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A systematic study on the kinetics of H-shift reactions in pristine acyl peroxy radicals

Prasenjit Seal,*[a] Shawon Barua,[a] Siddharth Iyer,[a] Avinash Kumar[a] and Matti Rissanen*[ab]

[a] *Aerosol Physics Laboratory, Physics Unit, Tampere University, 33720 Tampere, Finland. E-mail: prasenjit.seal@tuni.fi, matti.rissanen@tuni.fi*

[b] *Department of Chemistry, University of Helsinki, P.O. Box 55, FI-00014, Helsinki, Finland*

Contents

1. Master equation simulation (MESMER) methodology and results

One of the ways that can be used to estimate rate coefficients is the master equation simulations as were performed here with MESMER 6.0 code on the stationary points along the potential energy surface (PES) [*J. Phys. Chem. A*, 2012, **116**, 9545–9560]. Although MESMER is designed for pressure-dependent, multi-well reaction schemes, yet one can use the code to perform a single-well rate coefficient estimation as well. Transition states were treated using Rice-Ramsperger-Kassel-Marcus (RRKM) theory to calculate the micro-canonical rate coefficients and to determine the branching ratios of peracid radical formations via unimolecular isomerization. It is noteworthy to mention that in the present work, we considered the acyl peroxy radicals to be thermalized. Eckart tunneling was used in our calculations as tunneling has a profound impact on H-shift reaction rate coefficients. Energy transfer occurred *via* collisions between modeled species and N_2 bath gas. Such collisions were treated using Lennard-Jones (L-J) potential model and the L-J parameters (σ, ϵ) were used to account for the associated collisional frequency. MESMER utilizes the exponential down (ΔE_{down}) model as given in equation 1 for simulating the collisional energy transfer.

$$\Delta E_{down} = \Delta E_{down,\,ref} \left(\frac{T}{T_{ref}}\right)^{n} \qquad (1)$$

In equation 1, ΔE_{down} is the average downward energy transferred per collision, $\Delta E_{down,\,ref}$ is the value of ΔE_{down} at T_{ref} (=298 K) and n is an independent parameter associated with the temperature dependence of ΔE_{down}.The Lennard–Jones parameters were used for the reactant – AcOO radicals since they are the actual intermediates in the aldehyde autoxidation process. We used the L-J parameters [*J. Chem. Phys.*, 1983, **78**, 6709-6717] of the nearest alkanes for each of the –AcOO radicals and the corresponding values were tabulated in Table S1.

Table S1 The Lennard-Jones parameters used in the MESMER calculation

Reactant radicals	σ (Å)	ϵ (K)
Ethanal–AcOO	5.4	307

Propanal–AcOO	5.9	327
Butanal–AcOO	6.3	343
Pentanal–AcOO	6.7	351
Hexanal–AcOO	7.0	359
Heptanal–AcOO	7.3	362
Octanal–AcOO	7.7	363
Nonanal–AcOO	8.0	362

For N_2 bath gas, the MESMER recommended values for ΔE_{down} are between 175 and 275 cm^{-1}. We used a ΔE_{down} value of 225 cm^{-1} in our calculations. In addition, a grain size of 100 and a value of 25 k_BT for the energy spanned by the grains were used. All the MESMER input files for estimating the rate coefficients of these H-shift reactions are provided from pages S-88 upto S-249.

Hindered Rotor (HR) effect

We did not apply hindered rotation corrections (HR) in MESMER, as it has been suggested to have only a minor influence when used in combination with SS-TST [*J. Phys. Chem. A*, 2016, **120**, 10072−10087]. Nevertheless, we did perform a test computation with the 1,6 H-shift of pentanal-AcOO radical to illustrate the magnitude of this HR effect as given below. The results obtained with the HR reduces the MESMER derived rate coefficient from 1.0 s^{-1} to 0.45 s^{-1}, and thus decreases the difference between the other methodologies.

Reaction	$k_{MESMER}^{no\ HR}$	k_{MESMER}^{HR}
Pentanal-AcylOO-rad→ Pentanal-16-rad	1.00376	0.453425

2. **Table S2** Computed rate coefficients (in s^{-1}) obtained from MESMER, SS-TST and MC-TST (both IRC and GM approaches) rate equations and the SAR data obtained from Vereecken and Nozière's work (VN data) for all possible H-shifts in pristine –AcOO radicals.

Reactant radicals	Rate coefficients (s^{-1})	H-shifts					
		1,4	1,5	1,6	1,7	1,8	1,9
Ethanal-AcOO	k_{MESMER}	3.9×10^{-6}	–	–	–	–	–
	$k_{SS\text{-}TST}$	1.1×10^{-7}					
	$k_{GM\text{-}MC\text{-}TST}$	1.3×10^{-6}					
	$k_{IRC\text{-}MC\text{-}TST}$	7.3×10^{-8}					
	$k_{VN\ data}$	4.0×10^{-10}					
Propanal-AcOO	k_{MESMER}	2.1×10^{-5}	6.3×10^{-4}				
	$k_{SS\text{-}TST}$	1.1×10^{-5}	1.6×10^{-4}	–	–	–	–
	$k_{GM\text{-}MC\text{-}TST}$	7.8×10^{-6}	2.3×10^{-4}				
	$k_{IRC\text{-}MC\text{-}TST}$	5.7×10^{-6}	8.4×10^{-5}				
	$k_{VN\ data}$	1.2×10^{-7}	1.6×10^{-4}				
Butanal-AcOO	k_{MESMER}	2.9×10^{-5}	9.5×10^{-2}	9.7×10^{-3}			
	$k_{SS\text{-}TST}$	1.7×10^{-5}	3.0×10^{-2}	2.1×10^{-3}	–	–	–
	$k_{GM\text{-}MC\text{-}TST}$	7.0×10^{-6}	1.9×10^{-2}	1.9×10^{-3}			
	$k_{IRC\text{-}MC\text{-}TST}$	5.2×10^{-6}	9.3×10^{-3}	6.7×10^{-4}			
	$k_{VN\ data}$	1.2×10^{-7}	1.6×10^{-2}	8.1×10^{-5}			
Pentanal-AcOO	k_{MESMER}	3.5×10^{-5}	1.3×10^{-1}	1.00	7.5×10^{-2}		
	$k_{SS\text{-}TST}$	1.7×10^{-5}	5.0×10^{-2}	2.3×10^{-1}	1.1×10^{-2}	–	–
	$k_{GM\text{-}MC\text{-}TST}$	5.7×10^{-6}	2.5×10^{-2}	1.5×10^{-1}	1.9×10^{-2}		
	$k_{IRC\text{-}MC\text{-}TST}$	4.2×10^{-6}	1.3×10^{-2}	5.2×10^{-2}	4.4×10^{-3}		
	$k_{VN\ data}$	1.2×10^{-7}	1.6×10^{-2}	1.8×10^{-2}	2.1×10^{-5}		
Hexanal-AcOO	k_{MESMER}	5.2×10^{-6}	1.9×10^{-1}	2.03	1.62	4.7×10^{-3}	
	$k_{SS\text{-}TST}$	2.4×10^{-6}	9.5×10^{-2}	5.1×10^{-1}	3.9×10^{-1}	7.4×10^{-4}	–
	$k_{GM\text{-}MC\text{-}TST}$	5.0×10^{-7}	3.9×10^{-2}	2.6×10^{-1}	2.5×10^{-1}	7.5×10^{-4}	
	$k_{IRC\text{-}MC\text{-}TST}$	3.4×10^{-7}	1.9×10^{-2}	9.7×10^{-2}	8.8×10^{-2}	1.8×10^{-4}	
	$k_{VN\ data}$	1.2×10^{-7}	1.6×10^{-2}	1.8×10^{-2}	1.8×10^{-3}	1.7×10^{-6}	
Heptanal-AcOO	k_{MESMER}	9.1×10^{-6}	2.9×10^{-2}	3.41	2.41	3.0×10^{-1}	1.1×10^{-2}
	$k_{SS\text{-}TST}$	4.8×10^{-6}	1.0×10^{-2}	1.00	6.5×10^{-1}	7.8×10^{-2}	2.5×10^{-3}
	$k_{GM\text{-}MC\text{-}TST}$	1.3×10^{-6}	2.0×10^{-2}	5.9×10^{-1}	3.9×10^{-1}	5.9×10^{-2}	1.1×10^{-3}
	$k_{IRC\text{-}MC\text{-}TST}$	8.9×10^{-7}	1.0×10^{-2}	2.4×10^{-1}	1.5×10^{-1}	2.0×10^{-2}	4.2×10^{-4}
	$k_{VN\ data}$	1.2×10^{-7}	1.6×10^{-2}	1.8×10^{-2}	1.8×10^{-3}	2.1×10^{-5}	–
Octanal-AcOO	k_{MESMER}	6.3×10^{-6}	1.8×10^{-1}	3.1×10^{-1}	2.75	3.5×10^{-1}	2.2×10^{-2}
	$k_{SS\text{-}TST}$	3.8×10^{-6}	6.2×10^{-2}	9.1×10^{-2}	5.6×10^{-1}	9.0×10^{-2}	5.1×10^{-3}
	$k_{GM\text{-}MC\text{-}TST}$	2.1×10^{-6}	2.5×10^{-2}	2.6×10^{-1}	3.0×10^{-1}	7.4×10^{-2}	3.8×10^{-3}

	$k_{\text{IRC-MC-TST}}$	1.5×10^{-6}	1.3×10^{-2}	1.1×10^{-1}	9.5×10^{-2}	2.6×10^{-2}	1.3×10^{-3}
	$k_{\text{VN data}}$	1.2×10^{-7}	1.6×10^{-2}	1.8×10^{-2}	1.8×10^{-3}	2.1×10^{-5}	–
Nonanal-AcOO	k_{MESMER}	5.8×10^{-6}	1.4×10^{-1}	3.4×10^{-1}	2.19	5.1×10^{-1}	4.1×10^{-3}
	$k_{\text{SS-TST}}$	3.1×10^{-6}	5.3×10^{-2}	1.2×10^{-1}	4.9×10^{-1}	1.5×10^{-1}	7.6×10^{-4}
	$k_{\text{GM-MC-TST}}$	4.7×10^{-6}	4.6×10^{-2}	5.0×10^{-1}	5.5×10^{-1}	1.0×10^{-1}	2.1×10^{-3}
	$k_{\text{IRC-MC-TST}}$	3.3×10^{-6}	2.4×10^{-2}	2.1×10^{-1}	1.8×10^{-1}	3.6×10^{-2}	5.2×10^{-4}
	$k_{\text{VN data}}$	1.2×10^{-7}	1.6×10^{-2}	1.8×10^{-2}	1.8×10^{-3}	2.1×10^{-5}	–

3. **Table S3** The zero-point corrected forward barrier height (FBH) and reverse barrier height (RBH) for different H-shift reactions of –AcOO radical series along with the Eckart tunneling factor, κ computed using intrinsic coordinate (IRC) and global minimum (GM) approaches following multiconfromer transition state theory (MC-TST) treatment.

Reactant radicals	Approach	H-shifts											
		1,4		1,5		1,6		1,7		1,8		1,9	
		FBH	RBH	FBH	RBH	FBH	RBH	FBH	RBH	FBH	RBH	FBH	RBH
Ethanal–AcOO	GM	29.6	27.0										
	IRC	29.6	11.1										
	κ_{IRC}	115.3											
	κ_{GM}	2097.9											
Propanal–AcOO	GM	26.8	29.6	24.5	19.3								
	IRC	25.5	23.6	23.3	12.6								
	κ_{IRC}	99.2		93.6									
	κ_{GM}	136.1		257.0									
Butanal–AcOO	GM	26.5	28.7	21.0	18.6	22.8	18.2						
	IRC	25.6	22.8	19.8	12.2	22.5	12.3						
	κ_{IRC}	91.5		55.4		131.6							
	κ_{GM}	123.9		113.5		372.2							
Pentanal–AcOO	GM	26.5	28.8	20.6	17.9	19.5	17.8	20.7	16.4				
	IRC	25.6	22.9	19.5	11.7	19.3	10.0	19.7	9.0				
	κ_{IRC}	95.4		47.6		51.2		63.4					
	κ_{GM}	129.5		94.7		149.6		280.5					
Hexanal–AcOO	GM	27.1	29.2	20.5	17.6	19.1	17.3	18.1	16.7	22.2	17.5		
	IRC	25.5	22.5	18.9	11.3	17.7	9.7	15.9	8.8	21.3	9.8		
	κ_{IRC}	99.7		45.7		41.6		33.6		68.6			
	κ_{GM}	147.0		94.9		111.7		94.4		285.9			
Heptanal–AcOO	GM	27.0	29.2	20.9	18.1	19.0	17.1	17.4	16.0	18.7	17.2	20.9	16.2
	IRC	25.4	22.4	18.7	11.9	19.0	10.0	15.4	8.4	17.3	8.5	18.0	11.0
	κ_{IRC}	105.2		50.0		42.2		28.8		28.6		90.2	
	κ_{GM}	157.5		102.0		104.5		75.3		85.8		238.9	
Octanal–AcOO	GM	26.9	29.2	20.5	17.6	19.5	18.0	17.7	16.1	18.4	16.7	19.9	18.0
	IRC	26.0	22.8	19.5	11.5	18.2	11.2	16.1	8.3	16.8	8.0	18.9	9.1
	κ_{IRC}	89.2		44.6		55.9		34.4		23.6		32.9	

	κ_{GM}	122.9		85.7		129.0		107.1		68.1		98.4	
Nonanal–AcOO	GM	26.9	29.2	20.5	18.0	19.1	18.1	17.6	16.2	18.1	16.3	20.7	18.4
	IRC	25.9	22.8	19.4	11.6	18.0	11.0	16.2	8.3	16.6	8.0	17.0	9.1
	κ_{IRC}	95.6		43.5		54.9		34.4		24.8		42.0	
	κ_{GM}	133.7		85.5		130.2		107.1		69.3		166.2	

4. Variation in the GM-MC-TST, IRC-MC-TST rate coefficients and SAR data for pentanal – octanal acyl peroxy radicals with H-shift span

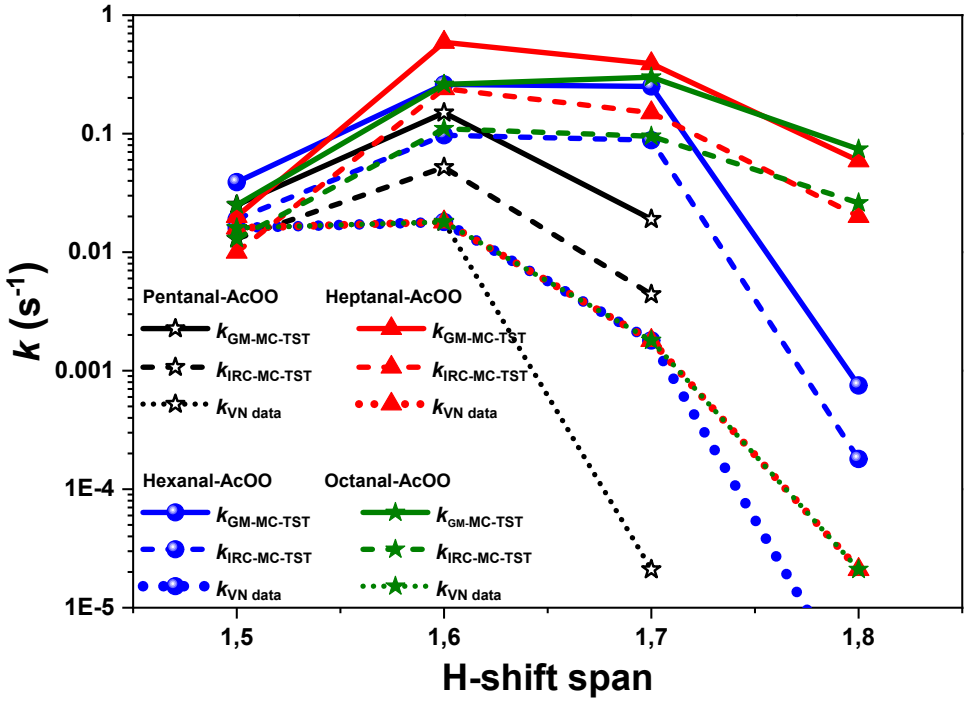

Fig. S1 Variation in the rate coefficients for pentanal – octanal acyl peroxy radicals with H-shift span. The solid (GM-MC-TST) and dashed lines (IRC-MC-TST) were obtained from the MC-TST equation 2. The values based on the SAR data by Vereecken and Nozière are presented in dotted lines.

5. **Variation in the rate coefficients for all the acyl peroxy radicals with H-shift span. The solid lines were obtained from the MESMER simulations while the dashed ones were obtained from the TST equations. The values based on the SAR data by Vereecken and Nozière are shown with dotted lines. For clarity, we also provided reaction schemes for some of the H-shifts in these acyl peroxy radicals.**

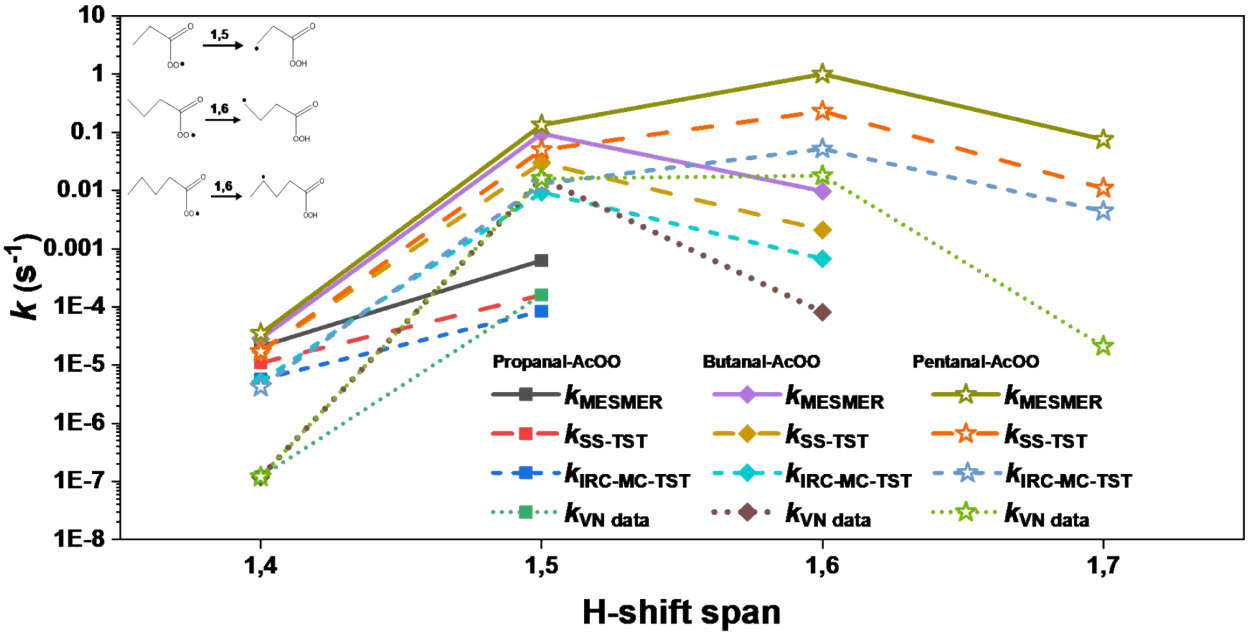

Fig. S2 Variation in the rate coefficients for the small-sized acyl peroxy radicals, *i.e.*, propanal, butanal, and pentanal with H-shift span. For clarity, we also provided the reaction schemes for 1,5 H-shift in propanal-AcOO, 1,6 H-shifts in butanal-AcOO, and 1,6 H-shift in pentanal-AcOO.

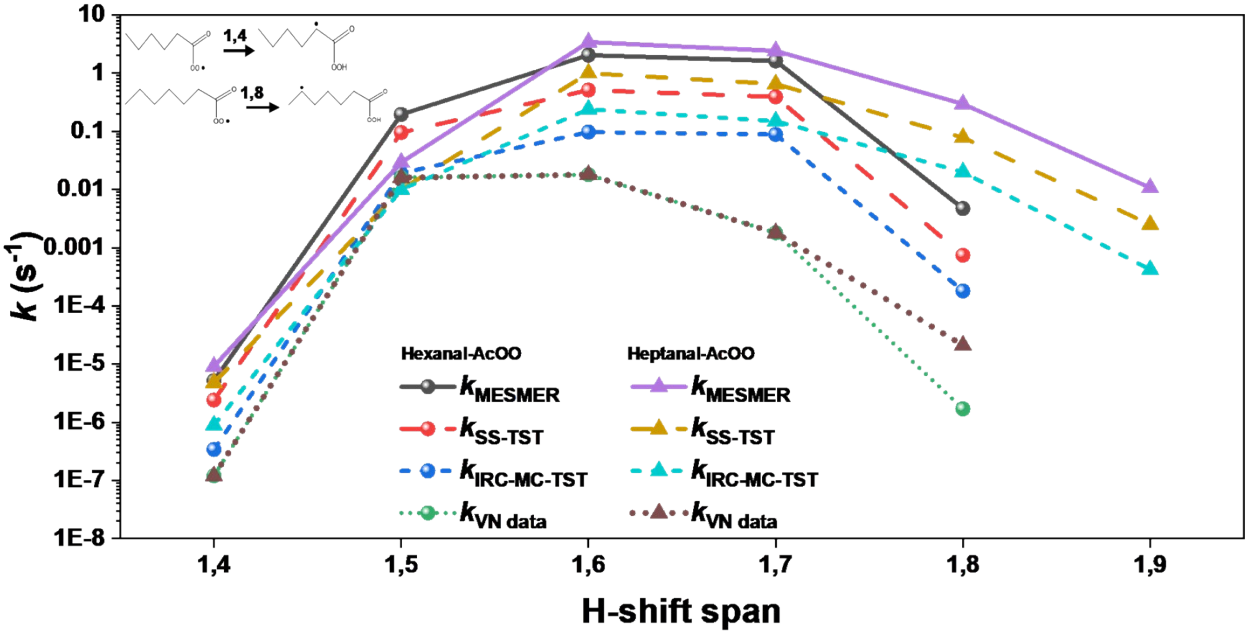

Fig. S3 Variation in the rate coefficients for the medium-sized acyl peroxy radicals, *i.e.*, hexanal and heptanal with H-shift span. For clarity, we also provide the reaction schemes for 1,4 H-shift in hexanal-AcOO, and 1,8 H-shift in heptanal-AcOO.

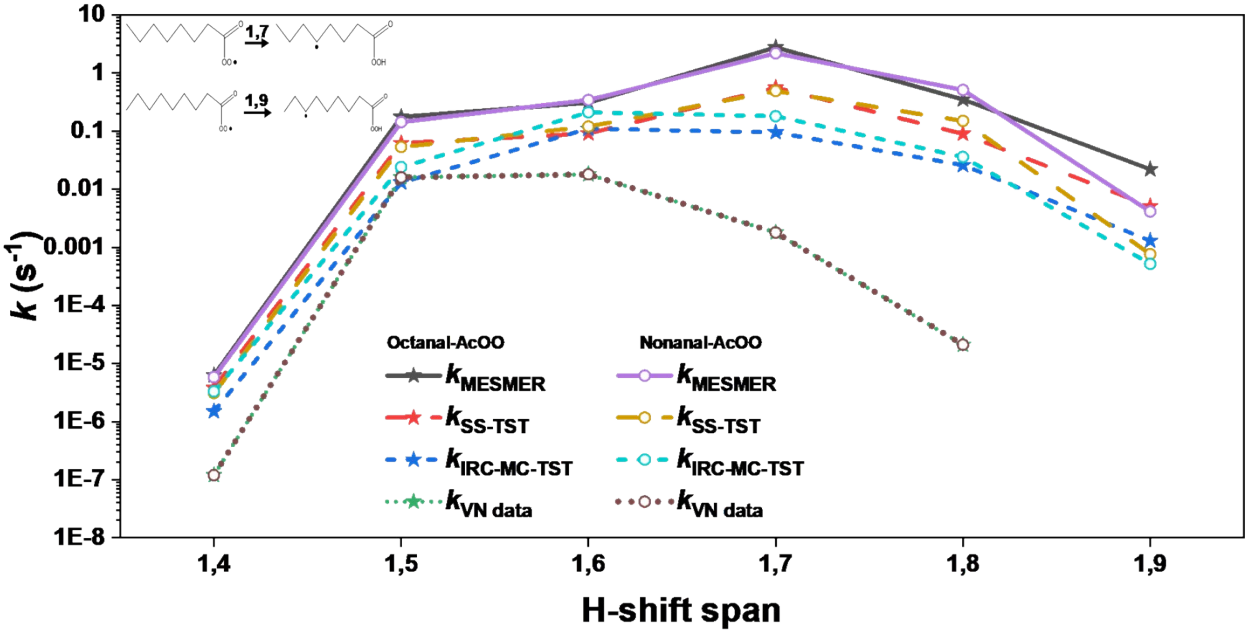

Fig. S4 Variation in the rate coefficients for the large sized acyl peroxy radicals octanal and nonanal with H-shift span. For clarity, we also provide the reaction schemes for 1,7 H-shift in octanal-AcOO, and 1,9 H-shift in nonanal-AcOO.

6. **Table S4** Ratio of the current best estimate $k_{\text{IRC-MC-TST}}$ and SAR data of Vereecken and Nozière with and without the new improved empirical correction factors for 1,4/1,7/1,8 H-shift spans. In the parentheses, are the factors obtained with the new empirical corrections for 1,4/1,7/1,8 H-shift spans.

Reactant radicals	**H-shifts**	$k_{\text{IRC-MC-TST}}$	$k_{\text{VN data}}$*	$k_{\text{VN data\_new ef}}$†	$k_{\text{IRC-MC-TST}}$: $k_{\text{VN data}}$	$k_{\text{IRC-MC-TST}}$: $k_{\text{VN data\_new ef}}$	**Avg$_{1,4}$**	**Avg$_{1,5}$**	**Avg$_{1,6}$**	**Avg$_{1,7}$**	**Avg$_{1,8}$**
Ethanal-AcOO	1,4	7.3×10^{-8}	4.0×10^{-10}	5.9×10^{-9}	182.5	12.3	44.8 (3.0)	0.9	7.9	98.9 (6.6)	1002.7 (4.6)
Propanal-AcOO	1,4	5.7×10^{-6}	1.2×10^{-7}	1.8×10^{-6}	47.5	3.2					
	1,5	8.4×10^{-5}	1.6×10^{-4}	1.6×10^{-4}	0.5	0.5					
Butanal-AcOO	1,4	5.2×10^{-6}	1.2×10^{-7}	1.8×10^{-6}	43.3	3.0					
	1,5	9.3×10^{-3}	1.6×10^{-2}	1.6×10^{-2}	0.6	0.6					
	1,6	6.7×10^{-4}	8.1×10^{-5}	8.1×10^{-5}	8.3	8.3					
Pentanal-AcOO	1,4	4.2×10^{-6}	1.2×10^{-7}	1.8×10^{-6}	35.0	2.4					
	1,5	1.3×10^{-2}	1.6×10^{-2}	1.6×10^{-2}	0.8	0.8					
	1,6	5.2×10^{-2}	1.8×10^{-2}	1.8×10^{-2}	2.9	2.9					
	1,7	4.4×10^{-3}	2.1×10^{-5}	3.1×10^{-4}	209.5	14.2					
Hexanal-AcOO	1,4	3.4×10^{-7}	1.2×10^{-7}	1.8×10^{-6}	2.8	0.2					
	1,5	1.9×10^{-2}	1.6×10^{-2}	1.6×10^{-2}	1.2	1.2					
	1,6	9.7×10^{-2}	1.8×10^{-2}	1.8×10^{-2}	5.4	5.5					
	1,7	8.8×10^{-2}	1.8×10^{-3}	2.7×10^{-2}	48.9	3.2					
	1,8	1.8×10^{-4}	1.7×10^{-6}	3.8×10^{-4}	105.9	0.5					
Heptanal-AcOO	1,4	8.9×10^{-7}	1.2×10^{-7}	1.8×10^{-6}	7.4	0.5					
	1,5	1.0×10^{-2}	1.6×10^{-2}	1.6×10^{-2}	0.6	0.6					
	1,6	2.4×10^{-1}	1.8×10^{-2}	1.8×10^{-2}	13.3	13.6					
	1,7	1.5×10^{-1}	1.8×10^{-3}	2.7×10^{-2}	83.3	5.5					

	1,8	2.0×10^{-2}	2.1×10^{-5}	4.5×10^{-3}	952.4	4.4
Octanal-AcOO	1,4	1.5×10^{-6}	1.2×10^{-7}	1.8×10^{-6}	12.5	0.9
	1,5	1.3×10^{-2}	1.6×10^{-2}	1.6×10^{-2}	0.8	0.8
	1,6	1.1×10^{-1}	1.8×10^{-2}	1.8×10^{-2}	6.1	6.2
	1,7	9.5×10^{-2}	1.8×10^{-3}	2.7×10^{-2}	52.8	3.5
	1,8	2.6×10^{-2}	2.1×10^{-5}	4.5×10^{-3}	1238.1	5.7
Nonanal-AcOO	1,4	3.3×10^{-6}	1.2×10^{-7}	1.8×10^{-6}	27.5	1.9
	1,5	2.4×10^{-2}	1.6×10^{-2}	1.6×10^{-2}	1.5	1.5
	1,6	2.1×10^{-1}	1.8×10^{-2}	1.8×10^{-2}	11.7	11.9
	1,7	1.8×10^{-1}	1.8×10^{-3}	2.7×10^{-2}	100.0	6.6
	1,8	3.6×10^{-2}	2.1×10^{-5}	4.5×10^{-3}	1714.3	7.9

*obtained from L. Vereecken and B. Nozière, *Atmos. Chem. Phys.*, 2020, **20**, 7429–7458.

†obtained from L. Vereecken and B. Nozière, *Atmos. Chem. Phys.*, 2020, **20**, 7429–7458 using the following modified equations

$k_{acyl\,peroxy}(T) = exp\frac{1700K}{T} k_{aliphatic}(T) = 300 * k_{aliphatic}(298)$, for 1,4 and 1,7 H-shift span

$k_{acyl\,peroxy}(T) = exp\frac{2500K}{T} k_{aliphatic}(T) = 4400 * k_{aliphatic}(298)$ for 1,8 H-shift span

7. Variation in $k_{\text{IRC-MC-TST}}$ and $k_{\text{VN data}}$ for all the acyl peroxy radicals with H-shift span. The dashed lines were obtained from the IRC-MC-TST approach while the SAR data obtained from Vereecken and Nozière with new empirical factors are shown here with dotted lines.

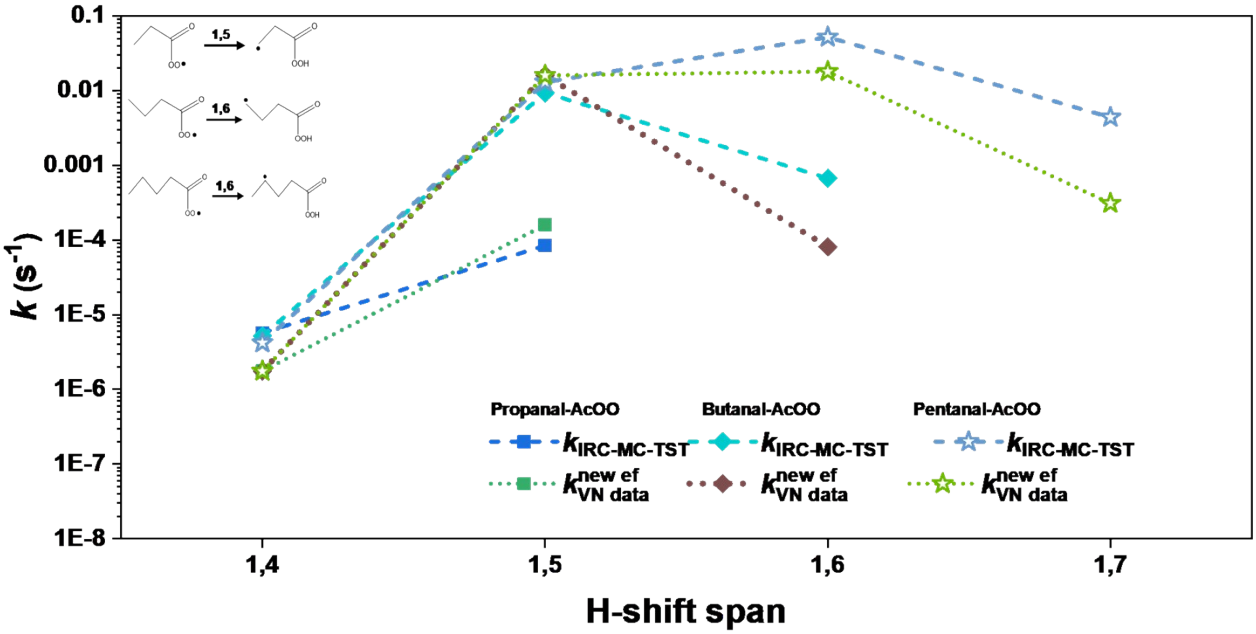

Fig. S5 Variation in the rate coefficients for the small-sized acyl peroxy radicals, *i.e.*, propanal, butanal, and pentanal with H-shift span. For clarity, we also provided the reaction schemes for 1,5 H-shift in propanal-AcOO, 1,6 H-shifts in butanal-AcOO, and 1,6 H-shift in pentanal-AcOO.

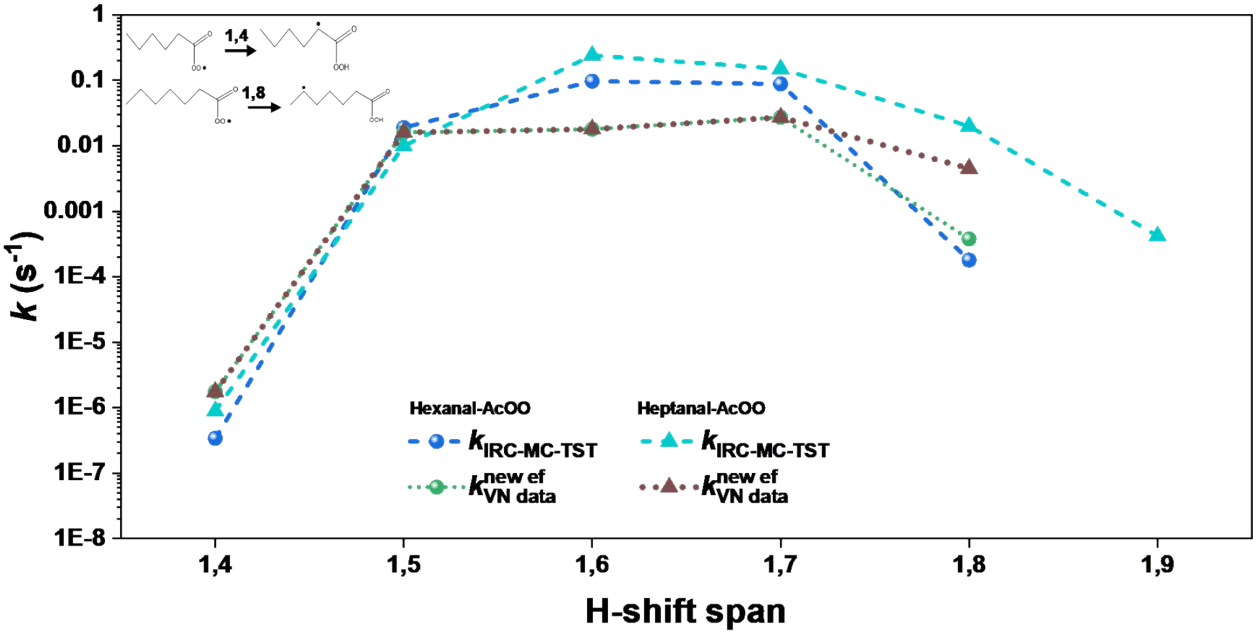

Fig. S6 Variation in the rate coefficients for the medium-sized acyl peroxy radicals, *i.e.*, hexanal and heptanal with H-shift span. For clarity, we also provide the reaction schemes for 1,4 H-shift in hexanal-AcOO, and 1,8 H-shift in heptanal-AcOO.

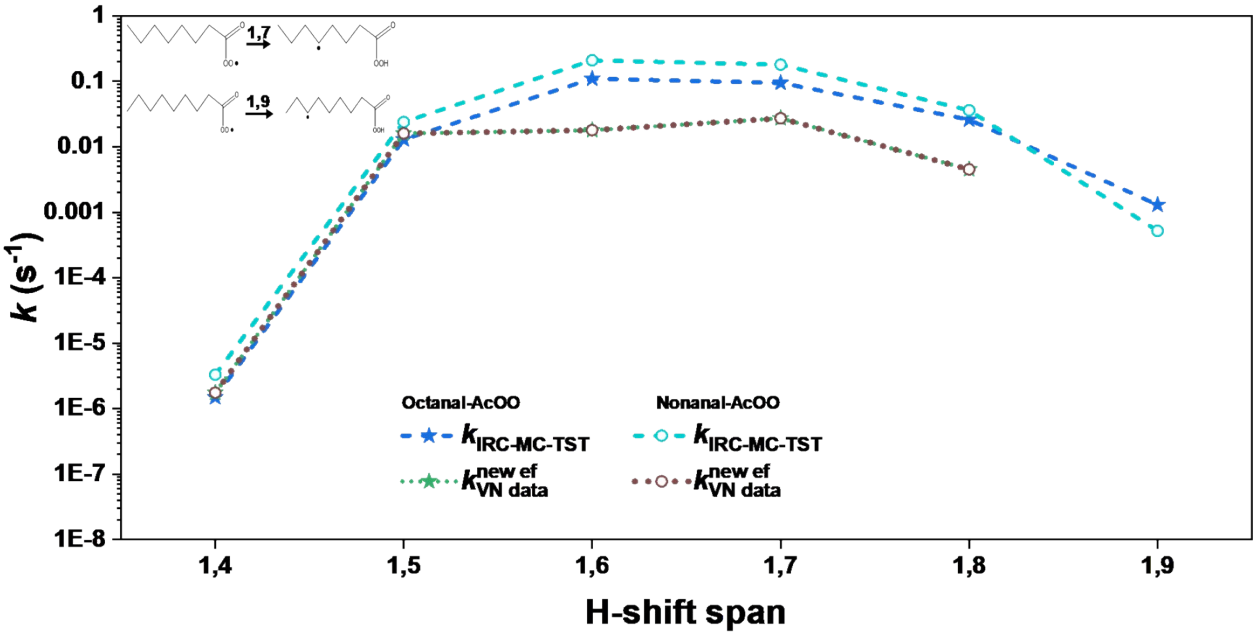

Fig. S7 Variation in the rate coefficients for the large sized acyl peroxy radicals octanal and nonanal with H-shift span. For clarity, we also provide the reaction schemes for 1,7 H-shift in octanal-AcOO, and 1,9 H-shift in nonanal-AcOO.

8. Table S5 Qualitative inspection of the influence of inductive effects in the determined H-shift rates investigated for a series of primary 1,n- H-shifts in comparison to the corresponding 1,n-secondary H-shifts with methyl and ethyl substitutions.

Reactions of interest	Addition of $-CH_3$		Addition of $-CH_2CH_3$	
(1º radical)	Reaction (2º radical)	$k_{IRC-MC-TST}^{secondary} / k_{IRC-MC-}^{primar}$	Reaction (2º radical)	$k_{IRC-MC-TST}^{secondary} / k_{IRC-MC-}^{primar}$
1,5 H-shift in Propanal-AcOO	1,5 H-shift in Butanal-AcOO	110.7	1,5 H-shift in Pentanal-AcOO	154.8
1,6 H-shift in Butanal-AcOO	1,6 H-shift in Pentanal-AcOO	77.6	1,6 H-shift in Hexanal-AcOO	144.8
1,7 H-shift in Pentanal-AcOO	1,7 H-shift in Hexanal-AcOO	20.0	1,7 H-shift in Heptanal-AcOO	34.1
1,8 H-shift in Hexanal-AcOO	1,8 H-shift in Heptanal-AcOO	111.1	1,8 H-shift in Octanal-AcOO	144.4
1,9 H-shift in Heptanal-AcOO	1,9 H-shift in Octanal-AcOO	3.1	1,9 H-shift in Nonanal-AcOO	1.2

9. Coupled cluster + zero-point correction energies (in a.u.), and frequencies (in cm^{-1}) obtained from ωB97X-D/aug-cc-pVTZ of the global minimum geometry of each of the species involved

Species	Formula	Energies (a.u.)	Frequencies (cm^{-1})
Ethanal-AcOO	$CH_3C(=O)OO•$	-303.1685493	143.92 211.58 339.42 500.44 543.44 574.84 786.97 993.82 1038.80 1178.35 1255.80 1386.05 1442.38 1450.85 1925.95 3099.79 3168.56 3208.93
Ethanal-1,4-TS		-303.121457	**-1903.81** 130.40 269.53 489.20 539.65 612.68 686.25 865.66 1024.10 1026.56 1033.63 1095.48 1199.02 1404.19 1741.14 1920.21 3156.26 3240.52
Ethanal-1,4-rad	$C•H_2C(=O)OOH$	-303.1644164	209.27 325.89 340.52 429.76 501.99 642.97 687.18 778.64 900.73 1025.38 1084.74 1308.29 1444.45 1491.46 1757.93 3225.87 3340.13 3507.38
Propanal-AcOO	$CH_3CH_2C(=O)OO•$	-342.3931836	95.05 137.99 219.09 234.67 332.22 526.80 553.24 602.71 766.85 813.39 1012.89 1057.92 1108.82 1120.59 1251.13 1285.07 1383.71 1432.36 1454.37 1503.45 1507.84 1923.28 3070.82 3083.19 3115.45 3149.46 3151.42
Propanal-1,4-TS		-342.3504947	**-1629.08** 79.65 180.88 196.44 247.34 502.32 562.36 673.81 690.16 800.16 819.13 1016.54 1043.57 1081.24 1129.30 1179.07 1188.00 1339.19 1411.38 1487.14 1495.06 1770.18 1917.31 3047.98 3119.88 3132.89 3152.86
Propanal-1,4-rad	$CH_3C•HC(=O)OOH$	-342.39756	85.91 118.81 215.18

			218.44 390.74 467.83 499.33 605.19 702.84 744.87 927.99 993.18 1004.26 1090.90 1156.55 1211.62 1404.21 1438.17 1476.12 1505.10 1533.05 1752.28 3028.46 3075.98 3155.81 3216.65 3539.89
Propanal-1,5-TS		-342.3540741	**-1798.87** 132.40 206.27 360.09 479.66 526.26 551.99 620.37 700.15 780.52 847.85 986.73 1056.44 1080.15 1112.84 1193.85 1212.10 1262.19 1330.06 1453.02 1473.83 1565.52 1877.05 3078.66 3117.34 3132.42 3212.65
Propanal-1,5-rad	C•$H_2CH_2C(=O)OOH$	-342.3848601	35.59 160.62 192.34 244.89 376.31 443.91 471.61 474.43 611.30 686.74 902.50 935.52 1004.06 1045.79 1122.72 1194.38 1239.11 1403.37 1444.93 1456.77 1524.80 1829.28 2981.39 3078.37 3181.75 3296.63 3567.84
Butanal-AcOO	$CH_3CH_2CH_2C(=O)OO$•	-381.6176886	78.03 103.47 139.47 156.21 251.57 304.63 366.30 530.20 562.11 591.26 752.98 826.26 889.29 931.07 1052.37 1074.42 1126.34 1143.83 1251.00 1257.41 1331.10 1335.83 1414.63 1427.83 1450.98 1499.31 1507.83 1514.25 1922.87 3047.03 3067.79 3075.72 3094.98 3109.16 3126.99 3131.93
Butanal-1,4-TS		-381.5753931	**-1623.87** 68.67 82.36 163.26 210.84 248.97 324.18 522.36 575.61 671.33 691.23 745.08 864.76 891.31 952.52

			1017.23 1068.93 1113.29 1146.37 1178.26 1188.67 1284.36 1300.45 1398.83 1427.05 1480.90 1506.28 1509.21 1763.78 1914.31 3038.94 3053.38 3086.87 3124.56 3128.02 3138.72
Butanal-1,4-rad	$CH_3CH_2C•HC(=O)OOH$	-381.6212488	24.46 90.12 172.42 200.53 255.35 349.19 380.97 460.99 501.03 609.59 707.72 764.72 807.61 925.29 970.79 1031.01 1058.09 1094.87 1169.18 1209.35 1279.93 1341.65 1418.29 1468.02 1484.26 1504.93 1511.11 1521.95 1749.60 3010.16 3054.16 3110.90 3132.37 3137.38 3204.15 3539.82
Butanal-1,5-TS		-381.584304	**-1716.03** 100.40 131.71 193.57 243.69 340.65 480.23 494.21 544.27 591.40 687.78 778.03 859.22 899.82 932.65 1042.04 1072.43 1106.57 1143.83 1195.13 1224.41 1251.10 1318.52 1372.02 1423.51 1457.16 1487.66 1497.24 1570.30 1874.76 3030.88 3076.03 3099.48 3128.02 3133.63 3146.41
Butanal-1,5-rad	$CH_3C•HCH_2C(=O)OOH$	-381.6139483	40.29 72.53 115.97 167.11 265.33 301.77 387.22 442.75 444.76 488.82 650.72 790.77 882.21 917.15 959.95 998.30 1024.33 1093.19 1155.33 1215.42 1283.08 1328.53 1389.87 1425.68 1470.57 1478.29 1487.49 1517.81 1813.55 2997.91 3055.07 3064.69 3131.11 3133.99 3205.11 3557.11
Butanal-1,6-TS		-381.58142	**-1878.23** 84.50 188.28 227.76 331.03 393.55

			459.04 513.47 581.24 641.73 721.01 767.95 886.14 898.79 933.53 1052.80 1061.61 1098.27 1117.25 1163.68 1220.28 1251.38 1297.27 1362.81 1371.95 1444.69 1468.58 1489.48 1498.88 1874.32 3050.47 3094.37 3104.76 3110.55 3162.39 3196.82
Butanal-1,6-rad	C•$H_2CH_2CH_2C(=O)OOH$	-381.610351	26.11 91.04 122.38 149.29 241.53 344.63 350.91 442.62 478.61 482.89 632.24 739.92 784.75 902.80 960.00 1005.19 1035.51 1104.34 1121.66 1172.68 1241.00 1301.10 1356.60 1416.79 1471.42 1475.06 1480.38 1512.01 1822.02 3001.65 3052.53 3064.73 3126.79 3161.59 3267.78 3566.02
Pentanal-AcOO	$CH_3CH_2CH_2CH_2C(=O)OO$•	-420.8424063	53.55 86.94 115.11 132.54 145.49 246.44 253.57 309.88 429.15 529.33 560.28 606.17 738.68 808.87 820.34 928.02 946.26 1041.25 1062.72 1088.34 1135.63 1146.75 1242.83 1250.30 1301.30 1321.05 1344.37 1382.75 1424.57 1426.61 1450.95 1496.41 1502.71 1506.13 1516.02 1921.44 3034.54 3045.83 3057.30 3064.55 3071.17 3093.72 3111.96 3117.58 3126.25
Pentanal-1,4-TS		-420.8002329	**-1628.40** 50.45 68.40 123.16 126.13 205.43 243.88 283.81 371.60 520.21 592.19 675.86 690.98 732.98 806.61 883.16 921.62 941.50 1017.35 1050.38 1082.67

			1129.50 1151.43 1175.84 1189.17 1263.74 1276.19 1335.25 1364.77 1414.03 1426.08 1477.46 1499.68 1506.55 1513.07 1765.74 1914.69 3026.74 3044.65 3048.10 3069.92 3089.27 3119.46 3126.69 3130.33
Pentanal-1,4-rad	$CH_3CH_2CH_2C•HC(=O)OOH$	-420.8460175	27.79 61.67 109.85 183.83 213.84 247.92 317.12 375.15 411.27 473.61 499.91 619.44 712.29 763.01 794.78 857.50 899.57 976.73 994.14 1059.29 1084.72 1103.69 1168.12 1204.07 1254.22 1289.11 1354.65 1379.27 1427.41 1461.50 1488.78 1499.29 1506.25 1509.97 1526.96 1749.92 3035.27 3047.47 3051.41 3088.98 3112.63 3120.80 3128.54 3204.73 3538.70
Pentanal-1,5-TS		-420.8095115	**-1699.90** 70.23 83.04 119.55 213.81 238.90 284.02 380.94 479.28 505.23 552.45 590.36 701.91 755.32 790.28 857.15 918.13 971.47 1035.16 1054.80 1076.28 1110.25 1155.22 1191.20 1221.72 1246.45 1289.94 1315.05 1336.86 1418.03 1426.75 1457.78 1477.91 1506.60 1509.35 1577.06 1873.91 3013.31 3050.84 3066.59 3076.36 3119.57 3122.99 3130.97 3134.84
Pentanal-1,5-rad	$CH_3CH_2C•HCH_2C(=O)OOH$	-420.838131	33.03 47.83 74.40 160.12 238.35 246.16 261.37 321.96 407.61 431.88 463.40 498.94 653.91 769.00 801.29 848.77 930.41 978.37 1026.98 1042.02 1069.11 1102.55

			1148.81 1207.86 1271.88 1285.60 1320.40 1348.15 1422.52 1430.28 1470.68 1475.25 1505.86 1509.90 1525.96 1813.58 2987.17 3012.57 3050.65 3066.10 3120.65 3130.58 3132.70 3190.34 3565.16
Pentanal-1,6-TS		-420.8113119	**-1778.60** 47.78 123.39 185.05 207.61 260.28 330.84 389.82 397.90 512.38 528.29 581.85 735.52 768.57 844.50 871.14 907.98 972.82 1017.39 1074.87 1105.17 1113.39 1134.64 1178.22 1218.14 1244.19 1298.72 1335.24 1365.91 1397.70 1417.15 1444.74 1477.51 1487.04 1495.39 1497.45 1872.18 3025.91 3045.88 3083.29 3095.08 3100.43 3105.67 3140.74 3161.88
Pentanal-1,6-rad	$CH_3C•HCH_2CH_2C(=O)OOH$	-420.8397415	26.19 41.88 83.08 116.08 194.26 219.94 296.95 339.20 384.37 429.27 469.65 504.66 631.20 718.69 855.77 897.95 949.58 980.52 1000.23 1021.16 1057.93 1120.75 1150.32 1195.85 1231.80 1284.22 1331.70 1397.57 1411.06 1438.05 1471.34 1480.21 1482.95 1489.55 1530.93 1823.17 2977.15 2983.51 3049.67 3056.43 3079.66 3127.64 3133.55 3180.74 3556.69
Pentanal-1,7-TS		-420.809389	**-1889.29** 89.88 151.68 199.17 281.15 307.68 363.74 460.51 480.33 504.51 581.80 589.02 730.13 772.75 810.75 831.35 918.14 967.17 984.75 1068.00 1081.39

			1100.13 1136.22 1150.70 1190.06 1240.35 1264.24 1305.74 1366.38 1383.92 1404.12 1448.80 1472.06 1482.28 1489.03 1502.99 1872.09 3021.63 3058.93 3070.08 3095.05 3109.41 3115.58 3169.18 3184.72
Pentanal-1,7-rad	C•$H_2CH_2CH_2CH_2C(=O)OOH$	-420.8355378	20.87 54.06 129.33 144.00 199.25 225.86 309.05 379.64 426.33 464.44 490.91 502.26 625.35 705.95 807.00 854.77 901.52 952.77 990.60 1003.02 1051.45 1105.78 1130.01 1181.47 1212.10 1273.81 1296.75 1372.34 1397.19 1410.52 1470.38 1471.32 1475.87 1496.20 1516.37 1817.50 2973.47 3053.69 3066.13 3073.35 3113.75 3128.69 3152.78 3259.78 3556.86
Hexanal-AcOO	$CH_3CH_2CH_2CH_2CH_2C(=O)OO$•	-460.0669611	52.98 61.04 86.53 128.84 137.68 148.07 221.32 244.60 248.42 397.87 435.34 529.57 562.51 610.25 735.20 769.36 821.66 861.61 921.48 984.03 1031.03 1061.10 1075.88 1090.14 1140.20 1149.43 1234.55 1250.68 1282.63 1300.24 1344.26 1346.00 1353.73 1408.19 1422.62 1430.11 1451.59 1493.98 1496.94 1506.03 1506.95 1516.41 1922.97 3022.86 3039.56 3044.47 3051.73 3059.64 3071.94 3076.86 3095.70 3113.64 3115.47 3123.97
Hexanal-1,4-TS		-460.0238594	**-1637.38** 34.78 63.86 102.14 153.56 182.85 210.20 287.08 300.13

			395.09 481.84 513.09 546.30 651.31 692.96 728.31 787.82 825.15 878.87 905.79 975.94 983.31 1018.45 1054.59 1103.44 1122.98 1145.37 1174.10 1183.67 1236.42 1270.30 1327.71 1341.97 1374.79 1402.92 1407.05 1427.44 1465.71 1499.90 1501.65 1512.82 1517.69 1768.73 1913.28 3032.52 3041.92 3051.44 3059.58 3080.80 3087.84 3100.13 3113.53 3125.31 3126.15
Hexanal-1,4-rad	$CH_3CH_2CH_2CH_2C•HC(=O)OOH$	-460.0703293	37.66 51.74 93.05 149.55 174.51 216.81 273.37 284.16 366.06 392.20 444.90 485.76 501.25 625.26 711.52 764.45 769.74 819.03 878.89 917.97 965.06 999.91 1016.43 1082.48 1109.90 1112.38 1158.11 1193.80 1239.85 1261.67 1321.75 1349.24 1385.11 1395.29 1429.11 1462.71 1484.79 1497.72 1501.54 1509.26 1521.89 1529.47 1747.02 3032.42 3037.77 3045.67 3046.20 3079.28 3087.89 3116.84 3123.78 3131.37 3204.30 3543.60
Hexanal-1,5-TS		-460.0343137	**-1704.50** 59.27 71.05 73.63 153.05 181.31 243.45 246.27 354.04 400.29 479.95 503.27 553.82 590.44 703.45 739.02 780.38 837.03 879.38 939.04 954.20 1029.87 1055.39 1069.36 1081.49 1127.64 1154.57 1190.28 1219.26 1239.85 1271.52 1294.14 1323.44 1343.54 1381.22 1425.26 1426.71 1457.98 1474.88

			1499.50 1506.78 1512.86 1574.94 1873.74 3001.29 3041.58 3046.11 3054.03 3075.72 3082.65 3116.94 3121.45 3127.91 3130.63
Hexanal-1,5-rad	$CH_3CH_2CH_2C•HCH_2C(=O)OOH$	-460.0623119	29.20 45.90 75.83 125.82 157.00 230.62 251.30 299.65 316.72 372.13 421.89 436.88 485.16 497.78 653.63 778.50 784.72 840.87 872.57 913.00 939.12 997.06 1030.46 1063.82 1080.45 1114.49 1151.85 1207.51 1248.00 1283.30 1296.40 1324.87 1354.04 1382.12 1421.37 1430.00 1473.27 1478.25 1498.62 1505.06 1512.35 1517.77 1813.82 2990.23 3044.64 3045.33 3063.37 3068.56 3085.60 3116.44 3126.15 3136.57 3189.86 3561.26
Hexanal-1,6-TS		-460.0365356	**-1743.82** 28.09 81.42 106.27 167.70 230.92 249.65 304.48 358.81 397.48 440.62 517.05 542.16 583.08 735.20 761.95 769.44 869.45 900.09 947.92 952.73 1021.62 1056.54 1075.45 1102.92 1125.52 1143.03 1174.72 1206.24 1231.96 1284.19 1307.01 1311.27 1367.47 1373.59 1412.27 1426.27 1447.72 1477.50 1488.58 1497.65 1506.64 1509.88 1871.60 3006.72 3049.45 3050.43 3063.66 3081.44 3095.04 3105.43 3122.01 3133.27 3161.17
Hexanal-1,6-rad	$CH_3CH_2C•HCH_2CH_2C(=O)OOH$	-460.0641677	21.39 27.54 41.76 101.07 163.98 196.55 234.63 260.38 328.62 366.85 408.01 417.24 460.38

			496.84 631.62 714.82 774.50 873.31 902.98 949.23 973.44 1008.97 1044.20 1066.17 1072.33 1126.38 1155.25 1191.84 1227.69 1273.50 1281.67 1305.02 1378.99 1400.15 1422.01 1444.25 1468.91 1478.68 1483.01 1504.71 1509.58 1511.51 1822.04 2962.70 2979.87 3017.16 3049.36 3062.24 3077.37 3119.36 3128.68 3132.20 3162.66 3551.15
Hexanal-1,7-TS		-460.0381727	**-1733.34** 70.32 118.03 167.80 175.57 214.42 284.12 326.82 336.22 411.22 505.55 518.79 569.28 603.29 711.75 760.77 805.75 846.64 886.77 916.62 960.47 1004.16 1034.29 1082.75 1097.69 1120.71 1134.00 1170.81 1210.45 1231.63 1272.14 1322.82 1361.80 1373.11 1393.38 1404.49 1423.83 1452.15 1475.24 1487.91 1491.51 1493.40 1514.02 1861.37 3014.20 3026.47 3064.70 3076.76 3097.83 3102.05 3108.01 3112.53 3143.95 3157.97
Hexanal-1,7-rad	$CH_3C•HCH_2CH_2CH_2C(=O)OOH$	-460.0646598	46.71 56.33 90.43 118.02 128.08 201.64 255.65 265.19 339.86 378.04 410.01 441.70 488.79 518.68 624.76 728.62 821.51 863.02 906.56 938.19 965.89 1000.04 1016.70 1020.56 1064.03 1120.32 1160.65 1195.56 1229.23 1257.78 1303.55 1359.88 1371.99 1401.04 1401.86 1426.29 1476.40 1479.06 1489.31 1490.89 1501.14 1523.95 1814.74

			2994.33 3012.72 3050.60 3064.36 3072.08 3077.43 3111.45 3119.93 3128.52 3198.56 3559.79
Hexanal-1,8-TS		-460.0315614	**-1858.46** 70.53 126.16 142.58 174.66 209.19 318.89 375.72 385.85 448.24 516.20 522.82 582.87 639.78 703.22 745.39 779.75 837.02 849.15 917.68 982.60 1006.61 1038.72 1076.43 1084.51 1112.95 1132.75 1149.19 1203.89 1239.79 1258.59 1282.14 1319.45 1363.64 1384.01 1398.65 1408.04 1430.71 1463.59 1476.72 1494.39 1503.77 1507.50 1866.45 3013.88 3045.87 3057.03 3066.00 3090.00 3097.05 3101.06 3107.50 3175.79 3176.29
Hexanal-1,8-rad	C•$H_2CH_2CH_2CH_2CH_2C(=O)OOH$	-460.0595377	27.85 40.59 75.71 144.09 168.81 214.05 236.98 308.91 339.92 403.11 438.53 481.49 501.20 515.75 636.03 714.97 791.71 818.68 870.96 928.96 946.37 954.84 1022.24 1030.86 1080.92 1112.90 1133.72 1157.78 1218.43 1235.78 1286.33 1321.45 1372.81 1387.92 1402.87 1407.96 1470.41 1473.94 1489.44 1494.85 1503.42 1508.39 1820.31 2971.57 3046.55 3053.20 3066.13 3083.99 3089.36 3113.17 3139.10 3152.04 3256.25 3553.57
Heptanal-AcOO	$CH_3CH_2CH_2CH_2CH_2CH_2C(=O)OO$•	-499.2916265	34.81 52.45 69.38 102.55 130.14 139.34 160.94 176.41 226.40 245.18 318.97 416.94 465.33

			529.95 563.74 609.24 733.32 749.85 809.39 826.79 901.65 913.07 1008.09 1033.20 1044.90 1077.91 1081.10 1091.06 1142.24 1152.73 1228.63 1249.61 1268.85 1284.78 1330.16 1330.38 1344.56 1350.82 1385.00 1419.33 1421.75 1430.53 1452.60 1493.85 1494.33 1501.19 1505.86 1510.29 1517.58 1921.65 3021.62 3026.30 3036.74 3043.01 3047.06 3058.68 3061.10 3073.10 3079.61 3095.97 3113.10 3115.12 3120.91
Heptanal-1,4-TS		-499.2485566	**-1645.41** 25.87 32.38 77.55 118.99 148.64 173.32 202.75 232.76 293.63 318.10 411.63 490.44 519.79 542.63 645.51 691.88 739.00 778.13 803.11 856.91 890.30 925.08 956.59 1003.80 1017.64 1024.16 1086.33 1111.04 1129.95 1145.18 1175.99 1182.54 1224.52 1263.24 1312.45 1323.83 1349.36 1360.65 1389.95 1392.36 1422.89 1428.23 1463.31 1494.46 1497.91 1509.67 1512.14 1515.52 1767.72 1912.86 3028.11 3031.72 3038.82 3047.05 3051.02 3070.87 3076.70 3081.73 3099.89 3118.78 3124.40 3127.89
Heptanal-1,4-rad	$CH_3CH_2CH_2CH_2CH_2C•HC(=O)OOH$	-499.2951792	29.04 36.53 79.44 90.44 144.08 181.22 236.42 244.17 261.93 307.12 371.11 394.98 456.95 498.75 503.02 624.94 711.69 745.50 769.04 805.45 850.20 890.95 930.75 956.75 1001.84

			1038.05 1049.47 1088.29 1107.59 1122.65 1160.41 1192.65 1237.36 1250.23 1302.68 1331.23 1346.60 1364.70 1389.76 1418.56 1422.44 1463.79 1489.13 1495.39 1500.62 1503.98 1506.79 1515.29 1532.28 1747.53 3023.63 3034.33 3038.25 3041.78 3046.29 3065.31 3085.29 3090.45 3113.39 3122.44 3126.68 3204.03 3531.90
Heptanal-1,5-TS		-499.258317	**-1706.73** 37.51 76.63 86.02 116.55 170.50 222.22 252.98 290.50 304.74 383.03 465.86 482.86 505.97 565.46 590.46 707.64 744.26 775.77 811.85 851.56 873.05 912.53 983.49 1003.58 1035.86 1059.92 1066.17 1110.82 1128.68 1147.55 1180.62 1222.45 1230.49 1252.85 1278.72 1314.97 1325.44 1342.05 1385.03 1398.34 1424.16 1429.23 1459.40 1475.18 1496.21 1499.42 1509.42 1518.76 1583.56 1875.09 3010.41 3038.04 3045.60 3047.31 3063.72 3076.64 3078.10 3088.19 3118.13 3118.48 3129.99 3131.64
Heptanal-1,5-rad	$CH_3CH_2CH_2CH_2C•HCH_2C(=O)OOH$	-499.2871682	28.15 40.23 61.23 91.69 136.57 179.15 226.58 253.02 262.91 294.63 330.03 398.13 424.62 439.52 487.33 561.27 644.72 747.16 783.50 822.81 846.91 901.07 924.04 952.63 986.50 1012.21 1040.14 1068.59 1115.12 1117.26 1157.97 1185.33 1248.53 1263.27 1282.45 1326.26 1337.08

			1341.48 1364.51 1404.04 1421.07 1423.07 1471.07 1486.44 1496.67 1503.14 1507.21 1515.43 1526.40 1817.45 3004.54 3034.19 3042.33 3045.82 3059.82 3062.46 3080.45 3094.87 3113.98 3122.10 3125.40 3206.66 3555.56
Heptanal-1,6-TS		-499.2613129	**-1736.78** 9.87 74.53 78.48 129.25 146.88 207.69 243.00 269.61 356.73 384.49 419.34 452.13 508.92 578.66 606.64 731.75 740.10 773.86 829.91 886.85 900.54 919.22 982.67 1001.10 1048.59 1074.64 1088.28 1106.21 1119.96 1138.40 1167.89 1182.20 1230.69 1270.09 1291.51 1297.01 1341.63 1349.18 1374.45 1386.87 1421.32 1424.36 1467.55 1478.08 1482.27 1499.78 1501.16 1506.71 1513.02 1872.31 2996.71 3040.96 3044.87 3050.80 3055.65 3084.15 3096.01 3103.50 3116.10 3117.02 3126.12 3163.28
Heptanal-1,6-rad	$CH_3CH_2CH_2C•HCH_2CH_2C(=O)OOH$	-499.2885605	38.09 46.17 73.72 93.59 154.55 181.61 217.83 239.30 274.65 327.38 341.40 373.98 430.68 463.05 495.18 510.14 633.46 725.15 770.22 848.92 857.53 895.95 914.87 960.62 992.59 1024.87 1041.42 1055.47 1090.40 1128.29 1149.60 1196.96 1216.44 1257.61 1287.41 1293.09 1336.16 1359.90 1380.57 1393.51 1423.07 1433.83 1477.51 1485.19 1488.62 1501.23 1503.49 1512.42 1520.30

			1820.03 2995.99 3010.05 3044.34 3049.93 3073.96 3077.43 3083.67 3089.89 3115.66 3125.45 3135.36 3179.95 3552.92
Heptanal-1,7-TS		-499.2639135	**-1710.89** 57.46 83.78 117.24 161.07 198.74 239.05 252.64 288.15 333.26 379.96 422.45 506.55 527.17 571.03 604.99 711.39 761.45 769.03 831.65 834.21 911.91 925.36 968.86 1010.05 1035.05 1063.20 1088.48 1098.01 1120.43 1137.92 1172.88 1206.98 1231.31 1263.60 1297.98 1319.00 1327.05 1371.87 1389.07 1402.87 1417.98 1427.17 1451.95 1475.85 1481.41 1490.09 1506.40 1508.14 1511.10 1860.87 3004.08 3015.60 3051.29 3064.64 3075.48 3078.26 3093.28 3097.77 3112.07 3124.38 3136.01 3157.47
Heptanal-1,7-rad	$CH_3CH_2C•HCH_2CH_2CH_2C(=O)OOH$	-499.2894119	43.98 57.44 82.77 104.19 116.92 191.92 233.72 237.86 255.14 295.73 341.50 366.91 427.40 445.09 494.03 533.19 621.37 724.59 778.32 813.33 867.93 907.73 937.46 964.05 1008.61 1034.93 1052.92 1062.97 1069.94 1121.97 1158.24 1195.99 1226.31 1253.48 1281.15 1297.27 1332.01 1364.24 1383.81 1403.08 1422.96 1434.99 1471.28 1477.33 1488.58 1497.54 1504.28 1508.83 1534.04 1812.87 2971.43 3007.28 3021.07 3049.62 3065.74 3071.25 3077.03 3112.37 3119.78 3127.27 3128.64

			3186.04 3555.41
Heptanal-1,8-TS		-499.2617743	**-1706.70** 59.61 84.33 121.23 141.13 196.52 235.02 241.44 284.80 366.18 383.12 416.94 465.90 521.82 555.56 592.22 694.97 770.74 779.10 859.33 880.79 896.13 916.28 957.29 1021.70 1049.68 1083.30 1096.10 1108.44 1123.23 1133.26 1159.97 1173.07 1237.40 1265.28 1286.53 1304.37 1332.81 1382.58 1394.10 1398.04 1410.38 1419.06 1447.77 1482.75 1490.22 1493.52 1497.55 1500.59 1503.21 1862.01 3015.57 3029.54 3044.88 3055.63 3061.72 3087.63 3092.94 3096.20 3102.03 3104.55 3140.11 3168.22
Heptanal-1,8-rad	$CH_3C•HCH_2CH_2CH_2CH_2C(=O)OOH$	-499.2892745	22.50 34.05 53.02 79.81 125.46 137.71 210.97 217.99 251.99 289.37 322.41 344.03 408.21 459.99 489.46 567.48 625.33 700.89 791.60 830.12 864.06 906.65 953.32 987.72 991.86 1009.11 1029.01 1069.52 1083.75 1133.48 1161.48 1177.89 1219.11 1251.98 1281.08 1327.45 1343.43 1376.93 1388.17 1405.01 1417.39 1429.07 1473.48 1476.38 1482.54 1489.77 1496.31 1509.70 1516.11 1816.93 2970.47 2991.86 3028.92 3042.50 3060.35 3066.01 3069.35 3082.03 3107.74 3123.97 3124.84 3203.82 3559.94
Heptanal-1,9-TS		-499.2584072	**-1867.51** 61.14 90.08 171.93 183.32 235.10

			275.36 293.34 327.49 330.97 397.20 445.08 479.17 515.67 560.36 618.60 668.74 738.65 796.98 840.44 875.57 887.55 931.26 965.10 1002.82 1045.50 1063.94 1074.31 1105.24 1122.19 1134.69 1140.72 1183.90 1216.79 1244.82 1266.04 1302.91 1326.48 1348.60 1374.14 1395.86 1406.79 1419.43 1453.79 1471.31 1472.33 1480.84 1493.91 1503.31 1521.34 1874.72 3017.37 3036.31 3060.12 3065.72 3072.01 3075.77 3081.26 3095.36 3107.28 3109.82 3132.44 3180.78
Heptanal-1,9-rad	C•$H_2CH_2CH_2CH_2CH_2CH_2C(=O)OOH$	-499.2841152	30.35 38.39 56.71 122.32 162.56 173.66 178.73 237.89 269.54 326.96 347.81 412.29 441.60 485.41 501.52 514.40 643.26 727.11 765.95 820.31 858.22 894.65 908.98 940.59 981.39 993.90 1034.18 1079.55 1091.31 1112.67 1135.29 1160.84 1211.79 1225.56 1283.96 1303.25 1337.14 1347.90 1380.00 1393.05 1394.90 1420.30 1470.52 1472.62 1488.69 1496.35 1498.90 1508.58 1514.10 1822.26 2965.90 3030.46 3036.19 3044.13 3056.77 3070.49 3088.82 3091.67 3108.00 3145.03 3153.16 3258.90 3555.44
Octanal-AcOO	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2C(=O)OO•$	-538.5162965	35.74 41.52 56.36 93.40 101.65 136.50 145.72 154.26 158.02 202.96 245.57 272.62 358.57

			435.13 481.75 529.94 563.25 611.25 733.64 740.98 777.19 826.73 846.25 912.60 933.65 1018.98 1025.86 1049.17 1060.61 1078.70 1090.42 1093.76 1142.21 1154.48 1223.57 1248.71 1259.69 1269.92 1311.76 1315.88 1336.52 1348.62 1351.19 1361.80 1401.87 1420.99 1423.63 1429.73 1451.81 1492.46 1493.32 1497.63 1503.82 1505.31 1512.18 1517.91 1921.74 3020.46 3022.46 3029.65 3037.26 3041.93 3044.75 3053.36 3059.15 3069.23 3072.80 3082.09 3096.11 3111.73 3115.02 3120.43
Octanal-1,4-TS		-538.473369	**-1618.87** 22.63 40.57 59.93 83.31 106.19 181.89 197.82 205.69 222.49 249.53 294.04 338.07 442.45 506.83 526.31 568.75 661.47 689.23 726.82 763.94 793.88 837.81 858.46 882.74 930.68 958.46 1016.90 1021.13 1042.55 1056.37 1080.25 1119.30 1134.89 1149.69 1170.79 1184.52 1218.46 1254.64 1298.97 1314.59 1335.95 1338.55 1349.38 1360.65 1401.53 1413.71 1421.57 1424.25 1467.78 1492.43 1498.86 1503.19 1505.49 1506.62 1516.80 1766.20 1912.45 3027.16 3030.47 3037.18 3039.79 3042.30 3050.98 3060.31 3074.78 3079.32 3085.18 3098.96 3111.45 3122.79 3135.06
Octanal-1,4-rad	$CH_3CH_2CH_2CH_2CH_2CH_2C•HC(=O)OOH$	-538.5200175	25.02 28.86 60.70 79.13 113.73 134.65 183.80

		201.17 237.74 254.50 287.47 364.57 384.37 405.86 450.68 494.44 500.54 621.72 711.71 739.31 769.12 776.13 841.35 868.93 905.83 933.28 970.17 996.48 1019.22 1059.68 1075.93 1089.99 1116.54 1127.67 1160.32 1191.65 1232.53 1245.06 1283.60 1308.19 1334.44 1348.88 1357.41 1387.14 1392.05 1421.68 1426.51 1464.49 1489.41 1494.89 1496.34 1503.86 1505.48 1506.34 1516.21 1522.78 1746.96 3021.03 3028.09 3035.04 3036.01 3042.02 3047.10 3060.58 3067.46 3086.49 3092.38 3112.37 3120.18 3126.96 3203.86 3526.83
Octanal-1,5-TS	-538.4836187	**-1688.96** 37.02 44.12 58.33 97.74 117.62 129.88 163.50 217.60 246.25 264.23 302.85 399.31 456.69 480.79 519.70 555.19 590.91 704.14 733.58 751.16 782.40 829.33 889.85 917.42 922.80 997.89 1020.86 1056.82 1059.82 1067.09 1081.92 1089.35 1139.06 1159.69 1192.35 1221.02 1232.26 1245.29 1273.31 1299.42 1318.37 1332.27 1344.98 1347.91 1381.86 1418.84 1422.54 1429.74 1458.10 1475.11 1494.03 1497.05 1506.36 1506.79 1516.37 1580.40 1873.66 3002.40 3023.22 3030.88 3038.16 3043.10 3050.16 3055.65 3072.08 3076.06 3086.40 3113.29 3121.41 3121.81 3130.94

Octanal-1,5-rad	$CH_3CH_2CH_2CH_2CH_2C•HCH_2C(=O)OOH$	-538.5116612	41.29 56.56 68.58 76.27 145.85 162.58 186.60 227.71 261.14 267.00 294.56 324.54 356.21 418.57 437.39 458.22 482.86 515.70 642.47 738.37 783.55 794.73 840.95 873.93 895.85 930.81 966.34 972.99 1012.44 1048.59 1052.18 1092.73 1116.73 1122.67 1152.78 1182.93 1224.12 1251.29 1299.47 1304.62 1323.07 1330.09 1341.82 1356.90 1392.26 1416.63 1419.47 1426.94 1470.80 1486.15 1492.40 1497.19 1502.89 1506.73 1517.89 1523.99 1817.58 2988.05 3030.69 3039.21 3041.49 3043.07 3058.04 3065.34 3068.84 3084.94 3092.71 3114.24 3122.27 3129.48 3194.81 3561.71
Octanal-1,6-TS		-538.485198	**-1753.64** 32.34 45.38 78.95 114.80 151.72 183.86 237.48 254.98 289.40 306.95 358.23 396.75 414.87 492.90 513.70 549.90 583.49 733.50 745.13 769.56 807.64 857.64 871.94 906.41 915.97 978.16 1011.07 1039.72 1047.97 1073.51 1090.01 1122.41 1134.01 1140.79 1170.87 1196.93 1249.00 1259.48 1271.96 1299.06 1312.63 1332.45 1366.18 1373.81 1390.98 1398.48 1417.35 1428.39 1457.47 1472.64 1483.71 1494.97 1496.19 1500.13 1512.16 1518.43 1872.16 3004.28 3036.62 3045.25 3047.24 3050.76 3059.94 3075.27 3079.24

			3088.10 3093.48 3104.15 3117.91 3129.43 3161.67
Octanal-1,6-rad	$CH_3CH_2CH_2CH_2C•HCH_2CH_2C(=O)OOH$	-538.5138592	41.99 51.51 69.73 91.30 136.26 159.79 173.79 221.56 254.11 259.29 294.93 333.57 349.26 403.67 430.76 457.55 480.30 535.93 633.52 726.15 747.70 815.81 843.15 887.45 904.07 939.79 964.90 977.25 1006.83 1046.65 1051.95 1070.06 1117.23 1130.61 1146.93 1196.59 1215.69 1249.28 1263.49 1289.74 1327.15 1333.19 1348.14 1362.48 1391.83 1408.65 1419.81 1432.54 1477.97 1485.86 1489.28 1498.41 1503.16 1506.10 1517.49 1537.67 1819.19 2997.99 3005.20 3036.73 3040.02 3043.26 3068.25 3077.34 3077.88 3086.40 3091.36 3110.78 3120.62 3135.50 3180.67 3565.15
Octanal-1,7-TS		-538.4881739	**-1766.33** 51.96 71.89 75.28 113.49 153.78 200.27 217.63 245.14 274.86 288.40 351.33 412.34 423.41 510.07 551.66 580.99 588.79 728.98 738.62 758.51 808.67 818.50 852.87 908.50 936.93 953.22 1004.93 1028.66 1065.62 1081.86 1087.35 1105.81 1137.49 1145.23 1173.87 1205.34 1234.73 1248.65 1276.56 1295.08 1315.04 1342.48 1362.66 1376.99 1388.75 1408.35 1419.32 1424.91 1462.18 1475.79 1485.95 1499.51 1501.67 1506.49 1510.39 1512.95 1869.45 2996.64 3020.43

			3043.68 3044.55 3059.12 3068.06 3076.29 3083.46 3097.96 3110.62 3114.66 3115.75 3125.62 3171.86
Octanal-1,7-rad	$CH_3CH_2CH_2C•HCH_2CH_2CH_2C(=O)OOH$	-538.5137578	39.54 66.47 76.46 87.35 112.73 161.94 194.52 212.79 247.04 260.97 301.52 320.49 353.38 366.35 432.27 457.06 478.21 543.56 620.73 726.77 773.69 827.76 851.57 873.35 905.75 934.25 943.24 987.98 1013.64 1055.91 1066.92 1077.86 1096.30 1128.85 1158.37 1188.78 1228.55 1244.98 1257.41 1293.81 1314.23 1342.54 1364.77 1383.80 1386.71 1403.78 1426.38 1436.98 1468.52 1476.97 1488.06 1496.46 1499.38 1507.38 1515.77 1522.51 1816.53 2975.68 2995.01 3005.96 3044.91 3045.19 3064.65 3070.82 3076.31 3080.65 3111.69 3117.81 3123.82 3127.30 3189.69 3564.11
Octanal-1,8-TS		-538.4870457	**-1677.33** 49.82 74.77 88.63 126.60 132.53 191.54 229.31 249.79 265.71 357.23 366.94 400.19 420.27 470.78 520.56 554.16 592.32 694.54 767.81 775.45 785.43 872.93 881.19 930.10 937.11 966.00 1004.37 1046.93 1064.93 1095.13 1097.51 1108.84 1131.01 1135.05 1168.24 1170.85 1228.93 1253.31 1280.78 1287.47 1310.39 1326.34 1367.84 1388.44 1397.99 1404.97 1419.89 1424.76 1447.50 1476.97 1488.85 1497.56 1502.14

			1504.25 1506.08 1511.49 1861.86 3008.47 3018.62 3046.24 3049.57 3055.27 3061.56 3067.32 3080.37 3092.15 3096.32 3103.67 3121.45 3133.32 3164.42
Octanal-1,8-rad	$CH_3CH_2C•HCH_2CH_2CH_2CH_2C(=O)OOH$	-538.5135741	19.23 25.64 31.38 73.84 81.70 131.27 203.84 211.76 230.83 232.11 272.58 302.07 321.48 362.84 419.89 469.26 494.01 581.69 625.05 700.17 773.73 801.40 839.65 851.02 911.96 947.52 979.66 1000.91 1040.99 1052.49 1063.33 1075.02 1087.04 1129.29 1163.01 1179.57 1216.24 1251.33 1280.17 1287.26 1317.99 1334.51 1349.00 1382.21 1404.29 1415.89 1420.19 1432.36 1475.62 1476.21 1479.89 1494.39 1504.31 1508.17 1508.88 1520.40 1817.18 2964.41 2971.71 3004.81 3042.33 3046.48 3060.33 3064.22 3070.04 3081.47 3108.30 3115.14 3124.73 3125.88 3182.62 3562.37
Octanal-1,9-TS		-538.4846642	**-1709.37** 51.06 74.07 128.55 149.87 180.55 192.20 207.19 248.68 292.58 316.00 365.67 414.79 424.11 490.11 515.01 555.67 600.03 699.07 742.23 772.15 825.33 845.54 888.58 892.71 950.37 970.28 1000.52 1045.09 1060.79 1082.76 1094.65 1119.15 1129.87 1132.41 1166.34 1174.31 1234.44 1247.47 1268.64 1307.90 1318.65 1341.96 1376.79 1390.34 1403.67 1405.03 1413.47

			1421.12 1457.08 1483.66 1486.45 1489.21 1496.58 1498.84 1504.79 1510.97 1860.85 3011.44 3030.43 3037.46 3055.80 3057.22 3060.27 3077.76 3083.95 3089.03 3099.12 3104.28 3108.02 3140.17 3157.49
Octanal-1,9-rad	$CH_3C•HCH_2CH_2CH_2CH_2CH_2C(=O)OOH$	-538.5133189	27.81 39.12 43.33 61.80 114.07 127.65 150.77 173.02 227.20 239.57 281.32 338.05 359.00 391.09 446.16 455.19 503.22 546.39 641.20 723.47 763.48 834.13 838.19 889.50 912.97 941.32 962.51 993.22 1009.54 1017.82 1046.97 1090.39 1101.14 1129.05 1159.22 1171.90 1199.17 1238.94 1281.80 1294.58 1331.48 1342.92 1366.41 1388.23 1394.69 1397.89 1416.69 1424.43 1476.87 1485.12 1488.03 1489.90 1496.35 1499.52 1508.47 1540.25 1823.56 2990.58 2994.45 3034.17 3041.36 3047.78 3056.13 3066.23 3076.41 3085.64 3092.64 3106.81 3116.23 3142.23 3196.71 3558.70
Nonanal-AcOO	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2C(=O)OO•$	-577.7409351	22.19 35.08 46.64 75.45 94.60 121.50 124.23 141.64 151.63 166.23 189.18 226.54 244.88 343.52 357.55 468.74 485.13 529.91 563.96 611.89 732.27 736.44 758.90 808.41 826.54 878.69 911.74 958.90 1014.70 1037.69 1038.43 1056.32 1072.17 1089.09 1090.61 1096.86 1143.54

			1155.87 1221.03 1246.84 1253.99 1261.41 1298.53 1303.92 1335.24 1336.81 1343.88 1350.60 1352.71 1384.31 1413.17 1420.55 1425.68 1430.03 1452.49 1491.68 1492.45 1495.97 1499.42 1505.51 1506.43 1513.58 1518.16 1921.68 3019.44 3021.81 3023.30 3030.94 3036.40 3042.01 3042.95 3049.31 3058.75 3059.43 3073.13 3073.27 3083.23 3096.15 3111.98 3115.13 3119.36
Nonanal-1,4-TS		-577.6981309	**-1628.11** 15.45 34.01 55.34 78.55 89.60 130.36 158.86 183.53 210.05 219.36 249.22 263.52 328.24 406.27 431.08 505.92 524.40 567.66 661.06 689.12 729.63 750.70 780.18 827.84 842.30 872.71 918.89 922.33 966.33 1007.76 1016.59 1032.72 1067.94 1078.10 1086.51 1119.19 1138.39 1152.25 1170.85 1184.14 1212.12 1242.26 1285.39 1301.49 1322.92 1325.50 1345.78 1350.48 1354.19 1385.97 1401.22 1419.96 1422.55 1427.15 1467.23 1492.21 1495.96 1500.98 1505.58 1506.80 1509.53 1518.49 1766.07 1911.25 3021.66 3027.00 3031.24 3035.16 3040.03 3042.81 3048.27 3052.86 3065.51 3075.45 3079.31 3086.38 3098.40 3113.23 3120.66 3134.99
Nonanal-1,4-rad	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2C•HC(=O)OOH$	-577.7446294	22.76 29.39 62.18 63.82 96.25 113.91 144.32 166.45 185.65 242.27 251.06 257.63 334.41

		367.38 384.08 417.44 468.23 500.90 512.30 621.67 711.52 738.26 757.18 769.21 811.44 852.15 892.00 913.16 927.55 985.50 999.76 1018.02 1047.29 1070.81 1088.26 1091.41 1118.32 1130.89 1159.82 1189.50 1227.47 1240.98 1269.35 1289.50 1317.79 1342.67 1344.53 1349.33 1367.62 1389.72 1408.81 1420.61 1427.03 1463.02 1488.69 1492.64 1495.23 1498.86 1503.33 1505.51 1508.98 1517.03 1532.85 1746.85 3017.85 3021.27 3030.17 3035.68 3036.10 3041.01 3046.73 3048.41 3064.81 3073.47 3086.14 3092.31 3110.82 3119.23 3125.26 3205.14 3539.70
Nonanal-1,5-TS	-577.7083104	**-1683.96** 26.95 37.57 52.43 75.42 98.00 113.57 144.64 164.33 194.77 235.15 244.05 284.87 332.33 431.94 471.12 483.89 520.18 555.33 590.52 704.29 732.22 740.51 773.65 794.62 864.05 894.70 916.08 940.94 1009.12 1021.88 1041.66 1061.22 1069.80 1076.50 1085.42 1090.11 1143.59 1159.99 1192.59 1221.00 1228.97 1238.31 1266.14 1285.96 1305.04 1321.48 1335.66 1343.82 1351.64 1359.39 1400.99 1421.19 1423.69 1429.44 1457.84 1474.69 1493.09 1493.78 1500.39 1505.67 1509.27 1516.84 1585.68 1873.69 3001.16 3021.02 3024.80 3032.50 3037.25

			3042.13 3046.44 3053.26 3061.56 3075.20 3076.01 3086.90 3112.05 3120.31 3122.09 3130.48
Nonanal-1,5-rad	$CH_3CH_2CH_2CH_2CH_2CH_2C•HCH_2C(=O)OOH$	-577.7370236	27.14 36.37 65.37 77.82 123.13 132.01 148.38 169.49 225.51 235.23 254.28 274.56 317.36 348.76 404.54 413.92 432.61 449.64 481.51 512.03 641.61 736.41 771.32 786.74 829.79 848.92 893.09 915.06 926.50 962.84 983.09 1003.37 1030.57 1064.33 1079.15 1096.56 1118.86 1129.09 1152.81 1179.99 1221.73 1240.57 1280.96 1298.45 1309.16 1325.01 1335.30 1341.45 1346.49 1387.96 1394.05 1419.84 1422.08 1426.16 1470.39 1485.22 1492.84 1497.56 1500.66 1504.19 1505.33 1511.97 1520.81 1817.70 2985.94 3024.12 3032.89 3036.83 3040.70 3041.93 3057.86 3059.27 3065.53 3070.39 3084.64 3088.24 3112.43 3120.74 3128.59 3195.10 3554.66
Nonanal-1,6-TS		-577.710426	**-1757.36** 30.34 37.14 44.98 107.89 119.72 159.57 212.81 226.65 248.08 278.43 295.19 305.96 370.54 401.02 433.26 502.28 512.97 556.82 583.15 733.03 737.16 769.23 783.00 846.41 860.63 892.04 902.97 937.14 959.72 1011.45 1050.09 1055.44 1062.50 1076.30 1090.84 1124.21 1137.03 1143.56 1172.24 1192.88 1234.17 1254.59 1263.11 1291.90

			1309.10 1320.00 1338.15 1352.87 1366.31 1380.89 1398.43 1413.25 1420.82 1420.87 1450.60 1479.26 1482.57 1495.84 1496.34 1498.12 1505.04 1507.91 1516.74 1872.70 3003.80 3032.06 3037.58 3042.21 3044.39 3048.20 3061.12 3066.64 3076.19 3084.95 3089.72 3093.33 3104.27 3115.43 3123.76 3161.66
Nonanal-1,6-rad	$CH_3CH_2CH_2CH_2CH_2C\bullet HCH_2CH_2C(=O)OOH$	-577.7392926	31.30 48.15 63.66 86.54 109.01 114.32 153.13 171.23 195.69 226.91 248.97 274.48 326.07 344.40 385.07 403.90 431.64 460.78 488.01 527.13 631.77 723.73 737.35 784.50 840.63 866.32 905.55 922.77 927.49 957.84 984.23 1002.28 1043.78 1053.30 1061.75 1086.79 1122.82 1134.82 1148.87 1194.59 1216.46 1242.54 1247.16 1285.76 1308.22 1318.36 1339.09 1340.14 1361.57 1382.90 1393.75 1416.76 1420.99 1433.07 1477.48 1484.92 1488.91 1493.37 1498.36 1505.47 1507.43 1518.42 1523.42 1820.02 2998.23 3006.66 3022.62 3032.69 3041.13 3042.01 3053.06 3068.39 3076.08 3077.56 3086.41 3090.75 3112.66 3119.64 3134.56 3180.07 3558.36
Nonanal-1,7-TS		-577.7129331	**-1765.73** 37.79 59.90 65.48 101.77 120.73 154.12 176.39 214.12 246.54 247.37 272.31 334.11 374.51 393.27 451.63 509.27 562.17 580.90 588.47 729.48

			734.76 753.73 777.56 819.16 828.53 882.15 912.46 939.37 969.88 1010.99 1017.99 1051.82 1079.78 1085.33 1093.02 1108.49 1139.03 1147.18 1175.36 1204.56 1231.13 1240.33 1266.91 1281.88 1310.53 1327.28 1342.68 1346.98 1368.78 1385.73 1398.19 1410.90 1423.18 1425.50 1462.04 1475.99 1484.26 1495.30 1500.42 1503.01 1505.74 1508.87 1515.01 1869.36 2997.74 3020.12 3029.41 3036.84 3044.29 3055.44 3063.55 3068.56 3076.43 3084.64 3099.18 3109.64 3114.77 3115.42 3122.73 3169.18
Nonanal-1,7-rad	$CH_3CH_2CH_2CH_2C\bullet HCH_2CH_2CH_2C(=O)OOH$	-577.7387381	29.97 56.05 71.24 77.16 103.30 105.92 149.29 182.10 230.17 242.04 253.39 260.05 299.57 311.50 353.54 371.85 439.19 469.69 488.12 563.72 618.25 724.96 758.18 815.01 820.93 864.78 878.21 931.40 940.27 943.97 985.18 1010.32 1042.59 1061.72 1073.65 1090.02 1104.48 1135.96 1158.75 1188.88 1227.47 1237.68 1249.70 1284.33 1303.19 1331.16 1339.54 1352.82 1366.48 1385.83 1404.14 1413.86 1421.11 1436.36 1468.85 1476.16 1487.88 1496.42 1497.24 1503.48 1505.49 1522.11 1528.95 1815.30 2977.37 2995.28 3004.38 3031.34 3039.92 3043.33 3064.50 3064.77 3070.23 3076.28 3086.14 3111.27 3111.73 3118.80 3126.59

			3188.73 3564.07
Nonanal-1,8-TS		-577.712077	**-1687.27** 37.63 65.50 69.48 88.74 105.42 144.18 165.21 232.89 243.98 255.48 296.70 343.91 369.33 394.57 461.09 472.91 518.78 559.32 593.83 694.13 741.94 774.54 782.30 841.60 873.84 884.14 914.34 945.95 988.55 1003.67 1037.14 1062.61 1088.64 1092.65 1096.82 1108.62 1132.00 1135.01 1169.28 1170.72 1224.07 1248.39 1273.04 1279.27 1295.16 1318.63 1340.72 1350.82 1382.61 1393.51 1398.37 1410.01 1423.71 1424.83 1448.16 1472.74 1483.74 1489.53 1500.23 1500.91 1502.05 1506.40 1513.66 1861.76 2997.28 3017.06 3040.57 3043.72 3045.45 3054.71 3055.24 3061.64 3078.93 3085.93 3091.56 3095.70 3103.18 3115.11 3124.54 3164.44
Nonanal-1,8-rad	$CH_3CH_2CH_2C•HCH_2CH_2CH_2CH_2C(=O)OOH$	-577.7380125	20.91 29.75 44.09 51.18 86.78 130.73 164.11 204.84 217.29 227.69 246.37 282.63 305.87 329.48 378.83 413.01 452.79 472.97 494.91 583.39 625.57 700.56 779.11 786.88 836.24 842.44 881.62 909.43 932.65 953.08 987.91 1013.80 1051.48 1067.46 1078.85 1083.72 1089.97 1133.14 1163.53 1181.65 1213.88 1246.29 1255.53 1279.96 1294.55 1326.15 1339.10 1351.80 1378.25 1386.77 1403.90 1415.78 1419.86 1436.62 1473.44

			1476.30 1477.00 1494.95 1499.04 1504.05 1507.95 1514.13 1524.79 1815.63 2954.12 2960.48 3037.91 3039.61 3044.51 3053.01 3059.89 3061.28 3070.39 3080.24 3082.87 3110.80 3111.46 3118.72 3125.44 3166.59 3559.23
Nonanal-1,9-TS		-577.7079898	**-1776.02** 49.77 72.65 85.44 131.30 139.97 176.62 187.84 217.04 242.27 274.57 336.00 365.10 377.45 385.91 441.28 460.64 512.73 577.86 600.85 699.06 754.61 766.37 779.73 799.91 856.63 882.23 896.98 950.10 986.54 993.77 1031.98 1046.10 1073.80 1082.75 1092.77 1106.96 1137.05 1152.93 1162.85 1193.39 1208.82 1234.15 1266.99 1289.24 1306.81 1329.67 1337.50 1375.17 1386.34 1394.52 1406.36 1417.06 1426.11 1428.61 1452.22 1476.65 1479.57 1491.36 1503.10 1504.14 1507.22 1507.90 1510.64 1865.74 3001.79 3010.73 3043.50 3047.29 3051.46 3056.69 3065.60 3073.28 3084.59 3087.40 3093.03 3100.98 3107.46 3124.77 3134.62 3198.23
Nonanal-1,9-rad	$CH_3CH_2C•HCH_2CH_2CH_2CH_2CH_2C(=O)OOH$	-577.7373221	34.54 36.49 57.99 62.58 81.39 92.49 162.18 202.66 225.21 228.65 251.88 295.95 328.94 338.17 368.80 427.40 445.18 457.82 484.86 531.66 638.26 719.28 765.46 786.51 821.76 844.49 873.57 912.43 952.00 970.60 990.45 1023.33

1048.92 1058.42 1061.12
1084.65 1095.97 1130.09
1158.38 1175.54 1201.09
1234.11 1279.42 1289.84
1292.71 1316.07 1341.19
1349.57 1369.56 1388.50
1394.14 1416.10 1419.58
1437.64 1480.39 1485.07
1492.06 1493.60 1500.18
1501.77 1502.79 1506.65
1512.30 1817.90 2962.38
3023.26 3035.65 3038.87
3043.53 3061.54 3065.13
3068.53 3074.55 3080.11
3087.28 3111.34 3114.73
3120.78 3135.49 3157.64
3555.62

10. Cartesian coordinates of the global minimum geometry of each of the species involved

Species		Coordinates		
Ethanal-AcOO	C	-1.441707000	0.186549000	0.000000000
	H	-1.672779000	-0.417565000	0.874873000
	H	-2.020645000	1.103483000	0.000000000
	H	-1.672779000	-0.417565000	-0.874873000
	C	0.000000000	0.558925000	0.000000000
	O	0.491666000	1.638754000	0.000000000
	O	0.916874000	-0.528970000	0.000000000
	O	0.343516000	-1.702434000	0.000000000
Ethanal-1,4-TS	C	0.000000000	0.583442000	0.000000000
	O	0.244666000	1.747616000	0.000000000
	C	-1.350373000	-0.066108000	0.000000000
	O	0.973883000	-0.366911000	0.000000000
	O	0.374846000	-1.632600000	0.000000000
	H	-1.922334000	0.076256000	0.909061000
	H	-0.800250000	-1.241358000	0.000000000
	H	-1.922334000	0.076256000	-0.909061000
Ethanal-1,4-rad	C	-0.473923000	0.132072000	-0.000057000
	O	-0.209785000	1.320234000	-0.000002000
	C	-1.777775000	-0.467027000	0.000033000
	O	0.504537000	-0.801697000	-0.000047000
	H	-1.884497000	-1.537757000	0.000145000
	H	-2.635330000	0.181296000	0.000004000
	O	1.769181000	-0.192974000	0.000029000
	H	1.518548000	0.761695000	0.000158000
Propanal-AcOO	C	-2.065742000	-0.896490000	0.000000000
	H	-2.429023000	-1.922372000	0.000000000
	H	-2.460857000	-0.390792000	0.878971000
	H	-2.460857000	-0.390792000	-0.878971000
	C	-0.545728000	-0.888667000	0.000000000
	H	-0.135805000	-1.410024000	0.865943000
	H	-0.135805000	-1.410024000	-0.865943000
	C	0.000000000	0.504177000	0.000000000
	O	-0.586155000	1.530979000	0.000000000
	O	1.427433000	0.628193000	0.000000000
	O	2.070117000	-0.507937000	0.000000000
Propanal-1,4-TS	C	0.273710000	0.650626000	0.083502000
	O	0.145549000	1.827929000	-0.012879000
	C	-0.761926000	-0.352274000	0.524879000
	O	1.438266000	0.022386000	-0.216026000

	O	1.268616000	-1.362571000	-0.040690000
	H	-0.930195000	-0.315651000	1.599266000
	H	0.050674000	-1.310465000	0.329910000
	C	-2.005140000	-0.447497000	-0.311085000
	H	-2.563130000	0.489297000	-0.242028000
	H	-1.768301000	-0.620723000	-1.359509000
	H	-2.648368000	-1.249536000	0.045347000
Propanal-1,4-rad	C	-0.058002000	0.066469000	-0.000144000
	O	-0.219161000	1.271229000	-0.000251000
	C	1.187978000	-0.647388000	-0.000004000
	O	-1.113721000	-0.783641000	0.000086000
	H	1.146638000	-1.727506000	0.000194000
	C	2.482763000	0.060148000	0.000080000
	H	3.074318000	-0.221806000	0.875729000
	H	3.075582000	-0.223822000	-0.874031000
	H	2.343236000	1.138285000	-0.001166000
	O	-2.330746000	-0.074036000	0.000113000
	H	-2.007196000	0.851050000	0.000088000
Propanal-1,5-TS	C	-0.822449000	-0.142568000	0.030371000
	O	-1.975823000	-0.391386000	-0.120103000
	C	0.274903000	-1.137140000	0.364581000
	H	0.420663000	-1.110569000	1.445302000
	H	-0.121657000	-2.116471000	0.099894000
	C	1.560440000	-0.816210000	-0.342249000
	O	-0.405446000	1.146366000	-0.182735000
	O	0.889257000	1.419991000	0.251084000
	H	2.476307000	-1.126164000	0.148068000
	H	1.519795000	0.482030000	-0.175904000
	H	1.563629000	-0.953083000	-1.419544000
Propanal-1,5-rad	C	0.031465000	0.083762000	0.065888000
	O	0.190152000	1.275561000	0.113709000
	C	-1.267891000	-0.668025000	0.169634000
	H	-1.197615000	-1.583896000	-0.421097000
	H	-1.333026000	-1.007878000	1.213990000
	C	-2.445253000	0.150905000	-0.200434000
	O	1.061810000	-0.765450000	-0.064251000
	O	2.297616000	-0.079784000	-0.098100000
	H	-2.369692000	1.225591000	-0.249448000
	H	1.998096000	0.849842000	-0.038098000
	H	-3.404310000	-0.326136000	-0.326733000
Butanal-AcOO	C	-1.561744000	2.519026000	0.000000000
	H	-2.604241000	2.833907000	0.000000000
	H	-1.083206000	2.949383000	0.881054000

	H	-1.083206000	2.949383000	-0.881054000
	C	-1.452454000	1.000379000	0.000000000
	H	-1.960128000	0.586731000	0.871799000
	H	-1.960128000	0.586731000	-0.871799000
	C	0.000000000	0.543723000	0.000000000
	H	0.541305000	0.929281000	-0.866332000
	H	0.541305000	0.929281000	0.866332000
	C	0.122519000	-0.946049000	0.000000000
	O	-0.732495000	-1.762655000	0.000000000
	O	1.455380000	-1.474761000	0.000000000
	O	2.396912000	-0.570979000	0.000000000
Butanal-1,4-TS	C	1.016152000	0.546451000	0.090614000
	O	1.382656000	1.674176000	0.012302000
	C	-0.346013000	0.049582000	0.497816000
	O	1.828092000	-0.499341000	-0.207259000
	O	1.111623000	-1.697599000	-0.035735000
	H	-0.534665000	0.176973000	1.562771000
	H	0.018092000	-1.158430000	0.335265000
	C	-1.497772000	0.422292000	-0.395656000
	H	-1.597566000	1.511851000	-0.366405000
	H	-1.256445000	0.163892000	-1.427988000
	C	-2.804302000	-0.235583000	0.029243000
	H	-2.728817000	-1.322217000	-0.015768000
	H	-3.069130000	0.042099000	1.050097000
	H	-3.618821000	0.071494000	-0.624540000
Butanal-1,4-rad	C	0.604381000	0.113777000	-0.078897000
	O	0.847616000	1.293984000	0.082231000
	C	-0.676224000	-0.489746000	-0.317447000
	O	1.590168000	-0.816504000	-0.045280000
	H	-0.711374000	-1.565372000	-0.430154000
	C	-1.914498000	0.313001000	-0.414158000
	H	-1.695141000	1.349544000	-0.161866000
	H	-2.248374000	0.307348000	-1.458968000
	C	-3.043008000	-0.237359000	0.462878000
	H	-3.275265000	-1.270765000	0.203987000
	H	-2.767269000	-0.206386000	1.516316000
	H	-3.947293000	0.354864000	0.330931000
	O	2.841756000	-0.214501000	0.191512000
	H	2.584494000	0.728903000	0.257786000
Butanal-1,5-TS	C	-1.026384000	-0.389335000	0.029845000
	O	-1.865319000	-1.153816000	-0.328541000
	C	0.143233000	-0.697869000	0.944327000
	H	-0.128525000	-0.370473000	1.948551000
	H	0.243025000	-1.783099000	0.952230000
	C	1.402474000	-0.001358000	0.490475000

	C	2.030001000	-0.483853000	-0.785841000
	H	2.417269000	-1.498751000	-0.653071000
	H	1.304719000	-0.515976000	-1.600144000
	O	-1.049265000	0.882803000	-0.481374000
	O	-0.203569000	1.781717000	0.162338000
	H	2.100553000	0.224756000	1.292481000
	H	0.853552000	1.139040000	0.255751000
	H	2.858687000	0.153369000	-1.088015000
Butanal-1,5-rad	C	0.488277000	0.042843000	0.364443000
	O	0.580958000	1.239245000	0.476282000
	C	-0.714871000	-0.805696000	0.702382000
	H	-0.404351000	-1.844390000	0.800000000
	H	-1.085391000	-0.448332000	1.664992000
	C	-1.752923000	-0.644086000	-0.359795000
	C	-2.626159000	0.552480000	-0.391028000
	H	-3.406497000	0.460031000	-1.144021000
	H	-3.098649000	0.723913000	0.580507000
	O	1.479795000	-0.701455000	-0.147908000
	H	-1.700432000	-1.300402000	-1.217178000
	H	-2.051674000	1.460936000	-0.613227000
	O	2.579163000	0.098064000	-0.538770000
	H	2.261723000	0.988158000	-0.283910000
Butanal-1,6-TS	C	-1.107266000	-0.186294000	0.036439000
	O	-2.151752000	-0.622031000	-0.338675000
	C	-0.013537000	-0.979569000	0.703821000
	H	0.284656000	-0.507797000	1.639048000
	H	-0.442201000	-1.954033000	0.919128000
	C	1.206256000	-1.129776000	-0.232358000
	H	0.857923000	-1.421923000	-1.222808000
	H	1.813382000	-1.956549000	0.143780000
	C	2.057515000	0.111355000	-0.316200000
	O	-0.836757000	1.125599000	-0.275854000
	O	0.261393000	1.652072000	0.391975000
	H	2.744682000	0.262416000	0.512668000
	H	1.209612000	1.090876000	-0.078954000
	H	2.491063000	0.347596000	-1.282640000
Butanal-1,6-rad	C	0.589404000	0.109965000	0.116190000
	O	0.843454000	1.284318000	0.206404000
	C	-0.758280000	-0.537267000	0.242670000
	H	-0.750140000	-1.492080000	-0.280963000
	H	-0.898807000	-0.758997000	1.304104000
	C	-1.885216000	0.365544000	-0.253764000
	H	-1.735256000	0.593417000	-1.312747000
	H	-1.806276000	1.332582000	0.258855000
	C	-3.226133000	-0.229683000	-0.041973000

	O	1.547130000	-0.805230000	-0.099651000
	O	2.827902000	-0.210406000	-0.164565000
	H	-3.392544000	-0.965897000	0.732231000
	H	2.601412000	0.734427000	-0.046996000
	H	-4.084929000	0.155741000	-0.570715000
Pentanal-AcOO	C	-3.366360000	-1.502871000	0.000000000
	H	-4.404385000	-1.171800000	0.000000000
	H	-3.214448000	-2.128789000	0.880707000
	H	-3.214448000	-2.128789000	-0.880707000
	C	-2.407713000	-0.320001000	0.000000000
	H	-2.599186000	0.307646000	-0.874578000
	H	-2.599186000	0.307646000	0.874578000
	C	-0.947000000	-0.754115000	0.000000000
	H	-0.746266000	-1.378855000	-0.872491000
	H	-0.746266000	-1.378855000	0.872491000
	C	0.000000000	0.436707000	0.000000000
	H	-0.164439000	1.080664000	0.866330000
	H	-0.164439000	1.080664000	-0.866330000
	C	1.434237000	0.016059000	0.000000000
	O	1.890196000	-1.075025000	0.000000000
	O	2.406140000	1.070605000	0.000000000
	O	1.900425000	2.273894000	0.000000000
Pentanal-1,4-TS	C	1.538458000	0.561188000	0.058368000
	O	1.864186000	1.699620000	-0.042328000
	C	0.242545000	0.021243000	0.603174000
	O	2.341105000	-0.457612000	-0.341309000
	O	1.680825000	-1.677691000	-0.109140000
	H	0.165438000	0.134854000	1.683451000
	H	0.620242000	-1.173657000	0.388225000
	C	-1.007301000	0.366019000	-0.158254000
	H	-1.138201000	1.452787000	-0.110087000
	H	-0.874201000	0.120276000	-1.214320000
	C	-2.248789000	-0.328271000	0.392604000
	H	-2.101701000	-1.410099000	0.355608000
	H	-2.367164000	-0.067111000	1.447164000
	C	-3.508101000	0.046196000	-0.376209000
	H	-4.382527000	-0.459143000	0.031755000
	H	-3.689991000	1.120920000	-0.330081000
	H	-3.421692000	-0.231609000	-1.427601000
Pentanal-1,4-rad	C	0.924169000	-0.195883000	0.164158000
	O	1.049269000	0.438813000	1.193579000
	C	-0.235420000	-0.914005000	-0.283376000
	O	1.940609000	-0.292553000	-0.728069000
	O	3.072145000	0.417716000	-0.280613000

	H	-0.179490000	-1.406213000	-1.245305000
	H	2.744922000	0.768872000	0.573830000
	C	-1.490167000	-0.938780000	0.498272000
	H	-1.797996000	-1.979878000	0.634370000
	H	-1.312800000	-0.510953000	1.484964000
	C	-2.635104000	-0.179507000	-0.198848000
	H	-2.817778000	-0.623945000	-1.179882000
	H	-3.543351000	-0.331511000	0.386212000
	C	-2.354683000	1.309961000	-0.344923000
	H	-1.480352000	1.489976000	-0.972357000
	H	-3.200983000	1.824245000	-0.799021000
	H	-2.161133000	1.766890000	0.626315000
Pentanal-1,5-TS	C	-1.496941000	-0.299314000	-0.128694000
	O	-2.322489000	-0.929553000	-0.710282000
	C	-0.572494000	-0.813085000	0.958231000
	H	-1.007834000	-0.536743000	1.919271000
	H	-0.585588000	-1.899799000	0.876549000
	C	0.814443000	-0.236157000	0.826538000
	C	1.644941000	-0.681881000	-0.345219000
	H	1.876304000	-1.745372000	-0.210584000
	H	1.050664000	-0.619570000	-1.260516000
	C	2.933427000	0.113964000	-0.503117000
	H	3.550558000	0.043170000	0.393669000
	H	2.717156000	1.167785000	-0.680274000
	O	-1.285671000	0.999543000	-0.513901000
	O	-0.499851000	1.745044000	0.360883000
	H	1.358738000	-0.151530000	1.765310000
	H	0.444342000	0.975469000	0.599916000
	H	3.519493000	-0.254841000	-1.343374000
Pentanal-1,5-rad	C	1.059070000	0.112695000	0.383158000
	O	1.107986000	-0.959505000	0.931413000
	C	-0.020386000	1.157880000	0.536148000
	H	-0.242017000	1.221830000	1.602956000
	H	0.359336000	2.117698000	0.190158000
	C	-1.229612000	0.739460000	-0.234037000
	C	-2.189812000	-0.243715000	0.325979000
	H	-1.662951000	-1.184004000	0.539873000
	H	-2.535629000	0.107842000	1.305884000
	C	-3.381553000	-0.516152000	-0.582879000
	H	-3.945704000	0.397503000	-0.772772000
	H	-4.057782000	-1.242899000	-0.134703000
	O	1.982910000	0.495596000	-0.511043000
	H	-1.281743000	1.007410000	-1.281524000
	H	-3.053277000	-0.912906000	-1.544298000
	O	2.953324000	-0.512498000	-0.717598000

	H	2.639773000	-1.202231000	-0.097966000
Pentanal-1,6-TS	C	-1.495809000	-0.099302000	-0.128717000
	O	-2.437841000	-0.402227000	-0.794551000
	C	-0.687425000	-1.040211000	0.727407000
	H	-0.597769000	-0.653997000	1.741728000
	H	-1.243623000	-1.972882000	0.751369000
	C	0.710068000	-1.266175000	0.114912000
	H	0.602024000	-1.456452000	-0.954591000
	H	1.128878000	-2.175841000	0.552279000
	C	1.672311000	-0.120177000	0.341143000
	C	2.657565000	0.182307000	-0.750662000
	H	3.328625000	-0.670012000	-0.899535000
	H	3.269907000	1.049835000	-0.511640000
	O	-1.039819000	1.191711000	-0.251056000
	O	-0.117849000	1.559959000	0.718544000
	H	2.099488000	-0.115997000	1.344351000
	H	0.887946000	0.895484000	0.465393000
	H	2.148346000	0.365660000	-1.697356000
Pentanal-1,6-rad	C	-0.984876000	0.369388000	0.203177000
	O	-1.114036000	0.036715000	1.354101000
	C	0.028410000	1.332064000	-0.344394000
	H	-0.050499000	1.365055000	-1.430011000
	H	-0.234648000	2.318024000	0.041596000
	C	1.442668000	0.950124000	0.094251000
	H	1.484406000	0.921754000	1.186843000
	H	2.120312000	1.761100000	-0.207723000
	C	1.898414000	-0.348860000	-0.466437000
	C	3.074164000	-1.050683000	0.101923000
	H	2.990317000	-1.146760000	1.188503000
	H	4.006137000	-0.500143000	-0.086210000
	O	-1.786193000	-0.105375000	-0.763155000
	O	-2.753455000	-0.994370000	-0.241613000
	H	1.476909000	-0.685408000	-1.405762000
	H	3.195281000	-2.046764000	-0.320159000
	H	-2.511425000	-0.994822000	0.707143000
Pentanal-1,7-TS	C	0.771040000	-1.507056000	0.264176000
	H	1.455106000	-1.876485000	1.030030000
	H	0.400548000	-2.376839000	-0.278273000
	C	1.531453000	-0.614505000	-0.718671000
	H	0.897717000	-0.380871000	-1.578445000
	C	2.063385000	0.660214000	-0.132447000
	H	2.578673000	1.320733000	-0.823772000
	C	-0.416464000	-0.831379000	0.979094000
	H	-1.031920000	-1.593052000	1.451172000
	H	-0.068651000	-0.139535000	1.739937000

	C	-1.295020000	-0.126275000	-0.018053000
	O	-2.183144000	-0.626700000	-0.637228000
	O	-0.996552000	1.183332000	-0.333646000
	H	2.371880000	-1.187094000	-1.126771000
	O	-0.080959000	1.794530000	0.511437000
	H	0.989632000	1.366711000	0.188205000
	H	2.565884000	0.571135000	0.828829000
Pentanal-1,7-rad	C	1.556315000	-0.989503000	0.196225000
	H	2.350273000	-1.258388000	0.895471000
	H	1.320832000	-1.882058000	-0.382773000
	C	2.055687000	0.113940000	-0.738634000
	H	1.273366000	0.374939000	-1.456829000
	C	2.530153000	1.329315000	-0.031632000
	H	3.021525000	1.246525000	0.929248000
	C	0.327765000	-0.581218000	1.005902000
	H	0.064134000	-1.368847000	1.715097000
	H	0.511249000	0.326416000	1.579760000
	C	-0.879032000	-0.378660000	0.136097000
	O	-1.204857000	-1.041887000	-0.816831000
	O	-1.616901000	0.660345000	0.555333000
	H	2.870462000	-0.303720000	-1.347055000
	O	-2.780046000	0.820429000	-0.231834000
	H	-2.666401000	0.095435000	-0.879990000
	H	2.523664000	2.295359000	-0.514018000
Hexanal-AcOO	C	-3.193143000	2.987216000	0.000000000
	H	-3.336055000	4.067432000	0.000000000
	H	-3.695744000	2.583990000	0.880737000
	H	-3.695744000	2.583990000	-0.880737000
	C	-1.714936000	2.621449000	0.000000000
	H	-1.227489000	3.060911000	0.874111000
	H	-1.227489000	3.060911000	-0.874111000
	C	-1.477911000	1.116145000	0.000000000
	H	-1.964980000	0.674237000	0.874975000
	H	-1.964980000	0.674237000	-0.874975000
	C	0.000000000	0.747098000	0.000000000
	H	0.490993000	1.182042000	-0.872396000
	H	0.490993000	1.182042000	0.872396000
	C	0.209251000	-0.760173000	0.000000000
	H	-0.260360000	-1.230390000	0.866221000
	H	-0.260360000	-1.230390000	-0.866221000
	C	1.657628000	-1.128832000	0.000000000
	O	2.605809000	-0.422566000	0.000000000
	O	1.956557000	-2.531626000	0.000000000
	O	0.908367000	-3.309111000	0.000000000

Hexanal-1,4-TS	C	1.633960000	-0.262020000	-0.078668000
	O	2.196212000	-1.169349000	-0.601553000
	C	0.610453000	-0.323579000	1.024727000
	O	1.862125000	1.028765000	-0.433857000
	O	1.006107000	1.864182000	0.304126000
	H	1.091616000	-0.400921000	1.998690000
	H	0.385368000	0.925720000	0.910566000
	C	-0.572876000	-1.235511000	0.850279000
	H	-0.212257000	-2.258645000	1.000317000
	H	-1.270512000	-1.046014000	1.668020000
	C	-1.281523000	-1.151393000	-0.500584000
	H	-0.597079000	-1.486352000	-1.282627000
	H	-2.104329000	-1.869870000	-0.485513000
	C	-1.828276000	0.229071000	-0.865285000
	H	-1.004931000	0.928051000	-1.025866000
	H	-2.339522000	0.144577000	-1.825639000
	C	-2.787201000	0.808556000	0.167533000
	H	-3.605660000	0.116986000	0.377724000
	H	-2.284467000	1.023691000	1.112130000
	H	-3.221001000	1.743248000	-0.185536000
Hexanal-1,4-rad	C	1.228654000	-0.205980000	0.203841000
	O	1.225750000	0.686980000	1.029921000
	C	0.198553000	-1.175495000	-0.037787000
	O	2.281668000	-0.383456000	-0.631061000
	O	3.284702000	0.575417000	-0.387132000
	H	0.360408000	-1.888943000	-0.835069000
	H	2.879514000	1.085648000	0.345012000
	C	-1.067945000	-1.180596000	0.724441000
	H	-1.203361000	-2.170314000	1.171787000
	H	-1.006846000	-0.460916000	1.539195000
	C	-2.291644000	-0.889100000	-0.165382000
	H	-2.371344000	-1.670568000	-0.924648000
	H	-3.185359000	-0.966018000	0.458164000
	C	-2.259545000	0.477889000	-0.845794000
	H	-1.389044000	0.534702000	-1.505661000
	H	-3.135194000	0.557363000	-1.492932000
	C	-2.237946000	1.652439000	0.125586000
	H	-1.320492000	1.672843000	0.713788000
	H	-2.304505000	2.599042000	-0.409886000
	H	-3.081503000	1.600692000	0.816992000
Hexanal-1,5-TS	C	-1.893790000	-0.404622000	-0.227985000
	O	-2.552360000	-1.209049000	-0.807831000
	C	-1.181726000	-0.609024000	1.095231000
	H	-1.814279000	-0.189617000	1.878496000
	H	-1.123408000	-1.687208000	1.243015000
	C	0.172754000	0.053711000	1.104679000

	C	1.240232000	-0.534212000	0.225181000
	H	1.502057000	-1.524740000	0.619758000
	H	0.838002000	-0.710402000	-0.777122000
	C	2.495193000	0.326234000	0.132035000
	H	2.888241000	0.498666000	1.137375000
	H	2.223236000	1.306224000	-0.266643000
	O	-1.675959000	0.807432000	-0.830949000
	O	-1.120671000	1.778127000	-0.001530000
	H	0.513847000	0.368054000	2.089249000
	H	-0.205564000	1.158842000	0.566050000
	C	3.571726000	-0.303655000	-0.740595000
	H	3.208514000	-0.458344000	-1.757617000
	H	4.456328000	0.329749000	-0.794939000
	H	3.878607000	-1.273888000	-0.346421000
Hexanal-1,5-rad	C	1.182166000	-0.510110000	0.292476000
	O	1.199883000	-0.008924000	1.388278000
	C	0.363879000	-1.701687000	-0.145222000
	H	0.893939000	-2.234296000	-0.932176000
	H	0.273943000	-2.348290000	0.729775000
	C	-0.974650000	-1.233315000	-0.614648000
	C	-2.006163000	-0.709201000	0.318036000
	H	-2.841277000	-1.419556000	0.375230000
	H	-1.592264000	-0.640726000	1.327469000
	C	-2.562223000	0.659128000	-0.098426000
	H	-3.377115000	0.925073000	0.577473000
	H	-3.001930000	0.575853000	-1.095703000
	O	1.880445000	0.001474000	-0.732973000
	H	-1.142844000	-1.157243000	-1.681169000
	C	-1.506345000	1.757132000	-0.090476000
	H	-1.051735000	1.852533000	0.896641000
	H	-0.706663000	1.542919000	-0.802124000
	H	-1.937625000	2.720964000	-0.359482000
	O	2.567833000	1.178395000	-0.354781000
	H	2.318303000	1.243524000	0.589424000
Hexanal-1,6-TS	C	1.882031000	-0.147797000	-0.184359000
	O	2.800408000	-0.113215000	-0.944786000
	C	1.377249000	1.011404000	0.635748000
	H	1.283075000	0.727924000	1.682758000
	H	2.128321000	1.790843000	0.544615000
	C	0.022924000	1.513223000	0.092244000
	H	0.103432000	1.636609000	-0.989408000
	H	-0.158332000	2.506557000	0.508266000
	C	-1.147657000	0.610896000	0.421747000
	C	-2.179500000	0.383831000	-0.648434000
	H	-1.679912000	0.031325000	-1.554444000
	H	-2.620422000	1.354400000	-0.908431000

	O	1.153747000	-1.312983000	-0.145461000
	O	0.256554000	-1.383829000	0.911159000
	H	-1.569116000	0.792833000	1.412021000
	H	-0.593814000	-0.527192000	0.650583000
	C	-3.274601000	-0.590214000	-0.237137000
	H	-3.802875000	-0.234687000	0.648684000
	H	-4.005357000	-0.717396000	-1.034467000
	H	-2.853349000	-1.569060000	-0.006314000
Hexanal-1,6-rad	C	-1.478951000	0.318188000	0.159405000
	O	-1.549901000	0.077280000	1.338001000
	C	-0.732586000	1.451922000	-0.481746000
	H	-0.771023000	1.345715000	-1.564878000
	H	-1.262237000	2.368041000	-0.215647000
	C	0.712534000	1.508179000	0.016293000
	H	0.713177000	1.614563000	1.104333000
	H	1.167408000	2.428844000	-0.374847000
	C	1.509637000	0.317908000	-0.379440000
	C	2.756388000	-0.049363000	0.337785000
	H	2.554119000	-0.086773000	1.414755000
	H	3.501816000	0.751468000	0.220410000
	O	-2.104919000	-0.438927000	-0.754941000
	H	1.266476000	-0.186914000	-1.308377000
	C	3.359983000	-1.370584000	-0.123067000
	H	4.272789000	-1.600023000	0.425600000
	H	2.658317000	-2.190972000	0.029792000
	H	3.606850000	-1.335729000	-1.185064000
	O	-2.826492000	-1.491848000	-0.147810000
	H	-2.619227000	-1.337754000	0.796545000
Hexanal-1,7-TS	C	0.419071000	1.675348000	0.177771000
	H	0.528040000	2.747147000	0.012357000
	H	0.345610000	1.545815000	1.259017000
	C	1.679286000	0.998405000	-0.364365000
	H	2.547202000	1.466717000	0.114895000
	C	1.789212000	-0.494129000	-0.161957000
	H	2.624383000	-0.927690000	-0.711395000
	C	-0.908542000	1.245080000	-0.477318000
	H	-1.646655000	2.026737000	-0.312613000
	H	-0.776538000	1.101942000	-1.547081000
	C	-1.513684000	0.020527000	0.161182000
	O	-2.254782000	0.039228000	1.097668000
	C	1.649079000	-1.038035000	1.232909000
	H	1.716246000	-2.124141000	1.241012000
	H	2.451728000	-0.645791000	1.866151000
	H	0.703958000	-0.758058000	1.697702000
	O	-1.178303000	-1.222774000	-0.317882000
	H	1.768748000	1.216261000	-1.430884000

	O	-0.285410000	-1.206213000	-1.375608000
	H	0.798700000	-0.974043000	-0.831928000
Hexanal-1,7-rad	C	1.358202000	-1.371831000	0.350536000
	H	1.437529000	-0.951559000	1.354147000
	H	1.898608000	-2.319209000	0.357149000
	C	2.016334000	-0.425473000	-0.671563000
	H	1.939690000	-0.877033000	-1.663202000
	C	1.449342000	0.950632000	-0.689490000
	H	0.766285000	1.232407000	-1.479128000
	C	-0.111290000	-1.663331000	0.044348000
	H	-0.239244000	-1.988929000	-0.987409000
	H	-0.472348000	-2.462206000	0.694481000
	C	-0.999442000	-0.483981000	0.310669000
	O	-1.082889000	0.137416000	1.341432000
	C	1.688535000	1.890687000	0.433737000
	H	1.464761000	2.919302000	0.154121000
	H	1.061651000	1.649979000	1.302433000
	H	2.726955000	1.844696000	0.775403000
	O	-1.767399000	-0.192039000	-0.751458000
	H	3.083449000	-0.376415000	-0.426956000
	O	-2.613665000	0.908854000	-0.488322000
	H	-2.365802000	1.114901000	0.436313000
Hexanal-1,8-TS	C	-1.516506000	-0.031659000	-0.072905000
	O	-2.328011000	-0.522146000	-0.797981000
	C	-0.754875000	-0.774349000	0.992426000
	H	-0.227260000	-0.093538000	1.651245000
	H	-1.500988000	-1.308487000	1.579241000
	C	0.198814000	-1.793445000	0.354811000
	H	-0.394938000	-2.529964000	-0.187274000
	H	0.704964000	-2.325350000	1.163002000
	C	1.243332000	-1.211723000	-0.598007000
	C	2.201873000	-0.184738000	0.028783000
	H	3.220438000	-0.385139000	-0.323128000
	H	2.242689000	-0.314842000	1.113275000
	C	1.911937000	1.250975000	-0.305390000
	H	0.737293000	1.598505000	0.172772000
	H	1.758316000	1.460309000	-1.362436000
	O	-1.241036000	1.299197000	-0.294258000
	O	-0.351500000	1.872470000	0.601007000
	H	0.742318000	-0.764773000	-1.461121000
	H	1.821418000	-2.047560000	-0.992688000
	H	2.552681000	1.984301000	0.178654000
Hexanal-1,8-rad	C	1.315647000	0.407440000	0.244453000
	O	1.977463000	1.082023000	-0.503863000
	C	0.082936000	0.831533000	0.985263000

	H	-0.283269000	0.003818000	1.589596000
	H	0.384350000	1.630971000	1.663144000
	C	-0.995279000	1.346895000	0.027294000
	H	-0.611178000	2.225291000	-0.491674000
	H	-1.842712000	1.674694000	0.631227000
	C	-1.460840000	0.317892000	-1.001576000
	C	-2.040589000	-0.965776000	-0.402095000
	H	-1.267829000	-1.515102000	0.142991000
	H	-2.315384000	-1.630737000	-1.233628000
	C	-3.220462000	-0.744892000	0.469371000
	H	3.005555000	-0.448252000	-0.684917000
	H	-3.894921000	0.080426000	0.281787000
	O	1.626332000	-0.874955000	0.496014000
	O	2.784042000	-1.275089000	-0.209435000
	H	-0.629995000	0.059708000	-1.662809000
	H	-2.217637000	0.786729000	-1.634640000
	H	-3.518150000	-1.481927000	1.200935000
Heptanal-AcOO	C	-5.062371000	0.050865000	0.000000000
	H	-5.151208000	0.689354000	0.880655000
	H	-5.151208000	0.689354000	-0.880655000
	H	-5.907645000	-0.637094000	0.000000000
	C	-3.735382000	-0.696169000	0.000000000
	H	-3.682864000	-1.350598000	0.874416000
	H	-3.682864000	-1.350598000	-0.874416000
	C	-2.530562000	0.236638000	0.000000000
	H	-2.581000000	0.892464000	0.874776000
	H	-2.581000000	0.892464000	-0.874776000
	C	-1.197997000	-0.500841000	0.000000000
	H	-1.147391000	-1.156323000	0.875138000
	H	-1.147391000	-1.156323000	-0.875138000
	C	0.000000000	0.439943000	0.000000000
	H	-0.042127000	1.094579000	0.872477000
	H	-0.042127000	1.094579000	-0.872477000
	C	1.318263000	-0.319829000	0.000000000
	H	1.401511000	-0.979124000	-0.866354000
	H	1.401511000	-0.979124000	0.866354000
	C	2.497676000	0.598299000	0.000000000
	O	2.520857000	1.780599000	0.000000000
	O	3.789367000	-0.025147000	0.000000000
	O	3.761781000	-1.330084000	0.000000000
Heptanal-1,4-TS	C	-1.857010000	-0.194584000	0.506138000
	O	-2.117997000	-0.054679000	1.657296000
	C	-1.521076000	0.876387000	-0.499837000
	O	-1.824996000	-1.417395000	-0.082151000

	O	-1.435004000	-1.269287000	-1.424347000
	H	-2.422328000	1.350240000	-0.885742000
	H	-1.246887000	-0.005594000	-1.376014000
	C	-0.416613000	1.838030000	-0.153037000
	H	-0.228089000	2.474355000	-1.020653000
	H	-0.810462000	2.498276000	0.627237000
	C	0.881413000	1.198027000	0.331648000
	H	1.536692000	1.993213000	0.694960000
	H	0.665400000	0.565805000	1.195519000
	C	1.616810000	0.399712000	-0.741282000
	H	0.996573000	-0.436084000	-1.075583000
	H	1.769344000	1.041783000	-1.613795000
	C	2.966285000	-0.147143000	-0.280505000
	H	3.469835000	-0.596163000	-1.138812000
	H	3.599762000	0.682157000	0.047046000
	C	2.861571000	-1.183096000	0.833471000
	H	3.838663000	-1.604831000	1.068055000
	H	2.462817000	-0.752776000	1.752403000
	H	2.204369000	-2.003491000	0.539430000
Heptanal-1,4-rad	C	-1.545960000	0.182322000	0.184131000
	O	-1.348860000	-0.579183000	1.112099000
	C	-0.789758000	1.351831000	-0.162022000
	O	-2.573204000	-0.016510000	-0.677727000
	O	-3.305471000	-1.169026000	-0.330374000
	H	-1.095819000	1.902634000	-1.041640000
	H	-2.814199000	-1.468661000	0.463073000
	C	0.405335000	1.767306000	0.602301000
	H	0.282731000	2.811658000	0.905110000
	H	0.484206000	1.171060000	1.509820000
	C	1.699447000	1.661054000	-0.228873000
	H	1.623928000	2.333703000	-1.086307000
	H	2.523900000	2.029476000	0.385774000
	C	2.015423000	0.250171000	-0.718510000
	H	1.203419000	-0.104596000	-1.361945000
	H	2.903965000	0.296052000	-1.353642000
	C	2.251710000	-0.766200000	0.393930000
	H	3.036497000	-0.392365000	1.058167000
	H	1.350628000	-0.867723000	1.001423000
	C	2.645051000	-2.134862000	-0.145700000
	H	1.862156000	-2.537274000	-0.790854000
	H	3.562640000	-2.077801000	-0.734204000
	H	2.808734000	-2.848146000	0.661707000
Heptanal-1,5-TS	C	2.097102000	-0.103401000	-0.269627000
	O	2.917083000	-0.133561000	-1.131743000
	C	1.609131000	1.126078000	0.470941000
	H	2.133213000	1.165617000	1.426575000

	H	1.918989000	1.982907000	-0.126811000
	C	0.117428000	1.080569000	0.693222000
	C	-0.760005000	1.234877000	-0.518285000
	H	-0.569276000	2.228682000	-0.941302000
	H	-0.448441000	0.525625000	-1.290088000
	C	-2.253203000	1.091097000	-0.233700000
	H	-2.799831000	1.300471000	-1.156190000
	H	-2.551938000	1.861192000	0.482681000
	O	1.455528000	-1.272291000	0.053624000
	O	0.700972000	-1.211079000	1.221847000
	H	-0.222454000	1.620182000	1.575641000
	H	0.072896000	-0.145531000	1.076872000
	C	-2.676966000	-0.279288000	0.294972000
	H	-2.209040000	-0.464741000	1.265316000
	H	-3.752074000	-0.252528000	0.482382000
	C	-2.355694000	-1.431521000	-0.649222000
	H	-2.767247000	-2.367234000	-0.272780000
	H	-2.779018000	-1.253680000	-1.639870000
	H	-1.281207000	-1.575983000	-0.762059000
Heptanal-1,5-rad	C	1.588095000	-0.316037000	0.082686000
	O	2.103867000	-0.071660000	1.143228000
	C	1.021068000	-1.643842000	-0.360744000
	H	0.834896000	-1.617487000	-1.433902000
	H	1.794355000	-2.386888000	-0.154928000
	C	-0.228449000	-1.951661000	0.399878000
	C	-1.572468000	-1.743859000	-0.201633000
	H	-1.662540000	-2.350527000	-1.110782000
	H	-2.337374000	-2.099961000	0.490401000
	C	-1.871687000	-0.280953000	-0.578749000
	H	-2.850524000	-0.240189000	-1.063133000
	H	-1.147296000	0.057860000	-1.323743000
	O	1.419267000	0.628468000	-0.856285000
	H	-0.124508000	-2.163775000	1.454595000
	C	-1.851428000	0.672587000	0.609593000
	H	-2.609337000	0.360287000	1.333596000
	H	-0.891084000	0.594445000	1.126464000
	C	-2.086204000	2.119993000	0.200852000
	H	-2.085769000	2.782400000	1.066276000
	H	-1.304159000	2.459716000	-0.479672000
	H	-3.045694000	2.233816000	-0.307098000
	O	1.879602000	1.889765000	-0.410688000
	H	2.213572000	1.660351000	0.480583000
Heptanal-1,6-TS	C	1.967194000	-0.567126000	-0.311747000
	O	2.459941000	-1.118706000	-1.247724000
	C	2.103559000	0.892298000	0.029879000
	H	2.336496000	1.005691000	1.086455000

	H	2.932027000	1.269857000	-0.562937000
	C	0.819486000	1.679725000	-0.315253000
	H	0.668079000	1.623108000	-1.395332000
	H	1.005652000	2.725515000	-0.072293000
	C	-0.436421000	1.192664000	0.389703000
	C	-1.479547000	0.520503000	-0.461517000
	H	-1.006672000	-0.267379000	-1.056652000
	H	-1.853003000	1.256210000	-1.186393000
	C	-2.645743000	-0.058866000	0.328935000
	H	-2.259797000	-0.791473000	1.041024000
	H	-3.109325000	0.735361000	0.920234000
	O	1.125796000	-1.316950000	0.477116000
	O	0.688051000	-0.658531000	1.617368000
	H	-0.844636000	1.892063000	1.119067000
	H	-0.014302000	0.257461000	1.162901000
	C	-3.690306000	-0.711396000	-0.565884000
	H	-4.108506000	0.008388000	-1.271755000
	H	-3.253181000	-1.527379000	-1.143212000
	H	-4.512466000	-1.120745000	0.020114000
Heptanal-1,6-rad	C	1.400142000	-0.426462000	0.283287000
	O	1.279884000	0.110404000	1.356053000
	C	0.915597000	-1.795318000	-0.091255000
	H	1.163079000	-1.998385000	-1.131895000
	H	1.456624000	-2.507146000	0.533891000
	C	-0.596221000	-1.920481000	0.147158000
	H	-0.808530000	-1.709580000	1.197049000
	H	-0.864343000	-2.971785000	-0.016724000
	C	-1.401680000	-1.029273000	-0.731449000
	C	-2.528407000	-0.217384000	-0.199984000
	H	-3.144695000	-0.836526000	0.461840000
	H	-3.172798000	0.108224000	-1.019335000
	C	-2.071698000	1.021632000	0.595456000
	H	-2.949627000	1.480624000	1.055026000
	H	-1.421096000	0.702866000	1.412716000
	O	2.008025000	0.183827000	-0.745735000
	H	-1.133444000	-0.966401000	-1.778900000
	C	-1.345133000	2.046728000	-0.264078000
	H	-1.033531000	2.906793000	0.328206000
	H	-0.452449000	1.620938000	-0.724266000
	H	-1.988416000	2.408902000	-1.068492000
	O	2.457310000	1.475477000	-0.388373000
	H	2.151873000	1.527151000	0.540517000
Heptanal-1,7-TS	C	-0.886238000	1.684260000	-0.541200000
	H	-0.670244000	1.348605000	-1.556919000
	H	-1.430574000	2.622786000	-0.645933000
	C	0.408478000	1.987624000	0.215396000

	H	0.159085000	2.412069000	1.190441000
	C	1.362578000	0.835266000	0.417379000
	H	2.180502000	1.082279000	1.096080000
	C	-1.838183000	0.677361000	0.134307000
	H	-1.857965000	0.833943000	1.210061000
	H	-2.839398000	0.825908000	-0.263862000
	C	-1.514374000	-0.757302000	-0.198155000
	O	-1.935581000	-1.345718000	-1.148369000
	C	1.815716000	0.048938000	-0.784173000
	H	0.956133000	-0.320159000	-1.347309000
	H	2.336744000	0.740688000	-1.458358000
	O	-0.646297000	-1.454990000	0.606697000
	H	0.941790000	2.775268000	-0.329819000
	O	-0.144486000	-0.728674000	1.673610000
	H	0.704061000	0.001674000	1.146216000
	C	2.727758000	-1.116726000	-0.426042000
	H	3.614336000	-0.771201000	0.107824000
	H	2.205190000	-1.829769000	0.211397000
	H	3.056834000	-1.643573000	-1.320394000
Heptanal-1,7-rad	C	-0.505553000	2.092378000	0.404841000
	H	-0.709270000	1.714766000	1.407591000
	H	-0.608479000	3.177257000	0.445941000
	C	-1.531649000	1.527171000	-0.594309000
	H	-1.362962000	1.994132000	-1.566939000
	C	-1.497091000	0.045332000	-0.729459000
	H	-1.109688000	-0.398526000	-1.637729000
	C	0.937919000	1.755676000	0.032101000
	H	1.142298000	1.992437000	-1.011539000
	H	1.625636000	2.339470000	0.646921000
	C	1.275658000	0.317208000	0.295051000
	O	1.104461000	-0.285763000	1.326171000
	C	-2.025745000	-0.844751000	0.336181000
	H	-1.629077000	-0.531509000	1.309071000
	H	-3.114496000	-0.712048000	0.415591000
	O	1.870781000	-0.255578000	-0.763819000
	H	-2.525101000	1.847286000	-0.258549000
	O	2.216179000	-1.599406000	-0.493969000
	C	-1.703617000	-2.316270000	0.109461000
	H	-2.106763000	-2.937642000	0.908381000
	H	-2.123435000	-2.665972000	-0.834789000
	H	-0.624956000	-2.471093000	0.071451000
	H	1.915390000	-1.683038000	0.434331000
Heptanal-1,8-TS	C	1.398882000	-0.872465000	-0.243383000
	O	1.899178000	-1.189442000	-1.280546000
	C	1.825737000	0.307921000	0.589062000
	H	1.482556000	0.214879000	1.614719000

	H	2.914162000	0.267870000	0.576109000
	C	1.386371000	1.652786000	-0.010339000
	H	1.640697000	1.665593000	-1.072432000
	H	1.993965000	2.425666000	0.462133000
	C	-0.084901000	2.023588000	0.176126000
	C	-1.090974000	1.161392000	-0.607865000
	H	-0.577991000	0.554200000	-1.359062000
	H	-1.760993000	1.811027000	-1.182454000
	C	-1.962848000	0.272745000	0.240952000
	H	-1.148290000	-0.473134000	0.896984000
	H	-2.452092000	0.804435000	1.058771000
	O	0.363873000	-1.669538000	0.191797000
	O	-0.265281000	-1.221908000	1.340662000
	H	-0.197255000	3.066185000	-0.122769000
	H	-0.328387000	1.988286000	1.241342000
	C	-2.854138000	-0.691714000	-0.489450000
	H	-2.270132000	-1.334607000	-1.149083000
	H	-3.414030000	-1.321706000	0.199281000
	H	-3.573150000	-0.147108000	-1.109462000
Heptanal-1,8-rad	C	1.627806000	-0.112568000	-0.347978000
	O	1.333762000	0.952418000	-0.831211000
	C	0.938678000	-1.427084000	-0.575230000
	H	1.300567000	-1.798707000	-1.536434000
	H	1.259161000	-2.135742000	0.187935000
	C	-0.579025000	-1.272984000	-0.602054000
	H	-1.017990000	-2.221160000	-0.918225000
	H	-0.847703000	-0.533545000	-1.357843000
	C	-1.159471000	-0.864602000	0.746503000
	C	-2.673099000	-0.619203000	0.690250000
	H	-3.012476000	-0.406088000	1.714182000
	H	-3.178321000	-1.539605000	0.389556000
	C	-3.071615000	0.498634000	-0.210617000
	H	-3.880334000	0.351398000	-0.912052000
	O	2.675041000	-0.243642000	0.480432000
	H	-0.663937000	0.044349000	1.098282000
	H	-0.946381000	-1.638648000	1.487823000
	C	-2.417436000	1.828938000	-0.115381000
	H	-2.940797000	2.579400000	-0.705084000
	H	-2.377567000	2.181201000	0.922305000
	H	-1.377479000	1.803029000	-0.464801000
	O	3.351511000	0.984661000	0.660094000
	H	2.805727000	1.579836000	0.106868000
Heptanal-1,9-TS	C	0.817524000	-1.240710000	0.221320000
	O	0.656480000	-1.786720000	1.266642000
	C	2.004163000	-0.404602000	-0.192202000
	H	2.640715000	-0.325233000	0.687642000

	H	2.555003000	-0.968717000	-0.947663000
	C	1.659426000	0.980153000	-0.755148000
	H	1.049317000	0.859247000	-1.650076000
	H	2.593664000	1.434944000	-1.087992000
	C	0.987265000	1.945182000	0.227001000
	C	-0.375069000	1.516966000	0.778036000
	H	-0.694286000	2.253411000	1.517973000
	H	-0.270024000	0.586289000	1.336009000
	C	-1.477991000	1.360168000	-0.276042000
	H	-1.972655000	2.324345000	-0.440546000
	H	-1.052678000	1.089029000	-1.244604000
	O	-0.086357000	-1.271957000	-0.813109000
	O	-1.305829000	-1.812996000	-0.449534000
	H	0.882373000	2.912093000	-0.272411000
	H	1.661610000	2.110466000	1.071168000
	C	-2.515503000	0.337809000	0.089331000
	H	-1.945986000	-0.831396000	-0.123053000
	H	-3.374471000	0.276257000	-0.573859000
	H	-2.785818000	0.282842000	1.141643000
Heptanal-1,9-rad	C	1.721753000	-0.200771000	-0.044727000
	O	2.366226000	-0.174395000	0.973173000
	C	1.089480000	-1.402927000	-0.679303000
	H	0.676354000	-1.127035000	-1.647217000
	H	1.883643000	-2.130818000	-0.844914000
	C	0.017264000	-2.003379000	0.239851000
	H	0.504183000	-2.367162000	1.145058000
	H	-0.406549000	-2.872987000	-0.266457000
	C	-1.094896000	-1.029643000	0.620398000
	C	-1.916521000	-0.514139000	-0.556497000
	H	-2.370859000	-1.360245000	-1.078869000
	H	-1.267208000	-0.011828000	-1.278145000
	C	-3.005922000	0.469004000	-0.128840000
	H	-3.646404000	0.681229000	-0.997278000
	H	-3.667857000	-0.006564000	0.602802000
	O	1.462917000	0.917844000	-0.743160000
	O	2.025620000	2.056894000	-0.123666000
	H	-0.669300000	-0.180646000	1.163544000
	H	-1.763212000	-1.527717000	1.327054000
	C	-2.473062000	1.741507000	0.419369000
	H	2.451077000	1.650651000	0.659144000
	H	-1.499938000	2.105395000	0.116418000
	H	-3.090608000	2.387079000	1.026575000
Octanal-AcOO	C	-2.475650000	5.169719000	0.000000000
	H	-1.933521000	5.518670000	0.880699000

	H	-3.455004000	5.648035000	0.000000000
	H	-1.933521000	5.518670000	-0.880699000
	C	-2.595983000	3.651623000	0.000000000
	H	-3.167903000	3.328950000	0.874281000
	H	-3.167903000	3.328950000	-0.874281000
	C	-1.243848000	2.949091000	0.000000000
	H	-0.670048000	3.271198000	-0.874955000
	H	-0.670048000	3.271198000	0.874955000
	C	-1.352856000	1.429942000	0.000000000
	H	-1.926035000	1.107756000	0.874813000
	H	-1.926035000	1.107756000	-0.874813000
	C	0.000000000	0.730191000	0.000000000
	H	0.573516000	1.051618000	-0.875105000
	H	0.573516000	1.051618000	0.875105000
	C	-0.118274000	-0.788453000	0.000000000
	H	-0.686379000	-1.116430000	0.872499000
	H	-0.686379000	-1.116430000	-0.872499000
	C	1.245205000	-1.463672000	0.000000000
	H	1.839990000	-1.167216000	-0.866327000
	H	1.839990000	-1.167216000	0.866327000
	C	1.135961000	-2.954294000	0.000000000
	O	0.165391000	-3.629849000	0.000000000
	O	2.371549000	-3.682639000	0.000000000
	O	3.441614000	-2.935265000	0.000000000
Octanal-1,4-TS	C	1.992776000	0.933592000	0.152956000
	O	1.453943000	1.992868000	0.189768000
	C	1.735979000	-0.257976000	1.040675000
	O	2.956494000	0.645556000	-0.756197000
	O	3.369520000	-0.687238000	-0.578638000
	H	2.167999000	-0.126887000	2.030737000
	H	2.575650000	-0.954198000	0.384086000
	C	0.341615000	-0.817833000	1.020066000
	H	0.294041000	-1.685282000	1.681335000
	H	-0.311122000	-0.058142000	1.464338000
	C	-0.153691000	-1.181064000	-0.376784000
	H	-0.087306000	-0.302296000	-1.022734000
	H	0.517204000	-1.926379000	-0.808936000
	C	-1.581892000	-1.722209000	-0.393172000
	H	-1.841515000	-1.965610000	-1.426223000
	H	-1.613457000	-2.664733000	0.160284000
	C	-2.641165000	-0.776698000	0.173667000
	H	-3.619032000	-1.253765000	0.068407000
	H	-2.492659000	-0.646744000	1.250073000
	C	-2.683320000	0.594267000	-0.493343000
	H	-1.740990000	1.121244000	-0.324848000
	H	-2.770418000	0.464112000	-1.575873000

	C	-3.832133000	1.455125000	0.014717000
	H	-4.794776000	0.978417000	-0.178401000
	H	-3.752686000	1.614572000	1.091653000
	H	-3.839603000	2.432970000	-0.466049000
Octanal-1,4-rad	C	1.850074000	-0.116100000	0.214268000
	O	1.349135000	-0.879862000	1.017856000
	C	1.526817000	1.266073000	0.003102000
	O	2.832891000	-0.528415000	-0.623344000
	O	3.138749000	-1.887103000	-0.409883000
	H	2.061672000	1.790213000	-0.777907000
	H	2.514259000	-2.106447000	0.313000000
	C	0.458558000	1.947118000	0.764771000
	H	0.128738000	1.308713000	1.582665000
	H	0.868866000	2.860752000	1.205260000
	C	-0.735850000	2.342585000	-0.126759000
	H	-1.456433000	2.877141000	0.496302000
	H	-0.391164000	3.050423000	-0.884046000
	C	-1.423255000	1.163640000	-0.810816000
	H	-2.202913000	1.553890000	-1.470047000
	H	-0.707225000	0.651009000	-1.461574000
	C	-2.040659000	0.152053000	0.147943000
	H	-1.264198000	-0.286065000	0.779568000
	H	-2.734628000	0.668585000	0.819724000
	C	-2.776700000	-0.971961000	-0.571018000
	H	-3.563198000	-0.546221000	-1.200492000
	H	-2.081967000	-1.476170000	-1.248301000
	C	-3.380969000	-1.989115000	0.387598000
	H	-4.099162000	-1.514796000	1.058946000
	H	-3.899875000	-2.783888000	-0.148258000
	H	-2.607081000	-2.449848000	1.003597000
Octanal-1,5-TS	C	-2.884537000	-0.424980000	-0.387313000
	O	-3.465563000	-1.279136000	-0.978906000
	C	-2.393678000	-0.496820000	1.045729000
	H	-3.129530000	0.008586000	1.672331000
	H	-2.387640000	-1.554159000	1.309815000
	C	-1.040297000	0.149606000	1.201507000
	C	0.135395000	-0.537332000	0.565487000
	H	0.312017000	-1.479269000	1.100900000
	H	-0.113965000	-0.821005000	-0.461390000
	C	1.407308000	0.301857000	0.573307000
	H	1.649398000	0.583799000	1.602570000
	H	1.221875000	1.234324000	0.033009000
	O	-2.543244000	0.714806000	-1.068724000
	O	-2.098715000	1.761652000	-0.265501000
	H	-0.848644000	0.562108000	2.190231000
	H	-1.300677000	1.195638000	0.500475000

	C	2.596958000	-0.416690000	-0.048989000
	H	2.781600000	-1.350228000	0.492186000
	H	2.348972000	-0.703362000	-1.075597000
	C	3.869087000	0.421905000	-0.054714000
	H	3.681687000	1.352967000	-0.596119000
	H	4.114689000	0.709241000	0.971328000
	C	5.053067000	-0.303546000	-0.679800000
	H	4.842325000	-0.574470000	-1.715709000
	H	5.949253000	0.316499000	-0.672936000
	H	5.278989000	-1.223252000	-0.137324000
Octanal-1,5-rad	C	1.606257000	-0.393545000	0.337872000
	O	1.534757000	0.272705000	1.338519000
	C	1.309749000	-1.869429000	0.202437000
	H	1.680788000	-2.209500000	-0.766707000
	H	1.867369000	-2.375448000	0.988991000
	C	-0.156269000	-2.115503000	0.338751000
	C	-1.124807000	-1.752926000	-0.729183000
	H	-0.625375000	-1.164557000	-1.502926000
	H	-1.475014000	-2.663847000	-1.232528000
	C	-2.353299000	-1.000884000	-0.197305000
	H	-2.877478000	-1.651845000	0.507091000
	H	-3.043254000	-0.822684000	-1.026049000
	O	1.938033000	0.143119000	-0.848062000
	H	-0.531397000	-2.460315000	1.293110000
	C	-2.025993000	0.321171000	0.493105000
	H	-2.934454000	0.708300000	0.962042000
	H	-1.316870000	0.140130000	1.306828000
	C	-1.457083000	1.392035000	-0.431566000
	H	-0.558478000	1.024344000	-0.930502000
	H	-2.178832000	1.601551000	-1.226252000
	C	-1.116543000	2.677752000	0.309585000
	H	-0.693414000	3.424120000	-0.362419000
	H	-2.003464000	3.108967000	0.777496000
	H	-0.389427000	2.483191000	1.100363000
	O	2.153976000	1.536962000	-0.745043000
	H	1.973098000	1.683280000	0.205977000
Octanal-1,6-TS	C	2.385301000	-0.476895000	-0.140175000
	O	3.254682000	-0.819295000	-0.881466000
	C	2.253928000	0.884965000	0.491375000
	H	2.121179000	0.796788000	1.568512000
	H	3.189934000	1.398110000	0.290065000
	C	1.076644000	1.661135000	-0.133008000
	H	1.136817000	1.578057000	-1.219952000
	H	1.205239000	2.719537000	0.105552000
	C	-0.289253000	1.211303000	0.340565000
	C	-1.402877000	1.236853000	-0.670364000

	H	-1.137895000	0.587884000	-1.509537000
	H	-1.446387000	2.250146000	-1.089564000
	C	-2.778078000	0.869807000	-0.118933000
	H	-3.053582000	1.594487000	0.652115000
	H	-3.510400000	0.982627000	-0.922241000
	O	1.354513000	-1.364441000	0.058394000
	O	0.507055000	-1.017355000	1.101080000
	H	-0.563008000	1.621075000	1.315021000
	H	-0.084746000	-0.008250000	0.698849000
	C	-2.887884000	-0.541720000	0.458052000
	H	-3.905974000	-0.677901000	0.828007000
	H	-2.236182000	-0.640051000	1.329409000
	C	-2.560215000	-1.644500000	-0.540953000
	H	-1.511302000	-1.623104000	-0.836953000
	H	-2.750059000	-2.626797000	-0.110129000
	H	-3.169021000	-1.549566000	-1.442567000
Octanal-1,6-rad	C	-1.595243000	0.027557000	0.307284000
	O	-1.181592000	0.549499000	1.312373000
	C	-1.805395000	-1.440191000	0.082788000
	H	-2.560048000	-1.767858000	0.799190000
	H	-2.193364000	-1.603858000	-0.921223000
	C	-0.497447000	-2.217989000	0.297480000
	H	-0.745702000	-3.285362000	0.246895000
	H	-0.137884000	-2.033442000	1.311413000
	C	0.556997000	-1.876745000	-0.696240000
	C	1.956587000	-1.583582000	-0.285284000
	H	2.612862000	-1.604829000	-1.157458000
	H	2.310182000	-2.367679000	0.394771000
	C	2.114155000	-0.228603000	0.429233000
	H	1.447530000	-0.197923000	1.295210000
	H	3.132669000	-0.150702000	0.818803000
	O	-1.918183000	0.746546000	-0.778655000
	H	0.277491000	-1.835231000	-1.741704000
	C	1.819920000	0.966464000	-0.468739000
	H	0.832081000	0.849731000	-0.920642000
	H	2.531129000	0.977216000	-1.299641000
	C	1.879002000	2.290230000	0.280025000
	H	2.870156000	2.458791000	0.705315000
	H	1.647582000	3.129381000	-0.375811000
	H	1.162909000	2.296472000	1.104109000
	O	-1.702428000	2.127575000	-0.568710000
	H	-1.341428000	2.123484000	0.341427000
Octanal-1,7-TS	C	0.969050000	1.683483000	0.366542000
	H	0.236368000	2.209758000	0.979383000
	H	1.804369000	2.368225000	0.219901000
	C	0.375754000	1.360940000	-1.007678000

	H	1.168282000	1.015949000	-1.676063000
	C	-0.748635000	0.355304000	-1.025251000
	H	-1.049923000	0.080108000	-2.036580000
	C	1.469859000	0.466410000	1.168579000
	H	2.078845000	0.811607000	2.000443000
	H	0.637898000	-0.112716000	1.557420000
	C	2.359722000	-0.396826000	0.316148000
	O	3.531057000	-0.236802000	0.154224000
	C	-1.914513000	0.560277000	-0.095056000
	H	-1.564504000	0.636470000	0.938056000
	H	-2.372452000	1.531334000	-0.326642000
	O	1.774977000	-1.402602000	-0.422439000
	H	0.006624000	2.294011000	-1.448784000
	O	0.449299000	-1.662423000	-0.110901000
	H	-0.193581000	-0.749255000	-0.632784000
	C	-2.970446000	-0.535340000	-0.192384000
	H	-2.505786000	-1.499022000	0.028242000
	H	-3.329172000	-0.595707000	-1.222953000
	C	-4.144289000	-0.302989000	0.748394000
	H	-4.640368000	0.644452000	0.530470000
	H	-4.885851000	-1.096125000	0.659530000
	H	-3.812426000	-0.272025000	1.787527000
Octanal-1,7-rad	C	-1.385975000	-1.928389000	0.398237000
	H	-0.937943000	-1.829386000	1.387798000
	H	-2.077343000	-2.770663000	0.443932000
	C	-0.298202000	-2.229470000	-0.648699000
	H	-0.776735000	-2.344494000	-1.623724000
	C	0.783575000	-1.210242000	-0.725812000
	H	0.832725000	-0.548773000	-1.581014000
	C	-2.189655000	-0.667756000	0.083647000
	H	-2.558137000	-0.682704000	-0.941559000
	H	-3.055172000	-0.605647000	0.746198000
	C	-1.410741000	0.593824000	0.315540000
	O	-0.815178000	0.901364000	1.318054000
	C	1.804585000	-1.098529000	0.348176000
	H	1.320942000	-0.816787000	1.294705000
	H	2.233972000	-2.092489000	0.533115000
	O	-1.489808000	1.419861000	-0.740741000
	H	0.136023000	-3.203533000	-0.393615000
	O	-0.807544000	2.634292000	-0.501319000
	C	2.926669000	-0.104036000	0.056065000
	H	3.391305000	-0.359661000	-0.899733000
	H	3.702137000	-0.216722000	0.816116000
	C	2.457126000	1.345146000	0.029567000
	H	1.706318000	1.511725000	-0.743690000
	H	2.010240000	1.619789000	0.986825000

	H	3.287134000	2.024593000	-0.164056000
	H	-0.439507000	2.467327000	0.390417000
Octanal-1,8-TS	C	-1.501773000	-1.144074000	0.238543000
	O	-1.951481000	-1.556080000	1.265445000
	C	-2.183913000	-0.142472000	-0.656029000
	H	-1.776592000	-0.167731000	-1.661931000
	H	-3.221761000	-0.471745000	-0.687267000
	C	-2.149454000	1.286590000	-0.092802000
	H	-2.456037000	1.260333000	0.955165000
	H	-2.913105000	1.856277000	-0.623897000
	C	-0.820687000	2.030627000	-0.226331000
	C	0.330405000	1.490501000	0.642184000
	H	-0.048319000	0.792716000	1.394152000
	H	0.770953000	2.312402000	1.217544000
	C	1.452196000	0.838740000	-0.123200000
	H	0.901581000	-0.105723000	-0.798687000
	H	1.844180000	1.460617000	-0.931703000
	O	-0.273266000	-1.649075000	-0.124155000
	O	0.273958000	-1.073644000	-1.258532000
	H	-1.005523000	3.073716000	0.032074000
	H	-0.515963000	2.030125000	-1.276195000
	C	2.516477000	0.145682000	0.683921000
	H	2.041822000	-0.595576000	1.331729000
	H	2.971385000	0.885327000	1.354145000
	C	3.592448000	-0.514091000	-0.167699000
	H	4.346491000	-0.992152000	0.456099000
	H	3.157021000	-1.275856000	-0.814423000
	H	4.095979000	0.218643000	-0.800392000
Octanal-1,8-rad	C	-1.934413000	-0.102501000	0.368613000
	O	-1.385639000	-1.142518000	0.635931000
	C	-1.526919000	1.272490000	0.813260000
	H	-2.048414000	2.013483000	0.208026000
	H	-1.885751000	1.379773000	1.839277000
	C	-0.013851000	1.460379000	0.756948000
	H	0.463942000	0.680830000	1.352022000
	H	0.234628000	2.413249000	1.228089000
	C	0.536719000	1.433579000	-0.663837000
	C	2.066350000	1.531455000	-0.707627000
	H	2.380928000	2.479229000	-0.264764000
	H	2.367018000	1.578248000	-1.764710000
	C	2.769793000	0.402061000	-0.037325000
	H	3.646013000	0.609580000	0.563747000
	O	-3.042847000	-0.066249000	-0.386500000
	H	0.106294000	2.256728000	-1.239341000
	H	0.222408000	0.512488000	-1.161898000
	C	2.406822000	-1.014547000	-0.309133000

	H	2.400850000	-1.189075000	-1.394889000
	H	1.373736000	-1.208287000	0.007356000
	C	3.333550000	-2.018528000	0.365093000
	H	4.362788000	-1.888242000	0.027806000
	H	3.318642000	-1.890157000	1.448251000
	H	3.033779000	-3.042725000	0.145545000
	O	-3.452926000	-1.364005000	-0.768984000
	H	-2.753868000	-1.909276000	-0.354053000
Octanal-1,9-TS	C	-1.353688000	-1.166166000	0.302773000
	O	-1.661325000	-1.559966000	1.387722000
	C	-2.089789000	-0.099842000	-0.462901000
	H	-1.912878000	-0.192837000	-1.530460000
	H	-3.138783000	-0.313701000	-0.261350000
	C	-1.791219000	1.334391000	0.009071000
	H	-1.760106000	1.347972000	1.101039000
	H	-2.659353000	1.930958000	-0.269477000
	C	-0.532138000	2.003389000	-0.574019000
	C	0.635049000	2.166293000	0.400108000
	H	0.277362000	2.694353000	1.287404000
	H	1.382784000	2.818066000	-0.060039000
	C	1.327524000	0.881350000	0.842563000
	H	2.075211000	1.132723000	1.604505000
	H	0.628714000	0.210589000	1.352068000
	O	-0.268424000	-1.785109000	-0.276000000
	O	0.207468000	-1.150702000	-1.410935000
	H	-0.804588000	3.002109000	-0.917821000
	H	-0.204775000	1.463371000	-1.464088000
	C	2.038751000	0.134115000	-0.256428000
	H	1.122692000	-0.441209000	-0.949171000
	H	2.496206000	0.784583000	-1.004313000
	C	2.909542000	-1.013340000	0.175404000
	H	3.311476000	-1.556037000	-0.678381000
	H	3.751544000	-0.643238000	0.768273000
	H	2.348557000	-1.712624000	0.796088000
Octanal-1,9-rad	C	-1.931078000	-0.066476000	-0.017323000
	O	-2.486443000	0.057568000	1.044868000
	C	-1.534764000	-1.349941000	-0.682946000
	H	-2.452999000	-1.911413000	-0.858219000
	H	-1.085080000	-1.132663000	-1.649543000
	C	-0.590212000	-2.164542000	0.208652000
	H	-0.351637000	-3.090181000	-0.318951000
	H	-1.126444000	-2.443426000	1.116101000
	C	0.697592000	-1.436203000	0.584458000
	C	1.572431000	-1.044182000	-0.600444000
	H	1.037399000	-0.345231000	-1.247881000
	H	1.788263000	-1.928994000	-1.206050000

	C	2.898526000	-0.393531000	-0.168878000
	H	3.468362000	-1.107820000	0.428927000
	H	3.485651000	-0.204778000	-1.076735000
	O	-1.571167000	1.000662000	-0.751202000
	O	-1.924493000	2.210837000	-0.111500000
	H	1.273547000	-2.079783000	1.254036000
	H	0.456888000	-0.542158000	1.167583000
	C	2.725183000	0.880634000	0.582090000
	H	-2.342305000	1.871721000	0.706846000
	H	2.991174000	0.922919000	1.629270000
	C	2.030481000	2.038918000	-0.035188000
	H	0.938240000	1.924920000	-0.023119000
	H	2.255400000	2.969940000	0.484066000
	H	2.311413000	2.156350000	-1.086197000
Nonanal-AcOO	C	-6.404728000	0.095781000	0.000000000
	H	-7.246056000	0.788757000	0.000000000
	H	-6.497563000	-0.542334000	0.880620000
	H	-6.497563000	-0.542334000	-0.880620000
	C	-5.072735000	0.834019000	0.000000000
	H	-5.016105000	1.488309000	0.874322000
	H	-5.016105000	1.488309000	-0.874322000
	C	-3.873062000	-0.105454000	0.000000000
	H	-3.928455000	-0.761279000	0.874811000
	H	-3.928455000	-0.761279000	-0.874811000
	C	-2.534971000	0.622086000	0.000000000
	H	-2.479969000	1.277567000	0.874979000
	H	-2.479969000	1.277567000	-0.874979000
	C	-1.337288000	-0.318944000	0.000000000
	H	-1.391246000	-0.974259000	0.874771000
	H	-1.391246000	-0.974259000	-0.874771000
	C	0.000000000	0.410091000	0.000000000
	H	0.054720000	1.065260000	-0.875105000
	H	0.054720000	1.065260000	0.875105000
	C	1.191981000	-0.538255000	0.000000000
	H	1.145738000	-1.192613000	0.872486000
	H	1.145738000	-1.192613000	-0.872486000
	C	2.514951000	0.213277000	0.000000000
	H	2.602225000	0.872065000	0.866347000
	H	2.602225000	0.872065000	-0.866347000
	C	3.688737000	-0.712012000	0.000000000
	O	3.704783000	-1.894432000	0.000000000
	O	4.984258000	-0.096425000	0.000000000
	O	4.964716000	1.208642000	0.000000000
Nonanal-1,4-TS	C	2.142869000	1.092467000	0.221033000

	O	1.410308000	2.019079000	0.357640000
	C	2.151458000	-0.194025000	1.007530000
	O	3.113500000	1.073355000	-0.725351000
	O	3.782422000	-0.162944000	-0.669778000
	H	2.583545000	-0.061740000	1.997396000
	H	3.087475000	-0.656826000	0.278679000
	C	0.892279000	-1.012763000	0.962848000
	H	1.036847000	-1.924626000	1.545639000
	H	0.121000000	-0.435359000	1.484630000
	C	0.427710000	-1.348049000	-0.451399000
	H	0.302196000	-0.422372000	-1.018183000
	H	1.213389000	-1.910788000	-0.959693000
	C	-0.870700000	-2.151498000	-0.489951000
	H	-1.117775000	-2.348262000	-1.535909000
	H	-0.701717000	-3.127418000	-0.026628000
	C	-2.067838000	-1.480793000	0.184395000
	H	-2.941847000	-2.123394000	0.051037000
	H	-1.906801000	-1.424808000	1.265251000
	C	-2.387821000	-0.087899000	-0.345927000
	H	-1.553046000	0.591243000	-0.148685000
	H	-2.493362000	-0.130183000	-1.435110000
	C	-3.653139000	0.505197000	0.261689000
	H	-4.497985000	-0.156758000	0.052356000
	H	-3.548602000	0.531296000	1.350067000
	C	-3.957344000	1.905004000	-0.254912000
	H	-4.864614000	2.308279000	0.194856000
	H	-3.138330000	2.590040000	-0.030024000
	H	-4.095064000	1.899898000	-1.337598000
Nonanal-1,4-rad	C	2.149851000	-0.508511000	0.203786000
	O	1.466395000	-1.058323000	1.046817000
	C	2.256700000	0.899428000	-0.052566000
	O	2.932221000	-1.226374000	-0.638866000
	O	2.815784000	-2.606479000	-0.380312000
	H	2.900179000	1.211701000	-0.864479000
	H	2.178171000	-2.602228000	0.364103000
	C	1.471963000	1.896374000	0.705979000
	H	0.990094000	1.413316000	1.554344000
	H	2.155012000	2.653435000	1.102707000
	C	0.426513000	2.611398000	-0.173708000
	H	-0.079164000	3.356075000	0.445094000
	H	0.945876000	3.160432000	-0.962469000
	C	-0.605646000	1.678307000	-0.801680000
	H	-1.250508000	2.268221000	-1.458029000
	H	-0.097914000	0.955366000	-1.448614000
	C	-1.470577000	0.927367000	0.204301000
	H	-0.843103000	0.295986000	0.837571000

	H	-1.959057000	1.648286000	0.868406000
	C	-2.527240000	0.054866000	-0.460644000
	H	-3.172142000	0.676131000	-1.090791000
	H	-2.035279000	-0.654497000	-1.133903000
	C	-3.385764000	-0.714862000	0.535293000
	H	-2.737675000	-1.334140000	1.160872000
	H	-3.875519000	-0.006783000	1.209597000
	C	-4.435463000	-1.589211000	-0.137511000
	H	-5.113258000	-0.988285000	-0.746622000
	H	-3.967606000	-2.325403000	-0.793550000
	H	-5.035335000	-2.129140000	0.595143000
Nonanal-1,5-TS	C	-3.435362000	-0.192371000	-0.543637000
	O	-4.024696000	-0.760036000	-1.408268000
	C	-2.989195000	-0.783240000	0.779758000
	H	-3.727218000	-0.502376000	1.532070000
	H	-3.023384000	-1.865234000	0.653856000
	C	-1.621673000	-0.286520000	1.176138000
	C	-0.449516000	-0.751866000	0.358780000
	H	-0.323002000	-1.829641000	0.524780000
	H	-0.674105000	-0.639312000	-0.706166000
	C	0.849152000	-0.027272000	0.690851000
	H	1.066394000	-0.143099000	1.757081000
	H	0.713766000	1.043941000	0.517815000
	O	-3.039369000	1.100124000	-0.773041000
	O	-2.586784000	1.778728000	0.355238000
	H	-1.446768000	-0.256389000	2.249912000
	H	-1.828367000	0.948718000	0.884690000
	C	2.033812000	-0.526919000	-0.125268000
	H	2.165702000	-1.599975000	0.046114000
	H	1.811205000	-0.413114000	-1.190561000
	C	3.333083000	0.198822000	0.198233000
	H	3.200013000	1.271742000	0.027519000
	H	3.555944000	0.085737000	1.264111000
	C	4.520408000	-0.296347000	-0.618416000
	H	4.296267000	-0.181950000	-1.682396000
	H	4.651348000	-1.368476000	-0.447888000
	C	5.814141000	0.435475000	-0.287262000
	H	6.075362000	0.310789000	0.765119000
	H	6.647082000	0.063948000	-0.883949000
	H	5.717450000	1.505587000	-0.478605000
Nonanal-1,5-rad	C	1.119867000	-1.447801000	0.322660000
	O	0.550674000	-1.524231000	1.381118000
	C	2.466129000	-0.815027000	0.054752000
	H	3.161132000	-1.240971000	0.776944000
	H	2.786951000	-1.096897000	-0.950227000
	C	2.380190000	0.667710000	0.200945000

	C	1.716163000	1.528113000	-0.813196000
	H	2.476697000	2.075906000	-1.385327000
	H	1.190465000	0.907884000	-1.543566000
	C	0.755170000	2.552585000	-0.194043000
	H	0.360080000	3.190926000	-0.988369000
	H	1.328095000	3.204235000	0.470629000
	O	0.570439000	-1.913182000	-0.811555000
	H	2.708891000	1.110840000	1.131553000
	C	-0.399796000	1.930893000	0.587889000
	H	0.000457000	1.268779000	1.361787000
	H	-0.935831000	2.724854000	1.114220000
	C	-1.393035000	1.154423000	-0.268857000
	H	-1.821862000	1.824195000	-1.021738000
	H	-0.882829000	0.363812000	-0.825526000
	C	-2.514901000	0.525005000	0.547844000
	H	-3.022984000	1.304058000	1.123125000
	H	-2.075995000	-0.156596000	1.282123000
	C	-3.526311000	-0.221625000	-0.311570000
	H	-4.310570000	-0.673521000	0.296169000
	H	-4.004612000	0.452492000	-1.024584000
	H	-3.039857000	-1.014957000	-0.880977000
	O	-0.712462000	-2.460359000	-0.579317000
	H	-0.808292000	-2.308525000	0.383244000
Nonanal-1,6-TS	C	2.474621000	-0.803265000	-0.148198000
	O	3.245669000	-1.320788000	-0.896621000
	C	2.664132000	0.530780000	0.526486000
	H	2.495906000	0.444864000	1.598824000
	H	3.699052000	0.809675000	0.350179000
	C	1.717690000	1.585598000	-0.082253000
	H	1.776787000	1.524898000	-1.170711000
	H	2.090727000	2.574221000	0.195149000
	C	0.275163000	1.459617000	0.360472000
	C	-0.781746000	1.767541000	-0.664605000
	H	-0.650187000	1.102224000	-1.522058000
	H	-0.587879000	2.777370000	-1.048073000
	C	-2.216471000	1.700708000	-0.146045000
	H	-2.347358000	2.462602000	0.627112000
	H	-2.889190000	1.973704000	-0.962706000
	O	1.259838000	-1.425221000	0.018270000
	O	0.506650000	-0.914466000	1.065612000
	H	0.085745000	1.900050000	1.341568000
	H	0.179320000	0.219034000	0.689414000
	C	-2.635985000	0.342772000	0.415287000
	H	-3.668153000	0.419730000	0.766851000
	H	-2.037876000	0.102124000	1.298840000
	C	-2.534952000	-0.809115000	-0.578153000

	H	-3.124706000	-0.569354000	-1.467966000
	H	-1.501514000	-0.924176000	-0.910987000
	C	-3.004235000	-2.129503000	0.016703000
	H	-2.391719000	-2.399092000	0.878225000
	H	-4.042230000	-2.065196000	0.348674000
	H	-2.933281000	-2.939681000	-0.708586000
Nonanal-1,6-rad	C	1.163550000	1.328559000	0.299031000
	O	0.585650000	1.220754000	1.351641000
	C	2.499781000	0.745798000	-0.052814000
	H	2.748050000	0.998745000	-1.082258000
	H	3.234096000	1.218826000	0.601097000
	C	2.507405000	-0.776299000	0.154711000
	H	2.250154000	-0.993999000	1.192870000
	H	3.541342000	-1.115126000	0.014591000
	C	1.589252000	-1.497600000	-0.768443000
	C	0.649967000	-2.543097000	-0.281033000
	H	1.189161000	-3.247513000	0.363263000
	H	0.264378000	-3.119692000	-1.124098000
	C	-0.534981000	-1.975175000	0.522318000
	H	-1.096328000	-2.806303000	0.957104000
	H	-0.153100000	-1.385736000	1.359989000
	O	0.637914000	2.017837000	-0.725466000
	H	1.609005000	-1.231182000	-1.817989000
	C	-1.470607000	-1.110783000	-0.312109000
	H	-1.907051000	-1.716606000	-1.113227000
	H	-0.898634000	-0.322029000	-0.810132000
	C	-2.584889000	-0.473112000	0.507255000
	H	-3.149458000	-1.256149000	1.021361000
	H	-2.135682000	0.141830000	1.292405000
	C	-3.529808000	0.372928000	-0.335835000
	H	-4.017125000	-0.233228000	-1.101758000
	H	-4.310242000	0.828533000	0.274058000
	H	-2.986686000	1.172275000	-0.842401000
	O	-0.621975000	2.563002000	-0.389557000
	H	-0.732607000	2.227292000	0.523696000
Nonanal-1,7-TS	C	1.592546000	1.614252000	0.513054000
	H	0.897147000	2.167906000	1.144925000
	H	2.503791000	2.209475000	0.454077000
	C	1.025678000	1.475982000	-0.902537000
	H	1.802967000	1.101951000	-1.573140000
	C	-0.199689000	0.607590000	-1.043742000
	H	-0.487367000	0.452728000	-2.084164000
	C	1.921255000	0.286245000	1.222662000
	H	2.527907000	0.490746000	2.101412000
	H	1.014652000	-0.224927000	1.531741000
	C	2.747222000	-0.599064000	0.329453000

	O	3.935009000	-0.559424000	0.222034000
	C	-1.373180000	0.863297000	-0.135889000
	H	-1.057489000	0.816862000	0.909886000
	H	-1.714625000	1.894312000	-0.298589000
	O	2.088514000	-1.468451000	-0.512512000
	H	0.778647000	2.478136000	-1.271536000
	O	0.729925000	-1.601263000	-0.269903000
	H	0.214680000	-0.581077000	-0.731671000
	C	-2.534256000	-0.098460000	-0.358360000
	H	-2.185910000	-1.124093000	-0.207479000
	H	-2.860205000	-0.035982000	-1.400991000
	C	-3.719210000	0.173346000	0.559547000
	H	-4.061940000	1.201073000	0.410460000
	H	-3.388903000	0.109122000	1.599892000
	C	-4.875887000	-0.790130000	0.330883000
	H	-5.243782000	-0.722713000	-0.694323000
	H	-4.564283000	-1.821623000	0.502775000
	H	-5.709746000	-0.577136000	0.999351000
Nonanal-1,7-rad	C	2.471112000	-1.185592000	0.346903000
	H	3.464620000	-1.635138000	0.364805000
	H	2.059207000	-1.282286000	1.352241000
	C	1.594725000	-1.949650000	-0.661771000
	H	1.634919000	-3.010750000	-0.387665000
	C	0.175778000	-1.503368000	-0.710150000
	H	-0.182602000	-0.960575000	-1.575222000
	C	2.622147000	0.296194000	0.008066000
	H	3.407334000	0.738960000	0.624310000
	H	2.904270000	0.435061000	-1.035115000
	C	1.384255000	1.092392000	0.300940000
	O	0.758426000	1.101298000	1.331752000
	C	-0.766313000	-1.828133000	0.392518000
	H	-0.730623000	-2.909695000	0.581756000
	H	-0.420345000	-1.364905000	1.327518000
	O	1.054269000	1.884738000	-0.732454000
	H	2.049053000	-1.863610000	-1.651233000
	O	-0.068481000	2.688788000	-0.430916000
	C	-2.209961000	-1.402265000	0.136910000
	H	-2.850094000	-1.829131000	0.913271000
	H	-2.549886000	-1.829746000	-0.811504000
	C	-2.406545000	0.109100000	0.110628000
	H	-1.768948000	0.551818000	-0.657865000
	H	-2.066001000	0.523839000	1.063438000
	C	-3.853297000	0.510853000	-0.140875000
	H	-4.204396000	0.126017000	-1.100094000
	H	-4.511266000	0.114034000	0.634592000
	H	-3.968994000	1.594614000	-0.155377000

	H	-0.291370000	2.365712000	0.466073000
Nonanal-1,8-TS	C	1.734188000	-1.285512000	-0.233067000
	O	2.053799000	-1.794640000	-1.265143000
	C	2.603624000	-0.352776000	0.568808000
	H	2.268110000	-0.285570000	1.598977000
	H	3.588393000	-0.817906000	0.548279000
	C	2.719902000	1.046204000	-0.055591000
	H	2.950176000	0.940343000	-1.118005000
	H	3.585425000	1.527439000	0.401666000
	C	1.512164000	1.966018000	0.124246000
	C	0.246613000	1.553784000	-0.649958000
	H	0.480850000	0.783269000	-1.389740000
	H	-0.117180000	2.405062000	-1.236122000
	C	-0.900672000	1.088395000	0.208225000
	H	-0.435365000	0.109619000	0.897609000
	H	-1.158356000	1.789950000	1.005283000
	O	0.476888000	-1.603799000	0.229125000
	O	0.089688000	-0.914421000	1.365772000
	H	1.815393000	2.965069000	-0.190299000
	H	1.278589000	2.043727000	1.189349000
	C	-2.091066000	0.506794000	-0.503371000
	H	-1.757943000	-0.322503000	-1.134648000
	H	-2.488215000	1.266377000	-1.189905000
	C	-3.199637000	0.033075000	0.429129000
	H	-2.791511000	-0.716489000	1.110212000
	H	-3.530517000	0.870629000	1.049200000
	C	-4.387426000	-0.548923000	-0.324501000
	H	-4.083687000	-1.406927000	-0.926127000
	H	-5.166931000	-0.881256000	0.360484000
	H	-4.826362000	0.189700000	-0.997763000
Nonanal-1,8-rad	C	2.032562000	-0.219898000	0.322302000
	O	1.397576000	-1.231182000	0.151978000
	C	1.642930000	0.958296000	1.167404000
	H	1.857527000	0.676167000	2.200507000
	H	2.285169000	1.803424000	0.921226000
	C	0.165390000	1.302955000	1.007140000
	H	-0.099219000	2.055550000	1.752275000
	H	-0.431127000	0.417262000	1.229079000
	C	-0.178530000	1.818037000	-0.385392000
	C	-1.680442000	2.060166000	-0.571806000
	H	-1.833619000	2.454625000	-1.587484000
	H	-2.001668000	2.855904000	0.104773000
	C	-2.533350000	0.856405000	-0.357827000
	H	-3.507239000	0.993173000	0.098272000
	O	3.233036000	-0.039756000	-0.248739000
	H	0.169841000	1.104802000	-1.136659000

	H	0.360717000	2.748901000	-0.576858000
	C	-2.244476000	-0.461615000	-0.984613000
	H	-1.165594000	-0.642355000	-1.018813000
	H	-2.571898000	-0.449218000	-2.035678000
	C	-2.913559000	-1.636341000	-0.269897000
	H	-3.992874000	-1.465452000	-0.228689000
	H	-2.766041000	-2.542306000	-0.860747000
	C	-2.369784000	-1.852736000	1.136990000
	H	-1.293103000	-2.030282000	1.109172000
	H	-2.546259000	-0.975625000	1.762414000
	H	-2.842772000	-2.708052000	1.619659000
	O	3.620591000	-1.166395000	-1.009691000
	H	2.844103000	-1.749479000	-0.886632000
Nonanal-1,9-TS	C	-1.870594000	-1.053754000	-0.074349000
	O	-2.643232000	-1.383216000	-0.922497000
	C	-2.014454000	0.172835000	0.788056000
	H	-3.002136000	0.114435000	1.244313000
	H	-1.276616000	0.188583000	1.580240000
	C	-1.942732000	1.423204000	-0.102179000
	H	-2.063785000	2.305410000	0.530199000
	H	-2.802858000	1.394610000	-0.770731000
	C	-0.670946000	1.557731000	-0.947837000
	C	0.517715000	2.257514000	-0.287789000
	H	0.198871000	3.255461000	0.023995000
	H	1.283040000	2.416307000	-1.051085000
	C	1.167363000	1.579526000	0.917394000
	H	1.972505000	2.235566000	1.269846000
	H	0.465321000	1.524754000	1.752718000
	O	-0.738828000	-1.830896000	0.040132000
	O	0.049057000	-1.560881000	1.145750000
	H	-0.922548000	2.134580000	-1.839068000
	H	-0.370598000	0.574303000	-1.319812000
	C	1.780261000	0.215059000	0.692971000
	H	0.851920000	-0.677936000	0.814202000
	H	2.362995000	-0.107996000	1.558629000
	C	2.484534000	-0.075692000	-0.606507000
	H	3.277603000	0.672504000	-0.733696000
	H	1.803863000	0.069968000	-1.446910000
	C	3.080561000	-1.476080000	-0.662333000
	H	3.596011000	-1.643658000	-1.607044000
	H	3.798901000	-1.627688000	0.144628000
	H	2.301284000	-2.231317000	-0.562069000
Nonanal-1,9-rad	C	-1.875234000	-0.450329000	0.392331000
	O	-1.724722000	0.405595000	1.228403000
	C	-1.373689000	-1.862196000	0.460744000
	H	-1.800000000	-2.301104000	1.363143000

H	-1.737791000	-2.422519000	-0.399365000
C	0.155930000	-1.891028000	0.528551000
H	0.471823000	-2.913149000	0.745535000
H	0.474862000	-1.276521000	1.371316000
C	0.810352000	-1.416192000	-0.764353000
C	2.334425000	-1.369385000	-0.707119000
H	2.716114000	-1.180484000	-1.712674000
H	2.723167000	-2.345777000	-0.403332000
C	2.895513000	-0.285757000	0.236385000
H	2.610559000	-0.513782000	1.266548000
H	3.987328000	-0.350312000	0.198756000
O	-2.524706000	-0.205797000	-0.755979000
O	-2.971445000	1.133778000	-0.823196000
H	0.438860000	-0.419756000	-1.022530000
H	0.499171000	-2.076273000	-1.577911000
C	2.445766000	1.087113000	-0.118389000
H	-2.631363000	1.485697000	0.024929000
H	2.865918000	1.551972000	-1.004328000
C	1.418465000	1.838869000	0.651060000
H	1.906046000	2.521836000	1.362049000
H	0.835157000	1.148645000	1.265548000
C	0.473522000	2.654560000	-0.229760000
H	-0.087072000	2.008650000	-0.907303000
H	-0.243235000	3.208492000	0.376686000
H	1.027135000	3.371839000	-0.837589000

11. MATLAB code for calculating ECKART tunneling coefficient

```
function [G,xa,Va]=eckart(e1,e2,w,mu,T,plotting)

%This program calculates the Eckart correction factor numerically.
%The following input is required:
%e1 is the energy difference between reactants and TS in kcal/mol
%e2 is the energy difference between TS and products in kcal/mol
%w is the numerical value of the imaginary frequency at the TS in cm-1
%mu is the reduced mass of the reaction coordinate (only required for
%plotting, set to 1 if no plotting) in amu
%T is the temperature and can be a vector or a scalar in K
%plotting is set to 1 if plotting of the potential is needed, otherwise it
%is set to 0
%e1 = left barrier = energy difference between transition state and
%product, positive (Sum of electronic and zero-point energies/kcal/mol)
%e2 = right barrier
%w = imaginary frequency of transition state
%mu = reduced mass of transition state
%T = temperature(K)
%plotting (1=on, 0=off)

%Constants
c=299792458 ; %SI
h=2*pi ; %atomic units
k=3.1668152*(10^(-6)); %atomic units

%Converting input to au
v1=e1*(1.5936*(10^(-3)));
v2=e2*(1.5936*(10^(-3)));
wau=w*c*100*(1/(4.134137*(10^16)));
m=mu*1822.888479;

%Calculate force constant, A, B and L
F=-4*(pi^2)*(wau^2)*m;
%F=-4*(pi^2)*(wau^2)*1822.888479;
A=v1-v2;
B=(sqrt(v2)+sqrt(v1))^2;
L=-pi*(A-B)*(B+A)/(sqrt(-2*F*B)*B);

%Defining reaction coordinate
x=-3:0.01:3;

%Removing reduced mass from reaction coordinate in order to get a well
%defined potential
```

```
x(:)=x(:)/sqrt(mu);

%Calculating potential
for i=1:numel(x)
   y(i)=-exp((2*pi*x(i))/L);
   V(i)=((-(y(i)*A)/(1-y(i)))-((y(i)*B)/((1-y(i))^2)));
   xa(i)=0.529177*x(i)*sqrt(mu); %reduced mass re-inserted for plotting
   Va(i)=V(i)*627.51; %potential converted to kcal/mol for plotting
end

%Calculating the correction factors for all T's
VB(1)=V(1); %value of potential at reactants
VB(2)=V(numel(x)); %value of potential at products
Emin=max(VB(:)); %minimum energy at which tunnelling can occur
Gdiff=1;    %initial convergence control set to 1
Gsize=max(V)/50;   %initial integration stepsize
[Gold,Eka,K,GK]=Gcalc(Emin,Gsize,V,A,B,L,h,k,m,T,v1); %calculate G
Gsize=Gsize/10; %reduce integration stepsize
runs=0; %initial number of runs
while Gdiff>=0.001  %convergence criteria
   [Gnew,Eka,K,GK]=Gcalc(Emin,Gsize,V,A,B,L,h,k,m,T,v1); %new G
   display(Gnew); %display new correction factor
   Gsize=Gsize/10; %reduce integration stepsize
   for j=1:numel(T)
      Gdiffcalc(j)=abs(Gnew(j)-Gold(j))/Gold(j); %calculate convergence
   end
   Gdiff=max(Gdiffcalc); %max convergence control value
   display(Gdiff); %display convergence control value
   Gold=Gnew; %replace old correction factor with new
   runs=runs+1;    %a run completed
   display(runs);  %display run number
end
[G,Eka,K,GK]=Gcalc(Emin,Gsize,V,A,B,L,h,k,m,T,v1); %final G


%If plotting needed run plot function
if plotting==1
   plotpotential;
end

%End of main program

function plotpotential
%Plotting function for numparabol program
%Plot potential, transmission and value of integrand in correction factor
%expression
```

```
subplot(2,2,[1 2])
plot(xa,Va) ;
xlabel('Reaction Coordinate in Å*amu^{1/2}'); ylabel('V in kcal/mol');title('Potential');
subplot(2,2,3)
plot(Eka,K);
xlabel('E in kcal/mol'); ylabel('KI');title('Transmission');
subplot(2,2,4)
plot(Eka,GK);
xlabel('E in kcal/mol'); ylabel('GKI');title('Integrand');

%End of plotting program

end
end
function [G,Eka,K,GK]=Gcalc(Emin,Gsize,V,A,B,L,h,k,m,T,v1)
%Sub-function to numparabol
%This program do the actual calculation of the correction factor

%Calculating correction factor
count=1; %index control
for E=Emin:Gsize:(2*max(V)) %interval where transmission may be less than 1
   C=(h^2)/(8*m*(L^2)); %calculation of C factor
   a=0.5*sqrt(E/C);    %calculation of a
   b=0.5*sqrt((E-A)/C); %calculation of b
   d=0.5*sqrt((B-C)/C); %calculation of d
   K(count)=1-((cosh(2*pi*(a-b))+cosh(2*pi*d))/(cosh(2*pi*(a+b))+cosh(2*pi*d))); %calc K
   EK(count)=E;    %save energy for later
   Eka(count)=E*627.51;    %convert energy to kcal/mol for plotting
   count=count+1;  %index control
end
for q=1:numel(T) %temperature XXXperat XXXperations begin
   GK=0; %clean variable
   for j=1:numel(K)
      GK(j)=K(j)*exp(-EK(j)/(k*T(q)));   %calculate integrand
   end
   GI=0; %sum control of integral
   for i=1:(numel(EK)-1) %numerical integration by using the areal of squares
      GI=GI+(0.5*(GK(i)+GK(i+1))*abs(EK(i)-EK(i+1)));
   end
   GI=GI*(exp(v1/(k*T(q)))/(k*T(q))); %multiplying integral with prefactor

   %For energies above the interval where transmission is less than 1, we use
   %analytical integration to obtain the final result
   G(q)=GI+exp(v1/(k*T(q)))*exp(-EK(numel(EK))/(k*T(q)));
end %temperature dependent operations end
```

```
%End of sub-function
End
```

12. MESMER Input files for all the possible H-shifts in pristine acyl peroxy radicals

Ethanal–AcOO ------> Ethanal–AcOOH

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
 <me:title>Project name</me:title>
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  </atomArray>
  <bondArray>
   <bond atomRefs2="a2 a1" order="3"/>
  </bondArray>
  <propertyList>
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    <scalar>48.0</scalar>
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   <property dictRef="me:sigma">
    <scalar>3.90</scalar>
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   <property dictRef="me:MW">
    <scalar units="amu">28.0</scalar>
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  </propertyList>
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    <atom id="a3" elementType="C" spinMultiplicity="2" x3="-1.777775" y3="-0.467027"
z3="0.000033" />
    <atom id="a4" elementType="O" x3="0.504537" y3="-0.801697" z3="-0.000047" />
    <atom id="a5" elementType="H" x3="-1.884497" y3="-1.537757" z3="0.000145" />
    <atom id="a6" elementType="H" x3="-2.635330" y3="0.181296" z3="0.000004" />
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```

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      <property title="basis">
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1084.74 1308.29 1444.45 1491.46 1757.93 3225.87 3340.13 3507.38</array>
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```

```
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     <atom id="a7" elementType="H" x3="-0.800250" y3="-1.241358" z3="0.000000" />
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     <property title="basis">
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1255.80 1386.05 1442.38 1450.85 1925.95 3099.79 3168.56 3208.93</array>
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       </property>
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      <me:DistributionCalcMethod  name="Boltzmann" />
      <me:energyTransferModel name="ExponentialDown"  />
      <me:deltaEDown >225.0</me:deltaEDown>
     </molecule>
    </moleculeList>
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       </reactant>
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      <productList>
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       </product>
      </productList>
      <me:transitionState>
       <molecule ref="14Hshift-TS" role="transitionState" />
      </me:transitionState>
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          <me:tunneling name="Eckart" />
  </reaction>
</reactionList>
<me:conditions>
  <me:bathGas>N2</me:bathGas>
  <me:PTs>
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    <!--<me:PTpair units="Torr" P="201.60" T="298." />-->
    <!--<me:PTpair units="Torr" P="10.06" T="298." />-->
    <!--<me:PTpair units="Torr" P="15.01" T="298." />-->
  </me:PTs>
        <me:InitialPopulation>
    <me:molecule ref="Ethanal-AcylOO-rad" population="1.0" />
  </me:InitialPopulation>
</me:conditions>
<me:modelParameters>
  <!--Specify grain size directly...-->
  <me:grainSize units="cm-1">100</me:grainSize>
  <!--...or by the total number of grains
     <me:numberOfGrains> 500 </me:numberOfGrains>-->
  <!--Specify increased energy range
     <me:maxTemperature>6000</me:maxTemperature>-->
  <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
</me:modelParameters>
<me:control>
  <me:printSpeciesProfile />
  <!--<me:testMicroRates />
        <me:testDOS />
  <me:testRateConstant />
  <me:printGrainDOS />-->
  <!--<me:printCellDOS />-->
  <!--<me:printReactionOperatorColumnSums />-->
  <!--<me:printTunnellingCoefficients />
  <me:printGrainkfE />-->
  <!--<me:printGrainBoltzmann />
  <me:printGrainkbE />-->
  <me:eigenvalues>3</me:eigenvalues>
  <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown
  <me:diagramEnergyOffset>0</me:diagramEnergyOffset>-->
  <!--Adjusts displayed energies to this values for the lowest species. -->
  <me:calcMethod  name="simpleCalc" />
  <me:ForceMacroDetailedBalance >true</me:ForceMacroDetailedBalance>
</me:control>
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  <dc:title>Project name</dc:title>
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   <dc:source>Acylperoxyrad-Ethanal.xml</dc:source>
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   <dc:date>20230618_144216</dc:date>
   <dc:contributor>ndprse</dc:contributor>
  </metadataList>
</me:mesmer>
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Propanal–AcOO ------> Propanal–AcOOH

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<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer                                                    xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>Project name</me:title>
  <moleculeList convention="">
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     <atom id="a2" elementType="N" />
   </atomArray>
   <bondArray>
     <bond atomRefs2="a2 a1" order="3"/>
   </bondArray>
   <propertyList>
     <property dictRef="me:epsilon">
       <scalar>48.0</scalar>
     </property>
     <property dictRef="me:sigma">
       <scalar>3.90</scalar>
     </property>
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       <scalar units="amu">28.0</scalar>
     </property>
   </propertyList>
  </molecule>
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       <atom id="a1" elementType="C" x3="-0.058002" y3="0.066469" z3="-0.000144" />
       <atom id="a2" elementType="O" x3="-0.219161" y3="1.271229" z3="-0.000251" />
       <atom  id="a3"  elementType="C"  spinMultiplicity="2"  x3="1.187978"  y3="-0.647388"  z3="-
0.000004" />
       <atom id="a4" elementType="O" x3="-1.113721" y3="-0.783641" z3="0.000086" />
       <atom id="a5" elementType="H" x3="1.146638" y3="-1.727506" z3="0.000194" />
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```
      <atom id="a6" elementType="C" x3="2.482763" y3="0.060148" z3="0.000080" />
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      <atom id="a8" elementType="H" x3="3.075582" y3="-0.223822" z3="-0.874031" />
      <atom id="a9" elementType="H" x3="2.343236" y3="1.138285" z3="-0.001166" />
      <atom id="a10" elementType="O" x3="-2.330746" y3="-0.074036" z3="0.000113" />
      <atom id="a11" elementType="H" x3="-2.007196" y3="0.851050" z3="0.000088" />
    </atomArray>
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      <bond atomRefs2="a1 a4" order="1" />
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      <bond atomRefs2="a3 a5" order="1" />
      <bond atomRefs2="a6 a7" order="1" />
      <bond atomRefs2="a4 a10" order="1" />
      <bond atomRefs2="a11 a10" order="1" />
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      </property>
      <property title="basis">
        <scalar>Aug-CC-pVTZ (5D, 7F)</scalar>
      </property>
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      </property>
      <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
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      </property>
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        <array units="cm-1">85.91 118.81 215.18 218.44 390.74 467.83 499.33 605.19 702.84 744.87
927.99 993.18 1004.26 1090.90 1156.55 1211.62 1404.21 1438.17 1476.12 1505.10 1533.05 1752.28
3028.46 3075.98 3155.81 3216.65 3539.89</array>
      </property>
      <property title="Rotational Constants" dictRef="me:rotConsts">
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    <atom id="a2" elementType="O" x3="0.145549" y3="1.827929" z3="-0.012879" />
    <atom id="a3" elementType="C" x3="-0.761926" y3="-0.352274" z3="0.524879" />
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0.040690" />
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    <atom id="a7" elementType="H" x3="0.050674" y3="-1.310465" z3="0.329910" />
    <atom id="a8" elementType="C" x3="-2.005140" y3="-0.447497" z3="-0.311085" />
    <atom id="a9" elementType="H" x3="-2.563130" y3="0.489297" z3="-0.242028" />
    <atom id="a10" elementType="H" x3="-1.768301" y3="-0.620723" z3="-1.359509" />
    <atom id="a11" elementType="H" x3="-2.648368" y3="-1.249536" z3="0.045347" />
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    </property>
    <property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
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    </property>
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```

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<scalar units="cm-1">1629.08</scalar>
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<property title="Rotational Constants" dictRef="me:rotConsts">
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<atom id="a5" elementType="H" x3="-1.333026" y3="-1.007878" z3="1.213990" />
<atom id="a6" elementType="C" spinMultiplicity="2" x3="-2.445253" y3="0.150905" z3="-0.200434" />
<atom id="a7" elementType="O" x3="1.061810" y3="-0.765450" z3="-0.064251" />
<atom id="a8" elementType="O" x3="2.297616" y3="-0.079784" z3="-0.098100" />
<atom id="a9" elementType="H" x3="-2.369692" y3="1.225591" z3="-0.249448" />
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902.50 935.52 1004.06 1045.79 1122.72 1194.38 1239.11 1403.37 1444.93 1456.77 1524.80 1829.28
2981.39 3078.37 3181.75 3296.63 3567.84</array>
      </property>
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</propertyList>
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      <atom id="a3" elementType="C" x3="0.274903" y3="-1.137140" z3="0.364581" />
      <atom id="a4" elementType="H" x3="0.420663" y3="-1.110569" z3="1.445302" />
      <atom id="a5" elementType="H" x3="-0.121657" y3="-2.116471" z3="0.099894" />
      <atom id="a6" elementType="C" spinMultiplicity="2" x3="1.560440" y3="-0.816210" z3="-
0.342249" />
      <atom id="a7" elementType="O" x3="-0.405446" y3="1.146366" z3="-0.182735" />
      <atom id="a8" elementType="O" x3="0.889257" y3="1.419991" z3="0.251084" />
      <atom id="a9" elementType="H" x3="2.476307" y3="-1.126164" z3="0.148068" />
      <atom id="a10" elementType="H" x3="1.519795" y3="0.482030" z3="-0.175904" />
      <atom id="a11" elementType="H" x3="1.563629" y3="-0.953083" z3="-1.419544" />
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<bond atomRefs2="a7 a1" order="1" />
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<atom id="a8" elementType="C" x3="0.000000" y3="0.504177" z3="0.000000" />
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</property>
<property title="SpinMultiplicity" dictRef="me:spinMultiplicity">
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</property>
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1012.89 1057.92 1108.82 1120.59 1251.13 1285.07 1383.71 1432.36 1454.37 1503.45 1507.84 1923.28
3070.82 3083.19 3115.45 3149.46 3151.42</array>
       </property>
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       <property dictRef="me:epsilon" >
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       </property>
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        <scalar>1</scalar>
       </property>
     </propertyList>
     <me:DOSCMethod  name="ClassicalRotors" />
     <me:DistributionCalcMethod  name="Boltzmann" />
     <me:energyTransferModel name="ExponentialDown"  />
     <me:deltaEDown >225.0</me:deltaEDown>
   </molecule>
  </moleculeList>
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       </reactant>
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     <me:transitionState>
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     <me:MCRCMethod name="RRKM" />
          <me:tunneling name="Eckart" />
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          <me:tunneling name="Eckart" />
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</reactionList>
<me:conditions>
  <me:bathGas>N2</me:bathGas>
  <me:PTs>
    <me:PTpair units="Torr" P="760." T="298." precision="qd"  bathGas="N2" />
  </me:PTs>
</me:conditions>
<me:modelParameters>
  <!--Specify grain size directly...-->
  <me:grainSize units="cm-1">100</me:grainSize>
  <!--...or by the total number of grains
      <me:numberOfGrains> 500 </me:numberOfGrains>-->
  <!--Specify increased energy range
      <me:maxTemperature>6000</me:maxTemperature>-->
  <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
</me:modelParameters>
<me:control>
  <me:printSpeciesProfile />
  <!--<me:testMicroRates />
        <me:testDOS />
  <me:testRateConstant />
  <me:printGrainDOS />-->
  <!--<me:printCellDOS />-->
  <!--<me:printReactionOperatorColumnSums />-->
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   <!--Adjusts displayed energies to this values for the lowest species. -->
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   <dc:source>Acylperoxyrad-Propanal.xml</dc:source>
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Butanal–AcOO ------> Butanal–AcOOH

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xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
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1414.63 1427.83 1450.98 1499.31 1507.83 1514.25 1922.87 3047.03 3067.79 3075.72 3094.98 3109.16
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Pentanal–AcOO ------> Pentanal–AcOOH

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1218.14 1244.19 1298.72 1335.24 1365.91 1397.70 1417.15 1444.74 1477.51 1487.04 1495.39 1497.45
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1181.47 1212.10 1273.81 1296.75 1372.34 1397.19 1410.52 1470.38 1471.32 1475.87 1496.20 1516.37
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1190.06 1240.35 1264.24 1305.74 1366.38 1383.92 1404.12 1448.80 1472.06 1482.28 1489.03 1502.99
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1189.17 1263.74 1276.19 1335.25 1364.77 1414.03 1426.08 1477.46 1499.68 1506.55 1513.07 1765.74
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  <!--...or by the total number of grains
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  <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown
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  <!--Adjusts displayed energies to this values for the lowest species. -->
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Hexanal–AcOO ------> Hexanal–AcOOH

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1063.82 1080.45 1114.49 1151.85 1207.51 1248.00 1283.30 1296.40 1324.87 1354.04 1382.12 1421.37
1430.00 1473.27 1478.25 1498.62 1505.06 1512.35 1517.77 1813.82 2990.23 3044.64 3045.33 3063.37
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1081.49 1127.64 1154.57 1190.28 1219.26 1239.85 1271.52 1294.14 1323.44 1343.54 1381.22 1425.26
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1426.71 1457.98 1474.88 1499.50 1506.78 1512.86 1574.94 1873.74 3001.29 3041.58 3046.11 3054.03 3075.72 3082.65 3116.94 3121.45 3127.91 3130.63</array>
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1066.17 1072.33 1126.38 1155.25 1191.84 1227.69 1273.50 1281.67 1305.02 1378.99 1400.15 1422.01
1444.25 1468.91 1478.68 1483.01 1504.71 1509.58 1511.51 1822.04 2962.70 2979.87 3017.16 3049.36
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1426.27 1447.72 1477.50 1488.58 1497.65 1506.64 1509.88 1871.60 3006.72 3049.45 3050.43 3063.66
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1097.69 1120.71 1134.00 1170.81 1210.45 1231.63 1272.14 1322.82 1361.80 1373.11 1393.38 1404.49
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1103.44 1122.98 1145.37 1174.10 1183.67 1236.42 1270.30 1327.71 1341.97 1374.79 1402.92 1407.05
1427.44 1465.71 1499.90 1501.65 1512.82 1517.69 1768.73 1913.28 3032.52 3041.92 3051.44 3059.58
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  <!--...or by the total number of grains
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  <!--Specify increased energy range
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  <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown
  <me:diagramEnergyOffset>0</me:diagramEnergyOffset>-->
  <!--Adjusts displayed energies to this values for the lowest species. -->
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Heptanal–AcOO ------> Heptanal–AcOOH


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398.13 424.62 439.52 487.33 561.27 644.72 747.16 783.50 822.81 846.91 901.07 924.04 952.63 986.50
1012.21 1040.14 1068.59 1115.12 1117.26 1157.97 1185.33 1248.53 1263.27 1282.45 1326.26 1337.08
1341.48 1364.51 1404.04 1421.07 1423.07 1471.07 1486.44 1496.67 1503.14 1507.21 1515.43 1526.40
1817.45 3004.54 3034.19 3042.33 3045.82 3059.82 3062.46 3080.45 3094.87 3113.98 3122.10 3125.40
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1003.58 1035.86 1059.92 1066.17 1110.82 1128.68 1147.55 1180.62 1222.45 1230.49 1252.85 1278.72
1314.97 1325.44 1342.05 1385.03 1398.34 1424.16 1429.23 1459.40 1475.18 1496.21 1499.42 1509.42
1518.76 1583.56 1875.09 3010.41 3038.04 3045.60 3047.31 3063.72 3076.64 3078.10 3088.19 3118.13
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1024.87 1041.42 1055.47 1090.40 1128.29 1149.60 1196.96 1216.44 1257.61 1287.41 1293.09 1336.16
1359.90 1380.57 1393.51 1423.07 1433.83 1477.51 1485.19 1488.62 1501.23 1503.49 1512.42 1520.30
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1021.70 1049.68 1083.30 1096.10 1108.44 1123.23 1133.26 1159.97 1173.07 1237.40 1265.28 1286.53
1304.37 1332.81 1382.58 1394.10 1398.04 1410.38 1419.06 1447.77 1482.75 1490.22 1493.52 1497.55
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1033.20 1044.90 1077.91 1081.10 1091.06 1142.24 1152.73 1228.63 1249.61 1268.85 1284.78 1330.16
1330.38 1344.56 1350.82 1385.00 1419.33 1421.75 1430.53 1452.60 1493.85 1494.33 1501.19 1505.86
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1001.84 1038.05 1049.47 1088.29 1107.59 1122.65 1160.41 1192.65 1237.36 1250.23 1302.68 1331.23
1346.60 1364.70 1389.76 1418.56 1422.44 1463.79 1489.13 1495.39 1500.62 1503.98 1506.79 1515.29
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411.63 490.44 519.79 542.63 645.51 691.88 739.00 778.13 803.11 856.91 890.30 925.08 956.59
1003.80 1017.64 1024.16 1086.33 1111.04 1129.95 1145.18 1175.99 1182.54 1224.52 1263.24 1312.45
1323.83 1349.36 1360.65 1389.95 1392.36 1422.89 1428.23 1463.31 1494.46 1497.91 1509.67 1512.14
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981.39 993.90 1034.18 1079.55 1091.31 1112.67 1135.29 1160.84 1211.79 1225.56 1283.96 1303.25
1337.14 1347.90 1380.00 1393.05 1394.90 1420.30 1470.52 1472.62 1488.69 1496.35 1498.90 1508.58
1514.10 1822.26 2965.90 3030.46 3036.19 3044.13 3056.77 3070.49 3088.82 3091.67 3108.00 3145.03
3153.16 3258.90 3555.44</array>
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1002.82 1045.50 1063.94 1074.31 1105.24 1122.19 1134.69 1140.72 1183.90 1216.79 1244.82 1266.04
1302.91 1326.48 1348.60 1374.14 1395.86 1406.79 1419.43 1453.79 1471.31 1472.33 1480.84 1493.91
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    <!--...or by the total number of grains
       <me:numberOfGrains> 500 </me:numberOfGrains>-->
    <!--Specify increased energy range
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    <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
  </me:modelParameters>
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    <!--<me:testMicroRates />
          <me:testDOS />
    <me:testRateConstant />
    <me:printGrainDOS />-->
    <!--<me:printCellDOS />-->
    <!--<me:printReactionOperatorColumnSums />-->
    <!--<me:printTunnellingCoefficients />
    <me:printGrainkfE />-->
    <!--<me:printGrainBoltzmann />
    <me:printGrainkbE />-->
    <me:eigenvalues>3</me:eigenvalues>
    <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown
    <me:diagramEnergyOffset>0</me:diagramEnergyOffset>-->
    <!--Adjusts displayed energies to this values for the lowest species. -->
    <me:calcMethod  name="simpleCalc" />
    <me:ForceMacroDetailedBalance >true</me:ForceMacroDetailedBalance>
  </me:control>
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    <dc:date>20220118_122459</dc:date>
    <dc:contributor>ndprse</dc:contributor>
  </metadataList>
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Octanal–AcOO ------> Octanal–AcOOH

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<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
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xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
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1403.78 1426.38 1436.98 1468.52 1476.97 1488.06 1496.46 1499.38 1507.38 1515.77 1522.51
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846.25 912.60 933.65 1018.98 1025.86 1049.17 1060.61 1078.70 1090.42 1093.76 1142.21
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1517.91 1921.74 3020.46 3022.46 3029.65 3037.26 3041.93 3044.75 3053.36 3059.15 3069.23
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838.19 889.50 912.97 941.32 962.51 993.22 1009.54 1017.82 1046.97 1090.39 1101.14 1129.05
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1397.89 1416.69 1424.43 1476.87 1485.12 1488.03 1489.90 1496.35 1499.52 1508.47 1540.25
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888.58 892.71 950.37 970.28 1000.52 1045.09 1060.79 1082.76 1094.65 1119.15 1129.87
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841.35 868.93 905.83 933.28 970.17 996.48 1019.22 1059.68 1075.93 1089.99 1116.54 1127.67
1160.32 1191.65 1232.53 1245.06 1283.60 1308.19 1334.44 1348.88 1357.41 1387.14 1392.05
1421.68 1426.51 1464.49 1489.41 1494.89 1496.34 1503.86 1505.48 1506.34 1516.21 1522.78
1746.96 3021.03 3028.09 3035.04 3036.01 3042.02 3047.10 3060.58 3067.46 3086.49 3092.38
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858.46 882.74 930.68 958.46 1016.90 1021.13 1042.55 1056.37 1080.25 1119.30 1134.89
1149.69 1170.79 1184.52 1218.46 1254.64 1298.97 1314.59 1335.95 1338.55 1349.38 1360.65
1401.53 1413.71 1421.57 1424.25 1467.78 1492.43 1498.86 1503.19 1505.49 1506.62 1516.80
1766.20 1912.45 3027.16 3030.47 3037.18 3039.79 3042.30 3050.98 3060.31 3074.78 3079.32
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  <!--Specify increased energy range
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Nonanal–AcOO ------> Nonanal–AcOOH

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844.49 873.57 912.43 952.00 970.60 990.45 1023.33 1048.92 1058.42 1061.12 1084.65 1095.97
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1388.50 1394.14 1416.10 1419.58 1437.64 1480.39 1485.07 1492.06 1493.60 1500.18 1501.77 1502.79
1506.65 1512.30 1817.90 2962.38 3023.26 3035.65 3038.87 3043.53 3061.54 3065.13 3068.53 3074.55
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1386.34 1394.52 1406.36 1417.06 1426.11 1428.61 1452.22 1476.65 1479.57 1491.36 1503.10 1504.14
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852.15 892.00 913.16 927.55 985.50 999.76 1018.02 1047.29 1070.81 1088.26 1091.41 1118.32
1130.89 1159.82 1189.50 1227.47 1240.98 1269.35 1289.50 1317.79 1342.67 1344.53 1349.33 1367.62
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     <me:numberOfGrains> 500 </me:numberOfGrains>-->
  <!--Specify increased energy range
     <me:maxTemperature>6000</me:maxTemperature>-->
  <me:energyAboveTheTopHill>25.0</me:energyAboveTheTopHill>
</me:modelParameters>
<me:control>
  <me:printSpeciesProfile />
  <!--<me:testMicroRates />-->
  <!--<me:testRateConstant />
  <me:printGrainDOS />
  <me:printCellDOS />
        <me:testDOS />-->
  <!--<me:printReactionOperatorColumnSums />-->
  <!--<me:printTunnellingCoefficients />
  <me:printGrainkfE />-->
  <!--<me:printGrainBoltzmann />
  <me:printGrainkbE />-->
  <me:eigenvalues>3</me:eigenvalues>
  <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown
  <me:diagramEnergyOffset>0</me:diagramEnergyOffset>-->
  <!--Adjusts displayed energies to this values for the lowest species. -->
  <me:calcMethod  name="simpleCalc" />
  <me:ForceMacroDetailedBalance >true</me:ForceMacroDetailedBalance>
</me:control>
```

```
  <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
    <dc:title>Project name</dc:title>
    <dc:source>Acylperoxyrad-Nonanal.xml</dc:source>
    <dc:creator>Mesmer v6.0</dc:creator>
    <dc:date>20220515_210950</dc:date>
    <dc:contributor>ndprse</dc:contributor>
  </metadataList>
</me:mesmer>
```