

## 烷烃与氢过氧自由基氢提取反应类反应能垒与速率常数的 精确计算

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## Accurate Calculation of the Energy Barriers and Rate Constants of Hydrogen Abstraction from Alkanes by Hydroperoxyl Radical

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表 S1 C<sub>5</sub> 以下反应体系反应物和过渡态的 $E_{\infty}^{\text{HF}}$ 和 $E_{\infty}^{\text{corr}}$ 值

Table S1  $E_{\infty}^{\text{HF}}$  and  $E_{\infty}^{\text{corr}}$  for reactants and transition states containing less than five carbon atoms

	$E_{\infty}^{\text{HF}}$ /Hartree	$E_{\infty}^{\text{corr}}$ /Hartree
CH <sub>4</sub>	-40.21680	-0.24564
HO <sub>2</sub>	-150.25210	-0.53658
TS <sub>1</sub>	-190.40114	-0.80874
C <sub>2</sub> H <sub>6</sub>	-79.26639	-0.45325
TS <sub>2</sub>	-229.45270	-1.02068
C <sub>3</sub> H <sub>8</sub>	-118.31741	-0.66273
TS <sub>3</sub>	-268.50354	-1.23025
TS <sub>4</sub>	-268.50576	-1.23247
<i>n</i> C <sub>4</sub> H <sub>10</sub>	-157.36832	-0.87251
<i>i</i> C <sub>4</sub> H <sub>10</sub>	-157.36881	-0.87426
TS <sub>5</sub>	-307.55447	-1.44035
TS <sub>6</sub>	-307.55548	-1.44322
TS <sub>7</sub>	-307.55478	-1.44287
TS <sub>8</sub>	-307.55966	-1.44573
<i>n</i> C <sub>5</sub> H <sub>12</sub>	-196.41914	-1.08236
<i>i</i> C <sub>5</sub> H <sub>12</sub>	-196.41768	-1.08538
<i>t</i> C <sub>5</sub> H <sub>12</sub>	-196.41948	-1.08791
TS <sub>9</sub>	-346.60510	-1.65669
TS <sub>10</sub>	-346.60533	-1.65029
TS <sub>11</sub>	-346.60631	-1.65334
TS <sub>12</sub>	-346.60595	-1.65400
TS <sub>13</sub>	-346.60358	-1.65349
TS <sub>14</sub>	-346.60777	-1.65756
TS <sub>15</sub>	-346.60495	-1.65665
TS <sub>16</sub>	-346.60398	-1.65353

表 S2 HF 方法修正前后反应势垒

Table S2 HF energy barriers ( $\Delta V$ ) before and after validation

Reaction	$\Delta V/(\text{kJ mol}^{-1})$	
	HF	IRM
R <sub>1</sub>	191.12	—
R <sub>2</sub>	178.97	—
R <sub>3</sub>	179.66	92.43
R <sub>4</sub>	169.73	82.50
R <sub>5</sub>	179.31	92.08
R <sub>6</sub>	172.64	85.42

R <sub>7</sub>	179.63	92.41
R <sub>8</sub>	160.93	73.70
R <sub>9</sub>	180.51	93.29
R <sub>10</sub>	179.08	91.85
R <sub>11</sub>	172.30	85.07
R <sub>12</sub>	173.46	86.24
R <sub>13</sub>	179.84	92.61
R <sub>14</sub>	162.14	74.92
R <sub>15</sub>	171.85	84.62
R <sub>16</sub>	178.42	91.19
R <sub>17</sub>	178.99	91.76
R <sub>18</sub>	169.72	82.49
R <sub>19</sub>	161.53	74.30
R <sub>20</sub>	179.49	92.26
R <sub>21</sub>	169.63	82.40
R <sub>22</sub>	161.38	74.15
R <sub>23</sub>	178.86	91.63
R <sub>24</sub>	169.59	82.36
R <sub>25</sub>	160.69	73.46

HF/6-31+G(d)水平优化得到的几何结构(TS<sub>n</sub>为对应的反应R<sub>n</sub>的过渡态)  
HO<sub>2</sub>·

	Cartesian Coordinates (Å)		
O	0.05393700	-0.60031100	0.00000000
H	-0.86298800	-0.86127700	0.00000000
O	0.05393700	0.70797100	0.00000000

H<sub>2</sub>O<sub>2</sub>

	Cartesian Coordinates (Å)		
O	0.00000000	0.69700700	-0.05493100
H	0.78361200	0.90258600	0.43944800
O	0.00000000	-0.69700700	-0.05493100
H	-0.78361200	-0.90258600	0.43944800

CH<sub>4</sub>

Cartesian Coordinates (Å)

C	0.00000000	0.00000000	0.00000000
H	0.62584000	0.62584000	0.62584000
H	-0.62584000	-0.62584000	0.62584000
H	-0.62584000	0.62584000	-0.62584000
H	0.62584000	-0.62584000	-0.62584000

TS<sub>1</sub>

Cartesian Coordinates (Å)			
C	-1.77475800	-0.15883000	0.00405100
H	-1.94470800	-0.51279600	1.00891500
H	-1.73194400	-0.93433000	-0.74413400
H	-2.36495700	0.70088300	-0.27214700
H	-0.50953900	0.31623500	0.01836700
O	0.59949100	0.69778900	0.01511400
O	1.34648500	-0.44595900	-0.11588500
H	1.63188700	-0.63165700	0.77085400

CH<sub>3</sub>

Cartesian Coordinates (Å)			
C	0.00000000	0.00000000	0.00000000
H	0.00000000	1.07269900	0.00000000
H	0.92898400	-0.53634900	0.00000000
H	-0.92898400	-0.53634900	0.00000000

C<sub>2</sub>H<sub>6</sub>

Cartesian Coordinates (Å)			
C	0.00000000	0.00000000	0.76358900
H	0.00000000	1.01217200	1.15667300
H	0.87656700	-0.50608600	1.15667300
H	-0.87656700	-0.50608600	1.15667300
C	0.00000000	0.00000000	-0.76358900
H	0.87656700	0.50608600	-1.15667300
H	0.00000000	-1.01217200	-1.15667300
H	-0.87656700	0.50608600	-1.15667300

TS<sub>2</sub>

Cartesian Coordinates (Å)			
C	-1.13762900	0.67722800	0.32439400
H	-1.48352400	1.59926100	-0.12247500
H	-1.02620900	0.75845000	1.39709600
H	0.13105100	0.62232900	-0.09569400

O	1.25167700	0.50951400	-0.47482200
O	1.72181500	-0.58669600	0.20565000
H	2.22024700	-0.21078800	0.92135300
C	-1.80795100	-0.58350100	-0.16902900
H	-1.79290700	-0.63698600	-1.25172900
H	-1.31538400	-1.46672000	0.22083500
H	-2.84772700	-0.61045100	0.15180500

C<sub>2</sub>H<sub>5</sub>

Cartesian Coordinates (Å)

C	0.01415200	-0.69918800	0.00000000
H	0.51517200	-1.09439900	0.87822600
H	-0.99962600	-1.10191300	0.00000000
H	0.51517200	-1.09439900	-0.87822600
C	0.01415200	0.79913400	0.00000000
H	-0.10026900	1.34551700	-0.91892400
H	-0.10026900	1.34551700	0.91892400

C<sub>3</sub>H<sub>8</sub>

Cartesian Coordinates (Å)

C	0.00000000	1.27250400	-0.25986800
H	-0.87701800	1.31715300	-0.90020800
H	0.87701800	1.31715300	-0.90020800
H	0.00000000	2.16175900	0.36351400
C	0.00000000	0.00000000	0.58595100
H	0.87009300	0.00000000	1.23825400
H	-0.87009300	0.00000000	1.23825400
C	0.00000000	-1.27250400	-0.25986800
H	0.87701800	-1.31715300	-0.90020800
H	0.00000000	-2.16175900	0.36351400
H	-0.87701800	-1.31715300	-0.90020800

TS<sub>3</sub>

Cartesian Coordinates (Å)

C	-0.41570400	0.80940300	0.31332800
H	-0.33232000	0.77571500	1.39197400
H	-0.64290600	1.80413500	-0.04757400
H	0.85307100	0.64818200	-0.08165800
O	1.96757400	0.44883000	-0.43978100
O	2.32613500	-0.70205400	0.21815200
H	2.83591700	-0.38992200	0.95614700
C	-1.21239000	-0.31344400	-0.31424700
H	-1.11803700	-0.26141600	-1.39454800
H	-0.79240100	-1.26650800	-0.00899700
C	-2.69457900	-0.25537600	0.07442100
H	-3.14954200	0.67765300	-0.24543800
H	-3.24465800	-1.06917200	-0.38791000

H	-2.82275500	-0.33638300	1.15002700
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*n*C<sub>3</sub>H<sub>7</sub>

Cartesian Coordinates (Å)

C	-1.17234000	-0.41500800	0.00000000
H	-2.12395500	0.10902300	0.00000000
H	-1.14184600	-1.05424100	0.87731000
H	-1.14184600	-1.05424100	-0.87731000
C	0.00000000	0.57948400	0.00000000
H	-0.08463900	1.22388300	-0.87132600
H	-0.08463900	1.22388300	0.87132600
C	1.34238300	-0.09167900	0.00000000
H	1.77833200	-0.44254600	-0.91901300
H	1.77833200	-0.44254600	0.91901300

TS<sub>4</sub>

Cartesian Coordinates (Å)

C	-0.86626200	0.04932000	0.42281700
H	-0.74991000	0.05839900	1.49945700
H	0.33786900	-0.37324400	0.05835900
O	1.42052800	-0.76303300	-0.28215800
O	2.28311300	0.17991000	0.22063600
H	2.47871100	0.72890200	-0.52917500
C	-1.81719600	-1.01846200	-0.07307300
H	-1.79218600	-1.09494300	-1.15560400
H	-1.57241800	-1.99007400	0.34151800
H	-2.83941600	-0.78031600	0.21766400
C	-1.02659400	1.42939100	-0.17606000
H	-1.98976900	1.85411300	0.10320100
H	-0.25525300	2.10610300	0.17526900
H	-0.98644400	1.39455800	-1.26062100

*i*C<sub>3</sub>H<sub>7</sub>

Cartesian Coordinates (Å)

C	-0.01511200	-0.20123400	1.30057100
H	0.94392400	-0.69138700	1.48285400
H	-0.77394200	-0.97981300	1.30686200
H	-0.20544800	0.45900500	2.14035900
C	-0.01511200	0.54612100	0.00000000
H	0.34294300	1.56246900	0.00000000
C	-0.01511200	-0.20123400	-1.30057100
H	-0.77394200	-0.97981300	-1.30686200
H	-0.20544800	0.45900500	-2.14035900
H	0.94392400	-0.69138700	-1.48285400

*n*C<sub>4</sub>H<sub>10</sub>

Cartesian Coordinates (Å)

C	0.70351400	1.82835800	0.00000000
H	0.19586500	2.22074000	0.87718500
H	1.71537400	2.22297600	0.00000000
H	0.19586500	2.22074000	-0.87718500
C	0.70351400	0.29999800	0.00000000
H	1.24772900	-0.06111000	-0.87071000
H	1.24772900	-0.06111000	0.87071000
C	-0.70351400	-0.29999800	0.00000000
H	-1.24772900	0.06111000	-0.87071000
H	-1.24772900	0.06111000	0.87071000
C	-0.70351400	-1.82835800	0.00000000
H	-0.19586500	-2.22074000	0.87718500
H	-1.71537400	-2.22297600	0.00000000
H	-0.19586500	-2.22074000	-0.87718500

TS<sub>5</sub>

Cartesian Coordinates (Å)

C	0.34498100	1.07345600	0.17182100
H	0.25963700	1.99423400	-0.39042000
H	0.49384500	1.25302200	1.22871700
H	1.54169700	0.61728200	-0.21572500
O	2.58522700	0.16000900	-0.55249500
O	2.79415600	-0.87299900	0.32790100
H	3.39173900	-0.50573800	0.96816900
C	-0.66138100	-0.00217400	-0.17275800
H	-0.63005800	-0.19485400	-1.24164900
H	-0.38034100	-0.92862900	0.31971200
C	-2.09066700	0.38188000	0.23463700
H	-2.36776900	1.31353900	-0.25391400
H	-2.12129000	0.57489200	1.30483800
C	-3.11069100	-0.70062800	-0.11711900
H	-4.11231100	-0.40638900	0.18146300
H	-3.12641900	-0.89200100	-1.18640300
H	-2.87724200	-1.63664400	0.38247800

*p*C<sub>4</sub>H<sub>9</sub>

Cartesian Coordinates (Å)

C	-1.44758100	1.21311900	0.00000000
H	-1.49572700	2.29816000	0.00000000
H	-1.98236000	0.85860400	0.87734400
H	-1.98236000	0.85860400	-0.87734400
C	0.00000000	0.72460600	0.00000000
H	0.51831400	1.11998600	-0.87071300
H	0.51831400	1.11998600	0.87071300
C	0.10792300	-0.81038100	0.00000000
H	-0.41551400	-1.19828600	-0.87159600

H	-0.41551400	-1.19828600	0.87159600
C	1.52301500	-1.30878600	0.00000000
H	2.07735200	-1.38506000	0.91933600
H	2.07735200	-1.38506000	-0.91933600

TS<sub>6</sub>

Cartesian Coordinates (Å)			
C	-0.32805800	0.21031800	0.34079600
H	-0.27914300	0.16493400	1.42276400
H	0.83002500	-0.35498800	0.02780100
O	1.87156400	-0.87837900	-0.26430800
O	2.82097800	-0.05969100	0.29623000
H	3.12449700	0.46608600	-0.43403600
C	-1.37025200	-0.72111100	-0.25121300
H	-1.28568100	-0.71445600	-1.33502500
H	-1.15917600	-1.73654500	0.07127100
C	-2.80466600	-0.35691100	0.15230200
H	-3.08668500	0.62703300	-0.20841500
H	-3.50885300	-1.07257300	-0.26045800
H	-2.92109200	-0.36277700	1.23238200
C	-0.25348400	1.62180600	-0.20151500
H	-1.13643500	2.19330600	0.07692700
H	0.60910100	2.14672000	0.19478100
H	-0.18814500	1.62320100	-1.28558400

sC<sub>4</sub>H<sub>9</sub>

Cartesian Coordinates (Å)			
C	1.93588100	0.16575300	-0.08062600
H	2.10363300	0.91697500	0.68614600
H	2.74106500	-0.55962000	-0.01446600
H	2.00614900	0.65700400	-1.04643400
C	0.57322700	-0.50525100	0.09558900
H	0.44632500	-1.27788500	-0.66098100
H	0.55470000	-1.02948200	1.05525400
C	-0.57858500	0.45613400	0.02136100
H	-0.42226800	1.45792100	0.39008800
C	-1.98812300	-0.04991800	-0.06339400
H	-2.31486000	-0.49140700	0.88072400
H	-2.68368200	0.74726300	-0.30450400
H	-2.08545800	-0.82108000	-0.82340500

iC<sub>4</sub>H<sub>10</sub>

Cartesian Coordinates (Å)			
C	0.00000000	1.45656300	-0.09628900
H	0.87760000	1.98693400	0.26254200
H	0.00000000	1.51481000	-1.18240400
H	-0.87760000	1.98693400	0.26254200



C	0.00000000	0.00000000	0.37374000
H	0.00000000	0.00000000	1.46273000
C	-1.26142000	-0.72828100	-0.09628900
H	-1.31186400	-0.75740500	-1.18240400
H	-1.28193500	-1.75349100	0.26254200
H	-2.15953500	-0.23344300	0.26254200
C	1.26142000	-0.72828100	-0.09628900
H	2.15953500	-0.23344300	0.26254200
H	1.28193500	-1.75349100	0.26254200
H	1.31186400	-0.75740500	-1.18240400

TS<sub>7</sub>

Cartesian Coordinates (Å)

C	-0.15150200	-0.70604100	0.77403100
H	-0.39791400	-0.49455700	1.80735900
H	0.04843800	-1.75690400	0.60893300
H	1.07020700	-0.16968600	0.65583600
O	2.15416100	0.29029200	0.49431200
O	2.53221400	-0.17977500	-0.73978500
H	3.09835000	-0.91482600	-0.53698800
C	-1.04156800	-0.04225500	-0.25963000
C	-2.41129200	-0.73625300	-0.29735100
H	-2.92304700	-0.64377800	0.65725100
H	-3.04541700	-0.29038200	-1.05804800
H	-2.31481200	-1.79417900	-0.52325300
C	-1.18914900	1.45739900	0.00866500
H	-1.80692500	1.92575000	-0.75170200
H	-1.66016000	1.63489000	0.97281100
H	-0.22502800	1.95382800	0.00954800
H	-0.57362500	-0.17139200	-1.23225500

*i*C<sub>4</sub>H<sub>9</sub>

Cartesian Coordinates (Å)

C	1.05102100	-0.96609800	0.13210600
H	2.05154200	-0.70544300	-0.19956700
H	1.06051100	-1.00629800	1.21806200
H	0.82464300	-1.96252600	-0.23808900
C	0.01432100	0.05401700	-0.37048900
H	0.04595000	0.03866000	-1.45886000
C	0.35622900	1.44716400	0.08289000
H	1.16752000	1.98485400	-0.37683000
H	-0.01728700	1.82338600	1.02025900
C	-1.39841100	-0.34204800	0.06929300
H	-2.13906200	0.35044100	-0.31863500
H	-1.65281100	-1.33757700	-0.28276200
H	-1.47996400	-0.34371000	1.15362200

TS<sub>8</sub>

Cartesian Coordinates (Å)			
C	0.75757500	-0.03458300	0.00033000
H	-0.47512400	0.43501000	-0.02427900
O	-1.60645800	0.86558500	-0.04681000
O	-2.38631700	-0.25365600	0.11337900
H	-2.66943600	-0.45965800	-0.76939500
C	0.78892600	-1.08207900	-1.09625300
H	0.07985500	-1.87995200	-0.90178300
H	0.56284600	-0.64934600	-2.06578400
H	1.78008600	-1.53069000	-1.15891500
C	0.90273200	-0.59271300	1.40309100
H	1.89800000	-1.01670400	1.53657000
H	0.76801000	0.18084600	2.15129700
H	0.17786500	-1.37662300	1.59259000
C	1.60541500	1.19209600	-0.28034000
H	1.45020000	1.95993800	0.47013000
H	2.66272300	0.92806000	-0.27127800
H	1.37928700	1.61735100	-1.25267700

*t*C<sub>4</sub>H<sub>9</sub>

Cartesian Coordinates (Å)			
C	0.00000000	1.48655800	-0.02286300
H	0.00000000	1.72683700	-1.08960300
H	-0.87877100	1.95551800	0.40993200
H	0.87877100	1.95551800	0.40993200
C	0.00000000	0.00000000	0.20345800
C	-1.28739700	-0.74327900	-0.02286300
H	-1.49548400	-0.86341800	-1.08960300
H	-1.25414300	-1.73879700	0.40993200
H	-2.13291400	-0.21672100	0.40993200
C	1.28739700	-0.74327900	-0.02286300
H	2.13291400	-0.21672100	0.40993200
H	1.25414300	-1.73879700	0.40993200
H	1.49548400	-0.86341800	-1.08960300

*t*C<sub>5</sub>H<sub>12</sub>

Cartesian Coordinates (Å)			
C	0.00000000	0.00000000	0.00000000
C	0.88614900	0.88614900	0.88614900
H	1.52648700	1.52648700	0.28533800
H	0.28533800	1.52648700	1.52648700
H	1.52648700	0.28533800	1.52648700
C	-0.88614900	-0.88614900	0.88614900
H	-1.52648700	-0.28533800	1.52648700
H	-1.52648700	-1.52648700	0.28533800

H	-0.28533800	-1.52648700	1.52648700
C	0.88614900	-0.88614900	-0.88614900
H	0.28533800	-1.52648700	-1.52648700
H	1.52648700	-0.28533800	-1.52648700
H	1.52648700	-1.52648700	-0.28533800
C	-0.88614900	0.88614900	-0.88614900
H	-1.52648700	1.52648700	-0.28533800
H	-0.28533800	1.52648700	-1.52648700
H	-1.52648700	0.28533800	-1.52648700

TS<sub>9</sub>

	Cartesian Coordinates (Å)		
C	-0.04526200	-0.14050200	-1.02579200
H	0.04771500	0.51076700	-1.88570600
H	-0.31803200	-1.15068700	-1.30332000
H	-1.18316200	0.29306100	-0.46279100
O	-2.20489000	0.65611900	0.02514400
O	-2.97603200	-0.47924700	0.07333400
H	-3.54333600	-0.39834700	-0.68400600
C	1.07447500	-0.02498400	-0.00068600
C	0.76264600	-0.90414400	1.21857400
H	0.64959900	-1.94608400	0.93194200
H	1.56657800	-0.84635700	1.94698100
H	-0.15485400	-0.59151600	1.70513100
C	2.37897600	-0.50684700	-0.66242200
H	2.62939600	0.09791900	-1.52956400
H	3.20749300	-0.44263400	0.03755700
H	2.29852400	-1.54039100	-0.98727800
C	1.23243100	1.43838400	0.43656100
H	0.32922300	1.80631200	0.91238700
H	2.04862000	1.54060600	1.14598500
H	1.45001000	2.08094300	-0.41254700

1-C<sub>5</sub>H<sub>11</sub>

	Cartesian Coordinates (Å)		
C	-0.02587700	0.04106000	0.00000000
C	1.51654300	0.04254600	0.00000000
H	1.90725100	0.54917000	0.87776600
H	1.90412100	-0.97330400	0.00000000
H	1.90725100	0.54917000	-0.87776600
C	-0.53120200	-0.68575600	-1.25572000
H	-0.17034500	-1.71030800	-1.28320700
H	-1.61655800	-0.71179700	-1.28193200
H	-0.18832900	-0.18961500	-2.15965300
C	-0.53120200	-0.68575600	1.25572000
H	-0.18832900	-0.18961500	2.15965300

H	-1.61655800	-0.71179700	1.28193200
H	-0.17034500	-1.71030800	1.28320700
C	-0.53120200	1.46335500	0.00000000
H	-0.57525800	2.02285200	-0.91919900
H	-0.57525800	2.02285200	0.91919900

$nC_5H_{12}$

Cartesian Coordinates (Å)

C	0.00000000	2.55077300	0.32416500
H	0.87715000	2.59593000	0.96421500
H	-0.87715000	2.59593000	0.96421500
H	0.00000000	3.44015800	-0.29928400
C	0.00000000	1.27870400	-0.52329800
H	-0.87072900	1.28089500	-1.17623900
H	0.87072900	1.28089500	-1.17623900
C	0.00000000	0.00000000	0.31599000
H	0.87106900	0.00000000	0.97015900
H	-0.87106900	0.00000000	0.97015900
C	0.00000000	-1.27870400	-0.52329800
H	0.87072900	-1.28089500	-1.17623900
H	-0.87072900	-1.28089500	-1.17623900
C	0.00000000	-2.55077300	0.32416500
H	-0.87715000	-2.59593000	0.96421500
H	0.00000000	-3.44015800	-0.29928400
H	0.87715000	-2.59593000	0.96421500

TS<sub>10</sub>

Cartesian Coordinates (Å)

C	1.00706100	1.08090700	0.18152200
H	0.95741000	2.01729200	-0.35880400
H	1.13053900	1.23057700	1.24631800
H	2.20362900	0.60820000	-0.18538100
O	3.24620400	0.13717400	-0.50660000
O	3.40580700	-0.92740300	0.34612900
H	3.99136200	-0.59399200	1.01535400
C	-0.01320500	0.03759300	-0.21764200
H	0.04484700	-0.12934100	-1.28965500
H	0.23341400	-0.90648300	0.25935700
C	-1.44367700	0.44656700	0.15985400
H	-1.68403400	1.39808100	-0.31162300
H	-1.49950700	0.61409700	1.23424900
C	-2.48675300	-0.59670300	-0.24489000
H	-2.43167300	-0.76252800	-1.31874300
H	-2.24465400	-1.54811600	0.22402200
C	-3.91110400	-0.19212400	0.13368400
H	-4.62765700	-0.95086300	-0.16625100

H	-4.00777300	-0.05231400	1.20699600
H	-4.19592800	0.73978700	-0.34724400

2-C<sub>5</sub>H<sub>11</sub>

	Cartesian Coordinates (Å)		
C	2.49848600	-0.16881100	0.00000000
H	3.24349400	-0.95902100	0.00000000
H	2.67193100	0.44881600	0.87709600
H	2.67193100	0.44881600	-0.87709600
C	1.08164700	-0.74233400	0.00000000
H	0.95177500	-1.38220200	0.87071800
H	0.95177500	-1.38220200	-0.87071800
C	0.00000000	0.33905600	0.00000000
H	0.12705800	0.97918600	-0.87107800
H	0.12705800	0.97918600	0.87107800
C	-1.42677400	-0.23710500	0.00000000
H	-1.54778600	-0.87642500	-0.87181400
H	-1.54778600	-0.87642500	0.87181400
C	-2.49430900	0.81752200	0.00000000
H	-2.80187300	1.28515400	-0.91887900
H	-2.80187300	1.28515400	0.91887900

TS<sub>11</sub>

	Cartesian Coordinates (Å)		
C	-0.28853900	0.39745700	-0.37363500
H	-0.37651500	0.41375400	-1.45390900
H	-1.32675000	-0.36650400	-0.06441900
O	-2.25888500	-1.06916800	0.22377900
O	-3.35178400	-0.36880400	-0.22431900
H	-3.69171000	0.04435600	0.56028800
C	0.91207800	-0.38962100	0.11889900
H	0.87574500	-0.46130800	1.20392900
H	0.84684700	-1.40587300	-0.26150900
C	2.25821900	0.21422900	-0.30658400
H	2.35412300	1.22053700	0.09250000
H	2.28333300	0.30791800	-1.39024500
C	-0.56647400	1.74032500	0.26799600
H	0.19810100	2.46638100	-0.00020300
H	-1.52022500	2.13928500	-0.06047600
H	-0.58150200	1.66246800	1.35117400
C	3.44646200	-0.62711300	0.15869900
H	3.40221800	-1.63103000	-0.25406200
H	4.38676700	-0.18215500	-0.15245900
H	3.46443800	-0.71572700	1.24145500

3-C<sub>5</sub>H<sub>11</sub>

Cartesian Coordinates (Å)

C	2.53172300	-0.29168600	-0.00408100
H	3.40668800	0.33701300	-0.14003900
H	2.55767300	-1.06338200	-0.76885000
H	2.62379100	-0.78169900	0.96158500
C	1.24401200	0.52655700	-0.08860400
H	1.19573700	1.03105200	-1.05070800
H	1.26327500	1.30904300	0.66724500
C	-0.01592000	-0.32264800	0.09712300
H	0.04356900	-0.84075600	1.05938500
H	-0.03736400	-1.10972200	-0.65614700
C	-1.29096100	0.46792100	0.02532600
H	-1.27781100	1.47986000	0.39894700
C	-2.61536200	-0.23042000	-0.06532500
H	-2.87666300	-0.72225900	0.87424200
H	-3.41629600	0.46319600	-0.29984400
H	-2.60355100	-1.00069200	-0.83245200

TS<sub>12</sub>

Cartesian Coordinates (Å)

C	0.36441900	0.05878600	0.27123800
H	0.32277900	0.09350200	1.35487700
H	-0.93257800	0.04143600	-0.01710700
O	-2.10133400	0.01225700	-0.30262400
O	-2.56022500	-1.13668600	0.29294500
H	-2.58403800	-1.76527500	-0.41849400
C	0.88011400	1.34234300	-0.35245600
C	0.90618700	-1.25609400	-0.25969700
H	0.28138000	-2.06640900	0.10511800
H	0.83404400	-1.26570700	-1.34468400
C	2.35695000	-1.52865800	0.15844600
H	2.68131500	-2.49884100	-0.20517500
H	3.03815700	-0.78407800	-0.23977000
H	2.45800700	-1.52967200	1.23999300
C	0.21701000	2.60038300	0.20954100
H	-0.85380100	2.59298700	0.03723100
H	0.38049600	2.68228500	1.28041800
H	0.62576100	3.49151500	-0.25654000
H	1.95588600	1.40433500	-0.19119400
H	0.73697100	1.29880100	-1.42966900

4-C<sub>5</sub>H<sub>11</sub>

Cartesian Coordinates (Å)

C	0.04278400	-0.41089200	2.51467800
H	0.83704300	-1.14729400	2.43724900
H	-0.89908600	-0.94665200	2.59396300
H	0.18739100	0.14177000	3.43807400

C	0.04278400	0.52575700	1.30573300
H	-0.73647700	1.28112700	1.44013000
H	0.98085300	1.07731000	1.27214800
C	-0.16208300	-0.18783700	0.00000000
H	-0.79377000	-1.06387300	0.00000000
C	0.04278400	0.52575700	-1.30573300
H	0.98085300	1.07731000	-1.27214800
H	-0.73647700	1.28112700	-1.44013000
C	0.04278400	-0.41089200	-2.51467800
H	-0.89908600	-0.94665200	-2.59396300
H	0.18739100	0.14177000	-3.43807400
H	0.83704300	-1.14729400	-2.43724900

*i*C<sub>5</sub>H<sub>12</sub>

Cartesian Coordinates (Å)

C	2.09635600	-0.02956400	-0.11177800
H	2.19529900	0.98473800	0.26014600
H	2.20857300	0.00072100	-1.19267300
H	2.92685200	-0.60383700	0.28828300
C	0.76196100	-0.66261100	0.28676500
H	0.77596900	-1.71049700	-0.00550300
H	0.66708100	-0.65235700	1.37193300
C	-0.48040700	-0.00281700	-0.33096100
H	-0.35255800	-0.00279300	-1.41349700
C	-1.73494900	-0.82054800	-0.00865600
H	-1.91180500	-0.85566300	1.06399400
H	-2.61677500	-0.38873400	-0.47353300
H	-1.64199100	-1.84376800	-0.36162900
C	-0.66104400	1.44979800	0.12178100
H	-0.75613700	1.50955700	1.20393500
H	0.17352300	2.07678800	-0.17307400
H	-1.55953000	1.88029800	-0.31128500

TS<sub>13</sub>

Cartesian Coordinates (Å)

C	-0.12285800	-0.69169100	0.41496800
H	0.15363500	-1.72054400	0.23350200
H	-0.34302700	-0.50224800	1.45848500
H	-1.34125200	-0.64235000	-0.13852400
O	-2.42020500	-0.60678200	-0.63873900
O	-3.21990800	-0.04074300	0.32337500
H	-3.65126800	-0.78554200	0.72475700
C	0.72815100	0.36308800	-0.26927600
H	0.72860300	0.15069200	-1.33699800
C	0.13799700	1.76085000	-0.05856000
H	0.13365800	2.02487700	0.99625100

H	0.72323500	2.50920900	-0.58452300
H	-0.88257600	1.81760100	-0.41924500
C	2.18995300	0.31316700	0.21857900
H	2.71928600	1.15049400	-0.22991400
H	2.21320000	0.48043300	1.29411200
C	2.94079500	-0.97650200	-0.11639100
H	3.98336900	-0.89752600	0.17643800
H	2.52601800	-1.83826400	0.39630400
H	2.91380300	-1.18010400	-1.18363800

5-C<sub>5</sub>H<sub>11</sub>

Cartesian Coordinates (Å)

C	1.79078200	-0.70727100	-0.02197400
H	1.73258900	-1.73292900	-0.37482700
H	1.97605000	-0.73541700	1.04911400
H	2.64823300	-0.23799800	-0.49400400
C	0.49918800	0.05887600	-0.33331500
H	0.35809600	0.05594700	-1.41335000
C	-0.71554500	-0.65989100	0.29116000
H	-0.61007200	-0.65677900	1.37453600
H	-0.69211100	-1.70323300	-0.01673900
C	-2.06790900	-0.05956800	-0.09229800
H	-2.20225800	-0.05351200	-1.17107800
H	-2.88167800	-0.63686500	0.33666900
H	-2.16870700	0.96176800	0.26026300
C	0.61144500	1.49066200	0.11738100
H	0.09548700	2.28177500	-0.39651600
H	1.03660500	1.72040200	1.08020700

TS<sub>14</sub>

Cartesian Coordinates (Å)

C	-0.32179600	0.40596300	0.05310900
H	0.93428600	0.27121200	-0.31751600
O	2.08937500	0.14670800	-0.67361900
O	2.56705100	-0.87659700	0.10758400
H	3.04008800	-0.43069200	0.79973400
C	-0.24086200	0.61034900	1.55546000
H	0.15810300	-0.26705300	2.05399000
H	0.38983800	1.45954000	1.80018500
H	-1.22630300	0.80957900	1.97259800
C	-0.76595900	1.63767900	-0.71659600
H	-0.14170600	2.49288100	-0.47848500
H	-0.71803100	1.47308800	-1.78799500
H	-1.79132800	1.90250000	-0.46481700
C	-0.94028800	-0.91196800	-0.39868000
H	-0.78553600	-1.02075300	-1.46836000



H	-0.40439900	-1.72944400	0.07444900
C	-2.43803800	-1.04891300	-0.09302800
H	-3.02217800	-0.27540500	-0.58151400
H	-2.80377000	-2.00741500	-0.44800000
H	-2.63880500	-0.99758900	0.97242900

6-C<sub>5</sub>H<sub>11</sub>

Cartesian Coordinates (Å)

C	2.06967500	-0.03478500	-0.18273900
H	2.08466000	0.07999800	-1.26274500
H	2.20948700	0.94610700	0.25904800
H	2.92428500	-0.64243900	0.09939300
C	0.76912800	-0.69447000	0.28401600
H	0.78575800	-0.76823900	1.37642100
H	0.74752500	-1.71949500	-0.07761700
C	-0.50185000	-0.00278400	-0.14757100
C	-0.63854200	1.48054300	0.06905600
H	0.20914200	2.03402800	-0.31996300
H	-1.53235200	1.86541500	-0.41193800
H	-0.71719900	1.71978700	1.13337800
C	-1.76609000	-0.81791400	-0.10946700
H	-1.61312200	-1.81265700	-0.51727200
H	-2.12851600	-0.94296300	0.91477600
H	-2.56358800	-0.34308400	-0.67325000

TS<sub>15</sub>

Cartesian Coordinates (Å)

C	0.14033800	0.67945100	-0.45646900
H	-0.03811100	0.81707000	-1.51768700
H	-1.09502300	0.44939800	-0.03067500
O	-2.21501100	0.23438600	0.35438300
O	-2.62403200	-0.83455900	-0.40529100
H	-3.14814100	-0.43724100	-1.09027700
C	0.90919600	-0.60727800	-0.17230000
H	0.33554600	-1.41303200	-0.62320400
C	0.54566900	1.96642000	0.23455300
H	1.55604800	2.25746600	-0.04596100
H	-0.11741400	2.77671300	-0.04901800
H	0.51479200	1.87349500	1.31382300
C	2.28542400	-0.58481900	-0.85600400
H	2.92767900	0.18414700	-0.43641200
H	2.78850900	-1.53843900	-0.72560700
H	2.19663700	-0.40114300	-1.92305800
C	1.04360200	-0.91453200	1.32217400
H	0.07675000	-0.91559700	1.81397500
H	1.48970800	-1.89437400	1.46400000

H	1.67998600	-0.19253900	1.82563500
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7-C<sub>5</sub>H<sub>11</sub>

Cartesian Coordinates (Å)

C	-1.64436400	-0.94585400	-0.03091900
H	-1.44416900	-1.95545500	-0.37618500
H	-1.85251600	-0.99451000	1.03526800
H	-2.54431100	-0.59328400	-0.52686200
C	-0.45851400	-0.01821000	-0.31443900
H	-0.29365100	-0.00215300	-1.39149700
C	0.80015500	-0.52931300	0.33848600
H	0.71480900	-0.92151400	1.34094900
C	2.15880900	-0.09122900	-0.12427900
H	2.40831800	0.91188700	0.22679500
H	2.93308100	-0.75783100	0.24256900
H	2.21940000	-0.07347400	-1.20938600
C	-0.78046300	1.42218600	0.12325200
H	-0.96211800	1.46985900	1.19399900
H	0.03633100	2.09966400	-0.10609300
H	-1.66890800	1.79132900	-0.38216500

TS<sub>16</sub>

Cartesian Coordinates (Å)

C	-0.60716500	-0.93607500	0.31615400
H	-0.44332300	-1.91823700	-0.10427100
H	-0.74151300	-0.96763100	1.38996600
H	-1.84056500	-0.65797300	-0.11895000
O	-2.92473200	-0.35725800	-0.50466500
O	-3.22551200	0.77953500	0.20430300
H	-3.78242700	0.46621200	0.90688700
C	0.28034600	0.17834000	-0.19594800
H	0.29641100	0.15457300	-1.28296500
H	-0.16124200	1.12928500	0.08707200
C	1.72671900	0.12663700	0.33439600
H	1.68272300	0.13367200	1.42307200
C	2.49371900	1.37457200	-0.11237500
H	3.50428900	1.37560600	0.28585000
H	2.56584800	1.41986500	-1.19637400
H	2.00299300	2.28281500	0.22485200
C	2.46369700	-1.14308200	-0.10256900
H	1.98533100	-2.04241800	0.27179200
H	2.50391100	-1.21453200	-1.18715400
H	3.48561600	-1.14179700	0.26516400

8-C<sub>5</sub>H<sub>11</sub>

Cartesian Coordinates (Å)

C	-2.12589900	-0.09040400	-0.10940600
H	-2.50376200	-0.24661400	-1.10506000
H	-2.64483700	0.61675300	0.51186200
C	-0.80719800	-0.67889700	0.29986300
H	-0.70866900	-0.63849700	1.38274500
H	-0.79150500	-1.73313000	0.02847900
C	0.42581300	-0.00052600	-0.33609900
H	0.29398600	-0.02285100	-1.41714300
C	1.69804800	-0.78244000	0.00103900
H	1.63312800	-1.81167000	-0.34052500
H	2.57002300	-0.33307400	-0.46572500
H	1.87160100	-0.80028300	1.07460400
C	0.55792300	1.46233200	0.09552900
H	-0.31811700	2.04171100	-0.17691800
H	0.68528600	1.53807800	1.17334000
H	1.42074100	1.92919100	-0.37120600

*n*C<sub>6</sub>H<sub>14</sub>

	Cartesian Coordinates (Å)		
C	-1.41219400	2.89190400	0.00000000
H	-0.90452900	3.28440400	0.87704600
H	-2.42402300	3.28671600	0.00000000
H	-0.90452900	3.28440400	-0.87704600
C	-1.41219400	1.36360200	0.00000000
H	-1.95709500	1.00354000	0.87050900
H	-1.95709500	1.00354000	-0.87050900
C	-0.00471600	0.76472400	0.00000000
H	0.53912400	1.12836600	0.87087400
H	0.53912400	1.12836600	-0.87087400
C	0.00471600	-0.76472400	0.00000000
H	-0.53912400	-1.12836600	-0.87087400
H	-0.53912400	-1.12836600	0.87087400
C	1.41219400	-1.36360200	0.00000000
H	1.95709500	-1.00354000	0.87050900
H	1.95709500	-1.00354000	-0.87050900
C	1.41219400	-2.89190400	0.00000000
H	0.90452900	-3.28440400	-0.87704600
H	2.42402300	-3.28671600	0.00000000
H	0.90452900	-3.28440400	0.87704600

TS<sub>17</sub>

	Cartesian Coordinates (Å)		
C	-4.42759600	-0.70547100	-0.09734800
H	-4.45652800	-0.94256200	-1.15742500
H	-5.39329200	-0.28972900	0.17460700
H	-4.30475900	-1.63873200	0.44556600

C	-3.29507500	0.27079100	0.21943900
H	-3.46575500	1.20532000	-0.31149000
H	-3.31527900	0.51420700	1.27996700
C	-1.91491900	-0.27645200	-0.14858300
H	-1.89662700	-0.52073600	-1.20955100
H	-1.74621700	-1.21201300	0.38238100
C	-0.77626400	0.69545700	0.16584200
H	-0.79334600	0.94166600	1.22620800
H	-0.94051100	1.62955100	-0.36869300
C	0.60427400	0.13449100	-0.20281100
H	0.62413000	-0.11268400	-1.26060900
H	0.77726500	-0.79152200	0.33770400
C	1.72070400	1.10836900	0.10369800
H	1.88024900	1.32138000	1.15279800
H	2.86302700	0.50654100	-0.24638700
H	1.74132300	2.00498900	-0.50203500
O	3.85660900	-0.07467900	-0.54165300
O	3.94259100	-1.07945800	0.39053600
H	4.56597700	-0.74569100	1.02447200

$pC_6H_{13}$

Cartesian Coordinates (Å)

C	-3.13859700	0.20940600	-0.00009000
H	-3.22545400	0.84582000	0.87652200
H	-3.98534100	-0.47071800	0.00048000
H	-3.22549400	0.84439800	-0.87772800
C	-1.81416100	-0.55358000	0.00049600
H	-1.77370800	-1.20449400	0.87168900
H	-1.77377500	-1.20596900	-0.86960000
C	-0.59299200	0.36770900	-0.00032600
H	-0.63632100	1.02091200	0.87024400
H	-0.63646700	1.01950500	-0.87194500
C	0.73606600	-0.38893300	0.00020100
H	0.78428900	-1.04011000	-0.87053100
H	0.78428300	-1.03912900	0.87167000
C	1.95862400	0.54578900	-0.00033100
H	1.90560100	1.19487100	0.87107100
H	1.90552200	1.19381400	-0.87255100
C	3.26807500	-0.18751700	-0.00002800
H	3.68510600	-0.56218400	-0.91844200
H	3.68966700	-0.55396200	0.91958400

TS<sub>18</sub>

Cartesian Coordinates (Å)

C	-3.79505900	-0.82060200	0.14680000
H	-3.48376700	-1.83867200	-0.06999500

H	-3.93447500	-0.74052100	1.22153300
C	-2.76289900	0.18970300	-0.35278500
H	-3.11861900	1.19847500	-0.15110400
H	-2.67310800	0.10784000	-1.43421800
C	-1.38608300	-0.00168200	0.28511200
H	-1.03065100	-1.00896100	0.08276900
H	-1.47701800	0.07951300	1.36716900
C	-0.35256300	1.01192500	-0.21032800
H	-0.70581900	2.02252000	0.00350300
H	-0.26157700	0.94796700	-1.29282000
C	1.01857800	0.84691600	0.41558400
H	1.43297600	-0.35907000	0.04039400
H	0.99120600	0.71914100	1.49155100
C	2.09320700	1.80756900	-0.04524300
H	1.84745200	2.82457800	0.25662000
H	3.05660000	1.56050700	0.38706500
H	2.18944800	1.80205300	-1.12694100
O	1.82276700	-1.43420900	-0.32943900
O	3.10111000	-1.51184200	0.16604400
H	3.64578700	-1.28777400	-0.57887100
H	-4.76054300	-0.66215900	-0.32433600

*s*C<sub>6</sub>H<sub>13</sub>

Cartesian Coordinates (Å)

C	3.17266100	0.23537100	-0.07411300
H	3.22852200	0.77436700	-1.01607000
H	3.27581200	0.96189600	0.72748500
C	1.85757000	-0.53441800	0.04433700
H	1.84820700	-1.08977300	0.98029700
H	1.80136100	-1.27563700	-0.75059100
C	0.62740300	0.37172800	-0.02014900
H	0.63607600	0.92773900	-0.95568300
H	0.68509300	1.11238300	0.77612100
C	-0.69380900	-0.39210000	0.09751400
H	-0.69496000	-0.96046000	1.03273500
H	-0.75575300	-1.13658100	-0.69564400
C	-1.90643500	0.49258900	0.04197300
H	-1.82844200	1.48118200	0.46664400
C	-3.27552600	-0.10157500	-0.10753600
H	-3.59212100	-0.61812900	0.80127500
H	-4.01894000	0.65949900	-0.32147300
H	-3.30283800	-0.83241000	-0.91198400
H	4.02680400	-0.43364600	-0.02526800

*i*C<sub>6</sub>H<sub>14</sub>

Cartesian Coordinates (Å)

C	2.83646200	-0.21739000	0.14316600
H	2.89738600	-0.29810100	1.22529100
H	3.66418200	0.40272400	-0.18845100
H	2.98224800	-1.21199700	-0.26964400
C	1.49396600	0.37142800	-0.29148900
H	1.40852100	1.38054200	0.10118400
H	1.47524600	0.46090700	-1.37633900
C	0.30556900	-0.47757400	0.16756400
H	0.29094700	-0.51567500	1.25703600
H	0.46586200	-1.50123100	-0.16735200
C	-1.06998000	-0.01358500	-0.33562500
H	-1.02485900	0.04341100	-1.42316100
C	-2.14580400	-1.04014100	0.03297800
H	-2.23450700	-1.14071200	1.11237000
H	-3.11855900	-0.74612300	-0.35120200
H	-1.91244800	-2.02086900	-0.37184600
C	-1.45542500	1.37208400	0.19313500
H	-1.47497100	1.38013000	1.28091700
H	-0.76343000	2.14146800	-0.13188200
H	-2.44433900	1.65658800	-0.15529700

TS<sub>19</sub>

	Cartesian Coordinates (Å)		
C	-3.11036100	0.60452000	0.21578500
H	-2.91862200	1.40144400	0.92932600
H	-3.61158700	-0.19929300	0.74822800
C	-1.81470500	0.11508900	-0.43165700
H	-1.35000700	0.93292400	-0.97740700
H	-2.05422900	-0.64635500	-1.16785900
C	-0.82909000	-0.44247000	0.59912200
H	-1.27328100	-1.31913300	1.07609700
H	-0.69156400	0.28833900	1.39254300
C	0.54417300	-0.84242600	0.07395100
H	1.07513000	0.27284300	-0.39495400
C	1.50972100	-1.24943600	1.17249200
H	1.18654900	-2.18552400	1.62769300
H	2.51031200	-1.39849000	0.78176000
H	1.56070100	-0.49846100	1.95280900
C	0.55953900	-1.77267200	-1.12656700
H	0.09567800	-2.72504900	-0.86957900
H	0.02327900	-1.36073400	-1.97298500
H	1.57659600	-1.97613100	-1.44377100
O	1.61688700	1.27721900	-0.80508700
O	1.59039000	2.12863700	0.27269300
H	0.85779900	2.70404000	0.08830400

H	-3.80063500	0.98710500	-0.52981100
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*t*C<sub>6</sub>H<sub>13</sub>

Cartesian Coordinates (Å)

C	2.82508000	-0.21915800	0.05856800
H	2.94630800	-1.20121500	-0.39060000
H	2.95298600	-0.33004500	1.13218200
C	1.45855600	0.37837900	-0.27651600
H	1.36820400	0.49598600	-1.35409800
H	1.39560300	1.37556400	0.14944800
C	0.30243200	-0.48715700	0.23677300
H	0.37079300	-0.54850800	1.32874500
H	0.44444700	-1.50450800	-0.12179200
C	-1.08364400	-0.02844100	-0.14890500
C	-2.18082300	-1.05681300	-0.09263500
H	-2.48328600	-1.26048100	0.93846800
H	-3.06722400	-0.72336000	-0.62410400
H	-1.86588100	-2.00182300	-0.52496600
C	-1.47710100	1.40350500	0.09878000
H	-1.55547800	1.61283600	1.16940500
H	-0.75939000	2.10580600	-0.31102400
H	-2.44393800	1.62547800	-0.34205000
H	3.62985800	0.41237500	-0.30600500

*n*C<sub>7</sub>H<sub>16</sub>

Cartesian Coordinates (Å)

C	-3.82877300	-0.35308000	-0.00000300
H	-3.87381300	-0.99321900	-0.87703900
H	-4.71853600	0.26984900	-0.00000700
H	-3.87382300	-0.99322200	0.87703100
C	-2.55703500	0.49449000	0.00000500
H	-2.55967000	1.14762400	-0.87050400
H	-2.55967100	1.14761200	0.87052200
C	-1.27808200	-0.34451600	0.00000000
H	-1.27912500	-0.99873200	-0.87084300
H	-1.27912200	-0.99873300	0.87084300
C	0.00000000	0.49585000	-0.00000200
H	0.00000000	1.14990900	0.87087500
H	0.00000000	1.14990300	-0.87088300
C	1.27808200	-0.34451600	0.00000200
H	1.27912300	-0.99873700	-0.87083800
H	1.27912400	-0.99872800	0.87084800
C	2.55703500	0.49449000	-0.00000300
H	2.55967100	1.14762200	0.87050700
H	2.55967000	1.14761300	-0.87051900

C	3.82877300	-0.35308000	0.00000100
H	3.87381800	-0.99322400	-0.87703100
H	4.71853600	0.26984900	-0.00000200
H	3.87381800	-0.99321600	0.87703900

TS<sub>20</sub>

Cartesian Coordinates (Å)			
C	-5.16802800	-0.11252500	0.12222300
H	-5.26136100	0.17964700	1.16473600
H	-5.94876300	-0.83730800	-0.08867900
H	-5.36155600	0.76764700	-0.48504300
C	-3.78288800	-0.68985500	-0.16764800
H	-3.63459800	-1.58768400	0.42922400
H	-3.73403000	-1.00398300	-1.20847100
C	-2.65148600	0.29962400	0.11640200
H	-2.70316900	0.61366900	1.15793700
H	-2.80288900	1.19807400	-0.48027300
C	-1.26181700	-0.27093100	-0.17159400
H	-1.20992900	-0.58380900	-1.21334200
H	-1.11098200	-1.16926500	0.42508500
C	-0.13239400	0.72040300	0.11468000
H	-0.18063800	1.03381200	1.15580700
H	-0.27830500	1.61799100	-0.48342100
C	1.25930700	0.14020300	-0.17447200
H	1.30988200	-0.16970300	-1.21543300
H	1.40835900	-0.75122100	0.42930100
C	2.36643100	1.13090100	0.11089800
H	2.50353200	1.39198900	1.15145800
H	3.53281400	0.53910800	-0.17289700
H	2.39505300	1.99747000	-0.53667700
O	4.55801300	-0.01199500	-0.40949100
O	4.56885800	-1.07983500	0.45371600
H	4.28685300	-1.80871100	-0.08604700

*p*C<sub>7</sub>H<sub>15</sub>

Cartesian Coordinates (Å)			
C	3.75772400	-0.34698200	0.00007400
H	3.80590500	-0.98661600	0.87733400
H	4.64422100	0.28048300	-0.00007800
H	3.80590000	-0.98703500	-0.87688000
C	2.48196800	0.49481300	-0.00012100
H	2.48124800	1.14800200	0.87038900
H	2.48125300	1.14760000	-0.87093300
C	1.20712200	-0.35061100	0.00007200
H	1.21105800	-1.00438300	0.87119600
H	1.21102400	-1.00471600	-0.87080100



C	-0.07462700	0.48422500	-0.00005600
H	-0.07788000	1.13780700	-0.87129000
H	-0.07782000	1.13813500	0.87093500
C	-1.34772400	-0.36348800	0.00014800
H	-1.35042700	-1.01570600	0.87140700
H	-1.35040500	-1.01622200	-0.87073300
C	-2.63259800	0.48351500	-0.00011900
H	-2.62494100	1.13398800	-0.87211500
H	-2.62511300	1.13442100	0.87153900
C	-3.88759100	-0.33953700	-0.00004800
H	-4.28083400	-0.73718100	0.91917400
H	-4.27882700	-0.74018000	-0.91884200

TS<sub>21</sub>

Cartesian Coordinates (Å)

C	-4.63842100	-0.34801700	-0.25587300
H	-4.97967200	0.66358100	-0.05241400
H	-5.37282200	-1.03338500	0.15681700
H	-4.63073700	-0.48236400	-1.33424600
C	-3.25332100	-0.59474500	0.34120900
H	-2.95608900	-1.62379600	0.15027600
H	-3.30285300	-0.48726400	1.42303900
C	-2.18665300	0.35090300	-0.21330500
H	-2.48607500	1.38070100	-0.02181200
H	-2.14098800	0.24328300	-1.29615200
C	-0.79752900	0.10666900	0.37799600
H	-0.49659200	-0.91995900	0.18521600
H	-0.84247900	0.21488400	1.46047900
C	0.26262200	1.05969700	-0.17813300
H	-0.03469000	2.09014300	0.02571300
H	0.30936400	0.96897700	-1.26150600
C	1.64736800	0.84289900	0.40021200
H	1.99002200	-0.38936200	0.03832600
H	1.65507900	0.73994400	1.47917100
C	2.74758600	1.74092000	-0.12241600
H	2.56168200	2.77474300	0.16477000
H	3.71415200	1.45725000	0.27924100
H	2.80189900	1.70779400	-1.20655100
O	2.31415200	-1.48979300	-0.32059400
O	3.60996800	-1.61314100	0.11679900
H	4.12793400	-1.43165200	-0.65814600

sC<sub>7</sub>H<sub>15</sub>

Cartesian Coordinates (Å)

C	3.79127500	-0.32931100	-0.00728900
H	3.86088600	-0.86602200	0.93513600

H	4.67394800	0.29722400	-0.09636700
H	3.82543100	-1.06378100	-0.80755700
C	2.51094800	0.50268500	-0.07570800
H	2.48877100	1.05320100	-1.01420800
H	2.52408600	1.24974200	0.71561600
C	1.24131600	-0.34167900	0.04615000
H	1.26666200	-0.89302100	0.98523600
H	1.23168400	-1.08985200	-0.74543400
C	-0.04399900	0.48396600	-0.02227400
H	-0.07233800	1.03472600	-0.96039800
H	-0.03504400	1.23039800	0.77050300
C	-1.31329000	-0.36304200	0.09966100
H	-1.27719400	-0.92663600	1.03704500
H	-1.32777800	-1.11302100	-0.69055300
C	-2.58036900	0.44154700	0.04196300
H	-2.56674100	1.43342500	0.46596000
C	-3.90821700	-0.23956000	-0.10882200
H	-4.19220900	-0.77474900	0.79998200
H	-4.69877400	0.47196300	-0.32435000
H	-3.88737800	-0.97123300	-0.91270100

*i*C<sub>7</sub>H<sub>16</sub>

Cartesian Coordinates (Å)

C	3.49317500	0.24499000	-0.12320400
H	3.56817500	0.37018900	-1.20017800
H	4.38170100	-0.28312500	0.21034800
H	3.50961000	1.23485900	0.32509800
C	2.22160900	-0.51297900	0.25727100
H	2.25425200	-1.51101800	-0.17530300
H	2.19308600	-0.64956200	1.33670800
C	0.94380400	0.19578400	-0.19730100
H	0.97046700	0.32046700	-1.27941500
H	0.92949600	1.19705500	0.22574100
C	-0.32767700	-0.56160100	0.19425800
H	-0.38827700	-0.62630400	1.28076500
H	-0.24217700	-1.58610400	-0.16432300
C	-1.63916500	0.03048700	-0.34474800
H	-1.54810600	0.11032200	-1.42794700
C	-2.81093600	-0.90940900	-0.04371300
H	-2.94896100	-1.02865400	1.02857900
H	-3.74011400	-0.52420100	-0.45430000
H	-2.64575400	-1.89619500	-0.46697600
C	-1.92632100	1.43047200	0.20819300
H	-1.98616500	1.41336800	1.29441300
H	-1.16022100	2.14585300	-0.07063300

H	-2.87394900	1.80658600	-0.16711600
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TS<sub>22</sub>

Cartesian Coordinates (Å)			
C	3.83563800	0.35723200	0.31005400
H	3.63197300	1.27105200	0.86184200
H	4.73613200	0.51842300	-0.27498900
H	4.04790400	-0.42411100	1.03471000
C	2.65582000	-0.02382500	-0.58353100
H	2.49531500	0.75899100	-1.32242100
H	2.90362400	-0.92366000	-1.14322600
C	1.36302700	-0.25488200	0.20195500
H	1.10730900	0.64996500	0.75007900
H	1.53937300	-1.02404200	0.94920000
C	0.19393000	-0.65901900	-0.70050900
H	0.42163200	-1.61943200	-1.16831600
H	0.10821100	0.05486200	-1.51617800
C	-1.16784000	-0.78022200	-0.02749400
H	-1.43969400	0.43010400	0.42683100
C	-2.29767300	-1.04351100	-1.00674700
H	-2.19537300	-2.03916200	-1.43818400
H	-3.26363600	-0.99192700	-0.51647600
H	-2.29280700	-0.32526000	-1.81889300
C	-1.22693600	-1.64673700	1.21848700
H	-0.96981100	-2.67693800	0.97184800
H	-0.54200900	-1.30915400	1.98698400
H	-2.22623400	-1.64811200	1.64020200
O	-1.74792300	1.53182800	0.82921100
O	-1.67271200	2.32392100	-0.29069100
H	-0.83261200	2.75819300	-0.20446000

*t*C<sub>7</sub>H<sub>15</sub>

Cartesian Coordinates (Å)			
C	3.45555700	0.25431000	-0.18577000
H	3.48163300	0.42924700	-1.25802400
H	4.35888400	-0.28559100	0.08273300
H	3.49078000	1.22245600	0.30669100
C	2.20361300	-0.52486400	0.21613300
H	2.21825200	-1.50172000	-0.26323800
H	2.22392900	-0.71110600	1.28834500
C	0.90663200	0.20011800	-0.14832600
H	0.87936700	0.37214600	-1.22293900
H	0.90926000	1.18084900	0.32060400
C	-0.34436700	-0.57952400	0.27126900
H	-0.33996000	-0.68766400	1.36162500

H	-0.27312400	-1.59120000	-0.12243100
C	-1.66372100	0.01398100	-0.16216700
C	-2.84810800	-0.91374000	-0.19547900
H	-3.21839500	-1.12323300	0.81206700
H	-3.67429700	-0.48543000	-0.75527200
H	-2.59582300	-1.86847200	-0.64716800
C	-1.94228500	1.46640500	0.11965300
H	-2.05456300	1.64697100	1.19250900
H	-1.14663600	2.11489100	-0.23061700
H	-2.86323900	1.78774100	-0.35677100

$n\text{C}_8\text{H}_{18}$

Cartesian Coordinates (Å)

C	-4.48121600	0.25660000	0.00000400
H	-4.55085000	0.89454300	-0.87702700
H	-4.55084000	0.89453600	0.87704200
H	-5.34639600	-0.40006700	0.00000600
C	-3.17781000	-0.54138200	-0.00000500
H	-3.15534800	-1.19413900	0.87050200
H	-3.15535000	-1.19412500	-0.87052300
C	-1.93200400	0.34612800	0.00000000
H	-1.95822400	0.99982000	0.87085200
H	-1.95822100	0.99982300	-0.87085000
C	-0.62251600	-0.44443100	0.00000100
H	-0.59743800	-1.09800800	-0.87084100
H	-0.59743700	-1.09800200	0.87084700
C	0.62251600	0.44443100	-0.00000300
H	0.59743700	1.09800900	0.87083900
H	0.59743800	1.09800100	-0.87085000
C	1.93200400	-0.34612800	0.00000200
H	1.95822300	-0.99982500	-0.87084600
H	1.95822200	-0.99981700	0.87085600
C	3.17781000	0.54138200	-0.00000200
H	3.15534900	1.19413600	0.87050800
H	3.15534900	1.19412800	-0.87051800
C	4.48121600	-0.25660000	0.00000200
H	4.55084500	-0.89454300	-0.87703000
H	5.34639600	0.40006700	-0.00000100
H	4.55084500	-0.89453600	0.87703900

TS<sub>23</sub>

Cartesian Coordinates (Å)

C	-5.73254600	-0.69094700	-0.08455200
H	-5.66546300	-1.60977300	0.49184400
H	-5.76625100	-0.96373900	-1.13593900
H	-6.67627400	-0.21392300	0.16319500

C	-4.55040400	0.23242400	0.20870600
H	-4.66563500	1.15560800	-0.35602400
H	-4.56550200	0.51420800	1.25983000
C	-3.19906200	-0.40101800	-0.12649800
H	-3.18699900	-0.68368100	-1.17825800
H	-3.08693000	-1.32568400	0.43800200
C	-2.01032700	0.51654100	0.16441800
H	-2.02289800	0.79818000	1.21639200
H	-2.12350100	1.44122100	-0.39974400
C	-0.66007600	-0.11870000	-0.17227000
H	-0.64591000	-0.39919400	-1.22417700
H	-0.54623200	-1.04324800	0.39134500
C	0.52779100	0.79980300	0.12062500
H	0.51522200	1.08347500	1.17164200
H	0.41993100	1.72229200	-0.44735900
C	1.87851400	0.15169800	-0.21390200
H	1.89351100	-0.13414200	-1.26200600
H	1.99629600	-0.76228600	0.36087500
C	3.04389400	1.07403400	0.06890900
H	3.20680400	1.31535200	1.11135500
H	4.15462900	0.40007000	-0.24946200
H	3.11770200	1.94616500	-0.56765300
O	5.11587800	-0.24347100	-0.52199700
O	5.14397400	-1.22173000	0.44142000
H	5.78198500	-0.90230700	1.06814700

*p*C<sub>8</sub>H<sub>17</sub>

Cartesian Coordinates (Å)

C	-4.40628700	0.26122700	-0.00004800
H	-4.47423300	0.89890100	-0.87743600
H	-4.47419300	0.89968000	0.87677600
H	-5.27300900	-0.39330900	0.00026300
C	-3.10512600	-0.54074100	0.00027900
H	-3.08425800	-1.19304300	0.87121600
H	-3.08430100	-1.19381800	-0.87007600
C	-1.85695400	0.34349500	-0.00015200
H	-1.88116300	0.99750200	0.87054600
H	-1.88114700	0.99664500	-0.87149100
C	-0.54999500	-0.45127800	0.00025400
H	-0.52679000	-1.10515300	-0.87036700
H	-0.52672100	-1.10410300	0.87165300
C	0.69739300	0.43436700	-0.00033500
H	0.67453600	1.08824200	0.87035500
H	0.67440600	1.08720000	-0.87180800
C	2.00342800	-0.36163700	0.00006900

H	2.03236100	-1.01373900	-0.87081300
H	2.03229500	-1.01322200	0.87134400
C	3.25332100	0.53619200	-0.00015200
H	3.21971100	1.18634900	0.87142700
H	3.21970900	1.18577400	-0.87219500
C	4.54029200	-0.23591800	0.00001500
H	4.94591500	-0.62273500	-0.91848700
H	4.95044400	-0.61541500	0.91952100

TS<sub>24</sub>

	Cartesian Coordinates (Å)		
C	5.22212200	0.74591300	0.15112600
H	5.04945400	1.79474800	-0.07466300
H	5.32962200	0.65463700	1.22868200
H	6.16834800	0.46227200	-0.30032200
C	4.07769600	-0.12559300	-0.36544400
H	4.01944300	-0.03855800	-1.44871400
H	4.29732000	-1.17061600	-0.15489500
C	2.72415500	0.24101000	0.24543900
H	2.78535000	0.15532100	1.32952400
H	2.50700500	1.28706700	0.03490700
C	1.57342300	-0.62678100	-0.26650700
H	1.79011400	-1.67303000	-0.05439400
H	1.51413200	-0.54142400	-1.35057300
C	0.22100800	-0.25476200	0.34341500
H	0.00127500	0.78819600	0.12986100
H	0.27863800	-0.34020200	1.42731300
C	-0.92454900	-1.13039900	-0.16883700
H	-0.70868700	-2.17659900	0.05623300
H	-0.98531800	-1.06249600	-1.25319500
C	-2.27508700	-0.78627000	0.42834100
H	-2.52265900	0.46097700	0.04111900
H	-2.25285000	-0.65700400	1.50426600
C	-3.45541500	-1.60292100	-0.05123400
H	-3.34930800	-2.64122700	0.25939600
H	-4.38731900	-1.23069100	0.35991600
H	-3.52822400	-1.59197800	-1.13474000
O	-2.76266200	1.57537800	-0.34019300
O	-4.03815800	1.81264600	0.10976800
H	-4.57988700	1.65523900	-0.65411500

sC<sub>8</sub>H<sub>17</sub>

	Cartesian Coordinates (Å)		
C	-4.43263100	0.27609100	0.06452000
H	-4.48379800	0.83939500	0.99248100
H	-4.51104700	0.98499600	-0.75545600

H	-5.30245000	-0.37308000	0.02400100
C	-3.13552200	-0.52770600	-0.02265600
H	-3.10439800	-1.25060700	0.79030700
H	-3.13133900	-1.10580000	-0.94476500
C	-1.88322400	0.34902100	0.03111100
H	-1.91822300	1.07353200	-0.78147800
H	-1.89017700	0.92715700	0.95416100
C	-0.58037500	-0.44746300	-0.05718500
H	-0.57426900	-1.02511100	-0.98052600
H	-0.54671600	-1.17207500	0.75524600
C	0.67015700	0.43119200	-0.00216600
H	0.66803100	1.00867500	0.92015500
H	0.63831100	1.15419200	-0.81576600
C	1.97350100	-0.36688400	-0.09018900
H	1.96849400	-0.95751300	-1.01148800
H	2.01111300	-1.09324700	0.72105400
C	3.20662900	0.48960800	-0.04543800
H	3.15716600	1.46749200	-0.49829900
C	4.55932800	-0.13248800	0.13630800
H	4.87340200	-0.68159500	-0.75411400
H	5.31848300	0.61639800	0.33774100
H	4.56024100	-0.84102500	0.96091700

*i*C<sub>8</sub>H<sub>18</sub>

Cartesian Coordinates (Å)

C	4.19311400	-0.22002400	0.15725600
H	4.24652000	-0.37237400	1.23197500
H	5.04677900	0.38540300	-0.13318600
H	4.29986200	-1.19130900	-0.31842500
C	2.87742800	0.44827300	-0.24094700
H	2.87035300	0.61739000	-1.31609200
H	2.81813400	1.43120100	0.22253400
C	1.64703500	-0.37176800	0.15073800
H	1.65563800	-0.53827100	1.22721800
H	1.71207000	-1.35677700	-0.30942600
C	0.32541700	0.28814200	-0.24850800
H	0.31290500	0.44073600	-1.32718400
H	0.27641900	1.27652500	0.20113300
C	-0.89740400	-0.53791600	0.15950700
H	-0.92258400	-0.63201300	1.24523600
H	-0.77525500	-1.54814300	-0.22770300
C	-2.25041200	0.00473500	-0.32625100
H	-2.19570200	0.11446800	-1.40929700
C	-3.36790800	-0.99605400	-0.01525700
H	-3.46864300	-1.14648900	1.05726100

H	-4.32567800	-0.64572200	-0.38982300
H	-3.16957000	-1.96389000	-0.46706900
C	-2.58524500	1.37617000	0.26977000
H	-2.61081100	1.33076400	1.35652500
H	-1.86217800	2.13329200	-0.01370200
H	-3.56041700	1.71587500	-0.06781700

TS<sub>25</sub>

	Cartesian Coordinates (Å)		
C	-4.81369800	0.37501700	-0.21018600
H	-5.13524500	-0.66307700	-0.21943700
H	-4.81870800	0.73050800	-1.23704100
H	-5.55585700	0.94563800	0.34029800
C	-3.42726700	0.51843200	0.41684600
H	-3.14981200	1.57034100	0.44141200
H	-3.46483400	0.18816200	1.45325600
C	-2.35001100	-0.27141800	-0.32816900
H	-2.31889600	0.05635900	-1.36602200
H	-2.62815400	-1.32452600	-0.34919900
C	-0.95821700	-0.12559300	0.29051900
H	-1.00188700	-0.43612200	1.33138200
H	-0.67256700	0.92374300	0.29083500
C	0.09988200	-0.94300000	-0.45601200
H	0.05355500	-0.69928200	-1.51450300
H	-0.14778100	-2.00420800	-0.38079600
C	1.54030100	-0.76574700	0.01061400
H	1.78670000	0.51462200	-0.20266500
C	2.55129700	-1.46751900	-0.87814300
H	2.39879400	-1.21925800	-1.92276800
H	3.56643400	-1.19584100	-0.61150500
H	2.45519700	-2.54821400	-0.77393800
C	1.79434200	-0.96647900	1.49412300
H	1.19539800	-0.30365100	2.10758600
H	1.55339200	-1.99015800	1.78081200
H	2.83875800	-0.79703800	1.73396200
O	2.04142800	1.67829700	-0.43160500
O	3.35072500	1.81254100	-0.03884900
H	3.28851500	2.20313800	0.82442200

*t*C<sub>8</sub>H<sub>17</sub>

	Cartesian Coordinates (Å)		
C	-4.16426300	-0.21779900	0.08009200
H	-4.25470100	-0.40009900	1.14765200
H	-4.25740400	-1.17489500	-0.42620800
H	-5.00583100	0.39871800	-0.22201700
C	-2.83401300	0.45662700	-0.25420400



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H	-2.78971400	0.65577600	-1.32323100
H	-2.78788700	1.42591100	0.23858900
C	-1.62002000	-0.37862100	0.15599500
H	-1.67198000	-1.35001300	-0.33383600
H	-1.66590100	-0.57523800	1.22648500
C	-0.28475200	0.28808000	-0.18010600
H	-0.24800900	1.26337000	0.29840500
H	-0.22989200	0.46802100	-1.25226400
C	0.92061200	-0.55399000	0.25282200
H	0.80872200	-1.55736300	-0.15241400
H	0.89200400	-0.67214800	1.34175100
C	2.27387200	-0.01942900	-0.15179200
C	3.41322000	-1.00219800	-0.17685400
H	3.12350400	-1.93863300	-0.64413700
H	4.26824300	-0.60753400	-0.71778600
H	3.75599600	-1.24054200	0.83401300
C	2.61635100	1.41485200	0.15173800
H	1.85871800	2.10444900	-0.20427500
H	2.71837500	1.57809300	1.22839300
H	3.55972000	1.69700700	-0.30526300

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