Supplementary Information for:

Detailed kinetic model for hexyl sulfide pyrolysis and its desulfurization by supercritical water

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S1 Additional Quantum Chemical Calculations

S1.1 Hydrogen Migration

Four intramolecular hydrogen abstraction (or hydrogen migration) reactions were chosen for this work, based on possible relevance to the hexyl sulfide decomposition mechanism. Due to the stabilization from the neighboring sulfur atom, the most stable product should be the hexyl sulfide alpha-radical produced from hydrogen abstraction of the initial

reactant. However, in a pyrolysis decomposition mechanism other hexyl sulfide radicals—particularly the beta radical—could also be important intermediates in some of the pathways. Thus, rate parameters were calculated for reactions with five- or six-membered cyclic transition states to convert between different hexyl sulfide radicals.

Rate parameters for four hydrogen migration reactions are presented in Table 1, and Figure 1 shows calculated transition state geometries. The ring size of the transition state had the greatest effect on the rate constant, as reactions S2 and S4 had greater Arrhenius pre-factors (ln *A*) but lower values for *n*, as well as activation energies approximately 22 kJ/mol less than the similar reactions (S1 and S3, respectively) with one fewer carbon in the cyclic transition state. Comparing reactions with the same number of atoms in the transition state ring, we see that the reaction rates at 400 °C will be similar (within a factor of 10) for reactions S1 and S3, and likewise for reactions S2 and S4.

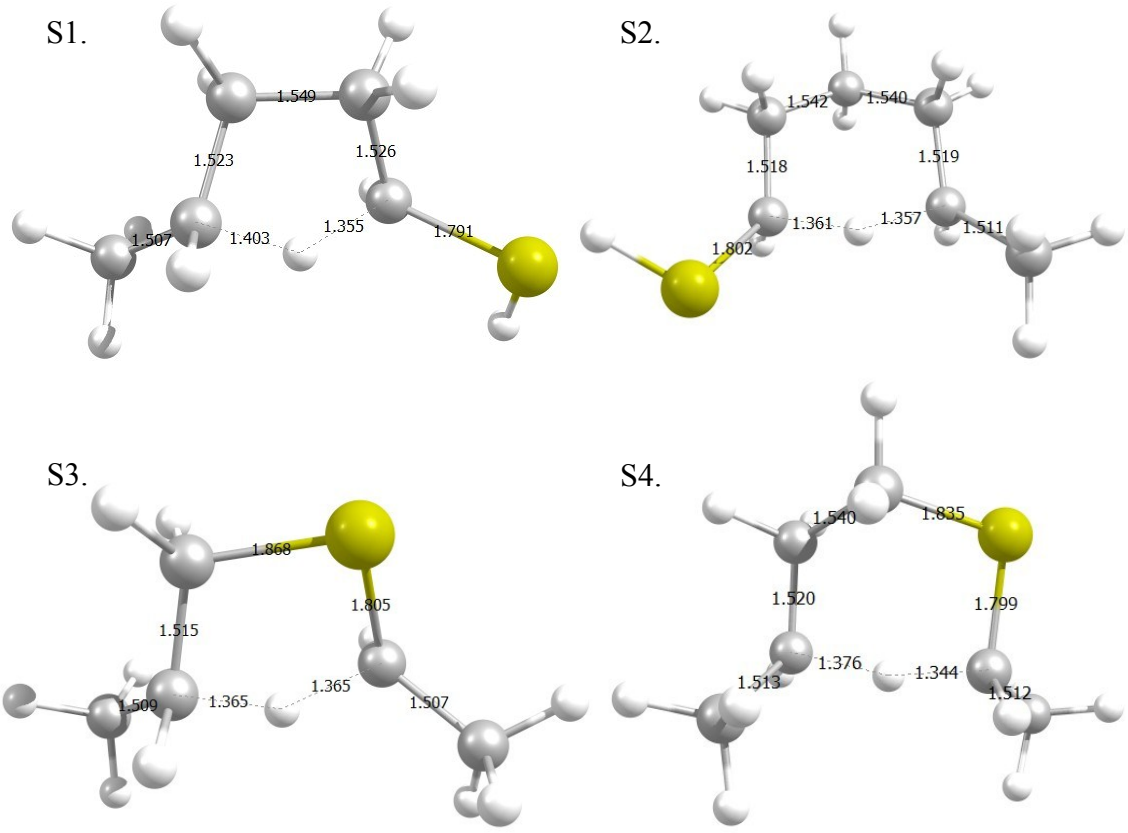
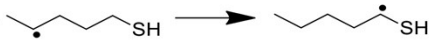
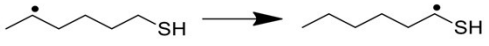
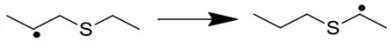


Figure 1. Transition state geometries for the four hydrogen migration reactions. Distances (Ångstroms).

Table 1. Calculated rate constants for hydrogen migration reactions. A (s^{-1}), n (unitless), and E_a (kJ/mol).

Reactions	Rate Parameters			Reverse		
	logA	*n*	*Ea*	*logA*	*n*	*Ea*
S1. 	-4.75	4.50	49.91	-3.34	4.07	69.27
S2. 	-1.29	3.24	29.04	0.11	2.82	48.56
S3. 	-2.94	3.95	46.73	-1.79	3.74	69.22
S4. 	-1.55	3.28	24.73	0.43	2.76	51.66

S1.2 Radical Addition to Multiple Bond

Six radical addition reactions—beta scission reactions in the reverse direction—were considered for this work. These proceed via the pathway shown in Figure 2, and the calculated modified Arrhenius parameters are presented in Table 2. Reactions S5 through S9 were chosen as possible consumption reactions for the thioaldehyde formed from hexyl sulfide decomposition. Radical addition to the sulfur atom in the C-S double bond were not calculated in this work, as rate parameters for many of these reactions have previously been calculated and added to the RMG database.[1] Reactions S10 through S12 are relevant to hexyl sulfide decomposition in the beta scission direction, as they are possible final steps in the production of thiophenic compounds from hexyl sulfide.

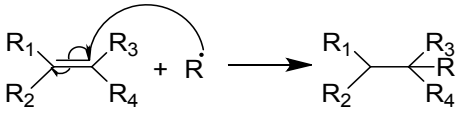
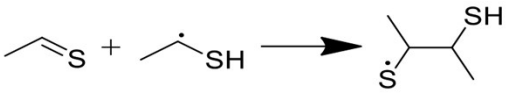
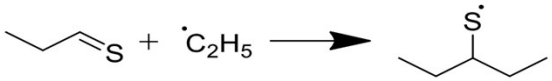
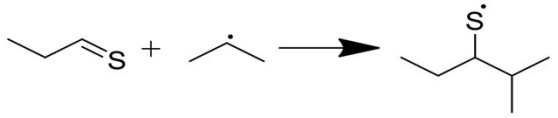
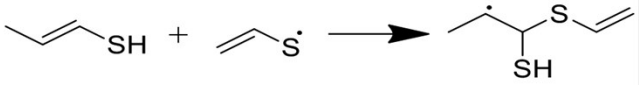
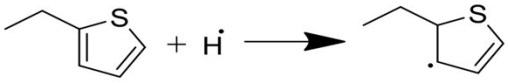
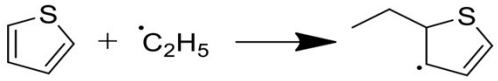
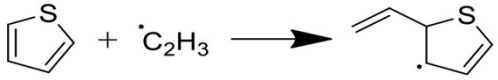


Figure 2. A radical addition reaction.

Activation energies for the four reactions involving addition of a radical to the thiocarbonyl group were all below 5 kJ/mol, and negative activation energies were fit to reactions S6 and S8 (although the overall rate constants exhibit the usual positive temperature dependence when including the temperature exponential n). This is due to the instability of thiocarbonyl compounds, which are known to polymerize at room temperature.[2] The energetics of reaction S9 reveal a submerged transition state, and a complex was optimized near this geometry. A rate constant for this reaction was estimated using the method described in section S1.3.

Table 2. Calculated rate constants for radical addition and beta scission reactions. *A* [cm^3/(mol*s)], *n* (unitless), and E_a (kJ/mol).

Reactions	Rate Parameters		
	logA	***n***	***Ea***
S5. 	9.07	1.46	4.92
S6. 	0.19	3.16	-6.73
S7. 	3.24	2.50	2.26
S8. 	1.58	2.82	-5.14
S9. 	12.2	0.03	2.10
S10. 	7.40	1.76	9.89
S11. 	1.99	3.25	24.33
S12. 	4.06	2.56	11.09

Larger activation energies were calculated for the addition of a radical to a stable thiophenic compound (reactions S10-S12). Of more interest to this work is the reverse direction for reactions S10 and S11, which can be estimated using thermodynamic consistency. Beta scission of the ethyl radical from the initial cyclic radical occurs via a significantly lower energy pathway than beta scission of hydrogen. Thus, if beta scission of this radical were the primary method of generating thiophenic compounds from hexyl sulfide, the production of thiophene over ethyl thiophene would be expected, in disagreement with experimental data. However, disproportionation reactions also promote the generation of ethyl thiophene, and this could help explain the experimental results. The beta scission of the vinyl radical to form thiophene, the reverse of reaction S12, has a high activation energy. This species would be more likely to undergo radical-mediated tautomerization to eventually form ethyl-thiophene, an experimentally observed pyrolysis product of hexyl sulfide. This mechanism is discussed further below.

S1.3 Calculation of Rate Constants for Reactions with Submerged Transition States

The reaction barrier was calculated to be significantly negative (i.e. greater than the uncertainty of the calculations) for two of the reactions studied in this work, implying the existence of reactive complexes at lower energy levels than the reactants of the respective reactions. This type of "submerged-barrier" reaction is illustrated in Figure 3. The same methods as discussed previously for reactants and products were used to calculate energies and frequencies for the reactive complex of each reaction.

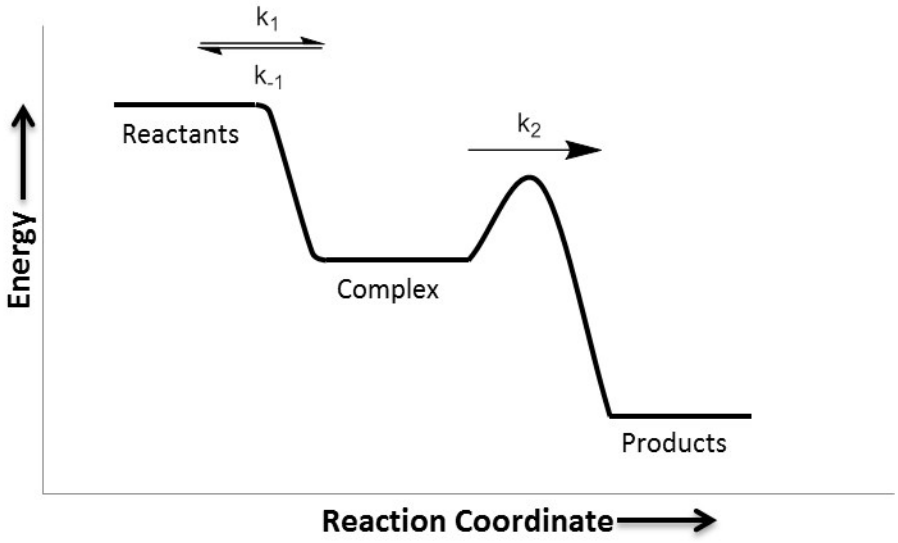


Figure 3. Potential energy surface for a generic reaction with a submerged transition state.

The parameters for each submerged reaction were calculated for the high-pressure limit using CanTherm. The rate k_1 for the formation of complex was assumed to be the collision rate, 10^{13} cm^3/(mol*s), and k_{-1} was calculated using thermochemical consistency. The rate of formation of products from the pre-reactive complex, k_2, was calculated using transition-state theory. The complex is short-lived, so it can be modeled using the quasi-steady-state approximation. The overall rate of product formation for a reaction with two reactants is therefore

$$\frac{dC_P}{dt} = \frac{k_1 k_2}{k_{-1} + k_2} C_{R_1} C_{R_2}$$

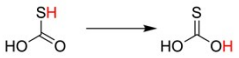
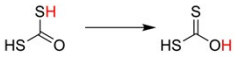
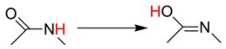
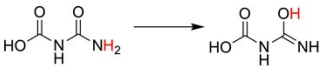
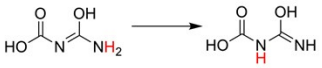
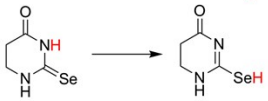
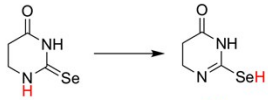
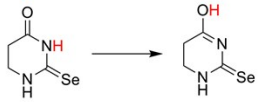
and the effective rate constant is

$$k_{eff}(T) = \frac{k_1 k_2}{k_{-1} + k_2}$$ The effective rate constant $k_{eff}(T)$ was calculated at temperatures between 300 and 2000 K, and modified Arrhenius parameters were fit to these calculations to obtain the values reported in the Tables for Reactions 21 and 37. As our primary interest is in supercritical water reactions (with pressures greater than 200 bar), rate constants are reported in the high pressure limit. In some gas-phase situations, the low-pressure limit might be more appropriate than the high-pressure limit values reported here.

S2 H_2O catalysis of hydrogen transfer reactions

We conducted a literature survey to better understand the impact of water on the rate of tautomerization reactions in organic compounds[3-9]. Reported activation energies and Gibbs free energies of activation are presented in Table 3. The assistance of one water molecule consistently decreases the activation barrier by about half, which would increase the reaction rate by multiple orders of magnitude at the SCW concentration in our study. While the tautomerization reactions of Deng *et al.* were included in the RMG database for this study, many more H_2O-assisted hydrogen transfer reactions are possible, and a thorough study of their reaction rates would likely improve the quantitative product predictions of our model.

Table 3. Reported activation energies (E_a) or Gibbs free energies of activation ($\Delta^{\ddagger}G$) for tautomerization reactions in the gas phase. Rate constants for the unimolecular reaction and the reaction assisted by one water molecule are presented, as well as the ratio of the two. Reactions are presented in the endothermic direction.

Reaction	Source	Unimolecular		H2O-Assisted		Ratio (H20-Assisted / Unimolecular)	
		E_a	$\Delta^{\ddagger}G$	E_a	$\Delta^{\ddagger}G$	E_a	$\Delta^{\ddagger}G$
	Deng *et al.* (2007)	132.1		63.2		0.48	
	Deng *et al.* (2008)		131.0		69.7		0.53
	Fu *et al.* (2003)	186.5		82.2		0.44	
	Li *et al.* (2008)		157.3		74.5		0.47
	Hajipour *et al.* (2016)	189.0		90.9		0.48	
	Hajipour *et al.* (2016)	184.9		121.2			
	Trujillo *et al.* (2007)	157.7		81.2		0.51	
	Trujillo *et al.* (2007)	128.9		69.5		0.54	
	Trujillo *et al.* (2007)	171.1		64.9		0.38	
					Average =	**0.47**	
					Std. Dev. =	**0.057**	

S3 References

1. A. G. Vandeputte, PhD Thesis. University of Ghent, 2012.
2. N. J. Cooper, *Compr. Org. Funct. Group Transform. II*, 2005, **3**, 355-396.
3. A.-P. Fu, H.-L. Li, D.-M. Du and Z.-Y. Zhou, *Chemical Physics Letters*, 2003, **382**, 332-337.
4. X.-C. Wang, J. Nichols, M. Feyereisen, M. Gutowski, J. Boatz, A. D. J. Haymet and J. Simons, *J. Phys. Chem.*, 1991, **95**, 10419-10424.
5. Q.-G. Li, Y. Xue and G.-s. Yan, *Journal of Molecular Structure (Theochem)*, 2008, **868**, 55-64.
6. A. R. Hajipour, M. Karimzadeh, S. Ghorbani, H. Farrokhpour and A. N. Chermahini, *Struct. Chem.*, 2016, **27**, 1345-1362.
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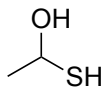
8. C. Deng, Q.-G. Li, Y. Ren, N.-B. Wong, S.-Y. Chu and H.-J. Zhu, *Journal of Computational Chemistry*, 2007, **29**, 466-480.
9. C. Deng, X.-P. Wu, X.-M. Sun, Y. Ren and Y.-H. Sheng, *Journal of Computational Chemistry*, 2008, **30**, 285-294.

S4 Optimized geometries



0 1

C						
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S	1	B2	2	A1		
H	1	B3	3	A2	2	D1
O	1	B4	3	A3	2	D2
H	3	B5	1	A4	5	D3
C	1	B6	5	A5	3	D4
H	7	B7	1	A6	5	D5
H	7	B8	1	A7	5	D6
H	7	B9	1	A8	5	D7

B1	1.08942056
B2	1.86212814
B3	1.93258637
B4	1.40618355
B5	1.34374699
B6	1.52450124
B7	1.09213032
B8	1.09216321
B9	1.09430327
A1	107.43710284
A2	95.69966608
A3	112.16537584
A4	95.43657376
A5	112.90485694
A6	111.56130222
A7	108.84778614
A8	110.84308365
D1	139.38757587
D2	115.43728334
D3	56.61660460
D4	-122.50257855
D5	-174.28312724
D6	-54.12186971
D7	64.87864161

H_2S

0 1
S
H 1 B1
H 1 B2 2 A1

B1 1.34327993
B2 1.34327993
A1 92.58329996

0 1
C
H 1 B1
C 1 B2 2 A1
H 3 B3 1 A2 2 D1
S 3 B4 1 A3 2 D2
H 1 B5 3 A4 5 D3
H 1 B6 3 A5 5 D4

B1 1.08911236
B2 1.49291678
B3 1.09300816
B4 1.61980609
B5 1.09733033
B6 1.09697723
A1 111.78326121
A2 114.81232591
A3 126.45725204
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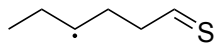
A5 109.77061696
D1 -179.94981833
D2 0.08504453
D3 -121.81265346
D4 121.94294055



0 2
C
H 1 B1
H 1 B2 2 A1
H 1 B3 2 A2 3 D1
C 1 B4 4 A3 3 D2
H 5 B5 1 A4 4 D3

H	5	B6	1	A5	4	D4	
C	5	B7	1	A6	4	D5	
H	8	B8	5	A7	1	D6	
C	8	B9	5	A8	1	D7	
H	10	B10	8	A9	5	D8	
H	10	B11	8	A10	5	D9	
C	10	B12	8	A11	5	D10	
H	13	B13	10	A12	8	D11	
H	13	B14	10	A13	8	D12	
C	13	B15	10	A14	8	D13	
H	16	B16	13	A15	10	D14	
S	16	B17	13	A16	10	D15	

B1	1.09310789
B2	1.09388454
B3	1.09285837
B4	1.53433172
B5	1.10523140
B6	1.09856903
B7	1.49260949
B8	1.08698919
B9	1.48920787
B10	1.09409912
B11	1.09704788
B12	1.57236339
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B16	1.09389876
B17	1.62211117
A1	107.75230659
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A9	110.49053739
A10	110.29638092
A11	112.78828438
A12	107.99698193
A13	109.85026660
A14	111.23421744
A15	114.75607469
A16	126.45855111

D1	116.19069085
D2	121.79168535
D3	-56.31432391
D4	57.74645191
D5	-179.14015813
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D8	158.94437424
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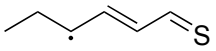

C

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H	1	B2	2	A1			
H	1	B3	3	A2	2	D1	
C	1	B4	4	A3	3	D2	
H	5	B5	1	A4	4	D3	
H	5	B6	1	A5	4	D4	
C	5	B7	1	A6	4	D5	
H	8	B8	5	A7	1	D6	
C	8	B9	5	A8	1	D7	
H	10	B10	8	A9	5	D8	
C	10	B11	8	A10	5	D9	
H	12	B12	10	A11	8	D10	
C	12	B13	10	A12	8	D11	
H	14	B14	12	A13	10	D12	
S	14	B15	12	A14	10	D13	

B1	1.09329581
B2	1.09329466
B3	1.09214141
B4	1.52908644
B5	1.09931982
B6	1.09931502
B7	1.49740746
B8	1.08885427
B9	1.35829549
B10	1.08675247

B11	1.42261083
B12	1.08674783
B13	1.39003439
B14	1.09069031
B15	1.67853720
A1	107.99430779
A2	107.64817564
A3	110.32516062
A4	109.76029717
A5	109.76146734
A6	116.58552993
A7	115.43508277
A8	126.86618093
A9	119.58564765
A10	123.22166677
A11	118.51329727
A12	123.71623936
A13	117.24519891
A14	124.46626726
D1	-115.96653981
D2	121.90303240
D3	-57.03802830
D4	57.03230689
D5	180.00000000
D6	-179.99100461
D7	0.00966225
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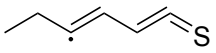

0 2

C							
C	1	B1					
H	2	B2	1	A1			
C	2	B3	1	A2	3	D1	
H	4	B4	2	A3	1	D2	
C	4	B5	2	A4	1	D3	
S	6	B6	4	A5	2	D4	
C	1	B7	2	A6	4	D5	
H	8	B8	1	A7	2	D6	

H	8	B9	1	A8	2	D7
C	8	B10	1	A9	2	D8
H	11	B11	8	A10	1	D9
H	11	B12	8	A11	1	D10
H	11	B13	8	A12	1	D11

B1	1.31885833
B2	1.08811509
B3	1.47379936
B4	1.08703509
B5	1.31492787
B6	1.56131445
B7	1.46895435
B8	1.09711358
B9	1.10378463
B10	1.53970500
B11	1.09284792
B12	1.09217522
B13	1.09214021
A1	119.45639330
A2	124.71545427
A3	118.70740921
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A5	179.32526106
A6	142.16379251
A7	109.36782904
A8	108.92444022
A9	113.74556529
A10	110.49832941
A11	110.88945985
A12	110.75361716
D1	-179.86895412
D2	0.06813492
D3	-179.94115088
D4	-4.78838976
D5	0.40776337
D6	-119.07667031
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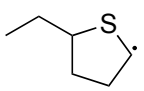

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H	5	B5	1	A4	3	D3	
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C	8	B9	5	A8	1	D7	
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C	10	B12	8	A11	5	D10	
H	13	B13	10	A12	8	D11	
H	13	B14	10	A13	8	D12	
C	13	B15	10	A14	8	D13	
H	16	B16	13	A15	10	D14	
S	16	B17	13	A16	10	D15	

B1	1.09471420
B2	1.09277114
B3	1.09296902
B4	1.52999159
B5	1.09468955
B6	1.09782627
B7	1.53471397
B8	1.09278337
B9	1.53971246
B10	1.09305808
B11	1.09405031
B12	1.54021476
B13	1.09584729
B14	1.10238912
B15	1.49603315
B16	1.08049121
B17	1.73613620
A1	107.95416388
A2	107.81988308
A3	111.17978170
A4	109.80171042
A5	109.17527314
A6	114.25851552
A7	109.38261641
A8	113.98506333

A9	109.02733813
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A11	108.27779757
A12	111.20914484
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A14	105.80134345
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D1	-116.07873164
D2	-121.76935181
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D5	-61.55283334
D6	-51.95613016
D7	-176.56511592
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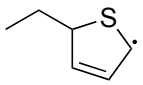

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H	5	B5 1	A4 4	D3
H	5	B6 1	A5 4	D4
C	5	B7 1	A6 4	D5
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C	8	B9 5	A8 1	D7
H	10	B10 8	A9 5	D8
C	10	B11 8	A10 5	D9
H	12	B12 10	A11 8	D10
C	12	B13 10	A12 8	D11
H	14	B14 12	A13 10	D12
S	14	B15 12	A14 10	D13

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B2	1.09452713
B3	1.09283973
B4	1.52992485
B5	1.09704274
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B7	1.54061370
B8	1.09829029
B9	1.50302029
B10	1.08281092
B11	1.37442074
B12	1.08385797
B13	1.39443268
B14	1.07937932
B15	1.74518083
A1	107.93349224
A2	107.58631454
A3	110.86328024
A4	109.50260223
A5	110.47582868
A6	114.05016022
A7	108.41977593
A8	114.14436943
A9	120.10383273
A10	115.41736635
A11	123.28737439
A12	114.86719086
A13	127.38854877
A14	112.91914707
D1	116.01549522
D2	-121.91987240
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D5	-177.97565910
D6	52.26207849
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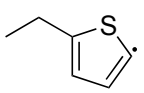

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C
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C 2 B3 1 A2 3 D1
H 4 B4 2 A3 1 D2
C 4 B5 2 A4 1 D3
S 6 B6 4 A5 2 D4
C 1 B7 2 A6 4 D5
H 8 B8 1 A7 2 D6
H 8 B9 1 A8 2 D7
C 8 B10 1 A9 2 D8
H 11 B11 8 A10 1 D9
H 11 B12 8 A11 1 D10
H 11 B13 8 A12 1 D11

B1 1.36771775
B2 1.08403064
B3 1.43923992
B4 1.08116358
B5 1.35056047
B6 1.71023818
B7 1.50243006
B8 1.09559470
B9 1.09508836
B10 1.53805348
B11 1.09341353
B12 1.09260633
B13 1.09290347
A1 122.49641228
A2 114.63590786
A3 124.66411964
A4 109.54424392
A5 115.52087672
A6 128.61758880
A7 110.07553893
A8 107.13671821
A9 114.29346718
A10 110.62424779
A11 110.79354998
A12 111.29558407
D1 179.86269832
D2 -179.86836979
D3 0.04713063

D4	-0.12037508
D5	-178.84548827
D6	-128.91797878
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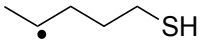

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H	5	B5	1	A4	4	D3	
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H	7	B7	5	A6	1	D5	
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C	7	B9	5	A8	1	D7	
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H	10	B11	7	A10	5	D9	
C	10	B12	7	A11	5	D10	
H	13	B13	10	A12	7	D11	
H	13	B14	10	A13	7	D12	
S	13	B15	10	A14	7	D13	
H	16	B16	13	A15	10	D14	

B1	1.10344680
B2	1.09688756
B3	1.09284247
B4	1.49021043
B5	1.08603472
B6	1.49291928
B7	1.09982298
B8	1.10619234
B9	1.53755681
B10	1.09452227
B11	1.09533725
B12	1.52748763
B13	1.09205797
B14	1.09340932
B15	1.83922317

B16	1.34458525
A1	106.06279594
A2	108.06352042
A3	111.88409959
A4	118.82372569
A5	121.44216973
A6	109.56922035
A7	110.04282722
A8	113.65266675
A9	109.71235487
A10	109.17588816
A11	112.60118503
A12	111.40707974
A13	110.62999925
A14	114.54062540
A15	96.88508918
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D2	122.95872821
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D4	167.52805164
D5	-42.67916127
D6	72.01003639
D7	-165.91445120
D8	-57.77797465
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D13	176.84768796
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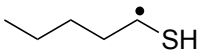

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C	1	B4	4	A3	2	D2
H	5	B5	1	A4	4	D3
H	5	B6	1	A5	4	D4
C	5	B7	1	A6	4	D5
H	8	B8	5	A7	1	D6
H	8	B9	5	A8	1	D7
C	8	B10	5	A9	1	D8

H	11	B11	8	A10	5	D9
H	11	B12	8	A11	5	D10
C	11	B13	8	A12	5	D11
H	14	B14	11	A13	8	D12
S	14	B15	11	A14	8	D13
H	16	B16	14	A15	11	D14

B1	1.09437594
B2	1.09434246
B3	1.09344181
B4	1.53140092
B5	1.09688813
B6	1.09683815
B7	1.53262511
B8	1.09583629
B9	1.09642010
B10	1.54719245
B11	1.09814658
B12	1.09706177
B13	1.49423924
B14	1.08383802
B15	1.74179628
B16	1.34694757
A1	107.54470796
A2	107.68860065
A3	111.39494765
A4	109.46023750
A5	109.45281685
A6	113.13486852
A7	109.74713976
A8	109.61532506
A9	113.03894380
A10	108.62925433
A11	108.63934999
A12	114.68883038
A13	120.52425296
A14	123.66799617
A15	97.79115791
D1	115.78053599
D2	122.13336018
D3	57.77066912
D4	-58.08762216
D5	179.80319741
D6	-58.30330375
D7	58.06802994
D8	179.83298302

D9	57.10961148
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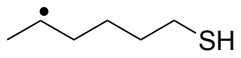

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C							
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H	1	B2	2	A1			
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C	1	B4	4	A3	3	D2	
H	5	B5	1	A4	4	D3	
C	5	B6	1	A5	4	D4	
H	7	B7	5	A6	1	D5	
H	7	B8	5	A7	1	D6	
C	7	B9	5	A8	1	D7	
H	10	B10	7	A9	5	D8	
H	10	B11	7	A10	5	D9	
C	10	B12	7	A11	5	D10	
H	13	B13	10	A12	7	D11	
H	13	B14	10	A13	7	D12	
C	13	B15	10	A14	7	D13	
H	16	B16	13	A15	10	D14	
H	16	B17	13	A16	10	D15	
S	16	B18	13	A17	10	D16	
H	19	B19	16	A18	13	D17	

B1	1.09693238
B2	1.10348692
B3	1.09290300
B4	1.49033418
B5	1.08619830
B6	1.49270223
B7	1.10603881
B8	1.09993724
B9	1.53564283
B10	1.09710444
B11	1.09637176
B12	1.53414845
B13	1.09648314
B14	1.09488872

B15	1.52808025
B16	1.09332001
B17	1.09194578
B18	1.83982196
B19	1.34451968
A1	106.04346481
A2	108.05402937
A3	111.92791697
A4	118.76751594
A5	121.44484735
A6	110.05285412
A7	109.55938955
A8	113.99338848
A9	108.98625678
A10	109.02040916
A11	113.18969024
A12	109.45846232
A13	110.00063668
A14	112.58148354
A15	110.61594876
A16	111.38030167
A17	114.60609155
A18	96.87412509
D1	-114.23310363
D2	-122.98873031
D3	26.90037035
D4	-167.42934462
D5	-71.00933683
D6	43.56428217
D7	166.75474009
D8	57.17748196
D9	-58.43056346
D10	179.11530404
D11	58.10182603
D12	-58.37953630
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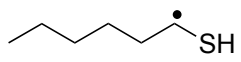

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C

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H	1	B2	2	A1			
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H	4	B4	1	A3	3	D2	
H	4	B5	1	A4	3	D3	
C	4	B6	1	A5	3	D4	
H	7	B7	4	A6	1	D5	
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H	10	B11	7	A10	4	D9	
C	10	B12	7	A11	4	D10	
H	13	B13	10	A12	7	D11	
S	13	B14	10	A13	7	D12	
H	15	B15	13	A14	10	D13	
C	1	B16	4	A15	7	D14	
H	17	B17	1	A16	4	D15	
H	17	B18	1	A17	4	D16	
H	17	B19	1	A18	4	D17	

B1	1.09661673
B2	1.09657838
B3	1.53321189
B4	1.09790255
B5	1.09785135
B6	1.53242581
B7	1.09565241
B8	1.09628750
B9	1.54743586
B10	1.09805638
B11	1.09708769
B12	1.49421358
B13	1.08386455
B14	1.74179327
B15	1.34700872
B16	1.53145901
B17	1.09449853
B18	1.09338835
B19	1.09450428
A1	106.06303098
A2	109.17762482
A3	109.16722148
A4	109.17009723
A5	113.51210679
A6	109.82911561
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A8	113.00371607
A9	108.65965733
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A11	114.63527869
A12	120.49436712
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A16	111.19706282
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D1	-117.50885833
D2	-64.58672729
D3	179.92559226
D4	57.63174729
D5	-58.54141708
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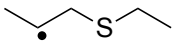

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C							
H	1	B1					
H	1	B2	2	A1			
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C	1	B4	3	A3	2	D2	
H	5	B5	1	A4	3	D3	
H	5	B6	1	A5	3	D4	
S	5	B7	1	A6	3	D5	
C	8	B8	5	A7	1	D6	
H	9	B9	8	A8	5	D7	
H	9	B10	8	A9	5	D8	
C	9	B11	8	A10	5	D9	
H	12	B12	9	A11	8	D10	

C	12	B13	9	A12	8	D11	
H	14	B14	12	A13	9	D12	
H	14	B15	12	A14	9	D13	
H	14	B16	12	A15	9	D14	

B1	1.09271677
B2	1.09265235
B3	1.09377436
B4	1.52724888
B5	1.09358729
B6	1.09195017
B7	1.83440046
B8	1.88287850
B9	1.09376194
B10	1.09183073
B11	1.47362455
B12	1.08519601
B13	1.49013393
B14	1.10109964
B15	1.09616604
B16	1.09284796
A1	108.04440509
A2	108.02089606
A3	111.31684300
A4	110.51930765
A5	110.43099396
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A7	100.42428937
A8	102.38060518
A9	106.53701036
A10	114.26470287
A11	118.20412467
A12	121.90791778
A13	111.64924626
A14	111.54057989
A15	111.65635220
D1	-116.56362123
D2	122.42908645
D3	59.65423445
D4	179.55725140
D5	-60.10680984
D6	178.34650360
D7	-168.86417849
D8	-55.16009491
D9	69.87717898
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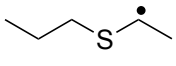

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C							
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C	1	B4	2	A3	3	D2	
H	5	B5	1	A4	2	D3	
S	5	B6	1	A5	2	D4	
C	7	B7	5	A6	1	D5	
H	8	B8	7	A7	5	D6	
H	8	B9	7	A8	5	D7	
C	8	B10	7	A9	5	D8	
H	11	B11	8	A10	7	D9	
H	11	B12	8	A11	7	D10	
C	11	B13	8	A12	7	D11	
H	14	B14	11	A13	8	D12	
H	14	B15	11	A14	8	D13	
H	14	B16	11	A15	8	D14	

B1	1.09414091
B2	1.10113021
B3	1.09443863
B4	1.49343645
B5	1.08541322
B6	1.73274522
B7	1.83218423
B8	1.09404430
B9	1.09332755
B10	1.52990294
B11	1.09436275
B12	1.09389399
B13	1.53259726
B14	1.09436449
B15	1.09307217
B16	1.09440605
A1	107.04957715
A2	107.80221581
A3	111.53048270

A4	120.11163500
A5	119.44121609
A6	101.69939229
A7	107.80488042
A8	104.66655539
A9	114.39970067
A10	108.95337647
A11	108.99046866
A12	112.23919385
A13	111.38796138
A14	110.93224589
A15	111.39177797
D1	114.64447126
D2	-123.94848813
D3	-162.88730087
D4	38.64174535
D5	-172.22751234
D6	-52.63115202
D7	-166.61697929
D8	71.74811612
D9	57.96880275
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D12	60.27050479
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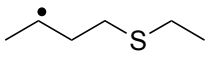

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H	5	B5	1	A4	3	D3	
H	5	B6	1	A5	3	D4	
S	5	B7	1	A6	3	D5	
C	8	B8	5	A7	1	D6	
H	9	B9	8	A8	5	D7	
H	9	B10	8	A9	5	D8	
C	9	B11	8	A10	5	D9	
H	12	B12	9	A11	8	D10	
C	12	B13	9	A12	8	D11	
H	14	B14	12	A13	9	D12	

H	14	B15	12	A14	9	D13
H	14	B16	12	A15	9	D14
C	12	B17	9	A16	8	D15
H	18	B18	12	A17	9	D16
H	18	B19	12	A18	9	D17

B1	1.09277969
B2	1.09258394
B3	1.09355656
B4	1.52728770
B5	1.09330684
B6	1.09216568
B7	1.83554925
B8	1.82975765
B9	1.09348989
B10	1.09348128
B11	2.52361492
B12	1.08652485
B13	1.49038817
B14	1.09294299
B15	1.09669765
B16	1.10333416
B17	1.49384392
B18	1.10347347
B19	1.09701908
A1	108.05652226
A2	108.07105361
A3	111.25158724
A4	110.56509957
A5	110.26314513
A6	109.93415826
A7	101.28609150
A8	104.38061938
A9	108.71896899
A10	148.30033026
A11	89.18202024
A12	151.84117362
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A14	111.60404590
A15	112.01505484
A16	34.07328091
A17	110.82148399
A18	109.58097577
D1	-116.54169504
D2	122.41178226
D3	59.39695844

D4	179.20590308
D5	-60.09399796
D6	176.30718585
D7	-165.22060035
D8	-51.26003947
D9	77.68420306
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D11	-45.12381613
D12	-142.80192222
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D16	121.40353523
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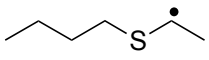

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H	5	B5	1	A4	2	D3	
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C	7	B7	5	A6	1	D5	
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C	8	B10	7	A9	5	D8	
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H	11	B12	8	A11	7	D10	
C	11	B13	8	A12	7	D11	
H	14	B14	11	A13	8	D12	
H	14	B15	11	A14	8	D13	
C	14	B16	11	A15	8	D14	
H	17	B17	14	A16	11	D15	
H	17	B18	14	A17	11	D16	
H	17	B19	14	A18	11	D17	

B1	1.09417480
B2	1.10114553
B3	1.09441266
B4	1.49333591
B5	1.08545919
B6	1.73257155

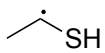
B7	1.83287366
B8	1.09388287
B9	1.09323468
B10	1.52927895
B11	1.09536572
B12	1.09492510
B13	1.53473135
B14	1.09666624
B15	1.09672862
B16	1.53156611
B17	1.09321828
B18	1.09419720
B19	1.09417456
A1	107.05733961
A2	107.80927635
A3	111.50377548
A4	120.14866064
A5	119.45938711
A6	101.71320892
A7	107.74684683
A8	104.61253389
A9	114.38482124
A10	109.07050443
A11	109.08349022
A12	112.60416440
A13	109.32998544
A14	109.38213880
A15	112.85006495
A16	111.34261075
A17	111.14471822
A18	111.16458092
D1	114.66094157
D2	-123.94575147
D3	-162.45049087
D4	38.99955256
D5	-171.86402179
D6	-52.73600745
D7	-166.66862975
D8	71.67086750
D9	58.39507582
D10	-57.38339994
D11	-179.47801396
D12	58.09498634
D13	-57.73335595
D14	-179.83162624
D15	-179.81884691

D16	-59.71958718
D17	60.07941503

0 2

S							
C	1	B1					
H	2	B2	1	A1			
H	2	B3	1	A2	3	D1	
C	2	B4	1	A3	4	D2	
H	5	B5	2	A4	1	D3	
H	5	B6	2	A5	1	D4	
H	5	B7	2	A6	1	D5	

B1	1.81255108
B2	1.09664263
B3	1.09673222
B4	1.52576377
B5	1.09500828
B6	1.09200972
B7	1.09200626
A1	105.99738868
A2	105.92913178
A3	115.64533741
A4	110.46961552
A5	110.99351663
A6	110.99466025
D1	111.39208323
D2	124.26821945
D3	-179.90021959
D4	-59.84034334
D5	60.04987358



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C							
H	1	B1					
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H	3	B3	1	A2	2	D1	
H	3	B4	1	A3	2	D2	
H	3	B5	1	A4	2	D3	
S	1	B6	3	A5	6	D4	

H	7	B7	1	A6	3	D5

B1	1.08280820
B2	1.49081581
B3	1.09616291
B4	1.10097693
B5	1.09318357
B6	1.74140765
B7	1.34672372
A1	120.84333401
A2	111.71416347
A3	112.40421945
A4	110.57850497
A5	123.18636190
A6	97.80640654
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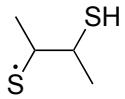

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C						
H	1	B1				
C	1	B2	2	A1		
H	3	B3	1	A2	2	D1
C	3	B4	1	A3	2	D2
H	5	B5	3	A4	1	D3
H	5	B6	3	A5	1	D4
H	5	B7	3	A6	1	D5
C	1	B8	3	A7	5	D6
H	9	B9	1	A8	3	D7
H	9	B10	1	A9	3	D8
H	9	B11	1	A10	3	D9
S	1	B12	9	A11	3	D10
S	3	B13	1	A12	9	D11
H	14	B14	3	A13	1	D12

B1	1.09677273
B2	1.54858189
B3	1.09597259
B4	1.52970739

B5	1.09423191
B6	1.09035918
B7	1.09300545
B8	1.53855186
B9	1.09053967
B10	1.09490589
B11	1.09171073
B12	1.82344416
B13	1.84476855
B14	1.34594172
A1	107.31927559
A2	106.44912693
A3	114.32764412
A4	111.10594690
A5	110.44375033
A6	110.69352243
A7	113.06099846
A8	110.34720317
A9	109.95583417
A10	111.91983440
A11	110.97018710
A12	112.13525299
A13	95.93838453
D1	-63.20774904
D2	176.46520742
D3	58.40099023
D4	178.44968498
D5	-61.87893476
D6	-64.50445401
D7	-171.05791344
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D9	68.71945001
D10	-129.66096727
D11	166.66358796
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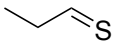

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C							
C	1	B1					
H	2	B2	1	A1			
S	2	B3	1	A2	3	D1	
H	1	B4	2	A3	4	D2	
H	1	B5	2	A4	4	D3	

C	1	B6	2	A5	4	D4
H	7	B7	1	A6	2	D5
H	7	B8	1	A7	2	D6
H	7	B9	1	A8	2	D7

B1	1.49928079
B2	1.09327780
B3	1.62101959
B4	1.10069884
B5	1.10021014
B6	1.52446846
B7	1.09248638
B8	1.09173182
B9	1.09173185
A1	113.68135958
A2	127.79107438
A3	106.54145479
A4	106.58648058
A5	117.20947132
A6	110.14116314
A7	111.21517133
A8	111.20612761
D1	-179.99577006
D2	-124.75872528
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D4	-0.03955432
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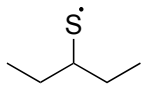
D6	-59.74443602
D7	59.81639596



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C						
H	1	B1				
C	1	B2	2	A1		
H	3	B3	1	A2	2	D1
C	3	B4	1	A3	2	D2
H	5	B5	3	A4	1	D3
H	5	B6	3	A5	1	D4
H	5	B7	3	A6	1	D5
C	1	B8	3	A7	5	D6
H	9	B9	1	A8	3	D7
H	9	B10	1	A9	3	D8

S	1	B11	3	A10	5	D9	
H	3	B12	1	A11	9	D10	
C	9	B13	1	A12	3	D11	
H	14	B14	9	A13	1	D12	
H	14	B15	9	A14	1	D13	
H	14	B16	9	A15	1	D14	

B1	1.10226194
B2	1.54217874
B3	1.09552624
B4	1.52889342
B5	1.09163168
B6	1.09304953
B7	1.09477542
B8	1.54224361
B9	1.09674518
B10	1.09551741
B11	1.82668254
B12	1.09674743
B13	1.52888430
B14	1.09304450
B15	1.09163860
B16	1.09476921
A1	108.20767624
A2	108.85232020
A3	114.86362812
A4	111.27992299
A5	110.67981624
A6	111.06857592
A7	112.57407314
A8	107.29811433
A9	108.85512092
A10	112.50692856
A11	107.29529495
A12	114.85603881
A13	110.68305025
A14	111.27634677
A15	111.06805461
D1	172.14354925
D2	48.29056594
D3	60.40166687
D4	-179.36508749
D5	-59.83547941
D6	167.82066401
D7	-46.01627889
D8	68.48402629

D9	-63.82350674
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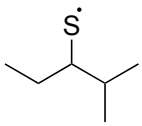

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C				
H	1	B1		
C	1	B2 2	A1	
H	3	B3 1	A2 2	D1
C	3	B4 1	A3 2	D2
H	5	B5 3	A4 1	D3
H	5	B6 3	A5 1	D4
H	5	B7 3	A6 1	D5
C	3	B8 1	A7 5	D6
H	9	B9 3	A8 1	D7
H	9	B10 3	A9 1	D8
H	9	B11 3	A10 1	D9
C	1	B12 3	A11 9	D10
H	13	B13 1	A12 3	D11
H	13	B14 1	A13 3	D12
S	1	B15 13	A14 3	D13
C	13	B16 1	A15 3	D14
H	17	B17 13	A16 1	D15
H	17	B18 13	A17 1	D16
H	17	B19 13	A18 1	D17

B1	1.10218121
B2	1.55164885
B3	1.09878610
B4	1.53481827
B5	1.09272600
B6	1.09322452
B7	1.09457122
B8	1.53281678
B9	1.09353216
B10	1.09448215
B11	1.09261846
B12	1.54430571

B13	1.09705083
B14	1.09409901
B15	1.82654627
B16	1.52928524
B17	1.09307241
B18	1.09186766
B19	1.09478297
A1	107.11280705
A2	104.98723958
A3	112.77395546
A4	112.14274269
A5	110.48388539
A6	110.62193320
A7	112.31484727
A8	110.46700015
A9	111.39030076
A10	111.07247889
A11	113.64817250
A12	107.40049987
A13	109.52119042
A14	112.15990143
A15	114.27562245
A16	110.76292126
A17	111.15104488
A18	111.09372904
D1	-68.49293314
D2	174.45997734
D3	56.57979906
D4	176.60450367
D5	-64.25409284
D6	-126.48145578
D7	-174.61120801
D8	-54.88378676
D9	65.47656012
D10	166.52714930
D11	-40.15018530
D12	74.87691404
D13	-130.90137495
D14	-161.58944563
D15	-179.96626754
D16	-59.81929570
D17	60.39724379

0 1
C
C 1 B1
C 2 B2 1 A1
C 3 B3 2 A2 1 D1
S 4 B4 3 A3 2 D2
H 1 B5 2 A4 3 D3
H 2 B6 1 A5 5 D4
H 3 B7 2 A6 1 D5
H 4 B8 3 A7 2 D6

B1 1.36629669
B2 1.42594200
B3 1.36629669
B4 1.72748369
B5 1.07892407
B6 1.08214933
B7 1.08214933
B8 1.07892407
A1 112.67431284
A2 112.67431284
A3 111.46777715
A4 128.49773050
A5 123.34875370
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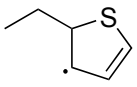
D6 180.00000000



0 1
C
C 1 B1
C 2 B2 1 A1
C 3 B3 2 A2 1 D1
S 1 B4 2 A3 3 D2
H 1 B5 2 A4 3 D3
H 2 B6 1 A5 5 D4

H	3	B7	2	A6 1 D5
C	4	B8	3	A7 2 D6
H	9	B9	4	A8 3 D7
C	9	B10	4	A9 3 D8
H	11	B11	9	A10 4 D9
H	11	B12	9	A11 4 D10

B1	1.36611175
B2	1.42064110
B3	1.37673881
B4	1.72772356
B5	1.07914062
B6	1.08196907
B7	1.08285374
B8	1.45312921
B9	1.08780089
B10	1.33683036
B11	1.08488250
B12	1.08259189
A1	112.50224180
A2	113.80240053
A3	111.74423143
A4	128.55273164
A5	123.43563801
A6	123.89791971
A7	126.46042820
A8	113.71410171
A9	127.60039470
A10	122.38504238
A11	120.93505612
D1	-0.05400000
D2	0.04834947
D3	-179.97564693
D4	-179.98496173
D5	179.97475778
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D7	0.02090095
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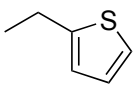

0 1

C							
C	1	B1					
C	2	B2	1	A1			
S	3	B3	2	A2	1	D1	
H	1	B4	2	A3	3	D2	
H	2	B5	1	A4	3	D3	
H	3	B6	2	A5	1	D4	
C	1	B7	2	A6	3	D5	
C	8	B8	1	A7	2	D6	
H	9	B9	8	A8	1	D7	
H	9	B10	8	A9	1	D8	
C	9	B11	8	A10	1	D9	
H	12	B12	9	A11	8	D10	
H	12	B13	9	A12	8	D11	
H	12	B14	9	A13	8	D12	

B1	1.42578418
B2	1.36439442
B3	1.72934976
B4	1.08324227
B5	1.08225864
B6	1.07896647
B7	1.36921688
B8	1.50344873
B9	1.09438600
B10	1.09530725
B11	1.53869801
B12	1.09356317
B13	1.09283609
B14	1.09270691
A1	112.65670388
A2	111.26732211
A3	123.70549689
A4	123.95416912
A5	128.73620126
A6	113.78736625
A7	128.32269395
A8	107.62052970
A9	109.99125910
A10	114.02454302
A11	110.66345777
A12	111.23090810
A13	110.77476270
D1	0.01527461
D2	-179.76812783
D3	179.79027523

D4	179.70276208
D5	0.01872080
D6	178.51084444
D7	17.68515127
D8	132.94238701
D9	-103.87392431
D10	178.33771372
D11	-61.63106025
D12	58.19018500

S4.1 Transition State Geometries

TS 1 and 2 are provided in Kida et al. (2014)

TS 3

0 1

O							
H	1	B1					
H	1	B2	2	A1			
H	1	B3	2	A2	3	D1	
S	1	B4	4	A3	2	D2	
O	1	B5	5	A4	2	D3	
H	6	B6	1	A5	5	D4	
C	6	B7	1	A6	5	D5	
H	8	B8	6	A7	1	D6	
C	8	B9	6	A8	1	D7	
H	10	B10	8	A9	6	D8	
H	10	B11	8	A10	6	D9	
H	10	B12	8	A11	6	D10	

B1	1.06952307
B2	1.22402479
B3	0.96583957
B4	2.87320980
B5	2.39424898
B6	0.97151059
B7	1.56861481
B8	1.09135899
B9	1.51406502
B10	1.09380187
B11	1.09131350
B12	1.09300096
A1	91.13577836
A2	107.96358827
A3	115.08383529

A4	62.22656177
A5	102.27360986
A6	94.79898146
A7	99.32302920
A8	106.09445059
A9	111.23288028
A10	108.86228927
A11	110.65211601
D1	-115.17820997
D2	-20.35986833
D3	-178.00133616
D4	79.67672631
D5	-26.50267574
D6	-76.23651761
D7	168.73864254
D8	52.18571138
D9	172.11796185
D10	-70.02134605

TS 4

0 1

C							
H	1	B1					
C	1	B2	2	A1			
H	3	B3	1	A2	2	D1	
H	3	B4	1	A3	2	D2	
H	3	B5	1	A4	2	D3	
S	1	B6	3	A5	4	D4	
H	7	B7	1	A6	3	D5	
O	1	B8	3	A7	7	D6	
H	9	B9	1	A8	3	D7	
H	7	B10	1	A9	9	D8	
H	9	B11	1	A10	3	D9	
S	9	B12	1	A11	3	D10	

B1	1.08970255
B2	1.50041074
B3	1.08939419
B4	1.09029759
B5	1.09718249
B6	2.46557561
B7	1.34468484
B8	1.27487254
B9	1.13118901

B10	1.48947314
B11	3.40733892
B12	2.84384951
A1	117.25337503
A2	111.66777376
A3	111.68528896
A4	106.82973355
A5	97.50660323
A6	92.73197867
A7	121.55246590
A8	112.88729008
A9	79.43731314
A10	94.12803678
A11	108.38953781
D1	38.72673208
D2	162.68957719
D3	-80.02410659
D4	-58.25202237
D5	-178.23359591
D6	-111.60040503
D7	50.14785862
D8	38.93279910
D9	45.53058497
D10	63.50347879

TS 5

0 1

H							
H	1	B1					
H	1	B2	2	A1			
S	1	B3	2	A2	3	D1	
O	4	B4	1	A3	2	D2	
H	5	B5	4	A4	1	D3	
C	5	B6	4	A5	1	D4	
H	7	B7	5	A6	4	D5	
C	7	B8	5	A7	4	D6	
H	9	B9	7	A8	5	D7	
H	9	B10	7	A9	5	D8	
H	9	B11	7	A10	5	D9	
S	5	B12	4	A11	1	D10	

B1	2.05725442
B2	2.19054211
B3	1.71556455

B4	2.76969204
B5	0.97396507
B6	1.64700051
B7	1.08938587
B8	1.50811532
B9	1.09244592
B10	1.09227723
B11	1.09181046
B12	2.94203736
A1	71.06737555
A2	97.35576949
A3	67.67516320
A4	79.57028984
A5	37.01955387
A6	96.85530280
A7	104.58134181
A8	111.09883852
A9	108.29857615
A10	111.20559006
A11	70.24551157
D1	-141.68526919
D2	0.36492204
D3	-106.76726622
D4	121.70178930
D5	-118.15448332
D6	126.54762855
D7	51.20802580
D8	170.48531821
D9	-71.44873318
D10	-0.99833723

TS 6

0 2

C							
H	1	B1					
H	1	B2	2	A1			
H	1	B3	3	A2	2	D1	
C	1	B4	3	A3	2	D2	
H	5	B5	1	A4	3	D3	
H	5	B6	1	A5	3	D4	
C	5	B7	1	A6	3	D5	
H	8	B8	5	A7	1	D6	
C	8	B9	5	A8	1	D7	
H	10	B10	8	A9	5	D8	

H	10	B11	8	A10	5	D9
C	10	B12	8	A11	5	D10
H	13	B13	10	A12	8	D11
H	13	B14	10	A13	8	D12
C	13	B15	10	A14	8	D13
H	16	B16	13	A15	10	D14
S	16	B17	13	A16	10	D15

B1	1.09421621
B2	1.09221317
B3	1.09291044
B4	1.53110961
B5	1.09763940
B6	1.10397803
B7	1.49446825
B8	1.08450417
B9	1.48657800
B10	1.09260693
B11	1.09817493
B12	1.58045077
B13	1.09353486
B14	1.09479214
B15	1.48691749
B16	1.08887009
B17	1.63777277
A1	107.97265689
A2	108.16009505
A3	110.70140393
A4	109.75360643
A5	109.02358494
A6	114.07839275
A7	117.46949565
A8	121.26339089
A9	110.62647261
A10	110.37626078
A11	113.95954997
A12	109.69691929
A13	107.73234650
A14	108.59120913
A15	118.98435067
A16	120.23454095
D1	-116.33591318
D2	121.69116766
D3	61.56429219
D4	176.20480896
D5	-62.14601144

D6	-28.33021231
D7	171.54037671
D8	161.12263718
D9	42.53945293
D10	-76.69114233
D11	-179.55659411
D12	63.10504633
D13	-56.66263629
D14	-114.27082759
D15	57.18413023

TS 7

0 2

C							
H	1	B1					
H	1	B2	2	A1			
H	1	B3	3	A2	2	D1	
C	1	B4	3	A3	2	D2	
H	5	B5	1	A4	3	D3	
H	5	B6	1	A5	3	D4	
C	5	B7	1	A6	3	D5	
H	8	B8	5	A7	1	D6	
C	8	B9	5	A8	1	D7	
H	10	B10	8	A9	5	D8	
C	10	B11	8	A10	5	D9	
H	12	B12	10	A11	8	D10	
C	12	B13	10	A12	8	D11	
H	14	B14	12	A13	10	D12	
S	14	B15	12	A14	10	D13	

B1	1.09356940
B2	1.09297820
B3	1.09324724
B4	1.54019775
B5	1.09365505
B6	1.09356292
B7	1.50754370
B8	1.08769500
B9	1.40911010
B10	1.08764618
B11	1.40285647
B12	1.08442076
B13	1.38382399
B14	1.08460362

B15	1.71190225
A1	107.79023255
A2	107.98846932
A3	111.35837338
A4	110.13452207
A5	108.99804449
A6	112.11429071
A7	114.09889451
A8	122.34290221
A9	120.24744832
A10	118.37026802
A11	122.19038962
A12	116.85809539
A13	121.60069215
A14	120.79559134
D1	-116.33040599
D2	122.09807742
D3	60.97572459
D4	177.71061351
D5	-61.55309639
D6	-61.22986216
D7	87.36788944
D8	-13.25143569
D9	154.65665621
D10	169.05476978
D11	-20.07596919
D12	-175.28685070
D13	0.88578625

TS 8

0 2

C							
C	1	B1					
H	2	B2	1	A1			
C	2	B3	1	A2	3	D1	
H	4	B4	2	A3	1	D2	
C	4	B5	2	A4	1	D3	
S	6	B6	4	A5	2	D4	
C	1	B7	2	A6	4	D5	
H	8	B8	1	A7	2	D6	
H	8	B9	1	A8	2	D7	
C	8	B10	1	A9	2	D8	
H	11	B11	8	A10	1	D9	
H	11	B12	8	A11	1	D10	

H	11	B13	8	A12	1	D11

B1	1.31753116
B2	1.09087804
B3	1.48363743
B4	1.07906737
B5	1.32369155
B6	1.58057883
B7	1.46698889
B8	1.09610558
B9	1.09610472
B10	1.54633067
B11	1.09269808
B12	1.09210292
B13	1.09210247
A1	119.26391461
A2	124.32526296
A3	121.54370792
A4	110.88645855
A5	140.32732762
A6	145.60831344
A7	109.69007715
A8	109.69043672
A9	112.50545531
A10	109.81239772
A11	110.96397649
A12	110.96424674
D1	180.00000000
D2	-180.00000000
D3	0.00000000
D4	-0.00000000
D5	-179.99486689
D6	121.76042525
D7	-121.81127277
D8	-0.02523913
D9	180.00000000
D10	-60.31786829
D11	60.31772054

TS S1

0 2

C	-2.70125100	-1.07993300	-0.14270700
H	-2.66773300	-1.06543300	-1.23700900
H	-3.68033300	-0.67506400	0.15268900

H	-2.67437600	-2.12394000	0.18168500
C	-1.56840400	-0.28482300	0.45280900
H	-1.45215100	-0.41761300	1.53151100
H	-0.30136800	-0.67983400	-0.00793900
C	-1.33315200	1.14848000	-0.00757700
H	-1.85005300	1.89202900	0.60867800
H	-1.70478200	1.26852400	-1.03199400
C	0.20202100	1.35086400	0.01434700
H	0.53482500	1.52783800	1.04285200
H	0.53326400	2.20517700	-0.58278900
C	0.76240400	0.01933800	-0.47677300
H	0.69627800	-0.12045500	-1.55734800
S	2.38541300	-0.52624200	0.03171700
H	2.23011200	-0.31491800	1.35159700

TS S2

0 2

S	2.42622400	-0.63513000	-0.06407900
H	2.03157000	-0.79863200	-1.33992600
C	0.96584300	0.23932700	0.51410900
H	-0.14939200	-0.49946200	0.50488700
H	1.11154800	0.41878600	1.58130900
C	0.50491400	1.47421500	-0.24623400
H	0.60570800	1.29797000	-1.32394900
H	1.14355400	2.33489300	-0.01359400
C	-0.96882700	1.79298500	0.06844000
H	-1.27299400	2.69221600	-0.47570900
H	-1.07654000	2.02275900	1.13591700
C	-1.89011400	0.61424100	-0.30054800
H	-1.81021900	0.42834600	-1.37962500
H	-2.93751400	0.89194900	-0.11607500
C	-1.52482700	-0.65027900	0.45710800
H	-1.77339000	-0.59158900	1.52026200
C	-1.87928900	-1.97815300	-0.16887800
H	-1.46249900	-2.07007300	-1.17724500
H	-1.50726000	-2.81671400	0.42562900
H	-2.96835900	-2.10239600	-0.26059000

TS S3

0 2

C		
H	1	B1

H	1	B2 2	A1	
H	1	B3 3	A2 2	D1
C	1	B4 3	A3 4	D2
H	5	B5 1	A4 3	D3
H	5	B6 1	A5 3	D4
S	5	B7 1	A6 3	D5
C	8	B8 5	A7 1	D6
H	9	B9 8	A8 5	D7
H	9	B10 8	A9 5	D8
C	9	B11 8	A10 5	D9
H	12	B12 9	A11 8	D10
C	12	B13 9	A12 8	D11
H	14	B14 12	A13 9	D12
H	14	B15 12	A14 9	D13
H	14	B16 12	A15 9	D14

B1	1.09480882
B2	1.09258500
B3	1.09725717
B4	1.50734084
B5	1.09170650
B6	1.36524488
B7	1.80529783
B8	1.86799990
B9	1.09271626
B10	1.09184974
B11	1.51465292
B12	1.09163965
B13	1.50866059
B14	1.09450653
B15	1.09363370
B16	1.09878829
A1	108.74419826
A2	107.41838456
A3	111.23972185
A4	114.48423616
A5	112.46673398
A6	117.08307974
A7	93.21780891
A8	108.97506695
A9	107.16252592
A10	107.11119200
A11	113.25632370
A12	118.36462180
A13	111.40783730
A14	111.34075730

A15	111.55534014
D1	-115.62166842
D2	-122.46664137
D3	-170.92287004
D4	-53.83526629
D5	52.88500053
D6	-137.05902963
D7	-90.23024721
D8	152.55890000
D9	29.89816647
D10	78.88891488
D11	-143.14446036
D12	51.97146622
D13	172.77056541
D14	-67.62619677

TS S4

0 2

C							
H	1	B1					
C	1	B2	2	A1			
H	3	B3	1	A2	2	D1	
H	3	B4	1	A3	2	D2	
C	3	B5	1	A4	2	D3	
H	6	B6	3	A5	1	D4	
H	6	B7	3	A6	1	D5	
S	6	B8	3	A7	1	D6	
C	9	B9	6	A8	3	D7	
H	10	B10	9	A9	6	D8	
C	10	B11	9	A10	6	D9	
H	12	B12	10	A11	9	D10	
H	12	B13	10	A12	9	D11	
H	12	B14	10	A13	9	D12	
C	1	B15	3	A14	6	D13	
H	16	B16	1	A15	3	D14	
H	16	B17	1	A16	3	D15	
H	16	B18	1	A17	3	D16	
H	1	B19	16	A18	3	D17	

B1	1.37640224
B2	1.51995145
B3	1.09314315
B4	1.10188181
B5	1.54010394

B6	1.09329063
B7	1.09169413
B8	1.83478723
B9	1.79946944
B10	1.09246129
B11	1.51201229
B12	1.09694401
B13	1.09417672
B14	1.09304587
B15	1.51335158
B16	1.09353662
B17	1.09494075
B18	1.09879067
B19	1.09073815
A1	100.20559402
A2	110.11799599
A3	110.17302488
A4	113.35224352
A5	111.42014628
A6	110.91499689
A7	112.37101362
A8	98.57117340
A9	112.15946625
A10	114.81280688
A11	111.99599206
A12	110.32117331
A13	111.21556643
A14	117.10737248
A15	111.52286423
A16	111.96317160
A17	111.33472958
A18	113.34110848
D1	86.33645864
D2	-156.11278372
D3	-35.18024324
D4	-59.36597607
D5	-179.10109788
D6	63.51325980
D7	-58.18113861
D8	-77.03809232
D9	150.82070880
D10	62.92416181
D11	-177.70819706
D12	-57.38166683
D13	79.44331404
D14	-174.17418690

D15	-53.61503362
D16	66.02096246
D17	-135.34582015

TS S5

0 2

C						
H	1	B1				
S	1	B2	2	A1		
C	1	B3	3	A2	2	D1
H	4	B4	1	A3	3	D2
H	4	B5	1	A4	3	D3
H	4	B6	1	A5	3	D4
H	1	B7	4	A6	3	D5

B1	1.09213187
B2	1.63134588
B3	1.49667803
B4	1.09424365
B5	1.09785510
B6	1.08936835
B7	2.22188373
A1	118.64372571
A2	125.83813399
A3	111.06196313
A4	108.51916885
A5	111.66246739
A6	98.13913227
D1	172.64770700
D2	136.99549110
D3	-106.20802067
D4	13.70759353
D5	-106.72242832

TS S6

0 2

C						
H	1	B1				
S	1	B2	2	A1		
C	1	B3	3	A2	2	D1
H	4	B4	1	A3	3	D2
H	4	B5	1	A4	3	D3

H	4	B6	1	A5	3	D4	
C	1	B7	4	A6	3	D5	
H	8	B8	1	A7	4	D6	
C	8	B9	1	A8	4	D7	
H	10	B10	8	A9	1	D8	
H	10	B11	8	A10	1	D9	
H	10	B12	8	A11	1	D10	
S	8	B13	1	A12	4	D11	
H	14	B14	8	A13	1	D12	

B1	1.08991844
B2	1.66145433
B3	1.50403259
B4	1.09280597
B5	1.09684199
B6	1.09116748
B7	2.38748706
B8	1.08496370
B9	1.49652974
B10	1.09056277
B11	1.09423053
B12	1.09758557
B13	1.74805416
B14	1.34599000
A1	118.13573458
A2	122.95673831
A3	112.13949620
A4	108.35316317
A5	111.26246996
A6	99.44720200
A7	89.76840188
A8	105.30927727
A9	110.33590774
A10	111.61894636
A11	110.60860326
A12	108.14287347
A13	97.50673530
D1	157.18493831
D2	157.63604353
D3	-84.39213120
D4	33.55340283
D5	-113.82146489
D6	54.92520640
D7	173.62806202
D8	-50.55543467
D9	69.50026006

D10	-170.66857985
D11	-56.76313587
D12	-90.00929782

TS S7

0 2

C								
H	1	B1						
H	1	B2	2	A1				
C	1	B3	3	A2	2	D1	0	
H	4	B4	1	A3	3	D2	0	
S	4	B5	1	A4	3	D3	0	
C	4	B6	1	A5	6	D4	0	
H	7	B7	4	A6	1	D5	0	
H	7	B8	4	A7	1	D6	0	
C	7	B9	4	A8	1	D7	0	
H	10	B10	7	A9	4	D8	0	
H	10	B11	7	A10	4	D9	0	
H	10	B12	7	A11	4	D10	0	
C	1	B13	4	A12	6	D11	0	
H	14	B14	1	A13	4	D12	0	
H	14	B15	1	A14	4	D13	0	
H	14	B16	1	A15	4	D14	0	

B1	1.09502
B2	1.09223
B3	1.50616
B4	1.09144
B5	1.64545
B6	2.5289
B7	1.08461
B8	1.08369
B9	1.48587
B10	1.09297
B11	1.09295
B12	1.10146
B13	1.54241
B14	1.09296
B15	1.09186
B16	1.09365
A1	108.24215
A2	109.39868
A3	115.235
A4	124.2771

A5	97.31934
A6	92.88555
A7	91.48118
A8	107.03109
A9	112.08981
A10	111.49719
A11	110.64999
A12	110.79459
A13	110.19314
A14	110.58347
A15	111.3769
D1	-119.70921
D2	164.92756
D3	-31.32699
D4	113.01704
D5	62.03939
D6	-54.2583
D7	-175.66352
D8	-65.65774
D9	56.05852
D10	175.00347
D11	89.69113
D12	178.05733
D13	-62.02162
D14	58.27573

TS S8

0 2

C							
H	1	B1					
H	1	B2	2	A1			
C	1	B3	3	A2	2	D1	
H	4	B4	1	A3	3	D2	
S	4	B5	1	A4	3	D3	
C	4	B6	1	A5	6	D4	
H	7	B7	4	A6	1	D5	
C	7	B8	4	A7	1	D6	
H	9	B9	7	A8	4	D7	
H	9	B10	7	A9	4	D8	
H	9	B11	7	A10	4	D9	
C	1	B12	4	A11	6	D10	
H	13	B13	1	A12	4	D11	
H	13	B14	1	A13	4	D12	
H	13	B15	1	A14	4	D13	

C	7	B16	4	A15	1	D14	
H	17	B17	7	A16	4	D15	
H	17	B18	7	A17	4	D16	
H	17	B19	7	A18	4	D17	

B1	1.09551170
B2	1.09237667
B3	1.50694639
B4	1.09089360
B5	1.64897012
B6	2.50820993
B7	1.08648269
B8	1.49077993
B9	1.09408913
B10	1.09193508
B11	1.10177260
B12	1.54208093
B13	1.09311886
B14	1.09178239
B15	1.09370740
B16	1.49090182
B17	1.09227570
B18	1.09431159
B19	1.10162104
A1	108.23912762
A2	109.38565719
A3	115.16305677
A4	123.85896901
A5	99.04499788
A6	89.06691479
A7	103.54936328
A8	111.37923689
A9	112.35712157
A10	110.29283969
A11	110.95445648
A12	110.25335173
A13	110.54058221
A14	111.35666395
A15	101.91012920
A16	112.33128469
A17	111.22022810
A18	110.40384184
D1	-119.82877677
D2	165.19146026
D3	-32.84450809
D4	114.45923806

D5	50.53452014
D6	-67.18927889
D7	-62.29556349
D8	59.72523582
D9	179.21191735
D10	88.09537572
D11	178.15226676
D12	-61.89095584
D13	58.34616105
D14	168.13771039
D15	-61.52732212
D16	60.19434528
D17	178.80367918

TS S9

0 2

C							
H	1	B1					
C	1	B2	2	A1			
H	3	B3	1	A2	2	D1	
S	3	B4	1	A3	2	D2	
H	5	B5	3	A4	1	D3	
C	1	B6	3	A5	5	D4	
H	7	B7	1	A6	3	D5	
H	7	B8	1	A7	3	D6	
H	7	B9	1	A8	3	D7	
S	3	B10	1	A9	7	D8	
C	11	B11	3	A10	1	D9	
H	12	B12	11	A11	3	D10	
C	12	B13	11	A12	3	D11	
H	14	B14	12	A13	11	D12	
H	14	B15	12	A14	11	D13	

B1	1.08783393
B2	1.40052145
B3	1.08717340
B4	1.80119224
B5	1.34851420
B6	1.49205251
B7	1.09932336
B8	1.09705966
B9	1.09350559
B10	2.25605884
B11	1.75558950

B12	1.09015062
B13	1.34336517
B14	1.08562336
B15	1.08680780
A1	118.16253204
A2	117.23375415
A3	115.98103957
A4	96.67195821
A5	123.44235473
A6	111.04544212
A7	110.82042895
A8	112.10152059
A9	105.21667198
A10	101.45762440
A11	116.73027105
A12	123.63580221
A13	121.55716276
A14	120.85033693
D1	-168.06535741
D2	-28.04367816
D3	165.15793688
D4	160.81714921
D5	104.09826465
D6	-137.45101571
D7	-16.26474640
D8	-84.31996164
D9	76.06788336
D10	57.63793470
D11	-126.34997845
D12	3.79654607
D13	-174.23052196

TS S10

0 2

C						
H	1	B1				
H	1	B2	2	A1		
H	1	B3	2	A2	3	D1
C	1	B4	2	A3	3	D2
H	5	B5	1	A4	2	D3
H	5	B6	1	A5	2	D4
C	5	B7	1	A6	2	D5
H	8	B8	5	A7	1	D6
C	8	B9	5	A8	1	D7

H	10	B10	8	A9	5	D8	
C	10	B11	8	A10	5	D9	
H	12	B12	10	A11	8	D10	
C	12	B13	10	A12	8	D11	
H	14	B14	12	A13	10	D12	
S	14	B15	12	A14	10	D13	

B1	1.09266972
B2	1.09267818
B3	1.09358359
B4	1.53794033
B5	1.09345525
B6	1.09387469
B7	1.50964421
B8	1.95125477
B9	1.38681361
B10	1.08282944
B11	1.41559576
B12	1.08214068
B13	1.36950861
B14	1.07915927
B15	1.72557593
A1	107.79375512
A2	108.20569344
A3	110.99518282
A4	109.78752725
A5	109.68591126
A6	113.40048793
A7	93.24614921
A8	127.20319729
A9	122.12414099
A10	113.86260816
A11	123.96464382
A12	112.79621087
A13	128.34498057
A14	111.62972487
D1	116.62505613
D2	-122.06621199
D3	-177.89090759
D4	-61.66298405
D5	58.85574903
D6	179.12940657
D7	-80.65092338
D8	-16.61293339
D9	165.76921181
D10	176.70435061

D11	-2.80270074
D12	178.35996518
D13	-0.27616375

TS S11

0 2

C							
H	1	B1					
H	1	B2	2	A1			
H	1	B3	2	A2	3	D1	
C	1	B4	2	A3	4	D2	
H	5	B5	1	A4	2	D3	
H	5	B6	1	A5	2	D4	
C	5	B7	1	A6	2	D5	
H	8	B8	5	A7	1	D6	
C	8	B9	5	A8	1	D7	
H	10	B10	8	A9	5	D8	
C	10	B11	8	A10	5	D9	
H	12	B12	10	A11	8	D10	
C	12	B13	10	A12	8	D11	
H	14	B14	12	A13	10	D12	
S	14	B15	12	A14	10	D13	

B1	1.09351560
B2	1.09371019
B3	1.10026893
B4	1.49371657
B5	1.08652584
B6	1.08664506
B7	2.28896361
B8	1.07932556
B9	1.39776252
B10	1.08208642
B11	1.41172261
B12	1.08266153
B13	1.37315331
B14	1.07889800
B15	1.73372688
A1	108.09618367
A2	107.05092794
A3	111.55977221
A4	117.62863563
A5	117.68353457
A6	107.88828379

A7	86.11963546
A8	106.27597828
A9	122.63867694
A10	113.20876335
A11	123.79578250
A12	113.26889758
A13	128.42580469
A14	111.52692059
D1	114.91444359
D2	122.23607554
D3	169.06089153
D4	-48.03655855
D5	60.42918947
D6	179.94298269
D7	-54.12274069
D8	-71.40898847
D9	106.17564513
D10	-175.60622045
D11	4.76761295
D12	-178.34182613
D13	0.29435173

TS S12

0 2

C							
H	1	B1					
C	1	B2	2	A1			
H	3	B3	1	A2	2	D1	
C	3	B4	1	A3	2	D2	
H	5	B5	3	A4	1	D3	
C	5	B6	3	A5	1	D4	
H	7	B7	5	A6	3	D5	
S	7	B8	5	A7	3	D6	
C	1	B9	3	A8	5	D7	
H	10	B10	1	A9	3	D8	
H	10	B11	1	A10	3	D9	
C	10	B12	1	A11	3	D10	
H	13	B13	10	A12	1	D11	

B1	1.07865811
B2	1.38937916
B3	1.08152683
B4	1.41464186
B5	1.08231295

B6	1.37192642
B7	1.07899279
B8	1.73035974
B9	3.19374227
B10	1.09268314
B11	1.08912179
B12	1.31098518
B13	1.08242146
A1	126.87218069
A2	122.71847006
A3	112.93956088
A4	123.87416652
A5	113.03292598
A6	128.36371588
A7	111.64474882
A8	111.18010049
A9	161.86944579
A10	82.70978552
A11	39.67478999
A12	132.88873577
D1	19.87009537
D2	-162.82821615
D3	-176.27562940
D4	3.88811982
D5	-178.89605868
D6	0.25085611
D7	124.16601971
D8	-66.65835113
D9	110.42358729
D10	-71.09615489
D11	177.86115145