

Supporting Information

1 **Formation of Low-volatile Products and Unexpected High**
2 **Formaldehyde Yield from the Atmospheric Oxidation of**
3 **Methylsiloxanes**

4 Zihao Fu[†], Hong-Bin Xie^{†*}, Jonas Elm[§], Xirui Guo[†], Zhiqiang Fu^{†,‡}, Jingwen Chen[†]

5 [†]Key Laboratory of Industrial Ecology and Environmental Engineering (Ministry of
6 Education), School of Environmental Science and Technology, Dalian University of
7 Technology, Dalian 116024, China

8 [§]Department of Chemistry and iClimate, Aarhus University, Langelandsgade 140, DK-
9 8000 Aarhus C, Denmark

10 [‡]Division of Analytical and Environmental Toxicology, Department of Laboratory
11 Medicine and Pathology, University of Alberta, Edmonton, Alberta T6G2R3, Canada

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29 **(1) Computational details for CBS-QB3 scheme**

30 The CBS-QB3 scheme requires three theoretical methods including CCSD(T)/6-
31 31+G(d'), MP4(SDQ)/CBSB4 and MP2/CBSB3 to perform accurate single-point
32 energy calculations.^{1,2} The total CBS-QB3 energy is calculated by:

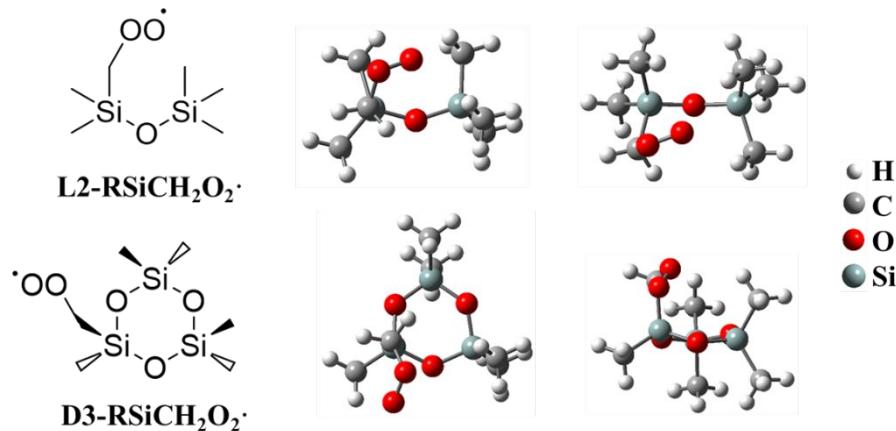
$$33 \quad E(\text{CBS-QB3}) = (E[\text{CCSD}(\text{T})/6-31+\text{G}(\text{d}')] - E[\text{MP4}(\text{SDQ})/6-31+\text{G}(\text{d}')]) \\ + (E[\text{MP4}(\text{SDQ})/\text{CBSB4}] - E[\text{MP2}/\text{CBSB4}]) \\ + E(\text{HF}) + E(\text{CBS-Int}) + \Delta E(\text{emp}) \\ + \Delta E(\text{spin}) + 0.974 \times \text{ZPE}$$

34 and the CBS-QB3 Gibbs free energy is calculated by:

$$35 \quad G(\text{CBS-QB3}) = (E[\text{CCSD}(\text{T})/6-31+\text{G}(\text{d}')] - E[\text{MP4}(\text{SDQ})/6-31+\text{G}(\text{d}')]) \\ + (E[\text{MP4}(\text{SDQ})/\text{CBSB4}] - E[\text{MP2}/\text{CBSB4}]) \\ + E(\text{HF}) + E(\text{CBS-Int}) + \Delta E(\text{emp}) \\ + \Delta E(\text{spin}) + \text{Gib}$$

36 where $E[\text{CCSD}(\text{T})/6-31+\text{G}(\text{d}')]$ and $E[\text{MP4}(\text{SDQ})/6-31+\text{G}(\text{d}')]$ are obtained from
37 CCSD(T)/6-31+G(d') single-point energy calculation; $E[\text{MP4}(\text{SDQ})/\text{CBSB4}]$ and
38 $E[\text{MP2}/\text{CBSB4}]$ are obtained from MP4(SDQ)/CBSB4 single-point energy calculation;
39 $E(\text{HF})$, the CBS interference correction $E(\text{CBS-Int})$, the empirical term
40 $\Delta E(\text{emp}) = -0.00579E(O_{ii})$ and the spin contamination correction
41 $\Delta E(\text{spin}) = -0.00953\Delta\langle S^2 \rangle$ are calculated from MP2/CBSB3 method; The zero-point
42 energy (ZPE), and Gibbs free energy correction (Gib) are obtained from M06-2X/6-
43 31+G(d,p) level of theory.

44 **(2) The global minima of L2-RSiCH₂O₂[·] and D3-RSiCH₂O₂[·]**



45

46 Figure S1. Global minima structures of L2-RSiCH₂O₂[·] and D3-RSiCH₂O₂[·] obtained at
47 CBS-QB3//M06-2X/6-31+G(d,p) level of theory.

48 **(3) The indoor NO concentration under steady-state conditions**

49 The indoor gas phase reaction



51 is very fast, as evidenced by its second-order reaction rate constant, $k = 4.43 \times 10^{-4} \text{ ppb}^{-1}$
52 $\text{s}^{-1} = 1.6 \text{ ppb}^{-1} \text{ h}^{-1}$ at 298 K.³

53 Under steady-state conditions and $[\text{O}_3 \text{ indoor}] \gg [\text{NO}_{\text{indoor}}]$, the ratio between the
54 indoor NO concentration and the outdoor NO concentration (I/O_{NO})^{3,4} can be calculated
55 by:

56
$$I/\text{O}_{\text{NO}} = \frac{[\text{NO}_{\text{indoor}}]}{[\text{NO}_{\text{outdoor}}]} = \frac{E_x}{k \times [\text{O}_3 \text{ indoor}] + E_x}$$

57 where $[\text{NO}_{\text{indoor}}]$ is the indoor NO concentration, $[\text{NO}_{\text{outdoor}}]$ is the outdoor NO
58 concentration, E_x is the air exchange rate, typically expressed in units of air changes per
59 hour (h^{-1}). The Table S1 presents the estimated indoor NO concentration under steady-
60 state conditions. As can be seen from Table S1, when the indoor O_3 concentration is
61 larger than 10 ppb, ourdoor NO concentration is 1 ppb and the air change rate (E_x) is
62 less than 1.0 h^{-1} , indoor NO concentration is less than 59 ppt. When outdoor O_3
63 concentration is elevated (>10 ppb) or outdoor NO concentration is decreased (< 1 ppb),
64 the indoor NO concentration is less than 50 ppt when there is no significant indoor

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65 source of NO.

66 Table S1. Estimated indoor NO concentration under steady-state conditions

E_x (h ⁻¹)	k (ppb ⁻¹ h ⁻¹)	[O ₃ <i>indoor</i>] (ppb)	$k \times [O_3 \text{ indoor}]$ (h ⁻¹)	I/O_{NO}	[NO _{outdoor}] (ppb)	[NO _{indoor}] (ppb)	[NO _{indoor}] (ppt)
0.3	1.6	10	16	0.018	1	0.018	18
0.5	1.6	10	16	0.030	1	0.030	30
1.0	1.6	10	16	0.059	1	0.059	59
1.5	1.6	10	16	0.086	1	0.086	86
2.0	1.6	10	16	0.111	1	0.111	111
0.3	1.6	20	32	0.009	1	0.009	9
0.5	1.6	20	32	0.015	1	0.015	15
1.0	1.6	20	32	0.030	1	0.030	30
1.5	1.6	20	32	0.045	1	0.045	45
2.0	1.6	20	32	0.059	1	0.059	59

67 **(4) Conformationally averaged unimolecular reaction rate constant**

68 To address the possible uncertainty resulting from employing the “single-
69 conformer” approximation, a conformationally averaged reaction rate constant
70 calculation was performed on the selected test pathways at CBS-QB3//M06-2X/6-
71 31+G(d,p) level of theory. The selected test pathways are the initial intramolecular Si-
72 C-O rearrangement of L2-RSiCH₂O₂[·] and D3-RSiCH₂O₂[·] to form L2-RSiOOCH₂[·] and
73 D3-RSiOOCH₂[·], respectively. These reactions are the key steps in determining the
74 competition between unimolecular and bimolecular reactions with NO/HO₂[·]. We used
75 a Boltzmann-weighted distribution⁵ to calculate the conformationally averaged reaction
76 rate constant (\bar{k})

$$77 \quad \bar{k} = \sum_i w_i k_i$$

78 where k_i represents the reaction rate constant of conformer i and w_i is the Boltzmann
79 weight of conformer i . w_i can be computed by

$$80 \quad w_i = \frac{\exp(-\Delta G_i / k_B T)}{\sum_i \exp(-\Delta G_i / k_B T)}$$

81 where ΔG_i is the relative free energy of conformer i with respect to the free energy of
82 global minimum, k_B is Boltzmann’s constant, and T is the absolute temperature (298 K
83 was used here). The ΔG_i , w_i and k_i for L2-RSiCH₂O₂[·] and D3-RSiCH₂O₂[·] reactions are

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84 shown in Table S2. The calculated conformationally averaged reaction rate constants
 85 for L2-RSiCH₂O₂[·], D3-RSiCH₂O₂[·] are 1.5×10^{-1} and 6.9×10^{-2} s⁻¹, respectively.

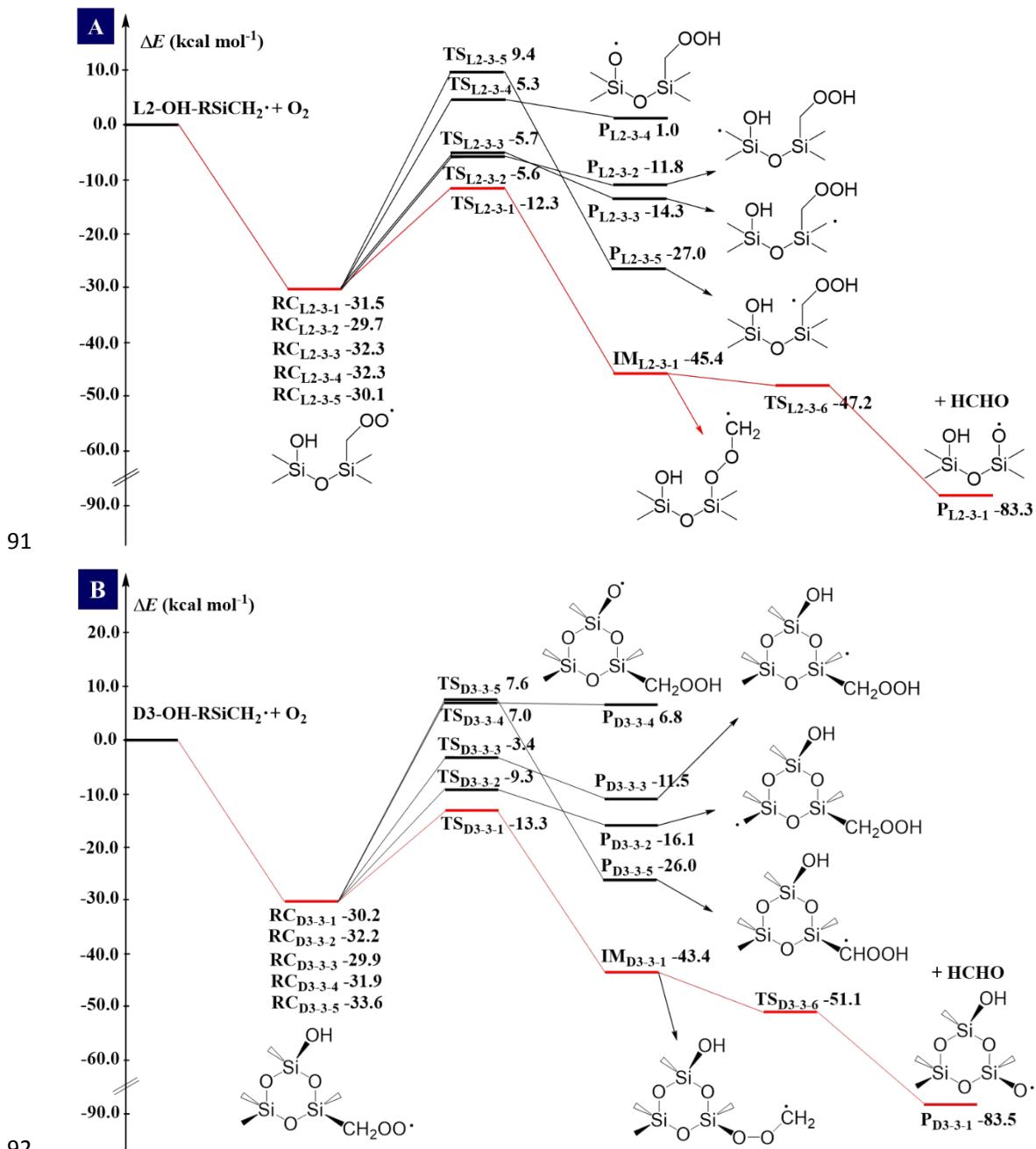
86 Table S2. The relative free energies, Boltzmann weight and conformationally averaged
 87 reaction rate constants of L2-RSiCH₂O₂[·] and D3-RSiCH₂O₂[·].

Conformer	ΔG_i (kcal mol ⁻¹)	w_i	k_i (s ⁻¹)	$\bar{k} = \sum_i w_i k_i$ (s ⁻¹)
L2-RSiCH ₂ O ₂ [·] -1	0.000	0.162	1.1×10^{-2}	1.5×10^{-1}
L2-RSiCH ₂ O ₂ [·] -2	0.003	0.161	1.0×10^{-2}	
L2-RSiCH ₂ O ₂ [·] -3	0.200	0.115	6.7×10^{-1}	
L2-RSiCH ₂ O ₂ [·] -4	0.205	0.114	1.1×10^{-2}	
L2-RSiCH ₂ O ₂ [·] -5	0.212	0.113	1.1×10^{-2}	
L2-RSiCH ₂ O ₂ [·] -6	0.213	0.113	1.6×10^{-2}	
L2-RSiCH ₂ O ₂ [·] -7	0.214	0.113	6.0×10^{-1}	
L2-RSiCH ₂ O ₂ [·] -8	0.226	0.110	1.4×10^{-2}	
D3-RSiCH ₂ O ₂ [·] -1	0.000	0.168	8.0×10^{-3}	6.9×10^{-2}
D3-RSiCH ₂ O ₂ [·] -2	0.002	0.167	7.8×10^{-3}	
D3-RSiCH ₂ O ₂ [·] -3	0.013	0.164	7.0×10^{-3}	
D3-RSiCH ₂ O ₂ [·] -4	0.018	0.163	6.9×10^{-3}	
D3-RSiCH ₂ O ₂ [·] -5	0.155	0.129	2.3×10^{-1}	
D3-RSiCH ₂ O ₂ [·] -6	0.171	0.126	2.8×10^{-1}	
D3-RSiCH ₂ O ₂ [·] -7	0.418	0.083	2.2×10^{-3}	

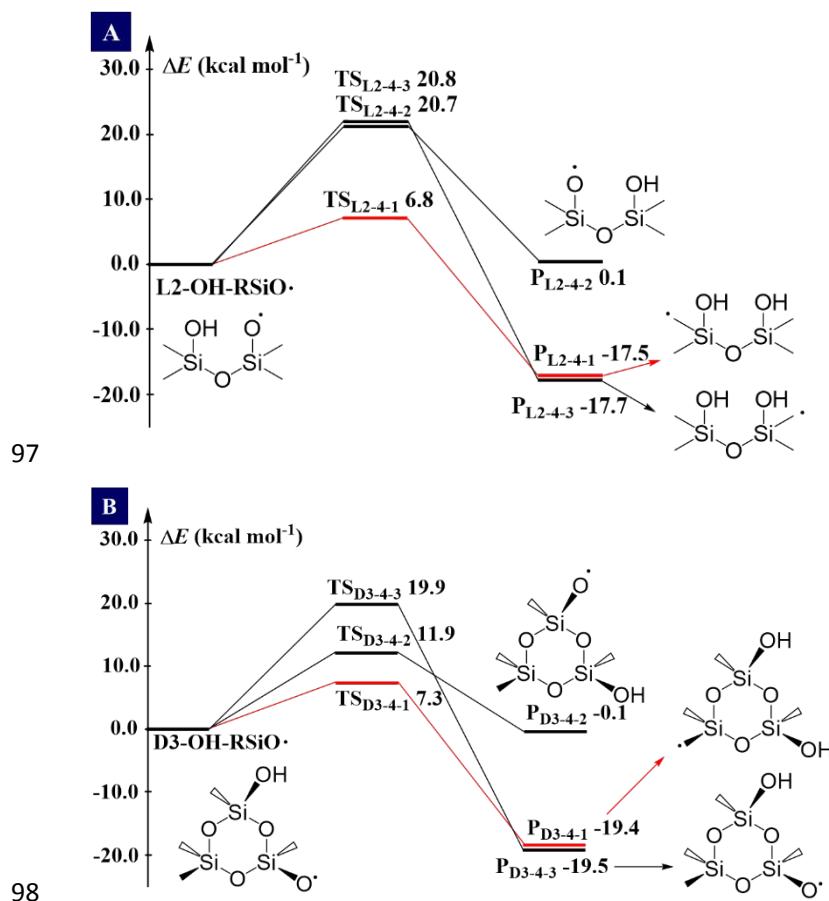
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89 (5) Calculated schematic potential energy surfaces for the chain reactions of L2-
 90 RSiCH₂O₂[·] and D3-RSiCH₂O₂[·] under low NO/HO₂[·] conditions (Figure S2 ~ S10)

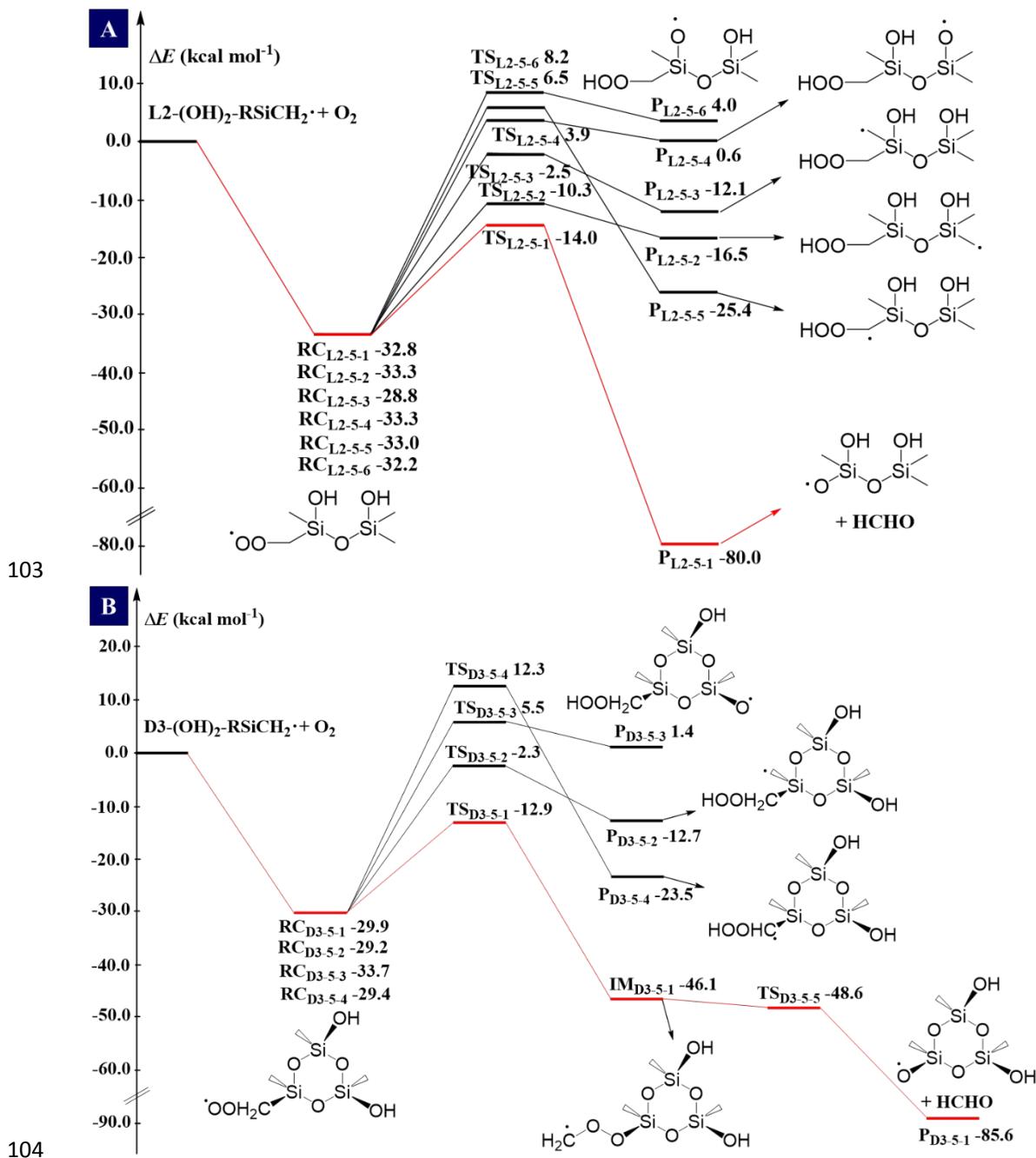


92
 93 Figure S2. The calculated schematic potential energy surfaces for unimolecular
 94 reactions of L2-OH-RSiCH₂O₂[·] (A) and D3-OH-RSiCH₂O₂[·] (B). The symbols TS_{R-3-m},
 95 IM_{R-3-m}, and P_{R-3-m} represent transition states, intermediates and products, respectively;
 96 R represents different parent compounds L2 or D3; m denotes different species.



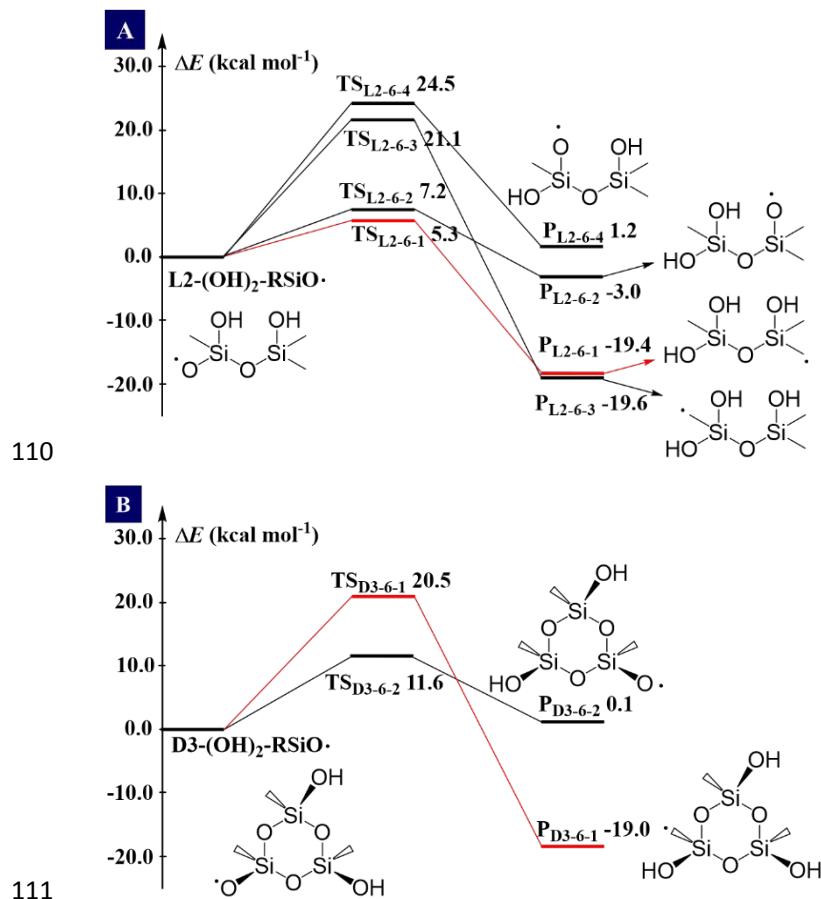
99 Figure S3. The calculated schematic potential energy surfaces for unimolecular
 100 reactions of L2-OH-RSiO[·] (A) and D3-OH-RSiO[·] (B). The symbols TS_{R-4-m} and P_{R-4-m}
 101 represent transition states and products, respectively; R represents different parent
 102 compounds L2 or D3; m denotes different species.

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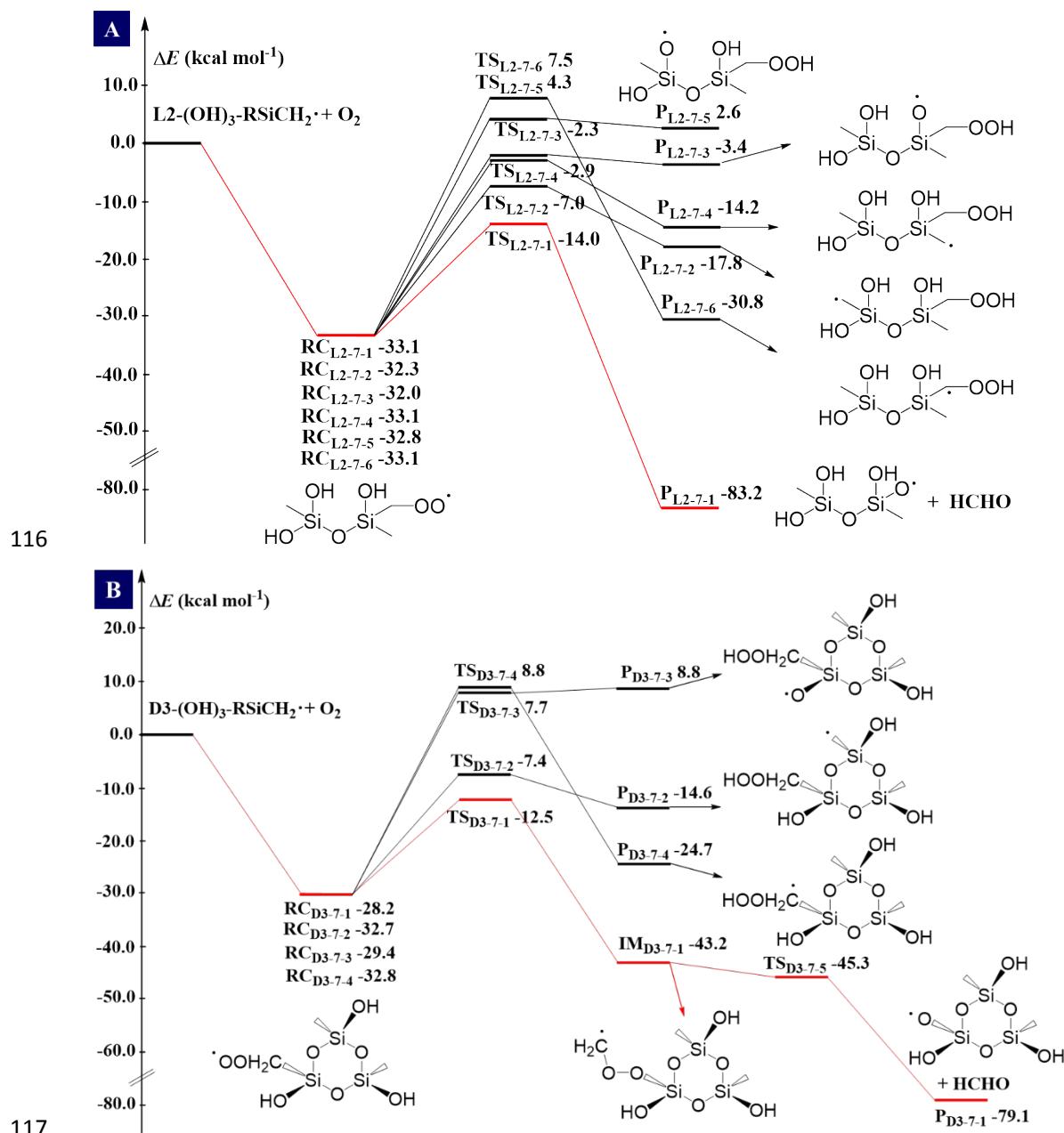
103 Figure S4. The calculated schematic potential energy surfaces for unimolecular
 104 reactions of L2-(OH)₂-RSiCH₂O₂· (A) and D3-(OH)₂-RSiCH₂O₂· (B). The symbols
 105 TS_{R-5-m}, IM_{R-5-m}, and P_{R-5-m} represent transition states, intermediates and products,
 106 respectively; R represents different parent compounds L2 or D3; m denotes different
 107 species.

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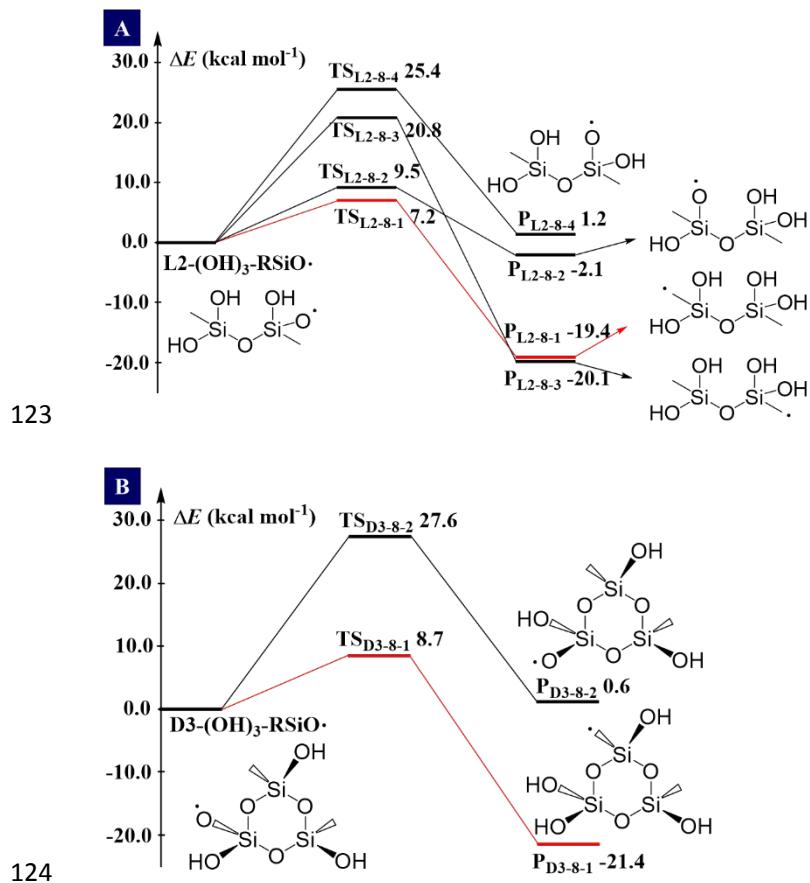
112 Figure S5. The calculated schematic potential energy surfaces for unimolecular
 113 reactions of $L_2\text{-(OH)}_2\text{-RSiO}\cdot$ (A) and $D_3\text{-(OH)}_2\text{-RSiO}\cdot$ (B). The symbols TS_{R-6-m} and
 114 P_{R-6-m} represent transition states and products, respectively; R represents different parent
 115 compounds L2 or D3; m denotes different species.

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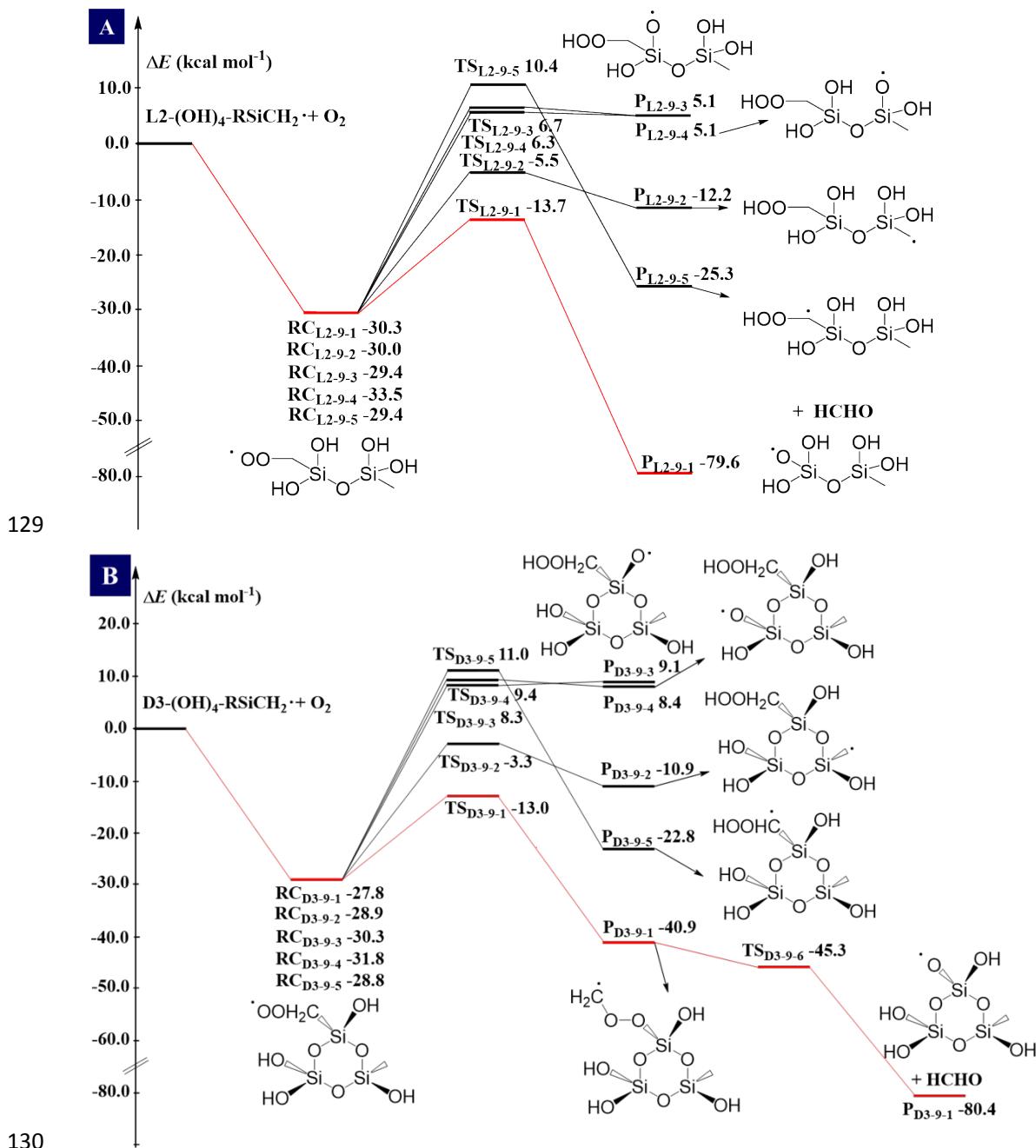
118 Figure S6. The calculated schematic potential energy surfaces for unimolecular
 119 reactions of L2-(OH)₃-RSiCH₂O₂· (A) and D3-(OH)₃-RSiCH₂O₂· (B). The symbols
 120 TS_{R-7-m}, IM_{R-7-m}, and P_{R-7-m} represent transition states, intermediates and products,
 121 respectively; R represents different parent compounds L2 or D3; m denotes different
 122 species.

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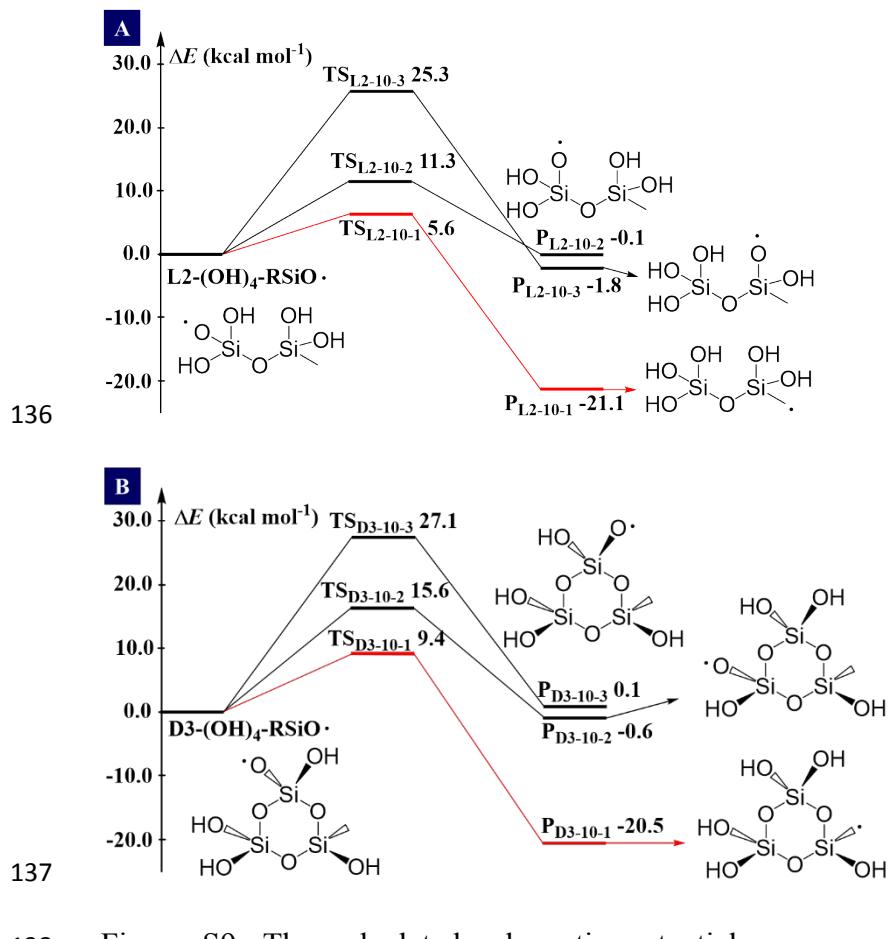


125 Figure S7. The calculated schematic potential energy surfaces for unimolecular
 126 reactions of $\text{L2}-(\text{OH})_3-\text{RSiO}\cdot$ (A) and $\text{D3}-(\text{OH})_3-\text{RSiO}\cdot$ (B). The symbols TS_{R-8-m} and
 127 P_{R-8-m} represent transition states and products, respectively; R represents different parent
 128 compounds L2 or D3; m denotes different species.

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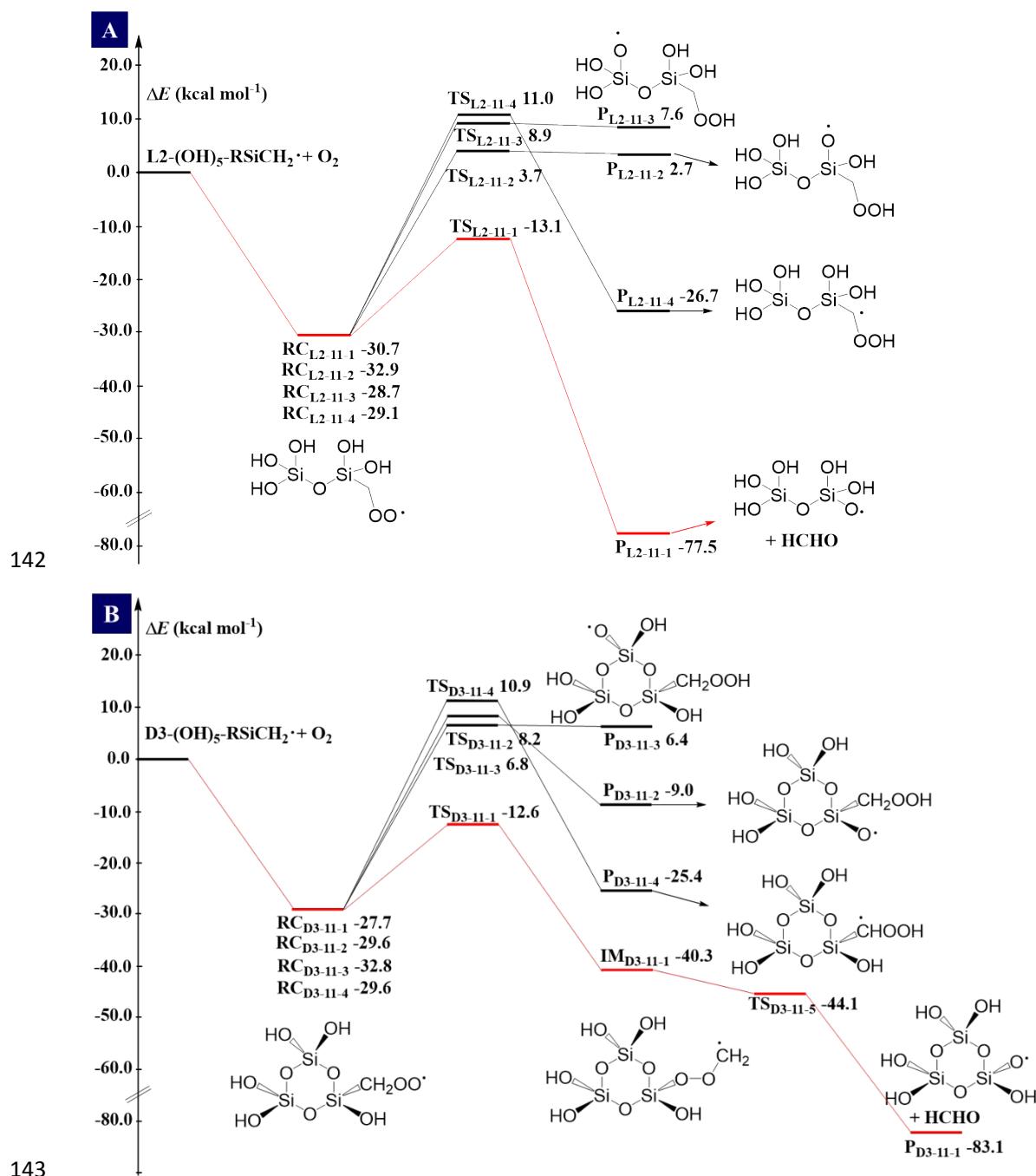


131 Figure S8. The calculated schematic potential energy surfaces for unimolecular
 132 reactions of L2-(OH)₄-RSiCH₂O₂· (A) and D3-(OH)₄-RSiCH₂O₂· (B). The symbols
 133 TS_{R-9-m}, IM_{R-9-m}, and P_{R-9-m} represent transition states, intermediates and products,
 134 respectively; R represents different parent compounds L2 or D3; m denotes different
 135 species.



138 Figure S9. The calculated schematic potential energy surfaces for unimolecular
 139 reactions of $L_2\text{-(OH)}_4\text{-RSiO}\cdot$ (A) and $D_3\text{-(OH)}_4\text{-RSiO}\cdot$ (B). The symbols TS_{R-10-m} and
 140 P_{R-10-m} represent transition states and products, respectively; R represents different
 141 parent compounds L2 or D3; m denotes different species.

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144 Figure S10. The calculated schematic potential energy surfaces for unimolecular
 145 reactions of $L2-(OH)_5-RSiCH_2O_2\cdot$ (A) and $D3-(OH)_5-RSiCH_2O_2\cdot$ (B). The symbols
 146 TS_{R-11-m} , IM_{R-11-m} , and P_{R-11-m} represent transition states, intermediates and products,
 147 respectively; R represents different parent compounds $L2$ or $D3$; m denotes different
 148 species.

149

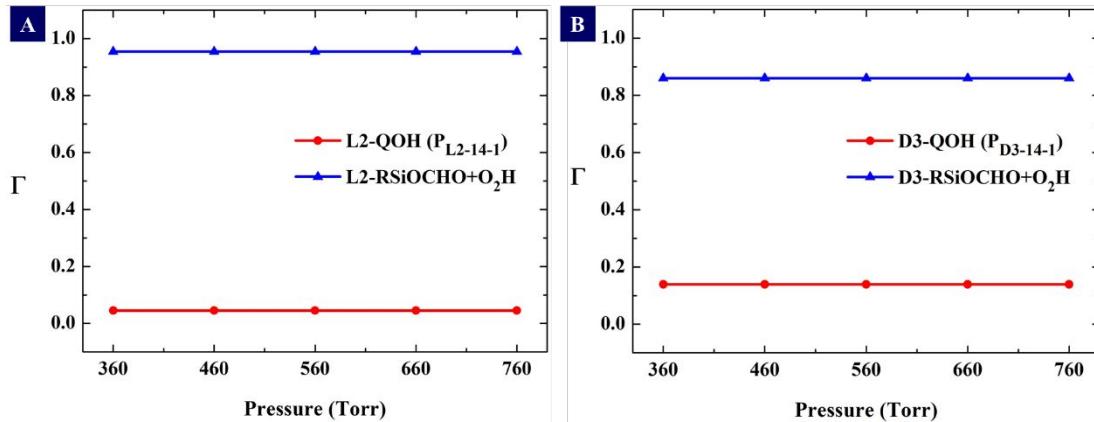
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150 **(6) Evaluation on the competition between the bimolecular reactions with O₂ and**
151 **unimolecular 1,7 H-shift reaction for both L2-RSiOCH₂O· and D3-RSiOCH₂O·.**

152 The master equation method within the MESMER program⁶ was employed to
153 perform the reaction kinetics and products branching ratio calculations for L2-
154 RSiOCH₂O· and D3-RSiOCH₂O· reactions based on the above two reaction pathways.
155 To account for the exothermic effect (-12.1 and -12.7 kcal mol⁻¹ for L2-RSiOCH₂O· and
156 D3-RSiOCH₂O·, respectively) from the reactions of corresponding peroxy radicals
157 with NO on the kinetics and product branching ratio of L2-RSiOCH₂O· and D3-
158 RSiOCH₂O· reactions, we employed a prior distribution model implemented in
159 MESMER to calculate the energy distribution of L2-RSiOCH₂O· and D3-RSiOCH₂O·
160 in the kinetics simulation. The reaction rate constants for the unimolecular 1,7 H-shift
161 reactions were calculated by Rice-Ramsperger-Kassel-Marcus (RRKM) theory,^{7,8}
162 based on the sum and density of rovibrational states from the M062X/6-31+G(d,p)
163 structures and CBS-QB3 energy barrier heights. A one-dimensional unsymmetrical
164 Eckart barrier was used to account for the tunneling correction.⁹ The bimolecular
165 reactions with O₂ are included by simply adding the pseudo-first-order rate constants
166 into the master equation calculation. The pseudo first-order rate constants with O₂ for
167 L2-RSiOCH₂O· and D3-RSiOCH₂O· are calculated to be 1.1×10^5 s⁻¹ and 2.1×10^4 s⁻¹,
168 respectively, based on the calculated high-pressure limit reaction rate constants of L2-
169 RSiOCH₂O· (2.1×10^{-14} cm³ molecules⁻¹ s⁻¹) and D3-RSiOCH₂O· (4.2×10^{-15} cm³
170 molecules⁻¹ s⁻¹) and the atmospheric concentration of O₂ (5.0×10^{18} molecules cm⁻³).
171 N₂ was employed as the buffer gas. The single exponential down model with an average
172 transfer energy of $\Delta E_d = 200$ cm⁻¹ was used to simulate the collision energy transfer
173 between active intermediates and N₂. An empirical method proposed by Gilbert and
174 Smith¹⁰ was applied to estimate the Lennard-Jones parameters of intermediates. To
175 evaluate the pressure effect, various pressures including 360, 460, 560, 660, 760 torr,
176 were set in the kinetics simulations. The variation of product branching ratios with
177 pressure for the reactions L2-RSiOCH₂O· and D3-RSiOCH₂O· were presented in
178 Figure S11. As can be seen in Figure S11, in the considered pressure range from 360

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179 torr to 760 torr, branching ratio of L2-RSiOCHO ($+\cdot\text{O}_2\text{H}$) and D3-RSiOCHO ($+\cdot\text{O}_2\text{H}$)
180 from L2-RSiOCH₂O \cdot and D3-RSiOCH₂O \cdot with O₂ are 0.95 and 0.86, respectively,
181 indicating that the bimolecular reactions with O₂ are the dominant pathway for both L2-
182 RSiOCH₂O \cdot and D3-RSiOCH₂O \cdot .



183
184 Figure S11. Variation of product branching ratios with pressure for the reactions of L2-
185 RSiOCH₂O \cdot (A) and D3-RSiOCH₂O \cdot (B). The symbols L2-RSiOCHO + ·O₂H/D3-
186 RSiOCHO + ·O₂H denote products from the bimolecular reaction with O₂ for
187 RSiOCH₂O \cdot /D3-RSiOCH₂O \cdot , and L2-QOH ($P_{\text{L}2-14-1}$)/D3-QOH ($P_{\text{D}3-14-1}$) for the
188 products from unimolecular 1,7 H-shift reactions for L2-RSiOCH₂O \cdot /D3-RSiOCH₂O \cdot .

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189 (7) Calculated branching ratios (Γ_R^i) of formaldehyde in the *i*-th Si-C-O
 190 rearrangement reaction of peroxy radicals from L2 and D3

191 The Γ_R^i ($i = 1 \sim 6$; $R = \text{L2 or D3}$) can be calculated by

$$192 \quad \Gamma_R^i = \frac{k_R^i}{k_R^i + k_{\text{NO}}[\text{NO}] + k_{\text{HO}_2^\cdot}[\text{HO}_2^\cdot]}$$

193 where k_R^i ($i = 1 \sim 6$; $R = \text{L2 or D3}$) is the unimolecular reaction rate constant (s^{-1}) of
 194 the *i*-th Si-C-O rearrangement reaction of peroxy radicals from L2 and D3, k_{NO} and
 195 $k_{\text{HO}_2^\cdot}$ are the typical reaction rate constants of peroxy radicals with NO ($9.0 \times 10^{-12} \text{ cm}^3$
 196 molecule $^{-1} \text{ s}^{-1}$)¹¹ and HO $_2^\cdot$ ($1.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$),¹¹ [NO] and [HO $_2^\cdot$] are the
 197 indoor concentration of NO and HO $_2^\cdot$, respectively. Here, [NO] = 50 ppt and [HO $_2^\cdot$] =
 198 1.6 ppt were used. It was found that the term $k_{\text{HO}_2^\cdot}[\text{HO}_2^\cdot]$ has little effect on Γ_R^i ,
 199 indicating that the Γ_R^i mainly depends on the competition between the bimolecular
 200 reaction with NO and unimolecular Si-C-O rearrangement reaction. The calculated Γ_R^i
 201 of peroxy radicals from L2 and D3 are shown in Table S3.

202 Table S3. Calculated branching ratios (Γ_R^i) of formaldehyde in the *i*-th Si-C-O
 203 rearrangement reaction of peroxy radicals from L2 and D3.

Parent compounds	L2	D3
Γ_R^1	$\Gamma_{\text{L2}}^1 = 0.49$	$\Gamma_{\text{D3}}^1 = 0.41$
Γ_R^2	$\Gamma_{\text{L2}}^2 = 0.58$	$\Gamma_{\text{D3}}^2 = 0.99$
Γ_R^3	$\Gamma_{\text{L2}}^3 = 0.55$	$\Gamma_{\text{D3}}^3 = 0.99$
Γ_R^4	$\Gamma_{\text{L2}}^4 = 0.58$	$\Gamma_{\text{D3}}^4 = 1.00$
Γ_R^5	$\Gamma_{\text{L2}}^5 = 0.95$	$\Gamma_{\text{D3}}^5 = 1.00$
Γ_R^6	$\Gamma_{\text{L2}}^6 = 0.90$	$\Gamma_{\text{D3}}^6 = 1.00$

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205 **(8) Uncertainty analysis for the model of the 8-h formaldehyde formation
206 concentration**

207 The uncertainty of the model of the 8-h formaldehyde formation concentration is
208 mainly coming from the calculated Γ_R^i . The Γ_R^i depends on the calculated reaction
209 rate constants of the Si-C-O rearrangement of peroxy radicals, and the employed NO
210 concentration (as discussed in Section (7) of SI). The 50 ppt NO concentration was used
211 when evaluating Γ_R^i . Reaction rate constants of the Si-C-O rearrangement of peroxy
212 radicals from CBS-QB3//M06-2X/6-31+G(d,p) level of theory and single-conformer
213 approximation were used in the model. As discussed in the section *Uncertainty Analysis*
214 of the *Unimolecular Reaction Rate Constants*, the reaction rate constants based on the
215 structural/energetic data from higher level computational methods are very close to
216 those at the CBS-QB3//M06-2X/6-31+G(d,p) level of theory. Therefore, the employed
217 computational method have negligible effect on the calculated 8-h formaldehyde
218 formation concentration. In addition, the conformationally averaged reaction rate
219 constants are 13.6 and 8.6 times higher than the corresponding values from the single-
220 conformer approximation for the tested Si-C-O rearrangement pathway of L2-
221 $\text{RSiCH}_2\text{O}_2\cdot$ and D3- $\text{RSiCH}_2\text{O}_2\cdot$, respectively. If such increased times in the test Si-C-
222 O rearrangement pathways were simply applied to other Si-C-O rearrangement
223 pathways in the chain reactions of peroxy radicals from L2 and D3, the calculated 8-h
224 formaldehyde formation concentration are increased to 0.31 ppb and 16.91 ppb,
225 contributing 1.1% and 62.6% to the 8-h RELs, under $[\cdot\text{OH}] = 1 \times 10^5$ and $[\cdot\text{Cl}] = 1 \times$
226 10^3 molecule cm^{-3} (corresponding to a normal indoor environment), and $[\cdot\text{OH}] = 2 \times$
227 10^6 and $[\cdot\text{Cl}] = 1 \times 10^5$ (corresponding to an indoor cleaning environment with
228 commercial bleach) conditions, respectively.

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(9) Cartesian coordinates of the transition states for all reactions

Table S4. Cartesian coordinates of the transition states for all reactions of L2-RSiCH₂O₂[·]

Species	Atoms	X	Y	Z
TS _{L2-1-1}	Si	1.773942951	-0.131028967	-0.02614475
	O	0.353225375	-0.994419745	-0.239030367
	Si	-1.258566759	-0.751433115	0.003608216
	C	3.138974992	-1.410134091	0.058372377
	H	3.17049128	-2.004086559	-0.860383211
	H	4.116973784	-0.93519052	0.18931023
	H	2.978650761	-2.095373706	0.896531395
	C	2.036161081	1.015741528	-1.48316977
	H	1.27849754	1.804627927	-1.49863998
	H	3.023125591	1.487826863	-1.429078393
	H	1.97757401	0.466503809	-2.428536811
	C	1.684863398	0.845847446	1.573089916
	H	1.465933136	0.192358837	2.424358786
	H	2.638759959	1.346371569	1.771967653
	H	0.906659549	1.61385813	1.515583884
	C	-1.814253452	-0.458076331	1.772943445
	H	-1.283293054	0.378998994	2.234430376
	H	-2.8851258	-0.224481671	1.79929668
	H	-1.657917581	-1.358487163	2.375115413
	C	-2.027314503	-2.437120679	-0.430617772
	H	-1.731192789	-2.771844626	-1.428437458
	H	-1.682378694	-3.180443052	0.296920598
	H	-3.12128256	-2.395154365	-0.382132883
	C	-2.100684898	0.145008443	-1.711562543
	H	-2.054507905	-0.259449383	-2.720843335
	H	-3.11217603	0.296946261	-1.315125102
	O	-1.328766061	1.261099436	-1.555718059
	O	-1.05870387	1.22290409	-0.207950234
TS _{L2-1-2}	Si	1.655982463	-0.30959052	-0.040204801
	O	0.14420239	-0.976154744	-0.230979337
	Si	-1.45286069	-0.582987211	-0.026751351
	C	2.813620661	-1.69525931	0.458103348
	H	2.841640344	-2.460102175	-0.325006604
	H	3.831933052	-1.324158346	0.610001674
	H	2.478462227	-2.169847927	1.385031044
	C	2.213654731	0.499861403	-1.628433793
	H	1.547894909	1.327663532	-1.889466844
	H	3.230673982	0.893689214	-1.527809835
	H	2.21192819	-0.222552224	-2.450764831

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	C	1.546915783	0.966454033	1.330297842
	H	1.251438859	0.621625456	2.324751156
	H	2.312154196	1.744042347	1.386646261
	H	0.451884962	1.705804422	0.946883857
	C	-1.894276492	-0.516582584	1.790927456
	H	-1.355121429	0.28528336	2.302337012
	H	-2.966090338	-0.327494191	1.9154353
	H	-1.661382864	-1.468105689	2.279813533
	C	-2.500224711	-1.852789882	-0.913478917
	H	-2.204202488	-1.939437298	-1.963221077
	H	-2.386215453	-2.836838169	-0.448288504
	H	-3.561795651	-1.585764589	-0.877043645
	C	-1.724902821	1.104014544	-0.880573326
	H	-1.772541145	0.962252472	-1.967341853
	H	-2.65734115	1.592497643	-0.565012088
	O	-0.63755846	2.023126787	-0.717020682
	O	-0.480647217	2.313584864	0.629676292
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TS _{L2-1-3}	Si	2.112912749	-0.222062885	-0.087165251
	O	0.594253683	0.201054931	-0.630692269
	Si	-0.869127655	0.699762674	-0.054711931
	C	3.035225665	1.338265228	0.394603287
	H	2.551283552	1.838489925	1.240196186
	H	4.0655272	1.109319463	0.687176417
	H	3.070818737	2.044144115	-0.441173455
	C	1.928176169	-1.335695344	1.414489724
	H	1.410044414	-2.26568856	1.158777369
	H	2.907512123	-1.601817217	1.826221061
	H	1.363160238	-0.837407086	2.21111867
	C	2.973094384	-1.111543601	-1.486399939
	H	3.069391952	-0.457251338	-2.358216599
	H	3.976704788	-1.435762279	-1.192712677
	H	2.403782926	-1.995089665	-1.790156624
	C	-1.955781033	1.18074546	-1.479292126
	H	-2.850264025	0.110533187	-1.336955105
	H	-2.62850168	2.033790198	-1.381930208
	H	-1.578293219	1.042145082	-2.492854773
	C	-0.66712592	2.028399535	1.251409064
	H	-0.133711736	1.63835544	2.125500951
	H	-0.100945191	2.878236262	0.85876864
	H	-1.642681521	2.392725548	1.588464523
	C	-1.784615262	-0.811028437	0.703759736
	H	-1.092433566	-1.505490862	1.192260577

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	H	-2.572874838	-0.530873977	1.41452216
	O	-2.358964218	-1.552936065	-0.374762085
	O	-3.395874413	-0.811923601	-0.909040772
TS _{L2-1-4}	Si	1.703477706	-0.194080586	-0.029861044
	O	0.298781613	-1.050075291	-0.354895273
	Si	-1.322879187	-0.884655449	-0.108683418
	C	3.117833711	-1.399289146	-0.248902239
	H	4.081786381	-0.909271695	-0.076938143
	H	3.030855271	-2.233799951	0.4536121
	H	3.121919133	-1.810243073	-1.263175203
	C	1.826791214	1.219552203	-1.253901779
	H	1.009624435	1.934625048	-1.110860905
	H	2.769654294	1.762826809	-1.129790877
	H	1.78560783	0.847434674	-2.282711925
	C	1.632183212	0.46415161	1.723108185
	H	2.560249957	0.987622947	1.977205148
	H	0.805962554	1.174596162	1.833232275
	H	1.494254046	-0.344928942	2.448119218
	C	-1.741904473	-0.986748524	1.705931443
	H	-1.278470826	-1.867759904	2.160464399
	H	-1.377384078	-0.09613998	2.227394507
	H	-2.823604096	-1.049159829	1.861887741
	C	-2.235904972	-2.122537634	-1.162055219
	H	-1.96860328	-3.141534785	-0.866367643
	H	-3.319412423	-2.011341344	-1.053882422
	H	-1.97929937	-2.003370868	-2.218744204
	C	-1.803213105	0.870626347	-0.669310642
	H	-1.954271388	1.196713737	-1.704199304
	H	-2.922447106	1.168929179	-0.037759707
	O	-1.216629464	1.875500727	0.118993065
	O	-2.541884567	2.184998855	0.650509005
TS _{L2-1-5}	C	-1.545964563	-0.327524511	1.352430151
	H	-2.629783696	-0.441230908	1.474491121
	H	-0.931036718	-0.58082594	2.227887972
	O	-1.096475244	0.603538773	0.521731839
	O	-1.099538706	2.601548419	1.356201867
	Si	-0.718803767	-1.271406741	-0.264891013
	O	0.90676019	-1.112568714	-0.17524796
	Si	1.982245724	0.174831046	-0.008684817
	C	-1.4998534	-0.778525443	-1.879306397
	H	-1.113866829	0.185331555	-2.218286699

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	H	-1.30402924	-1.536001112	-2.644607905
	H	-2.584001567	-0.684586673	-1.759523445
	C	-1.116243206	-3.066140402	0.127476843
	H	-0.698681085	-3.359613888	1.093897508
	H	-2.195450436	-3.244399382	0.137579837
	H	-0.668218282	-3.700050592	-0.646214769
	C	1.958018472	0.751886458	1.770647412
	H	1.00221588	1.234942679	1.996804823
	H	2.110059141	-0.087862358	2.456959471
	H	2.755387264	1.480715683	1.952063556
	C	1.498279159	1.55766778	-1.175540358
	H	2.216975469	2.381649365	-1.109842239
	H	1.480053812	1.21251851	-2.214841292
	H	0.509506383	1.949208438	-0.916520026
	C	3.659198585	-0.52311461	-0.462171732
	H	3.92588326	-1.352141417	0.20081752
	H	3.663608604	-0.898137858	-1.4902175
	H	4.437023195	0.242859973	-0.37668252
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TS _{L2-1-6}	Si	1.265903793	-1.839908454	1.60147942
	O	0.200275876	-2.007132021	0.318331025
	Si	-1.117926623	-1.183673654	-0.213968058
	C	2.428688038	-0.423014763	1.228200255
	H	1.858002307	0.499564372	1.08053041
	H	3.139242	-0.263665929	2.046120026
	H	2.999881151	-0.618495421	0.315164771
	C	0.274645892	-1.477985427	3.154332838
	H	-0.433294209	-2.285290479	3.369409882
	H	0.931321399	-1.365648491	4.023560014
	H	-0.288549226	-0.545428543	3.036036865
	C	2.185012758	-3.461943741	1.751032509
	H	2.727112989	-3.685312266	0.827089318
	H	2.910644498	-3.428291442	2.57023075
	H	1.492128567	-4.286811144	1.943684803
	C	-2.67491423	-1.767701494	0.630625716
	H	-2.577972949	-1.682971382	1.717926019
	H	-3.539418363	-1.176198825	0.31292763
	H	-2.873980759	-2.816697444	0.390251193
	C	-1.22843702	-1.24674715	-2.06575141
	H	-0.285464729	-0.919631174	-2.512165507
	H	-1.438885362	-2.263681584	-2.410281338
	H	-2.026322099	-0.589153891	-2.423118401
	C	-2.547663409	1.78078252	0.898917037

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	H	-2.643845541	1.214640806	1.818197565
	H	-2.710723081	2.850412057	0.836158246
	O	-1.986347847	1.199343831	-0.15083997
	O	-0.78611822	0.413598115	0.304336903
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TS _{L2-2-1}	Si	-1.751618611	0.092152221	-0.340441455
	O	-0.697274301	-1.129076905	0.100187281
	Si	0.953928369	-1.084772159	-0.079585281
	C	-2.965074976	0.362079469	1.055168876
	H	-2.437288325	0.594504399	1.985099758
	H	-3.648733613	1.187540943	0.83318941
	H	-3.563031321	-0.539104943	1.22278515
	C	-0.63890186	1.590966747	-0.617793953
	H	0.36127526	1.088286781	-1.039586384
	H	-0.93716198	2.293391525	-1.400636968
	H	-0.337509197	2.134667264	0.282245557
	C	-2.607755187	-0.373458353	-1.933987189
	H	-3.143776019	-1.321132608	-1.82445367
	H	-3.328699077	0.392417424	-2.238257523
	H	-1.873221206	-0.489739186	-2.737356568
	C	1.60528801	-2.697264139	-0.746612989
	H	1.106623526	-2.950208722	-1.685708789
	H	2.68189581	-2.639339537	-0.929761991
	H	1.421562181	-3.501650684	-0.027388718
	C	1.713879411	-0.613066753	1.557418579
	H	1.332867275	0.358328059	1.889385322
	H	1.47190772	-1.350105102	2.329304556
	H	2.802619933	-0.539184109	1.478503568
	O	1.287773237	0.07032384	-1.268098049
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TS _{L2-2-2}	Si	-1.8844616	0.155007829	0.084910939
	O	-0.549877205	-0.608940949	0.762305678
	Si	0.970923472	-0.897714654	0.223236494
	C	-3.329003952	-0.211162566	1.213486564
	H	-3.127888007	0.148353975	2.227278035
	H	-4.241870281	0.275849124	0.855424026
	H	-3.516796119	-1.287824492	1.268575833
	C	-1.525673369	1.988258615	-0.017691651
	H	-0.638874242	2.159145479	-0.637163099
	H	-2.364325804	2.533883939	-0.462629607
	H	-1.336586297	2.408587864	0.975020565
	C	-2.171794462	-0.547807188	-1.631033279

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	H	-2.314098944	-1.633060692	-1.595460358
	H	-3.065483458	-0.108611067	-2.086959761
	H	-1.321677889	-0.32897257	-2.286763903
	C	1.139771837	-2.102629145	-1.176804641
	H	1.440341986	-0.939622304	-1.703927732
	H	2.03821511	-2.704617157	-1.306383304
	H	0.270159271	-2.446198598	-1.735967217
	C	2.123623725	-1.01184159	1.669759785
	H	2.146809086	-0.059439245	2.207790609
	H	1.79202569	-1.785115853	2.368161323
	H	3.13928851	-1.245393955	1.340211805
	O	1.447854692	0.175988899	-0.991806635
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TS _{L2-3-1}	Si	-1.235674959	-0.812008964	-0.163748633
	O	0.334605918	-0.571524393	-0.628501243
	Si	1.721256161	0.069815696	0.009426493
	C	-1.246764905	-2.554949058	0.61497613
	H	-2.243149545	-2.813200111	0.991532127
	H	-0.971877953	-3.290995344	-0.148959351
	H	-0.534976846	-2.633136643	1.442876217
	C	-1.501223518	0.095335163	1.715462191
	H	-0.8647096	-0.100471529	2.57593283
	H	-2.572504397	-0.089491177	1.858199345
	C	-2.418267217	-0.979460213	-1.607151647
	H	-2.33661901	-0.125471766	-2.285049588
	H	-2.211680799	-1.899066221	-2.162629642
	H	-3.454743249	-1.028806004	-1.255126611
	C	1.749474451	1.915298333	-0.192200776
	H	1.604025493	2.187325164	-1.241769206
	H	0.949196035	2.378231127	0.391248786
	H	2.705342744	2.326502506	0.14586436
	C	3.150610913	-0.797397922	-0.817997728
	H	4.109444294	-0.432416998	-0.437709809
	H	3.102314969	-1.878922435	-0.653958702
	H	3.125602518	-0.628132386	-1.89868963
	O	1.741756554	-0.218188042	1.658675502
	H	2.018236612	-1.093996681	1.944665652
	O	-1.281591491	1.337335936	1.178745258
	O	-1.618269954	1.128922551	-0.135570214
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TS _{L2-3-2}	Si	-1.30778352	0.622840869	0.13454128
	O	0.31020459	0.809839717	0.499134025

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	Si	1.702328917	0.098457192	-0.034570448
	C	-1.773733282	1.959222488	-1.096454783
	H	-2.845438519	1.941006688	-1.320226425
	H	-1.529993178	2.948187324	-0.695834855
	H	-1.22924589	1.833564541	-2.038609071
	C	-1.553935419	-1.0227671	-0.799207562
	H	-0.810801842	-1.08727792	-1.611935992
	H	-2.547852298	-1.05693413	-1.262259073
	C	-2.325468886	0.741194211	1.69004557
	H	-2.017524548	-0.025082756	2.404869466
	H	-2.201415897	1.725086701	2.153320007
	H	-3.388954286	0.601863247	1.469967616
	C	1.684673339	-1.729881371	0.329725553
	H	0.383748173	-1.927850106	0.775268683
	H	1.741834636	-2.41881113	-0.515137429
	H	2.230855704	-2.096400753	1.200855351
	C	3.123292501	0.999816163	0.75891198
	H	4.083030204	0.593927572	0.427250614
	H	3.092169191	2.065552078	0.51087089
	H	3.068243254	0.91205708	1.848066469
	O	1.758093319	0.172847968	-1.698776101
	H	1.824912341	1.038859962	-2.111866871
	O	-1.46007869	-2.208611502	-0.002677657
	O	-0.703904686	-1.95504291	1.129972735
TS _{L2-3-3}	Si	1.327741774	-0.884774119	0.015487148
	O	-0.308170344	-1.10575733	-0.030014021
	Si	-1.637108463	-0.102255955	0.106902458
	C	2.186376102	-2.492852032	-0.380506608
	H	1.883353731	-3.271819576	0.324110355
	H	1.923526681	-2.825096718	-1.389384407
	H	3.273109864	-2.379052233	-0.324998207
	C	1.7974926	0.492610552	-1.247678816
	H	0.944333133	0.721723923	-1.899578072
	H	2.660393239	0.230496441	-1.868294407
	C	1.786124401	-0.108373927	1.647128274
	H	1.45241266	1.158269813	1.203131868
	H	1.156551753	-0.287949802	2.519620444
	H	2.835755109	0.055645889	1.898943469
	C	-1.865935728	0.311133022	1.91628503
	H	-1.056386342	0.956062442	2.276410694
	H	-2.807081271	0.847229861	2.072580965
	H	-1.880088241	-0.592753994	2.533302869

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	C	-3.089031773	-0.973178745	-0.651120219
	H	-2.902383163	-1.158464991	-1.712800774
	H	-3.269335782	-1.934681173	-0.162166852
	H	-3.994369717	-0.365541598	-0.566018664
	O	-1.385137725	1.282825769	-0.769726358
	H	-0.68746895	1.871789175	-0.448180712
	O	2.21402114	1.677825812	-0.555054089
	O	1.269364816	2.002641945	0.403563334
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TS _{L2-3-4}	Si	-1.351212626	0.832403868	0.129420336
	O	0.295684766	1.063487193	0.040066271
	Si	1.657585188	0.131858304	-0.072160936
	C	-2.215599753	2.297309981	-0.638215519
	H	-1.966585905	3.213823982	-0.094476325
	H	-1.91187479	2.43123993	-1.680480362
	H	-3.302846225	2.17344422	-0.609253496
	C	-1.64328773	-0.751200869	-0.8871617
	H	-1.268860249	-0.595316777	-1.906124182
	H	-2.671200311	-1.127131014	-0.953199776
	C	-1.851065014	0.554100576	1.907552557
	H	-1.34820499	-0.331809221	2.307994209
	H	-1.580417949	1.413043895	2.529172684
	H	-2.931111171	0.397516309	1.994188133
	C	1.851682978	-0.96866311	1.422853082
	H	1.090201654	-1.752428808	1.417898353
	H	2.839163637	-1.437780213	1.422131783
	H	1.742636983	-0.374889734	2.335983683
	C	3.098877209	1.277728511	-0.387231661
	H	2.949370291	1.833528419	-1.315963827
	H	3.168280059	1.995104514	0.436468296
	H	4.035071697	0.719274404	-0.455612542
	O	1.631919592	-0.844154914	-1.444397773
	H	0.643294224	-1.831747874	-1.48746014
	O	-0.815843455	-1.722428347	-0.227565924
	O	-0.09248578	-2.487167344	-1.147568746
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TS _{L2-3-5}	Si	1.287035393	-0.707675024	0.146100923
	O	-0.295749316	-0.954974998	0.581893276
	Si	-1.681577832	-0.053649713	0.425317354
	C	2.1563073	-2.358008411	0.116430007
	H	2.179628252	-2.792110588	1.121053713
	H	1.643599147	-3.060795292	-0.546185794

Supporting Information

	H	3.187552137	-2.243012054	-0.231288985
	C	1.270677852	0.069223424	-1.585981656
	H	0.737992109	1.254868687	-1.392557373
	H	0.760237786	-0.346139446	-2.462097916
	C	2.133075214	0.520236928	1.264985416
	H	1.617772311	1.485044381	1.246867002
	H	2.162992743	0.155259835	2.296222554
	H	3.15941208	0.691767846	0.92613328
	C	-2.67785174	-0.26203438	1.985501144
	H	-2.106303733	0.060437665	2.861884324
	H	-3.604913848	0.317342947	1.944724756
	H	-2.938752879	-1.314380868	2.132663775
	C	-2.573934724	-0.559971158	-1.124144955
	H	-1.975700585	-0.304443867	-2.004805531
	H	-2.760025911	-1.637639605	-1.137792535
	H	-3.532269552	-0.040250614	-1.212586607
	O	-1.255229108	1.543476817	0.184627803
	H	-1.052379027	2.095354449	0.945518961
	O	2.452659846	0.740400763	-1.925297138
	O	1.729230923	2.003018616	-1.773570758
TS _{L2-3-6}	Si	-1.307244427	-0.75383395	-0.06826087
	O	0.314658453	-0.875497244	-0.340227767
	Si	1.655728692	0.065344564	-0.077874309
	C	-1.609149254	-0.557550845	1.763597731
	H	-2.674367459	-0.424349155	1.975520522
	H	-1.260287457	-1.444136016	2.303803328
	H	-1.068136646	0.311434644	2.150127761
	C	-1.390504731	2.515252088	0.311573434
	H	-0.706330778	2.727225713	1.126924246
	H	-2.420707433	2.850824224	0.265392735
	C	-2.192385275	-2.208491899	-0.812177995
	H	-1.948815879	-2.296992613	-1.87418325
	H	-1.895309869	-3.135167283	-0.311527085
	H	-3.276360711	-2.098952732	-0.715585033
	C	2.074954787	1.032158536	-1.605749591
	H	2.246918639	0.357117112	-2.449552578
	H	1.253952577	1.70440139	-1.866477686
	H	2.979720396	1.62751982	-1.450757352
	C	3.028518709	-1.085718117	0.451762727
	H	3.958730525	-0.540065618	0.638898298
	H	2.759289695	-1.633919028	1.360900863
	H	3.223319889	-1.82595296	-0.330313181

Supporting Information

	O	1.346853984	1.152224192	1.160885165
	H	1.646227813	0.895875793	2.038199529
	O	-0.937782499	1.721844295	-0.63271531
	O	-1.9292145	0.582164848	-0.91058557
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TS _{L2-4-1}	Si	-1.112491345	-0.675488754	-0.023483348
	O	0.465066765	-1.142475934	0.246731919
	Si	1.753309906	-0.093238394	0.194735157
	C	-1.730574392	0.203546507	1.500197629
	H	-2.732371903	0.613563954	1.341874938
	H	-1.765766663	-0.474922566	2.358415854
	H	-1.058071188	1.029603931	1.755981681
	C	-2.153393101	-2.133449319	-0.525120995
	H	-1.716612259	-2.63067524	-1.39476545
	H	-2.211176875	-2.853788665	0.296932552
	H	-3.169908868	-1.82018659	-0.778817482
	C	1.216622977	1.34628721	-0.880083314
	H	1.739502697	1.459282995	-1.833019138
	H	0.100460944	1.079767969	-1.213087376
	H	1.156844111	2.304058287	-0.358053873
	C	3.239974429	-1.03237114	-0.409444198
	H	4.128035536	-0.394719925	-0.43477964
	H	3.447367842	-1.886060513	0.243596853
	H	3.061582254	-1.420879692	-1.416410011
	O	2.013296016	0.571706311	1.696386029
	H	2.248961683	-0.014155289	2.42165044
	O	-1.083101004	0.364092317	-1.356038667
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TS _{L2-4-2}	Si	1.353210082	0.427830047	-0.199370228
	O	-0.071183454	-0.282495463	-0.690038834
	Si	-1.581776262	-0.043956925	-0.030050255
	C	2.050550644	1.477511458	-1.574828719
	H	2.963623479	1.983324169	-1.249504126
	H	2.284999404	0.851175931	-2.441090319
	H	1.324248221	2.235049495	-1.880973387
	C	2.542877773	-0.876721698	0.403006425
	H	2.09563714	-1.452358317	1.217699608
	H	2.789151961	-1.563373604	-0.412795809
	H	3.466245138	-0.418630397	0.767588316
	C	-2.228630868	-1.643797904	0.678611963
	H	-2.338036734	-2.38766631	-0.116602557
	H	-1.535356903	-2.036005185	1.427379943

Supporting Information

	H	-3.201779053	-1.490639527	1.152851501
	C	-2.72167176	0.709428669	-1.300128285
	H	-3.704585721	0.910736253	-0.865687171
	H	-2.307527193	1.650020244	-1.67277451
	H	-2.844156557	0.025037274	-2.145275661
	O	-1.36414836	1.051863182	1.219411721
	H	-0.218991329	1.345219722	1.283366553
	O	0.945589182	1.422993196	1.086332692
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TS _{L2-4-3}	Si	1.53716159	-0.104043707	-0.051510615
	O	0.017922933	-0.737563124	-0.053880735
	Si	-1.501895753	-0.057586126	0.045966392
	C	1.763422293	1.42075407	-1.078531972
	H	2.712185388	1.675093989	-1.548418427
	H	0.888060838	1.950452505	-1.455164504
	H	1.881842754	1.834792995	0.161087148
	C	2.758631899	-1.495407476	-0.123134366
	H	2.667158251	-2.120304523	0.770236303
	H	2.5795973	-2.127749732	-0.996856891
	H	3.780576292	-1.110482504	-0.168453805
	C	-1.666923341	0.930218508	1.607215804
	H	-1.558169285	0.290636583	2.488067343
	H	-0.882045239	1.69154143	1.650903096
	H	-2.64036071	1.426635232	1.65437128
	C	-2.712210619	-1.463620558	-0.122077092
	H	-3.744042084	-1.100711695	-0.107757769
	H	-2.551024318	-2.007988004	-1.058266549
	H	-2.588284072	-2.176019296	0.699047822
	O	-1.67800598	1.03957461	-1.198828163
	H	-1.740173403	0.694481684	-2.094477844
	O	1.796421025	1.005887249	1.191529043
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TS _{L2-5-1}	Si	1.713646455	-0.209157087	-0.098866136
	O	0.250281255	-0.908836137	-0.481250151
	Si	-1.356240091	-0.639439982	-0.154109352
	C	3.065671067	-1.273208219	-0.795595584
	H	2.954512094	-1.35738175	-1.880388666
	H	4.047385636	-0.838018209	-0.587863538
	H	3.035816654	-2.278911949	-0.366517438
	C	1.791003374	-0.019516787	1.76048389
	H	1.713557246	-0.989726601	2.26195488
	H	2.730960691	0.449220243	2.066841944

Supporting Information

	H	0.969252329	0.612102794	2.116980399
	C	-1.782237191	-0.889531578	1.653363973
	H	-1.80301228	0.050093081	2.209773829
	H	-2.756606633	-1.377723575	1.732406779
	H	-1.028010376	-1.544155475	2.101840715
	C	-2.837733932	0.689572832	-0.724905625
	H	-2.623659869	0.742848394	-1.798287787
	H	-3.895640463	0.628608403	-0.478655443
	O	-2.21148153	1.7239039	-0.055507477
	O	-0.928507486	1.286583143	-0.00662309
	O	1.847483332	1.269415791	-0.841537129
	H	1.138758411	1.897970088	-0.660991888
	O	-2.020203964	-1.85557293	-1.092673579
	H	-1.37135151	-2.47039647	-1.452067845
TS _{L2-5-2}	Si	-1.222562448	0.691877657	-0.057420293
	O	0.414776196	0.892623775	-0.112438092
	Si	1.771511895	-0.057639361	-0.045838733
	C	-2.057522281	2.257348796	-0.586416852
	H	-3.140282813	2.122024655	-0.658694126
	H	-1.86633665	3.038550729	0.155505675
	H	-1.677548776	2.602910021	-1.55131976
	C	-1.595915282	-0.777183494	-1.213659715
	H	-1.440333086	-0.493570341	-2.261167312
	H	-2.620770737	-1.156140521	-1.11238528
	C	1.427819349	-1.342021568	1.274814411
	H	0.297728619	-1.888512422	0.761594001
	H	2.079204652	-2.21517315	1.347922312
	H	1.103776373	-0.987252159	2.256192577
	C	3.245304485	1.013172979	0.296347134
	H	4.154019461	0.411510534	0.3801111
	H	3.377783917	1.721324004	-0.527214773
	H	3.110828745	1.580032509	1.221190361
	O	2.041522535	-0.82701376	-1.484697905
	H	1.363036102	-1.466128025	-1.738890107
	O	-0.679558007	-1.871417698	-1.024579478
	O	-0.715717092	-2.283699057	0.303084521
	O	-1.754482709	0.321617484	1.466167155
	H	-1.72512338	-0.614915709	1.695035248
TS _{L2-5-3}	Si	1.265743069	-0.854572915	0.359726412
	O	-0.033000407	0.14989135	0.528178544

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	Si	-1.556636359	0.116376384	-0.152330553
	C	1.383603463	-1.629759866	-1.315132155
	H	1.681737476	-2.67532503	-1.394505286
	H	0.691909246	-1.302039436	-2.092693859
	H	2.560021251	-0.974223898	-1.664929379
	C	2.840758653	0.210154231	0.53655761
	H	3.248815013	0.211639909	1.552592264
	H	2.688397265	1.245595922	0.209873
	C	-2.554728279	1.422270978	0.720752049
	H	-2.070970048	2.400985757	0.639838272
	H	-3.559167388	1.499480326	0.294694538
	H	-2.651046937	1.188039252	1.785069812
	C	-2.248178988	-1.604657029	-0.045507871
	H	-3.233691264	-1.663331361	-0.515990127
	H	-1.585002959	-2.306185191	-0.56345937
	H	-2.337167811	-1.932182274	0.994310926
	O	-1.430555665	0.433616524	-1.781832535
	H	-1.166157219	1.315436456	-2.060053379
	O	3.856693359	-0.40307091	-0.266463123
	O	3.490237157	-0.283080112	-1.594469587
	O	1.23081209	-2.074911884	1.47813536
	H	1.21338451	-1.848221596	2.412478658
TS _{L2-5-4}	Si	1.371948516	-0.515753012	-0.001242359
	O	-0.198916537	-0.871194577	-0.388279679
	Si	-1.674674969	-0.286553902	0.077626383
	C	2.400763669	-2.052123243	-0.111988523
	H	3.463247207	-1.826606892	0.016317666
	H	2.108325817	-2.750531931	0.677725724
	H	2.260995916	-2.548944041	-1.075971675
	C	1.932696382	0.831009134	-1.220848811
	H	2.107394795	0.419575359	-2.220860406
	H	2.860933243	1.316947569	-0.886724683
	C	-1.914913407	-0.585035916	1.900512253
	H	-1.074848751	-0.175180332	2.468007434
	H	-2.841082785	-0.120825209	2.250321741
	H	-1.96317977	-1.659142707	2.105453284
	C	-3.016079461	-1.01140718	-0.996468113
	H	-3.99625393	-0.611978272	-0.725149724
	H	-2.823538706	-0.790980886	-2.04882798
	H	-3.030798427	-2.097755958	-0.862141545
	O	-1.752965013	1.364543441	-0.256137429
	H	-0.575049219	2.104086827	-0.317432461

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	O	0.928396608	1.823998743	-1.432818361
	O	0.447443047	2.254117492	-0.189620386
	O	1.489000925	0.078959695	1.542419077
	H	1.2966602	1.022713548	1.610904024
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TS _{L2-5-5}	Si	1.392675767	-0.750139467	0.031778903
	O	-0.151941286	-0.873868799	-0.476912664
	Si	-1.660717704	-0.198220856	-0.208988094
	C	2.511089591	-1.977842457	-0.775312942
	H	3.543665756	-1.844903762	-0.440791345
	H	2.198226147	-2.992153235	-0.512087842
	H	2.477667153	-1.880558978	-1.863725022
	C	1.916584455	1.03305099	-0.384171414
	H	1.502023981	1.282711214	-1.613254579
	H	2.937728524	1.424739421	-0.338797412
	C	-1.696725409	0.40557953	1.563447397
	H	-0.937405155	1.179371688	1.725029467
	H	-2.668370825	0.853046506	1.794242824
	H	-1.536562237	-0.41780602	2.26889522
	C	-2.949377361	-1.489144694	-0.551677103
	H	-3.952837785	-1.063022847	-0.460934046
	H	-2.835550422	-1.873288656	-1.569317384
	H	-2.865518977	-2.327678875	0.14573482
	O	-1.900719075	1.029402552	-1.281978306
	H	-1.166695311	1.64677947	-1.412427602
	O	0.970015651	1.991778081	0.016869106
	O	0.735726548	2.299474245	-1.393222608
	O	1.533220858	-0.93360506	1.670082067
	H	0.945959114	-0.425420602	2.240099977
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TS _{L2-5-6}	Si	0.813736386	0.558267527	0.378366232
	O	-0.792993716	0.558587886	0.653623974
	Si	-2.230801353	0.145186104	-0.105582508
	C	1.733950578	1.153509553	1.882006397
	H	1.474532567	2.194862392	2.090161667
	H	1.452448336	0.553459359	2.751706991
	H	2.814131242	1.088152321	1.733182428
	C	1.328118242	-1.223100944	-0.147844667
	H	1.029952194	-1.913415828	0.650549804
	H	2.411416766	-1.327514198	-0.309089918
	C	-2.534687542	-1.657071031	0.269026136
	H	-2.515172218	-1.844958427	1.347883489

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	H	-3.508627356	-1.97705562	-0.113265929
	H	-1.764047283	-2.274485964	-0.203861095
	C	-2.152828497	0.545067918	-1.911308203
	H	-3.101792548	0.301321308	-2.398359803
	H	-1.958770583	1.611986848	-2.055110618
	H	-1.351657246	-0.019213286	-2.398717427
	O	-3.416810778	1.102186377	0.552446906
	H	-3.530533521	1.089669605	1.506873149
	O	0.603511956	-1.665252089	-1.275876129
	O	0.913234362	-0.878075476	-2.421062346
	O	1.315824995	1.401978373	-0.964365862
	H	1.60259742	-0.244976508	-2.14651755
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TS _{L2-6-1}	Si	-1.195189478	-0.572367924	0.294685564
	O	0.414819789	-0.878212182	0.510896239
	Si	1.721462108	0.067233988	0.098302142
	C	-2.098521012	-0.339810516	1.888806932
	H	-3.137546075	-0.054387519	1.706875288
	H	-2.094254817	-1.274557846	2.456297176
	H	-1.621833158	0.438852471	2.48947013
	C	1.128670905	0.962869683	-1.43969086
	H	1.179201941	0.387422136	-2.368028449
	H	-0.029013629	1.095713537	-1.208584084
	H	1.500593636	1.977122686	-1.603773984
	O	-1.281162671	0.850308825	-0.609856608
	O	-1.919033396	-1.830971759	-0.48386493
	H	-1.675639469	-2.01832453	-1.394812566
	C	2.177678557	1.244205704	1.456090223
	H	2.380764491	0.700121406	2.382470521
	H	3.072596404	1.81490634	1.191553256
	H	1.361497119	1.950715714	1.638578067
	O	3.023354329	-0.917836769	-0.16624989
	H	2.868502617	-1.774141024	-0.575629276
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TS _{L2-6-2}	Si	1.370448921	0.169308602	0.122635895
	O	0.053788384	0.031149163	-0.87464449
	Si	-1.47412998	-0.042424814	-0.21084389
	C	2.549031873	1.494933549	-0.380241437
	H	3.350138333	1.594403827	0.356019737
	H	2.998599193	1.240500147	-1.343825111
	H	2.034663356	2.453941338	-0.473785983
	C	-2.258762536	1.642228232	-0.25092831

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	H	-1.645854222	2.355225779	0.309249393
	H	-2.352996124	2.006151133	-1.278492887
	H	-3.255566829	1.621691788	0.19943984
	O	0.698940417	0.580015442	1.617866867
	O	2.205428513	-1.245544167	0.193779389
	H	1.741649512	-2.04232491	0.46930668
	C	-2.499311005	-1.371853549	-1.007852935
	H	-1.97636387	-2.331021467	-0.978324118
	H	-3.458989821	-1.483492179	-0.495500071
	H	-2.697298596	-1.118157154	-2.053671283
	O	-1.186469656	-0.549424788	1.382739968
	H	-0.289559061	0.012008208	1.875977017
TS _{L2-6-3}	Si	1.538076688	-0.100053161	-0.152870827
	O	0.039690288	-0.365119022	-0.747596922
	Si	-1.49126569	-0.033609798	-0.150531335
	C	2.14775291	1.62454636	0.044425424
	H	3.205787571	1.859678813	-0.057933761
	H	1.474328989	2.478513538	-0.010742689
	H	2.01852883	1.162924968	1.267300883
	C	-1.883756491	-1.334652785	1.122033722
	H	-1.825196941	-2.340471616	0.693839627
	H	-1.16213841	-1.276079719	1.943869043
	H	-2.88768581	-1.196813336	1.533907456
	O	1.581157704	-0.070905926	1.519563
	O	2.566228701	-1.157864484	-0.864634892
	H	2.185599303	-1.818550054	-1.450639356
	C	-1.548301533	1.698403263	0.521993371
	H	-1.289321705	2.420343301	-0.258507037
	H	-2.553403595	1.939220725	0.88044747
	H	-0.852317801	1.815094512	1.359360584
	O	-2.539968266	-0.068502132	-1.432847629
	H	-2.589329892	-0.866749049	-1.966087662
TS _{L2-6-4}	Si	1.469156893	0.092308755	0.081120091
	O	0.078581886	0.817718486	0.496693995
	Si	-1.509277047	0.284298871	0.279650605
	C	2.872556242	1.280472891	0.063942514
	H	3.800777441	0.77004047	-0.200304954
	H	2.685871904	2.078856435	-0.658782053
	H	2.989113621	1.740842714	1.048802741
	C	-1.806460834	-1.074688693	1.518358471

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	H	-1.079968159	-1.882715973	1.382853514
	H	-1.702158565	-0.701351499	2.541866542
	H	-2.810820522	-1.493255713	1.405360054
	O	1.752226043	-1.41613338	0.780318476
	O	1.29824895	-0.974897299	-1.22157655
	H	1.577359013	-1.794250222	-0.360549746
	C	-2.636650598	1.742641446	0.46915507
	H	-2.364442703	2.52792633	-0.241187822
	H	-3.67355461	1.453054793	0.275511163
	H	-2.57770548	2.154910492	1.48049335
	O	-1.647454402	-0.260868795	-1.278077937
	H	-0.945595715	-0.83989556	-1.603197765
TS _{L2-7-1}	Si	1.664066843	0.015772515	-0.362710763
	O	0.133670058	-0.366819768	-0.84272194
	Si	-1.240083102	-0.728124325	0.051010248
	C	-2.198515051	-1.789962448	-1.134131321
	H	-1.534135508	-2.513629898	-1.612161319
	H	-3.018480053	-2.310703189	-0.632851782
	H	-2.631360627	-1.164225639	-1.92195315
	O	1.515356583	1.488511786	0.409793341
	H	2.192702273	1.690250521	1.062710352
	O	-0.52676889	-1.432578846	1.392874454
	H	-1.129298097	-1.651411613	2.112051984
	O	2.252869833	-1.106415181	0.692766556
	H	1.570869247	-1.484691007	1.267442134
	C	2.792904896	0.119636867	-1.822081595
	H	3.815630069	0.341508483	-1.503950018
	H	2.804414798	-0.829014974	-2.364895626
	H	2.466178236	0.908259667	-2.50486921
	C	-1.597621644	1.283757439	0.475936308
	H	-0.824016139	1.986501903	0.774578409
	H	-2.140469016	1.507800714	-0.451041281
	O	-2.440367138	0.922460449	1.483842353
	O	-2.862461483	-0.325552587	1.067930406
TS _{L2-7-2}	Si	-1.987589708	-0.127684039	0.221679002
	O	-0.645710941	0.469137327	-0.528789382
	Si	0.954413212	0.536095962	-0.083276056
	C	1.779553196	1.988034409	-0.889286051
	H	1.646506545	1.967163818	-1.974517677
	H	1.352435869	2.919502344	-0.507088427

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	H	2.851629319	1.997132124	-0.671163808
	O	-1.91788508	0.100810465	1.854304113
	H	-2.127388616	0.976377199	2.195214318
	O	1.089034485	0.740722044	1.549626026
	H	0.615378327	0.09706305	2.09250072
	O	-3.287299169	0.681852544	-0.385531746
	H	-3.158441445	1.157376707	-1.211798352
	C	-2.009652405	-1.959175693	0.020948796
	H	-2.635286066	-2.554894525	0.685356914
	H	-1.911132342	-2.385247653	-0.978426687
	H	-0.740679103	-2.186212493	0.483364241
	C	1.790221304	-1.068101316	-0.664719011
	H	1.966003983	-1.036932736	-1.746336185
	H	2.766095354	-1.17650281	-0.169921745
	O	1.03300133	-2.265572953	-0.465083811
	O	0.387526781	-2.207968564	0.763011848
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TS _{L2-7-3}	Si	-1.610284561	-0.259046024	-0.142837374
	O	-0.517936079	0.961964512	-0.512379551
	Si	0.965182958	1.177464702	0.164105243
	O	-1.022559511	-0.995987052	1.222380061
	H	-0.482941439	-0.41683598	1.792654498
	O	1.204677684	0.582591503	1.590442094
	H	1.02762493	-1.688974208	1.07947897
	C	2.034534108	-0.349403009	-0.91554082
	H	1.940387609	-0.006451461	-1.948931973
	H	3.024589735	-0.384986019	-0.461282974
	O	1.301153083	-1.477173554	-0.75413861
	O	1.656735955	-2.112691446	0.451956248
	O	-1.667431946	-1.372358016	-1.348987019
	H	-0.907399381	-1.960127204	-1.427123705
	C	-3.293110006	0.476161186	0.030980046
	H	-3.306649136	1.243721029	0.809084931
	H	-3.604846472	0.933727433	-0.911819967
	H	-4.018416437	-0.298014103	0.293876921
	C	1.7432319	2.743834385	-0.459426847
	H	1.245776167	3.594824492	0.015597475
	H	2.803492566	2.777316662	-0.200327175
	H	1.620360702	2.837443111	-1.541010921
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TS _{L2-7-4}	Si	-2.020746664	-0.126254116	0.000656519
	O	-0.798644811	0.811253243	-0.616273624

Supporting Information

	Si	0.776298682	0.672084396	-0.162009871
	C	1.830649731	2.106723465	-0.665137178
	H	2.120458127	2.84746	0.079817487
	H	2.971379154	1.318641538	-0.850234031
	H	1.725143788	2.514715851	-1.671152433
	O	-1.408870962	-1.664412726	-0.182280415
	H	-1.755294342	-2.3529949	0.392604929
	O	0.691542471	0.499681121	1.500729573
	H	1.487977118	0.247051838	1.978683726
	O	-2.25723177	0.206464958	1.596364319
	H	-1.438178317	0.339166509	2.095148318
	C	-3.595234292	0.158097971	-0.915627339
	H	-4.403400742	-0.443426927	-0.490428906
	H	-3.885634997	1.209837611	-0.851942488
	H	-3.481375845	-0.1092762	-1.96897499
	C	1.623167333	-0.852848397	-0.940114367
	H	2.0031225	-1.552478798	-0.183969589
	H	0.941643025	-1.393386826	-1.602861281
	O	2.700532969	-0.411143549	-1.774354239
	O	3.570248253	0.339799327	-1.001511761
TS _{L2-7-5}	Si	-1.99941305	-0.048501646	0.107859891
	O	-0.634897029	0.435336723	-0.68983666
	Si	0.917616173	0.521396231	-0.120781961
	C	1.729442419	2.087339224	-0.681446401
	H	1.244268744	2.944328016	-0.204810719
	H	2.788298871	2.105206389	-0.408177741
	H	1.644242646	2.206696925	-1.764896492
	O	-1.84034922	-1.707225838	0.385412952
	H	-0.582189786	-2.33988547	0.482389747
	O	0.86084931	0.515395145	1.54891491
	H	0.912424485	-0.370907888	1.931307998
	O	-2.126457353	0.79288038	1.513850255
	H	-1.293261639	0.971342934	1.971479548
	C	-3.538050402	0.14496476	-0.892235757
	H	-4.400768095	-0.252454248	-0.352446047
	H	-3.710746097	1.208303247	-1.081486801
	H	-3.448160906	-0.375931513	-1.847627463
	C	1.806063505	-1.046791898	-0.719230604
	H	2.049490653	-0.981988841	-1.785253765
	H	2.741343726	-1.229088813	-0.170220903
	O	0.967892757	-2.19998458	-0.63080529
	O	0.429961128	-2.25099359	0.663978652

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TS _{L2-7-6}	Si	-1.872312986	-0.152576844	-0.075201426
	O	-0.617856758	0.678842414	-0.773715445
	Si	0.932877025	0.66415948	-0.214764846
	C	1.812413161	2.206874332	-0.732662154
	H	2.857081275	2.179526775	-0.410848427
	H	1.781320198	2.329147505	-1.818624127
	H	1.332698504	3.076931192	-0.274707993
	O	-1.309418027	-1.721924001	-0.061661208
	H	-1.716079131	-2.337177861	0.556161701
	O	0.865494475	0.502306909	1.441360553
	H	1.345780735	-0.259098482	1.798689583
	O	-2.130999802	0.372191377	1.463763189
	H	-1.321272836	0.519579211	1.973448155
	C	-3.421755057	0.058796112	-1.053088652
	H	-4.252377957	-0.473488337	-0.58126928
	H	-3.689008268	1.116768552	-1.116302181
	H	-3.29194428	-0.330209268	-2.066077677
	C	1.788494325	-0.928940516	-0.76877572
	H	1.040072068	-1.81782724	-0.158689687
	H	1.943785943	-1.295967275	-1.786259703
	O	2.821225306	-1.295061123	0.110222188
	O	1.899735727	-2.250755903	0.727122165
TS _{L2-8-1}	Si	-0.968785577	-0.674220442	-0.166785384
	O	0.614909389	-1.115300608	-0.242413313
	Si	1.766630173	0.081048068	-0.11237354
	C	1.123793384	1.458900486	-1.198912609
	H	1.492042679	1.427938726	-2.22720636
	H	-0.043117883	1.244949108	-1.321303449
	H	1.197765013	2.467645042	-0.788236958
	O	-1.255360739	0.514741043	-1.314354299
	O	-1.075770847	-0.003683804	1.36023085
	H	-1.81761524	0.581224092	1.543595591
	O	3.234930554	-0.405511973	-0.647484131
	H	3.801223995	-0.873343589	-0.025768706
	O	1.896937405	0.49333121	1.47682413
	H	1.062958889	0.432768745	1.964145063
	C	-2.145868205	-2.065787691	-0.461001447
	H	-2.030623051	-2.820031493	0.322161398
	H	-3.181302026	-1.715286396	-0.455747357
	H	-1.944289854	-2.530238363	-1.429077407

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TS _{L2-8-2}	Si	-1.277241851	0.45175171	0.095062406
	O	0.12130897	1.027829432	-0.562294909
	Si	1.516813548	0.280940942	-0.045160505
	C	3.033956416	1.313621383	-0.197834174
	H	3.223844078	1.537495721	-1.250762497
	H	2.922277751	2.250555093	0.351760342
	H	3.89788015	0.77408653	0.198470922
	O	-1.003966508	0.354800865	1.746295196
	O	-1.401179035	-1.08970499	-0.517822859
	H	-1.90642898	-1.732066464	-0.009316688
	O	1.730159121	-1.120238569	-0.871743609
	H	0.92439045	-1.632809836	-1.022207813
	O	1.192521449	-0.018585069	1.591181252
	H	0.153927823	0.263948331	1.991991078
	C	-2.749027228	1.51408792	-0.234556267
	H	-3.639082304	1.113522256	0.257721743
	H	-2.576810789	2.528764182	0.131528234
	H	-2.939195251	1.555138255	-1.310404202
TS _{L2-8-3}	Si	-1.518064644	0.167770855	-0.038463396
	O	-0.020896133	-0.066270369	-0.606647017
	Si	1.554893136	-0.037887756	-0.054288815
	C	2.325674026	1.582114864	-0.487574914
	H	2.346122619	1.714726751	-1.572564066
	H	1.76425008	2.411687104	-0.049010823
	H	3.352755281	1.625315526	-0.116082816
	O	-2.361767471	1.500486151	-0.579059855
	O	-1.354047325	0.143123543	1.612486674
	H	-2.05850067	0.538811986	2.136044542
	O	2.424328616	-1.213602217	-0.803449034
	H	2.312138433	-2.11652146	-0.491263493
	O	1.504322218	-0.360843954	1.561209167
	H	0.657674038	-0.210226335	2.003879059
	C	-2.898324961	-0.741972685	-0.841779142
	H	-2.776040298	-1.170614487	-1.835137089
	H	-3.752056276	-1.114910054	-0.278757159
	H	-3.151968918	0.530581697	-1.048575201
TS _{L2-8-4}	Si	-1.455439045	-0.083616074	-0.06158675
	O	0.02423002	-0.513923452	-0.568037778

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	Si	1.547434028	-0.104208456	0.007816573
	C	2.030425892	1.538661722	-0.680093188
	H	2.125725581	1.485349719	-1.768089161
	H	1.272999359	2.289373517	-0.435548009
	H	2.988726501	1.861471675	-0.265693684
	O	-1.709843866	1.575157887	0.102015793
	O	-1.538294277	0.130840785	1.615522325
	H	-1.734134226	1.289525401	1.2825141
	O	2.638284349	-1.221781528	-0.494473917
	H	2.683665545	-2.050895931	-0.008792948
	O	1.460968453	-0.160778702	1.65352153
	H	0.603104858	0.010931544	2.065100019
	C	-2.766778893	-1.067423567	-0.892129026
	H	-2.633327361	-2.131618232	-0.681388021
	H	-3.754758701	-0.75674595	-0.547009657
	H	-2.709381218	-0.931147268	-1.975386941
TS _{L2-9-1}	Si	1.778447639	-0.46507246	0.431058501
	O	0.390686728	-0.934817634	-0.329984057
	Si	-1.202166385	-0.523088356	-0.021056461
	O	1.701928336	-0.776789905	2.0474416
	H	0.815829298	-0.657814097	2.420317993
	O	-1.124551759	-0.344780041	1.634861205
	H	-1.944702409	-0.077532831	2.064108234
	C	-1.042181058	1.336915502	-0.923037213
	H	-0.240606007	2.050539879	-0.753867203
	H	-1.179919295	0.975487694	-1.9501144
	O	-2.228556466	1.682883	-0.345752391
	O	-2.818941999	0.447375831	-0.153608982
	O	1.859694261	1.181685871	0.174002612
	H	2.379054484	1.683477699	0.809759286
	O	-1.983220893	-1.825200472	-0.656432627
	H	-1.408194713	-2.582514255	-0.810591661
	C	3.236009881	-1.346644581	-0.285313992
	H	4.153999969	-1.059878006	0.235575685
	H	3.11683602	-2.42892359	-0.190114263
	H	3.349973829	-1.099125068	-1.343888508
TS _{L2-9-2}	Si	-1.809130375	-0.280358875	-0.029140474
	O	-0.602922542	0.664940385	-0.66350328
	Si	0.925625776	0.940892111	-0.137691687
	O	-3.224535692	-0.024821142	-0.811636167
	H	-3.724621932	0.76896748	-0.597796057

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	O	0.909825554	0.757484979	1.518146598
	H	1.297043108	-0.071610372	1.826685347
	C	2.130718534	-0.23513713	-0.977780922
	H	2.253797529	0.042616984	-2.029532237
	H	3.12059746	-0.201543478	-0.5026445
	O	1.662490294	-1.587274905	-1.008090467
	O	1.15428397	-1.921069686	0.241650014
	O	-1.981035048	0.115550446	1.560182691
	H	-1.178902563	0.455118061	1.982038605
	O	1.436846176	2.445756541	-0.527036685
	H	1.106262291	3.209828013	-0.046249954
	C	-1.321303771	-2.051933219	-0.264991864
	H	-1.224840992	-2.424621913	-1.286767214
	H	-0.000895435	-2.020479657	0.063335831
	H	-1.725119791	-2.798839591	0.41936293
TS _{L2-9-3}	Si	1.925267723	0.304360332	-0.066141105
	O	0.769465142	-0.865192845	-0.419968375
	Si	-0.801636084	-0.927647799	0.008723255
	O	1.913408024	0.49899067	1.572437048
	H	1.145222847	0.189916663	2.065994232
	O	-0.985527783	-0.657384124	1.633205366
	H	-1.445946823	1.234439145	1.870478727
	C	-1.755859163	0.640019129	-0.577690723
	H	-1.490142075	0.759020313	-1.637070327
	H	-2.84030917	0.564103355	-0.465029835
	O	-1.260444235	1.791359353	0.073909265
	O	-1.904617542	1.907884802	1.323853311
	O	1.514027853	1.696561381	-0.837767391
	H	0.782944931	2.203322058	-0.459679355
	O	-1.502217586	-2.269422938	-0.600463194
	H	-0.942731419	-2.94213059	-1.001462953
	C	3.568550696	-0.250084915	-0.680429921
	H	3.829695008	-1.225709951	-0.263585352
	H	3.563657005	-0.322598133	-1.770962818
	H	4.338680602	0.468613096	-0.388849395
TS _{L2-9-4}	Si	1.956753331	0.115073109	0.127139119
	O	0.67882515	-0.599150632	-0.645936881
	Si	-0.897961379	-0.677913332	-0.188150175
	O	2.040830078	-0.470080025	1.660104757
	H	1.189116728	-0.655959283	2.079162507

Supporting Information

	O	-0.936805761	-0.526235698	1.468877651
	H	-1.164387781	0.35842779	1.782514111
	C	-1.855531383	0.689337243	-1.058886404
	H	-2.010855353	0.440151373	-2.113151594
	H	-2.839098247	0.865073019	-0.60205914
	O	-1.10897855	1.905783733	-1.084547376
	O	-0.653226325	2.158129244	0.21860172
	O	1.663282264	1.777350697	0.104325469
	H	0.356558537	2.314986192	0.0756711
	O	-1.588436297	-2.094283271	-0.626358283
	H	-1.421762728	-2.892229243	-0.116261576
	C	3.562105422	-0.130591939	-0.747184011
	H	4.366190325	0.403877643	-0.236037112
	H	3.80640235	-1.196696726	-0.752537248
	H	3.500198629	0.224335657	-1.777914984
TS _{L2-9-5}	Si	1.908538772	0.200219305	0.015576888
	O	0.77790149	-0.884147439	-0.590915617
	Si	-0.829064178	-0.802103459	-0.338005185
	O	1.86699043	0.085862111	1.657638388
	H	1.005827692	-0.142142599	2.034280549
	O	-1.014626258	-0.516665971	1.281457684
	H	-1.743777705	0.061495429	1.544558516
	C	-1.667500943	0.668244222	-1.159310262
	H	-1.779585645	0.862382627	-2.227741025
	H	-2.880084222	0.616635354	-0.645240505
	O	-1.506364504	1.841879673	-0.403020766
	O	-2.839463521	1.631026884	0.155659178
	O	1.467727923	1.703697311	-0.507083744
	H	0.806386386	2.198135368	-0.009312131
	O	-1.583725263	-2.134401663	-0.908636342
	H	-1.11245884	-2.97315225	-0.922148936
	C	3.575478206	-0.201425072	-0.650137051
	H	4.330659763	0.43190272	-0.177767635
	H	3.827396738	-1.246379345	-0.454410002
	H	3.60681595	-0.028251395	-1.728775402
TS _{L2-10-1}	Si	-0.989823525	-0.632565843	0.133368596
	O	0.568449118	-0.647937981	0.633319992
	Si	1.856337971	0.193630395	0.018207971
	C	1.118249255	1.424751681	-1.166079354
	H	1.664870353	1.575936604	-2.098793375

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	H	0.094981911	0.920414077	-1.48983383
	H	0.837888286	2.381132144	-0.719274327
	O	-1.023028601	0.056517292	-1.393917283
	O	-1.824774819	0.191015151	1.272889311
	H	-2.783277748	0.113770489	1.273673934
	O	2.885639185	-0.759600862	-0.831539935
	H	3.53242212	-1.273230533	-0.337986176
	O	2.685736493	0.822202259	1.294198083
	H	2.201547088	0.937923641	2.117769533
	O	-1.682925539	-2.108421455	-0.016801017
	H	-1.427689389	-2.650307069	-0.769933833
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TS _{L2-10-2}	Si	-1.428957405	-0.005471202	-0.061391694
	O	0.008083395	0.147803122	-0.858366076
	Si	1.4124257	-0.035539257	-0.021783324
	O	-1.195898255	0.723504051	1.432009206
	O	-1.622774208	-1.63640207	0.138216876
	H	-2.166859911	-1.945242258	0.868813627
	O	2.045126122	-1.535281645	-0.185872935
	H	1.455190229	-2.285288539	-0.054027204
	O	0.976486251	0.270597579	1.572712699
	H	-0.075020492	0.719775991	1.77160507
	C	-2.83275933	0.814802677	-0.932535434
	H	-3.749522792	0.758373552	-0.33965449
	H	-2.604154564	1.866459347	-1.119384193
	H	-3.011397449	0.317617732	-1.889908158
	O	2.566115902	1.014225944	-0.48567597
	H	3.365383265	0.643406858	-0.871920382
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TS _{L2-10-3}	Si	1.461598866	0.081203532	0.080918902
	O	-0.002705775	0.608294711	0.481856872
	Si	-1.579042738	0.328587893	0.04810424
	C	-1.779815014	-1.341191275	-0.715291316
	H	-2.829285926	-1.542815813	-0.948042736
	H	-1.202112071	-1.406256855	-1.641992714
	H	-1.427973245	-2.119051582	-0.031873779
	O	1.746884907	-1.564505871	0.192006543
	O	2.530163209	1.072005672	0.7950038
	H	3.466082551	0.884088629	0.67299565
	O	-1.911713089	1.576828462	-0.977784003
	H	-2.817916215	1.708296077	-1.269339413
	O	-2.516229614	0.385576798	1.400369579

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	H	-2.41176267	1.136616268	1.993001421
	O	1.719469302	-0.334973479	-1.519041023
	H	1.859805092	-1.438532716	-1.017370182
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TS _{L2-11-1}	Si	1.854630959	-0.107844256	0.306995104
	O	0.402755569	-0.14076942	1.062070611
	Si	-1.074460744	-0.511619858	0.401071833
	O	3.053032161	0.506092046	1.234275434
	H	3.504139706	-0.103203602	1.826115783
	O	-1.970209896	-0.835509492	1.73717683
	H	-2.901731479	-1.026151987	1.590490173
	C	-1.408892408	1.416001034	-0.276599901
	H	-1.32687689	2.337932852	0.292672831
	H	-0.729680538	1.323961406	-1.13682938
	O	-2.697444402	1.089911387	-0.58291097
	O	-2.624503789	-0.27809979	-0.728804419
	O	1.6117514	0.927913515	-0.959625575
	H	2.372165453	1.141436649	-1.5087217
	O	-0.57321191	-1.772177275	-0.574170811
	H	-1.178160037	-2.050534614	-1.269957854
	O	2.298628291	-1.616886674	-0.158405325
	H	1.544317233	-2.1539183	-0.441599544
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TS _{L2-11-2}	Si	-1.58674525	0.100610877	-0.073660412
	O	-0.250352455	0.976430073	-0.52547992
	Si	1.232227911	0.843300129	0.140188914
	O	-1.17725039	-0.733943854	1.289340015
	H	-0.542575968	-0.276701506	1.870563838
	O	1.38844725	0.282722462	1.579985202
	H	0.632668348	-1.930423185	1.156270602
	C	1.834200019	-0.937112065	-0.929798855
	H	1.766958492	-0.574813707	-1.95815292
	H	2.804295661	-1.200650722	-0.509770329
	O	0.850338237	-1.829693759	-0.692131263
	O	1.098457296	-2.513869621	0.515381284
	O	-2.050800583	-0.982750898	-1.207142112
	H	-1.547128017	-1.802853924	-1.251918873
	O	-2.784147828	1.190712549	0.107762531
	H	-3.689780925	0.883770754	0.007242852
	O	2.208657215	1.951627825	-0.554023767
	H	2.987589027	2.21732647	-0.053174288

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TS _{L2-11-3}	Si	-1.876287356	0.037091595	0.017637092
	O	-0.507836479	-0.297356598	-0.822740613
	Si	1.038757623	-0.465309187	-0.289611703
	O	-3.21858348	0.003056293	-0.900142939
	H	-3.879445962	-0.663062205	-0.68750038
	O	1.845874877	-1.620162851	-1.117179445
	H	1.708745961	-2.550459529	-0.916395297
	C	1.948840324	1.155795612	-0.575958591
	H	2.879599789	1.226365763	0.003001758
	H	2.198006423	1.27121659	-1.635323095
	O	1.108219765	2.272323628	-0.280848111
	O	0.521825462	2.044148584	0.973253111
	O	-1.738404512	1.627897081	0.53550484
	H	-0.478958165	2.218185623	0.798820215
	O	0.946806934	-0.890427422	1.317152771
	H	1.093555549	-0.16450993	1.936620806
	O	-2.043239874	-1.02893604	1.2499481
	H	-1.215656137	-1.32947676	1.650431062
TS _{L2-11-4}	Si	-1.980658183	0.146724702	-0.035421623
	O	-0.583761679	-0.409653563	-0.710859256
	Si	0.907921145	-0.437687172	-0.055048761
	O	-3.262425201	0.011381652	-1.035309648
	H	-3.750964529	-0.817040157	-1.019680064
	O	1.925972138	-1.519352178	-0.730555837
	H	2.666309485	-1.164475921	-1.240502004
	C	1.709674893	1.246422989	-0.27957052
	H	1.902859481	1.275184558	-1.581007047
	H	1.281919725	2.212477626	-0.002614648
	O	3.108459983	1.191973786	-0.166765311
	O	3.192065371	1.169147965	-1.626525021
	O	-1.661771396	1.738556082	0.222824041
	H	-2.368730776	2.2958287	0.56114939
	O	0.639588394	-0.822185262	1.533669591
	H	1.384822618	-1.127611528	2.061492632
	O	-2.306273061	-0.701307198	1.3290381
	H	-1.527837379	-0.938407471	1.852918047
TS _{L2-12-1}	Si	1.789908979	0.024759845	0.069359962
	O	0.329286908	-0.795132424	0.201998107
	Si	-1.255004762	-0.391053598	0.078525475

Supporting Information

	C	1.7606483	1.126696112	-1.445699506
	H	0.992392513	1.898891029	-1.341343221
	H	2.728195552	1.621609747	-1.58216609
	H	1.553096451	0.544792208	-2.350166896
	C	2.072002785	1.023032093	1.628257566
	H	1.99056517	0.388430145	2.517010835
	H	3.070297086	1.473517056	1.629421224
	H	1.332187393	1.82591977	1.700524697
	C	3.095367265	-1.306140007	-0.107844783
	H	2.905909103	-1.919446119	-0.994383419
	H	4.093929324	-0.867390383	-0.205856933
	H	3.099832703	-1.967371357	0.764225401
	C	-2.222504592	-1.826507363	0.818369335
	H	-1.926475922	-2.009297098	1.854544754
	H	-3.299752129	-1.638063945	0.786441369
	H	-2.011880173	-2.731339536	0.237016615
	C	-1.875628199	-0.048418132	-1.642857033
	H	-1.971859934	-0.981487218	-2.206777602
	H	-2.862284813	0.424274202	-1.596041139
	H	-1.204406916	0.628417331	-2.175531077
	C	-1.634512338	1.103031681	1.38271448
	H	-2.689228869	1.391591517	1.480364765
	H	-1.117294854	0.868327577	2.325100096
	O	-0.920392491	1.632361727	0.392405018
TS _{L2-12-2}	Si	0.425390353	-1.5134328	-2.381621691
	O	-0.704302726	-1.55840697	-1.148325709
	Si	-1.374841716	-0.396055485	-0.17277909
	C	-0.345838564	-0.635026181	-3.847541871
	H	-0.636280841	0.385492727	-3.571087894
	H	0.351619872	-0.567744299	-4.688876707
	H	-1.243538722	-1.158357363	-4.191361239
	C	1.922192774	-0.549245101	-1.786811922
	H	2.356589696	-1.005428133	-0.891377857
	H	2.700485745	-0.509095388	-2.556172419
	H	1.646376126	0.483432308	-1.541030344
	C	0.867123367	-3.281429805	-2.790390747
	H	-0.020475206	-3.839478815	-3.103374455
	H	1.601173158	-3.327411302	-3.601433053
	H	1.29223297	-3.786295527	-1.917537813
	C	-0.345677907	-0.121811145	1.368375104
	H	0.691390751	0.118329893	1.117314684
	H	-0.766064138	0.70484479	1.948983662

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	H	-0.347936207	-1.024373215	1.990361597
	C	-3.149546457	-0.837877685	0.20955486
	H	-3.188543322	-1.768956395	0.786362695
	H	-3.610876021	-0.039763973	0.798202326
	H	-3.726586404	-0.980380817	-0.707820863
	C	-1.965259726	2.375220576	-0.446419066
	H	-0.905866806	2.61824783	-0.647915312
	H	-2.594974478	2.173405399	-1.332039042
	O	-2.435769033	2.440017138	0.674966306
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TS _{L2-12-3}	Si	1.726128323	-0.416595529	0.334829857
	O	0.271434225	-1.239151228	0.357483813
	Si	-1.274097597	-0.749993436	-0.004021001
	C	2.510884079	-0.591036634	-1.355021039
	H	1.886153333	-0.119952261	-2.121357643
	H	3.493575774	-0.108396312	-1.381909426
	H	2.642787027	-1.644808975	-1.619178403
	C	1.296795099	1.381021119	0.616073982
	H	0.353352272	1.583495788	-0.270816617
	H	0.833744151	1.646989122	1.569641757
	H	2.022193433	2.137698718	0.307425815
	C	2.812024784	-1.138121156	1.674942621
	H	2.992010394	-2.201373745	1.486224258
	H	3.780496977	-0.629964859	1.715281726
	H	2.333778824	-1.043645598	2.654200499
	C	-2.078371211	0.013009134	1.503139733
	H	-1.603768512	0.965187126	1.75920721
	H	-3.139914712	0.20829777	1.319570659
	H	-1.997224198	-0.655013139	2.36614276
	C	-2.230280912	-2.218756585	-0.65097797
	H	-1.741958137	-2.643831288	-1.532872765
	H	-2.285731317	-3.001869355	0.11145004
	H	-3.252767205	-1.93912288	-0.923979307
	C	-1.206009256	0.567767486	-1.391515057
	H	-0.823184562	0.103490932	-2.315619749
	H	-2.262176596	0.836834115	-1.561195325
	O	-0.518760309	1.749091688	-1.095818469
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TS _{L2-12-4}	Si	1.666937938	-0.159130205	-0.109137775
	O	0.135608207	-0.786347582	-0.358395622
	Si	-1.423013945	-0.362082442	-0.031262077
	C	2.853998952	-1.601993283	-0.066657756

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	H	2.815244121	-2.162086879	-1.006041395
	H	3.883429174	-1.260583885	0.083504257
	H	2.60116448	-2.289066564	0.746604746
	C	2.071292142	0.999761188	-1.525319928
	H	1.390455641	1.856913028	-1.545562188
	H	3.091695674	1.386909174	-1.43411663
	H	1.991293217	0.481692851	-2.486046693
	C	1.677969313	0.776592013	1.518060989
	H	1.48872749	0.104753615	2.361830733
	H	2.648172029	1.256450138	1.684629444
	H	0.913745283	1.562432353	1.532896889
	C	-1.892271608	-0.277311516	1.787839497
	H	-2.52582676	0.846848734	1.504751304
	H	-2.582875431	-1.005373045	2.215708566
	H	-1.139557577	0.041165399	2.512281112
	C	-2.573097025	-1.478327893	-0.980047843
	H	-2.358511779	-1.439566903	-2.051889436
	H	-2.464403042	-2.5153828	-0.648279562
	H	-3.612666626	-1.173747721	-0.823040233
	C	-1.810236921	1.493601764	-0.341525864
	H	-0.915819765	2.133891395	-0.327551309
	H	-2.337195416	1.629802818	-1.295552983
	O	-2.673775075	1.791763099	0.725876277
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TS _{L2-12-5}	Si	-1.746026227	-0.054272914	-0.067853886
	O	-0.29136126	0.638885665	-0.499657489
	Si	1.312214863	0.476740259	-0.120420134
	C	-3.094027043	1.140306572	-0.569487925
	H	-3.050942957	1.338139738	-1.644982933
	H	-4.085332432	0.737593989	-0.337495278
	H	-2.983114376	2.095082899	-0.046597041
	C	-1.937542687	-1.689553008	-0.967592667
	H	-1.194680675	-2.419045979	-0.628194773
	H	-2.929775472	-2.117272534	-0.787857061
	H	-1.817536211	-1.558689525	-2.047727434
	C	-1.763069383	-0.352086323	1.786423221
	H	-1.600605608	0.577992264	2.340641919
	H	-2.724815372	-0.769489085	2.10347887
	H	-0.982872126	-1.063758102	2.080012977
	C	1.685536602	1.04573504	1.620157199
	H	2.742489028	0.877899157	1.850321359
	H	1.474740928	2.113638438	1.734238068
	H	1.089555528	0.501578761	2.359578384

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	C	2.311417983	1.428051884	-1.378572541
	H	2.09803602	1.079595505	-2.39302645
	H	2.071623514	2.494916463	-1.328340142
	H	3.382909448	1.307651696	-1.190616702
	C	1.72334463	-1.36913029	-0.212765775
	H	1.680913402	-1.931712794	0.910461447
	H	1.384138697	-2.012148857	-1.034917454
	O	2.827723205	-1.85410524	0.479114069
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TS _{L2-12-6}	Si	-1.719835086	-0.075908844	-0.020361985
	O	-0.229550329	-0.563850455	-0.615694347
	Si	1.297736632	-0.507976354	0.010974972
	C	-1.985296178	-0.872043465	1.656975269
	H	-1.213713134	-0.540350928	2.360933217
	H	-2.961137618	-0.603263747	2.074831736
	H	-1.936844055	-1.963647907	1.586031893
	C	-1.65507307	1.774371466	0.176845031
	H	-1.727486689	2.381648598	-0.728798007
	H	-2.208319134	2.22226611	1.004959463
	H	-0.327259221	1.986104051	0.548927362
	C	-2.993296085	-0.645809587	-1.266059639
	H	-2.966268395	-1.734724362	-1.375573077
	H	-4.002961474	-0.35578043	-0.958873887
	H	-2.794963225	-0.202215088	-2.246508157
	C	2.479362572	-0.127830945	-1.37928281
	H	2.458591296	-0.930232981	-2.123050194
	H	2.203929013	0.800069805	-1.88968641
	H	3.504805807	-0.028301795	-1.010844072
	C	1.716309613	-2.061388447	0.941081286
	H	1.663550017	-2.934869245	0.284623667
	H	2.72442427	-2.006171449	1.362138102
	H	1.012155576	-2.209458033	1.765419091
	O	1.338133806	0.714866612	1.16304702
	C	0.95445362	2.012217284	0.862377463
	H	1.031882816	2.654805808	1.740721558
	H	1.450702235	2.436398859	-0.019121337
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TS _{L2-12-7}	Si	-1.565984682	-0.07362632	-0.102550769
	O	-0.261431421	-1.10064207	-0.3140981
	Si	1.366655123	-0.926194719	-0.147208797
	C	-1.702375807	0.371094266	1.711350627
	H	-0.757023406	0.791205772	2.070132865

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	H	-2.498289043	1.103980171	1.881289693
	H	-1.921688961	-0.515194713	2.315029909
	C	-1.283462458	1.478875192	-1.122363629
	H	-1.177019222	1.238802341	-2.185340238
	H	-2.125949686	2.170725551	-1.016485082
	H	-0.378237101	2.008213299	-0.803266901
	C	-3.080187707	-0.994061167	-0.699128592
	H	-3.217982511	-1.916939308	-0.127422425
	H	-3.982988581	-0.385410136	-0.583787233
	H	-2.982607255	-1.263232846	-1.755243716
	C	2.108043045	0.157102576	-1.470212843
	H	2.28435745	1.157692963	-0.51916021
	H	3.11589739	-0.054041013	-1.831694045
	H	1.472086681	0.570692808	-2.253551047
	C	2.116264127	-2.598030151	0.140669589
	H	1.840460153	-3.291058119	-0.658725866
	H	3.206918088	-2.535449707	0.189489879
	H	1.754070976	-3.008734339	1.087892987
	C	2.160619407	1.338228914	0.826519356
	H	3.154763387	1.553988779	1.223497319
	H	1.433435347	2.139392856	0.990110776
	O	1.691173378	0.0777882	1.177719783
TS _{L2-12-8}	Si	-1.62140068	0.039892629	-0.028586919
	O	-0.109133109	-0.367836603	-0.615706043
	Si	1.370453374	-0.575249023	0.106516171
	C	-1.689730392	-0.357399595	1.804218706
	H	-0.90920404	0.195606951	2.338629784
	H	-2.658255277	-0.075453075	2.231044546
	H	-1.544557711	-1.427554757	1.987119112
	C	-1.93896431	1.866732722	-0.306723917
	H	-1.713161637	2.153017165	-1.33920347
	H	-2.989247484	2.109689874	-0.112827367
	H	-1.322220661	2.468813848	0.367147246
	C	-2.864462722	-0.981003581	-0.988440521
	H	-2.681721004	-2.050997224	-0.848386459
	H	-3.887795224	-0.764544827	-0.664002532
	H	-2.796311445	-0.765894201	-2.059538621
	C	2.702598102	-0.028905901	-1.094360453
	H	2.748102912	1.06173631	-1.189169889
	H	3.684737692	-0.386694109	-0.772137772
	H	2.493306272	-0.437252099	-2.089085252
	C	1.577579539	-2.391317675	0.568568414

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	H	1.475004336	-3.018960254	-0.325232274
	H	2.560652315	-2.57513431	1.011530085
	H	0.815498629	-2.699876158	1.289786123
	C	1.452256913	2.53277529	0.569237727
	H	2.344636366	3.093352863	0.880842725
	H	0.944944595	2.844765978	-0.356719012
	O	1.055037411	1.558570803	1.214621662
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TS _{L2-13-1}	Si	1.673214995	-0.13211412	0.039245195
	O	0.165180792	-0.830721925	0.082748754
	Si	-1.436715482	-0.45234329	0.032230298
	C	1.721748577	1.03938393	-1.42099288
	H	0.983438965	2.072346535	-1.005141189
	H	2.667807154	1.540414635	-1.642269835
	H	1.200860492	0.734851976	-2.331440865
	C	2.003812941	0.808076327	1.621249911
	H	1.924475748	0.145284136	2.488961844
	H	3.010905904	1.238517334	1.615066686
	H	1.286857886	1.626187156	1.739983832
	C	2.91198857	-1.516454379	-0.196345389
	H	2.721577766	-2.059965177	-1.126097749
	H	3.934581047	-1.127488609	-0.228253893
	H	2.842458629	-2.226950044	0.633979868
	C	-2.040119775	-0.104956803	1.764866431
	H	-1.466886733	0.709752232	2.220033642
	H	-3.101847837	0.161734255	1.78771137
	H	-1.903978621	-0.994383609	2.387745428
	C	-2.33855604	-1.828041672	-0.827382506
	H	-2.179560969	-2.780265052	-0.313220809
	H	-3.41340489	-1.628797348	-0.865452284
	H	-1.974848041	-1.930775456	-1.85388341
	O	-1.659378794	0.919950282	-0.914887281
	C	-1.740826279	2.200971766	-0.385642167
	H	-1.950978481	2.902023406	-1.196135586
	H	-2.492499353	2.26792804	0.410807178
	O	-0.542940118	2.592461809	0.259019454
	O	0.368918058	3.032425648	-0.689613185
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TS _{L2-13-2}	Si	1.676726851	-0.053915122	0.124467899
	O	0.139122044	-0.321650223	0.694476038
	Si	-1.466690947	-0.237780416	0.302582404
	C	1.79444846	-0.49826815	-1.68985784

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	H	1.157129269	0.151831084	-2.298113831
	H	2.82484593	-0.387891804	-2.044472311
	H	1.488494059	-1.534749603	-1.864180205
	C	2.032790422	1.780086428	0.297786026
	H	2.034278312	2.232253944	1.292710211
	H	2.7803713	2.238655961	-0.353311445
	H	0.864521465	2.233207367	-0.241297577
	C	2.845484395	-1.077917243	1.165079477
	H	2.623911316	-2.143891381	1.051380997
	H	3.885655899	-0.910717902	0.868493793
	H	2.74670766	-0.822609106	2.224217361
	C	-2.362478003	-1.591617778	1.210965829
	H	-2.141197831	-1.546229695	2.281228401
	H	-3.44442461	-1.489991823	1.082424287
	H	-2.065525295	-2.577787275	0.841046357
	C	-1.763533067	-0.326595133	-1.533567385
	H	-1.301321573	-1.219050192	-1.968041758
	H	-2.839770659	-0.377028867	-1.728583051
	H	-1.369200195	0.560122947	-2.036191137
	O	-2.07396958	1.207803238	0.907011269
	C	-1.30899555	2.273005479	1.325425065
	H	-1.905945421	2.932017922	1.960845613
	H	-0.404688009	1.930020097	1.850062543
	O	-0.906295026	3.129594148	0.263621466
	O	-0.210663215	2.388300728	-0.674041174
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TS _{L2-13-3}	Si	-1.737916484	-0.158210819	-0.159250298
	O	-0.263907523	0.571737727	-0.474203822
	Si	1.152838543	1.097246111	0.140953045
	C	-2.22271884	-1.163754066	-1.659105304
	H	-1.578126389	-2.038616833	-1.774102456
	H	-3.258385526	-1.50887322	-1.570109889
	H	-2.147344341	-0.555166583	-2.56592514
	C	-1.62843292	-1.195042305	1.396523795
	H	-1.497784035	-0.566185791	2.283859586
	H	-2.551573114	-1.769535986	1.531766136
	H	-0.793429103	-1.899123354	1.34104803
	C	-2.975642965	1.230518267	0.097517114
	H	-3.041856123	1.865455055	-0.791856739
	H	-3.975115526	0.832572805	0.303442354
	H	-2.687457161	1.863632415	0.94363874
	C	1.225327428	0.944660042	1.994141296
	H	1.104985349	-0.098349001	2.29984936

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	H	2.184459001	1.30905979	2.37523777
	H	0.43046275	1.537699672	2.459349552
	C	1.55704313	2.797101953	-0.481111899
	H	0.839140646	3.529293144	-0.099570156
	H	2.559217418	3.102476436	-0.166305235
	H	1.519198244	2.818335521	-1.573792236
	O	2.384931839	0.128038558	-0.548742222
	C	2.299886682	-1.201865665	-0.667499202
	H	1.389766899	-1.651200352	-1.486363708
	H	3.240534597	-1.678056553	-0.958694422
	O	1.6138321	-1.87760288	0.330283804
	O	0.642017392	-2.369363436	-0.644790132
TS _{L2-14-1}	Si	1.694543476	-0.138228226	0.027422519
	O	0.177131211	-0.792576881	-0.124731181
	Si	-1.428615028	-0.405919584	-0.047476682
	C	1.950150208	1.096941515	-1.359817636
	H	0.917621589	1.787074408	-1.474681213
	H	2.736229936	1.841364094	-1.206296652
	H	2.027275257	0.662808129	-2.360572224
	C	1.857209362	0.724691436	1.68589791
	H	1.599872907	0.042845731	2.50307003
	H	2.886526953	1.064975437	1.842236287
	H	1.206025821	1.601998709	1.759960536
	C	2.92792806	-1.537299344	-0.113111753
	H	2.799369868	-2.069363245	-1.060235244
	H	3.956059323	-1.164987492	-0.065849504
	H	2.78568327	-2.254923382	0.70121305
	C	-1.875368761	-0.129027921	1.74758528
	H	-1.282063296	0.678873757	2.189572005
	H	-2.932706317	0.132540491	1.852388918
	H	-1.686490797	-1.033789901	2.334009682
	C	-2.428525408	-1.736620924	-0.862853449
	H	-2.296243223	-2.693551197	-0.349822392
	H	-3.492248087	-1.482450093	-0.853388117
	H	-2.115707767	-1.8574961	-1.903582595
	O	-1.708614473	0.993244716	-0.913859786
	C	-1.03869712	2.20132715	-0.679368065
	H	-1.774395865	3.019132307	-0.722437376
	H	-0.580583201	2.208540833	0.326260699
	O	-0.115771508	2.518906269	-1.648099177

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TS _{L2-14-2}	Si	1.756447786	-0.179607294	-0.070330312
	O	0.251522528	-0.916260522	-0.094037508
	Si	-1.293471233	-0.372270835	0.019017948
	C	1.997882597	0.742702982	-1.680310719
	H	1.203969187	1.485820458	-1.806129276
	H	2.962836669	1.259673045	-1.704197094
	H	1.959819401	0.0564536	-2.532163591
	C	1.810524076	1.010494154	1.380708698
	H	1.622828163	0.490652599	2.326089705
	H	2.786101841	1.501959965	1.455745772
	H	1.053179761	1.7930382	1.261257736
	C	3.016915854	-1.544746488	0.140101777
	H	2.949745025	-2.263894169	-0.68189713
	H	4.0350723	-1.142289484	0.156885301
	H	2.849668312	-2.086348266	1.076208452
	C	-1.933095355	-0.318308779	1.78085841
	H	-2.694358664	0.675698856	1.630450729
	H	-2.600886323	-1.11245785	2.119852998
	H	-1.233240002	-0.015026023	2.563936769
TS _{L2-14-3}	C	-2.390777305	-1.366171573	-1.096110053
	H	-2.347467237	-2.430463659	-0.847737487
	H	-3.426044728	-1.023864489	-1.005190813
	H	-2.078889888	-1.24425183	-2.13742587
	O	-1.307645294	1.247898187	-0.433246413
	C	-1.926500144	2.188338326	0.412316607
	H	-1.206665931	2.517289204	1.178279473
	H	-2.230651075	3.054520002	-0.190423255
	O	-3.094059561	1.715923541	0.994428106
	Si	1.827314426	-0.234950979	-0.075047852
	O	0.276882183	-0.751627178	-0.429192228
	Si	-1.319719826	-0.619209461	-0.114033406
	C	2.237926662	1.24308175	-1.146371096
	H	1.583802006	2.085064692	-0.901901814
	H	3.275113046	1.558739183	-0.99039178
	H	2.114035979	1.000252694	-2.206447649
	C	1.951213497	0.19050833	1.745993824
	H	1.634155017	-0.651754779	2.370516375
	H	2.984491512	0.436178437	2.014243899
	H	1.322882952	1.05508343	1.978269453
	C	2.956863071	-1.673455007	-0.484975452
	H	2.851649259	-1.962173844	-1.535399872
	H	4.005317152	-1.410344901	-0.309107323

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	H	2.719859731	-2.546979134	0.130486185
	C	-1.666418266	-0.63919214	1.718965377
	H	-1.040602572	0.086803725	2.246014914
	H	-2.717696508	-0.407100477	1.919275748
	H	-1.455506002	-1.629260689	2.135762775
	C	-2.245838271	-1.914080381	-1.066051625
	H	-1.91493092	-2.916091955	-0.778349905
	H	-3.322293508	-1.839235567	-0.887028266
	H	-2.067566464	-1.791613896	-2.138099472
	O	-1.92384167	0.843843205	-0.751591732
	C	-1.608900592	2.044406185	-0.248166766
	H	-1.906434352	2.878724488	-0.886580215
	H	-1.56335587	2.34592841	1.005668714
	O	-0.466831792	2.177625169	0.498407939
TS _{L2-14-4}	Si	-1.835816053	0.080676147	0.002126062
	O	-0.371687804	-0.401751291	0.645358851
	Si	1.178868553	-0.599764006	0.13086291
	C	-2.970299138	0.443222123	1.442090036
	H	-2.536331814	1.213960323	2.086908889
	H	-3.947475236	0.796936543	1.097595006
	H	-3.126748233	-0.453145421	2.049679789
	C	-1.575983466	1.613617845	-1.052867273
	H	-0.763305398	1.467152656	-1.772653375
	H	-2.484627445	1.850998284	-1.616802305
	H	-1.328329622	2.488705485	-0.443491325
	C	-2.515224544	-1.306342716	-1.062455318
	H	-2.56824569	-2.241664994	-0.49613442
	H	-3.524851886	-1.066681092	-1.41287477
	H	-1.88848705	-1.47838414	-1.943719485
	C	1.230379238	-1.330542615	-1.595630879
	H	0.719271309	-0.689621801	-2.320350623
	H	2.261966406	-1.467970337	-1.930981784
	H	0.735191501	-2.307613907	-1.591307659
	C	2.127234656	-1.581134691	1.383288617
	H	2.029359855	-1.106567675	2.362559765
	H	1.746880569	-2.605219457	1.442917079
	H	3.18801918	-1.615725063	1.120134776
	O	1.869853908	0.923879625	-0.187463326
	C	1.609070239	2.212163996	1.187402366
	H	2.289067293	2.950870388	0.742575619
	H	0.533930233	2.361786116	1.006504934
	O	1.995177779	1.450578854	2.088288784

Supporting Information

Table S5. Cartesian coordinates of the transition states for all reactions of D3-RSiCH₂O₂[·]

Species	Atoms	X	Y	Z
TS _{D3-1-1}	O	-1.375956457	0.396667069	-0.936002354
	O	-0.267601592	-1.295552221	0.80798785
	Si	-1.384147295	-1.18668544	-0.423679581
	Si	0.910620324	-0.225848894	1.261511387
	Si	-0.85246419	1.781115753	-0.171179174
	O	0.256806504	1.304789151	0.968901758
	C	-0.049127536	2.886609709	-1.438214047
	H	-0.769722676	3.176729068	-2.209095354
	H	0.333992834	3.797870513	-0.968795725
	H	0.786513218	2.383162509	-1.934119235
	C	-2.280325949	2.616681833	0.684835111
	H	-1.947138821	3.516403774	1.21103476
	H	-3.05432732	2.904159567	-0.033218203
	H	-2.730008763	1.94272146	1.420745813
	C	2.118897409	-0.091636659	-0.463284194
	H	1.768936041	0.077206008	-1.481218268
	C	1.241238206	-0.128905107	3.087399316
	H	1.482915031	-1.112936917	3.497127564
	H	2.087239772	0.538286323	3.282378079
	H	0.368894138	0.28093815	3.602384648
	C	-3.056674765	-1.636762402	0.255982421
	H	-3.825422424	-1.56632837	-0.519485329
	H	-3.05512017	-2.65841809	0.647631554
	H	-3.331952052	-0.961411321	1.071947477
	C	-0.856088992	-2.271019155	-1.839907627
	H	-0.854030234	-3.323804386	-1.542175676
	H	-1.52811209	-2.154739579	-2.695384055
	H	0.157535197	-2.013712142	-2.163428402
	H	2.849005699	0.63671883	-0.09339467
	O	2.542981821	-1.376981978	-0.261133498
	O	2.355208382	-1.517319059	1.087200914
TS _{D3-1-2}	O	-1.007496832	1.196486472	-0.388792882
	O	-0.907010104	-1.34539725	0.431087718
	Si	-1.83786382	-0.248550979	-0.418187883
	Si	0.672068402	-1.233351547	0.914627191
	Si	0.391621478	1.681873977	0.347260896
	O	0.997251671	0.373002622	1.178378376
	C	1.620001708	2.165940015	-0.96082617
	H	1.253711852	2.68203219	-1.849965285
	H	2.592524568	2.541560316	-0.635510998
	H	1.98176691	0.936448862	-1.493991748

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	C	0.055285808	3.053454669	1.556019783
	H	0.976457654	3.359965003	2.059916538
	H	-0.369516714	3.925339366	1.050836519
	H	-0.655714554	2.71425547	2.315858499
	C	1.724969787	-1.785874426	-0.558074616
	H	2.804587897	-1.698168358	-0.404470072
	C	0.971942592	-2.225173346	2.451014894
	H	0.760640686	-3.28444068	2.278504519
	H	2.010318906	-2.127210825	2.78065061
	H	0.322524139	-1.875447186	3.258484467
	C	-3.453203383	-0.040851397	0.482305946
	H	-4.090024581	0.692196412	-0.022141188
	H	-3.99587882	-0.989849352	0.530838961
	H	-3.279605218	0.304443752	1.506038684
	C	-2.044987003	-0.806422778	-2.176277909
	H	-2.568220084	-1.766479568	-2.222490743
	H	-2.621512256	-0.074986643	-2.750793645
	H	-1.06281875	-0.92136982	-2.644049841
	H	1.505803568	-2.819782986	-0.852315535
	O	1.358289552	-0.972563015	-1.696430896
	O	2.34801946	-0.043587049	-1.96145281
TS _{D3-1-3}	O	-1.198845804	1.307815837	-0.160690089
	O	-0.636925656	-1.297155706	-0.189882009
	Si	-1.844798551	-0.184594375	-0.502579467
	Si	0.724345918	-1.163636114	0.738211699
	Si	0.333043307	1.794568323	0.264038514
	O	1.113567646	0.438475515	0.845974223
	C	1.233534447	2.395036504	-1.251224115
	H	0.732406025	3.264144476	-1.688012604
	H	2.262995424	2.677717606	-1.011324274
	H	1.266654582	1.607121443	-2.011267962
	C	0.229561196	3.069674008	1.608951354
	H	1.229616914	3.367182564	1.93827531
	H	-0.295615823	3.962724769	1.257248584
	H	-0.311610339	2.673421699	2.472909628
	C	2.147551627	-2.129476605	-0.079875119
	H	1.793780564	-2.961527088	-0.70030083
	C	0.532123392	-1.935213594	2.412507982
	H	1.461055763	-2.950735638	2.189781877
	H	0.967998228	-1.439405519	3.280259032
	H	-0.377499249	-2.493168924	2.63610439
	C	-3.280057576	-0.500234811	0.63695318
	H	-4.067459076	0.245462145	0.492278264

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	H	-3.709087202	-1.491246132	0.460857724
	H	-2.953761034	-0.450225992	1.680789683
	C	-2.293702056	-0.294721879	-2.302393821
	H	-2.672465015	-1.291508609	-2.54779609
	H	-3.065317267	0.43792673	-2.557154499
	H	-1.417652462	-0.09951652	-2.928315547
	H	2.792732692	-1.477123207	-0.676991946
	O	2.990819506	-2.630525153	0.964394605
	O	2.281884657	-3.582885694	1.673420186
TS _{D3-1-4}	O	1.632918599	0.36539932	-0.503124808
	O	-0.437102891	1.139575214	0.993591665
	Si	0.736193448	1.696259274	-0.065732484
	Si	-0.981937436	-0.388384867	1.266080371
	Si	1.405326456	-1.269528839	-0.333481876
	O	0.180481123	-1.459102281	0.79638985
	C	0.857749202	-2.004525066	-1.950507962
	H	1.619404114	-1.857557092	-2.722403528
	H	0.67288617	-3.078603297	-1.851497037
	H	-0.067660916	-1.525174446	-2.285942025
	C	2.951367677	-2.044570542	0.345451988
	H	2.815843247	-3.119977411	0.494569354
	H	3.789955228	-1.8973171	-0.341751975
	H	3.215567753	-1.595593746	1.30717223
	C	-2.447779096	-0.615013331	0.090463948
	H	-3.225434503	-1.382182249	0.152537183
	C	-1.483318612	-0.654250721	3.026697263
	H	-2.254689061	0.062356479	3.322992181
	H	-1.871835752	-1.666094468	3.17349648
	H	-0.621635577	-0.522054709	3.686957594
	C	1.823171729	2.890482061	0.855575859
	H	2.642545077	3.23766602	0.218931608
	H	1.250316949	3.763967632	1.181623934
	H	2.256033662	2.414977611	1.740487052
	C	-0.060579555	2.440909273	-1.567137081
	H	-0.71980667	3.269121907	-1.290231991
	H	0.699696835	2.818272123	-2.258214706
	H	-0.665145242	1.689541355	-2.083248353
	H	-3.081438483	0.541728804	0.076695047
	O	-2.096419108	-0.317280819	-1.236870592
	O	-2.962633765	0.856928061	-1.163207032
TS _{D3-1-5}	O	1.437124926	-0.341383374	0.35313802
	O	-0.421906442	-1.142434927	-1.39083095

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	Si	0.61783773	-1.681251154	-0.179617135
	Si	-0.921672346	0.408793655	-1.565824215
	Si	1.402647949	1.285757961	0.017265537
	O	0.274188606	1.473767654	-1.221082146
	C	0.88794985	2.238094931	1.522540858
	H	1.656752005	2.171254119	2.298823898
	H	0.737183109	3.294745083	1.280550108
	H	-0.04581507	1.830229361	1.920158846
	C	3.050093174	1.816611686	-0.66373355
	H	3.032856785	2.876260645	-0.936392206
	H	3.841658427	1.667230375	0.076656018
	H	3.302385382	1.237718061	-1.557037975
	C	-2.668472348	0.498806843	-0.483192643
	H	-3.31612965	1.374561742	-0.589245807
	C	-1.526944559	0.73738252	-3.290889499
	H	-2.314091998	0.032709979	-3.569908556
	H	-1.914348478	1.756025299	-3.374715856
	H	-0.689574552	0.626940147	-3.98726189
	C	1.808517863	-2.875336039	-0.963167133
	H	2.532888244	-3.240625866	-0.22905308
	H	1.278130005	-3.737367976	-1.379127812
	H	2.359303784	-2.389769728	-1.774097558
	C	-0.364632592	-2.428096852	1.2074907
	H	-0.94513739	-3.288398401	0.860047701
	H	0.295821787	-2.76314328	2.013044148
	H	-1.052727244	-1.681632359	1.616732678
	H	-3.136855028	-0.482644116	-0.636010172
	O	-1.637904164	0.574273457	0.34677939
	O	-2.083052075	0.344030912	2.33661605
TS _{D3-1-6}	O	-1.523067983	0.501935643	0.324099077
	O	0.510499906	1.076498234	-1.296470724
	Si	-0.61407022	1.764677623	-0.266065602
	Si	1.121144673	-0.443515687	-1.139149263
	Si	-1.42484341	-1.152094185	0.199203502
	O	-0.113368362	-1.473962319	-0.792755603
	C	-1.10888073	-1.877324772	1.881028974
	H	-0.171703458	-1.480266715	2.2839486
	H	-1.916419447	-1.628256284	2.57587413
	H	-1.022611874	-2.966846507	1.828227522
	C	-2.955273606	-1.816689676	-0.620390855
	H	-2.883718388	-2.899808614	-0.757511563
	H	-3.842914639	-1.605428219	-0.016592161
	H	-3.092275999	-1.355941694	-1.603137199

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	C	4.335875621	-0.137748573	0.006951725
	H	4.986347013	0.005840015	-0.850005011
	C	2.084402893	-0.934305466	-2.63384631
	H	1.432509122	-0.978823208	-3.510119916
	H	2.87172918	-0.201693039	-2.831718666
	H	2.543790502	-1.916085218	-2.491462011
	C	-1.694905951	2.91033195	-1.251608324
	H	-2.480062276	3.341127634	-0.623115519
	H	-1.1067325	3.729856415	-1.675349543
	H	-2.172575865	2.37144456	-2.075023273
	C	0.276578322	2.592488029	1.140214257
	H	0.886344911	3.426160706	0.778998519
	H	-0.423886169	2.973379076	1.889205707
	H	0.944138952	1.869986208	1.621351754
	H	4.541567841	-0.851447768	0.796714499
	O	3.185703927	0.494581893	0.003415615
	O	2.058246425	-0.519676182	0.270001176
TS _{D3-2-1}	O	1.721733289	-0.273694667	-0.244732551
	O	0.14988742	1.411151057	1.096324926
	Si	1.219642841	1.306661438	-0.183676772
	Si	-1.155279111	0.383453574	1.015742748
	Si	0.872427437	-1.652259335	0.173503898
	O	-0.517668901	-1.140366055	0.943934805
	C	0.401766688	-2.565643212	-1.37686417
	H	1.286264852	-2.837814819	-1.96048314
	H	-0.149437732	-3.480517327	-1.13897569
	H	-0.243171286	-1.937426136	-1.999972208
	C	1.890751604	-2.663645216	1.352062036
	H	1.340145998	-3.550409335	1.679660724
	H	2.821336737	-2.992489853	0.879971434
	H	2.146108266	-2.073069561	2.236625176
	C	-2.343865917	0.554381961	2.415189221
	H	-2.686424326	1.587829853	2.50160747
	H	-3.212223666	-0.090422756	2.258259531
	H	-1.860108837	0.260114859	3.350367057
	C	2.65349061	2.453540971	0.04519827
	H	3.354981168	2.369384646	-0.789273564
	H	2.312963806	3.490472979	0.110808863
	H	3.185129084	2.204829667	0.96780127
	C	0.121771729	1.614281009	-1.674520882
	H	-0.111589499	2.659825002	-1.891617805
	H	0.366021355	1.070840683	-2.590172292
	H	-0.9278673	1.173302942	-1.300716415

Supporting Information

	O	-1.94441753	0.751842649	-0.424384889
TS _{D3-2-2}	O	0.010402377	-1.492655461	0.117542959
	O	-1.320854677	0.801324854	-0.146581353
	Si	-1.51820416	-0.8478412	0.042647521
	Si	-0.002918145	1.774064625	-0.152332683
	Si	1.533750787	-0.832333767	0.079736261
	O	1.324298102	0.814742132	-0.114600052
	C	2.391259972	-1.143571127	1.698333661
	H	2.529787224	-2.215852745	1.866670053
	H	3.374008349	-0.663032909	1.717280854
	H	1.801337444	-0.741554663	2.527591511
	C	2.466877947	-1.492705894	-1.385456988
	H	3.453836239	-1.026497124	-1.461136899
	H	2.605120051	-2.574891268	-1.302704377
	H	1.921143225	-1.289110045	-2.311599219
	C	0.003694576	3.207995016	-1.299561996
	H	-0.9130889	3.55814858	-1.77020942
	H	-0.013557142	3.725678577	-0.092035496
	H	0.928003952	3.567510553	-1.747902826
TS _{D3-3-1}	C	-2.408646099	-1.517345998	-1.444799778
	H	-2.537956567	-2.600882384	-1.365352072
	H	-3.398113436	-1.061086856	-1.544535615
	H	-1.842594568	-1.308108174	-2.357390234
	C	-2.411656253	-1.168130366	1.639898351
	H	-3.399530791	-0.69786501	1.634778144
	H	-2.543064253	-2.241812436	1.804983223
	H	-1.846366152	-0.760053371	2.483232509
	O	-0.023058232	2.971335667	1.007786022
	O	-1.86730958	0.3931948	-0.439958846
	O	-0.244712209	-1.383203989	0.740824633
	Si	-1.513421805	-1.233138816	-0.323776261
	Si	0.879695984	-0.315149578	1.317970715
	Si	-0.899588243	1.681133456	-0.063409519

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	H	1.926335637	0.393000868	3.425538547
	H	0.213041046	0.029779644	3.656637698
	C	-2.989315952	-2.135403128	0.351136129
	H	-3.847473955	-2.029264362	-0.319396078
	H	-2.772091575	-3.201492754	0.465253855
	H	-3.268274811	-1.73610929	1.330301336
	C	-0.971307062	-1.851369726	-1.995583861
	H	-0.660776907	-2.89926452	-1.945025206
	H	-1.777261829	-1.764686689	-2.730647767
	H	-0.120153937	-1.263493339	-2.355707916
	H	2.842528967	0.725809471	0.193147789
	O	2.616469611	-1.267139468	-0.201252683
	O	2.354740248	-1.545662965	1.115864499
	O	0.036419566	2.054798926	-1.38987492
	H	-0.420844676	2.312195282	-2.19586704
TS _{D3-3-2}	O	-1.166298492	0.183337639	1.123034413
	O	1.067074773	-1.170779152	0.565500282
	Si	-0.548461597	-1.338222751	0.882729038
	Si	1.827725467	0.014135526	-0.324943832
	Si	-0.683051502	1.591230139	0.376339658
	O	0.847808519	1.350009162	-0.198763771
	C	-1.822951004	1.895738384	-1.063927409
	H	-2.885097463	2.036457912	-0.85207609
	H	-1.474945069	2.546107024	-1.868734835
	H	-1.8397568	0.672899728	-1.694664959
	C	-0.708406404	2.978885289	1.610324397
	H	-0.379994783	3.91548816	1.151387598
	H	-1.716554338	3.123260743	2.009280642
	H	-0.038231016	2.749482947	2.444274789
	C	3.509943271	0.353626443	0.348156423
	H	4.136868739	-0.53812942	0.266698468
	H	3.987831754	1.161238459	-0.212212953
	H	3.454957475	0.645012236	1.400154353
	C	-0.842541662	-2.419847798	2.355267774
	H	-1.912522652	-2.527032755	2.554644521
	H	-0.416071323	-3.41447558	2.197296866
	H	-0.372186224	-1.983991037	3.241121942
	H	1.15636235	-0.675893609	-2.337333325
	O	1.98300404	-0.441893013	-1.893766595
	C	-1.312992206	-1.987376852	-0.726161084
	H	-0.952930399	-2.986076763	-0.999611964
	H	-2.406208909	-2.001345769	-0.739079986
	O	-0.864091439	-1.097935322	-1.780751376

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	O	-1.911946917	-0.332853218	-2.261536436
TS _{D3-3-3}	O	-0.407737077	1.200884519	0.676412332
	O	-0.385093652	-1.410775642	0.111683927
	Si	-1.207406981	-0.2240419	0.918302993
	Si	1.149935629	-1.444676289	-0.524972028
	Si	0.971588086	1.579498537	-0.182430454
	O	1.565293816	0.137183929	-0.763234537
	C	0.52347726	2.676261366	-1.614124849
	H	0.108397258	3.625750318	-1.263100913
	H	1.403388575	2.893452798	-2.227108283
	H	-0.223543974	2.194006166	-2.252011048
	C	2.211852768	2.347532499	0.968648044
	H	3.140198805	2.583713815	0.440049496
	H	1.81972385	3.271755921	1.403580525
	H	2.450968852	1.661227148	1.786843015
	C	2.325511558	-2.298197465	0.613494644
	H	2.020295347	-3.33533634	0.774994637
	H	3.335221728	-2.297844518	0.19480816
	H	2.354863764	-1.792118406	1.583342449
	C	-1.419380288	-0.602186827	2.718236006
	H	-1.335413941	0.205884717	3.44530534
	H	-2.804794815	-0.755106038	2.652297794
	H	-1.090893172	-1.57054859	3.096072369
	H	0.597001765	-1.947171084	-2.666726574
	O	1.149464411	-2.265395435	-1.947034497
	C	-2.981785686	-0.106224469	0.23463031
	H	-3.082023192	0.690268952	-0.5097718
	H	-3.334413325	-1.052851214	-0.192081595
	O	-3.838653955	0.285027619	1.313864837
	O	-3.881066241	-0.751114936	2.22869785
TS _{D3-3-4}	O	-1.231776453	0.900415539	-0.340556364
	O	1.417538408	0.574423506	-0.291281028
	Si	0.199775276	1.687604773	-0.067978926
	Si	1.386792627	-1.043999411	0.024233861
	Si	-1.633784755	-0.696280112	-0.063347325
	O	-0.185947775	-1.522962037	0.022626381
	C	-2.532937996	-0.853109741	1.553247896
	H	-3.476943353	-0.299910804	1.531113872
	H	-2.755483324	-1.90081214	1.77675769
	H	-1.91354059	-0.452756175	2.361665596
	C	-2.60636533	-1.323143598	-1.516943886
	H	-2.863074192	-2.378844275	-1.387553545

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	H	-3.535710089	-0.75713856	-1.632642886
	H	-2.028317926	-1.221764253	-2.440016978
	C	2.387294094	-2.049905478	-1.156290354
	H	3.408411487	-1.665898086	-1.214524916
	H	2.427741383	-3.093387338	-0.832320654
	H	1.937165148	-2.018755553	-2.1522315
	C	0.402996455	3.117901469	-1.226673395
	H	-0.381540288	3.863463474	-1.067545457
	H	1.374262965	3.599080251	-1.080461139
	H	0.341624218	2.77642981	-2.263793349
	H	1.664552208	-0.284711413	2.603491968
	O	2.067292626	-1.241971498	1.55494209
	C	0.192430378	2.174970075	1.762005929
	H	1.005483559	2.837330883	2.076198158
	H	-0.756917631	2.656583286	2.025870508
	O	0.228757008	0.984591969	2.573010395
	O	1.577092374	0.697619727	2.835985268
TS _{D3-3-5}	O	-0.410331716	1.231021059	0.918635754
	O	-0.031724899	-1.416210497	0.89357051
	Si	-1.12934775	-0.222292373	1.193033324
	Si	1.141518704	-1.439925697	-0.298525811
	Si	0.923680187	1.598367502	-0.0313047
	O	1.556166824	0.142895959	-0.525650159
	C	0.391254483	2.584272266	-1.509078701
	H	-0.053499	3.536427331	-1.203690776
	H	1.248027738	2.796510743	-2.15603436
	H	-0.355888927	2.030033337	-2.084260222
	C	2.164877958	2.482668587	1.033780685
	H	3.066725286	2.719935042	0.46148079
	H	1.748830232	3.418344861	1.419326771
	H	2.45563291	1.861214186	1.886038213
	C	2.573293695	-2.465673582	0.244586684
	H	2.263598566	-3.503754462	0.390602303
	H	3.361617124	-2.445740569	-0.512277089
	H	2.983622875	-2.08901194	1.185024562
	C	-1.866166191	-0.346162555	2.882160496
	H	-2.617724334	0.433469202	3.035014626
	H	-2.338713518	-1.321167917	3.030165956
	H	-1.088769127	-0.224703892	3.64146067
	H	-0.177106563	-1.603472932	-2.110900485
	O	0.538606412	-2.089619657	-1.681782808
	C	-2.432188512	-0.412953138	-0.172937604
	H	-3.302938553	-1.07482979	-0.171740144

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	H	-2.895489122	0.790879944	-0.462755866
	O	-1.818039786	-0.351490222	-1.439126553
	O	-2.542715545	0.888592674	-1.692707446
TS _{D3-3-6}	O	-1.464850228	0.779150498	-0.423748267
	O	-0.357709034	-1.455588855	0.514497253
	Si	-1.671801238	-0.869970706	-0.333456401
	Si	1.072426235	-0.733406225	0.879645266
	Si	-0.32924471	1.827492686	0.158684905
	O	0.815238098	0.893380586	0.921685451
	C	-1.032300851	3.054255531	1.343636366
	H	-0.253592954	3.742551936	1.682992379
	H	-1.821878565	3.638684412	0.864450584
	H	-1.453001625	2.550476142	2.217940044
	C	2.39347594	0.412094722	-2.128124278
	H	2.921581566	1.099533296	-1.475920624
	C	1.823738762	-1.388596004	2.429979361
	H	2.013081724	-2.461114825	2.33965521
	H	2.768670204	-0.88320528	2.643869868
	H	1.145567122	-1.227770832	3.272349075
	C	-3.215154087	-1.249504484	0.630885186
	H	-4.098590093	-0.853885266	0.120742951
	H	-3.342969344	-2.329810455	0.748730902
	H	-3.16741595	-0.801184158	1.627708485
	C	-1.686718697	-1.58784015	-2.046173127
	H	-1.861689155	-2.667552947	-2.014539807
	H	-2.473379318	-1.129890737	-2.653451117
	H	-0.722465288	-1.413225487	-2.532038591
	H	2.675996449	0.238358137	-3.161904027
TS _{D3-4-1}	O	1.546532997	-0.442565452	-1.589093115
	O	2.19336255	-1.053430927	-0.344689618
	O	0.338730019	2.670755016	-1.088164397
	H	0.56948247	2.172032548	-1.880318279
	O	-1.277789896	0.766741647	-1.250845064
	O	1.350613161	0.468734673	-0.997932133
	Si	0.089488861	1.482394996	-0.643329239
	Si	1.335786134	-1.135818537	-0.548423954

Supporting Information

	C	-3.027128382	-1.541365377	-1.547373678
	H	-3.258270633	-2.523725528	-1.126791832
	H	-3.924351639	-0.918993756	-1.493678935
	H	-2.757688524	-1.671210442	-2.599145901
	C	2.495307109	-2.166752137	-1.53788953
	H	3.516632245	-1.790939934	-1.439578334
	H	2.473699437	-3.200519232	-1.182872502
	H	2.216564559	-2.15743839	-2.594312263
	C	0.389771883	3.193841979	-1.251456321
	H	-0.48284902	3.823327848	-1.063794248
	H	1.253861687	3.632710987	-0.746509204
	H	0.590258043	3.175016329	-2.325965017
	H	1.472052208	-0.464301894	1.58503658
	O	1.738157069	-1.22266124	1.049057383
	O	-0.099368013	1.470305161	1.041073724
TS _{D3-4-2}	O	0.181712277	-1.503366501	-0.110423897
	O	-1.388672527	0.5592198	-0.645729492
	Si	-1.305336844	-0.868228485	0.207631696
	Si	-0.240522861	1.644904918	-0.120497589
	Si	1.628709472	-0.667539141	-0.248904423
	O	1.22069246	0.948686661	-0.430370396
	C	2.595519805	-0.872165843	1.323069665
	H	2.838736495	-1.923619124	1.502595868
	H	3.528543758	-0.301828904	1.289628089
	H	2.002140493	-0.508809646	2.168275874
	C	2.516353934	-1.242517692	-1.773250986
	H	3.447312453	-0.685403483	-1.913803928
	H	2.760725912	-2.306493756	-1.702180196
	H	1.890638356	-1.09297733	-2.65777524
	C	-0.381082509	3.335652673	-0.832730378
	H	-0.175301851	3.30247686	-1.905816305
	H	-1.385116216	3.735360084	-0.675287495
	H	0.342243161	4.00703855	-0.363473249
	C	-2.667170468	-2.059250325	-0.127845691
	H	-2.592587033	-2.920040579	0.541214027
	H	-3.638349292	-1.582243056	0.020181812
	H	-2.599476262	-2.416664031	-1.158686872
	H	-1.086856687	0.771601373	1.958669428
	O	-0.490395091	1.689144926	1.546775171
	O	-1.356994806	-0.35709506	1.813983636
TS _{D3-4-3}	O	0.618049848	-1.12449684	-0.765578818
	O	-1.54973773	-0.410248448	0.556422219

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	Si	-0.740541694	-1.729691861	-0.021699492
	Si	-1.447275254	1.220273392	0.247571443
	Si	1.129326848	0.396529226	-1.10750485
	O	-0.069930322	1.426403065	-0.678536803
	C	1.986718418	0.675269429	-2.705650535
	H	2.897246855	0.876834112	-1.779792252
	H	2.362618398	-0.158396501	-3.295930226
	H	1.904870007	1.624125967	-3.232429478
	C	-2.915557872	1.770964845	-0.749474169
	H	-3.843845601	1.6246985	-0.189255401
	H	-2.83398385	2.831220574	-1.007211782
	H	-2.985419628	1.199365495	-1.679987084
	C	-1.773857799	-2.70317381	-1.199299518
	H	-1.208806442	-3.551629407	-1.593673355
	H	-2.664243721	-3.0882693	-0.695446492
	H	-2.095103699	-2.080051064	-2.038747053
	O	2.627686728	0.766547983	-0.477383152
	O	-0.305013475	-2.734848132	1.200563428
	H	0.338214243	-2.431238209	1.847842519
	C	-1.257090524	2.140203365	1.849199935
	H	-1.149313939	3.213887311	1.668908131
	H	-2.129049364	1.985205695	2.491573037
	H	-0.369819471	1.796407222	2.388838978
TS _{D3-5-1}	O	-1.244126401	0.834343658	-0.681007783
	O	1.37623411	0.516405419	-0.893772575
	Si	0.18528734	1.662299758	-0.661072903
	Si	1.365402518	-0.888100779	-0.034538809
	Si	-1.620340649	-0.692852171	-0.048668264
	O	-0.166387746	-1.506261552	-0.052538691
	C	-1.788191048	0.108421351	1.877216357
	H	-2.773901359	0.572592739	1.758597659
	H	-1.036244297	0.72183024	2.36730364
	C	-2.883436645	-1.281877193	-1.274711592
	H	-3.104213679	-2.343487839	-1.139489153
	H	-3.815566132	-0.721433461	-1.147931316
	H	-2.526151575	-1.104883238	-2.292072517
	C	2.574744756	-2.126106021	-0.668882768
	H	3.591647058	-1.728876537	-0.61921552
	H	2.530915819	-3.047849324	-0.082107912
	H	2.348983906	-2.375362807	-1.708896577
	C	0.20124037	2.970107651	-1.957751317
	H	-0.538717808	3.73972559	-1.721729971
	H	1.184533394	3.444459045	-2.007970279

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	H	-0.038644519	2.548920364	-2.936994921
	H	1.583729294	-1.012611476	2.23704103
	O	1.690175662	-0.374681832	1.523955816
	O	-1.883513622	-1.15619088	2.390012871
	O	-2.372808467	-1.849405873	1.310327936
	O	0.448756974	2.316534836	0.83800699
	H	1.062312563	1.805764973	1.384777759
TS _{D3-5-2}	O	0.113109323	-1.352280291	-0.34039199
	O	-2.102276943	0.074371863	-0.378117315
	Si	-1.497904986	-1.415286369	0.068956326
	Si	-1.343709472	1.474525438	0.035372817
	Si	1.155321257	-0.073147918	-0.428929591
	O	0.254955222	1.325761187	-0.376508313
	C	2.349333846	-0.113945408	1.057773375
	H	1.954822327	-0.730572366	1.871982077
	H	2.593889	0.885440462	1.437725578
	C	2.246014231	-0.142244816	-1.918131783
	H	3.443836674	-0.029056317	-1.200481143
	H	2.397211657	-1.098745466	-2.418700122
	H	2.280350136	0.717156094	-2.58712918
	C	-2.089620557	2.964639707	-0.750510624
	H	-3.141727476	3.056393131	-0.469296279
	H	-1.56629991	3.87311076	-0.43916421
	H	-2.025520258	2.892066612	-1.839145399
	C	-2.324247178	-2.813273212	-0.793175641
	H	-2.166969427	-2.751423328	-1.872576966
	H	-1.91617076	-3.76321688	-0.437512338
	H	-3.398121209	-2.804548124	-0.591322394
	H	-0.969350591	2.153111406	2.19467344
	O	-1.443140705	1.476441161	1.701584873
	O	3.548172684	-0.773416494	0.635778898
	O	4.171396558	0.02373607	-0.306976591
	O	-1.669055798	-1.558525124	1.700090279
	H	-1.702824935	-0.72242375	2.185679675
TS _{D3-5-3}	O	-0.613234707	-1.527491027	-0.24321252
	O	-1.484625556	0.954588251	0.149759833
	Si	-1.864607213	-0.631551336	0.351367445
	Si	-0.075447911	1.746722107	-0.24584857
	Si	0.959610999	-1.037234475	-0.489543731
	O	0.903646953	0.567513944	-0.895663678
	C	1.823811852	-1.089741721	1.1968403
	H	2.781000943	-0.555556119	1.170348163

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	H	1.997262439	-2.084812679	1.615099832
	C	1.769117475	-2.0447214	-1.81253187
	H	2.802057759	-1.721658115	-1.970328011
	H	1.772581052	-3.10532188	-1.54613417
	H	1.228999989	-1.930211169	-2.756526844
	C	-0.376842815	3.092519575	-1.466021047
	H	-1.064189091	3.834413991	-1.051923087
	H	0.562211614	3.594618248	-1.712767448
	H	-0.808407562	2.691788626	-2.386659468
	C	-3.50305335	-1.034231972	-0.393916248
	H	-3.696243085	-2.107561543	-0.331291772
	H	-4.302917303	-0.505253601	0.130920574
	H	-3.521557552	-0.728281867	-1.443503485
	O	1.00545639	-0.34443962	2.129980315
	O	0.233820584	-1.257390346	2.859734691
	O	-1.962165617	-1.005942069	1.995404107
	H	-0.732512315	-0.943793868	2.725501289
	O	0.605165437	2.399607257	1.097108716
	H	0.757752981	1.794471808	1.835075815
TS _{D3-5-4}	O	-0.380869696	1.166354392	-0.716791364
	O	2.034048199	0.163342637	-0.326096171
	Si	1.089313397	1.506305928	-0.019608746
	Si	1.507845026	-1.351346545	0.048504908
	Si	-1.197298151	-0.266082437	-0.604964321
	O	-0.066713281	-1.480316903	-0.455853695
	C	-2.168676891	-0.260125226	1.012911773
	H	-1.561361566	0.621110293	1.776630064
	H	-2.320178938	-1.143540972	1.641908283
	C	-2.296890153	-0.514441078	-2.068973727
	H	-2.801392175	-1.483069671	-2.018409959
	H	-3.05658047	0.2718952	-2.09484449
	H	-1.715902309	-0.469440561	-2.994317072
	C	2.542880408	-2.684120508	-0.691769263
	H	3.577939416	-2.598884653	-0.351706067
	H	2.164942148	-3.67142981	-0.411133826
	H	2.52823107	-2.613407344	-1.782444585
	C	1.790559024	3.052127146	-0.724279945
	H	1.859196679	2.98333382	-1.812563399
	H	1.148727117	3.900030207	-0.470654534
	H	2.787361752	3.239692661	-0.317766054
	H	1.161892939	-2.108371855	2.188370619
	O	1.515919259	-1.348429327	1.716874701
	O	-3.267514635	0.606834565	1.024985754

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	O	-2.554886503	1.42289727	2.004937799
	O	0.903694299	1.591021282	1.618301276
	H	1.199262615	0.8111317	2.109041133
TS _{D3-5-5}	O	0.207542923	1.098382117	1.024270915
	O	-1.77297752	0.025731486	-0.350823051
	Si	-1.004231783	1.465820015	-0.067664956
	Si	-1.427786408	-1.569481731	-0.078219655
	Si	0.961598034	-0.362114553	1.002208301
	O	-0.165590634	-1.557666683	1.024586228
	C	3.609006489	0.339455704	-1.244284255
	H	3.727514839	-0.465250339	-1.959987159
	H	4.43508366	0.797632644	-0.71140006
	C	2.257416918	-0.497926784	2.300272583
	H	2.728475182	-1.483323481	2.270301137
	H	3.024616413	0.265866227	2.144772953
	H	1.822260495	-0.346702289	3.291341457
	C	-2.882765663	-2.48539192	0.580802351
	H	-3.695474049	-2.474944005	-0.15014486
	H	-2.616766156	-3.525454159	0.785488723
	H	-3.241041224	-2.027105589	1.505894662
	C	-2.182727869	2.717235247	0.59380875
	H	-1.657065896	3.642863011	0.840991556
	H	-2.944369101	2.945087637	-0.156832419
	H	-2.682479579	2.345501327	1.491615814
	H	-0.115270838	-1.94911572	-1.850344741
TS _{D3-6-1}	O	-0.925519442	-2.302064894	-1.462602156
	O	2.390849555	0.685961612	-0.873529191
	O	1.577546314	-0.573276602	-0.579136388
	O	-0.309107719	2.053686649	-1.436491458
	H	0.564304057	1.708176313	-1.6614123
	O	0.593312557	-1.132080639	-0.850368197
	O	-1.467152159	-0.408650978	0.619701684
	Si	-0.718583964	-1.735951072	-0.025279513
	Si	-1.425196748	1.208169156	0.270104304
	Si	1.147392011	0.391194253	-1.098148705
	O	-0.020953117	1.425587365	-0.594394709
	C	2.011684155	0.756435761	-2.673565361
	H	2.9242452	0.881755548	-1.736302303
	H	2.3747411	-0.043820339	-3.315612317
	H	1.946649862	1.738925934	-3.137166869
	C	-2.897004335	1.744680431	-0.702197952
	H	-3.811050732	1.592873496	-0.122220132

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	H	-2.821595163	2.805725391	-0.953575506
	H	-2.977550462	1.173319471	-1.631271799
	C	-1.834092771	-2.682941097	-1.147020357
	H	-1.301127106	-3.528202206	-1.589933859
	H	-2.691705655	-3.070485298	-0.590951362
	H	-2.204589117	-2.045254175	-1.954616518
	H	-0.648598155	2.001343324	2.252782406
	O	-1.389107049	2.098908054	1.647144193
	O	2.650394112	0.686536432	-0.442727313
	O	-0.224371092	-2.75669439	1.159956466
	H	0.419940698	-2.452765503	1.805838929
TS _{D3-6-2}	O	0.218094145	-1.490205558	-0.221759079
	O	-1.395684958	0.524286476	-0.815682444
	Si	-1.317529148	-0.929051531	-0.00791337
	Si	-0.324755252	1.626436936	-0.17593943
	Si	1.632042462	-0.608524364	-0.147452261
	O	1.177464649	0.978930332	-0.383043946
	C	2.840556522	-1.161235548	-1.420372985
	H	3.749529432	-0.556750341	-1.363403134
	H	3.112149638	-2.206610762	-1.25214488
	H	2.419371845	-1.066171433	-2.424037316
	C	-0.462177089	3.332202551	-0.848010906
	H	-0.17116628	3.337461748	-1.90171779
	H	-1.487728552	3.697145983	-0.76065888
	H	0.200456767	4.009547921	-0.303799773
	C	-2.596915501	-2.159984817	-0.48556898
	H	-2.539063597	-3.038758368	0.161312282
	H	-3.595810806	-1.72656568	-0.402334114
	H	-2.432787357	-2.480016972	-1.517872643
	H	-1.307934674	0.662487356	1.798427626
TS _{D3-7-1}	O	-0.691374211	1.601312468	1.472145499
	O	-1.496783472	-0.47624509	1.608996694
	O	2.326559502	-0.78183607	1.331554538
	H	1.808969115	-0.530054998	2.104218352
	O	-1.141650362	0.847263223	-0.42433753
	O	1.272454043	0.753522391	0.615061753
	Si	0.262485682	1.720481792	-0.297259437
	Si	1.325229228	-0.869072149	0.327545445

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	H	-1.557145032	0.668478992	2.712172536
	O	-2.449884803	-1.155032646	2.418620473
	O	-2.679242841	-1.780497494	1.217327144
	C	-0.021987845	3.356723398	0.503606245
	H	0.92550066	3.883576638	0.641281967
	H	-0.67061893	3.97522195	-0.122537262
	H	-0.497677396	3.237160205	1.480963748
	C	2.478113281	-1.750333478	1.462473766
	H	3.497568434	-1.376912013	1.337700619
	H	2.176565036	-1.598121929	2.502068789
	H	2.47305019	-2.82526159	1.262043847
	O	0.930618286	1.950767761	-1.781274291
	H	1.363678487	1.165872709	-2.144587874
	O	-2.488675964	-1.188030705	-1.143105493
	H	-2.35222176	-0.658423842	-1.935630147
	O	1.761077227	-0.958933473	-1.280686422
	H	1.598628516	-1.786310718	-1.744774534
TS _{D3-7-2}	O	0.263904109	-1.423844518	0.452546625
	O	1.815961791	0.671827729	-0.099776077
	Si	1.817102328	-0.97160347	0.123493258
	Si	0.587570584	1.77100914	-0.183503862
	Si	-1.143859259	-0.570154773	0.437540509
	O	-0.74166693	1.02956472	0.469735595
	C	-2.208594722	-0.929854575	-1.070943764
	H	-3.246043605	-0.641847227	-0.87199064
	H	-2.193545491	-2.002924544	-1.303071961
	O	-1.848935182	-0.188033684	-2.239931587
	O	-0.470600021	-0.236445419	-2.405774345
	C	2.473453848	-1.808975874	-1.387523347
	H	3.492212234	-1.478198439	-1.611326329
	H	2.483543278	-2.89416805	-1.255458408
	H	1.838655454	-1.571032322	-2.246260028
	C	0.245574011	2.144791865	-1.954917406
	H	1.078295121	2.346797205	-2.628735197
	H	-0.128831521	0.872952445	-2.302357179
	H	-0.661222937	2.693322355	-2.212834705
	O	2.667912352	-1.344171108	1.485981692
	H	3.618111022	-1.200473242	1.487474567
	O	-2.067362311	-1.009416072	1.717771406
	H	-1.621780525	-1.282047075	2.526024609
	O	0.939445917	3.142934235	0.637158627
	H	1.032767835	3.097301496	1.593803296

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TS _{D3-7-3}	O	0.178588178	-1.384468861	-0.152881113
	O	-1.304299303	0.468351577	1.057305296
	Si	-1.347902639	-1.046114445	0.412467154
	Si	-0.734673888	1.766767976	0.178555132
	Si	1.257933447	-0.311152749	-0.785602392
	O	0.675390116	1.194344485	-0.515701633
	C	2.987513305	-0.504482481	0.062644315
	H	2.77085406	-0.595585425	1.135402827
	H	3.6169117	0.368505686	-0.135206665
	O	3.62057869	-1.694199177	-0.309943875
	O	4.194473315	-1.498724821	-1.582529075
	C	-0.38058934	3.236079419	1.225054025
	H	-1.290689208	3.570764602	1.728694536
	H	0.37458352	3.006072442	1.9803742
	H	-0.011297195	4.05615381	0.603538632
	O	-2.342152103	-0.868947556	-0.911871519
	H	-2.36517738	-1.569930491	-1.571115567
	O	1.726347068	-0.676969259	-2.306642498
	H	3.415614856	-1.567419951	-2.18004596
	O	-1.830160789	2.143832508	-0.982453723
	H	-2.31297355	1.391447855	-1.352105404
	C	-1.895900506	-2.328995901	1.612235246
	H	-2.902367417	-2.106405054	1.975067864
	H	-1.904184671	-3.318347273	1.146682923
	H	-1.216710487	-2.361938686	2.467897486
TS _{D3-7-4}	O	0.572265695	-1.535255089	0.548099571
	O	1.431882503	0.835149522	-0.227570355
	Si	1.745059311	-0.778948869	-0.374911539
	Si	0.14069139	1.73523605	0.29314096
	Si	-0.924359264	-0.98650892	0.941282542
	O	-0.847516926	0.643770447	1.078562031
	C	-2.112373116	-1.326929178	-0.464767095
	H	-3.066047669	-0.425943877	-0.349831586
	H	-2.610709664	-2.270164078	-0.698375321
	O	-1.716628138	-0.615288221	-1.611117905
	O	-2.894245358	0.232642884	-1.441519154
	C	-0.679459727	2.608943467	-1.102293396
	H	-1.59970058	3.091529363	-0.763861997
	H	-0.010594909	3.376398562	-1.501744904
	H	-0.933842976	1.904929293	-1.898144882
	O	3.231378948	-1.126457945	0.231229859
	H	3.505983055	-0.712408451	1.054262745
	O	-1.506647471	-1.733071309	2.271036097

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	H	-0.893279097	-2.074864929	2.92796195
	O	0.623688111	2.866755827	1.384048326
	H	0.885961981	2.578899688	2.262944403
	C	1.678190923	-1.37127715	-2.117725946
	H	2.40537293	-0.834272419	-2.732081481
	H	1.906865832	-2.439216541	-2.167563344
	H	0.680141007	-1.206301147	-2.534343199
TS _{D3-7-5}	O	0.671651746	1.200318288	0.685301064
	O	-1.155395111	0.2097697	-0.925953088
	Si	-0.797183523	1.559513899	-0.015665462
	Si	-1.144293031	-1.301188759	-0.254236119
	Si	1.374514409	-0.273344908	0.868415373
	O	0.212341521	-1.41743652	0.693710179
	C	1.797904336	0.412277148	-2.320067728
	H	2.764762814	0.878725379	-2.466094129
	H	0.860186159	0.802429686	-2.701227068
	O	1.714985921	-0.672628509	-1.577285701
	O	2.545973491	-0.50628272	-0.303295061
	C	-0.663062595	3.101993519	-1.011548557
	H	-1.561269735	3.247495246	-1.616941563
	H	-0.562338895	3.959854498	-0.340570034
	H	0.210551411	3.077749957	-1.667451197
	C	-1.214581782	-2.630888314	-1.525212908
	H	-2.124452829	-2.544126324	-2.12447462
	H	-0.345308567	-2.554279902	-2.18369123
	H	-1.200599487	-3.618193263	-1.055321081
	O	-1.96265559	1.727939083	1.131219482
	H	-2.453046734	0.920370003	1.341930711
	O	2.136570319	-0.389826367	2.301413083
	H	2.180871163	0.401769725	2.845528819
	O	-2.447828615	-1.282304553	0.782407288
	H	-2.466687874	-1.937764793	1.487091466
TS _{D3-8-1}	O	1.627070044	-0.169248001	-0.341240734
	O	0.075582475	1.447179893	1.037359397
	Si	1.085850791	1.392050068	-0.284498252
	Si	-1.18880176	0.388564487	0.968427568
	Si	0.87099755	-1.583006352	0.109870791
	O	-0.514088785	-1.11486845	0.905409538
	C	0.492469543	-2.626887007	-1.35920355
	H	1.410789913	-2.887149913	-1.891790552
	H	-0.005448952	-3.550999035	-1.055177305
	H	-0.168667022	-2.088628223	-2.044647443

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	C	-0.040796585	1.738921723	-1.720892924
	H	-0.291614041	2.789758777	-1.880060549
	H	0.181026312	1.235420965	-2.663426241
	H	-1.073222169	1.261588643	-1.326571432
	O	-2.017784212	0.736844245	-0.441710537
	O	-2.220388556	0.490860314	2.219499885
	H	-2.301701096	-0.27729067	2.792442623
	O	2.321700895	2.452420892	-0.193603045
	H	3.055656465	2.267955032	0.400239928
	O	1.831650434	-2.44945214	1.121115861
	H	2.074098477	-2.070017118	1.970843465
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TS _{D3-8-2}	O	-0.114793239	-1.417259078	-0.198687094
	O	-1.263315283	0.941321927	-0.030358635
	Si	-1.591711311	-0.695930689	-0.016114592
	Si	0.118219526	1.794416804	-0.050993077
	Si	1.447255536	-0.917776966	0.01440603
	O	1.360505084	0.749750497	-0.004521618
	C	2.166140295	-1.525957358	1.596353158
	H	2.199332436	-2.618509799	1.602861136
	H	3.184579619	-1.149689997	1.720903965
	H	1.56795485	-1.192499187	2.448909141
	C	-2.42292696	-1.191152148	1.550121038
	H	-3.377853322	-0.670197058	1.655161632
	H	-2.615259303	-2.267168537	1.553885993
	H	-1.799586123	-0.947659699	2.415008565
	O	0.205162174	3.121000921	0.946576694
	O	0.219318239	3.027574681	-1.163548207
	H	0.257599949	3.692177229	-0.134931931
	O	-2.587882815	-1.073582028	-1.260031042
	H	-2.350147072	-0.82848054	-2.158679373
	O	2.402761424	-1.438183722	-1.209728998
	H	2.221243527	-1.162597543	-2.112652024
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TS _{D3-9-1}	O	-1.199871417	0.753697045	-0.809409981
	O	1.390439239	0.53722662	-0.382949219
	Si	0.163389217	1.617768869	-0.546835971
	Si	1.374196236	-1.059239006	0.076471991
	Si	-1.632304649	-0.721371664	-0.099320923
	O	-0.205316842	-1.546015854	-0.005878164
	C	-1.844750221	0.13149164	1.7946668
	H	-2.776077094	0.67823321	1.60543589
	H	-1.098359655	0.675937025	2.368866813
	O	-2.091095083	-1.127210448	2.276703978

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	O	-2.533481261	-1.774678836	1.152434079
	C	2.076486603	-1.231146078	1.773042787
	H	2.002531579	-2.265852962	2.116912873
	H	3.129677775	-0.937766933	1.782402687
	H	1.537548441	-0.590581374	2.477605978
	O	0.515605623	2.680365917	-1.739710786
	H	1.049385031	2.370018547	-2.476784216
	O	-2.7061236	-1.250449055	-1.227503962
	H	-2.679424196	-0.761668833	-2.056401007
	O	2.268188774	-1.96763165	-0.959925556
	H	1.838362724	-2.30596871	-1.750955651
	O	-0.077572258	2.486752808	0.828527287
	H	0.422714623	3.302637992	0.924861393
TS _{D3-9-2}	O	-0.299944804	-1.548752522	-0.220836841
	O	-1.911600562	0.512934992	0.084810844
	Si	-1.824805824	-1.125524503	0.220619386
	Si	-0.773044731	1.683129262	-0.181934205
	Si	1.074141167	-0.646946137	-0.3897271
	O	0.568691015	0.885740326	-0.73727548
	C	2.056340004	-0.648725192	1.205624338
	H	3.050100817	-0.200143314	1.1152194
	H	2.177185494	-1.675121376	1.569517883
	O	1.329020705	0.019655456	2.254384301
	O	1.639224112	1.367571052	2.242696789
	C	-0.414620613	2.574557534	1.388920318
	H	-0.029152411	3.592577086	1.326320641
	H	-1.08537604	2.424133889	2.234887163
	H	0.708990235	1.897754675	1.835947052
	O	-2.971981747	-1.802741224	-0.734711877
	H	-3.286207049	-1.295517149	-1.488261069
	O	2.023040144	-1.274288851	-1.564772074
	H	1.617433024	-1.720930904	-2.313612397
	O	-1.259440203	2.750805563	-1.327460646
	H	-1.058465587	2.553117932	-2.247179002
	O	-2.066005086	-1.663180677	1.740062324
	H	-2.96218319	-1.908956489	1.986709436
TS _{D3-9-3}	O	0.066442874	-1.324308355	-0.579706657
	O	-1.678248447	0.521830387	0.197687536
	Si	-1.368961087	-1.08354023	0.18702886
	Si	-0.748072296	1.856460162	-0.122255651
	Si	1.252281064	-0.268931937	-0.998590831
	O	0.676525877	1.240435085	-0.729512971

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	C	2.834530726	-0.552800601	0.079774835
	H	2.460019102	-0.667283979	1.106447709
	H	3.519231892	0.297549303	0.007654276
	O	3.468237559	-1.757233234	-0.241413233
	O	4.235503611	-1.543317951	-1.404863639
	C	-0.444126605	2.864412804	1.38640968
	H	-1.386328292	3.263585532	1.770513229
	H	0.016520408	2.256598236	2.169750356
	H	0.217573474	3.703972157	1.15869085
	O	-2.481231105	-1.93011642	-0.658047868
	H	-3.398512727	-1.898951784	-0.37161565
	O	1.925357697	-0.571967273	-2.452048382
	H	3.556709866	-1.574797146	-2.115153852
	O	-1.479128736	2.809946002	-1.235656563
	H	-1.701749056	2.450256417	-2.099423922
	O	-1.279835622	-1.545778815	1.757547718
	H	-1.159976567	-2.480779829	1.949249212
TS _{D3-9-4}	O	0.577117838	-1.536300177	0.558824624
TS _{D3-9-4}	O	1.496812576	0.857097349	-0.126654905
TS _{D3-9-4}	Si	1.735007364	-0.755545633	-0.29820126
TS _{D3-9-4}	Si	0.186187359	1.740721538	0.398899726
TS _{D3-9-4}	Si	-0.939565477	-0.995846195	0.946944327
TS _{D3-9-4}	O	-0.790797237	0.634165395	1.162323647
TS _{D3-9-4}	C	-2.096463156	-1.28255807	-0.500312965
TS _{D3-9-4}	H	-3.008135941	-0.683737414	-0.404746543
TS _{D3-9-4}	H	-2.383376078	-2.322861943	-0.674139012
TS _{D3-9-4}	O	-1.441985086	-0.770523177	-1.680054453
TS _{D3-9-4}	O	-0.717027295	-1.827511142	-2.247725624
TS _{D3-9-4}	C	-0.655617971	2.58364937	-1.003019761
TS _{D3-9-4}	H	-1.518544535	3.152065388	-0.646641647
TS _{D3-9-4}	H	0.029249841	3.273951764	-1.502375353
TS _{D3-9-4}	H	-0.99702447	1.841534784	-1.730319821
TS _{D3-9-4}	O	3.251253125	-1.13500686	0.158296103
TS _{D3-9-4}	H	3.802932465	-0.425605488	0.500586025
TS _{D3-9-4}	O	-1.532517704	-1.746300075	2.268485513
TS _{D3-9-4}	H	-1.039974741	-1.748979955	3.0943053
TS _{D3-9-4}	O	0.669249799	2.87937915	1.477793511
TS _{D3-9-4}	H	0.990538943	2.601537573	2.340341948
TS _{D3-9-4}	O	1.557356515	-1.254258249	-1.884343296
TS _{D3-9-4}	H	0.201720387	-1.429776712	-2.416451733
TS _{D3-9-5}	O	0.583117546	-1.566590033	0.469886728
TS _{D3-9-5}	O	1.435726626	0.811048907	-0.287263229

Supporting Information

	Si	1.769666454	-0.791592459	-0.376440222
	Si	0.143201665	1.70331089	0.259209876
	Si	-0.913607395	-1.025520913	0.885865739
	O	-0.817696565	0.601549925	1.059934815
	C	-2.139224362	-1.313794056	-0.494845516
	H	-3.107003298	-0.449466683	-0.267156756
	H	-2.621113828	-2.255130596	-0.766160834
	O	-1.818797399	-0.516182669	-1.604824636
	O	-2.987573834	0.306712644	-1.302006648
	C	-0.683829077	2.580305354	-1.127940417
	H	-1.607946395	3.052063122	-0.785427067
	H	-0.020728698	3.35655169	-1.520361823
	H	-0.928879729	1.878577587	-1.928186741
	O	3.259669596	-1.071435136	0.245564008
	H	3.61099946	-0.422268061	0.861594267
	O	-1.463451771	-1.799567491	2.212368528
	H	-0.833562591	-2.148459527	2.84988785
	O	0.644075383	2.817737398	1.360328825
	H	0.753548664	2.538262467	2.273690764
	O	1.730902195	-1.394994304	-1.890254285
	H	2.544409443	-1.376873357	-2.402159976
TS _{D3-9-6}	O	-1.134991667	0.566059579	-0.770176634
	O	1.228869756	1.153780013	0.226007675
	Si	-0.247299333	1.783366636	-0.109172701
	Si	1.87277554	-0.376059336	0.195485817
	Si	-0.860503167	-1.052575844	-0.795810507
	O	0.733311511	-1.308030123	-0.578460273
	C	-2.249761879	-0.422122201	2.233123731
	H	-2.887351174	0.210376558	1.628444549
	H	-2.124641312	-0.329127027	3.302579541
	O	-1.228101019	-1.061700954	1.630943503
	O	-1.752487068	-1.751522088	0.439307754
	C	2.26531436	-0.954215775	1.897576926
	H	2.629738819	-1.984375822	1.874310366
	H	3.041220448	-0.324297732	2.340924749
	H	1.373654719	-0.912276584	2.527894069
	O	-0.093957028	3.06968081	-1.111852183
	H	0.617062511	3.060112335	-1.758715999
	O	-1.337066856	-1.754067293	-2.182355964
	H	-2.267123175	-1.728413401	-2.42453214
	O	3.246785856	-0.406146549	-0.705099694
	H	3.16561285	-0.538678768	-1.654203758
	O	-1.04299468	2.315372146	1.216014691

Supporting Information

	H	-0.954250774	3.250440741	1.424256122
TS _{D3-10-1}	O	1.642338055	0.013912221	-0.433091692
	O	-0.01247223	1.450016229	1.015457032
	Si	1.039306242	1.547133389	-0.270522779
	Si	-1.199903371	0.318609841	0.845357642
	Si	1.085723787	-1.425712848	0.136908803
	O	-0.417787027	-1.134034198	0.75580426
	C	-0.062410281	1.946960177	-1.709763552
	H	-0.387512897	2.986957226	-1.779747685
	H	0.219852881	1.549323003	-2.685766504
	H	-1.061342978	1.357340386	-1.391223959
	O	-1.980164909	0.661887002	-0.593141876
	O	-2.307853355	0.29125027	2.030806081
	H	-2.232579444	-0.39509394	2.700695407
	O	2.223579332	2.644157521	-0.05575045
	H	2.939156959	2.450726698	0.558163263
	O	2.132627322	-1.963466276	1.266871001
	H	2.275799226	-2.913176314	1.315791548
	O	0.990249049	-2.576734895	-1.022351107
	H	0.215567527	-2.586330293	-1.592211571
TS _{D3-10-2}	O	-0.137600339	-1.580334237	0.007105623
	O	-1.081144508	0.859368461	-0.447066272
	Si	-1.554340347	-0.728591625	-0.21989354
	Si	0.399855107	1.510900034	-0.177019531
	Si	1.360592	-0.987684052	0.277483317
	O	1.499454917	0.372875279	-0.657748023
	C	-2.675207206	-0.869305391	1.23089337
	H	-3.593020606	-0.299988869	1.063095521
	H	-2.941858814	-1.913895828	1.409610004
	H	-2.180565398	-0.476714383	2.123980963
	O	0.68246635	1.656496913	1.469172055
	O	0.554599181	2.96381771	-0.873668434
	H	-0.147841078	3.265904669	-1.457438524
	O	-2.327005251	-1.288114647	-1.552245654
	H	-1.821743752	-1.43550867	-2.357390118
	O	2.459003045	-2.145884564	0.010315886
	H	3.37701151	-1.99235096	0.252537804
	O	1.489409616	-0.393304513	1.842089908
	H	1.262554724	0.755444773	1.929244706
TS _{D3-10-3}	O	-1.176372246	-0.775385035	0.713744886
	O	-0.041530997	1.465398971	-0.036670108

Supporting Information

	Si	-1.537651452	0.721465635	0.073159673
	Si	1.478340506	0.926608952	0.13437211
	Si	0.081106359	-1.669961412	0.171972654
	O	1.421060321	-0.70108337	0.278505435
	C	-2.670110731	1.69922709	1.136673607
	H	-2.891435578	2.659396032	0.663585922
	H	-3.61028233	1.16199006	1.282765809
	H	-2.217255768	1.889861696	2.112537614
	O	2.465694065	1.719171331	1.211796551
	O	2.636663902	1.541886244	-0.885690557
	H	3.067315648	1.975037712	0.175147397
	O	-2.175431589	0.521771024	-1.422669206
	H	-1.832231921	-0.218398723	-1.941104341
	O	-0.277017444	-1.98834716	-1.399863934
	H	0.246881597	-2.639013729	-1.87746044
	O	0.343671906	-3.059519615	0.972749588
	H	0.861901791	-3.040354561	1.782804039
TS _{D3-11-1}	O	-1.267422215	0.788332548	-0.853744396
TS _{D3-11-1}	O	1.316178207	0.636315075	-0.358253846
TS _{D3-11-1}	Si	0.071007896	1.692094823	-0.596219303
TS _{D3-11-1}	Si	1.302808996	-0.930501902	0.132043288
TS _{D3-11-1}	Si	-1.637161544	-0.699520267	-0.138003774
TS _{D3-11-1}	O	-0.199327674	-1.524841868	-0.180946673
TS _{D3-11-1}	C	-1.621470575	0.074968375	1.799697461
TS _{D3-11-1}	H	-2.540236713	0.671352114	1.747847876
TS _{D3-11-1}	H	-0.789343264	0.545220439	2.320016434
TS _{D3-11-1}	O	-1.878852309	-1.196604836	2.24980945
TS _{D3-11-1}	O	-2.452787725	-1.775742368	1.152072924
TS _{D3-11-1}	O	0.447893022	2.698261331	-1.82823636
TS _{D3-11-1}	H	0.983614182	2.350140579	-2.546695397
TS _{D3-11-1}	O	-2.781541445	-1.221516466	-1.197146769
TS _{D3-11-1}	H	-2.813596653	-0.720805045	-2.018712523
TS _{D3-11-1}	O	2.409470966	-1.858063353	-0.634055765
TS _{D3-11-1}	H	2.121413742	-2.331027305	-1.420534659
TS _{D3-11-1}	O	-0.225097622	2.605629474	0.732903802
TS _{D3-11-1}	H	0.326837173	3.379983929	0.877400556
TS _{D3-11-1}	O	1.64633907	-0.907835691	1.732153168
TS _{D3-11-1}	H	1.945256833	-1.728607336	2.134906226
TS _{D3-11-2}	O	-0.662350388	-1.516021884	-0.127230921
TS _{D3-11-2}	O	-1.790366446	0.849514048	0.078121273
TS _{D3-11-2}	Si	-2.033918786	-0.753322906	0.370601579
TS _{D3-11-2}	Si	-0.418558673	1.735256281	-0.076488652

Supporting Information

	Si	0.840058932	-0.972464841	-0.493940895
	O	0.759158618	0.669429001	-0.531075839
	C	2.10253086	-1.584693329	0.830955664
	H	1.933774659	-2.638005024	1.074582244
	H	1.929715709	-0.95081042	1.711279701
	O	3.423509771	-1.350744036	0.430651006
	O	3.77997221	-2.363940401	-0.482694213
	O	-3.374852233	-1.246300057	-0.416766873
	H	-3.574475894	-0.86436231	-1.276113226
	O	1.547678213	-1.610283861	-1.821143313
	H	3.382359267	-2.043274983	-1.32202265
	O	-0.535547976	2.917603845	-1.196920555
	H	-0.31400767	2.711087301	-2.109433912
	O	-2.196912442	-1.1066349	1.951676779
	H	-3.050013702	-0.961516846	2.370882671
	O	-0.106470602	2.42156608	1.367954035
	H	0.408324364	3.233853052	1.381328107
TS _{D3-11-3}	O	-0.524357894	-1.581069988	-0.248880673
TS _{D3-11-3}	O	-1.802911319	0.701714908	0.073248699
TS _{D3-11-3}	Si	-1.958017442	-0.932971557	0.225204022
TS _{D3-11-3}	Si	-0.491038116	1.649003653	-0.171929241
TS _{D3-11-3}	Si	0.954590952	-0.901543982	-0.507301226
TS _{D3-11-3}	O	0.688348031	0.698480162	-0.81654216
TS _{D3-11-3}	C	2.100411	-1.047316406	0.980260061
TS _{D3-11-3}	H	3.145736527	-1.047587369	0.657225671
TS _{D3-11-3}	H	1.912514338	-1.966584985	1.549165446
TS _{D3-11-3}	O	2.007575548	0.08275048	1.849024349
TS _{D3-11-3}	O	0.64661447	0.270721168	2.14205438
TS _{D3-11-3}	O	-3.214821241	-1.421380781	-0.704637047
TS _{D3-11-3}	H	-3.446706731	-0.87613899	-1.462212123
TS _{D3-11-3}	O	1.710705432	-1.668530013	-1.737669209
TS _{D3-11-3}	H	1.189186675	-1.999807965	-2.475004414
TS _{D3-11-3}	O	-0.921711913	2.868139986	-1.163237961
TS _{D3-11-3}	H	-0.273415581	3.546594143	-1.373775741
TS _{D3-11-3}	O	-2.242946609	-1.424267593	1.751467907
TS _{D3-11-3}	H	-3.160689953	-1.499790751	2.028552592
TS _{D3-11-3}	O	0.059589784	2.316615848	1.249531334
TS _{D3-11-3}	H	0.568254731	1.275947871	2.224321534
TS _{D3-11-4}	O	-0.411493556	-1.376410132	0.041195002
TS _{D3-11-4}	O	-1.87694307	0.803373944	0.049873721
TS _{D3-11-4}	Si	-1.912174475	-0.805866744	0.395443871
TS _{D3-11-4}	Si	-0.647204899	1.882984714	-0.062842545

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	Si	1.016412514	-0.63156833	-0.264318452
	O	0.723028139	0.985828377	-0.261828715
	C	2.277659366	-1.112486825	1.03710242
	H	2.387050644	-2.411856359	0.854522812
	H	2.200682229	-0.95821327	2.115728233
	O	3.593544136	-1.025657836	0.557600753
	O	3.591734409	-2.479331323	0.391900288
	O	-3.100784543	-1.518648255	-0.466706675
	H	-3.2503109	-1.231973673	-1.372125579
	O	1.639497637	-1.101593233	-1.696890432
	H	2.531476763	-1.471722677	-1.683834081
	O	-0.81121742	2.909032424	-1.325574932
	H	-0.449495211	2.644681023	-2.176547447
	O	-2.16411534	-1.123809624	1.973317617
	H	-3.065508291	-1.094663675	2.306649733
	O	-0.621856983	2.769448586	1.304135707
	H	-0.317133269	3.679299779	1.240050873
TS _{D3-11-5}	O	-0.542284471	-1.376924561	-0.414716615
	O	-1.41780693	1.054563838	0.036584209
	Si	-1.83872327	-0.534464179	0.136375963
	Si	0.029343346	1.796679334	-0.172472037
	Si	1.006354745	-0.956359118	-0.734596856
	O	1.033925259	0.68120896	-0.856897971
	C	0.95869003	-0.660523064	2.370301422
	H	0.720257447	-1.679334577	2.649140627
	H	0.400062349	0.2193536	2.669719317
	O	2.003437984	-0.432968948	1.583454221
	O	2.056632062	-1.446742254	0.46773773
	O	-3.198217107	-0.80746393	-0.729136093
	H	-3.297356912	-0.393914378	-1.59102583
	O	1.474799982	-1.712793031	-2.096186799
	H	2.415512117	-1.858923325	-2.233426296
	O	-0.045316327	3.098526896	-1.15665885
	H	0.064284547	2.954198303	-2.101004282
	O	-2.154758956	-1.010877048	1.665060364
	H	-3.080425778	-1.054842537	1.923731687
	O	0.512456508	2.28512398	1.308824711
	H	1.300459776	2.833722599	1.369050698
TS _{D3-12-1}	O	1.425671059	0.205306164	0.447608734
	O	-0.453759047	-1.362262398	-0.608224305
	Si	1.094444096	-1.366228064	0.015397097
	Si	-1.634233867	-0.19415644	-0.454083567

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	Si	0.682892242	1.645102502	0.067030392
	O	-0.856026544	1.253584283	-0.447269109
	C	0.579639727	2.692350431	1.597243682
	H	1.577751088	2.920069827	1.983309193
	H	0.067172108	3.635699161	1.387017796
	H	0.020717229	2.172356834	2.381112934
	C	1.577429288	2.47714354	-1.335902941
	H	1.068065553	3.399936524	-1.629496218
	H	2.603958059	2.727039885	-1.0514527
	H	1.615393419	1.818202198	-2.208912959
	C	-2.311642624	-0.50393248	1.400405646
	H	-2.669710289	-1.524942082	1.589762731
	C	-2.855891332	-0.432852227	-1.811389662
	H	-3.474815395	-1.311110069	-1.607593706
	H	-3.511023786	0.43704876	-1.8848851
	H	-2.336332092	-0.588190634	-2.760545882
	C	2.264050934	-1.936505242	-1.312558993
	H	3.29838227	-1.91766793	-0.956372462
	H	2.026931235	-2.957945382	-1.625222679
	H	2.193161928	-1.288309654	-2.191309535
	C	1.15413732	-2.427571493	1.542934384
	H	0.891404602	-3.463698508	1.309393688
	H	2.154146814	-2.418347704	1.986788029
	H	0.449300995	-2.057697998	2.294640437
	H	-1.544097908	-0.141627841	2.103490789
	O	-3.148285651	0.381640966	0.875507364
TS _{D3-12-2}	O	1.323123638	0.183137744	0.428975668
	O	-0.651841831	-1.420749681	-0.403600417
	Si	0.939638907	-1.401498324	0.12694929
	Si	-1.771678793	-0.213504323	-0.540901823
	Si	0.548919248	1.620270008	0.131028668
	O	-1.007157527	1.239096787	-0.366321172
	C	0.499774112	2.670714585	1.658366156
	H	1.51471935	2.928664739	1.976623867
	H	-0.045327911	3.600715905	1.469220353
	H	0.005380047	2.124357844	2.465161263
	C	1.388247517	2.474792984	-1.298595972
	H	0.862080369	3.396796303	-1.564782381
	H	2.421971631	2.731395394	-1.047057875
	H	1.405230165	1.826051555	-2.180265712
	C	-2.230557228	-0.393301648	2.260350148
	H	-3.037568633	0.36031205	2.270878584
	C	-2.641614161	-0.30635323	-2.192503018

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	H	-3.146066831	-1.268157601	-2.311625394
	H	-3.377460228	0.495607768	-2.287809554
	H	-1.898426845	-0.19800775	-2.990390232
	C	1.994219766	-2.030503741	-1.274935033
	H	3.05340022	-2.025543666	-0.999804636
	H	1.715507348	-3.054202598	-1.543416785
	H	1.871329404	-1.400559079	-2.161708196
	C	1.111212633	-2.427458856	1.66303753
	H	0.773047522	-3.452747605	1.483260153
	H	2.156049011	-2.46451474	1.986641944
	H	0.512956607	-1.986459615	2.464247263
	H	-2.538595989	-1.446458513	2.131431913
	O	-1.071105039	-0.090229899	2.47344404
TS _{D3-12-3}	O	-1.803503118	0.669558003	-0.25955601
	O	0.792065826	1.059282166	-0.775144449
	Si	-0.604408214	1.813894501	-0.254247919
	Si	1.242028561	-0.451920366	-0.250381536
	Si	-1.717724127	-0.985197174	-0.060948795
	O	-0.113191161	-1.401900359	-0.271592064
	C	-2.259098314	-1.431250043	1.659788118
	H	-3.281841806	-1.090597576	1.848145453
	H	-2.224714705	-2.514146939	1.814243718
	H	-1.590786146	-0.959827642	2.387766811
	C	-2.724961845	-1.808397628	-1.389428409
	H	-2.645243128	-2.897180616	-1.314670532
	H	-3.781013191	-1.535999925	-1.302311087
	H	-2.373782813	-1.50666015	-2.380355233
	C	1.78719539	-0.30527822	1.566697392
	H	1.962189366	-1.34344581	1.894069479
	C	2.576822108	-1.153135307	-1.327377824
	H	3.460146296	-0.508255471	-1.322792562
	H	2.870952659	-2.148834829	-0.983240743
	H	2.221269326	-1.239044553	-2.357941598
	C	-1.038062578	3.205143219	-1.400366796
	H	-1.964014087	3.692557178	-1.082183115
	H	-0.241932441	3.954611594	-1.421418584
	H	-1.181314596	2.824057367	-2.415710354
	C	-0.268714583	2.293261522	1.510246315
	H	0.488088958	3.061290085	1.686461768
	H	-1.125167658	2.413727391	2.177063353
	H	0.28748197	1.230019202	1.988422434
	H	2.733099795	0.245257547	1.685705352
	O	0.785842536	0.185495335	2.422299316

Supporting Information

TS _{D3-12-4}	O	1.59815604	0.209633137	0.266388126
	O	-0.474606338	-1.406407747	-0.185717657
	Si	1.167917084	-1.387880963	0.116808183
	Si	-1.614964167	-0.21695351	-0.255562949
	Si	0.759132153	1.637865734	0.143561574
	O	-0.851791608	1.224552331	-0.011918576
	C	0.980719253	2.630487598	1.698520245
	H	2.030027165	2.908777195	1.835323575
	H	0.384913928	3.547505046	1.662048224
	H	0.665054553	2.052511742	2.572079086
	C	1.300406052	2.544080485	-1.387729449
	H	0.729831222	3.468258283	-1.51951081
	H	2.362417651	2.802004946	-1.334145953
	H	1.147232715	1.920497184	-2.274221273
	C	-3.066175582	-0.496912461	0.950539734
	H	-2.951805965	-1.442929519	1.49601614
	C	-2.648066294	-0.254628919	-1.809619764
	H	-3.70607566	-0.415105766	-1.03743472
	H	-2.791610865	0.669657278	-2.370770138
	H	-2.593762199	-1.129072051	-2.45954786
	C	2.054458991	-2.14405231	-1.330960706
	H	3.138260121	-2.11048423	-1.184515965
	H	1.759519866	-3.188904132	-1.466466354
	H	1.817949027	-1.601680922	-2.251398287
	C	1.499941693	-2.271523494	1.718682592
	H	1.170432657	-3.31354365	1.664347652
	H	2.568333271	-2.261980609	1.954697306
	H	0.9662593	-1.787977919	2.54263843
	H	-3.156351269	0.336076628	1.65973228
	O	-4.177388934	-0.542297835	0.092565384
TS _{D3-12-5}	O	-1.407910197	0.787560078	-0.49654887
	O	-0.182880691	-1.500851265	0.132370128
	Si	-1.661599024	-0.838774015	-0.267737684
	Si	1.283545001	-0.785825889	0.413049378
	Si	-0.191965572	1.811845312	-0.005467045
	O	1.01690238	0.837586532	0.604589997
	C	0.440217612	2.750204024	-1.481425119
	H	-0.352192133	3.360333178	-1.925338523
	H	1.265449139	3.410479536	-1.198503523
	H	0.806644632	2.058872114	-2.246891566
	C	-0.802497904	2.918632036	1.358506874
	H	-0.001881212	3.572903257	1.716330616

Supporting Information

	H	-1.628897335	3.546049077	1.011364899
	H	-1.158271753	2.322716542	2.204602875
	C	2.315826889	-1.082962679	-1.130506415
	H	3.174037024	-1.985300818	-0.97352725
	C	2.132874382	-1.467258882	1.909781352
	H	3.147524591	-1.064204787	1.980467617
	H	1.588669877	-1.193010218	2.817715438
	H	2.195368576	-2.558255634	1.859790276
	C	-2.837071872	-1.100056841	1.152258591
	H	-3.813555167	-0.654294924	0.940390009
	H	-2.981549712	-2.166404141	1.350425501
	H	-2.441997151	-0.636802587	2.062135489
	C	-2.26244988	-1.588502903	-1.858741586
	H	-2.399737217	-2.66887457	-1.753953274
	H	-3.218717579	-1.148047462	-2.156960637
	H	-1.541798808	-1.411360078	-2.662713731
	H	1.880942753	-1.078673624	-2.13803755
	O	3.688776991	-0.87599754	-1.084419587
TS _{D3-12-6}	O	1.646891115	-0.599425599	-0.56976388
	O	0.220542667	1.356385074	0.569061169
	Si	1.46728368	1.052089683	-0.499127401
	Si	-0.736640187	0.36412342	1.481157773
	Si	0.635811861	-1.780483689	0.025749129
	O	-0.051705787	-1.138739381	1.410668953
	C	-0.743803618	-2.02659073	-1.18800038
	H	-0.502888083	-1.951639889	-2.250444884
	H	-1.449964439	-2.835591153	-0.987895867
	H	-1.565843841	-0.911862594	-0.970518597
	C	1.620759379	-3.284177027	0.48262755
	H	0.970994114	-4.056068746	0.904996301
	H	2.124859827	-3.699440096	-0.394429777
	H	2.378954195	-3.026114989	1.227821559
	C	-0.961587233	0.949045773	3.211440753
	H	-1.363103127	1.965460921	3.221223989
	H	-1.659271047	0.296185487	3.742288008
	H	-0.008192027	0.944208354	3.745548244
	C	3.031818539	1.820927959	0.144172814
	H	3.871962822	1.611968504	-0.524812533
	H	2.925297846	2.906357161	0.231941156
	H	3.275653697	1.419950349	1.132370776
	C	0.98439323	1.69182349	-2.180476094
	H	0.712310509	2.750782471	-2.137623831
	H	1.809751421	1.577906853	-2.889985295

Supporting Information

	H	0.128000002	1.132680824	-2.571074555
	O	-2.23044263	0.304184863	0.75017879
	C	-2.32766248	0.119723715	-0.621396898
	H	-3.340979364	-0.165058252	-0.906988909
	H	-1.932742901	0.961438962	-1.201344608
TS _{D3-12-7}	O	1.653938811	-0.578920293	-0.517829633
	O	0.482073986	1.458268445	0.744402079
	Si	1.57098918	1.079580263	-0.462295228
	Si	-0.603483104	0.543412613	1.573182122
	Si	0.734246022	-1.773175609	0.181897248
	O	-0.18371198	-1.030828695	1.362446297
	C	-0.406438262	-2.49955597	-1.095893651
	H	0.156426133	-2.930204451	-1.929426117
	H	-1.034557185	-3.283451222	-0.662052933
	H	-1.066612914	-1.721534909	-1.493294767
	C	1.844382972	-3.028874293	0.981968259
	H	1.257051797	-3.809881269	1.473991856
	H	2.491509537	-3.504023952	0.238690786
	H	2.479563527	-2.553421509	1.734853526
	C	-0.885670893	1.078434724	3.315552609
	H	-2.193017055	1.413247687	2.966498912
	H	-0.9748251	0.320978895	4.093988842
	H	-0.416915985	1.994791418	3.672988435
	C	3.236599701	1.771313662	-0.015406374
	H	3.981102556	1.508912571	-0.773060257
	H	3.197367021	2.86197828	0.062315938
	H	3.572287606	1.372094169	0.946056295
	C	0.920456318	1.721051493	-2.082905863
	H	0.83461636	2.811772058	-2.067792869
	H	1.578852287	1.438840935	-2.910018252
	H	-0.073579697	1.306869496	-2.279855441
TS _{D3-12-8}	O	-2.142791132	0.796208535	0.959685714
	C	-3.01540726	1.368803092	1.881519237
	H	-3.288258747	2.398069406	1.638763196
	H	-3.85950181	0.723471582	2.131998725
	O	1.192703589	0.09637721	0.751183005
	O	-0.843583328	-1.399140119	-0.113925955
	Si	0.800732985	-1.412609781	0.162996382

Supporting Information

	H	1.222402695	2.845161729	2.194171633
	H	-0.009673576	3.684488754	1.235061911
	H	-0.471683269	2.298172733	2.233302511
	C	1.89511858	2.271396735	-1.025511302
	H	1.535178974	3.213874144	-1.449253078
	H	2.845541574	2.464737421	-0.518469865
	H	2.083346339	1.578144331	-1.850848182
	C	-2.588176501	-0.378746316	-2.173722218
	H	-1.803813927	-0.52092013	-2.926404273
	H	-3.213295218	-1.274238812	-2.141330265
	H	-3.205831324	0.472883094	-2.468537231
	C	1.677912937	-1.702769248	-1.458007294
	H	2.763168887	-1.61927336	-1.344618096
	H	1.447679042	-2.696012824	-1.855582308
	H	1.355009433	-0.963572564	-2.199601717
	C	1.208881736	-2.700622576	1.439340864
	H	0.949851398	-3.697385255	1.06957982
	H	2.278277954	-2.688143684	1.670408934
	H	0.658250126	-2.532053967	2.369189459
	O	-2.115739733	0.399904488	1.76955962
	C	-1.574825584	-0.339280506	2.59656609
	H	-0.479577936	-0.372081813	2.692896233
	H	-2.174546664	-0.996071474	3.241402879
TS _{D3-13-1}	O	1.424806706	-0.568471308	-0.690652898
	O	0.340589007	1.469279327	0.657674897
	Si	1.439079965	1.09350453	-0.542834642
	Si	-0.782120319	0.564538155	1.444296514
	Si	0.633203716	-1.75428707	0.139986624
	O	-0.374199257	-1.028489454	1.24913509
	C	-0.395373439	-2.743409031	-1.060396876
	H	0.128121906	-3.215133157	-1.895240412
	H	-1.17755589	-3.389325346	-0.656061803
	H	-1.093580255	-1.774082071	-1.722019926
	C	1.850022124	-2.831784289	1.043443564
	H	1.338095284	-3.615509952	1.609134644
	H	2.543120717	-3.306735301	0.343185024
	H	2.43314786	-2.226986918	1.745406587
	C	-0.913789624	1.060632352	3.213741637
	H	-1.259123379	2.095436847	3.287179231
	H	-1.628548168	0.421617028	3.738308394
	H	0.056220871	0.985573725	3.711263063
	C	3.123707656	1.621514094	0.049989387
	H	3.893743367	1.361629074	-0.682724999

Supporting Information

	H	3.157614288	2.703288739	0.212055798
	H	3.371830609	1.128605655	0.995126846
	C	0.974037059	1.883712396	-2.155191256
	H	0.917401034	2.971228427	-2.045959122
	H	1.724272121	1.65670962	-2.919119055
	H	0.00363634	1.515672611	-2.496401408
	O	-2.296818319	0.762027248	0.764634882
	C	-2.665652275	-0.006751755	-0.320904297
	H	-2.766020834	-1.070855846	-0.066888399
	H	-3.589549923	0.385550905	-0.753915473
	O	-1.598935935	0.103481723	-1.277532557
	O	-1.717605041	-0.918675665	-2.200713889
TS _{D3-13-2}	O	1.645587718	-0.559675123	-0.639162876
	O	0.766229529	1.449341297	0.876713188
	Si	1.745163136	1.079554397	-0.417260329
	Si	-0.667745794	0.732510934	1.27142675
	Si	0.614955587	-1.696360336	0.013086556
	O	-0.563905727	-0.858415975	0.85515447
	C	-0.17330138	-2.706361699	-1.328637292
	H	-0.71450193	-2.058053887	-2.022447814
	H	0.585265853	-3.260813842	-1.889512449
	H	-0.87563673	-3.42891537	-0.900987448
	C	1.567720769	-2.737161108	1.228688915
	H	0.914032471	-3.47445151	1.704935227
	H	2.381700438	-3.272944428	0.730994172
	H	2.003091443	-2.111331205	2.014184038
	C	-1.018315706	0.98594327	3.063966961
	H	-1.137333783	2.051429717	3.278432099
	H	-1.938209754	0.471522268	3.353875599
	H	-0.19653174	0.601428177	3.673730508
	C	3.492845128	1.577561733	-0.043311935
	H	4.156465734	1.306689275	-0.869343708
	H	3.564949435	2.656642897	0.118631407
	H	3.841933347	1.06829784	0.860065257
	C	1.013009862	1.909122899	-1.912818412
	H	0.59061813	2.908781451	-1.792937781
	H	1.487639399	1.770767229	-2.885965683
	H	-0.083659894	1.153081899	-2.047729621
	O	-1.890260091	1.421742661	0.380031555
	C	-2.627148312	0.820191008	-0.630545765
	H	-2.638308386	-0.27055853	-0.52189878
	H	-3.635744841	1.240747296	-0.633598456
	O	-2.139296297	1.139620668	-1.919252934

Supporting Information

	O	-0.991519717	0.401857778	-2.153901759
TS _{D3-13-3}	O	1.451443999	-0.464409753	-0.738964974
	O	-0.018041894	1.432638648	0.455632862
	Si	1.278565776	1.17441226	-0.575477765
	Si	-0.90969069	0.392504517	1.360998867
	Si	0.742622653	-1.761728113	0.018375399
	O	-0.367286451	-1.127890305	1.102409062
	C	-0.083564526	-2.879187552	-1.212012174
	H	0.669877753	-3.447042872	-1.76732004
	H	-0.739734645	-3.589429267	-0.699798762
	H	-0.684456557	-2.309533926	-1.924405657
	C	2.034823783	-2.656728108	1.017073437
	H	1.599001965	-3.508830791	1.547756084
	H	2.834374493	-3.030368296	0.370002302
	H	2.482286036	-1.987007237	1.758069578
	C	-0.957546091	0.826056595	3.149980176
	H	-1.334689088	1.842404904	3.28881551
	H	-1.610974311	0.136854128	3.691381026
	H	0.04372148	0.763814972	3.584329744
	C	2.79959816	1.866607522	0.248273913
	H	3.689898437	1.685040013	-0.361518731
	H	2.705818897	2.94558501	0.405163043
	H	2.956721635	1.393941251	1.223327327
	C	0.951801812	1.982150325	-2.216668606
	H	0.149239301	1.478225598	-2.76124431
	H	0.675556043	3.032123826	-2.076806645
	H	1.853386695	1.950652394	-2.836757034
TS _{D3-14-1}	O	-2.511596349	0.558605708	0.834870408
	C	-2.883569942	0.431978543	-0.450101193
	H	-3.911841278	0.743726827	-0.647487563
	H	-2.068001422	1.051284693	-1.275366268
	O	-2.513276166	-0.732805799	-1.094201648
	O	-1.488711757	0.005167334	-1.843178649
	O	-1.663683522	0.735453065	-0.426965267
	O	-0.377958424	-1.477700116	0.358323819
	Si	-1.77585026	-0.930072025	-0.363235996

Supporting Information

	H	0.808083105	1.014207664	-1.953753066
	C	-1.044990336	3.22874228	0.894728824
	H	-0.222233677	3.898819982	1.159462933
	H	-1.77109305	3.789032656	0.298984344
	H	-1.534712682	2.903959978	1.817441757
	C	1.557257369	-1.336245159	2.492597593
	H	1.79183186	-2.402422041	2.435266069
	H	2.454047149	-0.803047274	2.818284915
	H	0.774055133	-1.194123166	3.241618711
	C	-3.219960654	-1.382329823	0.720860429
	H	-4.1572745	-1.014120637	0.292492508
	H	-3.297582179	-2.468325118	0.830157066
	H	-3.105629111	-0.946335209	1.7178281
	C	-1.927367234	-1.618788137	-2.080895769
	H	-1.988194193	-2.711279802	-2.0541979
	H	-2.827532716	-1.238520052	-2.57370138
	H	-1.05354085	-1.33537512	-2.673674371
	O	2.248013208	-0.986924346	-0.207995455
	C	2.338017957	-0.493336004	-1.516856183
	H	2.978974393	0.400848922	-1.52192369
	H	2.814073715	-1.270225163	-2.131842642
	O	1.123726552	-0.221632437	-2.118802049
TS _{D3-14-2}	O	-1.647670743	0.696833568	-0.36724648
	O	-0.403912275	-1.498754049	0.499868778
	Si	-1.728297609	-0.962901356	-0.368195037
	Si	0.972455699	-0.694070871	0.91463849
	Si	-0.517751517	1.790592829	0.170723325
	O	0.625220618	0.903042061	1.011332114
	C	0.30030548	2.597575165	-1.289827638
	H	-0.427118868	3.143398106	-1.898164274
	H	1.075792124	3.298350796	-0.966635238
	H	0.774028859	1.837110867	-1.91906227
	C	-1.308841068	2.994817194	1.34198111
	H	-0.567057163	3.697684081	1.732918742
	H	-2.092785561	3.568212197	0.838370288
	H	-1.759570704	2.467462785	2.187698105
	C	1.730414472	-1.427176824	2.442590933
	H	1.263413067	-2.326370602	2.847341148
	H	2.836996568	-1.80093593	1.962604341
	H	2.036305493	-0.730110691	3.224114923
	C	-3.275206026	-1.51560805	0.500051435
	H	-4.165110705	-1.155416945	-0.024763136
	H	-3.326179281	-2.607326597	0.55035349

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	H	-3.299858819	-1.124677514	1.521471514
	C	-1.599169313	-1.583973971	-2.116321334
	H	-1.633584886	-2.677148916	-2.148804245
	H	-2.415578933	-1.196049412	-2.732835426
	H	-0.652125123	-1.260184096	-2.559985281
	O	2.122329746	-0.90213618	-0.273171529
	C	2.981378066	-2.008110564	-0.111508262
	H	2.398831491	-2.941919805	-0.160139225
	H	3.716656875	-2.000796739	-0.926259976
	O	3.725568086	-1.934303707	1.057542355
TS _{D3-14-3}	O	-1.714081956	-0.058005268	-0.648408948
	O	0.326403315	-1.267116698	0.596863465
	Si	-1.078053877	-1.541046277	-0.27202929
	Si	1.079162369	0.127814865	1.034835648
	Si	-1.250594385	1.502740701	-0.31567029
	O	0.118060527	1.39552694	0.64038868
	C	-0.876362459	2.419792812	-1.884799394
	H	-1.77387765	2.494261623	-2.506908366
	H	-0.528439131	3.434023233	-1.665345741
	H	-0.100028516	1.899126132	-2.451372389
	C	-2.583310612	2.327542913	0.689906895
	H	-2.294087276	3.34793489	0.959329464
	H	-3.519979346	2.375234011	0.126130179
	H	-2.770075518	1.771278213	1.613563127
	C	1.559954276	0.159602886	2.812701728
	H	2.207222945	-0.688358931	3.050277187
	H	2.099212416	1.082007991	3.044087111
	H	0.672814126	0.110311416	3.449406126
	C	-2.262460052	-2.459264698	0.832234398
	H	-3.226797747	-2.604286862	0.336199153
	H	-1.864795354	-3.442201121	1.102610156
	H	-2.435987171	-1.897509604	1.755424861
	C	-0.678545979	-2.480650117	-1.826726595
	H	-0.041724558	-3.343995526	-1.608682753
	H	-1.594783909	-2.848647055	-2.299011238
	H	-0.166893054	-1.832437922	-2.543629757
	O	2.533192328	0.212268431	0.180776387
	C	2.595521175	-0.052366907	-1.134686745
	H	3.555628255	0.197876418	-1.588387678
	H	1.954126411	-1.011060564	-1.715936037
	O	1.461655886	0.088901856	-1.890402502
TS _{D3-14-4}	O	1.333818355	-0.387423198	-0.467836063

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O	-0.273309523	1.377807186	0.728895669
Si	1.050829208	1.239599851	-0.286556358
Si	-1.330051569	0.259599387	1.287676286
Si	0.635340962	-1.741973216	0.179596488
O	-0.680011315	-1.23672025	1.085133855
C	0.076848168	-2.896027217	-1.167519803
H	0.942487825	-3.348676157	-1.661495335
H	-0.538376055	-3.704352935	-0.759420216
H	-0.499105586	-2.351583769	-1.920066469
C	1.8379612	-2.564292271	1.34017328
H	1.394213189	-3.453911873	1.797898749
H	2.744004336	-2.869712249	0.807935641
H	2.130382962	-1.879564001	2.142298142
C	-1.820472637	0.596196214	3.041054318
H	-2.294531776	1.576674099	3.129389299
H	-2.512384152	-0.164812439	3.409183684
H	-0.92599309	0.58789029	3.671060722
C	2.505069218	2.013713356	0.582102581
H	3.411787838	1.924458013	-0.024071267
H	2.325044727	3.076342269	0.77226745
H	2.688458234	1.522075028	1.542454972
C	0.70108588	2.03278475	-1.926745063
H	0.506416261	3.102523637	-1.801947241
H	1.558680461	1.917601537	-2.596891796
H	-0.173722857	1.569572575	-2.388698397
O	-2.81849233	0.319301206	0.47233245
C	-2.751908093	-0.676989171	-1.161277526
H	-2.747901362	-1.67340679	-0.694658733
H	-3.712604735	-0.304281757	-1.539141741
O	-1.684735547	-0.139507277	-1.503414399

230

231

Supporting Information

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