   -0.7637   -1.1864   -2.0163
 H   -4.4409   -3.1610   -2.7713
 C    3.5205   -0.8578   -0.0550
 C    3.0032   -0.4068   -1.2700
 C    1.6694   -0.6783   -1.5636
 C    0.8453   -1.3693   -0.6598
 C    1.4138   -1.8495    0.5347
 C    2.7436   -1.5893    0.8481
 N    4.9152   -0.5709    0.2739
 H    3.6374    0.1358   -1.9699
 H    1.2643   -0.3551   -2.5245
 H    0.7969   -2.4192    1.2262
 H    3.1828   -1.9460    1.7792
 C   -3.7877   -2.3699   -2.3408
 H   -4.3681   -1.4222   -2.4168
 H   -2.9317   -2.2658   -3.0480
 O    5.3597   -0.9848    1.3376
 O    5.5816    0.0739   -0.5269
 H    0.0931    3.3557    2.0313
 H    1.4804    2.7460    1.1021
 N    0.0911    3.8731    0.0042
 H    1.4635    2.9311   -1.2615
 H    0.3066    4.0017   -2.0846
 H   -1.5742    4.8438   -0.8101
 H   -1.5641    4.7400    0.9644
 H   -1.8419   -3.1052   -1.0526
 H   -2.6657   -1.6270   -0.5281
 O   -3.3977   -2.6699   -1.0358

r1-TS7-62
Final geometry with  54 atoms:
 O   -0.4736    2.3751   -1.9552
 C    2.3714    0.7265   -0.3417
 H    3.0149    1.2023    0.4067
 H    2.8212    0.8890   -1.3294
 N    2.5513   -0.7844   -0.0892
 C    1.6180   -1.3081    0.9717
 H    0.5981   -1.1450    0.6157
 C    1.9272   -2.8057    1.2181
 H    1.7793   -0.6913    1.8602
 C    3.9650   -1.0268    0.3855
 H    4.0662   -0.5028    1.3436
 C    4.1932   -2.5547    0.5182
 H    4.6346   -0.5615   -0.3484
 C    2.3759   -1.5576   -1.3730
 C    2.4964   -3.0698   -1.0756
 H    3.1614   -1.2017   -2.0506
 H    1.4086   -1.2826   -1.7988
 C    1.0159    1.3817   -0.2617
 C    0.5854    1.7049    1.1062
 O   -0.6263    2.2894    1.1499
 O    1.2607    1.5748    2.1241
 C   -1.0976    2.7315    2.4217
 H   -1.1328    1.8996    3.1412
 H   -0.4529    3.5284    2.8237
 H   -2.1092    3.1214    2.2517
 C   -0.0494    1.1514   -1.3819
 H    0.4647    0.5459   -2.1524
 H    0.0199    4.7922   -0.2258
 C   -3.5867   -1.0402   -0.2179
 C   -2.4464   -1.7504   -0.5973
 C   -1.3141   -1.0380   -0.9825
 C   -1.2946    0.3673   -0.9777
 C   -2.4746    1.0471   -0.6260
 C   -3.6178    0.3570   -0.2398
 N   -4.7787   -1.7747    0.1924
 H   -2.4534   -2.8396   -0.6006
 H   -0.4395   -1.5995   -1.3071
 H   -2.4864    2.1341   -0.6621
 H   -4.5274    0.8869    0.0413
 C    1.1273    4.7145   -0.3032
 H    1.4973    5.7330   -0.5527
 H    1.4951    4.5008    0.7259
 O   -5.7761   -1.1375    0.5105
 O   -4.7341   -2.9997    0.2050
 H    1.5247   -3.5656   -1.2099
 H    3.2088   -3.5264   -1.7770
 N    2.9508   -3.2946    0.2957
 H    4.9402   -2.8925   -0.2135
 H    4.5748   -2.7839    1.5228
 H    2.2794   -2.9523    2.2486
 H    1.0122   -3.3996    1.0849
 H    0.2846    3.0316   -1.8364
 H    1.3909    2.5465   -0.6352
 O    1.5487    3.7634   -1.2364

r1-TS7-63
Final geometry with  54 atoms:
 O   -1.0721   -2.7045   -1.3652
 C   -2.2446    0.6995   -0.2855
 H   -2.5824    0.8592   -1.3164
 H   -3.0934    0.8717    0.3844
 N   -1.2947    1.8965   -0.0101
 C   -0.6418    2.3480   -1.2921
 H   -1.4552    2.6565   -1.9602
 C    0.3384    3.5039   -0.9850
 H   -0.1400    1.4820   -1.7267
 C   -0.2279    1.5883    1.0105
 H    0.3960    0.7951    0.5915
 C    0.5820    2.8779    1.2950
 H   -0.7392    1.2072    1.8982
 C   -2.1191    3.0479    0.5124
 C   -1.2146    4.2996    0.6387
 H   -2.9463    3.1958   -0.1926
 H   -2.5265    2.7232    1.4774
 C   -1.7754   -0.7173   -0.0960
 C   -1.7945   -1.1602    1.3061
 O   -1.4545   -2.4559    1.4718
 O   -2.1957   -0.4951    2.2586
 C   -1.5150   -2.9780    2.8002
 H   -1.1891   -4.0235    2.7292
 H   -0.8455   -2.4213    3.4737
 H   -2.5415   -2.9319    3.1942
 C   -0.7927   -1.3359   -1.1317
 H   -0.9744   -0.7508   -2.0543
 H   -4.7017   -0.8675   -2.1376
 C    3.4132   -0.8855   -0.2957
 C    2.8644   -0.2476   -1.4087
 C    1.5087   -0.4264   -1.6735
 C    0.6950   -1.2073   -0.8367
 C    1.2932   -1.8731    0.2492
 C    2.6451   -1.7108    0.5310
 N    4.8309   -0.6976    0.0048
 H    3.4904    0.3674   -2.0540
 H    1.0765    0.0475   -2.5566
 H    0.6880   -2.5179    0.8826
 H    3.1082   -2.2136    1.3793
 C   -4.1075   -1.7988   -2.2782
 H   -3.3143   -1.5520   -3.0219
 H   -4.7854   -2.5191   -2.7863
 O    5.3024   -1.2794    0.9741
 O    5.4885    0.0359   -0.7235
 H   -1.5224    5.0670   -0.0852
 H   -1.3148    4.7254    1.6468
 N    0.1880    3.9613    0.3954
 H    0.4209    3.2044    2.3320
 H    1.6545    2.6749    1.1666
 H    1.3757    3.1724   -1.1341
 H    0.1479    4.3410   -1.6713
 H   -2.0763   -2.7745   -1.3179
 H   -2.8086   -1.3832   -0.5050
 O   -3.6076   -2.3138   -1.0815

r1-TS7-64
Final geometry with  54 atoms:
 O   -0.2213   -2.5504   -1.8007
 C    1.0025   -0.1563    0.8133
 H   -0.0007    0.0138    1.2196
 H    1.6515   -0.4693    1.6375
 N    1.5115    1.2530    0.4652
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C	0.6276	1.9429	-0.5384
H	-0.3800	1.9658	-0.1096
C	1.1892	3.3609	-0.8173
H	0.6257	1.3248	-1.4397
C	2.9193	1.2389	-0.0746
H	2.8886	0.7115	-1.0336
C	3.4057	2.7016	-0.2452
H	3.5299	0.6690	0.6331
C	1.5011	2.0561	1.7464
C	1.9306	3.5108	1.4405
H	0.4833	1.9926	2.1490
H	2.1877	1.5493	2.4348
C	0.9705	-1.2343	-0.2456
C	2.2937	-1.6603	-0.7606
O	3.1854	-1.8612	0.2356
O	2.5898	-1.8673	-1.9277
C	4.5060	-2.2509	-0.1461
H	5.0752	-2.3509	0.7866
H	4.4919	-3.2117	-0.6821
H	4.9707	-1.4873	-0.7889
C	-0.0874	-1.1958	-1.3558
H	0.2443	-0.5743	-2.2069
H	0.5345	-3.9091	3.2700
C	-3.9922	0.0951	-0.1125
C	-3.3975	0.7171	-1.2112
C	-2.1237	0.3049	-1.5981
C	-1.4503	-0.7048	-0.8972
C	-2.0802	-1.3234	0.1988
C	-3.3508	-0.9246	0.5988
N	-5.3276	0.5216	0.3053
H	-3.9262	1.5034	-1.7484
H	-1.6452	0.7795	-2.4577
H	-1.5461	-2.1167	0.7344
H	-3.8472	-1.3895	1.4500
C	0.6773	-3.0327	2.5894
H	1.7765	-2.8238	2.6204
H	0.2035	-2.1736	3.1323
O	-5.8398	-0.0320	1.2702
O	-5.8783	1.4148	-0.3266
H	1.0998	4.2014	1.6410
H	2.7713	3.7936	2.0890
N	2.3337	3.6524	0.0429
H	4.2465	2.8999	0.4339
H	3.7570	2.8549	-1.2748
H	1.5060	3.4391	-1.8664
H	0.4050	4.1104	-0.6426
H	-0.7547	-2.5469	-2.6096
H	0.6278	-2.2097	0.4681
O	0.1831	-3.2548	1.3191

r1-TS7-65
Final geometry with 54 atoms:

O	0.0635	-2.6337	-1.3426
C	-0.9911	0.0590	1.0695
H	-1.6289	-0.1655	1.9321
H	0.0214	0.2553	1.4406
N	-1.4855	1.4243	0.5744
C	-0.5458	2.0217	-0.4400
H	-0.5328	1.3448	-1.2984
C	-1.0545	3.4330	-0.8325
H	0.4478	2.0424	0.0206
C	-1.5392	2.3388	1.7782
H	-0.5334	2.3378	2.2147
C	-1.9953	3.7484	1.3317
H	-2.2345	1.8757	2.4885
C	-2.8603	1.3590	-0.0399
C	-3.3117	2.7964	-0.4112
H	-2.7827	0.7205	-0.9262
H	-3.5191	0.8821	0.6929
C	-1.0158	-1.1404	0.1492
C	-2.4000	-1.6136	-0.1147
O	-2.6477	-1.9551	-1.3920
O	-3.2612	-1.7091	0.7505
C	-3.9388	-2.5006	-1.6770
H	-4.1141	-3.4142	-1.0890
H	-3.9384	-2.7378	-2.7483
H	-4.7305	-1.7695	-1.4534
C	-0.0372	-1.2400	-1.0252
H	-0.4130	-0.6980	-1.9109
H	-1.6769	-4.4095	2.2490
C	3.9660	0.0787	-0.1893
C	3.3512	-0.8299	0.6787
C	2.0489	-1.2367	0.4098
C	1.3603	-0.7326	-0.7086
C	2.0082	0.1657	-1.5676
C	3.3136	0.5823	-1.3157
N	5.3351	0.5124	0.0883
H	3.8922	-1.2057	1.5465
H	1.5412	-1.9458	1.0710
H	1.4841	0.5479	-2.4466
H	3.8229	1.2825	-1.9767
C	-0.8081	-4.0850	1.6188
H	-0.0941	-4.9470	1.6386
H	-1.2033	-4.0755	0.5704
O	5.8632	1.3036	-0.6834
O	5.8967	0.0669	1.0812
H	-3.5428	2.8460	-1.4841
H	-4.2225	3.0570	0.1451
N	-2.2723	3.7764	-0.1029
H	-2.9042	4.0367	1.8775
H	-1.2139	4.4868	1.5582
H	-0.2817	4.1825	-0.6128
H	-1.2639	3.4663	-1.9105
H	0.5593	-2.7137	-2.1714
H	-0.6344	-1.9689	0.9895
O	-0.2454	-2.8890	2.0099

r1-TS7-66
Final geometry with 54 atoms:

O	-0.2620	2.5825	-1.8849
C	2.3237	0.3151	-0.5730
H	2.6813	0.3499	-1.6096
H	3.1396	0.6518	0.0740
N	2.1855	-1.1939	-0.2679
C	1.1732	-1.4831	0.8107
H	0.2040	-1.1320	0.4485
C	1.1738	-3.0041	1.1055
H	1.4629	-0.8897	1.6822
C	3.5206	-1.7172	0.2059
H	3.7339	-1.2072	1.1534
C	3.4265	-3.2566	0.3664
H	4.2671	-1.4149	-0.5387
C	1.8327	-1.9457	-1.5276
C	1.6261	-3.4392	-1.1872
H	0.9445	-1.4809	-1.9609
H	2.6704	-1.7893	-2.2180
C	1.1581	1.2530	-0.3892
C	0.8481	1.6903	0.9790
O	1.8369	1.4167	1.8702
O	-0.1381	2.3265	1.3234
C	1.6716	1.9379	3.1898
H	1.6125	3.0370	3.1732
H	0.7616	1.5362	3.6605
H	2.5570	1.6200	3.7550
C	-0.0163	1.2679	-1.4171
H	0.3277	0.6318	-2.2553
H	0.9503	4.7348	-0.1955
C	-3.7773	-0.3668	-0.0681
C	-3.5430	1.0061	0.0503
C	-2.3308	1.5208	-0.3952
C	-1.3431	0.6854	-0.9466
C	-1.6310	-0.6827	-1.0877
C	-2.8360	-1.2213	-0.6448
N	-5.0434	-0.9178	0.4039
H	-4.3038	1.6531	0.4858
H	-2.1376	2.5883	-0.3216
H	-0.9137	-1.3473	-1.5669
H	-3.0524	-2.2832	-0.7541
C	2.0001	4.4581	-0.4411
H	2.4676	4.1430	0.5195
H	2.5135	5.3997	-0.7352
O	-5.2287	-2.1253	0.3021
O	-5.8698	-0.1518	0.8856
H	0.5668	-3.7137	-1.2896
H	2.2049	-4.0585	-1.8867
N	2.0514	-3.7223	0.1830
H	4.0693	-3.7563	-0.3715
H	3.7750	-3.5432	1.3684
H	1.5132	-3.1885	2.1343
H	0.1522	-3.3979	1.0101
H	0.6271	3.0622	-1.8659
H	1.7420	2.3038	-0.8120
O	2.0925	3.4790	-1.4334

r1-TS7-67
Final geometry with 54 atoms:

O	-0.7588	-2.7953	1.0533
C	-0.9564	0.1794	-1.2396
H	0.0587	0.0215	-1.6151
H	-1.6162	0.3056	-2.1058
N	-0.8989	1.5735	-0.6175
C	-2.2626	2.0434	-0.1682
H	-2.5650	1.3650	0.6362
C	-2.1446	3.5064	0.3255
H	-2.9338	1.9348	-1.0265
C	-0.3863	2.5274	-1.6670
H	-1.1094	2.5046	-2.4918
C	-0.2413	3.9360	-1.0406
H	0.5707	2.1272	-2.0236
C	0.0433	1.6116	0.5579
C	0.0409	3.0417	1.1509
H	-0.3270	0.8703	1.2695
H	1.0267	1.3133	0.1790
C	-1.4228	-0.9694	-0.3582
C	-2.7789	-1.3988	-0.7666
O	-3.0658	-2.6821	-0.4757
O	-3.6206	-0.6675	-1.2789
C	-4.3915	-3.1301	-0.7638
H	-4.6109	-3.0504	-1.8397
H	-4.4312	-4.1814	-0.4512
H	-5.1346	-2.5438	-0.2020
C	-0.4230	-2.1403	-0.1658
H	-0.5351	-2.8534	-1.0034
H	-0.5113	-0.0163	3.2797
C	3.6701	-0.8302	-0.1056
C	2.9467	-0.8560	1.0895
C	1.6276	-1.2972	1.0624
C	1.0305	-1.7041	-0.1408
C	1.7925	-1.6920	-1.3200
C	3.1124	-1.2499	-1.3156
N	5.0531	-0.3555	-0.0888
H	3.4145	-0.5281	2.0170
H	1.0465	-1.3241	1.9836
H	1.3434	-2.0303	-2.2568
H	3.7074	-1.2325	-2.2278
C	-1.5385	-0.4557	3.2040
H	-2.0802	-0.0848	4.1055
H	-1.4028	-1.5514	3.3642
O	5.6731	-0.3320	-1.1448
O	5.5325	0.0015	0.9800
H	-0.3841	3.0256	2.1643
H	1.0713	3.4180	1.2200
N	-0.7518	3.9561	0.3288
H	0.8156	4.2373	-1.0287
H	-0.7954	4.6694	-1.6430
H	-2.7295	4.1768	-0.3200
H	-2.5453	3.5829	1.3463
H	-0.2512	-3.6193	1.0985
H	-1.7056	-0.5843	0.8569
O	-2.1995	-0.1379	2.0319

r1-TS7-68
Final geometry with 54 atoms:

O	1.0271	-2.7850	-1.4109
C	2.0287	0.7915	-0.8067
H	2.9764	1.0755	-0.3409
H	2.1333	0.9154	-1.8919
N	1.0422	1.9151	-0.3878
C	1.8376	3.1581	-0.0693
H	2.5002	3.3427	-0.9237
C	0.8569	4.3313	0.1856

H	2.4482	2.9196	0.8104
C	0.2192	1.5635	0.8258
H	0.9176	1.2725	1.6146
C	-0.6346	2.7927	1.2267
H	-0.3980	0.7023	0.5557
C	0.1191	2.2459	-1.5328
C	-0.8947	3.3206	-1.0768
H	0.7586	2.5952	-2.3528
H	-0.3686	1.3193	-1.8390
C	1.7320	-0.6432	-0.4659
C	1.9728	-1.0637	0.9231
O	2.7264	-0.1758	1.6253
O	1.6513	-2.1316	1.4282
C	3.1399	-0.5757	2.9324
H	3.7677	-1.4789	2.8866
H	2.2708	-0.7743	3.5777
H	3.7215	0.2628	3.3362
C	0.6650	-1.4201	-1.2887
H	0.6823	-0.9328	-2.2835
H	3.8136	-3.5447	-0.0624
C	-3.4283	-1.1653	0.0361
C	-2.5075	-1.8664	0.8203
C	-1.1907	-1.9663	0.3837
C	-0.7795	-1.3591	-0.8173
C	-1.7432	-0.7042	-1.6019
C	-3.0663	-0.5899	-1.1825
N	-4.8094	-1.0411	0.4978
H	-2.8260	-2.3223	1.7572
H	-0.4610	-2.5050	0.9840
H	-1.4563	-0.2805	-2.5664
H	-3.8096	-0.0737	-1.7886
C	4.3138	-2.7155	-0.6114
H	5.2714	-3.1273	-1.0002
H	4.5984	-1.9667	0.1627
O	-5.5981	-0.4038	-0.1897
O	-5.1203	-1.5765	1.5546
H	-0.9248	4.1358	-1.8134
H	-1.9028	2.8875	-1.0085
N	-0.5273	3.8592	0.2325
H	-1.6873	2.4927	1.3235
H	-0.3028	3.1824	2.1992
H	0.9457	5.0820	-0.6120
H	1.1065	4.8184	1.1386
H	2.0198	-2.7641	-1.5831
H	2.7324	-1.2390	-1.0150
O	3.5251	-2.1689	-1.6256

r1-TS7-69
Final geometry with 54 atoms:

O	0.6046	-3.0431	0.8490
C	1.0911	0.0679	-1.2204
H	1.8630	0.2348	-1.9792
H	0.1411	-0.0559	-1.7498
N	0.9500	1.4299	-0.5383
C	2.2507	1.8798	0.0836
H	3.0052	1.8492	-0.7099
C	2.0547	3.2996	0.6701
H	2.4871	1.1465	0.8617
C	-0.1188	1.4074	0.5239
H	0.1926	0.6525	1.2496
C	-0.2270	2.8174	1.1552
H	-1.0450	1.0985	0.0280
C	0.5515	2.4331	-1.5915
C	0.3642	3.8186	-0.9256
H	1.3482	2.4308	-2.3455
H	-0.3727	2.0613	-2.0505
C	1.4082	-1.1388	-0.3481
C	2.7371	-1.7176	-0.6415
O	3.6808	-0.7697	-0.8594
O	3.0326	-2.9046	-0.6450
C	5.0176	-1.2249	-1.0690
H	5.0787	-1.8834	-1.9490
H	5.3894	-1.7694	-0.1874
H	5.6239	-0.3248	-1.2338
C	0.3358	-2.2532	-0.3044
H	0.4362	-2.8848	-1.2077
H	1.1050	-1.9404	3.2660
C	-3.6638	-0.6828	-0.1977
C	-3.0822	-0.9671	-1.4354
C	-1.7971	-1.5021	-1.4580
C	-1.0901	-1.7357	-0.2680
C	-1.7158	-1.4684	0.9597
C	-3.0010	-0.9388	1.0055
N	-5.0082	-0.1089	-0.1606
H	-3.6321	-0.7753	-2.3559
H	-1.3345	-1.7419	-2.4182
H	-1.1807	-1.6706	1.8865
H	-3.4871	-0.7164	1.9547
C	1.2695	-0.8383	3.2238
H	0.2501	-0.3812	3.2853
H	1.7679	-0.5710	4.1846
O	-5.5714	0.1230	-1.2232
O	-5.5132	0.1195	0.9313
H	1.0207	4.5564	-1.4076
H	-0.6741	4.1572	-1.0487
N	0.6772	3.7629	0.5011
H	-1.2582	3.1875	1.0683
H	0.0275	2.7685	2.2232
H	2.2953	3.2918	1.7428
H	2.7304	4.0120	0.1761
H	0.0704	-3.8495	0.7909
H	1.6089	-0.8077	0.9094
O	2.0040	-0.4248	2.1258

r1-TS7-70
Final geometry with 54 atoms:

O	-0.0725	0.8600	-2.2503
C	0.5952	-0.5422	0.3394
H	0.2089	-0.8306	1.3242
H	0.0365	-1.0943	-0.4243
N	1.9915	-1.1551	0.2788
C	2.9602	-0.4402	1.1854
H	2.5123	-0.4324	2.1842
C	4.3226	-1.1753	1.1390
H	3.0333	0.5897	0.8267
C	2.5228	-1.1444	-1.1346
H	2.5094	-0.1044	-1.4761
C	3.9408	-1.7658	-1.1385
H	1.8084	-1.7230	-1.7327
C	1.8966	-2.5918	0.7330
C	3.2902	-3.2556	0.6038
H	1.5354	-2.5705	1.7683
H	1.1388	-3.0734	0.1031
C	0.4903	0.9563	0.1190
C	0.3916	1.6834	1.3934
O	0.1841	3.0276	1.4298
O	0.5121	1.1554	2.4972
C	0.4135	3.9390	0.3505
H	0.9149	4.8171	0.7847
H	1.0502	3.5062	-0.4320
H	-0.5468	4.2633	-0.0799
C	-0.5546	1.2777	-0.9846
H	-0.7365	2.3624	-0.9976
H	3.9698	3.0521	-1.9083
C	-4.3345	-0.5712	-0.1184
C	-3.5940	-1.0400	-1.2048
C	-2.3755	-0.4312	-1.4986
C	-1.8960	0.6291	-0.7153
C	-2.6707	1.0866	0.3668
C	-3.8883	0.4931	0.6734
N	-5.6112	-1.2042	0.1984
H	-3.9711	-1.8662	-1.8065
H	-1.7868	-0.7772	-2.3477
H	-2.3167	1.9238	0.9719
H	-4.4930	0.8442	1.5085
C	3.5211	2.3686	-1.1580
H	3.5528	2.9076	-0.1852
H	4.2163	1.5050	-1.0651
O	-6.2513	-0.7793	1.1530
O	-5.9909	-2.1357	-0.5018
H	3.5873	-3.6862	1.5703
H	3.2549	-4.0696	-0.1336
N	4.2965	-2.2819	0.1831
H	3.9859	-2.5867	-1.8681
H	4.6842	-1.0118	-1.4322
H	5.1150	-0.4713	0.8489
H	4.5703	-1.5723	2.1334
H	0.8205	1.2589	-2.3385
H	1.5449	1.4892	-0.5792
O	2.2280	1.9950	-1.5209

r1-TS7-71
Final geometry with 54 atoms:

O	-0.0919	-2.5915	-1.5921
C	1.0366	-0.0186	1.0056
H	0.0337	0.1542	1.4117
H	1.7050	-0.2445	1.8425
N	1.4967	1.3605	0.5201
C	1.5960	2.2444	1.7453
H	2.3127	1.7615	2.4199
C	2.0443	3.6631	1.3212
H	0.6045	2.2351	2.2135
C	0.5100	1.9814	-0.4349
H	-0.4657	1.9684	0.0624
C	0.9829	3.4138	-0.7940
H	0.4749	1.3401	-1.3185
C	2.8453	1.3221	-0.1525
C	3.2616	2.7705	-0.5222
H	3.5396	0.8460	0.5471
H	2.7408	0.6915	-1.0423
C	1.0435	-1.2012	0.0584
C	2.4206	-1.6944	-0.2190
O	2.5723	-2.2179	-1.4543
O	3.3351	-1.7049	0.5894
C	3.8357	-2.8218	-1.7631
H	4.6418	-2.0761	-1.7020
H	4.0486	-3.6490	-1.0704
H	3.7464	-3.1992	-2.7889
C	0.0690	-1.2454	-1.1404
H	0.4498	-0.6327	-1.9771
H	0.5332	-3.5633	3.7805
C	-3.9291	0.0362	-0.2405
C	-3.2917	-0.8561	0.6261
C	-1.9905	-1.2586	0.3384
C	-1.3313	-0.7671	-0.8019
C	-2.0020	0.1147	-1.6609
C	-3.3039	0.5276	-1.3878
N	-5.2948	0.4682	0.0615
H	-3.8129	-1.2238	1.5094
H	-1.4629	-1.9569	1.0015
H	-1.4981	0.4890	-2.5549
H	-3.8307	1.2160	-2.0474
C	0.6406	-2.7459	3.0208
H	1.7406	-2.5328	2.9924
H	0.1896	-1.8450	3.5166
O	-5.8444	1.2432	-0.7111
O	-5.8305	0.0373	1.0747
H	4.2057	3.0242	-0.0208
H	3.4214	2.8461	-1.6065
N	2.2401	3.7370	-0.1249
H	1.1244	3.4958	-1.8804
H	0.2203	4.1457	-0.4941
H	1.2859	4.4010	1.6169
H	2.9863	3.9232	1.8233
H	0.7974	-2.8959	-1.8395
H	0.6399	-2.0705	0.8010
O	0.0980	-3.0657	1.7954

r1-TS7-72
Final geometry with 54 atoms:

O	-0.0572	-2.6899	-1.4600
C	1.0184	-0.0718	1.0085
H	0.0121	0.0997	1.4066
H	1.6804	-0.3010	1.8499
N	1.4853	1.3178	0.5436
C	1.5459	2.1967	1.7727
H	2.2572	1.7225	2.4593
C	1.9786	3.6246	1.3620
H	0.5463	2.1705	2.2226
C	0.5245	1.9346	-0.4377
H	-0.4616	1.9332	0.0388

C	1.0140	3.3613	-0.7982
H	0.5036	1.2836	-1.3151
C	2.8520	1.2860	-0.0910
C	3.2834	2.7387	-0.4245
H	3.5259	0.7938	0.6177
H	2.7685	0.6740	-0.9954
C	1.0407	-1.2369	0.0472
C	2.4218	-1.6900	-0.2567
O	2.6486	-1.9779	-1.5505
O	3.3002	-1.8210	0.5870
C	3.9427	-2.4870	-1.8863
H	4.7243	-1.7462	-1.6587
H	4.1531	-3.4154	-1.3345
H	3.9189	-2.6882	-2.9647
C	0.0509	-1.3013	-1.1226
H	0.4249	-0.7471	-2.0018
H	0.5370	-3.6186	3.7442
C	-3.9332	0.0530	-0.2480
C	-3.3133	-0.8482	0.6241
C	-2.0177	-1.2694	0.3443
C	-1.3412	-0.7871	-0.7913
C	-1.9949	0.1027	-1.6554
C	-3.2933	0.5336	-1.3917
N	-5.2937	0.5038	0.0441
H	-3.8453	-1.2071	1.5045
H	-1.5043	-1.9769	1.0062
H	-1.4798	0.4688	-2.5465
H	-3.8062	1.2281	-2.0557
C	0.6820	-2.7911	3.0051
H	1.7861	-2.6120	2.9889
H	0.2487	-1.8861	3.5052
O	-5.8275	1.2865	-0.7324
O	-5.8428	0.0811	1.0539
H	4.1983	2.9929	0.1282
H	3.5005	2.8229	-1.4982
N	2.2373	3.6975	-0.0745
H	1.2098	3.4259	-1.8773
H	0.2365	4.0964	-0.5489
H	1.1908	4.3459	1.6189
H	2.8904	3.9088	1.9052
H	-0.5580	-2.7559	-2.2869
H	0.6477	-2.1370	0.8252
O	0.1441	-3.0787	1.7654

r1-TS7-73
Final geometry with 54 atoms:

O	0.4798	1.7714	-1.7053
C	-1.2874	-1.0502	-0.1937
H	-1.0880	-1.4885	-1.1783
H	-1.0606	-1.8016	0.5715
N	-2.8139	-0.9337	-0.1568
C	-3.3849	-2.3308	-0.1693
H	-3.0219	-2.8258	0.7397
C	-4.9302	-2.2450	-0.2198
H	-2.9603	-2.8396	-1.0432
C	-3.3301	-0.2003	-1.3713
H	-2.9881	-0.7701	-2.2442
C	-4.8740	-0.1149	-1.2845
H	-2.8634	0.7902	-1.3651
C	-3.3022	-0.2360	1.0872
C	-4.8518	-0.2591	1.0945
H	-2.8619	-0.7617	1.9403
H	-2.9055	0.7821	1.0552
C	-0.4733	0.2176	0.0258
C	0.0213	0.2605	1.4175
O	0.9595	1.1544	1.8215
O	-0.3560	-0.5143	2.2952
C	1.1742	2.4600	1.2821
H	0.8652	2.5511	0.2384
H	2.2511	2.6650	1.3583
H	0.6283	3.1907	1.8990
C	0.5325	0.4692	-1.1438
H	0.2307	-0.2442	-1.9329
H	-1.7850	2.9212	1.4306
C	4.5995	-0.6261	-0.2481
C	4.3475	0.6228	-0.8181
C	3.0309	0.9766	-1.1042
C	1.9724	0.1023	-0.8194
C	2.2603	-1.1545	-0.2554
C	3.5666	-1.5263	0.0354
N	5.9752	-1.0038	0.0594
H	5.1727	1.3014	-1.0312
H	2.8145	1.9464	-1.5499
H	1.4507	-1.8518	-0.0315
H	3.7930	-2.4955	0.4779
C	-1.9711	3.3408	0.4193
H	-1.3049	4.2215	0.3118
H	-3.0127	3.7233	0.4247
O	6.1794	-2.1014	0.5652
O	6.8711	-0.2090	-0.2004
H	-5.2161	-0.8364	1.9558
H	-5.2368	0.7661	1.1868
N	-5.3810	-0.8574	-0.1306
H	-5.1874	0.9346	-1.1910
H	-5.3241	-0.5224	-2.2006
H	-5.3035	-2.6785	-1.1580
H	-5.3607	-2.8181	0.6133
H	-0.3839	2.1830	-1.4220
H	-1.2473	1.3432	-0.1526
O	-1.7785	2.3913	-0.5903

r1-TS7-74
Final geometry with 54 atoms:

O	0.0300	0.5368	2.3700
C	-0.6647	-0.5971	-0.1897
H	-0.2462	-0.8859	-1.1610
H	-0.1726	-1.1916	0.5867
N	-2.0882	-1.1328	-0.2061
C	-2.9292	-0.4428	-1.2483
H	-2.4248	-0.5998	-2.2081
C	-4.3573	-1.0404	-1.2149
H	-2.9201	0.6243	-1.0194
C	-2.7389	-0.9918	1.1503
H	-2.7577	0.0798	1.3864
C	-4.1558	-1.6140	1.0889
H	-2.0817	-1.5069	1.8609
C	-2.0332	-2.6023	-0.5500
C	-3.4764	-3.1648	-0.5889
H	-1.5239	-2.6822	-1.5179
H	-1.4136	-3.0804	0.2184
C	-0.4885	0.8932	0.0734
C	-0.2649	1.6346	-1.1888
O	0.0268	2.9609	-1.1866
O	-0.3495	1.1277	-2.3030
C	-0.1326	3.8585	-0.0817
H	-0.5238	4.7969	-0.5014
H	-0.8379	3.4733	0.6653
H	0.8464	4.0633	0.3792
C	0.5656	1.1047	1.1850
H	0.7256	2.1802	1.3360
H	-3.6706	3.7239	0.6522
C	4.3502	-0.6068	0.0489
C	3.5778	-1.2621	1.0094
C	2.3625	-0.6977	1.3900
C	1.9154	0.5032	0.8178
C	2.7226	1.1452	-0.1398
C	3.9382	0.5977	-0.5311
N	5.6260	-1.1903	-0.3566
H	3.9288	-2.1949	1.4491
H	1.7508	-1.1897	2.1470
H	2.3958	2.0878	-0.5827
H	4.5675	1.0902	-1.2715
C	-3.3502	2.6969	0.3631
H	-2.9069	2.8022	-0.6560
H	-4.2917	2.1149	0.2226
O	6.2965	-0.5997	-1.1950
O	5.9735	-2.2470	0.1573
H	-3.7024	-3.5484	-1.5935
H	-3.5728	-3.9976	0.1217
N	-4.4520	-2.1319	-0.2466
H	-4.2407	-2.4357	1.8141
H	-4.9075	-0.8550	1.3476
H	-5.0836	-0.2622	-0.9419
H	-4.6253	-1.4201	-2.2109
H	0.6146	0.7602	3.1101
H	-1.5381	1.4770	0.6396
O	-2.4812	2.1307	1.2860

r1-TS7-75
Final geometry with 54 atoms:

O	0.1799	2.6571	1.6072
C	-0.9849	0.0407	-0.8445
H	0.0609	-0.1167	-1.1264
H	-1.5389	0.2393	-1.7684
N	-1.4812	-1.3769	-0.4366
C	-1.1428	-1.7203	0.9888
H	-1.6830	-1.0131	1.6262
C	-1.5525	-3.1907	1.2624
H	-0.0672	-1.5693	1.1066
C	-0.8081	-2.3818	-1.3398
H	0.2675	-2.3069	-1.1377
C	-1.3682	-3.7936	-1.0367
H	-1.0000	-2.0626	-2.3716
C	-2.9733	-1.5064	-0.6223
C	-3.4177	-2.9255	-0.1900
H	-3.4532	-0.7266	-0.0239
H	-3.1709	-1.3114	-1.6829
C	-1.0691	1.1611	0.1572
C	-2.3863	1.4803	0.7432
O	-3.4609	1.7061	-0.0653
O	-2.6056	1.5926	1.9431
C	-3.3946	1.9395	-1.4736
H	-3.6723	1.0271	-2.0229
H	-4.1300	2.7252	-1.6975
H	-2.4021	2.2758	-1.7949
C	0.0476	1.2873	1.2288
H	-0.2243	0.7498	2.1499
H	-0.7023	5.4435	-0.6003
C	3.9277	-0.1285	-0.0025
C	3.3169	-0.7056	1.1115
C	2.0588	-0.2438	1.4935
C	1.4089	0.7726	0.7772
C	2.0624	1.3464	-0.3304
C	3.3172	0.8994	-0.7284
N	5.2447	-0.6074	-0.4183
H	3.8218	-1.4957	1.6658
H	1.5758	-0.6781	2.3716
H	1.5768	2.1543	-0.8816
H	3.8242	1.3342	-1.5890
C	-1.2003	4.4718	-0.8003
H	-1.7858	4.6067	-1.7356
H	-1.9395	4.3285	0.0187
O	5.7744	-0.0831	-1.3903
O	5.7635	-1.5142	0.2213
H	-4.0595	-2.8663	0.6998
H	-3.9988	-3.3922	-0.9975
N	-2.2622	-3.7644	0.1202
H	-1.9247	-4.1769	-1.9033
H	-0.5372	-4.4838	-0.8348
H	-0.6595	-3.7980	1.4654
H	-2.2006	-3.2339	2.1486
H	0.1659	3.1580	0.7470
H	-0.7642	2.2996	-0.5337
O	-0.2687	3.4308	-0.8807

r1-TS7-76
Final geometry with 54 atoms:

O	-0.2498	0.5474	-2.3865
C	1.9362	0.9466	-0.4890
H	2.3397	1.8541	-0.0253
H	1.9512	1.0951	-1.5745
N	3.0398	-0.1002	-0.2277
C	3.3833	-0.1969	1.2380
H	2.4999	-0.5836	1.7524
C	4.5945	-1.1501	1.4102
H	3.5880	0.8213	1.5888
C	4.2691	0.3551	-0.9803
H	4.5193	1.3512	-0.5944
C	5.4085	-0.6698	-0.7729
H	3.9747	0.4468	-2.0323
C	2.6604	-1.4745	-0.7090

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C    3.8472   -2.4409   -0.4499
H    2.4132   -1.3821   -1.7733
H    1.7666   -1.7695   -0.1510
C    0.5072    0.6647   -0.0848
C    0.2636    0.2809    1.3098
O    0.6693    1.1120    2.3125
O   -0.2703   -0.7618    1.6725
C    0.7546    2.5265    2.1390
H    1.5446    2.8249    1.4365
H   -0.2106    2.9338    1.8071
H    0.9954    2.9364    3.1294
C   -0.2916   -0.1439   -1.1370
H    0.1441   -1.1337   -1.3344
H   -1.3638    4.5894   -1.4538
C   -4.4045   -0.8126   -0.0537
C   -3.5735   -1.9135   -0.2786
C   -2.2436   -1.6847   -0.6181
C   -1.7401   -0.3805   -0.7332
C   -2.6032    0.7047   -0.5093
C   -3.9354    0.4995   -0.1666
N   -5.8012   -1.0396    0.3061
H   -3.9686   -2.9243   -0.1846
H   -1.5788   -2.5344   -0.7896
H   -2.2207    1.7188   -0.6125
H   -4.6075    1.3378    0.0124
C   -0.9020    3.9727   -0.6536
H   -1.7385    3.6694    0.0164
H   -0.2619    4.6617   -0.0588
O   -6.5189   -0.0659    0.5029
O   -6.2002   -2.1948    0.3975
H    3.5336   -3.2377    0.2384
H    4.1585   -2.9098   -1.3935
N    4.9893   -1.7377    0.1320
H    5.6959   -1.1128   -1.7365
H    6.2917   -0.1693   -0.3524
H    5.4503   -0.6015    1.8272
H    4.3334   -1.9555    2.1105
H   -0.3907    1.5069   -2.1753
H    0.0676    1.9189   -0.4119
O   -0.1935    2.8993   -1.1867

r1-TS7-77
Final geometry with  54 atoms:
O   -0.0448   -0.4315    2.0306
C    1.9882    0.9637    0.4952
H    2.3955    1.8770    0.0502
H    2.0240    1.0739    1.5842
N    3.0626   -0.1003    0.1884
C    4.4157    0.5562    0.3380
H    4.4327    1.0266    1.3285
C    5.5196   -0.5146    0.1631
H    4.4681    1.3391   -0.4287
C    2.9521   -0.6331   -1.2151
H    2.9330    0.2337   -1.8858
C    4.1610   -1.5645   -1.4901
H    1.9975   -1.1629   -1.2883
C    3.0021   -1.2469    1.1701
C    4.0658   -2.2992    0.7735
H    3.1881   -0.8111    2.1591
H    1.9891   -1.6520    1.1574
C    0.5712    0.7442    0.0155
C    0.3583    0.9517   -1.4171
O    0.8333    2.1078   -1.9817
O   -0.1978    0.1660   -2.1735
C    0.6865    3.3614   -1.3073
H    1.1308    3.3727   -0.3029
H    1.1948    4.1082   -1.9324
H   -0.3808    3.6237   -1.2292
C   -0.1695   -0.4612    0.6079
H    0.2671   -1.4197    0.2798
H   -2.3184    2.4403    2.1874
C   -4.4043   -0.8081   -0.1218
C   -3.8097    0.4461   -0.2784
C   -2.4378    0.5680   -0.0788
C   -1.6563   -0.5441    0.2699
C   -2.2876   -1.7909    0.4191
C   -3.6571   -1.9368    0.2251
N   -5.8430   -0.9443   -0.3321
H   -4.4166    1.3079   -0.5537
H   -1.9785    1.5457   -0.2096
H   -1.6900   -2.6637    0.6931
H   -4.1459   -2.9039    0.3368
C   -1.3801    3.0084    2.0016
H   -1.3167    3.7775    2.8020
H   -1.5383    3.5672    1.0527
O   -6.3488   -2.0530   -0.2040
O   -6.4865    0.0558   -0.6273
H    4.6660   -2.5666    1.6546
H    3.5770   -3.2123    0.4061
N    4.9451   -1.7860   -0.2757
H    3.8007   -2.5309   -1.8689
H    4.8136   -1.1223   -2.2556
H    6.2514   -0.1700   -0.5807
H    6.0508   -0.6761    1.1116
H   -0.2240    0.5196    2.2768
H    0.0456    1.6833    0.8301
O   -0.2401    2.2058    1.9733

r1-TS7-78
Final geometry with  54 atoms:
O    0.0645   -1.0866   -1.8481
C    1.8496    0.7173   -0.8265
H    2.2023    1.7458   -0.7235
H    1.7629    0.5034   -1.8965
N    3.0541   -0.1255   -0.3635
C    3.1858   -0.1617    1.1363
H    2.3148   -0.7030    1.5189
C    4.5153   -0.8690    1.5069
H    3.1504    0.8744    1.4898
C    4.2938    0.5247   -0.9378
H    4.3432    1.5320   -0.5070
C    5.5323   -0.3303   -0.5803
H    4.1334    0.6086   -2.0197
C    2.9923   -1.5446   -0.8742
C    4.2373   -2.3149   -0.3650
H    2.9494   -1.4807   -1.9674
H    2.0629   -1.9870   -0.5106
C    0.4948    0.5486   -0.1669
C    0.3792    0.8927    1.2686
O    0.8476    2.0726    1.7471
O   -0.1450    0.1632    2.1032
C    1.2563    3.1937    0.9542
H    0.7881    3.1864   -0.0385
H    0.9386    4.0914    1.5036
H    2.3540    3.2080    0.8633
C   -0.2127   -0.7877   -0.4826
H    0.1842   -1.5891    0.1672
H   -2.7062    2.9679   -1.1272
C   -4.4834   -0.7352    0.0380
C   -3.7029   -1.4560    0.9450
C   -2.3210   -1.4610    0.7764
C   -1.7201   -0.7516   -0.2737
C   -2.5331   -0.0493   -1.1785
C   -3.9155   -0.0319   -1.0284
N   -5.9347   -0.7185    0.2076
H   -4.1754   -2.0012    1.7610
H   -1.6964   -2.0190    1.4756
H   -2.0658    0.5127   -1.9863
H   -4.5516    0.5198   -1.7193
C   -1.6861    2.9967   -0.6757
H   -1.7826    2.4362    0.2875
H   -1.5183    4.0606   -0.3784
O   -6.6077   -0.0796   -0.5924
O   -6.4202   -1.3433    1.1432
H    3.9299   -3.1064    0.3324
H    4.7498   -2.7904   -1.2129
N    5.1684   -1.4216    0.3212
H    5.9769   -0.7570   -1.4900
H    6.2903    0.3015   -0.0969
H    5.2001   -0.1576    1.9887
H    4.3128   -1.6811    2.2187
H   -0.3266   -1.9497   -2.0519
H   -0.1246    1.4754   -0.8172
O   -0.6995    2.4954   -1.5075

r1-TS7-79
Final geometry with  54 atoms:
O    0.3378    2.5085    1.7354
C   -0.9825    0.1052   -0.8079
H    0.0450   -0.1719   -1.0652
H   -1.4805    0.3910   -1.7408
N   -1.6591   -1.2373   -0.4387
C   -1.4268   -1.6399    0.9937
H   -1.9051   -0.8813    1.6211
C   -2.0255   -3.0522    1.2220
H   -0.3467   -1.6244    1.1609
C   -1.0772   -2.3064   -1.3335
H   -0.0098   -2.3661   -1.0888
C   -1.8180   -3.6421   -1.0784
H   -1.1862   -1.9514   -2.3657
C   -3.1470   -1.1791   -0.6876
C   -3.7800   -2.5382   -0.2987
H   -3.5507   -0.3509   -0.0979
H   -3.2721   -0.9488   -1.7521
C   -0.9448    1.2327    0.1986
C   -2.2376    1.6730    0.7877
O   -3.2627    2.0633   -0.0109
O   -2.4639    1.7180    1.9905
C   -3.1533    2.3460   -1.4125
H   -3.4922    1.4776   -1.9981
H   -3.8318    3.1884   -1.6093
H   -2.1291    2.6243   -1.6957
C    0.1388    1.1621    1.2921
H   -0.1989    0.5597    2.1513
H    0.5612    4.7677   -0.2157
C    3.9420   -0.3834    0.0100
C    3.2948   -0.9888    1.0877
C    2.0579   -0.4850    1.4867
C    1.4693    0.5987    0.8189
C    2.1528    1.1963   -0.2568
C    3.3875    0.7070   -0.6687
N    5.2379   -0.9062   -0.4229
H    3.7554   -1.8316    1.6015
H    1.5442   -0.9404    2.3364
H    1.6834    2.0325   -0.7846
H    3.9213    1.1537   -1.5070
C   -0.3056    4.3769   -0.7997
H   -0.5608    5.1730   -1.5374
H   -1.1585    4.3524   -0.0784
O    5.8006   -0.3599   -1.3634
O    5.7058   -1.8691    0.1722
H   -4.4454   -2.4121    0.5664
H   -4.3803   -2.9183   -1.1370
N   -2.7500   -3.5172    0.0413
H   -2.3797   -3.9432   -1.9735
H   -1.0874   -4.4317   -0.8543
H   -1.2237   -3.7680    1.4500
H   -2.7122   -3.0263    2.0793
H    0.8572    2.4792    2.5528
H   -0.5225    2.2011   -0.5720
O   -0.0631    3.1508   -1.4022

r1-TS7-80
Final geometry with  54 atoms:
O    0.4507    2.3758    1.8549
C   -0.9993    0.0827   -0.8164
H    0.0143   -0.2478   -1.0680
H   -1.4777    0.3855   -1.7540
N   -1.7397   -1.2159   -0.4335
C   -1.4796   -1.6435    0.9870
H   -1.9111   -0.8731    1.6343
C   -2.1285   -3.0323    1.2198
H   -0.3947   -1.6719    1.1215
C   -1.2491   -2.3089   -1.3561
H   -0.1807   -2.4361   -1.1416
C   -2.0640   -3.5986   -1.0942
H   -1.3636   -1.9362   -2.3813
C   -3.2303   -1.0758   -0.6280
C   -3.9210   -2.3976   -0.2104
H   -3.5670   -0.2266   -0.0260
H   -3.3813   -0.8421   -1.6886
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 C  -0.8942   1.2234   0.1741
 C  -2.1373   1.8014   0.7414
 O  -3.1641   2.1810  -0.0503
 O  -2.2924   2.0032   1.9450
 C  -3.0601   2.4072  -1.4649
 H  -3.4033   1.5203  -2.0182
 H  -3.7373   3.2438  -1.6872
 H  -2.0341   2.6744  -1.7551
 C   0.1718   1.0910   1.2942
 H  -0.1936   0.4382   2.1035
 H  -0.1761   5.1912  -1.4413
 C   3.9637  -0.4644   0.0053
 C   3.3085  -1.0745   1.0756
 C   2.0759  -0.5627   1.4767
 C   1.5000   0.5336   0.8186
 C   2.1869   1.1310  -0.2535
 C   3.4201   0.6347  -0.6657
 N   5.2571  -0.9948  -0.4294
 H   3.7596  -1.9269   1.5819
 H   1.5553  -1.0229   2.3194
 H   1.7232   1.9692  -0.7848
 H   3.9589   1.0836  -1.4996
 C  -0.0859   4.3193  -0.7514
 H  -1.0026   4.3549  -0.1112
 H   0.7601   4.5606  -0.0642
 O   5.8272  -0.4440  -1.3624
 O   5.7141  -1.9676   0.1576
 H  -4.5311  -2.2386   0.6895
 H  -4.5869  -2.7346  -1.0170
 N  -2.9343  -3.4383   0.0700
 H  -2.6850  -3.8414  -1.9676
 H  -1.3772  -4.4388  -0.9217
 H  -1.3497  -3.7883   1.3899
 H  -2.7662  -2.9938   2.1136
 H  -0.3886   2.6626   2.2545
 H  -0.4306   2.1411  -0.5855
 O   0.0672   3.1193  -1.4271

r1-TS7-81
Final geometry with  54 atoms:
 O  -0.1711  -1.8341  -1.1368
 C  -1.7419   0.3529  -1.0214
 H  -2.0028   1.3501  -1.3912
 H  -1.5711  -0.2889  -1.8897
 N  -3.0573  -0.1663  -0.4035
 C  -3.9748  -0.5534  -1.5397
 H  -3.4916  -1.3938  -2.0524
 C  -5.3619  -0.9290  -0.9657
 H  -4.0174   0.3033  -2.2232
 C  -3.7463   0.9051   0.4063
 H  -3.9648   1.7252  -0.2878
 C  -5.0281   0.3114   1.0400
 H  -3.0413   1.2622   1.1627
 C  -2.8566  -1.3732   0.4786
 C  -4.2441  -1.9304   0.8840
 H  -2.2624  -2.0918  -0.0936
 H  -2.2831  -1.0320   1.3464
 C  -0.4740   0.3607  -0.1907
 C  -0.4981   1.0999   1.0939
 O  -0.8784   2.4008   1.1385
 O  -0.1789   0.6123   2.1728
 C  -1.0616   3.2553  -0.0004
 H  -0.4747   2.9139  -0.8637
 H  -2.1308   3.3138  -0.2553
 H  -0.7194   4.2528   0.3096
 C   0.2039  -1.0301  -0.0243
 H  -0.1338  -1.5073   0.9099
 H   3.0608   2.1423  -1.4117
 C   4.4865  -0.6365   0.1496
 C   3.8608  -0.7619  -1.0941
 C   2.4788  -0.9060  -1.1348
 C   1.7206  -0.9122   0.0476
 C   2.3796  -0.8078   1.2824
 C   3.7633  -0.6640   1.3437
 N   5.9367  -0.4733   0.2013
 H   4.4542  -0.7420  -2.0072
 H   1.9735  -0.9966  -2.0954
 H   1.7992  -0.8259   2.2043
 H   4.2808  -0.5764   2.2982
 C   2.0265   2.3426  -1.0432
 H   1.9470   3.4548  -0.9597
 H   2.0173   1.9719   0.0118
 O   6.4737  -0.3656   1.2976
 O   6.5588  -0.4486  -0.8543
 H  -4.4196  -2.9021   0.4013
 H  -4.2734  -2.0830   1.9719
 N  -5.3156  -1.0144   0.4939
 H  -4.9095   0.2244   2.1291
 H  -5.8775   0.9804   0.8435
 H  -6.1103  -0.1765  -1.2507
 H  -5.6800  -1.8967  -1.3781
 H   0.2300  -2.7092  -1.0237
 H   0.2784   1.0361  -0.9897
 O   1.0435   1.7762  -1.8339

r1-TS7-82
Final geometry with  54 atoms:
 O  -0.5083   2.2609  -1.8051
 C   2.2818   0.8485  -0.2025
 H   2.5922   1.1542  -1.2102
 H   2.9637   1.3160   0.5166
 N   2.6699  -0.6437  -0.1521
 C   4.1477  -0.7134  -0.4781
 H   4.6581  -0.0355   0.2156
 C   4.6352  -2.1753  -0.3418
 H   4.2586  -0.3268  -1.4983
 C   1.9319  -1.4742  -1.1711
 H   2.0246  -0.9630  -2.1359
 C   2.5395  -2.9003  -1.2015
 H   0.8828  -1.4974  -0.8667
 C   2.4643  -1.2615   1.2071
 C   2.8730  -2.7543   1.1502
 H   3.0713  -0.6821   1.9098
 H   1.4140  -1.1278   1.4714
 C   0.8745   1.3545   0.0462
 C   0.5115   1.4551   1.4741
 O  -0.7083   1.8972   1.8662
 O   1.2851   1.1803   2.3862
 C  -1.5557   2.7893   1.1362
 H  -1.2518   2.9152   0.0935
 H  -2.5771   2.3860   1.1711
 H  -1.5382   3.7662   1.6444
 C  -0.1596   1.0859  -1.0843
 H   0.3502   0.4144  -1.7966
 H   0.0801   5.2619  -0.2601
 C  -3.7546  -1.1004  -0.1370
 C  -2.5799  -1.4069   0.5529
 C  -1.4270  -0.6847   0.2630
 C  -1.4282   0.3330  -0.7047
 C  -2.6279   0.6150  -1.3803
 C  -3.7930  -0.0937  -1.1044
 N  -4.9717  -1.8492   0.1625
 H  -2.5763  -2.1921   1.3077
 H  -0.5173  -0.9178   0.8127
 H  -2.6427   1.4073  -2.1274
 H  -4.7230   0.1261  -1.6277
 C   1.0500   4.7689  -0.0277
 H   0.9744   4.4232   1.0287
 H   1.8176   5.5739  -0.0304
 O  -5.9975  -1.5596  -0.4415
 O  -4.9172  -2.7373   1.0050
 H   3.5694  -2.9750   1.9712
 H   1.9879  -3.3937   1.2758
 N   3.5093  -3.0828  -0.1244
 H   1.7351  -3.6415  -1.0962
 H   3.0414  -3.0783  -2.1626
 H   5.1708  -2.4724  -1.2543
 H   5.3304  -2.2665   0.5043
 H   0.1908   2.9623  -1.5918
 H   1.1671   2.5605  -0.2598
 O   1.3705   3.7359  -0.9088

r1-TS7-83
Final geometry with  54 atoms:
 O   0.4944   1.6612  -1.9483
 C  -1.2587  -1.0082  -0.2728
 H  -1.0940  -1.4642  -1.2550
 H  -0.9673  -1.7338   0.4963
 N  -2.7766  -0.9346  -0.1673
 C  -3.3217  -2.3385  -0.2842
 H  -2.8428  -2.9326   0.5033
 C  -4.8633  -2.2931  -0.1397
 H  -3.0011  -2.7186  -1.2618
 C  -3.3577  -0.1063  -1.2896
 H  -2.9728  -0.5378  -2.2220
 C  -4.9023  -0.1599  -1.2013
 H  -2.9669   0.9117  -1.1601
 C  -3.2225  -0.3772   1.1589
 C  -4.7694  -0.3073   1.1742
 H  -2.8197  -1.0451   1.9282
 H  -2.7627   0.6052   1.2740
 C  -0.4655   0.2928  -0.1352
 C   0.0762   0.4110   1.2489
 O   0.8874   1.4370   1.5906
 O  -0.1673  -0.3844   2.1501
 C   1.0069   2.6868   0.8994
 H   0.2861   2.7843   0.0824
 H   2.0320   2.7849   0.5173
 H   0.8287   3.4783   1.6428
 C   0.5758   0.4056  -1.2887
 H   0.2953  -0.3729  -2.0171
 H  -1.8270   2.4825   1.6791
 C   4.6025  -0.6264  -0.1486
 C   4.3746   0.5975  -0.7787
 C   3.0718   0.9312  -1.1418
 C   2.0043   0.0624  -0.8762
 C   2.2687  -1.1694  -0.2491
 C   3.5613  -1.5211   0.1193
 N   5.9648  -0.9857   0.2361
 H   5.2059   1.2726  -0.9784
 H   2.8781   1.8828  -1.6368
 H   1.4537  -1.8659  -0.0438
 H   3.7707  -2.4722   0.6072
 C  -2.3188   2.9906   0.8150
 H  -2.0755   4.0721   0.9376
 H  -3.4150   2.9053   1.0092
 O   6.1491  -2.0653   0.7853
 O   6.8674  -0.1936  -0.0063
 H  -5.1550  -0.8297   2.0609
 H  -5.0980   0.7399   1.2277
 N  -5.3399  -0.9157  -0.0271
 H  -5.3045   0.8609  -1.1362
 H  -5.3216  -0.6324  -2.1008
 H  -5.3332  -2.7663  -1.0131
 H  -5.1742  -2.8497   0.7555
 H   0.9174   1.5732  -2.8158
 H  -1.2231   1.3665  -0.2719
 O  -1.9342   2.4862  -0.4164

r1-TS7-84
Final geometry with  54 atoms:
 O   1.0429  -3.0904   0.5984
 C   1.3304   0.2188  -1.3068
 H   2.2180   0.6037  -1.8176
 H   0.5987  -0.0180  -2.0909
 N   0.7301   1.4835  -0.6118
 C   0.9530   1.4995   0.8734
 H   2.0180   1.3365   1.0475
 C   0.4594   2.8505   1.4467
 H   0.3937   0.6527   1.2757
 C  -0.7546   1.5864  -0.8653
 H  -1.2065   0.6680  -0.4970
 C  -1.3148   2.8324  -0.1374
 H  -0.8842   1.6374  -1.9529
 C   1.3754   2.7107  -1.2140
 C   0.7071   3.9813  -0.6326
 H   2.4431   2.6546  -0.9736
 H   1.2526   2.6325  -2.3010
 C   1.7100  -1.0077  -0.4922
 C   3.0196  -1.5354  -0.9458
 O   4.1073  -0.7038  -0.9790
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 O   3.2285  -2.6830  -1.3130
 C   4.3153   0.3309  -0.0141
 H   3.8211   1.2706  -0.2991
 H   5.4000   0.5077   0.0147
 H   3.9687   0.0096   0.9775
 C   0.7018  -2.1947  -0.4497
 H   0.7876  -2.7617  -1.3927
 H   2.0305  -1.1788   4.0947
 C  -3.3938  -0.9570  -0.0638
 C  -2.9118  -1.3062  -1.3273
 C  -1.5858  -1.7174  -1.4431
 C  -0.7486  -1.7763  -0.3188
 C  -1.2766  -1.4571   0.9436
 C  -2.5942  -1.0357   1.0814
 N  -4.7747  -0.4946   0.0664
 H  -3.5660  -1.2490  -2.1963
 H  -1.1913  -1.9908  -2.4243
 H  -0.6381  -1.5397   1.8226
 H  -3.0046  -0.7672   2.0540
 C   1.7594  -0.6242   3.1727
 H   2.1676   0.4020   3.2939
 H   0.6522  -0.5276   3.1841
 O  -5.1664  -0.1387   1.1710
 O  -5.4799  -0.4771  -0.9347
 H   1.4800   4.6501  -0.2289
 H   0.1689   4.5234  -1.4227
 N  -0.2362   3.6384   0.4302
 H  -1.8944   3.4436  -0.8433
 H  -1.9888   2.5210   0.6731
 H  -0.2217   2.6624   2.2884
 H   1.3100   3.4351   1.8242
 H   1.4761  -2.5487   1.3140
 H   1.9620  -0.8800   0.8826
 O   2.2559  -1.2737   2.0397

r1-TS7-85
Final geometry with  54 atoms:
 O  -0.1213  -1.2150   1.1904
 C  -1.7448   0.1237  -1.2994
 H  -2.1146   1.0162  -1.8142
 H  -1.5890  -0.6489  -2.0700
 N  -2.9611  -0.3920  -0.5268
 C  -2.8286  -1.8609  -0.1949
 H  -1.9111  -1.9703   0.3906
 C  -4.0801  -2.3083   0.5998
 H  -2.7262  -2.3850  -1.1532
 C  -4.1687  -0.2210  -1.4206
 H  -3.9297  -0.7031  -2.3762
 C  -5.4047  -0.8456  -0.7297
 H  -4.2823   0.8575  -1.5861
 C  -3.2017   0.3668   0.7484
 C  -4.5456  -0.0987   1.3622
 H  -2.3508   0.1521   1.3945
 H  -3.2005   1.4330   0.4991
 C  -0.4358   0.4453  -0.5769
 C   0.3196   1.3421  -1.4757
 O  -0.2227   2.5630  -1.7804
 O   1.3884   1.1018  -2.0190
 C  -1.0430   3.2794  -0.8572
 H  -2.0389   2.8300  -0.7395
 H  -1.1616   4.2878  -1.2775
 H  -0.5516   3.3497   0.1229
 C   0.3377  -0.8111  -0.1112
 H   0.1110  -1.6596  -0.7793
 H  -0.6619   2.6231   3.4664
 C   4.6276  -0.5490   0.1377
 C   3.8477   0.3080   0.9225
 C   2.4640   0.2300   0.8276
 C   1.8529  -0.6875  -0.0470
 C   2.6624  -1.5386  -0.8143
 C   4.0501  -1.4780  -0.7315
 N   6.0806  -0.4743   0.2321
 H   4.3278   1.0216   1.5913
 H   1.8365   0.8914   1.4282
 H   2.1964  -2.2564  -1.4934
 H   4.6835  -2.1350  -1.3265
 C  -1.1919   2.1343   2.6234
 H  -1.6386   2.9508   2.0196
 H  -2.0385   1.5694   3.0692
 O   6.7519  -1.2326  -0.4592
 O   6.5756   0.3448   0.9988
 H  -4.3903  -0.3731   2.4149
 H  -5.2823   0.7161   1.3298
 N  -5.0883  -1.2492   0.6391
 H  -6.2248  -0.1141  -0.7130
 H  -5.7486  -1.7279  -1.2873
 H  -4.5144  -3.2048   0.1353
 H  -3.8006  -2.5639   1.6316
 H  -0.2127  -0.3785   1.7173
 H  -0.5334   1.1125   0.6880
 O  -0.3187   1.3297   1.8854

r1-TS7-86
Final geometry with  54 atoms:
 O  -0.1634  -1.6573  -0.0567
 C  -1.8656   0.6331  -1.1512
 H  -2.2529   1.6504  -1.2403
 H  -1.8168   0.2250  -2.1730
 N  -3.0142  -0.1481  -0.4986
 C  -3.1013  -1.5534  -1.0513
 H  -2.1130  -2.0047  -0.9268
 C  -4.2087  -2.3180  -0.2888
 H  -3.3249  -1.4480  -2.1202
 C  -4.3090   0.5542  -0.8395
 H  -4.3131   0.7160  -1.9244
 C  -5.4956  -0.3171  -0.3640
 H  -4.2742   1.5269  -0.3336
 C  -2.8973  -0.2293   0.9999
 C  -4.2055  -0.8259   1.5679
 H  -2.0326  -0.8644   1.1956
 H  -2.6850   0.7765   1.3733
 C  -0.4764   0.6714  -0.5099
 C   0.1802   1.9063  -1.0046
 O  -0.3855   3.1204  -0.7556
 O   1.2150   1.9389  -1.6588
 C  -1.2882   3.3878   0.3249
 H  -2.3326   3.1836   0.0418
 H  -1.1922   4.4622   0.5367
 H  -1.0223   2.8062   1.2166
 C   0.3611  -0.5693  -0.8405
 H   0.2454  -0.8227  -1.9119
 H   0.3313   0.1457   3.8868
 C   4.5810  -0.5136  -0.0090
 C   3.7081   0.0821   0.9079
 C   2.3458   0.0925   0.6315
 C   1.8524  -0.4792  -0.5551
 C   2.7530  -1.0698  -1.4546
 C   4.1203  -1.0929  -1.1930
 N   6.0127  -0.5271   0.2773
 H   4.1014   0.5319   1.8191
 H   1.6477   0.5713   1.3238
 H   2.3776  -1.5154  -2.3790
 H   4.8232  -1.5473  -1.8902
 C  -0.3069  -0.0280   2.9914
 H  -1.3295  -0.2352   3.3869
 H   0.0482  -0.9826   2.5445
 O   6.7660  -1.0558  -0.5323
 O   6.4046  -0.0094   1.3167
 H  -3.9580  -1.6055   2.3024
 H  -4.7904  -0.0513   2.0837
 N  -5.0298  -1.3998   0.5025
 H  -6.2129   0.3103   0.1840
 H  -6.0196  -0.7554  -1.2249
 H  -4.8451  -2.8545  -1.0071
 H  -3.7641  -3.0606   0.3888
 H   0.2628  -2.4769  -0.3523
 H  -0.4437   0.7977   0.8686
 O  -0.2590   1.0458   2.1106

r1-TS7-87
Final geometry with  54 atoms:
 O   0.8160  -3.3169  -0.1144
 C   1.5710   0.2583  -1.2568
 H   2.5632   0.6144  -1.5465
 H   1.0215   0.0913  -2.1945
 N   0.8877   1.5130  -0.6481
 C   0.9032   1.5288   0.8550
 H   1.9503   1.4942   1.1621
 C   0.1839   2.8066   1.3565
 H   0.4080   0.6159   1.1851
 C  -0.5490   1.6216  -1.1013
 H  -1.0714   0.7666  -0.6760
 C  -1.1487   2.9610  -0.6081
 H  -0.5489   1.5347  -2.1937
 C   1.6238   2.7357  -1.1490
 C   0.9835   4.0075  -0.5393
 H   2.6725   2.6195  -0.8519
 H   1.5596   2.7123  -2.2440
 C   1.6947  -1.0417  -0.4621
 C   3.0341  -1.6380  -0.6924
 O   4.1594  -0.9117  -0.4835
 O   3.2237  -2.7956  -1.0660
 C   4.2388   0.1436   0.4804
 H   3.9420   1.1113   0.0522
 H   5.2944   0.2027   0.7794
 H   3.6216  -0.0920   1.3551
 C   0.6180  -2.1065  -0.8345
 H   0.6947  -2.3061  -1.9219
 H   1.9589  -0.9644   4.1667
 C  -3.4098  -0.9003   0.0099
 C  -3.0413  -1.1264  -1.3171
 C  -1.7322  -1.5237  -1.5842
 C  -0.8050  -1.6838  -0.5458
 C  -1.2144  -1.4797   0.7839
 C  -2.5152  -1.0799   1.0700
 N  -4.7760  -0.4615   0.3012
 H  -3.7669  -0.9886  -2.1177
 H  -1.4228  -1.6971  -2.6170
 H  -0.4839  -1.6221   1.5830
 H  -2.8400  -0.9027   2.0946
 C   1.7436  -0.4623   3.1947
 H   2.5275   0.3275   3.0946
 H   0.7846   0.0890   3.3533
 O  -5.0833  -0.2563   1.4684
 O  -5.5519  -0.3153  -0.6344
 H   1.7083   4.5151   0.1123
 H   0.7020   4.7039  -1.3412
 N  -0.2026   3.6749   0.2456
 H  -1.4065   3.5999  -1.4642
 H  -2.0694   2.7632  -0.0417
 H  -0.7191   2.5293   1.9180
 H   0.8478   3.3611   2.0341
 H   1.7254  -3.5859  -0.3442
 H   1.6829  -1.0056   0.8780
 O   1.7143  -1.3662   2.1469

r1_MA.1S
Final geometry with  18 atoms:
 C   2.7003  -1.2013   0.1397
 O   2.0803   0.0789   0.4223
 C   0.8840   0.3106  -0.1350
 O   0.3220  -0.5105  -0.8608
 C   0.3616   1.6430   0.2301
 C  -0.7889   2.1069  -0.2714
 H   0.9645   2.2245   0.9212
 H   3.6427  -1.1889   0.6862
 H   2.0605  -2.0136   0.4931
 H   2.8790  -1.3023  -0.9337
 H  -1.1609   3.0892   0.0045
 H  -1.3837   1.5220  -0.9677
 H  -1.5154  -0.8190  -0.7588
 O  -2.4349  -1.0686  -0.5438
 C  -2.6607  -0.7645   0.8378
 H  -2.6914   0.3191   1.0134
 H  -3.6283  -1.1929   1.1148
 H  -1.8850  -1.2044   1.4785

r1_MA.2S
Final geometry with  24 atoms:
 C   1.7173   2.4792   0.1830
 C   2.3050   1.2772   0.1470
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 C   1.5257   0.0383  -0.0370
 O   0.3065  -0.0237  -0.2169
 O   2.2983  -1.0503   0.0117
 C   1.6472  -2.3355  -0.1708
 H   3.3785   1.1571   0.2586
 H   2.4550  -3.0664  -0.1603
 H   0.9507  -2.5205   0.6498
 H   1.1208  -2.3548  -1.1276
 H   2.3063   3.3808   0.3235
 H   0.6422   2.5940   0.0739
 H  -0.9608  -1.1020   0.6922
 H  -1.0031   1.1895  -0.7276
 O  -1.7597  -1.6190   0.9020
 O  -1.7600   1.7937  -0.8493
 C  -2.3885  -1.9413  -0.3448
 H  -1.7520  -2.5922  -0.9591
 H  -3.3165  -2.4729  -0.1159
 H  -2.6315  -1.0377  -0.9189
 C  -2.4589   1.8682   0.3995
 H  -2.9534   0.9192   0.6433
 H  -1.7833   2.1368   1.2226
 H  -3.2203   2.6477   0.3035

r1_MA.3S
Final geometry with  30 atoms:
 C   0.7727   2.6113  -0.0746
 C  -0.3000   1.8661   0.2173
 C  -0.1951   0.6263   1.0102
 O   0.8479   0.0889   1.3860
 O  -1.4026   0.1196   1.3007
 C  -1.4535  -1.0752   2.1250
 H  -2.5144  -1.2928   2.2404
 H  -0.9417  -1.9018   1.6292
 H  -0.9928  -0.8709   3.0942
 H   0.6699   3.5241  -0.6541
 H   1.7695   2.3393   0.2597
 H  -1.2988   2.1468  -0.1023
 C   3.2336   0.1508  -1.2723
 H   4.2007   0.3419  -1.7465
 H   2.9074  -0.8634  -1.5336
 H   2.5040   0.8730  -1.6616
 H   2.5458   0.2204   0.5758
 O   3.4163   0.2961   0.1412
 C   0.1566  -1.9228  -1.1175
 H  -0.8614  -1.9345  -0.7103
 H   0.4032  -0.9048  -1.4423
 H   0.1944  -2.5862  -1.9857
 H   1.1429  -1.7843   0.5731
 O   1.1072  -2.4167  -0.1641
 C  -2.7634   0.1051  -1.9941
 H  -2.5643  -0.9714  -2.0696
 H  -3.4191   0.3981  -2.8189
 H  -1.8168   0.6520  -2.0862
 H  -2.8320   0.2829  -0.0345
 O  -3.4440   0.4322  -0.7751

r1_MA.4S
Final geometry with  36 atoms:
 C  -0.1917  -2.4706   2.4348
 C  -0.8293  -1.9344   1.3876
 C  -0.0954  -1.1923   0.3470
 O   1.1214  -1.0029   0.3271
 O  -0.9196  -0.7131  -0.5960
 C  -0.3353   0.0296  -1.7011
 H  -1.1846   0.3879  -2.2804
 H   0.2566   0.8629  -1.3210
 H   0.2831  -0.6408  -2.3022
 H  -0.7360  -3.0122   3.2026
 H   0.8854  -2.3787   2.5484
 H  -1.9047  -2.0142   1.2605
 C   4.2549  -1.0579  -0.8467
 H   5.1563  -0.8970  -1.4450
 H   4.3524  -0.5008   0.0938
 H   4.1705  -2.1290  -0.6181
 H   2.3417  -0.6963  -1.0638
 O   3.1380  -0.5971  -1.6176
 C   3.0957   2.1872   0.5673
 H   3.4087   1.9253  -0.4509
 H   3.2067   3.2664   0.7050
 H   3.7461   1.6730   1.2868
 H   1.5849   0.9197   0.6566
 O   1.7139   1.8741   0.7900
 C  -1.7492   2.8252   0.3390
 H  -1.4515   3.7008   0.9219
 H  -1.0781   2.7301  -0.5227
 H  -2.7767   2.9716  -0.0184
 H  -1.8481   0.8951   0.6910
 O  -1.6537   1.6889   1.2097
 C  -4.1526   0.2128  -0.8716
 H  -3.5213   0.9226  -1.4207
 H  -5.1816   0.3096  -1.2284
 H  -4.1272   0.4606   0.1975
 H  -2.8033  -1.2108  -0.8770
 O  -3.7452  -1.1427  -1.1074

r1_MeO.1S
Final geometry with  11 atoms:
 C  -1.7749   0.5310   0.1586
 H  -1.5771   0.6764   1.2328
 H  -2.8632   0.4945   0.0204
 H  -1.3981   1.4184  -0.3759
 O  -1.1976  -0.6720  -0.3295
 H  -0.1693  -0.6819  -0.0445
 O   1.2004  -0.6701   0.3379
 C   1.7882   0.5085  -0.1557
 H   1.5315   1.4043   0.4461
 H   2.8936   0.4509  -0.1674
 H   1.4808   0.7373  -1.1967

r1_MeO.2S
Final geometry with  17 atoms:
 C  -1.1246   1.9105   0.2687
 H  -2.2045   1.7598   0.0844
 H  -0.9399   2.9980   0.1953
 H  -0.9423   1.6292   1.3240
 O  -0.3252   1.1748  -0.6303
 H   0.9769   0.7771   0.0615
 O   1.8452   0.4626   0.5174
 C   2.3142  -0.6816  -0.1906
 H   2.4683  -0.4657  -1.2590
 H   3.2759  -0.9889   0.2363
 H   1.6173  -1.5294  -0.1115
 H  -0.9037  -0.2245  -0.7369
 O  -1.2777  -1.1867  -0.7448
 C  -1.3711  -1.6164   0.6105
 H  -2.1994  -1.1220   1.1416
 H  -1.5543  -2.6972   0.6273
 H  -0.4433  -1.4181   1.1669

r1_MeO.3S
Final geometry with  23 atoms:
 C  -0.5705   0.1990   1.8588
 H  -1.0605   1.1863   1.7916
 H   0.3372   0.3301   2.4736
 H  -1.2516  -0.4615   2.4233
 O  -0.2662  -0.3270   0.5827
 H   1.1091  -1.0746   0.5682
 O   2.0177  -1.5262   0.4923
 C   2.3987  -1.4839  -0.8819
 H   2.5549  -0.4535  -1.2331
 H   3.3396  -2.0332  -0.9983
 H   1.6430  -1.9555  -1.5277
 H  -1.5652  -0.8386  -0.1019
 O  -2.4451  -1.0976  -0.5479
 C  -3.2388   0.0850  -0.6243
 H  -2.7042   0.9022  -1.1308
 H  -4.1448  -0.1392  -1.1984
 H  -3.5437   0.4384   0.3725
 H   0.1722   0.8661  -0.3334
 O   0.5142   1.6598  -0.8713
 C   1.5710   2.2506  -0.1172
 H   2.0886   2.9788  -0.7516
 H   1.1938   2.7775   0.7723
 H   2.3035   1.5004   0.2143

r1_MeO.4S
Final geometry with  29 atoms:
 C   0.3415  -0.5374   1.7525
 H   0.1718  -1.5991   1.9992
 H  -0.3162   0.0594   2.4071
 H   1.3817  -0.3010   2.0316
 O   0.0942  -0.2748   0.3816
 H  -1.0212   0.9190   0.3097
 O  -1.7033   1.6470   0.2002
 C  -1.8264   1.8848  -1.2009
 H  -2.1283   0.9760  -1.7421
 H  -2.5957   2.6490  -1.3535
 H  -0.8841   2.2484  -1.6363
 H   1.0358  -1.3422  -0.4532
 O   1.6379  -1.9970  -0.9163
 C   2.9606  -1.8102  -0.4100
 H   3.0228  -2.0462   0.6624
 H   3.6305  -2.4879  -0.9499
 H   3.3122  -0.7804  -0.5612
 H  -1.1144  -1.2569  -0.1274
 O  -1.8511  -1.8841  -0.3953
 C  -3.0410  -1.4896   0.2880
 H  -3.7908  -2.2762   0.1498
 H  -2.8664  -1.3642   1.3661
 H  -3.4480  -0.5487  -0.1079
 H   1.1414   0.8717  -0.1378
 O   1.7945   1.5863  -0.4048
 C   1.5801   2.7159   0.4414
 H   1.6508   2.4459   1.5049
 H   2.3552   3.4580   0.2221
 H   0.5979   3.1766   0.2671

r1_3
Final geometry with  32 atoms:
 C  -4.6967   0.7956   0.2348
 O  -3.6179  -0.0047   0.7350
 C  -2.5425  -0.2367  -0.1378
 O  -2.5725   0.3030  -1.2847
 C  -1.5696  -1.0645   0.4070
 C  -0.3727  -1.4483  -0.3503
 N   0.9089  -0.5383  -0.1246
 C   1.3349  -0.5807   1.3208
 C   0.6261   0.8926  -0.5100
 C   2.0437  -1.0487  -0.9781
 H  -1.7076  -1.4399   1.4151
 H  -5.4181   0.8618   1.0526
 H  -4.3595   1.8016  -0.0372
 H  -5.1729   0.3292  -0.6348
 H  -0.0002  -2.4412  -0.0845
 H  -0.5186  -1.3941  -1.4325
 H   0.2407   0.8793  -1.5301
 H  -0.1585   1.2470   0.1587
 C   1.9400   1.7123  -0.3831
 H   1.7287  -0.9396  -2.0179
 C   3.3225  -0.2264  -0.6579
 H   2.1674  -2.1102  -0.7536
 C   2.5339   0.3866   1.5199
 H   0.4681  -0.2966   1.9185
 H   1.5953  -1.6187   1.5401
 H   2.2392   1.2341   2.1445
 H   3.3536  -0.1356   2.0201
 H   4.0655  -0.8569  -0.1626
 H   3.7619   0.1538  -1.5838
 N   3.0162   0.9107   0.2288
 H   2.2763   2.0434  -1.3692
 H   1.7679   2.5994   0.2321

r1_3.1S
Final geometry with  38 atoms:
 C  -4.3958  -1.2214   0.8738
 O  -3.2254  -1.7546   0.2382
 C  -2.2880  -0.8335  -0.2402
 O  -2.5237   0.4032  -0.0403
 C  -1.2123  -1.4223  -0.8828
 C  -0.1212  -0.6291  -1.4654
 N   1.1396  -0.4096  -0.5341
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 C   1.8184  -1.7250  -0.2474
 C   0.7414   0.2325   0.7720
 C   2.1216   0.4995  -1.2317
 H  -1.1826  -2.5040  -0.9542
 H  -4.9922  -2.0894   1.1638
 H  -4.1385  -0.6397   1.7653
 H  -4.9733  -0.5930   0.1874
 H   0.3199  -1.0986  -2.3486
 H  -0.4220   0.3901  -1.7154
 H   0.1834   1.1337   0.5235
 H   0.0782  -0.4698   1.2771
 C   2.0259   0.5397   1.5891
 H   1.6223   1.4625  -1.3556
 C   3.4082   0.6067  -0.3676
 H   2.3183   0.0715  -2.2169
 C   2.9929  -1.4785   0.7387
 H   1.0624  -2.3942   0.1654
 H   2.1578  -2.1184  -1.2081
 H   2.7768  -1.9334   1.7089
 H   3.9074  -1.9316   0.3472
 H   4.2474   0.1207  -0.8720
 H   3.6655   1.6580  -0.2145
 N   3.2220  -0.0369   0.9462
 H   2.1703   1.6200   1.6751
 H   1.9341   0.1282   2.5977
 H  -1.7341   1.8169  -0.5757
 O  -1.3417   2.7049  -0.7733
 C  -1.4741   3.5084   0.4017
 H  -0.9419   3.0690   1.2575
 H  -1.0380   4.4896   0.1895
 H  -2.5281   3.6475   0.6803

r1_3.2S
Final geometry with  44 atoms:
 N   3.4171   0.5736   0.9352
 C   2.0725   0.8912   1.4543
 C   3.5188   1.0770  -0.4473
 C   3.5774  -0.8925   0.9155
 N   1.6024  -0.5087  -0.5480
 C   0.9663   0.3780   0.4952
 C   2.5325   0.3327  -1.3884
 C   2.4127  -1.5748   0.1473
 H   1.9688   0.4305   2.4402
 H   1.9832   1.9739   1.5744
 H   3.3012   2.1481  -0.4391
 H   4.5438   0.9405  -0.8018
 H   4.5346  -1.1263   0.4419
 H   3.6081  -1.2603   1.9444
 H   0.2142  -0.2195   1.0082
 H   0.4713   1.1855  -0.0434
 H   1.9131   1.0214  -1.9662
 H   3.0427  -0.3481  -2.0729
 H   2.7681  -2.2650  -0.6203
 H   1.7284  -2.1045   0.8110
 C   0.5068  -1.1588  -1.4733
 C  -0.4734  -2.0162  -0.7864
 C  -1.6847  -1.5287  -0.3402
 O  -2.1438  -0.3356  -0.4382
 O  -2.4891  -2.4764   0.2878
 C  -3.8038  -2.0583   0.6885
 H  -4.2776  -2.9500   1.1043
 H  -3.7602  -1.2769   1.4533
 H  -4.3855  -1.6982  -0.1664
 H   1.1035  -1.7069  -2.2067
 H   0.0492  -0.2976  -1.9633
 H  -0.2425  -3.0624  -0.6194
 C  -2.5945   2.6958  -1.6697
 H  -2.9647   2.8516  -0.6474
 H  -2.3839   3.6718  -2.1179
 H  -3.3833   2.2052  -2.2572
 H  -1.5733   1.0616  -1.2655
 O  -1.3819   1.9371  -1.6817
 C  -1.5932   2.1293   1.9749
 H  -1.2478   2.6203   1.0565
 H  -1.9420   2.8983   2.6712
 H  -0.7457   1.6052   2.4369
 H  -2.4564   0.6413   0.9783
 O  -2.6888   1.2445   1.7240

r1_3.3S
Final geometry with  50 atoms:
 N  -3.9786  -0.2016   0.5113
 C  -2.8858   0.2160   1.4121
 C  -3.7921  -1.6276   0.1805
 C  -3.8798   0.5832  -0.7346
 N  -1.6833  -0.5755  -0.6140
 C  -1.5035  -0.1818   0.8336
 C  -2.5057  -1.8410  -0.6623
 C  -2.4451   0.5215  -1.3205
 H  -2.9468   1.2997   1.5449
 H  -3.0252  -0.2547   2.3888
 H  -3.7338  -2.1909   1.1155
 H  -4.6620  -1.9837  -0.3775
 H  -4.6036   0.1827  -1.4493
 H  -4.1471   1.6225  -0.5262
 H  -0.7944   0.6434   0.8579
 H  -1.0673  -1.0445   1.3385
 H  -1.8847  -2.6497  -0.2721
 H  -2.7246  -2.0344  -1.7144
 H  -2.4403   0.2878  -2.3870
 H  -1.8888   1.4447  -1.1547
 C  -0.2959  -0.8198  -1.3093
 C   0.5643   0.3721  -1.3948
 C   1.5094   0.6727  -0.4404
 O   1.8661  -0.0013   0.5883
 O   2.1378   1.9092  -0.6503
 C   3.2066   2.2737   0.2411
 H   3.4873   3.2892  -0.0448
 H   2.8784   2.2608   1.2840
 H   4.0641   1.6056   0.1194
 H  -0.5788  -1.2075  -2.2916
 H   0.1471  -1.6255  -0.7229
 H   0.3969   1.0873  -2.1920
 C   1.8026  -3.4484   0.8625
 H   1.5399  -4.4080   1.3187
 H   1.5029  -3.4746  -0.1945
 H   2.8912  -3.3203   0.9167
 H   1.3403  -1.5497   1.1827
 O   1.1129  -2.4233   1.5830
 C   4.2650  -1.3802  -1.1467
 H   3.4092  -2.0296  -1.3745
 H   4.1734  -0.4589  -1.7386
 H   5.1838  -1.8953  -1.4433
 H   3.5044  -0.6690   0.5060
 O   4.3536  -1.0991   0.2533
 C  -0.0284   3.5139   1.3778
 H  -0.9877   3.8587   1.7745
 H   0.1469   2.4873   1.7219
 H   0.7682   4.1594   1.7715
 H   0.6727   3.1128  -0.4108
 O  -0.1026   3.5856  -0.0521

r1_3.4S
Final geometry with  56 atoms:
 N   4.0556  -0.5329   0.9249
 C   3.0022   0.4057   1.3581
 C   4.6310  -0.0401  -0.3406
 C   3.4377  -1.8498   0.6788
 N   2.2202  -0.3445  -0.8824
 C   1.8141   0.4129   0.3616
 C   3.5203   0.2332  -1.3903
 C   2.4459  -1.7915  -0.5140
 H   2.6489   0.1132   2.3502
 H   3.4427   1.4033   1.4350
 H   5.1890   0.8794  -0.1455
 H   5.3319  -0.7910  -0.7143
 H   4.2240  -2.5800   0.4696
 H   2.9191  -2.1597   1.5898
 H   0.9357  -0.0888   0.7634
 H   1.5367   1.4185   0.0478
 H   3.3478   1.2998  -1.5474
 H   3.7346  -0.2387  -2.3512
 H   2.8342  -2.2847  -1.4077
 H   1.4737  -2.2167  -0.2631
 C   1.1223  -0.2186  -1.9948
 C  -0.2107  -0.7233  -1.6141
 C  -1.1447   0.0940  -1.0257
 O  -1.0617   1.3410  -0.7621
 O  -2.3139  -0.5782  -0.6215
 C  -3.4405   0.2256  -0.2196
 H  -4.2160  -0.4859   0.0679
 H  -3.1873   0.8620   0.6309
 H  -3.7930   0.8394  -1.0541
 H   1.5519  -0.7682  -2.8358
 H   1.1168   0.8491  -2.2280
 H  -0.4459  -1.7723  -1.7510
 C  -1.6040   4.5048  -1.1589
 H  -2.0157   5.5124  -1.0453
 H  -0.6737   4.4394  -0.5790
 H  -1.3684   4.3412  -2.2200
 H  -2.1731   2.6808  -0.7243
 O  -2.5844   3.5748  -0.6891
 C  -0.2018   3.0174   2.1267
 H  -0.8744   3.8192   1.7937
 H   0.0076   3.1585   3.1916
 H   0.7443   3.0958   1.5735
 H  -0.9196   1.5673   1.0064
 O  -0.7999   1.7284   1.9697
 C  -2.2139  -1.5566   2.7360
 H  -1.8164  -1.9038   3.6939
 H  -2.4419  -0.4865   2.8170
 H  -3.1400  -2.1058   2.5204
 H  -1.5591  -1.4868   0.8887
 O  -1.2120  -1.8054   1.7418
 C  -3.4834  -3.7068  -0.1750
 H  -4.2477  -3.1110   0.3412
 H  -3.8917  -4.7028  -0.3697
 H  -2.6072  -3.8058   0.4776
 H  -2.7932  -2.2302  -1.2716
 O  -3.1346  -3.1308  -1.4409

r1_4
Final geometry with  33 atoms:
 C  -4.2151   1.2540   0.0446
 O  -3.2165   0.4244   0.6960
 C  -2.4913  -0.3763  -0.0921
 O  -2.6232  -0.4255  -1.3071
 C  -1.5354  -1.2369   0.7066
 C  -0.2641  -1.6253  -0.0420
 N   0.8559  -0.5986  -0.0065
 C   1.5299  -0.5653   1.3553
 C   0.3756   0.8009  -0.3478
 C   1.9043  -0.9982  -1.0352
 H  -1.3434  -0.7782   1.6778
 H  -4.6886   1.8155   0.8492
 H  -3.7321   1.9302  -0.6649
 H  -4.9464   0.6259  -0.4695
 H   0.1603  -2.5356   0.3833
 H  -0.4883  -1.8014  -1.0957
 H  -0.2188   0.7284  -1.2587
 H  -0.2541   1.1323   0.4787
 C   1.6176   1.7153  -0.5265
 H   1.4362  -0.8716  -2.0131
 C   3.1495  -0.0943  -0.8513
 H   2.1284  -2.0543  -0.8767
 C   2.5617   0.5921   1.3645
 H   0.7595  -0.4310   2.1139
 H   1.9971  -1.5430   1.4869
 H   2.1869   1.4332   1.9531
 H   3.4920   0.2441   1.8202
 H   3.9625  -0.6524  -0.3806
 H   3.4939   0.2521  -1.8289
 N   2.8339   1.0687  -0.0031
 H   1.7748   1.9393  -1.5844
 H   1.4521   2.6575   0.0016
 H  -2.0790  -2.1691   0.9072

r1_5
Final geometry with  48 atoms:
 C  -4.4119  -0.2416   0.2541
 C  -3.5789  -0.8819   1.1826
```

C	-2.3171	-1.2898	0.7724
C	-1.8718	-1.0612	-0.5410
C	-2.7320	-0.4226	-1.4479
C	-4.0039	-0.0078	-1.0628
C	-0.4672	-1.5021	-0.9613
O	-0.1527	-2.7639	-0.5466
N	-5.7343	0.1883	0.6707
O	-6.4668	0.7586	-0.1519
O	-6.0923	-0.0251	1.8390
C	0.5837	-0.4213	-0.3776
C	1.9422	-0.7663	-0.9736
N	3.1595	-0.2994	-0.1934
C	3.3170	-1.0703	1.1058
C	4.4934	-0.4502	1.9034
C	0.1260	0.9692	-0.7275
O	-0.4818	1.5817	0.2999
C	-1.0897	2.8684	0.0276
O	0.2250	1.4748	-1.8408
C	4.3940	-0.5594	-1.0452
C	5.6549	-0.2999	-0.1831
C	3.1138	1.1833	0.1244
C	4.4984	1.6088	0.6812
H	2.0368	-0.3376	-1.9732
H	-1.5347	3.1805	0.9720
H	-0.3294	3.5846	-0.2940
H	-1.8586	2.7635	-0.7419
H	2.0337	-1.8514	-1.0367
H	0.5615	-0.5507	0.7058
H	-0.4108	-1.3733	-2.0630
H	-2.4014	-0.2441	-2.4670
H	-4.6664	0.4844	-1.7645
H	-3.9174	-1.0489	2.1980
H	-1.6607	-1.7917	1.4760
H	2.3764	-1.0073	1.6513
H	3.4992	-2.1087	0.8244
H	2.8578	1.7074	-0.7975
H	2.3217	1.3268	0.8599
H	4.3334	-1.5906	-1.3966
H	4.3240	0.1166	-1.8995
N	5.3075	0.4326	1.0482
H	4.1171	0.1384	2.7439
H	5.1227	-1.2500	2.3016
H	6.1269	-1.2441	0.0998
H	6.3770	0.2830	-0.7604
H	5.0491	2.1855	-0.0660
H	4.3564	2.2390	1.5626

r1_5.1S
Final geometry with 54 atoms:

C	-4.4161	-0.0409	-0.1177
C	-3.5534	0.8702	-0.7429
C	-2.2929	1.0733	-0.1982
C	-1.8820	0.3793	0.9533
C	-2.7701	-0.5227	1.5581
C	-4.0404	-0.7420	1.0319
C	-0.4809	0.6026	1.5228
O	-0.1674	1.9351	1.6617
N	-5.7366	-0.2644	-0.6809
O	-6.4926	-1.0790	-0.1307
O	-6.0676	0.3644	-1.6970
C	0.5718	-0.1418	0.5711
C	1.9365	-0.0415	1.2447
N	3.1448	-0.1602	0.3329
C	3.3121	1.0772	-0.5344
C	4.4753	0.8243	-1.5276
C	0.1290	-1.5697	0.3666
O	-0.4502	-1.7591	-0.8267
C	-1.0197	-3.0681	-1.0788
O	0.2251	-2.4523	1.2120
C	4.3842	-0.2900	1.2066
C	5.6391	-0.1786	0.3064
C	3.0788	-1.3781	-0.5698
C	4.4589	-1.5541	-1.2572
H	2.0423	-0.8240	1.9986
H	-1.4483	-3.0056	-2.0786
H	-0.2380	-3.8311	-1.0425
H	-1.7957	-3.2874	-0.3413
H	2.0251	0.9338	1.7242
H	0.5423	0.3840	-0.3846
H	-0.4332	0.0610	2.4867
H	-2.4628	-1.0639	2.4483
H	-4.7249	-1.4390	1.4999
H	-3.8663	1.3981	-1.6355
H	-1.6111	1.7709	-0.6721
H	2.3699	1.2637	-1.0465
H	3.5141	1.9035	0.1486
H	2.8148	-2.2338	0.0528
H	2.2874	-1.1922	-1.2957
H	4.3362	0.5013	1.9562
H	4.3091	-1.2600	1.7012
N	5.2816	-0.3390	-1.1150
H	4.0862	0.6333	-2.5309
H	5.1132	1.7106	-1.5718
H	6.1173	0.7959	0.4323
H	6.3587	-0.9510	0.5891
H	5.0026	-2.3916	-0.8130
H	4.3096	-1.7682	-2.3183
H	0.2590	2.6910	0.3719
O	0.5195	3.2517	-0.4426
C	-0.3100	4.4112	-0.4472
H	-1.3787	4.1508	-0.4772
H	-0.1363	5.0413	0.4382
H	-0.0770	5.0035	-1.3392

r1_5.2S
Final geometry with 60 atoms:

C	4.5299	-0.2143	0.2071
C	3.6778	0.2810	1.2031
C	2.3948	0.6725	0.8451
C	1.9540	0.5723	-0.4855
C	2.8321	0.0777	-1.4611
C	4.1238	-0.3201	-1.1264
C	0.5274	0.9788	-0.8449
O	0.1649	2.1860	-0.2802
N	5.8749	-0.6290	0.5711
O	6.6274	-1.0641	-0.3127
O	6.2276	-0.5372	1.7559
C	-0.4623	-0.1841	-0.3795
C	-1.8671	0.2058	-0.8285
N	-3.0139	-0.4394	-0.0718
C	-3.1195	0.1003	1.3447
C	-4.2190	-0.6985	2.0908
C	0.0047	-1.4906	-0.9768
O	0.6709	-2.2441	-0.0925
C	1.2823	-3.4584	-0.5963
O	-0.1458	-1.8081	-2.1505
C	-4.3071	-0.0966	-0.7969
C	-5.5020	-0.5544	0.0764
C	-2.8963	-1.9505	-0.0103
C	-4.2269	-2.5253	0.5425
H	-2.0125	-0.0430	-1.8813
H	1.7820	-3.9045	0.2630
H	0.5155	-4.1313	-0.9879
H	2.0060	-3.2145	-1.3778
H	-1.9952	1.2785	-0.6912
H	-0.3817	-0.2370	0.7075
H	0.4573	1.0095	-1.9474
H	2.5015	-0.0017	-2.4926
H	4.8018	-0.7029	-1.8794
H	4.0161	0.3513	2.2297
H	1.7200	1.0559	1.6025
H	-2.1459	-0.0019	1.8202
H	-3.3587	1.1606	1.2505
H	-2.6822	-2.3030	-1.0199
H	-2.0549	-2.1762	0.6451
H	-4.3038	0.9805	-0.9698
H	-4.2674	-0.6166	-1.7555
N	-5.0531	-1.4643	1.1460
H	-3.7684	-1.3999	2.7973
H	-4.8508	-0.0065	2.6532
H	-5.9907	0.3064	0.5395
H	-6.2362	-1.0663	-0.5507
H	-4.8018	-2.9957	-0.2591
H	-4.0069	-3.2855	1.2959
H	-0.2977	2.1887	1.2424
O	-0.5690	2.2619	2.2146
C	0.1929	3.3195	2.7944
H	1.2730	3.1136	2.7594
H	0.0090	4.2786	2.2882
H	-0.1028	3.4228	3.8441
H	-0.2997	3.2061	-1.3772
O	-0.5997	3.8588	-2.0954
C	-1.9555	3.5715	-2.4296
H	-2.3012	4.3237	-3.1472
H	-2.0623	2.5801	-2.8940
H	-2.6120	3.6129	-1.5479

r1_5.3S
Final geometry with 66 atoms:

C	5.0753	-0.6797	0.3528
C	4.2290	-0.1887	1.3558
C	3.0303	0.4042	0.9824
C	2.6676	0.5079	-0.3713
C	3.5394	0.0136	-1.3526
C	4.7473	-0.5838	-1.0026
C	1.3280	1.1303	-0.7548
O	1.0801	2.3074	-0.0765
N	6.3303	-1.3082	0.7323
O	7.0719	-1.7493	-0.1575
O	6.6191	-1.3859	1.9352
C	0.1761	0.0591	-0.4772
C	-1.1348	0.6715	-0.9586
N	-2.4084	0.0847	-0.3766
C	-2.5650	0.4432	1.0923
C	-3.8025	-0.3031	1.6477
C	0.5232	-1.2252	-1.1925
O	1.0075	-2.1562	-0.3610
C	1.4847	-3.3865	-0.9624
O	0.4333	-1.3876	-2.4035
C	-3.5866	0.6839	-1.1324
C	-4.8951	0.2825	-0.4113
C	-2.4741	-1.4244	-0.5200
C	-3.9055	-1.8917	-0.1542
H	-1.2215	0.5787	-2.0426
H	1.8395	-3.9928	-0.1295
H	0.6681	-3.8903	-1.4852
H	2.3013	-3.1705	-1.6555
H	-1.1490	1.7251	-0.6846
H	0.1731	-0.1175	0.5996
H	1.3347	1.2862	-1.8488
H	3.2685	0.0913	-2.4015
H	5.4202	-0.9669	-1.7601
H	4.5060	-0.2774	2.3993
H	2.3612	0.7878	1.7449
H	-1.6521	0.1580	1.6113
H	-2.6740	1.5278	1.1321
H	-2.2126	-1.6683	-1.5500
H	-1.7291	-1.8401	0.1588
H	-3.4398	1.7645	-1.1564
H	-3.5317	0.2899	-2.1485
N	-4.6376	-0.8156	0.5424
H	-3.4992	-1.1511	2.2662
H	-4.3983	0.3756	2.2627
H	-5.3097	1.1269	0.1443
H	-5.6362	-0.0455	-1.1437
H	-4.4676	-2.1614	-1.0515
H	-3.8530	-2.7679	0.4961
H	0.4783	2.2022	1.3895
O	0.1322	2.2010	2.3409
C	0.9678	3.0723	3.1007
H	2.0177	2.7442	3.0914
H	0.9273	4.1055	2.7251
H	0.6167	3.0702	4.1383
H	0.7306	3.4847	-1.0517
O	0.5221	4.2533	-1.6825
C	-0.8447	4.1638	-2.0779
H	-1.0830	5.0368	-2.6956
H	-1.0414	3.2597	-2.6724
H	-1.5222	4.1638	-1.2113
H	-6.1669	-1.4214	1.1746
O	-7.0537	-1.7507	1.4930

```
 C  -8.0115  -1.4863   0.4643
 H  -8.9788  -1.8781   0.7943
 H  -8.1205  -0.4087   0.2770
 H  -7.7412  -1.9819  -0.4789

r1_5.4S
Final geometry with  72 atoms:
 C   4.3222  -1.0421  -0.4501
 C   3.3959  -2.0901  -0.5379
 C   2.1250  -1.8989  -0.0122
 C   1.7722  -0.6812   0.5929
 C   2.7243   0.3452   0.6757
 C   4.0042   0.1775   0.1542
 C   0.3583  -0.4716   1.1232
 O  -0.0772  -1.5160   1.9147
 N   5.6533  -1.2283  -1.0056
 O   6.4662  -0.2954  -0.9366
 O   5.9335  -2.3145  -1.5330
 C  -0.6221  -0.2476  -0.1170
 C  -1.9909   0.1120   0.4522
 N  -3.1804  -0.0817  -0.4689
 C  -3.4341  -1.5505  -0.7652
 C  -4.5802  -1.6471  -1.8055
 C  -0.0331   0.8263  -0.9934
 O   0.4862   0.3508  -2.1220
 C   1.1929   1.2857  -2.9810
 O   0.0295   2.0156  -0.6774
 C  -4.4081   0.4722   0.2412
 C  -5.6676   0.0939  -0.5762
 C  -3.0265   0.6585  -1.7841
 C  -4.3886   0.6267  -2.5281
 H  -2.0138   1.1561   0.7665
 H   1.4594   0.7101  -3.8664
 H   0.5406   2.1214  -3.2435
 H   2.0898   1.6465  -2.4727
 H  -2.1827  -0.5233   1.3164
 H  -0.6446  -1.1871  -0.6703
 H   0.3544   0.4819   1.6761
 H   2.4623   1.2868   1.1473
 H   4.7375   0.9726   0.2130
 H   3.6681  -3.0245  -1.0133
 H   1.3920  -2.6960  -0.0758
 H  -2.5099  -1.9875  -1.1388
 H  -3.6889  -2.0149   0.1886
 H  -2.7035   1.6746  -1.5530
 H  -2.2484   0.1442  -2.3487
 H  -4.4183   0.0474   1.2457
 H  -4.2603   1.5515   0.3083
 N  -5.2980  -0.3654  -1.9274
 H  -4.1816  -1.9118  -2.7881
 H  -5.2811  -2.4281  -1.5006
 H  -6.2201  -0.7077  -0.0801
 H  -6.3248   0.9635  -0.6555
 H  -4.8701   1.6066  -2.4830
 H  -4.2214   0.3756  -3.5783
 H  -0.6785  -2.7901   1.1682
 O  -1.0412  -3.6330   0.7434
 C  -0.3341  -4.7364   1.3069
 H   0.7474  -4.6697   1.1173
 H  -0.4892  -4.8074   2.3937
 H  -0.7075  -5.6573   0.8460
 H  -0.3680  -0.9051   3.3501
 O  -0.5365  -0.4509   4.2392
 C  -1.6924   0.3759   4.1080
 H  -1.8624   0.8815   5.0649
 H  -1.5634   1.1429   3.3328
 H  -2.5902  -0.2129   3.8685
 H   1.7241   2.9250  -0.5071
 O   2.4165   3.5908  -0.3506
 C   1.8001   4.8809  -0.4529
 H   1.0083   5.0095   0.2962
 H   2.5780   5.6291  -0.2767
 H   1.3745   5.0434  -1.4523
 H  -0.3327   2.7214   1.0260
 O  -0.5527   3.2194   1.8364
 C   0.5613   3.1659   2.7362
 H   0.7391   2.1473   3.1043
 H   1.4784   3.5411   2.2655
 H   0.3183   3.8044   3.5904

r1_9
Final geometry with  49 atoms:
 C  -4.4272  -0.2225   0.2400
 C  -3.6032  -0.8375   1.1889
 C  -2.3296  -1.2373   0.8020
 C  -1.8849  -1.0292  -0.5124
 C  -2.7339  -0.4170  -1.4441
 C  -4.0123  -0.0053  -1.0757
 C  -0.4747  -1.4269  -0.9130
 O  -0.1082  -2.6984  -0.3750
 N  -5.7656   0.2031   0.6375
 O  -6.4872   0.7557  -0.2022
 O  -6.1321  -0.0024   1.8015
 C   0.5809  -0.4187  -0.3667
 C   1.9425  -0.7591  -0.9846
 N   3.1562  -0.2966  -0.2058
 C   3.3248  -1.0797   1.0866
 C   4.5034  -0.4605   1.8818
 C   0.1261   0.9910  -0.7181
 O  -0.4203   1.6162   0.3250
 C  -0.9749   2.9357   0.0792
 O   0.2153   1.4771  -1.8358
 C   4.3879  -0.5459  -1.0690
 C   5.6523  -0.2926  -0.2104
 C   3.1091   1.1847   0.1258
 C   4.4978   1.6075   0.6746
 H   2.0199  -0.3136  -1.9781
 H  -1.3759   3.2590   1.0389
 H  -0.1878   3.6133  -0.2599
 H  -1.7684   2.8696  -0.6690
 H   2.0445  -1.8405  -1.0725
 H   0.5841  -0.5275   0.7200
 H  -0.4048  -1.4431  -2.0077
 H  -2.3945  -0.2567  -2.4629
 H  -4.6727   0.4680  -1.7918
 H  -3.9519  -0.9923   2.2025
 H  -1.6742  -1.7127   1.5240
 H   2.3890  -1.0255   1.6410
 H   3.5102  -2.1145   0.7937
 H   2.8450   1.7167  -0.7893
 H   2.3256   1.3199   0.8720
 H   4.3275  -1.5739  -1.4295
 H   4.3106   0.1390  -1.9154
 N   5.3098   0.4298   1.0278
 H   4.1289   0.1216   2.7275
 H   5.1366  -1.2613   2.2715
 H   6.1259  -1.2387   0.0627
 H   6.3707   0.2953  -0.7870
 H   5.0419   2.1893  -0.0735
 H   4.3608   2.2320   1.5606
 H  -0.6374  -3.3832  -0.8125

(b) Structures in reaction II.

r2_DABCO
Final geometry with  20 atoms:
 N  -1.2896   0.0001  -0.0001
 C  -0.7822   1.3841  -0.1131
 C  -0.7821  -0.7899  -1.1421
 C  -0.7824  -0.5941   1.2549
 N   1.2896   0.0000   0.0002
 C   0.7823   1.3841  -0.1128
 C   0.7823  -0.7898  -1.1420
 C   0.7821  -0.5943   1.2550
 H  -1.1809   1.9631   0.7274
 H  -1.1803   1.8188  -1.0367
 H  -1.1801  -0.3512  -2.0639
 H  -1.1804  -1.8071  -1.0571
 H  -1.1807  -1.6117   1.3355
 H  -1.1809  -0.0122   2.0934
 H   1.1806   1.9630   0.7280
 H   1.1807   1.8190  -1.0362
 H   1.1804  -0.3509  -2.0636
 H   1.1808  -1.8070  -1.0571
 H   1.1802  -1.6119   1.3355
 H   1.1806  -0.0126   2.0936

r2_MA
Final geometry with  12 atoms:
 C   2.5028  -0.0212   0.0001
 C   1.3186  -0.6427  -0.0001
 C   0.0454   0.1203  -0.0002
 O  -1.0139  -0.7153   0.0000
 O  -0.0588   1.3371  -0.0001
 C  -2.3203  -0.0972   0.0002
 H  -3.0323  -0.9227   0.0004
 H  -2.4514   0.5193  -0.8932
 H  -2.4511   0.5195   0.8935
 H   3.4323  -0.5828   0.0002
 H   2.5669   1.0639   0.0000
 H   1.2387  -1.7260  -0.0000

r2_pNBA
Final geometry with  16 atoms:
 C   3.1852   0.3427   0.0000
 H   3.5625   1.3839   0.0000
 C   1.7068   0.2084   0.0000
 C   0.9213   1.3702  -0.0000
 C  -0.4687   1.2793  -0.0000
 C  -1.0462   0.0092  -0.0000
 C  -0.2869  -1.1659   0.0000
 C   1.0986  -1.0582   0.0000
 H   1.3977   2.3464  -0.0000
 H  -1.0903   2.1658  -0.0000
 H  -0.7745  -2.1327   0.0000
 H   1.7181  -1.9489   0.0000
 N  -2.5162  -0.0976  -0.0000
 O  -3.1750   0.9459  -0.0000
 O  -3.0174  -1.2251  -0.0000
 O   3.9598  -0.6014   0.0000

r2_THF
Final geometry with  13 atoms:
 C   1.1727   0.4245   0.1343
 O  -0.0000   1.2577  -0.0001
 C  -1.1727   0.4245  -0.1342
 C  -0.7319  -0.9947   0.2330
 C   0.7319  -0.9947  -0.2331
 H   1.9571   0.8211  -0.5197
 H   1.5277   0.4734   1.1743
 H  -1.9570   0.8210   0.5200
 H  -1.5280   0.4734  -1.1742
 H  -0.7857  -1.1432   1.3181
 H  -1.3442  -1.7612  -0.2513
 H   1.3443  -1.7611   0.2512
 H   0.7858  -1.1431  -1.3182

r2_TS1
Final geometry with  32 atoms:
 N  -3.0374   0.9398   0.1774
 C  -1.8999   1.7452  -0.3063
 C  -3.3087  -0.1387  -0.7911
 C  -2.6730   0.3398   1.4741
 N  -0.9660  -0.5388  -0.0935
 C  -0.6316   0.8557  -0.4879
 C  -2.0539  -1.0552  -0.9633
 C  -1.4092  -0.5638   1.3248
 H  -1.7135   2.5450   0.4166
 H  -2.1825   2.2079  -1.2565
 H  -3.5857   0.3167  -1.7464
 H  -4.1635  -0.7196  -0.4322
 H  -3.5233  -0.2454   1.8366
 H  -2.4890   1.1475   2.1887
 H   0.2027   1.1771   0.1391
 H  -0.2855   0.8281  -1.5229
 H  -1.6835  -1.0551  -1.9920
 H  -2.2549  -2.0883  -0.6659
 H  -1.6166  -1.6053   1.5864
 H  -0.5705  -0.2147   1.9325
 C   0.5484  -1.6051  -0.2739
 C   1.6723  -1.1615   0.4490
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```
 C    2.6048   -0.2580   -0.1392
 O    3.6349    0.0684    0.7274
 O    2.5828    0.2178   -1.2861
 C    4.6415    0.9427    0.2046
 H    5.3592    1.0875    1.0154
 H    4.2174    1.9080   -0.0919
 H    5.1454    0.4990   -0.6607
 H    0.0576   -2.5164    0.0657
 H    0.6029   -1.5175   -1.3584
 H    1.8213   -1.4569    1.4821

r2_3
Final geometry with  32 atoms:
 N   -2.9970    0.9171    0.2492
 C   -1.8933    1.7385   -0.2793
 C   -3.3005   -0.1511   -0.7181
 C   -2.5649    0.3050    1.5180
 N   -0.9130   -0.5423   -0.1356
 C   -0.5909    0.9008   -0.4191
 C   -2.0243   -0.9804   -1.0477
 C   -1.3747   -0.6697    1.2875
 H   -1.7292    2.5818    0.3973
 H   -2.1981    2.1385   -1.2504
 H   -3.7009    0.3016   -1.6295
 H   -4.0748   -0.7934   -0.2895
 H   -3.4102   -0.2311    1.9584
 H   -2.2776    1.1067    2.2038
 H    0.1800    1.1916    0.2946
 H   -0.1584    0.9427   -1.4189
 H   -1.6772   -0.8195   -2.0709
 H   -2.1729   -2.0514   -0.8906
 H   -1.6573   -1.7147    1.4357
 H   -0.5152   -0.4438    1.9210
 C    0.4064   -1.4767   -0.3858
 C    1.5868   -1.1275    0.3831
 C    2.5378   -0.2351   -0.1420
 O    3.6224   -0.0363    0.7188
 O    2.5143    0.3602   -1.2421
 C    4.6506    0.8298    0.2371
 H    5.4006    0.8732    1.0314
 H    4.2706    1.8379    0.0361
 H    5.1103    0.4422   -0.6794
 H   -0.0021   -2.4661   -0.1627
 H    0.5444   -1.3556   -1.4634
 H    1.7472   -1.5565    1.3659

r2_TS2_SS
Final geometry with  48 atoms:
 H   -0.4344   -0.9798   -2.3890
 C   -4.3739   -0.3167    0.2893
 C   -3.9148    0.3421   -0.8571
 C   -2.6945   -0.0403   -1.4016
 C   -1.9303   -1.0629   -0.8164
 C   -2.4265   -1.7213    0.3206
 C   -3.6408   -1.3520    0.8849
 H   -4.5045    1.1336   -1.3034
 H   -2.3218    0.4669   -2.2873
 H   -1.8409   -2.5270    0.7511
 H   -4.0244   -1.8507    1.7668
 C    1.8985   -0.6183   -0.9551
 H    1.9110   -1.7079   -1.0533
 H    2.0675   -0.1591   -1.9318
 N    3.1591   -0.2824   -0.1318
 C    4.3846   -0.6681   -0.9394
 H    4.4091    0.0031   -1.8002
 H    4.2342   -1.6908   -1.2898
 C    3.1891   -1.0575    1.1693
 H    3.2667   -2.1122    0.8991
 H    2.2398   -0.8904    1.6775
 C    3.2466    1.1963    0.1850
 H    3.0647    1.7392   -0.7433
 H    2.4394    1.4132    0.8850
 C    0.5930   -0.1793   -0.3888
 H    0.3646   -0.5226    0.6162
 C    0.1778    1.1855   -0.6654
 O   -0.6852    1.6650    0.2775
 O    0.4838    1.8520   -1.6584
 C   -1.2797    2.9457    0.0067
 H   -0.5178    3.7310   -0.0210
 H   -1.8188    2.9356   -0.9443
 H   -1.9745    3.1267    0.8283
 C   -0.5997   -1.4641   -1.4036
 O   -0.1586   -2.6457   -1.2159
 C    5.6400   -0.5243   -0.0379
 H    6.0156   -1.5071    0.2591
 H    6.4323   -0.0092   -0.5875
 C    4.3991   -0.5623    2.0078
 H    4.0597    0.0598    2.8404
 H    4.9366   -1.4199    2.4208
 C    4.6449    1.4872    0.7937
 H    5.2781    2.0092    0.0714
 H    4.5371    2.1256    1.6746
 N    5.3191    0.2365    1.1808
 N   -5.6479    0.0802    0.8745
 O   -6.0420   -0.5103    1.8903
 O   -6.2872    0.9957    0.3368

r2_TS2_SR
Final geometry with  48 atoms:
 N   -5.0325   -0.9526   -0.8065
 C   -4.2974   -0.1260   -1.7790
 C   -4.3353   -2.2397   -0.6548
 C   -5.0427   -0.2632    0.4940
 N   -2.6177   -0.5537    0.0086
 C   -2.9025    0.2765   -1.2258
 C   -2.8324   -2.0153   -0.3381
 C   -3.6096   -0.1742    1.0881
 H   -4.8805    0.7720   -1.9992
 H   -4.1922   -0.6977   -2.7049
 H   -4.4367   -2.8145   -1.5791
 H   -4.8190   -2.8001    0.1494
 H   -5.6949   -0.8056    1.1835
 H   -5.4592    0.7371    0.3486
 H   -2.8662    1.3207   -0.9136
 H   -2.0920    0.0940   -1.9315
 H   -2.1897   -2.2255   -1.1950
 H   -2.4909   -2.6032    0.5158
 H   -3.4501   -0.8698    1.9140
 H   -3.3660    0.8335    1.4222
 C   -1.1670   -0.3747    0.4914
 C   -0.7131    1.0166    0.7675
 C   -0.1682    1.7683   -0.3539
 O   -0.0252    3.0925   -0.0488
 O    0.2061    1.3123   -1.4355
 C    0.6083    3.9097   -1.0494
 H    0.6481    4.9145   -0.6258
 H    0.0254    3.9154   -1.9754
 H    1.6192    3.5521   -1.2651
 H   -1.1042   -0.9615    1.4141
 H   -0.5508   -0.8341   -0.2834
 H   -1.3477    1.6072    1.4214
 C    0.6549    0.7346    2.1805
 H    0.7722    1.8173    2.3827
 C    1.8233    0.2098    1.3747
 C    2.6971    1.0877    0.7113
 C    3.7629    0.6071   -0.0395
 C    3.9544   -0.7773   -0.1239
 C    3.1086   -1.6769    0.5372
 C    2.0534   -1.1733    1.2886
 H    2.5336    2.1595    0.7821
 H    4.4366    1.2821   -0.5531
 H    3.2872   -2.7430    0.4642
 H    1.3929   -1.8422    1.8302
 N    5.0641   -1.2942   -0.9143
 O    5.8197   -0.4867   -1.4734
 O    5.2082   -2.5221   -1.0000
 O    0.1361   -0.0138    3.0789

r2_5_SS
Final geometry with  48 atoms:
 H   -0.4447   -0.7456   -2.4150
 C    1.9376   -0.4697   -1.1345
 H    1.9641   -1.5242   -1.4203
 H    2.1111    0.1629   -2.0072
 N    3.1376   -0.2582   -0.2160
 C    4.4017   -0.3795   -1.0509
 H    4.3922    0.4636   -1.7439
 H    4.3231   -1.3083   -1.6179
 C    3.1911   -1.3178    0.8699
 H    3.3228   -2.2720    0.3575
 H    2.2300   -1.3223    1.3820
 C    3.1297    1.1093    0.4382
 H    2.9582    1.8446   -0.3486
 H    2.2877    1.1203    1.1308
 C    0.5733   -0.1864   -0.5399
 C   -0.4731   -1.1784   -1.3836
 O   -0.0910   -2.4455   -1.2876
 C   -4.3866   -0.3576    0.2563
 C   -3.5591   -1.3049    0.8752
 C   -2.3120   -1.5641    0.3211
 C   -1.8704   -0.8834   -0.8247
 C   -2.7291    0.0461   -1.4322
 C   -3.9867    0.3189   -0.9008
 H   -3.8967   -1.8199    1.7667
 H   -1.6562   -2.3081    0.7616
 H   -2.4073    0.5667   -2.3303
 H   -4.6488    1.0385   -1.3671
 C    0.1703    1.2509   -0.6404
 O   -0.5307    1.6592    0.4404
 O    0.3800    1.9757   -1.6052
 C   -1.1083    2.9799    0.3718
 H   -0.3257    3.7385    0.2814
 H   -1.7910    3.0559   -0.4784
 H   -1.6541    3.1080    1.3071
 C    4.3656   -0.9823    1.8296
 H    3.9864   -0.6173    2.7876
 H    4.9544   -1.8835    2.0187
 C    4.4863    1.3167    1.1680
 H    5.1001    2.0470    0.6344
 H    4.3063    1.6956    2.1772
 C    5.6310   -0.3580   -0.1040
 H    6.0864   -1.3497   -0.0436
 H    6.3807    0.3384   -0.4887
 N    5.2368    0.0542    1.2523
 H    0.4804   -0.5331    0.4897
 N   -5.6963   -0.0738    0.8289
 O   -6.4146    0.7718    0.2762
 O   -6.0405   -0.6848    1.8508

r2_5_SR
Final geometry with  48 atoms:
 N   -5.0908   -0.9006   -0.7242
 C   -4.4665    0.1430   -1.5539
 C   -4.3583   -2.1624   -0.9178
 C   -4.9906   -0.5064    0.6908
 N   -2.6158   -0.5946   -0.0562
 C   -3.0377    0.4766   -1.0438
 C   -2.8357   -1.9500   -0.7070
 C   -3.5125   -0.5149    1.1653
 H   -5.0860    1.0431   -1.5261
 H   -4.4313   -0.2136   -2.5866
 H   -4.5421   -2.5350   -1.9289
 H   -4.7468   -2.8971   -0.2078
 H   -5.5756   -1.1995    1.3010
 H   -5.4237    0.4913    0.8004
 H   -3.0061    1.4265   -0.5087
 H   -2.2942    0.4924   -1.8406
 H   -2.2825   -1.9324   -1.6476
 H   -2.3933   -2.6986   -0.0478
 H   -3.2716   -1.3840    1.7796
 H   -3.2500    0.3865    1.7172
 C   -1.1438   -0.4820    0.3295
 C   -0.6741    0.8715    0.8132
 C   -0.2196    1.7782   -0.2848
 O   -0.1067    3.0533    0.1517
 O    0.0799    1.4448   -1.4246
 C    0.4327    4.0076   -0.7878
 H    0.4607    4.9579   -0.2538
 H   -0.2097    4.0861   -1.6692
 H    1.4398    3.7161   -1.0976
 H   -1.0017   -1.1937    1.1473
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 H  -0.5794  -0.7957  -0.5493
 H  -1.4205   1.3828   1.4216
 C   0.5216   0.5926   1.9749
 H   0.7187   1.6329   2.3217
 C   1.7886   0.1379   1.2299
 C   2.6848   1.0648   0.6713
 C   3.8231   0.6483  -0.0106
 C   4.0667  -0.7246  -0.1313
 C   3.2030  -1.6740   0.4291
 C   2.0765  -1.2308   1.1138
 H   2.4881   2.1287   0.7742
 H   4.5125   1.3637  -0.4423
 H   3.4221  -2.7307   0.3318
 H   1.4036  -1.9370   1.5888
 N   5.2520  -1.1757  -0.8504
 O   6.0214  -0.3239  -1.3173
 O   5.4430  -2.3940  -0.9710
 O   0.0751  -0.2484   2.8931

r2_TS3_SSR
Final geometry with  64 atoms:
 H   0.2173  -0.8089  -1.0484
 C   2.7509  -0.5612  -0.6314
 H   2.4374  -1.5665  -0.3415
 H   2.8273  -0.5152  -1.7191
 N   4.1611  -0.3877  -0.0962
 C   5.0777  -1.3320  -0.8611
 H   5.1091  -0.9622  -1.8877
 H   4.6064  -2.3157  -0.8492
 C   4.2361  -0.7530   1.3754
 H   3.9901  -1.8140   1.4377
 H   3.4724  -0.1840   1.9037
 C   4.6840   1.0246  -0.2772
 H   4.4939   1.3118  -1.3124
 H   4.1055   1.6646   0.3893
 C   1.7200   0.4538  -0.1409
 C   0.3371  -0.3262  -0.0612
 O   0.4325  -1.2536   0.9520
 C   0.0951  -2.9483   0.3463
 H   0.3433  -3.3616   1.3419
 O   0.8177  -3.2309  -0.6504
 C  -4.1065  -2.2488  -0.1968
 C  -3.2789  -2.3441  -1.3197
 C  -1.9261  -2.6111  -1.1307
 C  -1.3977  -2.7610   0.1588
 C  -2.2570  -2.6856   1.2667
 C  -3.6121  -2.4300   1.1017
 H  -3.6912  -2.2082  -2.3122
 H  -1.2552  -2.6962  -1.9790
 H  -1.8499  -2.8008   2.2672
 H  -4.2786  -2.3570   1.9524
 C  -2.9732   2.3739   0.4970
 C  -2.2904   1.8857   1.6166
 C  -1.2267   1.0120   1.4209
 C  -0.8352   0.6306   0.1293
 C  -1.5460   1.1283  -0.9730
 C  -2.6159   2.0025  -0.8018
 H  -2.5946   2.1838   2.6125
 H  -0.6971   0.5990   2.2722
 H  -1.2669   0.8216  -1.9765
 H  -3.1699   2.3822  -1.6516
 C   1.6171   1.6565  -1.0564
 O   1.3647   2.7828  -0.3686
 O   1.6976   1.6151  -2.2735
 C   1.0904   3.9685  -1.1516
 H   0.8821   4.7534  -0.4249
 H   1.9573   4.2328  -1.7627
 H   0.2219   3.8034  -1.7940
 C   5.6670  -0.4350   1.8878
 H   5.6598   0.4599   2.5154
 H   6.0348  -1.2699   2.4898
 C   6.1971   1.0386   0.0764
 H   6.8010   1.1363  -0.8293
 H   6.4139   1.8919   0.7240
 C   6.4728  -1.3261  -0.1827
 H   6.6366  -2.2559   0.3680
 H   7.2519  -1.2391  -0.9444

 N   6.5869  -0.2031   0.7618
 H   1.9144   0.7972   0.8764
 N  -5.5245  -1.9547  -0.3816
 O  -6.2487  -1.8873   0.6207
 O  -5.9472  -1.7808  -1.5326
 N  -4.0936   3.2933   0.6915
 O  -4.6745   3.7341  -0.3082
 O  -4.4123   3.5965   1.8483

r2_TS3_SSS
Final geometry with  64 atoms:
 H   1.2813  -0.4062   1.9424
 C  -0.5079   1.3083   1.0619
 H  -0.9266   0.3875   1.4676
 H  -0.3406   2.0067   1.8831
 N  -1.6048   1.9147   0.2036
 C  -2.7999   2.1946   1.1056
 H  -2.4331   2.7846   1.9468
 H  -3.1398   1.2245   1.4705
 C  -2.0506   0.9588  -0.8911
 H  -2.2223  -0.0067  -0.4215
 H  -1.2233   0.8654  -1.5925
 C  -1.1771   3.2202  -0.4362
 H  -0.9631   3.9124   0.3803
 H  -0.2609   3.0311  -0.9958
 C   0.8111   1.0086   0.3461
 C   1.2974  -0.4230   0.8391
 O   0.3965  -1.3504   0.3587
 C  -0.3593  -2.2799   1.6243
 H   0.1855  -3.2219   1.4105
 O  -0.2230  -1.7472   2.7726
 C  -4.2536  -2.1650  -0.2061
 C  -4.0764  -1.6060   1.0636
 C  -2.8180  -1.6823   1.6547
 C  -1.7471  -2.2967   0.9926
 C  -1.9645  -2.8856  -0.2630
 C  -3.2113  -2.8193  -0.8756
 H  -4.9058  -1.1221   1.5654
 H  -2.6381  -1.2540   2.6353
 H  -1.1392  -3.3722  -0.7737
 H  -3.3807  -3.2517  -1.8543
 C   5.3299  -1.1061  -0.4988
 C   4.2651  -1.4464  -1.3407
 C   2.9660  -1.2411  -0.8890
 C   2.7223  -0.6995   0.3821
 C   3.8102  -0.3868   1.2111
 C   5.1194  -0.5835   0.7800
 H   4.4581  -1.8581  -2.3238
 H   2.1231  -1.5059  -1.5181
 H   3.6313   0.0166   2.2035
 H   5.9611  -0.3419   1.4172
 C   1.8513   2.0796   0.6115
 O   2.6488   2.2650  -0.4541
 O   1.9909   2.6734   1.6680
 C   3.7809   3.1465  -0.2695
 H   3.4442   4.1562  -0.0207
 H   4.4287   2.7664   0.5242
 H   4.3078   3.1438  -1.2235
 C  -3.3209   1.5401  -1.5688
 H  -3.2066   1.5071  -2.6551
 H  -4.2009   0.9486  -1.3021
 C  -2.3268   3.7134  -1.3615
 H  -2.5342   4.7674  -1.1603
 H  -2.0369   3.6175  -2.4110
 C  -3.8852   2.9409   0.2848
 H  -4.8556   2.4599   0.4319
 H  -3.9665   3.9799   0.6140
 N  -3.5538   2.9307  -1.1476
 H   0.6906   0.9078  -0.7338
 N   6.7008  -1.3080  -0.9672
 O   7.6323  -0.9877  -0.2182
 O   6.8730  -1.7868  -2.0951
 N  -5.5570  -2.0513  -0.8563
 O  -5.7075  -2.5678  -1.9710
 O  -6.4563  -1.4341  -0.2703

r2_TS3_SRR
Final geometry with  64 atoms:
 H  -1.0420  -0.0493  -1.9274
 C   0.8531   0.9670  -0.3179
 H   1.3520   0.3075   0.3901
 H   1.0592   0.6117  -1.3288
 N   1.5391   2.3187  -0.2104
 C   1.2192   3.0391   1.0844
 H   1.3729   2.3280   1.8960
 H   0.1653   3.3150   1.0405
 C   1.1694   3.2165  -1.3776
 H   0.0822   3.2751  -1.4224
 H   1.5358   2.7151  -2.2750
 C   3.0414   2.0806  -0.2601
 H   3.2942   1.5307   0.6481
 H   3.2346   1.4443  -1.1244
 C  -0.6525   0.9453  -0.0668
 C  -1.1939  -0.3313  -0.8666
 O  -0.4647  -1.4470  -0.5623
 C   0.5097  -2.0130  -2.0281
 H  -0.1084  -2.9210  -2.1510
 O   0.5192  -1.1437  -2.9467
 C   4.0901  -2.7291   0.2338
 C   4.1040  -1.7666  -0.7811
 C   2.9415  -1.5574  -1.5161
 C   1.7750  -2.2838  -1.2406
 C   1.7967  -3.2600  -0.2324
 C   2.9471  -3.4885   0.5142
 H   5.0082  -1.2066  -0.9867
 H   2.9183  -0.8254  -2.3165
 H   0.8951  -3.8260  -0.0197
 H   2.9662  -4.2306   1.3031
 C  -5.4225  -0.7860  -0.1862
 C  -4.5329  -1.6716   0.4296
 C  -3.1697  -1.5252   0.1889
 C  -2.6920  -0.5073  -0.6476
 C  -3.6105   0.3581  -1.2623
 C  -4.9768   0.2293  -1.0401
 H  -4.9054  -2.4529   1.0810
 H  -2.4547  -2.2003   0.6458
 H  -3.2517   1.1427  -1.9231
 H  -5.6880   0.8941  -1.5149
 C  -0.9979   0.8265   1.4025
 O  -2.2199   1.3330   1.6556
 O  -0.2991   0.3097   2.2572
 C  -2.7404   1.1288   2.9882
 H  -2.1079   1.6260   3.7285
 H  -3.7372   1.5698   2.9803
 H  -2.7990   0.0608   3.2124
 C   1.8250   4.6072  -1.1572
 H   2.3086   4.9356  -2.0806
 H   1.0687   5.3486  -0.8868
 C   3.7622   3.4516  -0.3515
 H   4.5798   3.4877   0.3730
 H   4.1839   3.5977  -1.3492
 C   2.1385   4.2880   1.1959
 H   1.5409   5.1610   1.4703
 H   2.8959   4.1363   1.9692
 N   2.8242   4.5522  -0.0788
 H  -1.1569   1.8243  -0.4754
 N   5.3021  -2.9492   1.0185
 O   5.2902  -3.8284   1.8896
 O   6.2933  -2.2438   0.7844
 N  -6.8553  -0.9268   0.0631
 O  -7.6304  -0.1343  -0.4884
 O  -7.2368  -1.8298   0.8187

r2_TS3_SRS
Final geometry with  64 atoms:
 N  -5.7466  -1.9555  -0.5912
 C  -5.5736  -1.4739   0.7889
 C  -5.8319  -0.7918  -1.4890
 C  -4.5671  -2.7581  -0.9629
 N  -3.6007  -0.5352  -0.4075
 C  -4.1865  -0.8003   0.9680
 C  -4.6536   0.1850  -1.2328
 C  -3.3072  -1.8653  -1.0876
 H  -5.6629  -2.3160   1.4799
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H	-6.3767	-0.7657	1.0099
H	-6.7801	-0.2741	-1.3219
H	-5.8177	-1.1512	-2.5212
H	-4.7561	-3.2605	-1.9153
H	-4.4215	-3.5269	-0.1991
H	-3.4854	-1.4512	1.4906
H	-4.2438	0.1575	1.4857
H	-4.9534	1.0603	-0.6529
H	-4.1724	0.5154	-2.1548
H	-3.0722	-1.6200	-2.1253
H	-2.4214	-2.3072	-0.6255
C	-2.3549	0.3322	-0.3447
C	-1.2938	-0.1365	0.6432
C	-1.4033	0.5512	1.9854
O	-0.5819	-0.0198	2.8852
O	-2.1129	1.5100	2.2465
C	-0.5388	0.5872	4.1974
H	0.1968	0.0108	4.7585
H	-1.5187	0.5261	4.6778
H	-0.2306	1.6334	4.1254
H	-1.9442	0.3091	-1.3542
H	-2.6952	1.3406	-0.1063
H	-1.3443	-1.2136	0.8109
C	0.1636	0.0034	-0.0088
H	0.8470	-0.4099	0.7518
C	0.5386	1.4688	-0.2017
C	1.0568	2.2182	0.8679
C	1.3681	3.5657	0.7172
C	1.1580	4.1652	-0.5281
C	0.6616	3.4427	-1.6172
C	0.3594	2.0951	-1.4444
H	1.2297	1.7405	1.8278
H	1.7707	4.1427	1.5406
H	0.5216	3.9287	-2.5752
H	-0.0028	1.5074	-2.2802
N	1.4743	5.5831	-0.6976
O	1.9125	6.2086	0.2758
O	1.2872	6.0995	-1.8063
O	0.2061	-0.6920	-1.1935
C	0.4092	-2.5260	-0.9445
H	0.1760	-2.6823	-2.0135
C	1.8970	-2.4760	-0.6797
C	2.8085	-2.3104	-1.7342
C	4.1751	-2.2442	-1.4908
C	4.6252	-2.3398	-0.1678
C	3.7408	-2.5124	0.9016
C	2.3770	-2.5890	0.6333
H	2.4391	-2.2229	-2.7521
H	4.8846	-2.1163	-2.2992
H	4.1190	-2.5895	1.9138
H	1.6644	-2.7439	1.4364
N	6.0590	-2.2630	0.1014
O	6.8326	-2.1297	-0.8560
O	6.4439	-2.3330	1.2762
O	-0.3651	-2.9904	-0.0604

r2_6_SSR

Final geometry with 64 atoms:

H	0.1906	-0.6519	-1.2178
C	2.7735	-0.3677	-0.9108
H	2.3791	-1.3890	-0.8560
H	3.0250	-0.1368	-1.9473
N	4.0834	-0.3850	-0.1483
C	5.0524	-1.2992	-0.8844
H	5.2716	-0.8111	-1.8358
H	4.5279	-2.2364	-1.0749
C	3.8917	-0.9448	1.2512
H	3.5769	-1.9810	1.1202
H	3.0779	-0.3993	1.7248
C	4.7163	0.9905	-0.0562
H	4.7204	1.4104	-1.0641
H	4.0738	1.5961	0.5822
C	1.7247	0.6220	-0.3815
C	0.3666	-0.1629	-0.2488
O	0.5561	-1.1075	0.7638
C	0.2701	-2.6312	0.2867
H	0.5360	-3.0945	1.2618
O	0.9618	-2.9722	-0.7484
C	-4.0155	-2.4327	-0.1696
C	-3.2097	-2.5244	-1.3091
C	-1.8311	-2.6259	-1.1442
C	-1.2560	-2.6173	0.1329
C	-2.0913	-2.5430	1.2585
C	-3.4713	-2.4508	1.1210
H	-3.6586	-2.5153	-2.2951
H	-1.1729	-2.7096	-2.0030
H	-1.6506	-2.5351	2.2516
H	-4.1204	-2.3830	1.9856
C	-2.9473	2.4496	0.5838
C	-2.1597	1.9885	1.6440
C	-1.0942	1.1404	1.3632
C	-0.8085	0.7563	0.0450
C	-1.6205	1.2283	-0.9962
C	-2.6933	2.0780	-0.7385
H	-2.3849	2.2865	2.6606
H	-0.4835	0.7522	2.1708
H	-1.4205	0.9197	-2.0179
H	-3.3269	2.4377	-1.5399
C	1.5765	1.8305	-1.2870
O	1.3644	2.9536	-0.5818
O	1.5977	1.7928	-2.5056
C	1.0654	4.1470	-1.3453
H	0.8950	4.9286	-0.6052
H	1.9076	4.4079	-1.9912
H	0.1690	3.9919	-1.9508
C	5.2335	-0.8100	2.0178
H	5.1767	-0.0050	2.7555
H	5.4482	-1.7416	2.5477
C	6.1450	0.8374	0.5359
H	6.9000	1.0037	-0.2366
H	6.2963	1.5781	1.3252
C	6.3185	-1.4880	-0.0070
H	6.3402	-2.4921	0.4240
H	7.2142	-1.3613	-0.6204
N	6.3399	-0.5104	1.0930
H	1.9480	0.9756	0.6263
N	-5.4623	-2.3183	-0.3280
O	-6.1644	-2.2513	0.6900
O	-5.9314	-2.2904	-1.4739
N	-4.0722	3.3422	0.8677
O	-4.7486	3.7562	-0.0815
O	-4.2972	3.6481	2.0451

r2_6_SSS

Final geometry with 64 atoms:

H	1.2311	-0.6406	1.7981
C	-0.5644	1.1852	1.0571
H	-0.9773	0.2149	1.3319
H	-0.4830	1.8076	1.9489
N	-1.6260	1.8281	0.1798
C	-2.8799	2.0177	1.0215
H	-2.5832	2.5679	1.9159
H	-3.2088	1.0195	1.3097
C	-1.9712	0.9346	-1.0013
H	-2.1323	-0.0672	-0.6078
H	-1.0959	0.9121	-1.6485
C	-1.2045	3.1873	-0.3385
H	-1.0719	3.8243	0.5380
H	-0.2472	3.0716	-0.8455
C	0.8064	0.9961	0.4069
C	1.2592	-0.5175	0.6941
O	0.3813	-1.3452	0.0715
C	-0.3624	-2.6931	1.4514
H	0.2221	-3.4732	0.9382
O	-0.0651	-2.3260	2.6028
C	-4.2651	-2.0239	-0.1709
C	-3.9934	-1.6173	1.1398
C	-2.7279	-1.8582	1.6652
C	-1.7421	-2.4918	0.8944
C	-2.0542	-2.9261	-0.4042
C	-3.3104	-2.6909	-0.9498
H	-4.7591	-1.1222	1.7248
H	-2.4829	-1.5482	2.6757
H	-1.2920	-3.4216	-0.9973
H	-3.5520	-3.0019	-1.9589
C	5.3411	-0.9849	-0.6089
C	4.3002	-1.2027	-1.5194
C	2.9889	-1.0688	-1.0770
C	2.7069	-0.7130	0.2504
C	3.7712	-0.5214	1.1447
C	5.0924	-0.6516	0.7258
H	4.5220	-1.4685	-2.5459
H	2.1610	-1.2454	-1.7554
H	3.5641	-0.2645	2.1798
H	5.9155	-0.5020	1.4138
C	1.8088	2.0077	0.9141
O	2.6891	2.3567	-0.0417
O	1.8621	2.4286	2.0592
C	3.7954	3.1905	0.3722
H	3.4329	4.1543	0.7392
H	4.3732	2.6920	1.1545
H	4.4050	3.3271	-0.5211
C	-3.2133	1.5253	-1.7210
H	-3.0279	1.5729	-2.7970
H	-4.0900	0.8930	-1.5572
C	-2.3083	3.7074	-1.3036
H	-2.5634	4.7392	-1.0487
H	-1.9482	3.6911	-2.3353
C	-3.9404	2.7792	0.1819
H	-4.8990	2.2567	0.2338
H	-4.0820	3.7903	0.5723
N	-3.5195	2.8767	-1.2233
H	0.7689	1.0596	-0.6812
N	-5.5731	-1.7256	-0.7483
O	-5.8041	-2.0938	-1.9071
O	-6.3943	-1.1055	-0.0588
N	6.7237	-1.1144	-1.0628
O	7.6339	-0.8998	-0.2514
O	6.9304	-1.4290	-2.2422

r2_6_SRR

Final geometry with 64 atoms:

N	-1.6307	4.4653	-1.6593
C	-0.4519	4.9889	-0.9505
C	-1.1769	3.7594	-2.8688
C	-2.3227	3.5053	-0.7790
N	-0.0471	2.5329	-1.0180
C	0.4045	3.8304	-0.3719
C	-0.0559	2.7419	-2.5231
C	-1.4732	2.2265	-0.5778
H	-0.7795	5.6417	-0.1374
H	0.1347	5.5877	-1.6525
H	-0.8009	4.4866	-3.5932
H	-2.0357	3.2497	-3.3129
H	-3.2872	3.2400	-1.2203
H	-2.5133	3.9965	0.1793
H	0.2601	3.7175	0.7020
H	1.4681	3.9440	-0.5828
H	0.9378	3.1059	-2.7922
H	-0.2182	1.7668	-2.9855
H	-1.8069	1.4024	-1.2110
H	-1.4514	1.8792	0.4604
C	0.8775	1.3746	-0.6900
C	1.1762	1.1972	0.7980
C	2.4954	1.8248	1.1997
O	2.6886	1.7308	2.5262
O	3.2954	2.3538	0.4449
C	3.9290	2.2710	3.0399
H	3.9095	2.0700	4.1109
H	3.9805	3.3468	2.8538
H	4.7841	1.7761	2.5724
H	0.3699	0.4919	-1.0778
H	1.7935	1.5421	-1.2566
H	0.3919	1.6352	1.4241
C	1.0527	-0.3259	1.2150
H	1.2384	-0.3632	2.2978
C	2.0889	-1.1900	0.5159
C	3.4168	-1.2059	0.9756
C	4.3932	-1.9503	0.3219
C	4.0271	-2.6901	-0.8059
C	2.7124	-2.7087	-1.2777

```
 C    1.7495   -1.9577   -0.6083
 H    3.6904   -0.6402    1.8609
 H    5.4160   -1.9640    0.6774
 H    2.4524   -3.3010   -2.1465
 H    0.7200   -1.9756   -0.9462
 N    5.0475   -3.4732   -1.5055
 O    6.2032   -3.4586   -1.0655
 O    4.7108   -4.1140   -2.5083
 O   -0.2346   -0.7742    0.9073
 C   -1.2908   -0.4266    2.0192
 H   -0.9431   -1.0951    2.8457
 C   -2.5390   -1.0604    1.3831
 C   -3.6478   -0.2609    1.0837
 C   -4.7892   -0.8078    0.5017
 C   -4.8098   -2.1794    0.2301
 C   -3.7222   -3.0078    0.5339
 C   -2.5937   -2.4366    1.1129
 H   -3.5963    0.7963    1.3222
 H   -5.6492   -0.1932    0.2643
 H   -3.7678   -4.0680    0.3161
 H   -1.7372   -3.0607    1.3501
 N   -5.9988   -2.7649   -0.3859
 O   -6.0045   -3.9807   -0.6194
 O   -6.9521   -2.0216   -0.6536
 O   -1.3642    0.8386    2.3177

r2_6_SRS
Final geometry with  64 atoms:
 N   -5.6007   -2.1737   -0.6751
 C   -5.3871   -1.9247    0.7597
 C   -5.8252   -0.8848   -1.3490
 C   -4.3847   -2.7950   -1.2331
 N   -3.5638   -0.6271   -0.3341
 C   -4.0494   -1.1732    0.9971
 C   -4.7154    0.1325   -0.9716
 C   -3.2061   -1.7888   -1.2512
 H   -5.3690   -2.8785    1.2929
 H   -6.2298   -1.3399    1.1378
 H   -6.8009   -0.4873   -1.0570
 H   -5.8373   -1.0588   -2.4281
 H   -4.5886   -3.1397   -2.2504
 H   -4.1364   -3.6683   -0.6238
 H   -3.2724   -1.8396    1.3711
 H   -4.1525   -0.3247    1.6739
 H   -5.0516    0.8632   -0.2335
 H   -4.3159    0.6589   -1.8401
 H   -3.0534   -1.3470   -2.2384
 H   -2.2604   -2.2261   -0.9125
 C   -2.3876    0.3197   -0.1715
 C   -1.2394   -0.2260    0.6743
 C   -1.2976    0.2549    2.1095
 O   -0.3218   -0.3062    2.8445
 O   -2.1093    1.0417    2.5692
 C   -0.2491    0.0896    4.2345
 H    0.6025   -0.4529    4.6447
 H   -1.1676   -0.1882    4.7578
 H   -0.0911    1.1680    4.3171
 H   -2.0437    0.5195   -1.1863
 H   -2.7913    1.2367    0.2598
 H   -1.2352   -1.3208    0.6908
 C    0.1570    0.0515   -0.0191
 H    0.9150   -0.3629    0.6584
 C    0.4306    1.5384   -0.1750
 C    0.8451    2.2959    0.9339
 C    1.0631    3.6653    0.8261
 C    0.8633    4.2789   -0.4138
 C    0.4655    3.5516   -1.5381
 C    0.2539    2.1811   -1.4093
 H    1.0145    1.8102    1.8900
 H    1.3880    4.2483    1.6790
 H    0.3292    4.0497   -2.4902
 H   -0.0351    1.5950   -2.2738
 N    1.0876    5.7199   -0.5394
 O    1.4371    6.3497    0.4660
 O    0.9152    6.2473   -1.6448
 O    0.1825   -0.5758   -1.2679
 C    0.4980   -2.1360   -1.2193
 H    0.3756   -2.3075   -2.3120
 C    1.9992   -2.1673   -0.8880
 C    2.9504   -1.7140   -1.8149
 C    4.3075   -1.7218   -1.5106
 C    4.7079   -2.1888   -0.2523
 C    3.7835   -2.6512    0.6899
 C    2.4314   -2.6420    0.3569
 H    2.6205   -1.3439   -2.7817
 H    5.0458   -1.3721   -2.2220
 H    4.1226   -3.0099    1.6543
 H    1.6833   -3.0077    1.0526
 N    6.1296   -2.1951    0.0839
 O    6.4709   -2.6089    1.1999
 O    6.9379   -1.7848   -0.7597
 O   -0.2778   -2.8151   -0.4281

r2_TS4_SSR
Final geometry with  64 atoms:
 H    0.1204    0.6332   -0.3389
 C    0.1878   -1.8846   -0.9110
 H    0.1184   -1.1257   -1.6934
 H    0.8687   -2.6692   -1.2448
 N   -1.2013   -2.5535   -0.9356
 C   -1.3620   -3.2900   -2.2500
 H   -0.6440   -4.1122   -2.2362
 H   -1.0903   -2.5954   -3.0474
 C   -2.3016   -1.5167   -0.8357
 H   -2.2311   -0.9031   -1.7363
 H   -2.0939   -0.9103    0.0434
 C   -1.3694   -3.5534    0.1926
 H   -0.4827   -4.1869    0.1946
 H   -1.3950   -2.9813    1.1185
 C    0.6173   -1.3043    0.4172
 C    0.8338    0.2423    0.4030
 O    0.5658    0.8456    1.6671
 C   -0.7827    0.6526    2.1649
 H   -0.7028    1.0311    3.1996
 O   -1.1833   -0.6592    2.1378
 C   -3.5493    3.2715    0.1215
 C   -4.0206    2.0869    0.6953
 C   -3.1122    1.2509    1.3388
 C   -1.7524    1.5858    1.4159
 C   -1.3123    2.7894    0.8448
 C   -2.2016    3.6371    0.1893
 H   -5.0714    1.8309    0.6340
 H   -3.4484    0.3193    1.7803
 H   -0.2623    3.0544    0.9050
 H   -1.8629    4.5613   -0.2628
 C    4.7865    1.3671   -0.8732
 C    4.4747    1.4242    0.4882
 C    3.1927    1.0739    0.9004
 C    2.2233    0.6706   -0.0309
 C    2.5638    0.6331   -1.3937
 C    3.8408    0.9756   -1.8257
 H    5.2242    1.7349    1.2059
 H    2.9334    1.1047    1.9503
 H    1.8223    0.3385   -2.1298
 H    4.1003    0.9509   -2.8769
 C    1.6060   -2.1477    1.0955
 O    2.2573   -1.5111    2.1006
 O    1.8114   -3.3413    0.8527
 C    3.2196   -2.2853    2.8350
 H    3.6401   -1.6013    3.5742
 H    2.7402   -3.1313    3.3364
 H    4.0096   -2.6568    2.1756
 C   -3.6620   -2.2555   -0.7239
 H   -4.0488   -2.1882    0.2965
 H   -4.3913   -1.7936   -1.3948
 C   -2.6894   -4.3367   -0.0427
 H   -2.4797   -5.3573   -0.3741
 H   -3.2544   -4.3919    0.8914
 C   -2.8291   -3.7842   -2.3664
 H   -3.3801   -3.1869   -3.0976
 H   -2.8422   -4.8253   -2.6993
 N   -3.5172   -3.6798   -1.0697
 H   -0.3836   -1.1742    1.3272
 N   -4.4923    4.1521   -0.5698
 O   -4.0643    5.2051   -1.0579
 O   -5.6779    3.8058   -0.6392
 N    6.1308    1.7335   -1.3136
 O    6.3900    1.6783   -2.5228
 O    6.9556    2.0832   -0.4599

r2_TS4_SSS
Final geometry with  64 atoms:
 H    0.8049    0.0926   -1.6661
 C    2.5566   -1.2103   -0.3062
 H    2.6941   -0.9387   -1.3549
 H    3.4793   -0.9954    0.2360
 N    2.4971   -2.7532   -0.3411
 C    3.8632   -3.2755   -0.7398
 H    4.5412   -3.0247    0.0781
 H    4.1711   -2.7324   -1.6356
 C    1.4887   -3.2413   -1.3619
 H    1.8589   -2.9158   -2.3368
 H    0.5393   -2.7549   -1.1403
 C    2.1447   -3.3390    1.0136
 H    2.7832   -2.8507    1.7490
 H    1.1088   -3.0687    1.2115
 C    1.3681   -0.5100    0.3128
 C    0.6223    0.4712   -0.6460
 O   -0.7857    0.4930   -0.4278
 C   -1.4016   -0.8136   -0.5872
 H   -1.2182   -1.1068   -1.6469
 O   -0.8968   -1.7364    0.2868
 C   -5.6206   -0.1083   -0.1555
 C   -4.9967   -1.0183    0.7012
 C   -3.6283   -1.2418    0.5571
 C   -2.8965   -0.5680   -0.4257
 C   -3.5488    0.3369   -1.2771
 C   -4.9125    0.5776   -1.1490
 H   -5.5708   -1.5328    1.4621
 H   -3.1111   -1.9391    1.2064
 H   -2.9800    0.8608   -2.0391
 H   -5.4223    1.2779   -1.7992
 C    2.1569    4.4885   -0.4789
 C    0.8525    4.2480   -0.0389
 C    0.3486    2.9520   -0.1019
 C    1.1329    1.9001   -0.5964
 C    2.4394    2.1734   -1.0356
 C    2.9614    3.4606   -0.9813
 H    0.2497    5.0606    0.3478
 H   -0.6558    2.7446    0.2441
 H    3.0597    1.3717   -1.4239
 H    3.9680    3.6705   -1.3211
 C    1.6402   -0.0564    1.6808
 O    0.7413    0.8543    2.1292
 O    2.5472   -0.4755    2.4063
 C    0.9263    1.3342    3.4714
 H    0.8388    0.5173    4.1939
 H    1.9032    1.8135    3.5845
 H    0.1306    2.0634    3.6315
 C    1.3856   -4.7865   -1.2477
 H    0.4446   -5.0696   -0.7682
 H    1.4073   -5.2340   -2.2450
 C    2.3419   -4.8775    0.9474
 H    3.2336   -5.1771    1.5048
 H    1.4786   -5.3772    1.3943
 C    3.7626   -4.8064   -0.9770
 H    3.8102   -5.0358   -2.0449
 H    4.5973   -5.3110   -0.4834
 N    2.4946   -5.3313   -0.4464
 H    0.2707   -1.3051    0.4318
 N   -7.0574    0.1345   -0.0117
 O   -7.5934    0.9554   -0.7663
 O   -7.6761   -0.4905    0.8582
 N    2.6938    5.8456   -0.4152
 O    3.8499    6.0410   -0.8130
 O    1.9719    6.7447    0.0342

r2_TS4_SRR
Final geometry with  64 atoms:
 N   -1.3000    3.9212   -2.3472
 C   -0.8528    4.5623   -1.0980
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 C  -0.1256   3.6957  -3.2057
 C  -1.9020   2.6170  -2.0197
 N   0.4122   2.4196  -1.1325
 C   0.0147   3.5905  -0.2532
 C   0.9994   2.9754  -2.4154
 C  -0.8304   1.6287  -1.4930
 H  -1.7280   4.8686  -0.5188
 H  -0.2869   5.4611  -1.3580
 H   0.2422   4.6562  -3.5760
 H  -0.4375   3.0972  -4.0658
 H  -2.3797   2.2039  -2.9122
 H  -2.6768   2.7776  -1.2648
 H  -0.5407   3.1772   0.5861
 H   0.9359   4.0409   0.1164
 H   1.8022   3.6539  -2.1209
 H   1.4280   2.1373  -2.9682
 H  -0.5211   0.9034  -2.2484
 H  -1.1521   1.1052  -0.5965
 C   1.4705   1.5203  -0.4645
 C   1.2286   1.1333   0.9796
 C   2.0562   1.8974   1.9127
 O   2.1393   1.3393   3.1556
 O   2.5879   2.9839   1.6687
 C   2.8248   2.1127   4.1575
 H   2.7853   1.5110   5.0668
 H   2.3239   3.0717   4.3189
 H   3.8646   2.2921   3.8695
 H   1.5175   0.6493  -1.1213
 H   2.3999   2.0830  -0.5684
 H  -0.0467   1.3583   1.3984
 C   1.0638  -0.3896   1.2370
 H   1.1874  -0.5567   2.3148
 C   2.0887  -1.2419   0.5156
 C   3.4460  -1.0936   0.8524
 C   4.4297  -1.8225   0.1968
 C   4.0450  -2.7091  -0.8159
 C   2.7057  -2.8793  -1.1710
 C   1.7323  -2.1422  -0.4983
 H   3.7328  -0.3985   1.6355
 H   5.4747  -1.7121   0.4589
 H   2.4333  -3.5737  -1.9565
 H   0.6878  -2.2653  -0.7580
 N   5.0727  -3.4760  -1.5188
 O   6.2544  -3.3150  -1.1893
 O   4.7185  -4.2522  -2.4149
 O  -0.2450  -0.8202   0.8519
 C  -1.2742  -0.2394   1.7154
 H  -1.0821  -0.6479   2.7297
 C  -2.5835  -0.8243   1.1986
 C  -3.5832   0.0087   0.6852
 C  -4.7750  -0.5271   0.2007
 C  -4.9516  -1.9121   0.2436
 C  -3.9717  -2.7679   0.7591
 C  -2.7893  -2.2115   1.2358
 H  -3.4160   1.0797   0.6754
 H  -5.5538   0.1102  -0.1999
 H  -4.1388  -3.8378   0.7831
 H  -2.0149  -2.8582   1.6372
 N  -6.2012  -2.4851  -0.2621
 O  -6.3520  -3.7111  -0.2025
 O  -7.0527  -1.7191  -0.7291
 O  -1.2408   1.1276   1.7015

r2_TS4_SRS
Final geometry with  64 atoms:
 N  -4.3963  -3.5908  -0.9431
 C  -3.6745  -3.9916   0.2776
 C  -5.2849  -2.4645  -0.6151
 C  -3.4152  -3.1413  -1.9465
 N  -3.0165  -1.6103  -0.0278
 C  -2.6832  -2.8844   0.7262
 C  -4.5021  -1.3476   0.1253
 C  -2.7292  -1.8230  -1.5013
 H  -3.1258  -4.9167   0.0823
 H  -4.4108  -4.1927   1.0607
 H  -6.1029  -2.8214   0.0165
 H  -5.7156  -2.0831  -1.5448
 H  -3.9218  -2.9898  -2.9036
 H  -2.6720  -3.9326  -2.0774
 H  -1.6540  -3.1343   0.4755
 H  -2.7441  -2.6525   1.7892
 H  -4.7067  -1.3372   1.1975
 H  -4.7005  -0.3553  -0.2841
 H  -3.1285  -0.9485  -2.0185
 H  -1.6484  -1.8586  -1.6189
 C  -2.2506  -0.3944   0.5261
 C  -0.7625  -0.5652   0.7470
 C  -0.4215  -0.7618   2.1562
 O   0.8990  -0.5557   2.4312
 O  -1.1995  -1.1487   3.0325
 C   1.3345  -0.8749   3.7644
 H   2.4018  -0.6486   3.7833
 H   1.1704  -1.9341   3.9839
 H   0.8074  -0.2667   4.5052
 H  -2.4698   0.3996  -0.1908
 H  -2.7614  -0.1664   1.4637
 H  -0.2348  -1.6551   0.1213
 C   0.1480   0.3828  -0.0832
 H   1.1315   0.3938   0.3992
 C  -0.3489   1.8133  -0.1282
 C  -0.3996   2.5452   1.0715
 C  -0.8789   3.8485   1.0951
 C  -1.3210   4.4222  -0.1030
 C  -1.2823   3.7208  -1.3094
 C  -0.7930   2.4155  -1.3136
 H  -0.0588   2.0874   1.9952
 H  -0.9120   4.4151   2.0175
 H  -1.6276   4.1885  -2.2234
 H  -0.7515   1.8583  -2.2417
 N  -1.8354   5.7908  -0.0897
 O  -1.8552   6.4006   0.9867
 O  -2.2315   6.2818  -1.1543
 O   0.2872  -0.0954  -1.4248
 C   0.9829  -1.3837  -1.4983
 H   0.9235  -1.6183  -2.5750
 C   2.4591  -1.1522  -1.1450
 C   3.2077  -0.2117  -1.8700
 C   4.5419   0.0291  -1.5603
 C   5.1227  -0.6892  -0.5085
 C   4.4026  -1.6336   0.2267
 C   3.0674  -1.8595  -0.1030
 H   2.7359   0.3436  -2.6751
 H   5.1251   0.7558  -2.1126
 H   4.8787  -2.1739   1.0357
 H   2.4771  -2.5811   0.4494
 N   6.5261  -0.4443  -0.1711
 O   7.1579   0.3785  -0.8452
 O   7.0225  -1.0697   0.7738
 O   0.3737  -2.3395  -0.7339

r2_7_SSR
Final geometry with  64 atoms:
 N   4.1443  -3.1791  -0.8444
 C   3.6373  -3.1184   0.5376
 C   3.6312  -4.3994  -1.4877
 C   3.6444  -2.0074  -1.5823
 N   1.5652  -3.1637  -0.8395
 C   2.0904  -2.9695   0.5637
 C   2.0818  -4.4756  -1.3739
 C   2.0949  -2.0469  -1.7078
 H   4.1004  -2.2684   1.0459
 H   3.9449  -4.0309   1.0559
 H   4.0827  -5.2718  -1.0078
 H   3.9401  -4.3914  -2.5365
 H   4.1009  -1.9910  -2.5758
 H   3.9596  -1.1063  -1.0490
 H   1.7687  -1.9776   0.8841
 H   1.6049  -3.7153   1.1934
 H   1.7562  -5.2492  -0.6753
 H   1.5993  -4.6461  -2.3389
 H   1.7658  -2.2622  -2.7269
 H   1.6315  -1.1229  -1.3635
 C  -0.0329  -3.1902  -0.8588
 C  -0.7037  -2.1372  -0.0778
 C  -1.0120  -2.3494   1.2731
 O  -0.8578  -3.6529   1.7173
 O  -1.3979  -1.4757   2.0994
 C  -1.0500  -3.8723   3.1202
 H  -0.8497  -4.9341   3.2804
 H  -2.0744  -3.6386   3.4258
 H  -0.3564  -3.2696   3.7160
 H  -0.2487  -3.1471  -1.9305
 H  -0.2563  -4.1898  -0.4874
 H  -0.0615  -0.4624   2.0845
 C  -0.9348  -0.8025  -0.7214
 O   0.1117   0.2211  -0.4975
 C   0.1769   0.8954   0.7485
 O   0.6909   0.1133   1.7919
 H  -0.8081  -0.9579  -1.8001
 H  -0.8320   1.2385   1.0267
 C  -2.3274  -0.1775  -0.5915
 C  -3.4459  -0.9370  -0.2164
 C  -2.5260   1.1620  -0.9729
 C  -4.7226  -0.3827  -0.2039
 H  -3.3163  -1.9733   0.0700
 C  -3.7918   1.7381  -0.9636
 H  -1.6770   1.7624  -1.2793
 C  -4.8814   0.9546  -0.5747
 H  -5.5811  -0.9726   0.0933
 H  -3.9363   2.7711  -1.2553
 C   1.0615   2.1165   0.5537
 C   1.1929   2.7244  -0.7038
 C   1.7135   2.6819   1.6601
 C   1.9657   3.8719  -0.8631
 H   0.6968   2.2895  -1.5629
 C   2.4889   3.8294   1.5208
 H   1.6166   2.2121   2.6317
 C   2.6053   4.4108   0.2556
 H   2.0730   4.3409  -1.8334
 H   2.9954   4.2666   2.3724
 N  -6.2178   1.5466  -0.5609
 O  -7.1755   0.8312  -0.2410
 O  -6.3363   2.7394  -0.8684
 N   3.4206   5.6175   0.0979
 O   3.9700   6.0899   1.0999
 O   3.5246   6.1129  -1.0305

r2_7_SSS
Final geometry with  64 atoms:
 H   1.1276   0.6212  -1.8343
 C   0.6118   2.8236  -0.6473
 H   0.8389   2.8251  -1.7172
 H   1.0214   3.7257  -0.1909
 N  -0.9519   3.1214  -0.6437
 C  -1.2032   4.4761  -1.2578
 H  -0.7449   5.2125  -0.5948
 H  -0.6872   4.4977  -2.2202
 C  -1.6910   2.0873  -1.4551
 H  -1.3496   2.1990  -2.4868
 H  -1.3854   1.1088  -1.0905
 C  -1.4991   3.1260   0.7629
 H  -0.8649   3.7866   1.3533
 H  -1.3865   2.1108   1.1424
 C   1.0549   1.5904   0.0266
 C   1.2076   0.3324  -0.7787
 O   0.1257  -0.6646  -0.6829
 C  -0.4517  -0.8895   0.5901
 H  -0.7577   0.0849   1.0068
 O   0.4082  -1.5239   1.4944
 C  -4.0681  -3.1632   0.1142
 C  -3.3693  -3.2297   1.3222
 C  -2.1866  -2.5067   1.4512
 C  -1.7016  -1.7272   0.3901
 C  -2.4220  -1.6832  -0.8134
 C  -3.6068  -2.3994  -0.9607
 H  -3.7437  -3.8353   2.1385
 H  -1.6260  -2.5509   2.3775
 H  -2.0450  -1.0996  -1.6441
 H  -4.1624  -2.3719  -1.8899
 C   5.0918  -1.5532  -0.6321
 C   3.9516  -2.3593  -0.5873
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 C    2.6972   -1.7554   -0.6100
 C    2.5686   -0.3603   -0.6635
 C    3.7351    0.4229   -0.7154
 C    4.9965   -0.1589   -0.6986
 H    4.0481   -3.4370   -0.5350
 H    1.8066   -2.3669   -0.5632
 H    3.6483    1.5042   -0.7499
 H    5.8925    0.4487   -0.7306
 C    1.4705    1.6120    1.3709
 O    1.4354    2.8572    1.9713
 O    1.8661    0.6300    2.0533
 C    1.8104    2.9077    3.3543
 H    2.8492    2.5953    3.4980
 H    1.1610    2.2729    3.9654
 H    1.6936    3.9526    3.6502
 C   -3.2172    2.3348   -1.3070
 H   -3.6752    1.5544   -0.6931
 H   -3.6952    2.3155   -2.2901
 C   -2.9820    3.5883    0.7173
 H   -3.0864    4.5856    1.1533
 H   -3.6055    2.8997    1.2938
 C   -2.7389    4.6804   -1.4005
 H   -3.0360    4.6383   -2.4519
 H   -3.0219    5.6599   -1.0064
 N   -3.4767    3.6363   -0.6694
 H    1.0540   -0.8274    1.7835
 N   -5.3163   -3.9153   -0.0309
 O   -5.9178   -3.8522   -1.1099
 O   -5.7170   -4.5800    0.9316
 N    6.4108   -2.1774   -0.6120
 O    7.4101   -1.4468   -0.6543
 O    6.4794   -3.4124   -0.5554

r2_7_SRR
Final geometry with  64 atoms:
 N   -0.2411   -2.7675    3.3211
 C   -0.4964   -3.5579    2.1042
 C    1.1638   -2.9498    3.7219
 C   -0.4648   -1.3455    3.0118
 N    1.3297   -2.0153    1.4191
 C    0.3280   -3.0195    0.9013
 C    2.1223   -2.6517    2.5334
 C    0.5812   -0.8315    1.9850
 H   -1.5638   -3.5152    1.8712
 H   -0.2370   -4.5996    2.3123
 H    1.3067   -3.9780    4.0652
 H    1.3710   -2.2799    4.5608
 H   -0.4003   -0.7634    3.9352
 H   -1.4769   -1.2374    2.6121
 H   -0.2843   -2.4967    0.1661
 H    0.8911   -3.8028    0.3936
 H    2.5689   -3.5599    2.1235
 H    2.9205   -1.9569    2.8038
 H    1.3296   -0.1807    2.4422
 H    0.1146   -0.3176    1.1474
 C    2.3347   -1.5511    0.2646
 C    1.7311   -1.3011   -1.0533
 C    1.6136   -2.3318   -1.9991
 O    2.2710   -3.5065   -1.6786
 O    0.9676   -2.2816   -3.0850
 C    2.1140   -4.5947   -2.5981
 H    2.6741   -5.4264   -2.1649
 H    2.5212   -4.3475   -3.5834
 H    1.0610   -4.8729   -2.7094
 H    2.8062   -0.6724    0.7114
 H    3.0556   -2.3670    0.2345
 H   -0.5883   -1.8309   -2.6493
 C    1.0689    0.0005   -1.3930
 H    1.0467    0.0894   -2.4869
 C    1.8109    1.2187   -0.8642
 C    3.1435    1.4195   -1.2678
 C    3.8759    2.5099   -0.8154
 C    3.2637    3.4118    0.0627
 C    1.9417    3.2441    0.4775
 C    1.2219    2.1475    0.0056
 H    3.6083    0.7045   -1.9397
 H    4.9007    2.6637   -1.1302
 H    1.4870    3.9574    1.1542
 H    0.1927    2.0128    0.3133
 N    4.0268    4.5575    0.5552
 O    5.2006    4.6845    0.1850
 O    3.4684    5.3514    1.3227
 O   -0.3239    0.0956   -0.9332
 C   -1.3203   -0.1808   -1.9097
 H   -1.0781    0.3966   -2.8195
 C   -2.6196    0.3317   -1.3166
 C   -3.6833   -0.5280   -1.0203
 C   -4.8541   -0.0337   -0.4468
 C   -4.9456    1.3335   -0.1801
 C   -3.9007    2.2159   -0.4752
 C   -2.7403    1.7032   -1.0436
 H   -3.5923   -1.5845   -1.2418
 H   -5.6810   -0.6928   -0.2123
 H   -4.0006    3.2730   -0.2620
 H   -1.9161    2.3709   -1.2739
 N   -6.1708    1.8608    0.4261
 O   -6.2363    3.0742    0.6556
 O   -7.0859    1.0704    0.6847
 O   -1.4353   -1.5369   -2.2179

r2_7_SRS
Final geometry with  64 atoms:
 N   -5.3937   -0.1178   -1.7743
 C   -5.2388   -1.4106   -1.0849
 C   -5.7347    0.9141   -0.7807
 C   -4.1104    0.2366   -2.4036
 N   -3.5415    0.0400    0.0125
 C   -4.0324   -1.3826   -0.1049
 C   -4.7093    0.9176    0.3880
 C   -3.0155    0.4858   -1.3301
 H   -5.0944   -2.1955   -1.8322
 H   -6.1656   -1.6237   -0.5451
 H   -6.7390    0.7204   -0.3944
 H   -5.7461    1.8845   -1.2845
 H   -4.2476    1.1340   -3.0131
 H   -3.8165   -0.5820   -3.0664
 H   -3.1878   -1.9746   -0.4577
 H   -4.2935   -1.7162    0.8991
 H   -5.1286    0.5064    1.3085
 H   -4.3152    1.9151    0.5936
 H   -2.7646    1.5437   -1.2276
 H   -2.1044   -0.0799   -1.5227
 C   -2.4173    0.1715    1.1313
 C   -1.2634   -0.7358    1.0191
 C   -1.2642   -1.9935    1.6448
 O   -2.3684   -2.2622    2.4322
 O   -0.3629   -2.8747    1.5519
 C   -2.4246   -3.5649    3.0267
 H   -3.3689   -3.5958    3.5751
 H   -1.5905   -3.7262    3.7167
 H   -2.4113   -4.3502    2.2641
 H   -2.1450    1.2271    1.0576
 H   -2.9824    0.0133    2.0507
 H    0.0443   -3.0802   -0.0482
 C   -0.0245   -0.3814    0.2496
 H    0.8113   -0.9120    0.7180
 C    0.3126    1.0977    0.3033
 C    0.7406    1.6449    1.5255
 C    1.0432    2.9961    1.6416
 C    0.9041    3.8137    0.5138
 C    0.4836    3.2999   -0.7144
 C    0.1950    1.9401   -0.8107
 H    0.8345    0.9992    2.3937
 H    1.3807    3.4145    2.5819
 H    0.3906    3.9508   -1.5752
 H   -0.1149    1.5250   -1.7614
 N    1.2083    5.2390    0.6240
 O    1.6049    5.6733    1.7125
 O    1.0544    5.9531   -0.3753
 O   -0.0522   -0.7884   -1.1683
 C    0.7124   -1.9397   -1.5115
 H    0.6430   -1.9814   -2.6051
 C    2.1875   -1.7467   -1.1368
 C    2.8338   -0.5578   -1.5130
 C    4.1723   -0.3445   -1.2057
 C    4.8655   -1.3429   -0.5130
 C    4.2517   -2.5377   -0.1331
 C    2.9094   -2.7332   -0.4551
 H    2.2752    0.2121   -2.0344
 H    4.6726    0.5734   -1.4889
 H    4.8124   -3.2941    0.4021
 H    2.4175   -3.6561   -0.1709
 N    6.2754   -1.1294   -0.1788
 O    6.8066   -0.0676   -0.5257
 O    6.8752   -2.0195    0.4354
 O    0.1715   -3.1333   -1.0371

r2_11
Final geometry with  28 atoms:
 C   -3.0284   -0.9850    1.7064
 C   -2.3301   -0.6849    0.6027
 C   -2.5517    0.5893   -0.1507
 O   -3.7251    1.1772    0.1521
 O   -1.7567    1.0558   -0.9483
 C   -3.9893    2.4410   -0.4996
 H   -4.9637    2.7588   -0.1286
 H   -4.0173    2.3115   -1.5847
 H   -3.2221    3.1740   -0.2369
 H   -2.8352   -1.9041    2.2536
 H   -3.7952   -0.3242    2.0963
 H   -2.4296   -2.5860   -1.1852
 C   -1.2631   -1.6271    0.0622
 H   -1.2167   -2.4820    0.7521
 C    0.1271   -1.0137    0.0312
 C    0.6653   -0.5017    1.2224
 C    1.9436    0.0436    1.2509
 C    2.6872    0.0672    0.0671
 C    2.1784   -0.4429   -1.1295
 C    0.8956   -0.9844   -1.1392
 H    0.0772   -0.5232    2.1351
 H    2.3603    0.4423    2.1674
 H    2.7746   -0.4116   -2.0332
 H    0.4838   -1.3742   -2.0615
 N    4.0338    0.6385    0.0838
 O    4.4638    1.0991    1.1486
 O    4.6867    0.6367   -0.9668
 O   -1.6013   -2.0887   -1.2486

r2_11a
Final geometry with  28 atoms:
 C   -2.9518   -0.5824    1.9275
 C   -2.3356   -0.5783    0.7387
 C   -2.6278    0.4472   -0.3051
 O   -3.3131    1.5046    0.1413
 O   -2.2716    0.3220   -1.4735
 C   -3.6689    2.5068   -0.8433
 H   -4.2226    3.2660   -0.2915
 H   -4.2943    2.0659   -1.6236
 H   -2.7681    2.9365   -1.2881
 H   -2.7374   -1.3540    2.6621
 H   -3.6827    0.1733    2.1953
 H   -1.8580   -1.6928   -1.5080
 C   -1.2970   -1.6245    0.3491
 H   -1.2556   -2.3646    1.1556
 C    0.1007   -1.0088    0.2247
 C    0.5922   -0.1860    1.2520
 C    1.8685    0.3620    1.1808
 C    2.6571    0.0787    0.0622
 C    2.1975   -0.7390   -0.9716
 C    0.9172   -1.2807   -0.8805
 H   -0.0280    0.0321    2.1158
 H    2.2473    0.9966    1.9725
 H    2.8288   -0.9458   -1.8270
 H    0.5538   -1.9226   -1.6743
 N    4.0024    0.6510   -0.0254
 O    4.3932    1.3746    0.8981
 O    4.6899    0.3856   -1.0182
 O   -1.6875   -2.3516   -0.8123

r2_11b
Final geometry with  28 atoms:
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```
 C    3.0961   -1.8430   -1.0298
 C    2.4714   -0.9106   -0.2998
 C    2.7227    0.5312   -0.6158
 O    2.1630    1.3460    0.3075
 O    3.3514    0.9458   -1.5725
 C    2.3092    2.7714    0.0952
 H    1.7805    3.2416    0.9239
 H    1.8587    3.0565   -0.8584
 H    3.3660    3.0485    0.1053
 H    2.9411   -2.9013   -0.8400
 H    3.7741   -1.5660   -1.8314
 H    2.0525    0.1438    2.0461
 C    1.5033   -1.2733    0.8200
 H    1.4962   -2.3658    0.8979
 C    0.0685   -0.8357    0.5131
 C   -0.4685   -1.0462   -0.7675
 C   -1.7800   -0.6868   -1.0610
 C   -2.5575   -0.1094   -0.0536
 C   -2.0535    0.1049    1.2305
 C   -0.7389   -0.2640    1.5058
 H    0.1429   -1.4915   -1.5459
 H   -2.1937   -0.8467   -2.0491
 H   -2.6779    0.5497    1.9957
 H   -0.3407   -0.1086    2.5017
 N   -3.9385    0.2769   -0.3518
 O   -4.3707    0.0751   -1.4925
 O   -4.6125    0.7881    0.5500
 O    1.9604   -0.8213    2.0942

r2_11c
Final geometry with  28 atoms:
 C    3.2190   -1.6301   -1.1469
 C    2.5149   -0.8088   -0.3563
 C    2.7420    0.6692   -0.4856
 O    1.8298    1.3853    0.1865
 O    3.6445    1.1715   -1.1370
 C    1.9509    2.8231    0.1119
 H    1.1248    3.2125    0.7067
 H    1.8680    3.1593   -0.9249
 H    2.9084    3.1463    0.5285
 H    3.0916   -2.7077   -1.0927
 H    3.9316   -1.2400   -1.8669
 H    2.7754   -1.4232    2.1745
 C    1.5274   -1.3573    0.6667
 H    1.5345   -2.4508    0.5521
 C    0.0951   -0.9048    0.4328
 C   -0.4987   -1.1572   -0.8138
 C   -1.8122   -0.7787   -1.0679
 C   -2.5324   -0.1413   -0.0532
 C   -1.9674    0.1161    1.1978
 C   -0.6509   -0.2711    1.4345
 H    0.0732   -1.6481   -1.5955
 H   -2.2723   -0.9709   -2.0293
 H   -2.5472    0.6121    1.9665
 H   -0.1960   -0.0704    2.3963
 N   -3.9151    0.2647   -0.3084
 O   -4.4011    0.0278   -1.4209
 O   -4.5391    0.8281    0.5988
 O    1.9143   -1.0160    2.0005

r2_11d
Final geometry with  28 atoms:
 C    1.3764   -1.4311   -1.2463
 C    1.9519   -0.5449   -0.4229
 C    3.4441   -0.5924   -0.2829
 O    3.9038    0.3936    0.5225
 O    4.1783   -1.4050   -0.8156
 C    5.3365    0.4467    0.7311
 H    5.4995    1.2950    1.3955
 H    5.8512    0.5985   -0.2207
 H    5.6834   -0.4784    1.1972
 H    0.3029   -1.4644   -1.3957
 H    1.9818   -2.1500   -1.7896
 H    2.4961    1.9588    0.1280
 C    1.2018    0.5197    0.3828
 H    1.4876    0.4041    1.4370
 C   -0.3021    0.3748    0.2899
 C   -0.9653   -0.5026    1.1604
 C   -2.3414   -0.6889    1.0728
 C   -3.0503    0.0215    0.1005
 C   -2.4173    0.9067   -0.7747
 C   -1.0385    1.0769   -0.6740
 H   -0.4009   -1.0461    1.9126
 H   -2.8572   -1.3649    1.7436
 H   -2.9922    1.4458   -1.5176
 H   -0.5312    1.7615   -1.3436
 N   -4.5003   -0.1681   -0.0027
 O   -5.0447   -0.9593    0.7758
 O   -5.1152    0.4693   -0.8649
 O    1.5536    1.8388   -0.0614
```

(c) Structures in react. III.

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r3_DABCO
Final geometry with  20 atoms:
 N   -1.2896    0.0001   -0.0001
 C   -0.7822    1.3841   -0.1131
 C   -0.7821   -0.7899   -1.1421
 C   -0.7824   -0.5941    1.2549
 N    1.2896    0.0000    0.0002
 C    0.7823    1.3841   -0.1128
 C    0.7823   -0.7898   -1.1420
 C    0.7821   -0.5943    1.2550
 H   -1.1809    1.9631    0.7274
 H   -1.1803    1.8188   -1.0367
 H   -1.1801   -0.3512   -2.0639
 H   -1.1804   -1.8071   -1.0571
 H   -1.1807   -1.6117    1.3355
 H   -1.1809   -0.0122    2.0934
 H    1.1806    1.9630    0.7280
 H    1.1807    1.8190   -1.0362
 H    1.1804   -0.3509   -2.0636
 H    1.1808   -1.8070   -1.0571
 H    1.1802   -1.6119    1.3355
 H    1.1806   -0.0126    2.0936

r3_MA
Final geometry with  12 atoms:
 C    2.5028   -0.0212    0.0001
 C    1.3186   -0.6427   -0.0001
 C    0.0454    0.1203   -0.0002
 O   -1.0139   -0.7153    0.0000
 O   -0.0588    1.3371   -0.0001
 C   -2.3203   -0.0972    0.0002
 H   -3.0323   -0.9227    0.0004
 H   -2.4514    0.5193   -0.8932
 H   -2.4511    0.5195    0.8935
 H    3.4323   -0.5828    0.0002
 H    2.5669    1.0639    0.0000
 H    1.2387   -1.7260   -0.0000

r3_BA
Final geometry with  14 atoms:
 C   -1.9897    0.4679   -0.0000
 H   -2.2697    1.5410    0.0000
 C   -0.5367    0.2044   -0.0000
 C   -0.0374   -1.1106   -0.0000
 C    1.3377   -1.3302   -0.0000
 C    2.2221   -0.2413    0.0000
 C    1.7311    1.0685    0.0000
 C    0.3528    1.2913   -0.0000
 H   -0.7355   -1.9422   -0.0000
 H    1.7263   -2.3444   -0.0000
 H    2.4188    1.9091    0.0000
 H   -0.0384    2.3061    0.0000
 H    3.2943   -0.4168    0.0000
 O   -2.8594   -0.3942    0.0000

r3_THF
Final geometry with  13 atoms:
 C    1.1727    0.4245    0.1343
 O   -0.0000    1.2577   -0.0001
 C   -1.1727    0.4245   -0.1342
 C   -0.7319   -0.9947    0.2330
 C    0.7319   -0.9947   -0.2331
 H    1.9571    0.8211   -0.5197
 H    1.5277    0.4734    1.1743
 H   -1.9570    0.8210    0.5200
 H   -1.5280    0.4734   -1.1742
 H   -0.7857   -1.1432    1.3181
 H   -1.3442   -1.7612   -0.2513
 H    1.3443   -1.7611    0.2512
 H    0.7858   -1.1431   -1.3182

r3_TS1
Final geometry with  32 atoms:
 N   -3.0374    0.9398    0.1774
 C   -1.8999    1.7452   -0.3063
 C   -3.3087   -0.1387   -0.7911
 C   -2.6730    0.3398    1.4741
 N   -0.9660   -0.5388   -0.0935
 C   -0.6316    0.8557   -0.4879
 C   -2.0539   -1.0552   -0.9633
 C   -1.4092   -0.5638    1.3248
 H   -1.7135    2.5450    0.4166
 H   -2.1825    2.2079   -1.2565
 H   -3.5857    0.3167   -1.7464
 H   -4.1635   -0.7196   -0.4322
 H   -3.5233   -0.2454    1.8366
 H   -2.4890    1.1475    2.1887
 H    0.2027    1.1771    0.1391
 H   -0.2855    0.8281   -1.5229
 H   -1.6835   -1.0551   -1.9920
 H   -2.2549   -2.0883   -0.6659
 H   -1.6166   -1.6053    1.5864
 H   -0.5705   -0.2147    1.9325
 C    0.5484   -1.6051   -0.2739
 C    1.6723   -1.1615    0.4490
 C    2.6048   -0.2580   -0.1392
 O    3.6349    0.0684    0.7274
 O    2.5828    0.2178   -1.2861
 C    4.6415    0.9427    0.2046
 H    5.3592    1.0875    1.0154
 H    4.2174    1.9080   -0.0919
 H    5.1454    0.4990   -0.6607
 H    0.0576   -2.5164    0.0657
 H    0.6029   -1.5175   -1.3584
 H    1.8213   -1.4569    1.4821

r3_3
Final geometry with  32 atoms:
 N   -2.9970    0.9171    0.2492
 C   -1.8933    1.7385   -0.2793
 C   -3.3005   -0.1511   -0.7181
 C   -2.5649    0.3050    1.5180
 N   -0.9130   -0.5423   -0.1356
 C   -0.5909    0.9008   -0.4191
 C   -2.0243   -0.9804   -1.0477
 C   -1.3747   -0.6697    1.2875
 H   -1.7292    2.5818    0.3973
 H   -2.1981    2.1385   -1.2504
 H   -3.7009    0.3016   -1.6295
 H   -4.0748   -0.7934   -0.2895
 H   -3.4102   -0.2311    1.9584
 H   -2.2776    1.1067    2.2038
 H    0.1800    1.1916    0.2946
 H   -0.1584    0.9427   -1.4189
 H   -1.6772   -0.8195   -2.0709
 H   -2.1729   -2.0514   -0.8906
 H   -1.6573   -1.7147    1.4357
 H   -0.5152   -0.4438    1.9210
 C    0.4064   -1.4767   -0.3858
 C    1.5868   -1.1275    0.3831
 C    2.5378   -0.2351   -0.1420
 O    3.6224   -0.0363    0.7188
 O    2.5143    0.3602   -1.2421
 C    4.6506    0.8298    0.2371
 H    5.4006    0.8732    1.0314
 H    4.2706    1.8379    0.0361
 H    5.1103    0.4422   -0.6794
 H   -0.0021   -2.4661   -0.1627
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 H   0.5444  -1.3556  -1.4634
 H   1.7472  -1.5565   1.3659

r3_TS2_SS
Final geometry with  46 atoms:
 H  -1.5321  -0.8062  -2.1030
 C   0.9855  -0.5936  -0.9427
 H   0.9496  -1.6811  -1.0595
 H   1.0689  -0.1220  -1.9245
 N   2.3378  -0.3148  -0.2514
 C   3.4554  -0.7271  -1.1892
 H   3.4072  -0.0483  -2.0431
 H   3.2358  -1.7411  -1.5281
 C   2.4731  -1.1157   1.0269
 H   2.4692  -2.1672   0.7337
 H   1.5927  -0.9149   1.6360
 C   2.5121   1.1532   0.0756
 H   2.2664   1.7168  -0.8250
 H   1.7809   1.3891   0.8489
 O  -1.1438  -2.5216  -1.0385
 C  -5.1837  -0.2263   1.0177
 C  -4.3798  -1.2780   1.4773
 C  -3.2214  -1.6323   0.7819
 C  -2.8409  -0.9367  -0.3743
 C  -3.6559   0.1068  -0.8336
 C  -4.8191   0.4627  -0.1443
 H  -4.6617  -1.8234   2.3749
 H  -2.5973  -2.4548   1.1200
 H  -3.3719   0.6476  -1.7340
 C  -0.2396  -0.1260  -0.2380
 H  -5.4409   1.2744  -0.5140
 C  -0.6301   1.2565  -0.4495
 O  -1.3558   1.7571   0.5937
 O  -0.4205   1.9258  -1.4663
 C  -1.9495   3.0499   0.3955
 H  -1.1806   3.8187   0.2683
 H  -2.6059   3.0508  -0.4790
 H  -2.5307   3.2480   1.2976
 C  -1.5789  -1.3201  -1.1181
 C   3.7889  -0.6946   1.7359
 H   3.5716  -0.0927   2.6223
 H   4.3368  -1.5848   2.0563
 C   3.9712   1.3827   0.5578
 H   4.5491   1.9133  -0.2037
 H   3.9681   1.9900   1.4669
 C   4.8056  -0.6326  -0.4296
 H   5.1886  -1.6305  -0.2002
 H   5.5446  -0.1190  -1.0501
 N   4.6407   0.1005   0.8360
 H  -0.3679  -0.4725   0.7839
 H  -6.0878   0.0470   1.5553

r3_TS2_SR
Final geometry with  46 atoms:
 N  -4.5430  -0.1912  -0.4351
 C  -3.8258   0.8703  -1.1619
 C  -4.0608  -1.4989  -0.9080
 C  -4.2477  -0.0676   1.0020
 N  -2.0035  -0.3922  -0.0284
 C  -2.3175   0.8770  -0.7910
 C  -2.5118  -1.5729  -0.8325
 C  -2.7495  -0.3625   1.2890
 H  -4.2720   1.8372  -0.9144
 H  -3.9572   0.7004  -2.2339
 H  -4.3888  -1.6504  -1.9398
 H  -4.5145  -2.2776  -0.2893
 H  -4.8752  -0.7688   1.5585
 H  -4.5071   0.9458   1.3195
 H  -2.0569   1.7063  -0.1328
 H  -1.6608   0.9025  -1.6607
 H  -2.0417  -1.5020  -1.8152
 H  -2.1583  -2.4771  -0.3340
 H  -2.5938  -1.3377   1.7541
 H  -2.2879   0.4024   1.9127
 C  -0.4883  -0.5663   0.1938
 C   0.2387   0.5704   0.8221
 C   0.7441   1.5980  -0.0742
 O   1.1682   2.7027   0.6133
 O   0.8726   1.5174  -1.2978
 C   1.8005   3.7300  -0.1685
 H   2.0929   4.5038   0.5434
 H   1.1066   4.1436  -0.9071
 H   2.6830   3.3423  -0.6857
 H  -0.4023  -1.4495   0.8362
 H  -0.0800  -0.7845  -0.7941
 H  -0.1891   0.9635   1.7397
 C   1.7099  -0.3478   1.7613
 H   2.0661   0.5774   2.2579
 C   2.6530  -0.7455   0.6411
 C   3.5949   0.1623   0.1350
 C   4.4631  -0.2066  -0.8961
 C   4.4003  -1.4955  -1.4387
 C   3.4686  -2.4114  -0.9342
 C   2.6073  -2.0390   0.1017
 H   3.6434   1.1662   0.5516
 H   5.1884   0.5088  -1.2759
 H   3.4209  -3.4177  -1.3436
 H   1.8955  -2.7458   0.5180
 H   5.0746  -1.7852  -2.2404
 O   1.1800  -1.2680   2.4814

r3_5_SS
Final geometry with  46 atoms:
 H  -1.4936  -0.9142  -2.0408
 C   0.9951  -0.6226  -1.0198
 H   0.9821  -1.7050  -1.1707
 H   1.0645  -0.1101  -1.9817
 N   2.3010  -0.3182  -0.2904
 C   3.4504  -0.5990  -1.2441
 H   3.3693   0.1380  -2.0454
 H   3.2868  -1.5950  -1.6587
 C   2.4743  -1.2059   0.9291
 H   2.5290  -2.2303   0.5572
 H   1.5828  -1.1022   1.5459
 C   2.3945   1.1291   0.1502
 H   2.1292   1.7478  -0.7078
 H   1.6509   1.2667   0.9354
 C  -0.2900  -0.2465  -0.3155
 C  -1.4439  -1.2728  -0.9809
 O  -1.0681  -2.5365  -0.8284
 C  -5.2102  -0.1905   0.9262
 C  -4.3620  -1.1425   1.5077
 C  -3.1634  -1.4916   0.8802
 C  -2.7819  -0.8924  -0.3279
 C  -3.6430   0.0487  -0.9083
 C  -4.8479   0.4008  -0.2886
 H  -6.1465   0.0774   1.4090
 H  -4.6412  -1.6161   2.4462
 H  -2.5075  -2.2450   1.3076
 H  -3.3671   0.5122  -1.8534
 H  -5.5045   1.1308  -0.7562
 C  -0.6672   1.1865  -0.4932
 O  -1.2289   1.7109   0.6199
 O  -0.5505   1.8228  -1.5345
 C  -1.7856   3.0349   0.4947
 H  -1.0048   3.7614   0.2516
 H  -2.5568   3.0551  -0.2796
 H  -2.2233   3.2603   1.4677
 C   3.7617  -0.7679   1.6785
 H   3.5077  -0.2480   2.6062
 H   4.3550  -1.6493   1.9354
 C   3.8372   1.3988   0.6623
 H   4.3880   2.0166  -0.0517
 H   3.7950   1.9350   1.6138
 C   4.7874  -0.4875  -0.4657
 H   5.2253  -1.4767  -0.3089
 H   5.4991   0.1128  -1.0385
 N   4.5730   0.1378   0.8491
 H  -0.2905  -0.5148   0.7411

r3_5_SR
Final geometry with  46 atoms:
 N  -4.5239  -0.2198  -0.3760
 C  -3.8451   0.9118  -1.0294
 C  -4.0370  -1.4734  -0.9752
 C  -4.1809  -0.2171   1.0558
 N  -1.9672  -0.4120  -0.0682
 C  -2.3313   0.9243  -0.6835
 C  -2.4863  -1.5086  -0.9827
 C  -2.6775  -0.5432   1.2660
 H  -4.3052   1.8469  -0.6995
 H  -3.9918   0.8234  -2.1092
 H  -4.4118  -1.5548  -1.9989
 H  -4.4396  -2.3098  -0.3980
 H  -4.7930  -0.9589   1.5753
 H  -4.4219   0.7680   1.4641
 H  -2.0891   1.6871   0.0572
 H  -1.6943   1.0624  -1.5568
 H  -2.0690  -1.3038  -1.9704
 H  -2.0842  -2.4535  -0.6138
 H  -2.5120  -1.5685   1.6005
 H  -2.1997   0.1374   1.9694
 C  -0.4582  -0.5917   0.0837
 C   0.2895   0.5110   0.7955
 C   0.7455   1.6101  -0.1047
 O   1.1409   2.6921   0.6077
 O   0.8257   1.5674  -1.3268
 C   1.7127   3.7805  -0.1462
 H   1.9906   4.5332   0.5925
 H   0.9811   4.1909  -0.8481
 H   2.5958   3.4465  -0.6976
 H  -0.3337  -1.5065   0.6694
 H  -0.0741  -0.7310  -0.9272
 H  -0.2724   0.9301   1.6303
 C   1.5604  -0.2282   1.6393
 H   1.9967   0.6548   2.1612
 C   2.6067  -0.6900   0.6061
 C   3.5775   0.1882   0.1020
 C   4.5129  -0.2374  -0.8468
 C   4.4926  -1.5590  -1.3073
 C   3.5374  -2.4486  -0.8003
 C   2.6097  -2.0159   0.1526
 H   3.6030   1.2163   0.4583
 H   5.2593   0.4584  -1.2227
 H   3.5232  -3.4813  -1.1417
 H   1.8825  -2.7012   0.5784
 H   5.2195  -1.8944  -2.0426
 O   1.0717  -1.1778   2.4228

r3_TS3_SSR
Final geometry with  60 atoms:
 H  -0.9870  -0.2846  -1.0759
 C   1.6521  -0.2280  -0.9119
 H   1.1910  -1.2195  -0.9353
 H   1.8828   0.0844  -1.9318
 N   2.9892  -0.4171  -0.2180
 C   3.8634  -1.3003  -1.0933
 H   4.0875  -0.7198  -1.9904
 H   3.2676  -2.1708  -1.3713
 C   2.8197  -1.1179   1.1196
 H   2.4529  -2.1188   0.8906
 H   2.0448  -0.5973   1.6793
 C   3.7175   0.8959  -0.0083
 H   3.6920   1.4335  -0.9579
 H   3.1562   1.4593   0.7357
 C   0.7073   0.7744  -0.2391
 C  -0.7019   0.0518  -0.0614
 O  -0.5100  -1.0028   0.7992
 C  -0.9147  -2.6512  -0.0026
 H  -0.6339  -3.1498   0.9443
 O  -0.2074  -2.8263  -1.0348
 C  -5.1758  -2.0257  -0.3873
 C  -4.3520  -1.9837  -1.5171
 C  -2.9769  -2.2075  -1.3913
 C  -2.4086  -2.4605  -0.1367
 C  -3.2422  -2.5108   0.9898
 C  -4.6164  -2.2973   0.8687
 H  -4.7809  -1.7771  -2.4947
 H  -2.3242  -2.1870  -2.2590
 H  -2.8027  -2.6963   1.9672
 H  -5.2518  -2.3333   1.7501
```

```
 C  -3.6957   2.8893   1.2986
 C  -2.8703   2.2329   2.2205
 C  -1.9178   1.3115   1.7785
 C  -1.7684   1.0349   0.4130
 C  -2.6050   1.6879  -0.5014
 C  -3.5625   2.6102  -0.0652
 H  -2.9754   2.4357   3.2836
 H  -1.2899   0.7818   2.4887
 H  -2.5131   1.4662  -1.5620
 H  -4.2083   3.1020  -0.7884
 C   0.5922   2.0549  -1.0331
 O   0.5067   3.1343  -0.2338
 O   0.5364   2.1202  -2.2516
 C   0.2372   4.3965  -0.8836
 H   0.1732   5.1294  -0.0791
 H   1.0461   4.6551  -1.5723
 H  -0.7089   4.3473  -1.4285
 C   4.1941  -1.1286   1.8366
 H   4.2178  -0.3872   2.6400
 H   4.3681  -2.1131   2.2788
 C   5.1618   0.5866   0.4716
 H   5.8816   0.7686  -0.3307
 H   5.4165   1.2379   1.3116
 C   5.1385  -1.6792  -0.2951
 H   5.0891  -2.7192   0.0373
 H   6.0194  -1.5672  -0.9326
 N   5.2829  -0.8193   0.8920
 H   1.0125   1.0272   0.7771
 H  -6.2445  -1.8518  -0.4826
 H  -4.4416   3.6013   1.6418

r3_TS3_SSS
Final geometry with  60 atoms:
 H  -1.4955  -1.0008  -1.5312
 C   0.3903   0.7757  -0.9848
 H   0.7750  -0.2187  -1.2068
 H   0.2568   1.3197  -1.9213
 N   1.5056   1.4857  -0.2380
 C   2.6914   1.6207  -1.1802
 H   2.3703   2.2869  -1.9828
 H   2.8843   0.6301  -1.5933
 C   1.9610   0.6856   0.9724
 H   2.3588  -0.2504   0.5848
 H   1.0841   0.4634   1.5767
 C   1.0982   2.8751   0.2087
 H   0.6767   3.3830  -0.6607
 H   0.3236   2.7514   0.9653
 C  -0.9377   0.6613  -0.2334
 C  -1.4716  -0.8268  -0.4409
 O  -0.5677  -1.6721   0.1632
 C   0.1907  -2.8028  -0.9878
 H  -0.3588  -3.6858  -0.6028
 O   0.0018  -2.4519  -2.1955
 C   4.1984  -2.5331   0.6511
 C   3.9517  -2.1747  -0.6787
 C   2.6587  -2.2791  -1.2050
 C   1.5985  -2.7348  -0.4127
 C   1.8579  -3.1134   0.9123
 C   3.1455  -3.0088   1.4451
 H   5.2009  -2.4529   1.0634
 H   4.7659  -1.8182  -1.3053
 H   2.4480  -2.0060  -2.2349
 H   1.0380  -3.4702   1.5300
 H   3.3312  -3.2961   2.4771
 C  -5.5050  -1.1418   1.1320
 C  -4.4012  -1.3214   1.9752
 C  -3.1042  -1.2365   1.4624
 C  -2.8876  -0.9690   0.1036
 C  -3.9980  -0.8017  -0.7352
 C  -5.2992  -0.8858  -0.2273
 H  -6.5142  -1.2111   1.5293
 H  -4.5534  -1.5312   3.0311
 H  -2.2446  -1.3897   2.1082
 H  -3.8424  -0.6058  -1.7935
 H  -6.1488  -0.7580  -0.8934
 C  -1.9429   1.6873  -0.7071
 O  -2.6692   2.1844   0.3107
 O  -2.1201   2.0052  -1.8726
 C  -3.7600   3.0626  -0.0468
 H  -3.3832   3.9578  -0.5487
 H  -4.4656   2.5431  -0.6999
 H  -4.2403   3.3272   0.8954
 C   3.0202   1.5172   1.7412
 H   2.6069   1.8963   2.6795
 H   3.8781   0.8832   1.9797
 C   2.3532   3.6025   0.7698
 H   2.6692   4.3980   0.0900
 H   2.1154   4.0552   1.7357
 C   3.8993   2.1816  -0.3837
 H   4.6549   1.4050  -0.2393
 H   4.3583   3.0044  -0.9380
 N   3.4749   2.6657   0.9398
 H  -0.8162   0.7660   0.8458

r3_TS3_SRR
Final geometry with  60 atoms:
 N  -2.9285   3.2526  -0.7219
 C  -1.9426   3.8695   0.1782
 C  -2.3781   3.2179  -2.0846
 C  -3.1893   1.8733  -0.2752
 N  -0.7377   1.8918  -0.7442
 C  -0.5690   3.1469   0.0880
 C  -1.1203   2.3076  -2.1539
 C  -1.8735   1.0566  -0.1737
 H  -2.3306   3.8192   1.1987
 H  -1.8246   4.9227  -0.0901
 H  -2.1248   4.2392  -2.3810
 H  -3.1443   2.8445  -2.7688
 H  -3.8762   1.4053  -0.9852
 H  -3.6816   1.9061   0.7001
 H  -0.2026   2.8490   1.0695
 H   0.1925   3.7500  -0.4097
 H  -0.2580   2.8206  -2.5835
 H  -1.3000   1.3849  -2.7088
 H  -1.8979   0.1318  -0.7481
 H  -1.6125   0.7978   0.8521
 C   0.5479   1.0824  -0.8165
 C   1.1084   0.6365   0.5318
 C   2.3458   1.4144   0.9157
 O   2.6955   1.1618   2.1919
 O   2.9851   2.1609   0.1904
 C   3.9102   1.7850   2.6639
 H   4.0287   1.4459   3.6933
 H   3.8208   2.8742   2.6301
 H   4.7639   1.4698   2.0580
 H   0.2954   0.2123  -1.4213
 H   1.2662   1.7034  -1.3520
 H   0.3845   0.7485   1.3404
 C   1.3246  -0.9542   0.5441
 H   1.6388  -1.1785   1.5788
 C   2.4644  -1.3682  -0.3855
 C   3.8009  -1.2683   0.0328
 C   4.8496  -1.6181  -0.8226
 C   4.5766  -2.0790  -2.1154
 C   3.2479  -2.1965  -2.5370
 C   2.2018  -1.8470  -1.6763
 H   4.0228  -0.9237   1.0401
 H   5.8775  -1.5378  -0.4780
 H   3.0251  -2.5676  -3.5344
 H   1.1682  -1.9637  -1.9860
 H   5.3900  -2.3546  -2.7813
 O   0.1356  -1.5596   0.2146
 C  -0.9141  -1.7778   1.7597
 H  -0.2552  -2.5988   2.1070
 C  -2.1401  -2.2897   1.0328
 C  -3.3578  -1.6067   1.1360
 C  -4.4956  -2.0709   0.4674
 C  -4.4269  -3.2340  -0.3074
 C  -3.2154  -3.9316  -0.4030
 C  -2.0824  -3.4622   0.2662
 H  -3.3978  -0.7103   1.7476
 H  -5.4352  -1.5307   0.5558
 H  -3.1566  -4.8385  -0.9998
 H  -1.1372  -3.9915   0.1835
 H  -5.3096  -3.5989  -0.8262
 O  -0.9793  -0.7201   2.4492

r3_TS3_SRS
Final geometry with  60 atoms:
 N  -4.9875  -1.4944  -0.2366
 C  -4.7573  -0.7582   1.0174
 C  -5.0697  -0.5253  -1.3416
 C  -3.8400  -2.3899  -0.4751
 N  -2.8007  -0.1334  -0.3901
 C  -3.3461  -0.1106   1.0254
 C  -3.8620   0.4489  -1.3065
 C  -2.5639  -1.5774  -0.8089
 H  -4.8489  -1.4458   1.8622
 H  -5.5326   0.0066   1.1153
 H  -6.0009   0.0415  -1.2590
 H  -5.0909  -1.0790  -2.2839
 H  -4.0732  -3.0645  -1.3032
 H  -3.6873  -2.9957   0.4223
 H  -2.6452  -0.6722   1.6426
 H  -3.3582   0.9298   1.3512
 H  -4.1233   1.4260  -0.8957
 H  -3.4046   0.5853  -2.2878
 H  -2.3612  -1.5457  -1.8814
 H  -1.6715  -1.9506  -0.2999
 C  -1.5284   0.6887  -0.5302
 C  -0.4488   0.3806   0.4979
 C  -0.4952   1.3093   1.6854
 O   0.3370   0.8894   2.6580
 O  -1.1678   2.3250   1.7840
 C   0.4396   1.7309   3.8275
 H   1.1610   1.2364   4.4784
 H  -0.5295   1.8135   4.3269
 H   0.7950   2.7277   3.5530
 H  -1.1511   0.4588  -1.5269
 H  -1.8335   1.7344  -0.4816
 H  -0.5214  -0.6445   0.8649
 C   0.9907   0.3460  -0.2182
 H   1.6899   0.0785   0.5932
 C   1.3854   1.7348  -0.7189
 C   1.9375   2.6791   0.1607
 C   2.2668   3.9644  -0.2791
 C   2.0510   4.3258  -1.6137
 C   1.5143   3.3873  -2.5019
 C   1.1878   2.1020  -2.0569
 H   2.1201   2.4027   1.1965
 H   2.6978   4.6798   0.4167
 H   1.3568   3.6542  -3.5441
 H   0.7960   1.3612  -2.7466
 H   2.3093   5.3231  -1.9594
 O   0.9699  -0.5863  -1.2241
 C   1.1336  -2.3580  -0.5749
 H   0.9213  -2.7096  -1.6017
 C   2.6114  -2.3194  -0.2688
 C   3.5582  -2.3842  -1.3008
 C   4.9250  -2.3464  -1.0162
 C   5.3620  -2.2368   0.3107
 C   4.4230  -2.1731   1.3460
 C   3.0553  -2.2204   1.0564
 H   3.2171  -2.4538  -2.3312
 H   5.6499  -2.3995  -1.8246
 H   4.7564  -2.0910   2.3777
 H   2.3140  -2.1889   1.8494
 H   6.4253  -2.2050   0.5339
 O   0.3056  -2.6039   0.3491

r3_6_SSR
Final geometry with  60 atoms:
 H  -0.9868  -0.3261  -1.0643
 C   1.6380  -0.2252  -0.9135
 H   1.1812  -1.2246  -0.9299
 H   1.8522   0.0930  -1.9351
 N   2.9841  -0.4013  -0.2338
 C   3.7923  -1.3977  -1.0528
 H   3.7798  -1.0496  -2.0866
 H   3.2607  -2.3480  -0.9907
 C   2.8244  -0.9690   1.1680
```

H	2.1271	-1.8034	1.0933
H	2.3690	-0.1889	1.7759
C	3.7688	0.8899	-0.1545
H	3.9701	1.1927	-1.1840
H	3.1363	1.6402	0.3193
C	0.6844	0.7682	-0.2335
C	-0.7139	0.0590	-0.0719
O	-0.5232	-0.9868	0.8412
C	-0.8571	-2.4373	0.2618
H	-0.6872	-2.9759	1.2221
O	-0.0930	-2.7673	-0.7365
C	-5.1310	-2.1926	-0.5339
C	-4.2226	-2.3385	-1.5877
C	-2.8516	-2.4392	-1.3234
C	-2.3692	-2.3832	-0.0118
C	-3.2874	-2.2440	1.0387
C	-4.6580	-2.1509	0.7845
H	-6.1966	-2.1158	-0.7349
H	-4.5822	-2.3762	-2.6134
H	-2.1294	-2.5626	-2.1255
H	-2.9200	-2.1895	2.0611
H	-5.3574	-2.0381	1.6094
C	-3.7520	2.8696	1.2167
C	-2.9039	2.2673	2.1547
C	-1.9347	1.3520	1.7385
C	-1.7960	1.0262	0.3827
C	-2.6539	1.6248	-0.5484
C	-3.6263	2.5427	-0.1368
H	-4.5099	3.5779	1.5405
H	-3.0030	2.5083	3.2101
H	-1.2879	0.8681	2.4641
H	-2.5679	1.3632	-1.6001
H	-4.2895	2.9926	-0.8711
C	0.5565	2.0540	-1.0267
O	0.4883	3.1307	-0.2252
O	0.4858	2.1174	-2.2431
C	0.2223	4.3975	-0.8702
H	0.1772	5.1294	-0.0636
H	1.0243	4.6479	-1.5697
H	-0.7320	4.3570	-1.4012
C	4.2275	-1.3672	1.6982
H	4.3557	-0.9924	2.7171
H	4.3357	-2.4547	1.7202
C	5.0654	0.6278	0.6621
H	5.9224	1.0647	0.1430
H	4.9941	1.0902	1.6502
C	5.2280	-1.4739	-0.4718
H	5.5282	-2.5196	-0.3659
H	5.9400	-0.9810	-1.1391
N	5.2925	-0.8152	0.8427
H	0.9944	1.0242	0.7805

r3_6_SSS
Final geometry with 60 atoms:

H	-1.3570	0.5933	1.7971
C	0.1927	-1.4315	1.0670
H	0.6410	-0.6056	1.6352
H	-0.1048	-2.2279	1.7511
N	1.3140	-2.0047	0.2207
C	2.3464	-2.6140	1.1557
H	1.8697	-3.4786	1.6212
H	2.5625	-1.8697	1.9230
C	2.0106	-0.9176	-0.5813
H	2.4799	-0.2601	0.1499
H	1.2514	-0.3391	-1.1040
C	0.8346	-3.0904	-0.7225
H	0.2098	-3.7715	-0.1413
H	0.2240	-2.6064	-1.4843
C	-1.0187	-0.9156	0.2739
C	-1.2848	0.5802	0.7004
O	-0.1674	1.3031	0.2652
C	0.6148	2.0406	1.4357
H	-0.1324	2.8227	1.7181
O	0.9751	1.2389	2.3945
C	3.7901	3.9092	-0.8809
C	4.0941	2.9643	0.1053
C	3.0669	2.3720	0.8499
C	1.7295	2.7059	0.6160
C	1.4336	3.6615	-0.3662
C	2.4532	4.2597	-1.1126
H	4.5853	4.3748	-1.4577
H	5.1302	2.6959	0.2989
H	3.2797	1.6468	1.6303
H	0.3954	3.9285	-0.5488
H	2.2091	4.9978	-1.8729
C	-5.0017	2.0084	-1.0126
C	-3.8104	2.0909	-1.7439
C	-2.6099	1.6467	-1.1840
C	-2.5811	1.1144	0.1122
C	-3.7757	1.0446	0.8419
C	-4.9804	1.4865	0.2845
H	-5.9352	2.3563	-1.4470
H	-3.8179	2.5032	-2.7497
H	-1.6815	1.7197	-1.7420
H	-3.7628	0.6440	1.8527
H	-5.8975	1.4298	0.8652
C	-2.2384	-1.7888	0.4881
O	-2.9542	-1.9318	-0.6403
O	-2.5629	-2.2818	1.5559
C	-4.2120	-2.6350	-0.5211
H	-4.0456	-3.6651	-0.1948
H	-4.8654	-2.1232	0.1898
H	-4.6495	-2.6173	-1.5193
C	3.0300	-1.5963	-1.5307
H	2.6537	-1.6123	-2.5571
H	3.9670	-1.0333	-1.5218
C	2.0763	-3.7874	-1.3418
H	2.2268	-4.7746	-0.8969
H	1.9247	-3.9178	-2.4165
C	3.5989	-2.9985	0.3253
H	4.4131	-2.2927	0.5087
H	3.9409	-3.9958	0.6147
N	3.2911	-2.9869	-1.1144
H	-0.8249	-0.8668	-0.7987

r3_6_SRR
Final geometry with 60 atoms:

N	2.1695	3.9412	0.7249
C	0.9676	4.3973	0.0068
C	1.7897	3.5987	2.1054
C	2.6842	2.7287	0.0598
N	0.3763	2.0864	0.7199
C	-0.0330	3.2266	-0.1933
C	0.5604	2.6514	2.1173
C	1.7196	1.5343	0.2600
H	1.2592	4.7984	-0.9673
H	0.5064	5.2042	0.5828
H	1.5530	4.5141	2.6543
H	2.6464	3.1234	2.5902
H	3.6668	2.4804	0.4699
H	2.8084	2.9498	-1.0040
H	-0.0066	2.8434	-1.2128
H	-1.0582	3.4957	0.0637
H	-0.3663	3.1718	2.3679
H	0.6899	1.8050	2.7942
H	2.0495	0.8630	1.0548
H	1.5633	0.9448	-0.6506
C	-0.6695	0.9867	0.7738
C	-1.1230	0.4614	-0.5869
C	-2.4344	1.0717	-1.0297
O	-2.7722	0.6495	-2.2616
O	-3.1187	1.8515	-0.3854
C	-4.0262	1.1368	-2.7903
H	-4.1286	0.6687	-3.7694
H	-4.0021	2.2252	-2.8890
H	-4.8552	0.8463	-2.1396
H	-0.2011	0.1870	1.3466
H	-1.5092	1.3918	1.3391
H	-0.3802	0.6608	-1.3677
C	-1.1247	-1.1230	-0.5994
H	-1.4268	-1.4184	-1.6144
C	-2.1197	-1.7022	0.3963
C	-3.4877	-1.7380	0.0823
C	-4.4213	-2.2207	1.0031
C	-3.9993	-2.6806	2.2554
C	-2.6373	-2.6618	2.5716
C	-1.7047	-2.1777	1.6479
H	-3.8246	-1.3958	-0.8928
H	-5.4756	-2.2442	0.7403
H	-2.2977	-3.0294	3.5366
H	-0.6458	-2.1824	1.8834
H	-4.7233	-3.0593	2.9719
O	0.1696	-1.5693	-0.3126
C	1.1122	-1.5853	-1.5678
H	0.6408	-2.4093	-2.1610
C	2.4040	-2.1240	-0.9314
C	3.5755	-1.3615	-0.9700
C	4.7604	-1.8386	-0.3967
C	4.7859	-3.0954	0.2175
C	3.6195	-3.8715	0.2502
C	2.4399	-3.3865	-0.3222
H	3.5389	-0.3952	-1.4644
H	5.6639	-1.2342	-0.4347
H	3.6323	-4.8520	0.7203
H	1.5330	-3.9856	-0.2916
H	5.7052	-3.4713	0.6593
O	1.1956	-0.4380	-2.1888

r3_6_SRS
Final geometry with 60 atoms:

N	-4.9654	-1.4966	-0.3185
C	-4.7322	-0.8882	1.0018
C	-5.0741	-0.4217	-1.3187
C	-3.8060	-2.3446	-0.6569
N	-2.8019	-0.0906	-0.3540
C	-3.3323	-0.2192	1.0622
C	-3.8814	0.5628	-1.1981
C	-2.5458	-1.4824	-0.9180
H	-4.8013	-1.6604	1.7723
H	-5.5196	-0.1524	1.1863
H	-6.0127	0.1188	-1.1692
H	-5.0987	-0.8774	-2.3121
H	-4.0380	-2.9362	-1.5466
H	-3.6346	-3.0359	0.1729
H	-2.6165	-0.8275	1.6139
H	-3.3573	0.7828	1.4911
H	-4.1533	1.4905	-0.6909
H	-3.4368	0.8023	-2.1656
H	-2.3585	-1.3354	-1.9839
H	-1.6369	-1.8885	-0.4566
C	-1.5454	0.7601	-0.4257
C	-0.4494	0.3731	0.5630
C	-0.4637	1.2353	1.8049
O	0.4634	0.8236	2.6885
O	-1.2041	2.1840	2.0139
C	0.5848	1.5934	3.9059
H	1.3892	1.1195	4.4686
H	-0.3484	1.5610	4.4743
H	0.8390	2.6319	3.6780
H	-1.1839	0.6404	-1.4465
H	-1.8649	1.7916	-0.2744
H	-0.5382	-0.6725	0.8768
C	0.9637	0.3379	-0.1559
H	1.6847	0.0455	0.6187
C	1.3657	1.7047	-0.6913
C	1.8831	2.6753	0.1814
C	2.2160	3.9509	-0.2818
C	2.0397	4.2761	-1.6313
C	1.5379	3.3116	-2.5108
C	1.2051	2.0355	-2.0437
H	2.0394	2.4280	1.2283
H	2.6205	4.6866	0.4084
H	1.4107	3.5495	-3.5639
H	0.8369	1.2793	-2.7290
H	2.3015	5.2662	-1.9945
O	0.9198	-0.6011	-1.1912
C	1.1026	-2.1092	-0.7228
H	0.9555	-2.5538	-1.7340
C	2.5954	-2.1974	-0.3657
C	3.5795	-2.0809	-1.3574
C	4.9370	-2.1394	-1.0298

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 C    5.3290   -2.3115    0.3045
 C    4.3533   -2.4317    1.3001
 C    2.9958   -2.3803    0.9623
 H    3.2762   -1.9343   -2.3919
 H    5.6891   -2.0492   -1.8100
 H    4.6500   -2.5689    2.3375
 H    2.2210   -2.4857    1.7163
 H    6.3841   -2.3557    0.5625
 O    0.2611   -2.4829    0.2014

r3_TS4_SSR
Final geometry with  60 atoms:
 H   -0.6241    0.9025    0.7305
 C    0.3112   -1.5005    0.8785
 H    0.1473   -0.9289    1.7946
 H    0.0818   -2.5485    1.0764
 N    1.8433   -1.4752    0.7046
 C    2.4784   -2.2441    1.8436
 H    2.1923   -3.2897    1.7115
 H    2.0410   -1.8714    2.7721
 C    2.3676   -0.0549    0.7417
 H    2.1670    0.3215    1.7469
 H    1.8009    0.5193    0.0115
 C    2.2717   -2.1201   -0.6003
 H    1.7469   -3.0726   -0.6746
 H    1.9299   -1.4664   -1.4007
 C   -0.4889   -0.9663   -0.2860
 C   -1.2722    0.3462    0.0357
 O   -1.4832    1.1437   -1.1292
 C   -0.2615    1.6028   -1.7715
 H   -0.6477    2.0164   -2.7205
 O    0.6371    0.5878   -1.9988
 C    1.4794    4.9277    0.4448
 C    2.2881    4.0904   -0.3318
 C    1.7220    3.0178   -1.0293
 C    0.3450    2.7670   -0.9648
 C   -0.4600    3.6177   -0.1939
 C    0.1022    4.6867    0.5116
 H    3.3586    4.2708   -0.3923
 H    2.3438    2.3549   -1.6230
 H   -1.5273    3.4262   -0.1372
 H   -0.5340    5.3304    1.1139
 C   -5.0481   -0.3136    2.0665
 C   -5.0166   -0.1864    0.6730
 C   -3.8076    0.0406    0.0095
 C   -2.6081    0.1456    0.7292
 C   -2.6521    0.0376    2.1277
 C   -3.8592   -0.1978    2.7936
 H   -5.9374   -0.2635    0.1002
 H   -3.7795    0.1358   -1.0688
 H   -1.7360    0.1487    2.7029
 H   -3.8715   -0.2767    3.8777
 C   -1.1374   -2.0395   -1.0414
 O   -2.1193   -1.6068   -1.8724
 O   -0.8069   -3.2314   -1.0141
 C   -2.7677   -2.6069   -2.6729
 H   -3.5301   -2.0735   -3.2438
 H   -2.0579   -3.0866   -3.3537
 H   -3.2361   -3.3710   -2.0451
 C    3.8817   -0.0840    0.4076
 H    4.0549    0.2881   -0.6058
 H    4.4278    0.5588    1.1031
 C    3.8175   -2.2625   -0.5887
 H    4.1098   -3.3055   -0.4380
 H    4.2231   -1.9313   -1.5483
 C    4.0159   -2.0374    1.7851
 H    4.3453   -1.3636    2.5806
 H    4.5226   -2.9965    1.9214
 N    4.4134   -1.4561    0.4920
 H    0.2355   -0.3203   -1.2267
 H    1.9169    5.7593    0.9908
 H   -5.9894   -0.4906    2.5800

r3_TS4_SSS
Final geometry with  60 atoms:
 H   -0.2091    0.6509   -1.6582
 C    1.8982    1.1303   -0.2591
 H    1.8219    1.4738   -1.2940
 H    2.3981    1.9016    0.3301
 N    2.9373   -0.0118   -0.3300
 C    4.2807    0.5826   -0.7017
 H    4.5871    1.2074    0.1396
 H    4.1247    1.2165   -1.5768
 C    2.5620   -1.0326   -1.3857
 H    2.6023   -0.5115   -2.3446
 H    1.5434   -1.3567   -1.1748
 C    3.0861   -0.7226    1.0023
 H    3.1900    0.0475    1.7666
 H    2.1582   -1.2651    1.1725
 C    0.5530    0.7700    0.3273
 C   -0.6375    0.8767   -0.6635
 O   -1.6467   -0.1011   -0.4036
 C   -1.1554   -1.4673   -0.5285
 H   -0.8441   -1.5751   -1.5934
 O   -0.1150   -1.7175    0.3287
 C   -4.6551   -3.9286    0.1501
 C   -3.7062   -3.7616    1.1652
 C   -2.5701   -2.9766    0.9428
 C   -2.3723   -2.3507   -0.2923
 C   -3.3231   -2.5238   -1.3063
 C   -4.4607   -3.3071   -1.0893
 H   -3.8514   -4.2434    2.1289
 H   -1.8209   -2.8419    1.7164
 H   -3.1718   -2.0407   -2.2694
 H   -5.1916   -3.4355   -1.8837
 C   -2.5498    4.7548   -1.1271
 C   -3.2655    3.5773   -1.3671
 C   -2.6536    2.3314   -1.1985
 C   -1.3174    2.2374   -0.7814
 C   -0.6095    3.4237   -0.5407
 C   -1.2167    4.6713   -0.7133
 H   -4.3046    3.6267   -1.6828
 H   -3.2148    1.4206   -1.3757
 H    0.4202    3.3837   -0.1989
 H   -0.6494    5.5770   -0.5141
 C    0.3826    1.2834    1.6885
 O   -0.9125    1.3352    2.0855
 O    1.3018    1.5933    2.4555
 C   -1.1517    1.7657    3.4348
 H   -0.6823    1.0858    4.1525
 H   -0.7714    2.7788    3.5973
 H   -2.2359    1.7490    3.5578
 C    3.5685   -2.2122   -1.3039
 H    3.0921   -3.0867   -0.8527
 H    3.9005   -2.4866   -2.3088
 C    4.3073   -1.6769    0.9116
 H    5.1514   -1.2822    1.4839
 H    4.0413   -2.6520    1.3282
 C    5.2796   -0.5728   -0.9754
 H    5.4754   -0.6689   -2.0469
 H    6.2289   -0.3659   -0.4741
 N    4.7398   -1.8515   -0.4866
 H    0.3749   -0.5581    0.4639
 H   -5.5368   -4.5406    0.3215
 H   -3.0254    5.7234   -1.2550

r3_TS4_SRR
Final geometry with  60 atoms:
 N   -1.9434    3.7675   -1.0674
 C   -1.2834    4.0286    0.2245
 C   -0.9488    3.9217   -2.1413
 C   -2.4320    2.3764   -1.0745
 N    0.0130    2.1210   -0.7110
 C   -0.2473    2.9202    0.5523
 C    0.3282    3.0967   -1.8276
 C   -1.2502    1.3740   -1.0911
 H   -2.0400    4.0658    1.0128
 H   -0.8013    5.0088    0.1709
 H   -0.6880    4.9785   -2.2446
 H   -1.4015    3.5909   -3.0800
 H   -3.0632    2.2183   -1.9531
 H   -3.0480    2.2251   -0.1838
 H   -0.6248    2.2171    1.2920
 H    0.7138    3.3101    0.8879
 H    1.1504    3.7214   -1.4727
 H    0.6699    2.5123   -2.6841
 H   -1.0704    0.9547   -2.0831
 H   -1.3783    0.5675   -0.3745
 C    1.2067    1.1601   -0.5494
 C    1.2362    0.3131    0.7045
 C    2.2032    0.7986    1.6863
 O    2.5143   -0.1184    2.6498
 O    2.6665    1.9428    1.7310
 C    3.3518    0.3450    3.7229
 H    3.4800   -0.5136    4.3843
 H    2.8738    1.1672    4.2638
 H    4.3235    0.6779    3.3465
 H    1.1737    0.5482   -1.4533
 H    2.0805    1.8120   -0.6023
 H    0.0675    0.2968    1.3779
 C    1.1442   -1.2195    0.4622
 H    1.4550   -1.7180    1.3897
 C    2.0351   -1.7212   -0.6628
 C    3.4263   -1.5655   -0.5475
 C    4.2797   -1.9910   -1.5669
 C    3.7542   -2.5760   -2.7264
 C    2.3714   -2.7327   -2.8492
 C    1.5168   -2.3093   -1.8231
 H    3.8417   -1.1068    0.3462
 H    5.3540   -1.8677   -1.4573
 H    1.9523   -3.1867   -3.7436
 H    0.4439   -2.4360   -1.9165
 H    4.4171   -2.9069   -3.5213
 O   -0.2089   -1.5885    0.1782
 C   -1.0808   -1.4036    1.3425
 H   -0.7022   -2.1126    2.1096
 C   -2.4569   -1.8666    0.8771
 C   -3.5367   -0.9793    0.8351
 C   -4.7912   -1.4079    0.3852
 C   -4.9755   -2.7324   -0.0234
 C   -3.8992   -3.6280    0.0240
 C   -2.6492   -3.1958    0.4745
 H   -3.3801    0.0435    1.1619
 H   -5.6236   -0.7091    0.3569
 H   -4.0361   -4.6602   -0.2878
 H   -1.8125   -3.8892    0.5081
 H   -5.9493   -3.0673   -0.3711
 O   -1.0568   -0.1104    1.7939

r3_TS4_SRS
Final geometry with  60 atoms:
 N   -4.6780   -1.5671   -0.8543
 C   -4.1490   -2.0950    0.4159
 C   -5.1347   -0.1854   -0.6330
 C   -3.5893   -1.5505   -1.8481
 N   -2.7190   -0.1063   -0.0220
 C   -2.8423   -1.3623    0.8203
 C   -4.0295    0.6501    0.0665
 C   -2.5089   -0.5045   -1.4700
 H   -3.9490   -3.1641    0.3048
 H   -4.9178   -1.9721    1.1840
 H   -6.0355   -0.1964   -0.0133
 H   -5.3944    0.2508   -1.6015
 H   -4.0029   -1.3165   -2.8330
 H   -3.1521   -2.5518   -1.8924
 H   -1.9585   -1.9618    0.6117
 H   -2.8230   -1.0511    1.8645
 H   -4.2310    0.7995    1.1291
 H   -3.8773    1.6224   -0.4062
 H   -2.5938    0.4146   -2.0535
 H   -1.4993   -0.9004   -1.5530
 C   -1.5901    0.8165    0.4755
 C   -0.2513    0.1714    0.7602
 C   -0.0044    0.0092    2.1912
 O    1.3097   -0.1907    2.5023
 O   -0.8735   -0.0234    3.0692
 C    1.6016   -0.5109    3.8725
 H    2.6836   -0.6458    3.9155
 H    1.0960   -1.4333    4.1740
 H    1.2971    0.3011    4.5395
 H   -1.5164    1.5799   -0.3022
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 H  -2.0027   1.2763   1.3755
 H  -0.1299  -1.0783   0.2499
 C   0.9232   0.6750  -0.1265
 H   1.8539   0.3683   0.3630
 C   0.9624   2.1842  -0.2959
 C   1.1812   2.9858   0.8368
 C   1.1981   4.3778   0.7346
 C   0.9889   4.9952  -0.5056
 C   0.7689   4.2049  -1.6365
 C   0.7572   2.8079  -1.5325
 H   1.3401   2.5133   1.8029
 H   1.3761   4.9813   1.6208
 H   0.6079   4.6729  -2.6044
 H   0.5940   2.1954  -2.4123
 H   1.0009   6.0787  -0.5868
 O   0.8583   0.0678  -1.4215
 C   1.0801  -1.3814  -1.3819
 H   0.9016  -1.6639  -2.4349
 C   2.5569  -1.6498  -1.0603
 C   3.5597  -1.0081  -1.8023
 C   4.9091  -1.2427  -1.5276
 C   5.2725  -2.1295  -0.5056
 C   4.2775  -2.7760   0.2339
 C   2.9263  -2.5361  -0.0445
 H   3.2762  -0.3108  -2.5865
 H   5.6768  -0.7348  -2.1059
 H   4.5518  -3.4642   1.0296
 H   2.1423  -3.0235   0.5257
 H   6.3218  -2.3136  -0.2902
 O   0.2002  -2.0078  -0.5379

r3_7_SSR
Final geometry with  60 atoms:
 N   4.3183   1.3153  -0.5148
 C   3.8876   0.8101   0.8016
 C   4.9139   0.2059  -1.2783
 C   3.1322   1.8044  -1.2388
 N   2.6023  -0.5890  -0.8025
 C   2.7378  -0.2250   0.6566
 C   3.9507  -1.0137  -1.3232
 C   2.1598   0.6375  -1.5651
 H   3.5526   1.6531   1.4122
 H   4.7533   0.3587   1.2944
 H   5.8587  -0.0831  -0.8096
 H   5.1320   0.5627  -2.2887
 H   3.4531   2.2944  -2.1622
 H   2.6349   2.5526  -0.6152
 H   1.7710   0.1696   0.9720
 H   2.9322  -1.1482   1.2025
 H   4.2912  -1.8318  -0.6851
 H   3.8048  -1.3937  -2.3369
 H   2.1768   0.3681  -2.6236
 H   1.1371   0.8581  -1.2610
 C   1.5601  -1.7941  -1.0025
 C   0.2971  -1.6785  -0.2557
 C   0.2097  -2.1859   1.0483
 O   1.2699  -2.9968   1.4378
 O  -0.7108  -1.9702   1.8839
 C   1.2741  -3.4169   2.8063
 H   2.1884  -4.0022   2.9309
 H   0.4036  -4.0381   3.0392
 H   1.2876  -2.5594   3.4877
 H   1.4301  -1.8006  -2.0885
 H   2.1484  -2.6611  -0.7034
 H  -0.6129  -0.3033   2.0070
 C  -0.8171  -0.8777  -0.8677
 O  -0.8564   0.5596  -0.4984
 C  -1.3798   0.9604   0.7676
 O  -0.5224   0.6701   1.8420
 H  -0.5610  -0.7772  -1.9295
 H  -2.3471   0.4661   0.9292
 C  -2.2300  -1.4719  -0.8610
 C  -2.4757  -2.8221  -0.5802
 C  -3.3133  -0.6724  -1.2641
 C  -3.7654  -3.3551  -0.6802
 H  -1.6540  -3.4616  -0.2788
 C  -4.6037  -1.1986  -1.3627
 H  -3.1395   0.3741  -1.4947
 C  -4.8375  -2.5461  -1.0677
 H  -3.9303  -4.4045  -0.4492
 H  -5.4249  -0.5568  -1.6719
 C  -1.5693   2.4586   0.6598
 C  -2.8300   2.9917   0.3695
 C  -0.4765   3.3241   0.8047
 C  -3.0000   4.3729   0.2215
 H  -3.6816   2.3248   0.2596
 C  -0.6423   4.7030   0.6556
 H   0.4985   2.9117   1.0444
 C  -1.9056   5.2318   0.3621
 H  -3.9846   4.7759   0.0000
 H   0.2108   5.3666   0.7717
 H  -2.0355   6.3048   0.2490
 H  -5.8400  -2.9592  -1.1414

r3_7_SSS
Final geometry with  60 atoms:
 H  -0.9972  -0.5266  -1.9565
 C   0.2997  -2.2953  -0.6614
 H   0.1608  -2.4206  -1.7395
 H   0.3058  -3.2746  -0.1813
 N   1.8418  -1.8736  -0.5832
 C   2.6956  -2.9906  -1.1270
 H   2.5667  -3.8428  -0.4563
 H   2.3023  -3.2536  -2.1111
 C   2.0933  -0.6371  -1.4084
 H   1.8857  -0.9088  -2.4460
 H   1.3737   0.1168  -1.0950
 C   2.2552  -1.6094   0.8430
 H   1.9544  -2.4766   1.4308
 H   1.6773  -0.7495   1.1805
 C  -0.6716  -1.3671  -0.0622
 C  -1.2813  -0.2947  -0.9224
 O  -0.7169   1.0627  -0.7901
 C  -0.3934   1.5273   0.5068
 H   0.2325   0.7647   0.9974
 O  -1.5169   1.7665   1.3145
 C   2.0498   5.0950   0.1974
 C   1.3243   4.8262   1.3633
 C   0.5188   3.6865   1.4441
 C   0.4238   2.8002   0.3614
 C   1.1510   3.0768  -0.8051
 C   1.9578   4.2168  -0.8868
 H   1.3829   5.5050   2.2100
 H  -0.0497   3.4816   2.3453
 H   1.0720   2.4064  -1.6535
 H   2.5101   4.4201  -1.8006
 C  -5.6319  -0.1948  -1.1432
 C  -4.9082   0.9998  -1.0865
 C  -3.5123   0.9801  -0.9871
 C  -2.8149  -0.2327  -0.9303
 C  -3.5495  -1.4269  -0.9934
 C  -4.9425  -1.4122  -1.0983
 H  -5.4294   1.9536  -1.1160
 H  -2.9574   1.9079  -0.9281
 H  -3.0224  -2.3758  -0.9412
 H  -5.4898  -2.3508  -1.1376
 C  -1.1123  -1.5438   1.2623
 O  -0.5800  -2.6512   1.9092
 O  -1.9214  -0.8188   1.8969
 C  -0.9763  -2.8390   3.2723
 H  -2.0562  -2.9953   3.3584
 H  -0.6933  -1.9817   3.8921
 H  -0.4459  -3.7321   3.6113
 C   3.5640  -0.1857  -1.1978
 H   3.6012   0.7358  -0.6103
 H   4.0376   0.0100  -2.1637
 C   3.7880  -1.3535   0.8780
 H   4.3035  -2.1798   1.3753
 H   4.0010  -0.4370   1.4349
 C   4.1720  -2.5038  -1.1887
 H   4.4875  -2.3673  -2.2266
 H   4.8291  -3.2473  -0.7295
 N   4.3325  -1.2205  -0.4843
 H  -1.8352   0.8700   1.5890
 H   2.6760   5.9808   0.1337
 H  -6.7160  -0.1791  -1.2184

r3_7_SRR
Final geometry with  60 atoms:
 N  -1.0244  -3.0121  -2.4057
 C  -1.0501  -3.3217  -0.9646
 C  -2.3724  -2.5953  -2.8261
 C  -0.0933  -1.8926  -2.6270
 N  -1.7782  -0.9463  -1.0565
 C  -1.3445  -2.0499  -0.1217
 C  -2.9077  -1.4535  -1.9156
 C  -0.6198  -0.5925  -1.9594
 H  -0.0833  -3.7432  -0.6759
 H  -1.8151  -4.0841  -0.7925
 H  -3.0448  -3.4562  -2.7766
 H  -2.3206  -2.2659  -3.8676
 H   0.0319  -1.7372  -3.7022
 H   0.8791  -2.1680  -2.2095
 H  -0.4696  -1.6791   0.4130
 H  -2.1521  -2.1989   0.5955
 H  -3.6899  -1.7994  -1.2363
 H  -3.2882  -0.6044  -2.4881
 H  -1.0019   0.1252  -2.6883
 H   0.1375  -0.1162  -1.3410
 C  -2.2794   0.3407  -0.2379
 C  -1.5014   0.6804   0.9607
 C  -1.8351   0.1374   2.2097
 O  -3.0401  -0.5512   2.2544
 O  -1.1487   0.2089   3.2692
 C  -3.3757  -1.1611   3.5054
 H  -4.3273  -1.6711   3.3370
 H  -3.4925  -0.4148   4.2978
 H  -2.6151  -1.8863   3.8128
 H  -2.2712   1.1160  -1.0077
 H  -3.3097   0.0815   0.0023
 H   0.3658  -0.4248   2.8300
 C  -0.2092   1.4394   0.8728
 H   0.0032   1.8572   1.8651
 C  -0.2316   2.6021  -0.1163
 C  -1.2488   3.5658  -0.0106
 C  -1.2964   4.6589  -0.8779
 C  -0.3264   4.8083  -1.8772
 C   0.6906   3.8572  -1.9888
 C   0.7397   2.7656  -1.1122
 H  -2.0102   3.4493   0.7563
 H  -2.0906   5.3939  -0.7748
 H   1.4530   3.9622  -2.7567
 H   1.5371   2.0366  -1.1969
 H  -0.3633   5.6566  -2.5553
 O   0.9344   0.5826   0.5246
 C   1.7689   0.1746   1.6027
 H   2.0071   1.0654   2.2084
 C   3.0267  -0.3746   0.9624
 C   3.1010  -1.7150   0.5628
 C   4.2391  -2.1948  -0.0913
 C   5.3161  -1.3384  -0.3491
 C   5.2481   0.0000   0.0523
 C   4.1065   0.4780   0.7037
 H   2.2685  -2.3775   0.7757
 H   4.2883  -3.2368  -0.3965
 H   6.0821   0.6699  -0.1391
 H   4.0523   1.5196   1.0112
 H   6.2025  -1.7127  -0.8541
 O   1.1775  -0.8106   2.4079

r3_7_SRS
Final geometry with  60 atoms:
 N  -4.3334  -0.0883  -1.9764
 C  -3.8027  -1.3960  -1.5491
 C  -5.0280   0.5384  -0.8391
 C  -3.2045   0.7708  -2.3713
 N  -2.7075   0.2073   0.0030
 C  -2.7071  -1.2294  -0.4601
 C  -4.1072   0.5862   0.4131
 C  -2.2928   1.0854  -1.1532
 H  -3.3866  -1.9102  -2.4197
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 H  -4.6353  -1.9949  -1.1695
 H  -5.9328  -0.0328  -0.6140
 H  -5.3290   1.5473  -1.1345
 H  -3.5949   1.6994  -2.7973
 H  -2.6368   0.2537  -3.1499
 H  -1.7018  -1.4374  -0.8282
 H  -2.8883  -1.8499   0.4179
 H  -4.4155  -0.1276   1.1798
 H  -4.0581   1.5824   0.8585
 H  -2.3945   2.1180  -0.8132
 H  -1.2444   0.8720  -1.3544
 C  -1.7229   0.4123   1.2520
 C  -0.4358  -0.2911   1.1783
 C  -0.2998  -1.5873   1.6942
 O  -1.3950  -2.0609   2.4064
 O   0.7014  -2.3480   1.5635
 C  -1.3006  -3.4032   2.8942
 H  -2.2505  -3.6003   3.3971
 H  -0.4763  -3.5151   3.6059
 H  -1.1592  -4.1169   2.0757
 H  -1.6310   1.5005   1.2934
 H  -2.3311   0.0689   2.0881
 H   0.9307  -2.3981  -0.1130
 C   0.7460   0.2842   0.4496
 H   1.6453  -0.2034   0.8403
 C   0.9152   1.7845   0.6609
 C   1.1237   2.2584   1.9669
 C   1.2836   3.6219   2.2204
 C   1.2299   4.5447   1.1677
 C   1.0249   4.0836  -0.1348
 C   0.8734   2.7136  -0.3855
 H   1.1571   1.5468   2.7879
 H   1.4509   3.9648   3.2382
 H   0.9866   4.7876  -0.9624
 H   0.7286   2.3626  -1.4005
 H   1.3514   5.6068   1.3626
 O   0.7232   0.0412  -1.0046
 C   1.4472  -1.0853  -1.4856
 H   1.3132  -1.0235  -2.5724
 C   2.9443  -0.9770  -1.1714
 C   3.5876   0.2659  -1.2734
 C   4.9592   0.3793  -1.0369
 C   5.7102  -0.7533  -0.6999
 C   5.0773  -1.9957  -0.6037
 C   3.7024  -2.1065  -0.8414
 H   3.0043   1.1478  -1.5179
 H   5.4408   1.3508  -1.1109
 H   5.6510  -2.8809  -0.3415
 H   3.2132  -3.0717  -0.7655
 H   6.7772  -0.6662  -0.5132
 O   0.8908  -2.3122  -1.1034

r3_11
Final geometry with  26 atoms:
 C   1.7761   1.5620   1.4751
 C   1.1939   0.9257   0.4486
 C   1.7623  -0.3417  -0.1102
 O   3.0508  -0.5325   0.2438
 O   1.1419  -1.1264  -0.8052
 C   3.6587  -1.7612  -0.2135
 H   4.6804  -1.7370   0.1660
 H   3.6587  -1.8045  -1.3058
 H   3.1230  -2.6259   0.1875
 H   1.3410   2.4703   1.8845
 H   2.6842   1.1926   1.9392
 H   0.7789   2.4454  -1.6413
 C  -0.0840   1.4574  -0.1861
 H  -0.3300   2.3898   0.3422
 C  -1.2774   0.5251  -0.0280
 C  -1.6353   0.0952   1.2579
 C  -2.7436  -0.7330   1.4490
 C  -3.5124  -1.1400   0.3527
 C  -3.1619  -0.7090  -0.9301
 C  -2.0517   0.1208  -1.1208
 H  -1.0400   0.4049   2.1134
 H  -3.0057  -1.0600   2.4517
 H  -3.7513  -1.0203  -1.7886
 H  -1.7784   0.4453  -2.1180
 O   0.1156   1.7434  -1.5757
 H  -4.3741  -1.7858   0.4978

r3_11a
Final geometry with  26 atoms:
 C   1.7823   1.1029   1.8749
 C   1.2047   0.8374   0.6963
 C   1.7981  -0.1282  -0.2743
 O   2.7170  -0.9437   0.2578
 O   1.4762  -0.1657  -1.4580
 C   3.3651  -1.8653  -0.6521
 H   4.0709  -2.4252  -0.0389
 H   3.8904  -1.3169  -1.4381
 H   2.6284  -2.5374  -1.0987
 H   1.3462   1.8301   2.5546
 H   2.6978   0.6119   2.1881
 H   0.4427   1.6179  -1.6177
 C  -0.0880   1.5075   0.2467
 H  -0.3475   2.2554   1.0035
 C  -1.2463   0.5057   0.1584
 C  -1.4633  -0.4104   1.1995
 C  -2.5354  -1.3053   1.1502
 C  -3.4076  -1.2981   0.0563
 C  -3.2001  -0.3850  -0.9814
 C  -2.1275   0.5121  -0.9295
 H  -0.7904  -0.4277   2.0525
 H  -2.6868  -2.0089   1.9644
 H  -3.8722  -0.3686  -1.8353
 H  -1.9768   1.2213  -1.7363
 O   0.1000   2.2475  -0.9600
 H  -4.2398  -1.9954   0.0149

r3_11b
Final geometry with  26 atoms:
 C   1.9847  -2.1990  -0.5381
 C   1.4081  -1.1021  -0.0310
 C   1.9512   0.2350  -0.4308
 O   1.4521   1.2282   0.3391
 O   2.7501   0.4327  -1.3292
 C   1.8740   2.5757   0.0198
 H   1.3620   3.2161   0.7377
 H   1.5764   2.8298  -1.0005
 H   2.9575   2.6691   0.1255
 H   1.6239  -3.1912  -0.2822
 H   2.8278  -2.1277  -1.2187
 H   0.7601   0.2786   2.0929
 C   0.2136  -1.1761   0.9119
 H   0.0094  -2.2381   1.0859
 C  -1.0490  -0.5498   0.3104
 C  -1.3551  -0.7365  -1.0461
 C  -2.5240  -0.2001  -1.5935
 C  -3.4057   0.5313  -0.7910
 C  -3.1097   0.7157   0.5628
 C  -1.9401   0.1774   1.1098
 H  -0.6769  -1.2998  -1.6810
 H  -2.7427  -0.3517  -2.6472
 H  -3.7888   1.2792   1.1972
 H  -1.7197   0.3208   2.1624
 O   0.5274  -0.6565   2.2075
 H  -4.3131   0.9513  -1.2160

r3_11c
Final geometry with  26 atoms:
 C   2.0611  -2.0514  -0.7643
 C   1.4481  -1.0371  -0.1382
 C   1.9928   0.3471  -0.3411
 O   1.1840   1.2948   0.1512
 O   3.0509   0.5934  -0.9010
 C   1.6163   2.6626  -0.0113
 H   0.8336   3.2678   0.4463
 H   1.7178   2.9077  -1.0719
 H   2.5710   2.8242   0.4963
 H   1.7098  -3.0736  -0.6536
 H   2.9203  -1.8788  -1.4049
 H   1.2470  -1.4091   2.4444
 C   0.2456  -1.2815   0.7655
 H   0.0639  -2.3659   0.7532
 C  -1.0321  -0.6111   0.2789
 C  -1.4766  -0.8660  -1.0263
 C  -2.6569  -0.2895  -1.5016
 C  -3.4106   0.5503  -0.6737
 C  -2.9735   0.8022   0.6301
 C  -1.7914   0.2241   1.1055
 H  -0.8936  -1.5141  -1.6759
 H  -2.9865  -0.4954  -2.5164
 H  -3.5517   1.4524   1.2815
 H  -1.4516   0.4282   2.1142
 O   0.5166  -0.8685   2.1107
 H  -4.3281   1.0014  -1.0414

r3_11d
Final geometry with  26 atoms:
 C  -0.3930   1.8199  -0.6193
 C  -0.9215   0.6658  -0.1901
 C  -2.4148   0.5875  -0.0817
 O  -2.8244  -0.6255   0.3606
 O  -3.1933   1.4862  -0.3480
 C  -4.2527  -0.8147   0.5051
 H  -4.3736  -1.8384   0.8588
 H  -4.7515  -0.6786  -0.4575
 H  -4.6549  -0.1072   1.2342
 H   0.6786   1.9575  -0.7098
 H  -1.0341   2.6549  -0.8842
 H  -1.3559  -1.8902  -0.5224
 C  -0.1103  -0.5715   0.2068
 H  -0.3881  -0.8323   1.2371
 C   1.3857  -0.3415   0.1665
 C   2.0493   0.1119   1.3140
 C   3.4219   0.3757   1.2841
 C   4.1465   0.1820   0.1034
 C   3.4900  -0.2760  -1.0440
 C   2.1162  -0.5335  -1.0138
 H   1.4889   0.2612   2.2339
 H   3.9243   0.7252   2.1820
 H   4.0469  -0.4326  -1.9639
 H   1.6073  -0.8892  -1.9036
 O  -0.4205  -1.6789  -0.6588
 H   5.2142   0.3820   0.0791
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