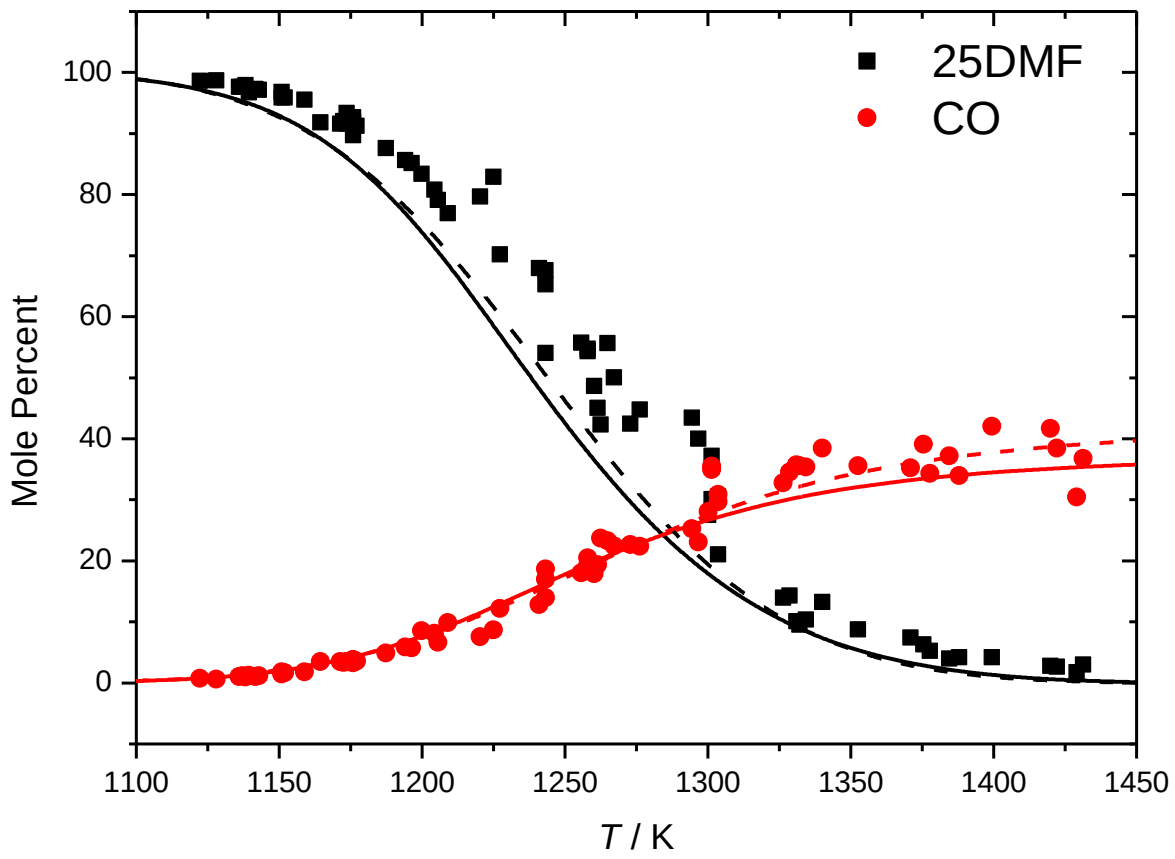
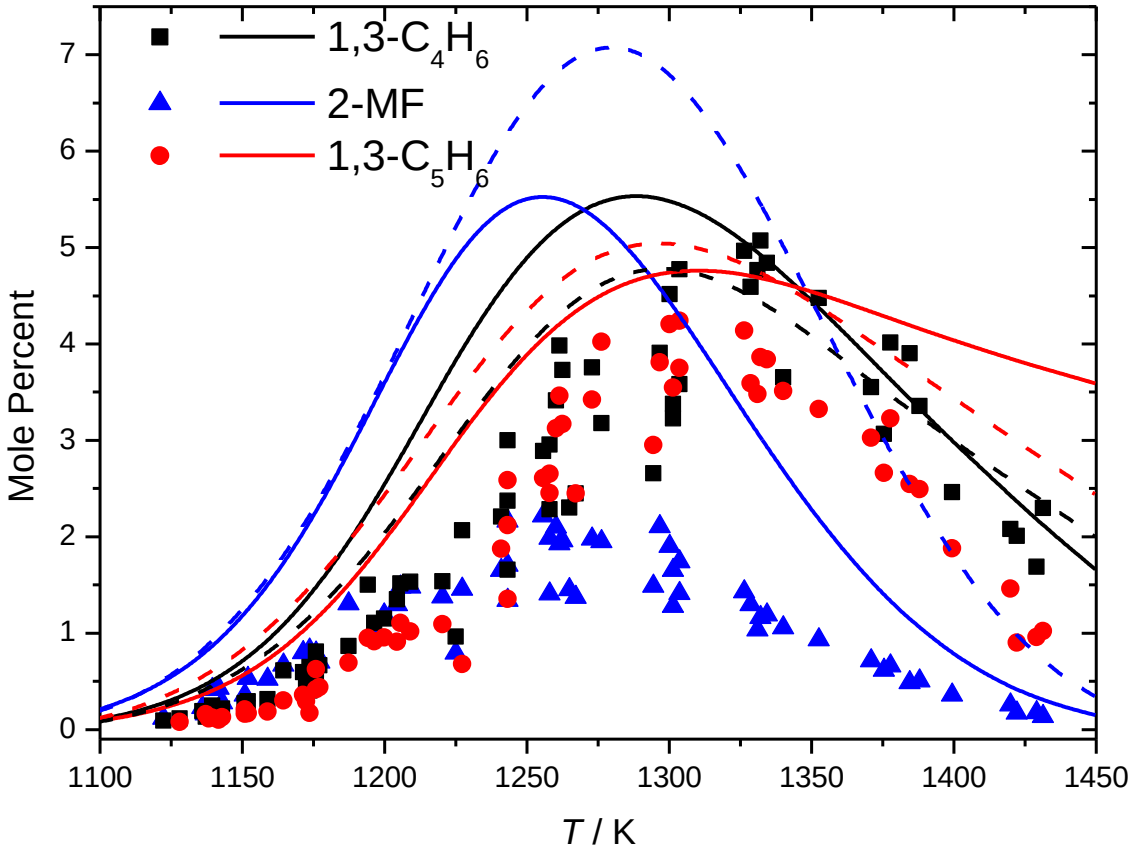
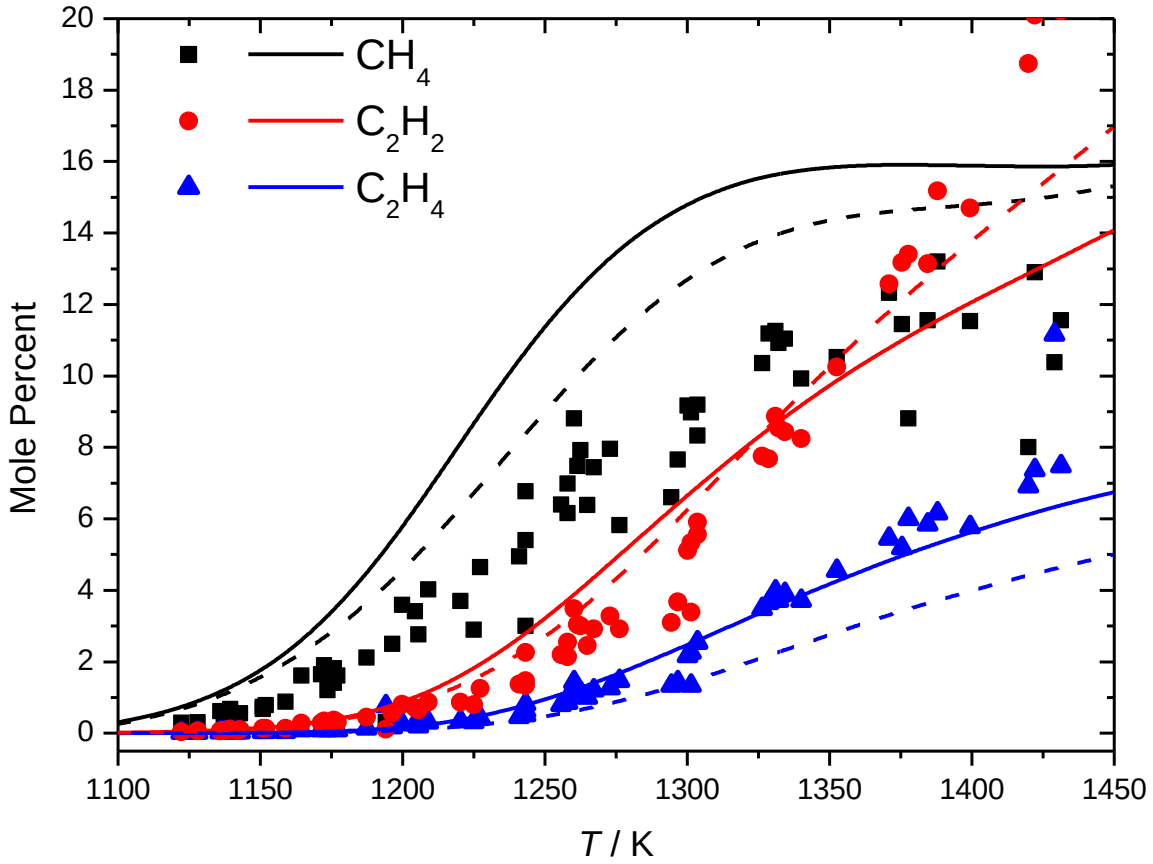
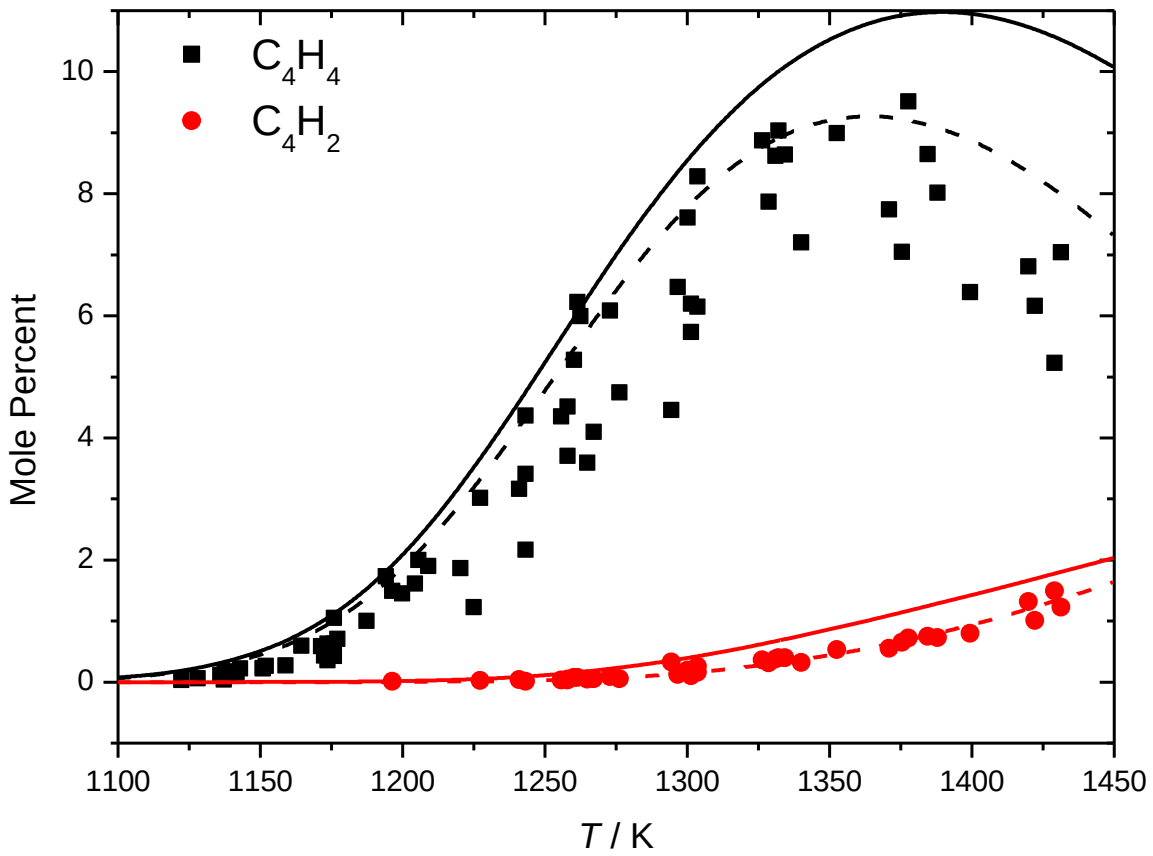
Kinetic Modelling Supplementary

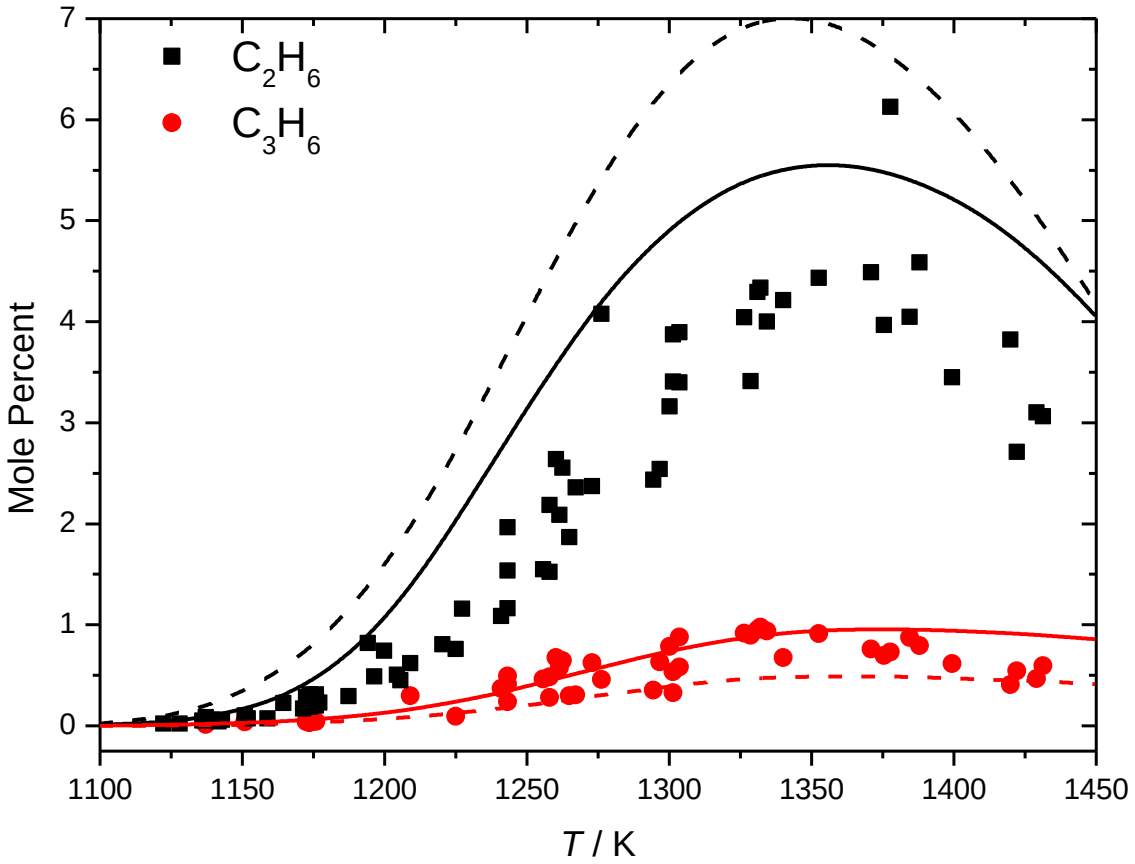
Data from Lifshitz et al. with temperature correction from Sirjean et al. Lines are model calculations; Solid lines (this study), dashed lines (Sirjean et al.).

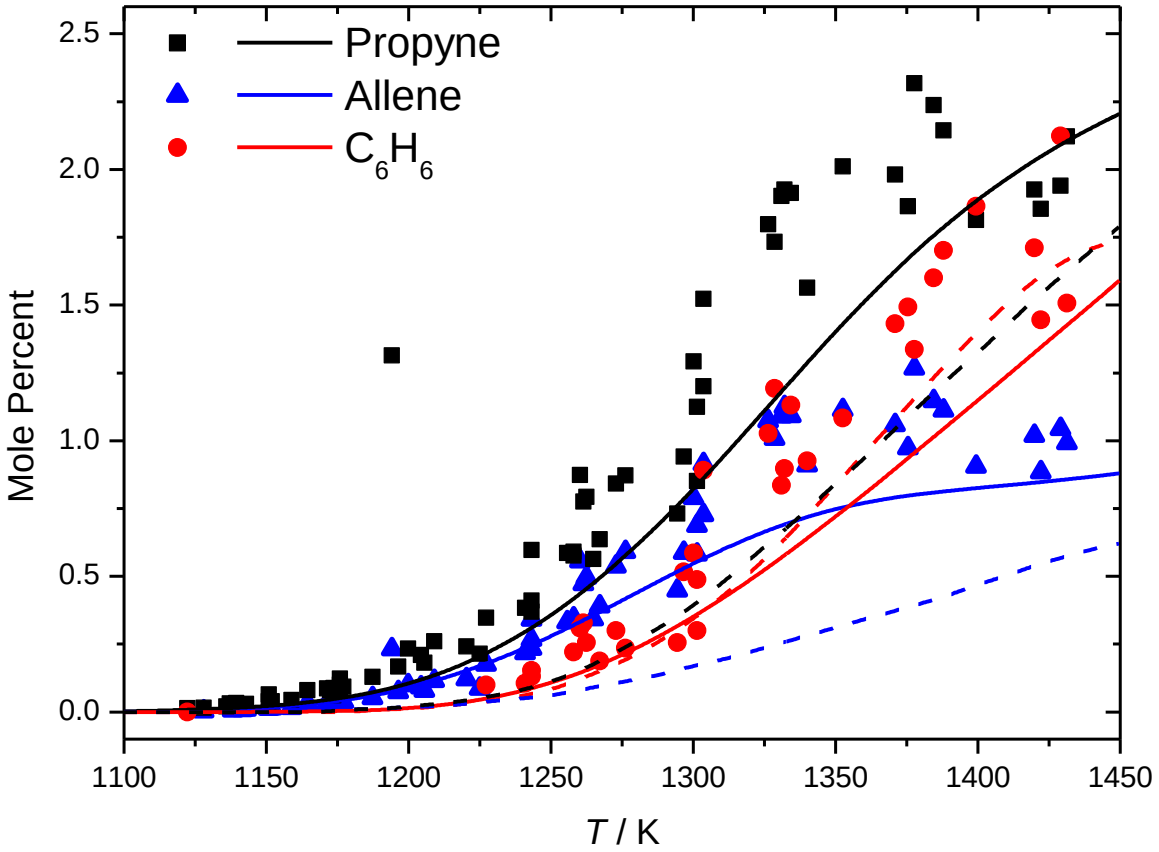



1,3-C4H6
2-MF
1,3-C5H6
Mole Percent
T / K
0
1
2
3
4
5
6
7
1100
1150
1200
1250
1300
1350
1400
1450


CH4
C2H2
C2H4
Mole Percent
T / K
0
2
4
6
8
10
12
14
16
18
20
1100
1150
1200
1250
1300
1350
1400
1450

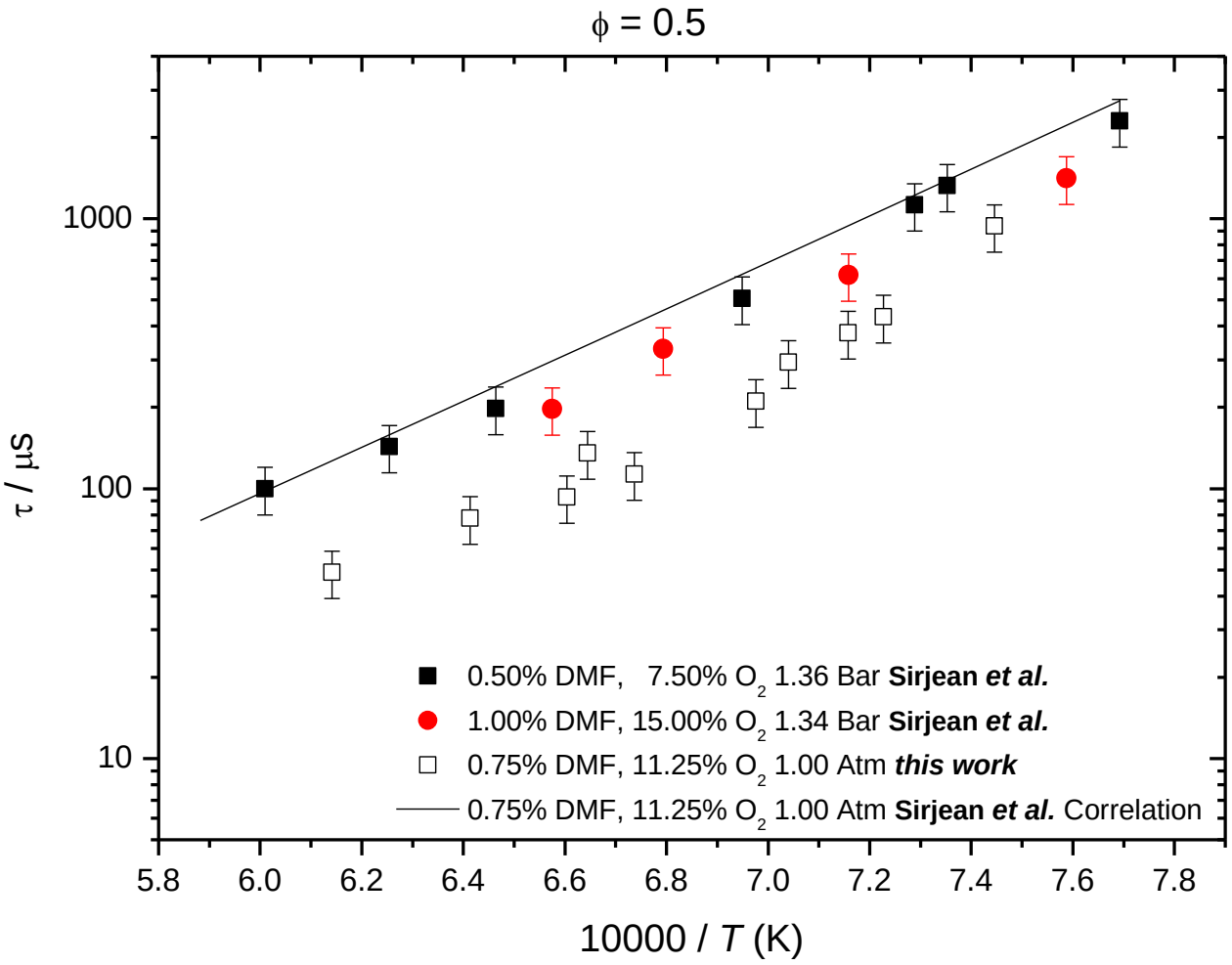

C4H4
C4H2
Mole Percent
T / K
0
2
4
6
8
10
1100
1150
1200
1250
1300
1350
1400
1450

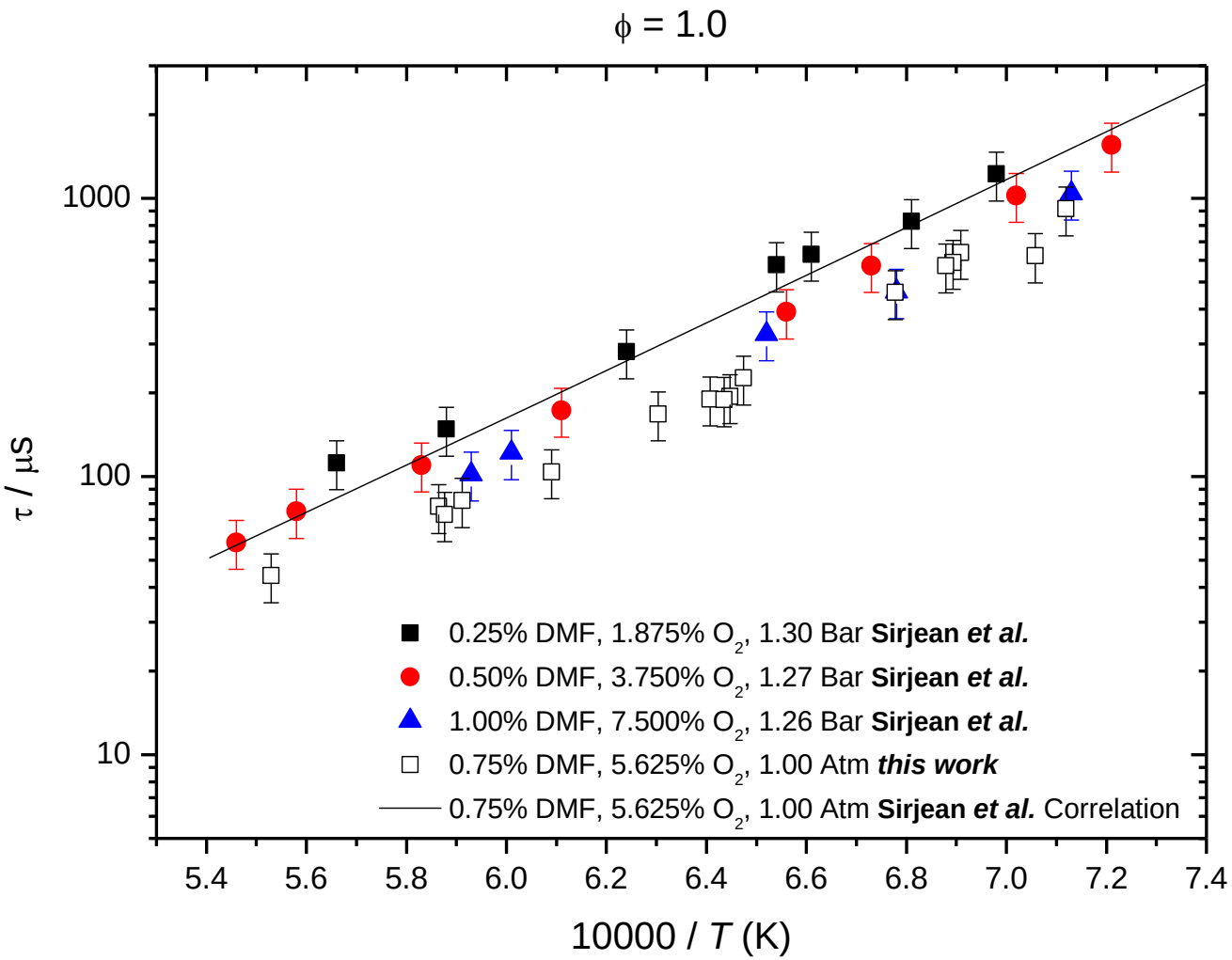

C2H6
C3H6
Mole Percent
T / K
0
1
2
3
4
5
6
7
1100
1150
1200
1250
1300
1350
1400
1450


Propyne
Allene
C6H6
Mole Percent
T / K
2.5
2.0
1.5
1.0
0.5
0.0
1100
1150
1200
1250
1300
1350
1400
1450

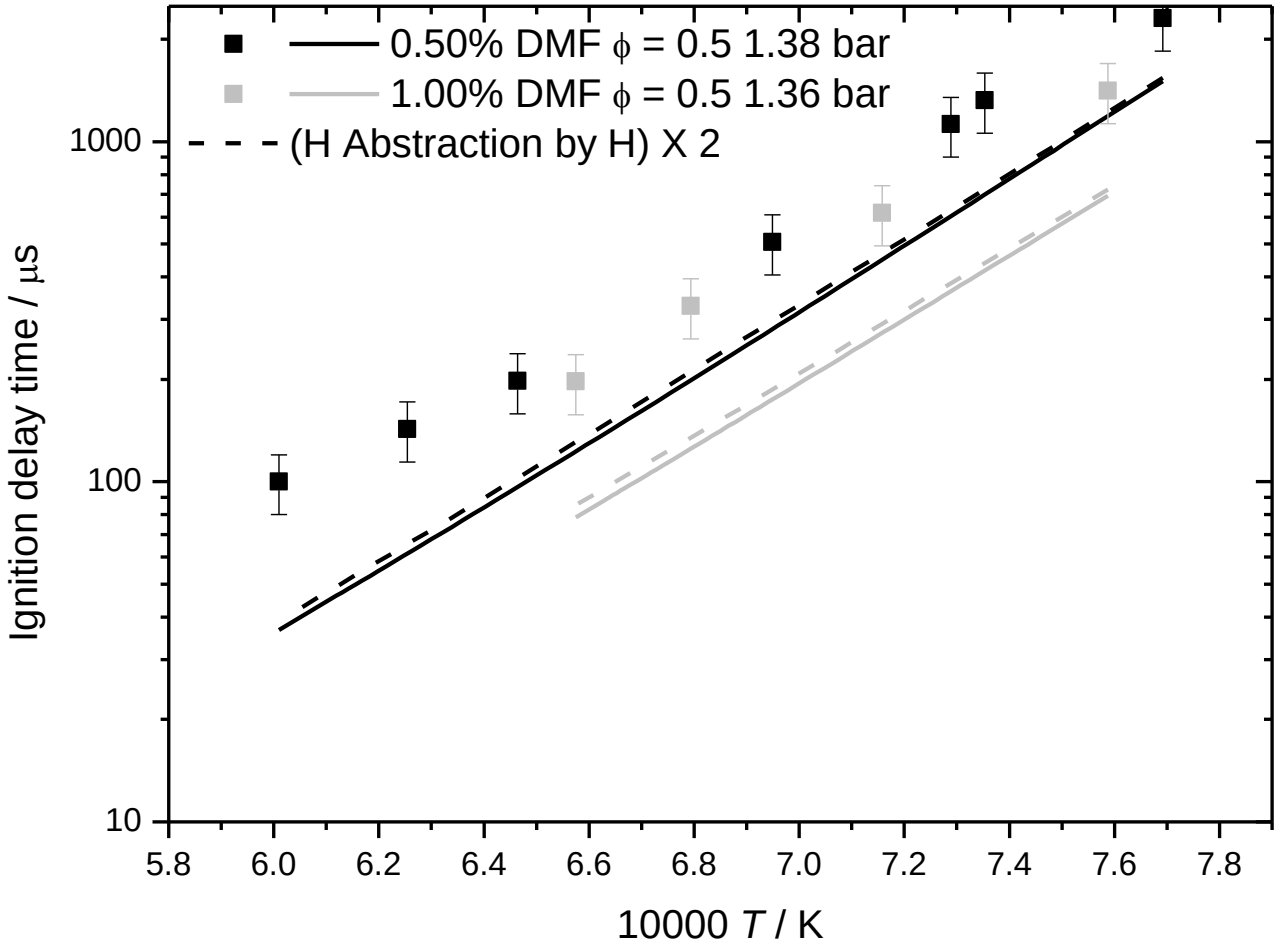
Ignition delay times from Sirjean et al., *J. Phys. Chem. A*, 2013, 117 (7), pp 1371–1392

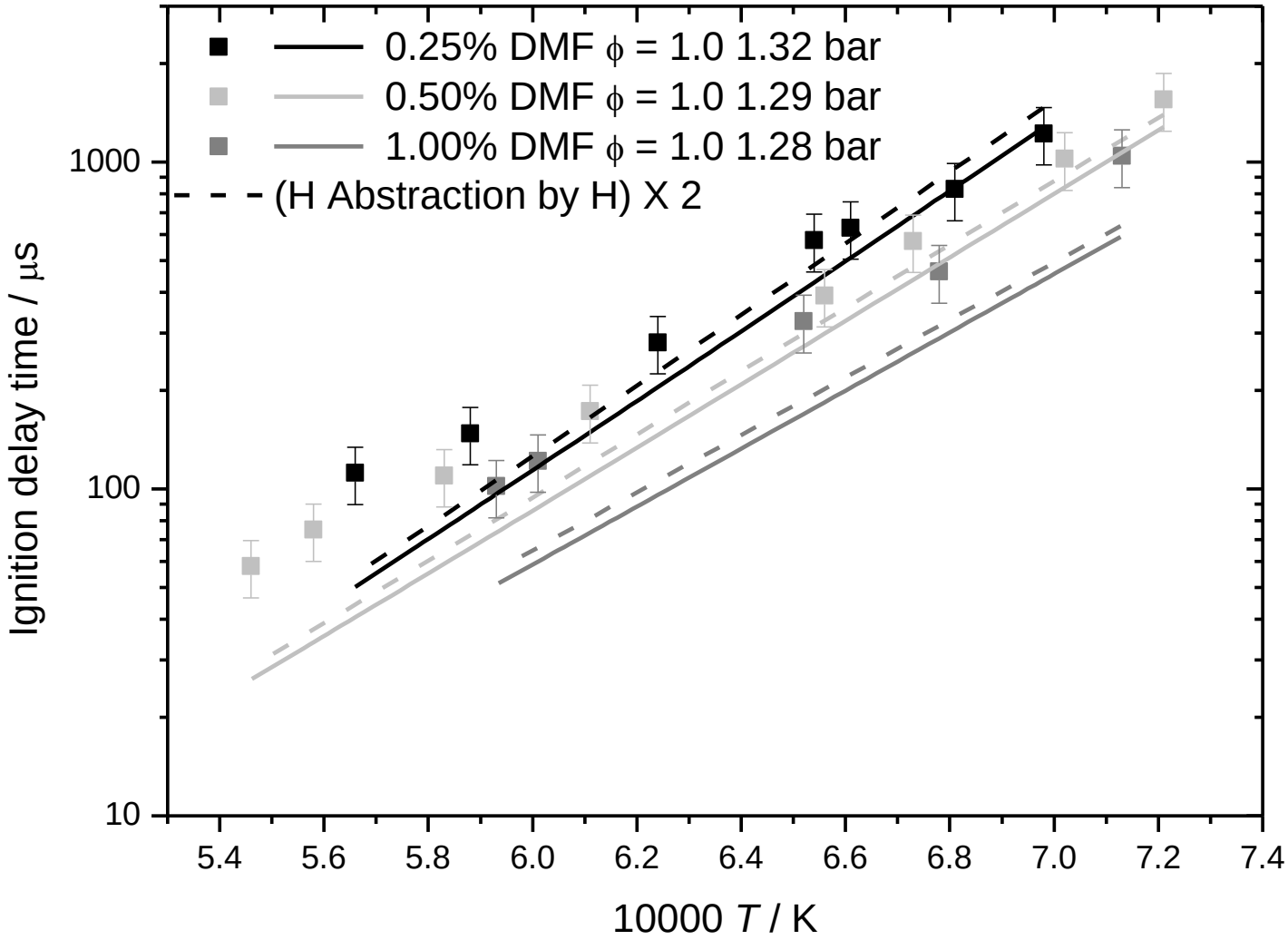
Experimental Comparison

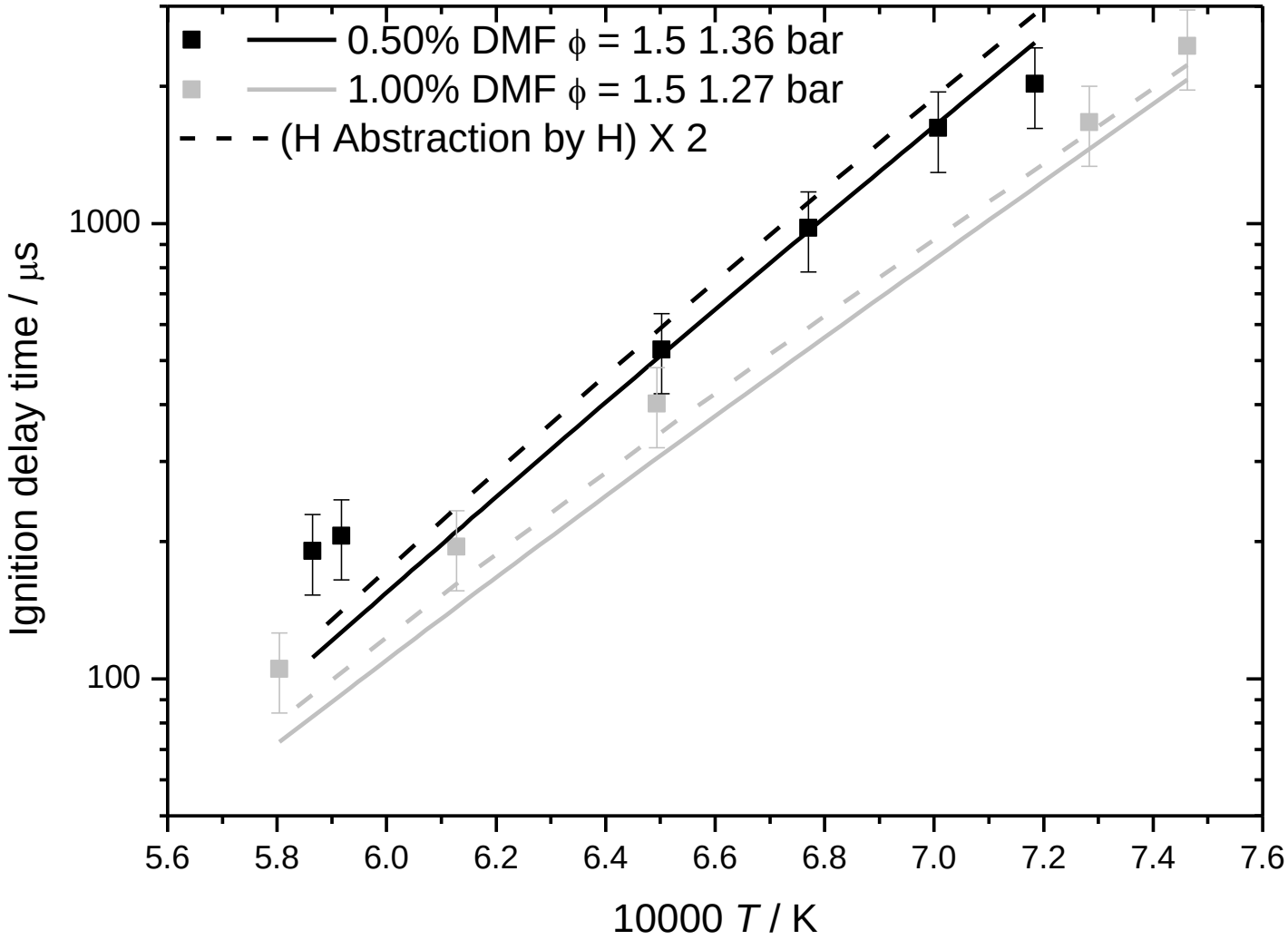


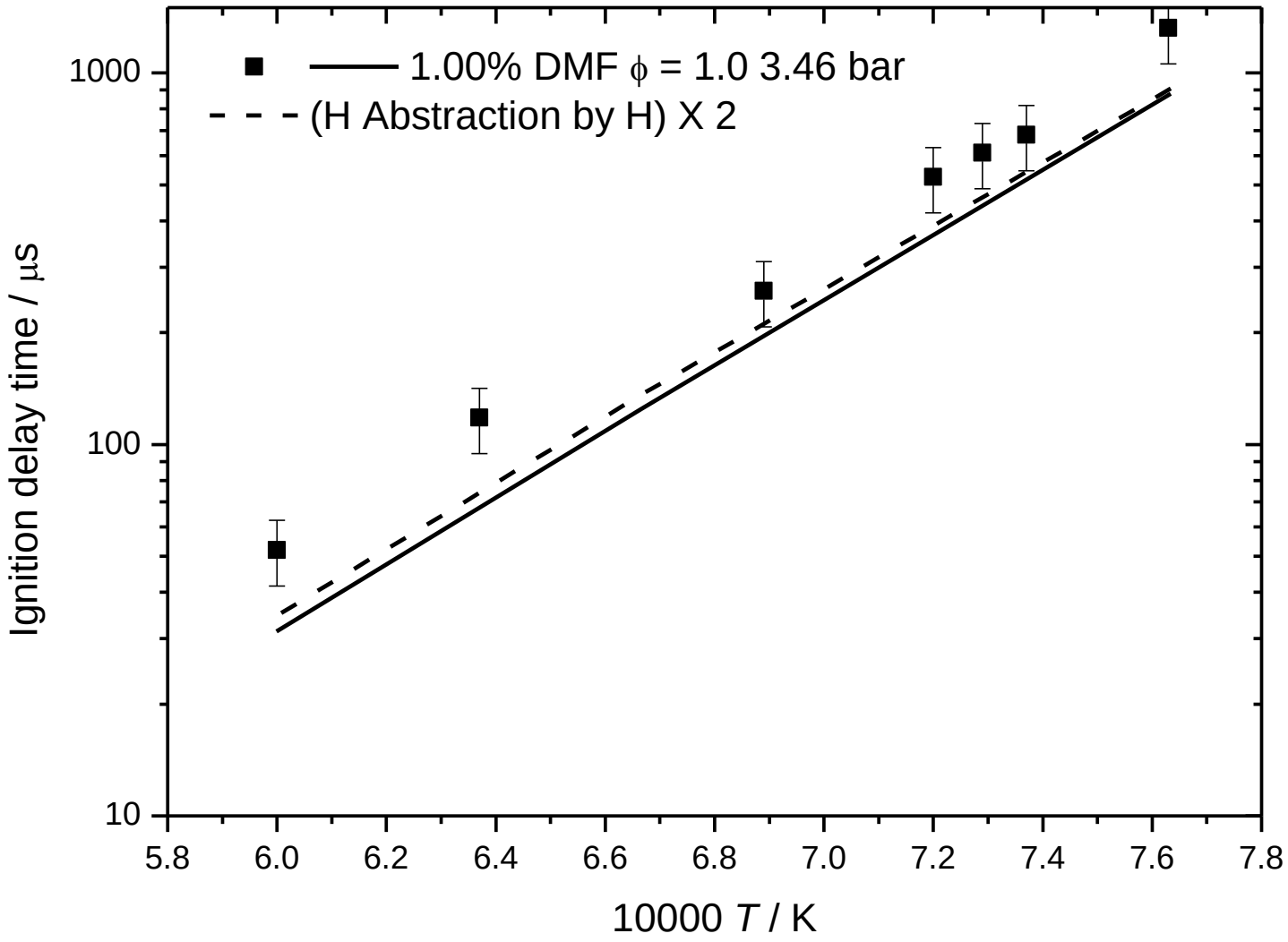

ϕ = 1.0
1000
100
10
τ / μs
5.4
5.6
5.8
6.0
6.2
6.4
6.6
6.8
7.0
7.2
7.4
10000 / T (K)
0.25% DMF, 1.875% O2, 1.30 Bar Sirjean et al.
0.50% DMF, 3.750% O2, 1.27 Bar Sirjean et al.
1.00% DMF, 7.500% O2, 1.26 Bar Sirjean et al.
0.75% DMF, 5.625% O2, 1.00 Atm this work
0.75% DMF, 5.625% O2, 1.00 Atm Sirjean et al. Correlation

Influence of adopting rate constant for H atom abstraction by H from Sirjean *et al.*

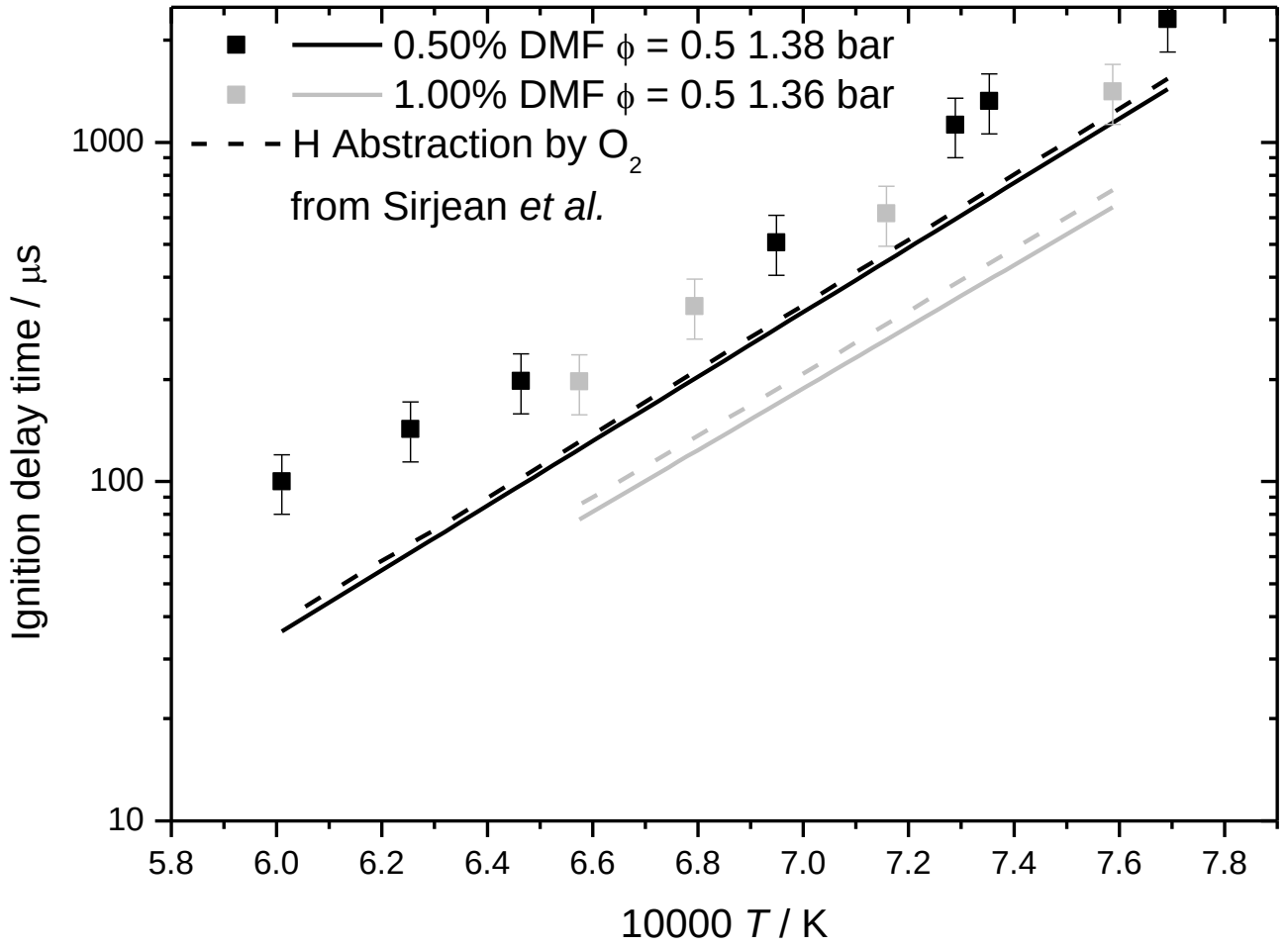


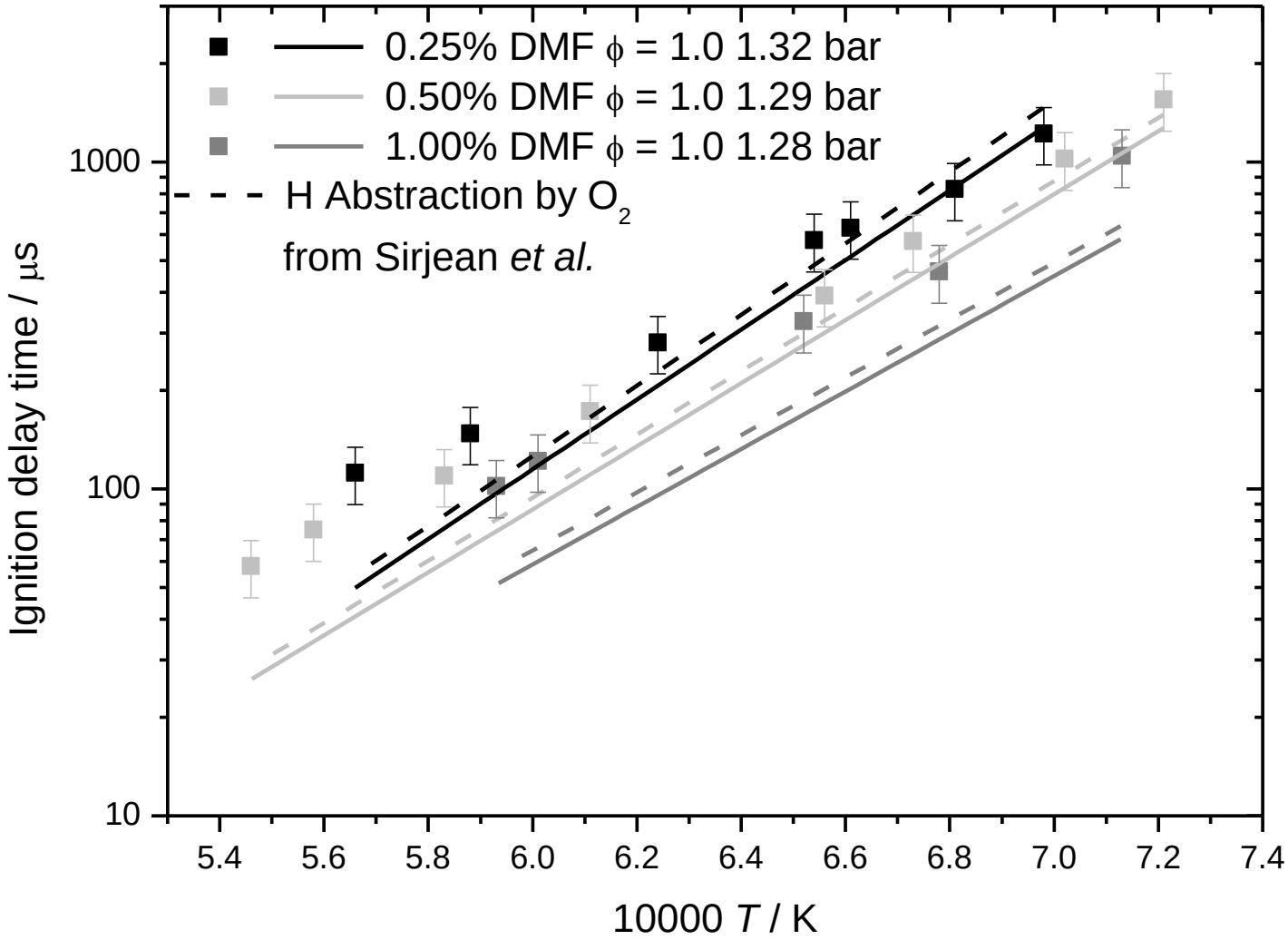

0.25% DMF ϕ = 1.0 1.32 bar
0.50% DMF ϕ = 1.0 1.29 bar
1.00% DMF ϕ = 1.0 1.28 bar
(H Abstraction by H) X 2
Ignition delay time / μs
1000
100
10
5.4
5.6
5.8
6.0
6.2
6.4
6.6
6.8
7.0
7.2
7.4
10000 T / K

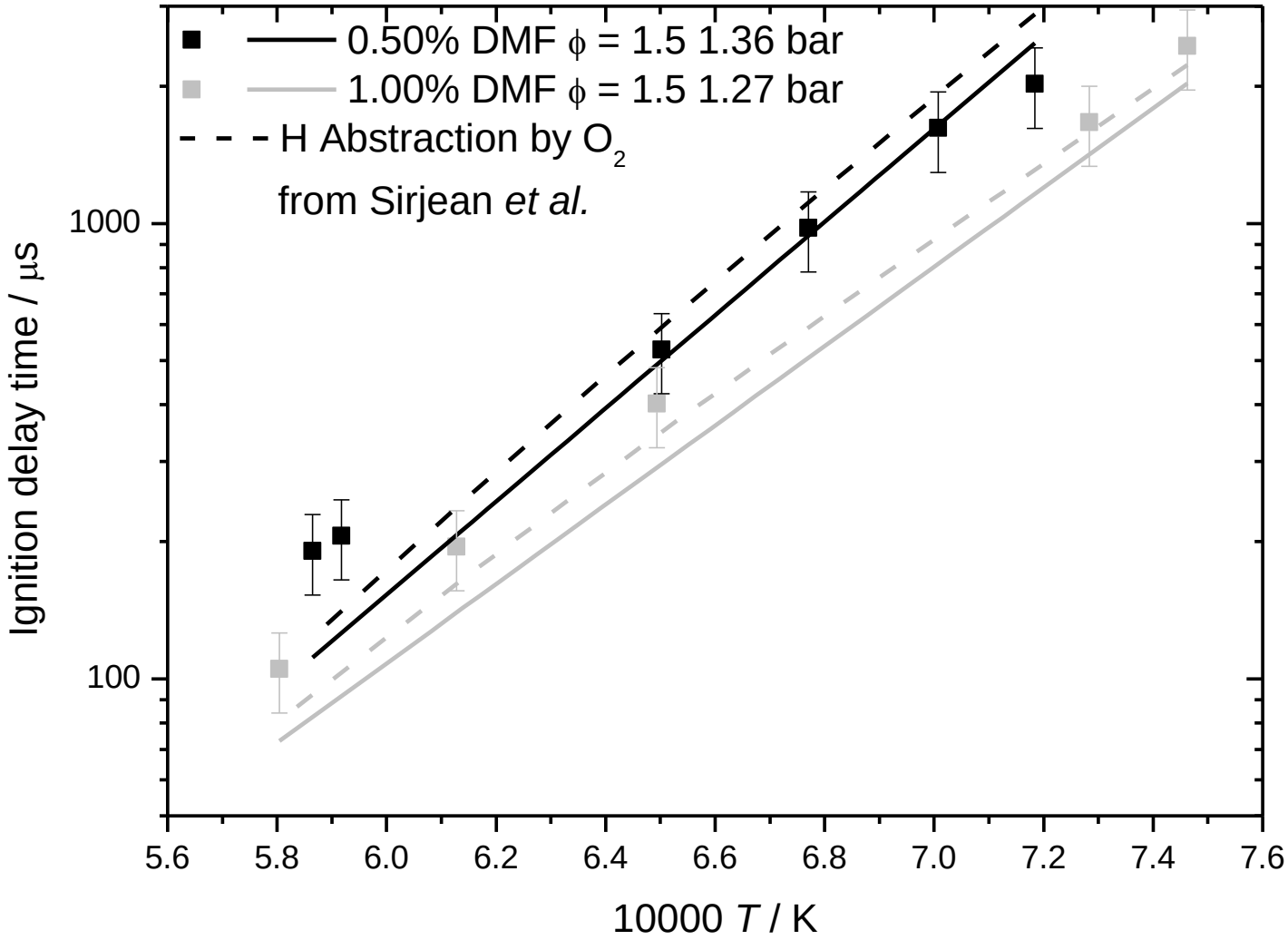

0.50% DMF ϕ = 1.5 1.36 bar
1.00% DMF ϕ = 1.5 1.27 bar
(H Abstraction by H) X 2
Ignition delay time / μs
1000
100
5.6
5.8
6.0
6.2
6.4
6.6
6.8
7.0
7.2
7.4
7.6
10000 T / K

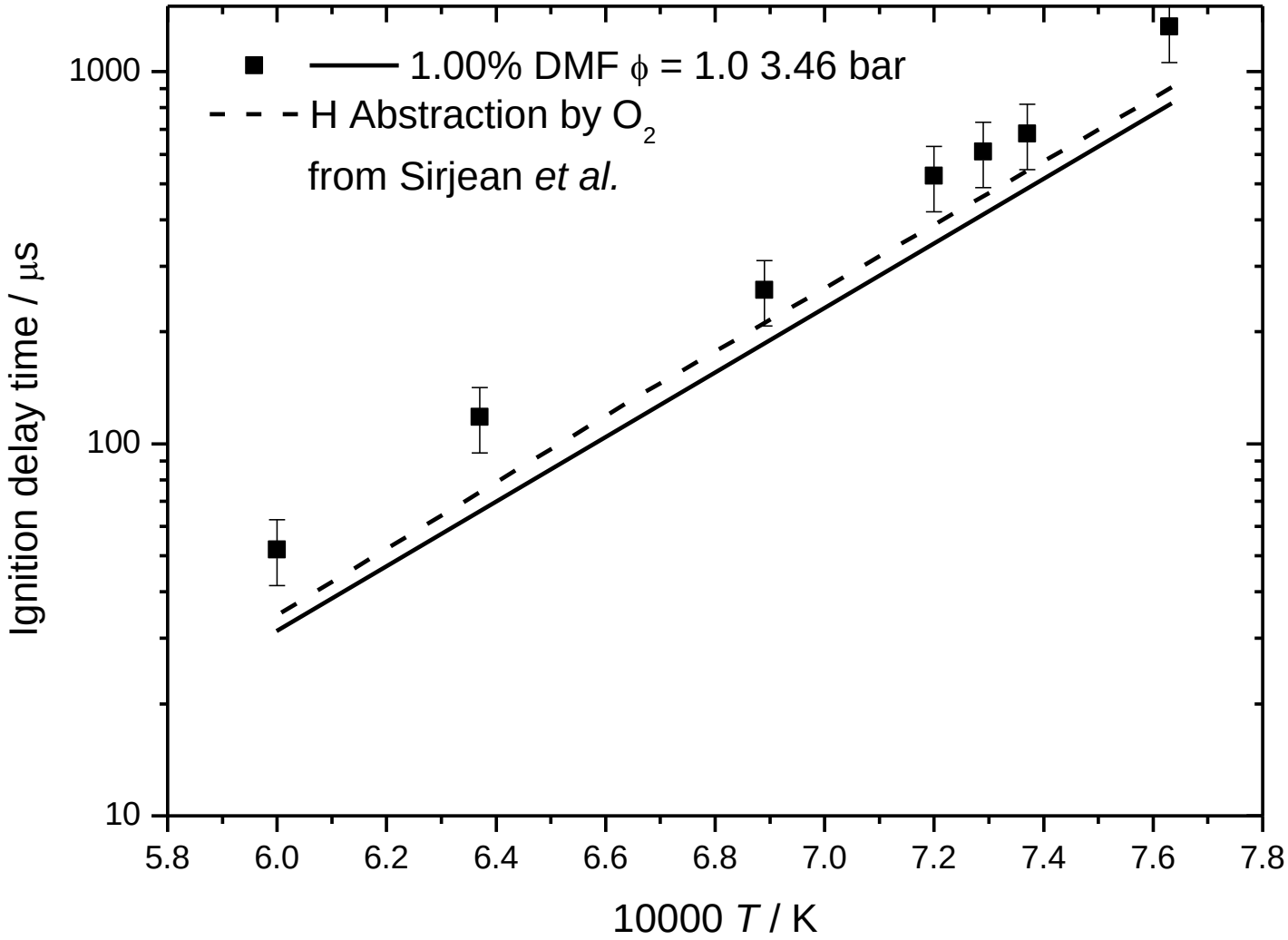

1.00% DMF ϕ = 1.0 3.46 bar
(H Abstraction by H) X 2
Ignition delay time / μs
1000
100
10
5.8
6.0
6.2
6.4
6.6
6.8
7.0
7.2
7.4
7.6
7.8
10000 T / K

Influence of adopting rate constant for H atom abstraction by O_2 from Sirjean *et al.*

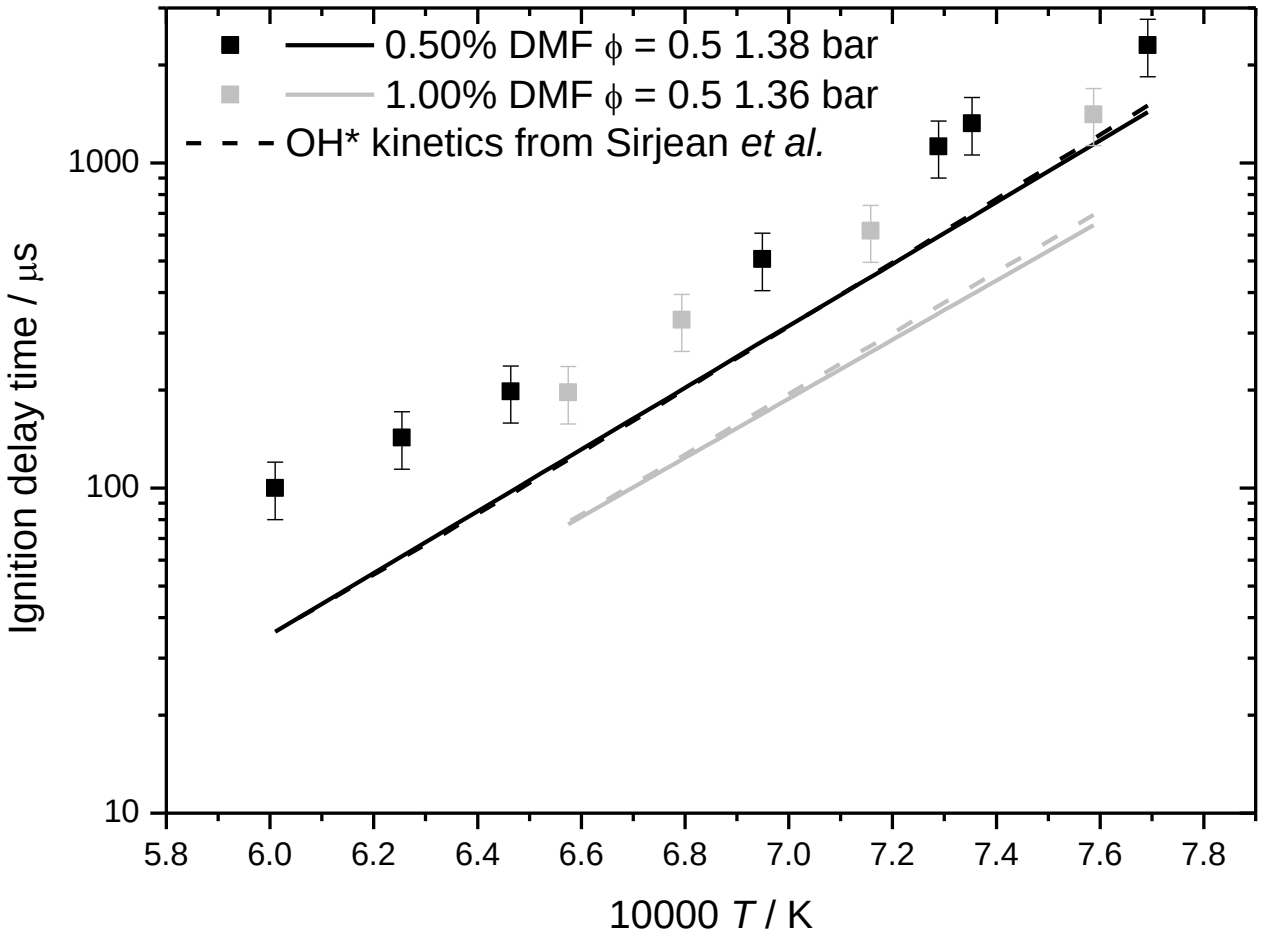


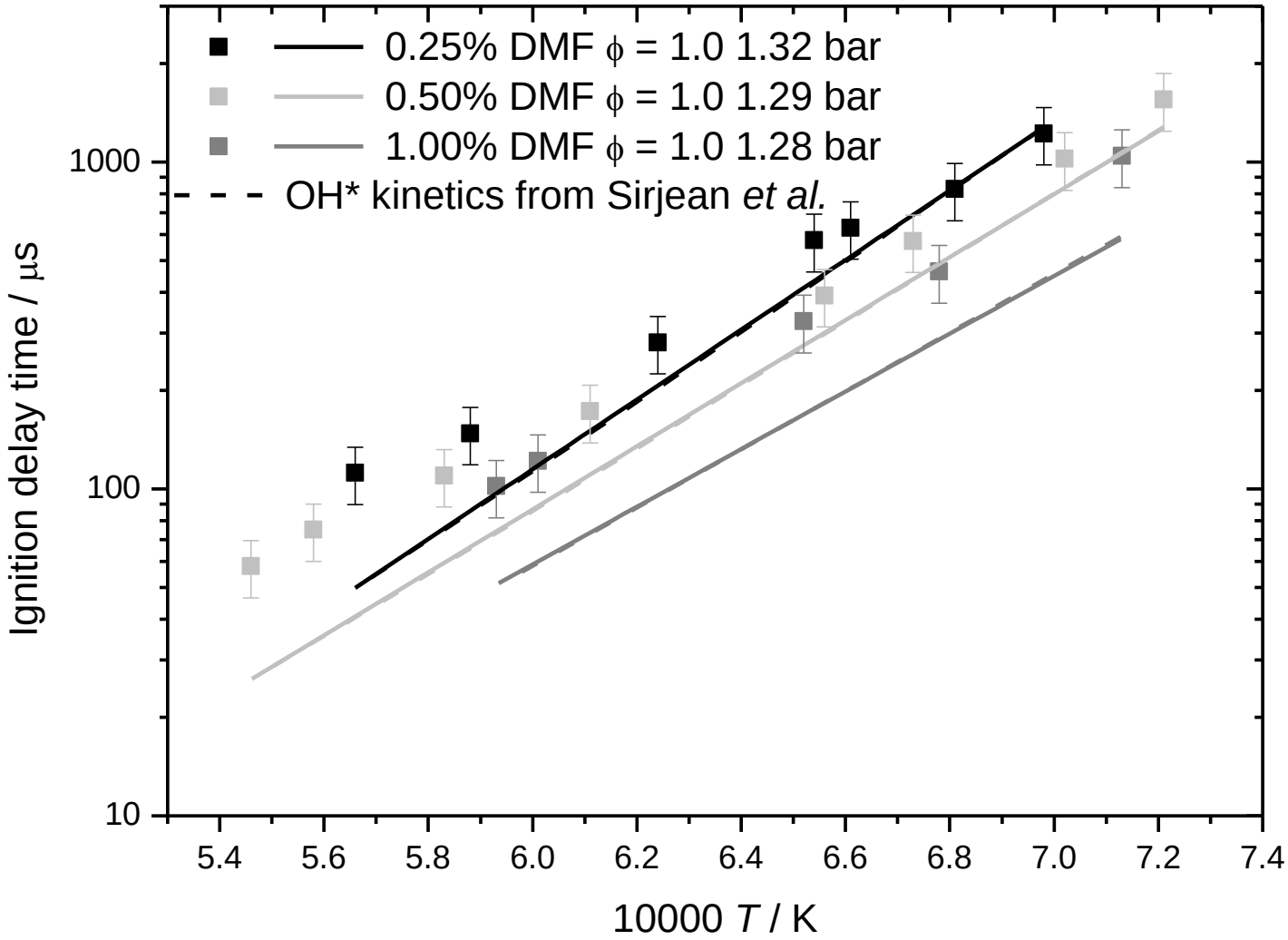

0.25% DMF ϕ = 1.0 1.32 bar
0.50% DMF ϕ = 1.0 1.29 bar
1.00% DMF ϕ = 1.0 1.28 bar
H Abstraction by O2
from Sirjean et al.
Ignition delay time / μs
1000
100
10
5.4
5.6
5.8
6.0
6.2
6.4
6.6
6.8
7.0
7.2
7.4
10000 T / K

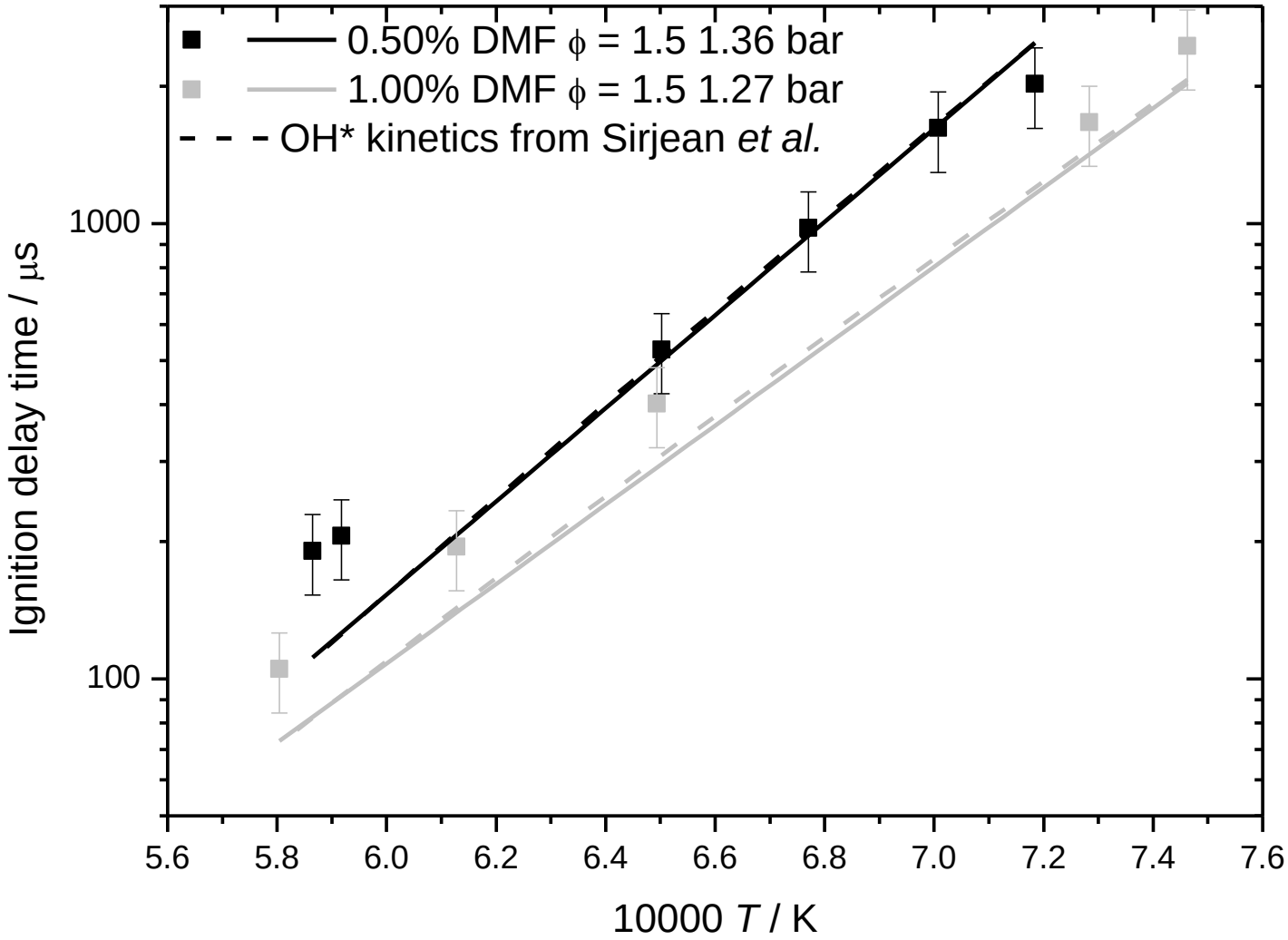

0.50% DMF ϕ = 1.5 1.36 bar
1.00% DMF ϕ = 1.5 1.27 bar
H Abstraction by O2
from Sirjean et al.
Ignition delay time / μs
1000
100
5.6
5.8
6.0
6.2
6.4
6.6
6.8
7.0
7.2
7.4
7.6
10000 T / K

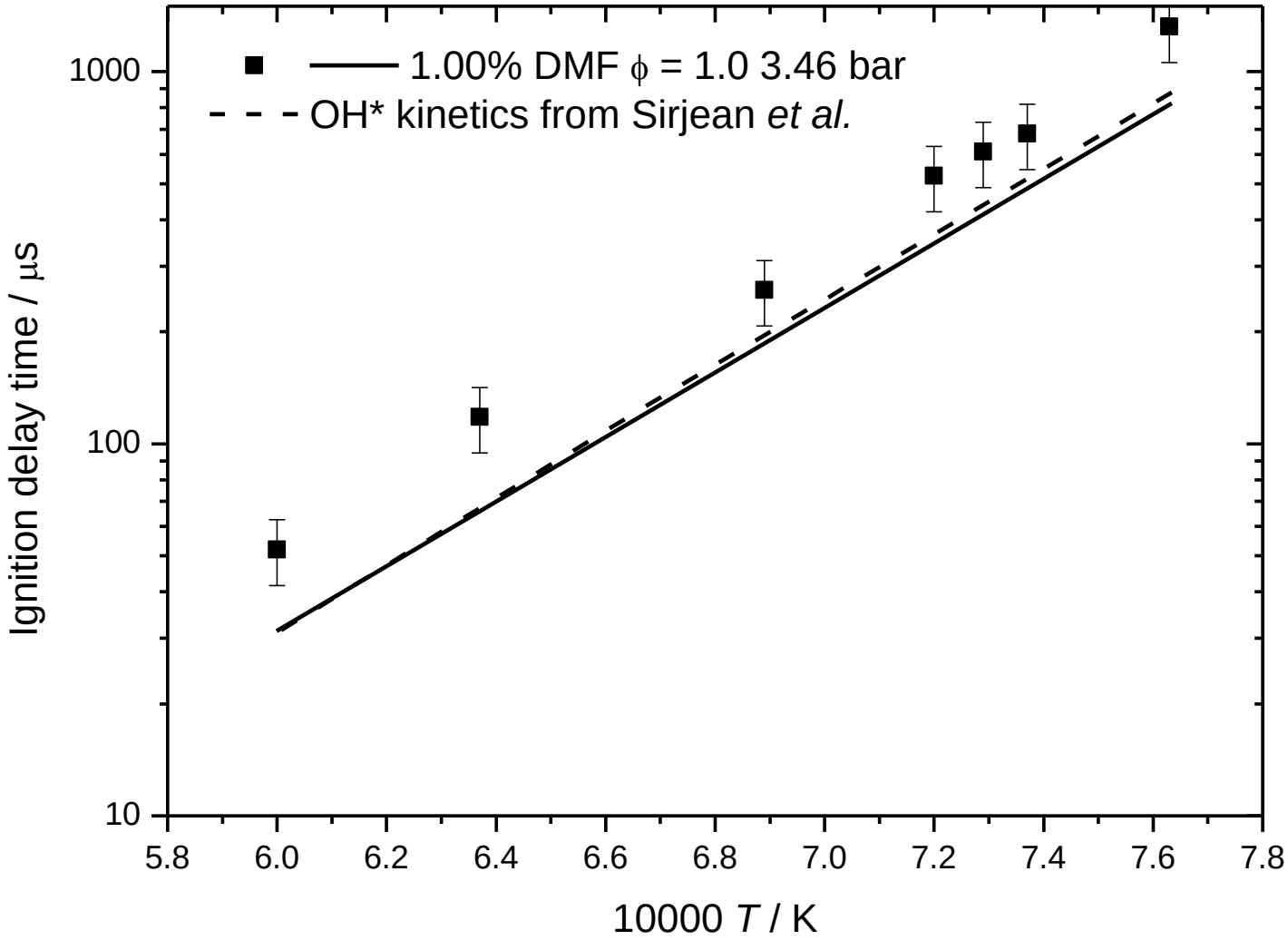

1.00% DMF ϕ = 1.0 3.46 bar
H Abstraction by O2
from Sirjean et al.
Ignition delay time / μs
1000
100
10
5.8
6.0
6.2
6.4
6.6
6.8
7.0
7.2
7.4
7.6
7.8
10000 T / K

Influence of adopting OH* submechanism from mechanism of Sirjean *et al.*

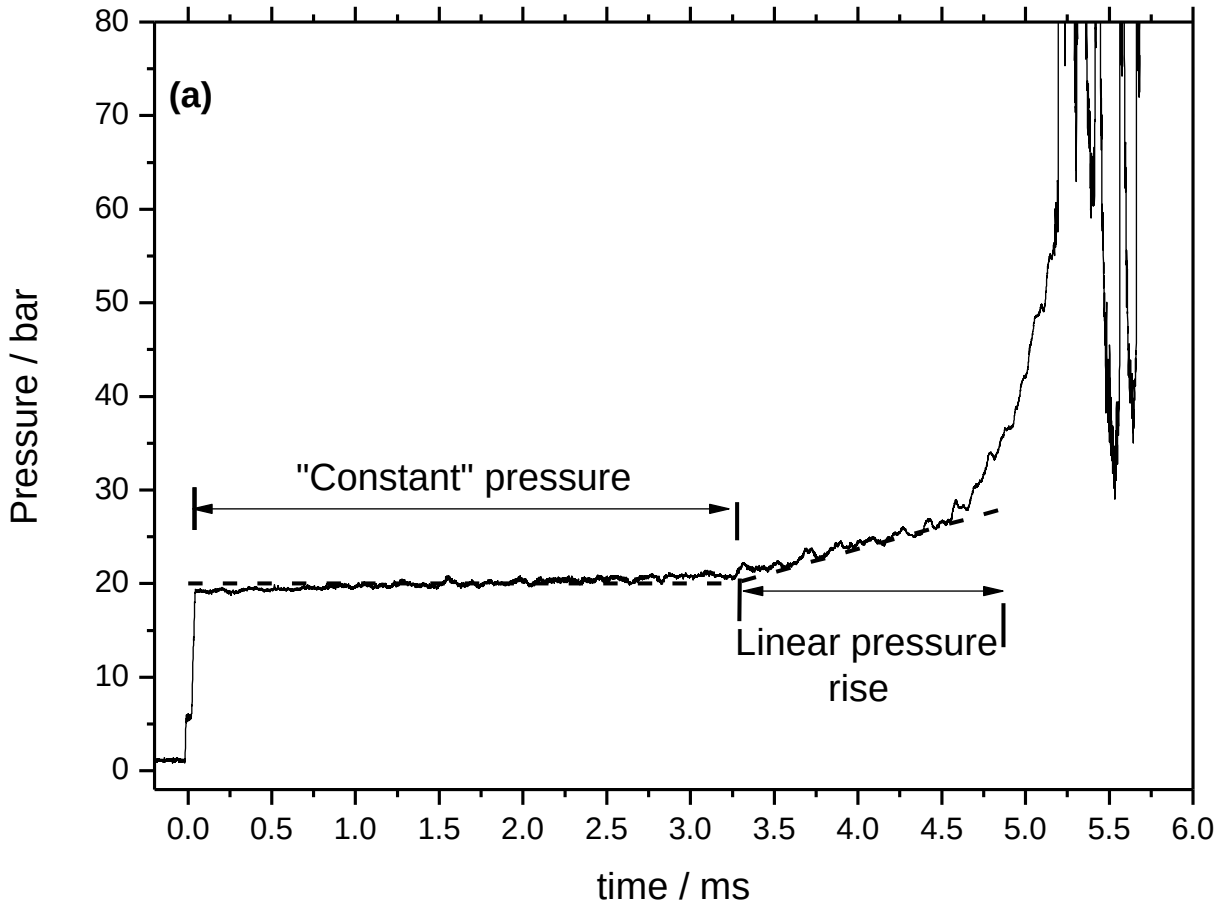



0.25% DMF ϕ = 1.0 1.32 bar
0.50% DMF ϕ = 1.0 1.29 bar
1.00% DMF ϕ = 1.0 1.28 bar
OH* kinetics from Sirjean *et al.*
Ignition delay time / μs
1000
100
10
5.4
5.6
5.8
6.0
6.2
6.4
6.6
6.8
7.0
7.2
7.4
10000 *T* / K


0.50% DMF ϕ = 1.5 1.36 bar
1.00% DMF ϕ = 1.5 1.27 bar
OH* kinetics from Sirjean et al.
Ignition delay time / μs
1000
100
5.6
5.8
6.0
6.2
6.4
6.6
6.8
7.0
7.2
7.4
7.6
10000 T / K


1.00% DMF ϕ = 1.0 3.46 bar
OH* kinetics from Sirjean et al.
Ignition delay time / μs
1000
100
10
5.8
6.0
6.2
6.4
6.6
6.8
7.0
7.2
7.4
7.6
7.8
10000 T / K

High Pressure Shock Tube Ignition Delay Times Example Pressure Profiles



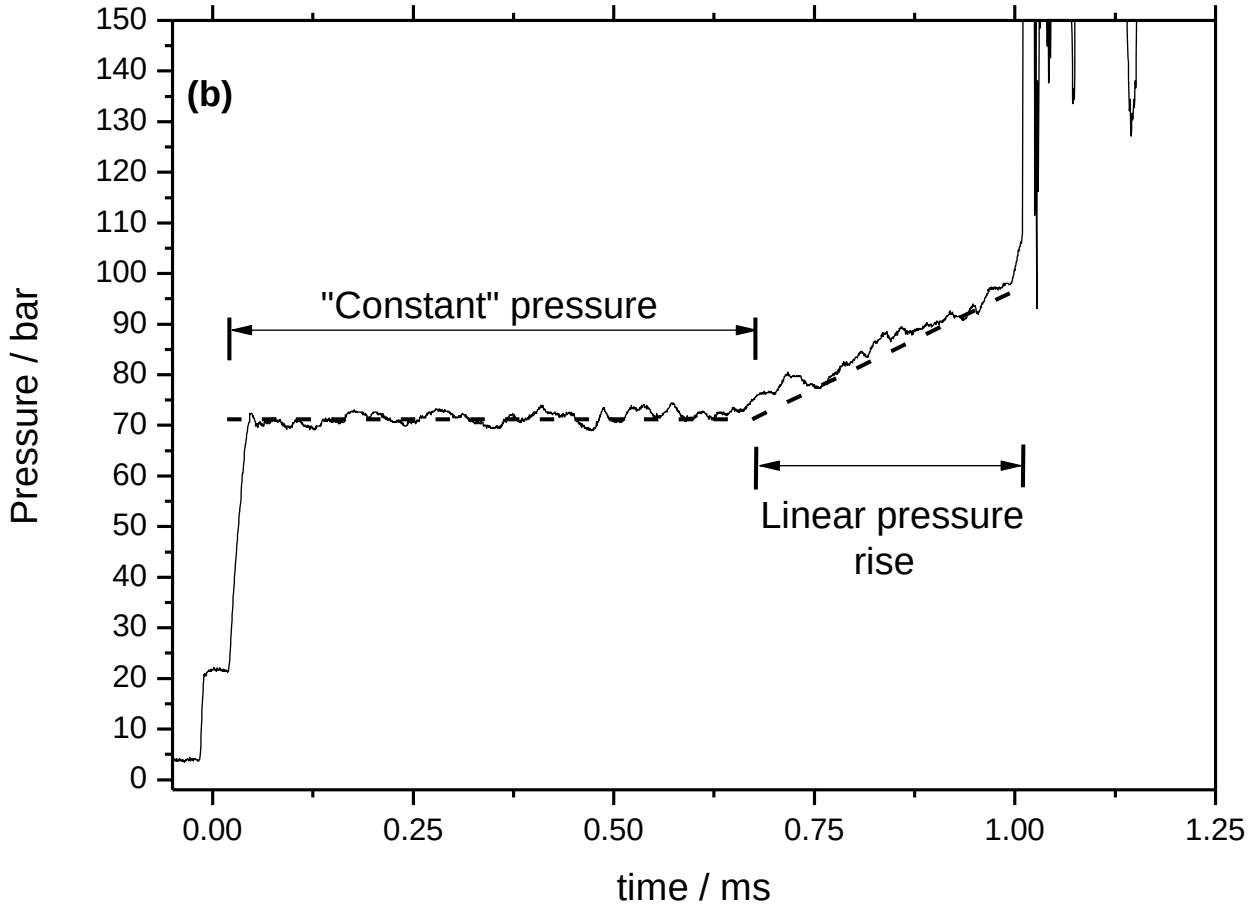
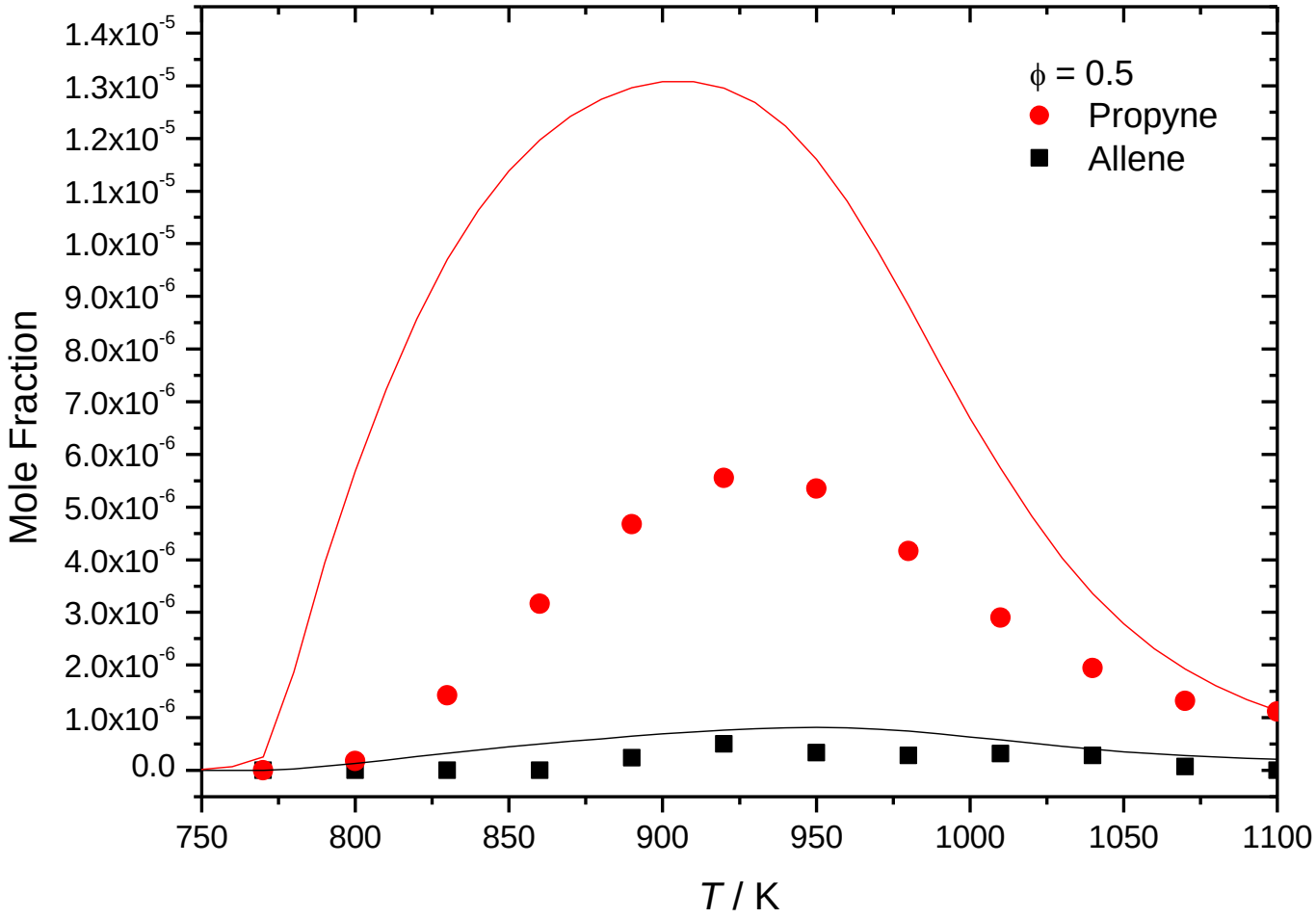
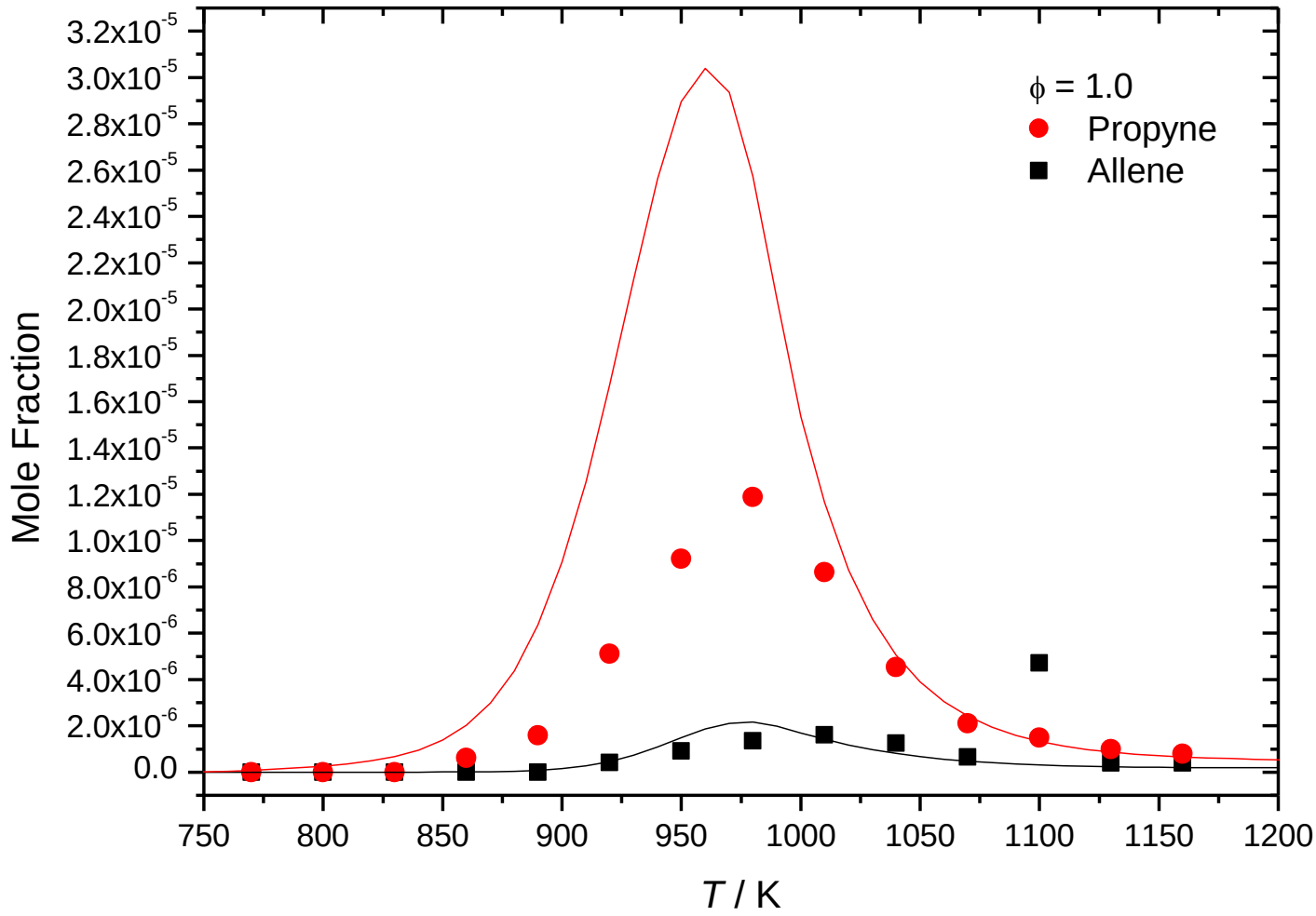
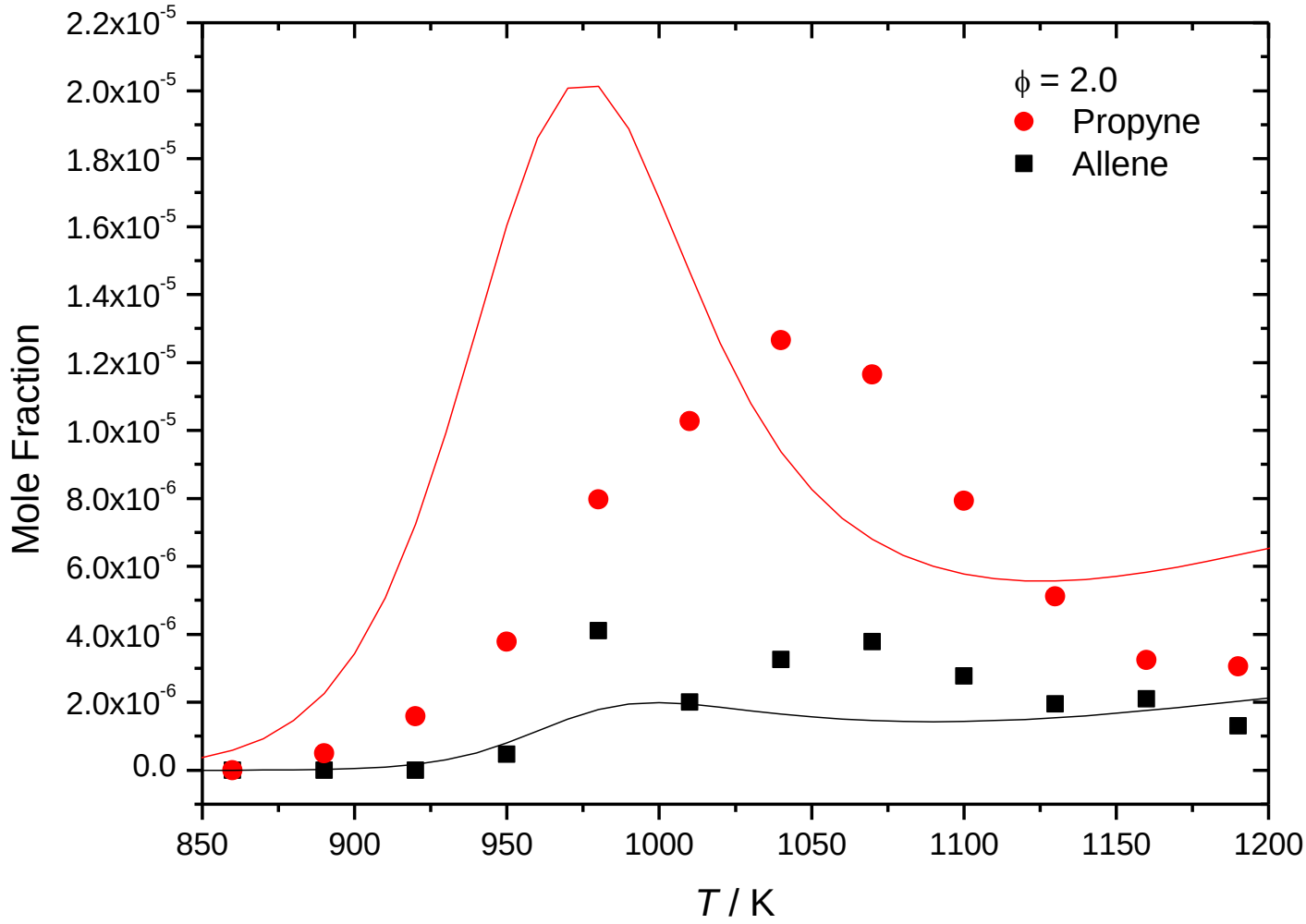


Figure 1: Example pressure-time profiles for stoichiometric 2.66% 2,5-dimethylfuran-'air' mixtures showing "constant" pressure region behind reflected shock wave and pre-ignition pressure rise prior to autoignition at (a) 852 K and 20.4 bar and (b) 913 K and 74.1 bar.

Jet Stirred Reactor Propyne-Allene Profiles




ϕ = 1.0
Propyne
Allene
Mole Fraction
3.2x10-5
3.0x10-5
2.8x10-5
2.6x10-5
2.4x10-5
2.2x10-5
2.0x10-5
1.8x10-5
1.6x10-5
1.4x10-5
1.2x10-5
1.0x10-5
8.0x10-6
6.0x10-6
4.0x10-6
2.0x10-6
0.0
750
800
850
900
950
1000
1050
1100
1150
1200
T / K


2.2x10-5
2.0x10-5
1.8x10-5
1.6x10-5
1.4x10-5
1.2x10-5
1.0x10-5
8.0x10-6
6.0x10-6
4.0x10-6
2.0x10-6
0.0
Mole Fraction
850
900
950
1000
1050
1100
1150
1200
T / K
ϕ = 2.0
Propyne
Allene

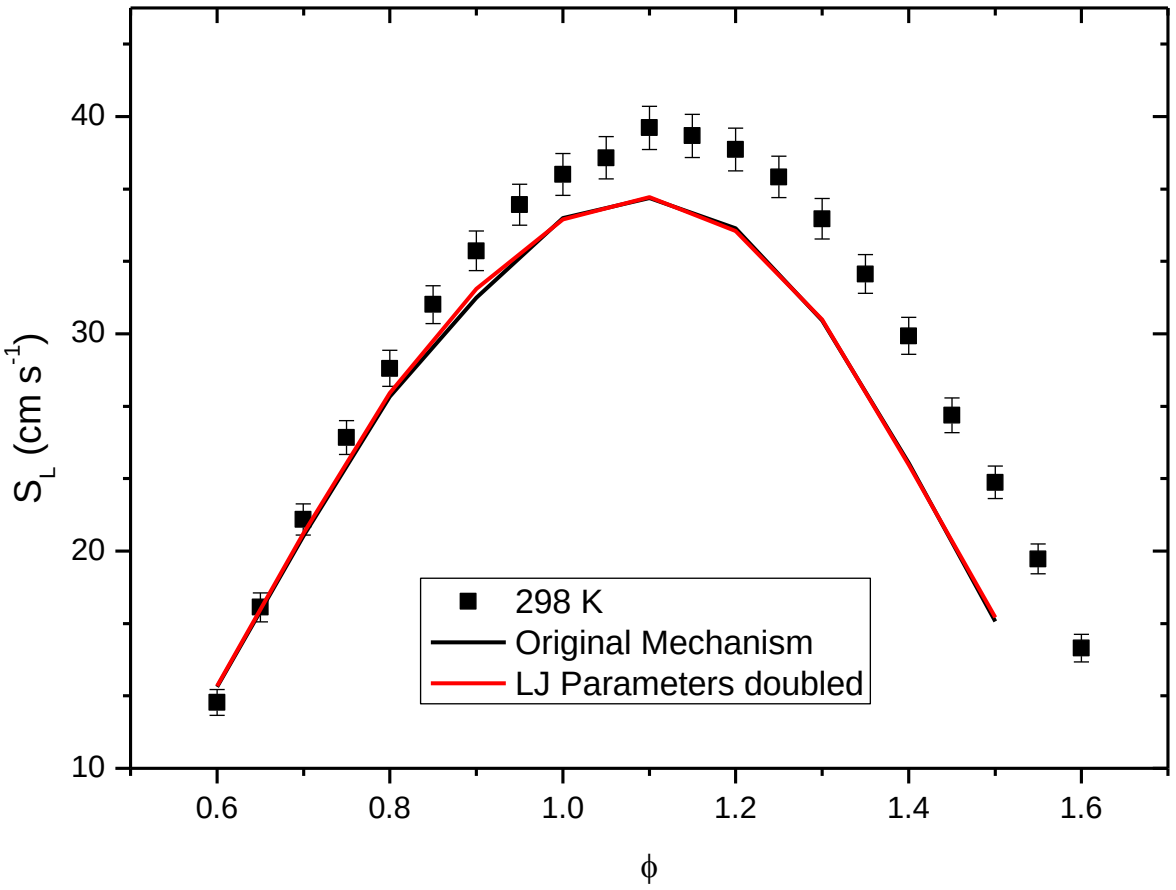


Figure 2: Effect of doubling the LJ parameters (σ and ε/k for all furanic intermediates) on atmospheric pressure laminar burning velocities. Black lines are computations from unmodified mechanism.

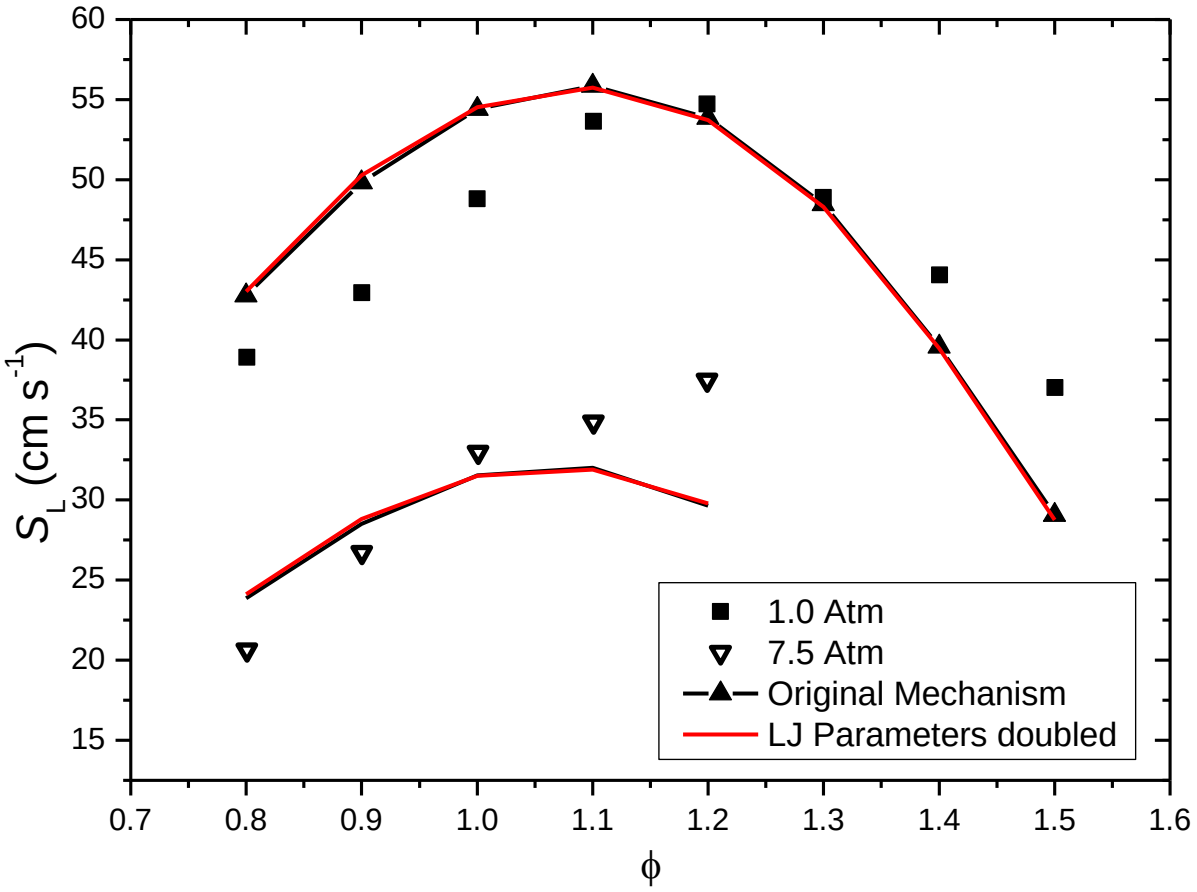


Figure 3: Effect of doubling the LJ parameters (σ and ε/k) for all furanic intermediates on atmospheric and high pressure pressure laminar burning velocities at 393 K. Black lines are computations from unmodified mechanism.

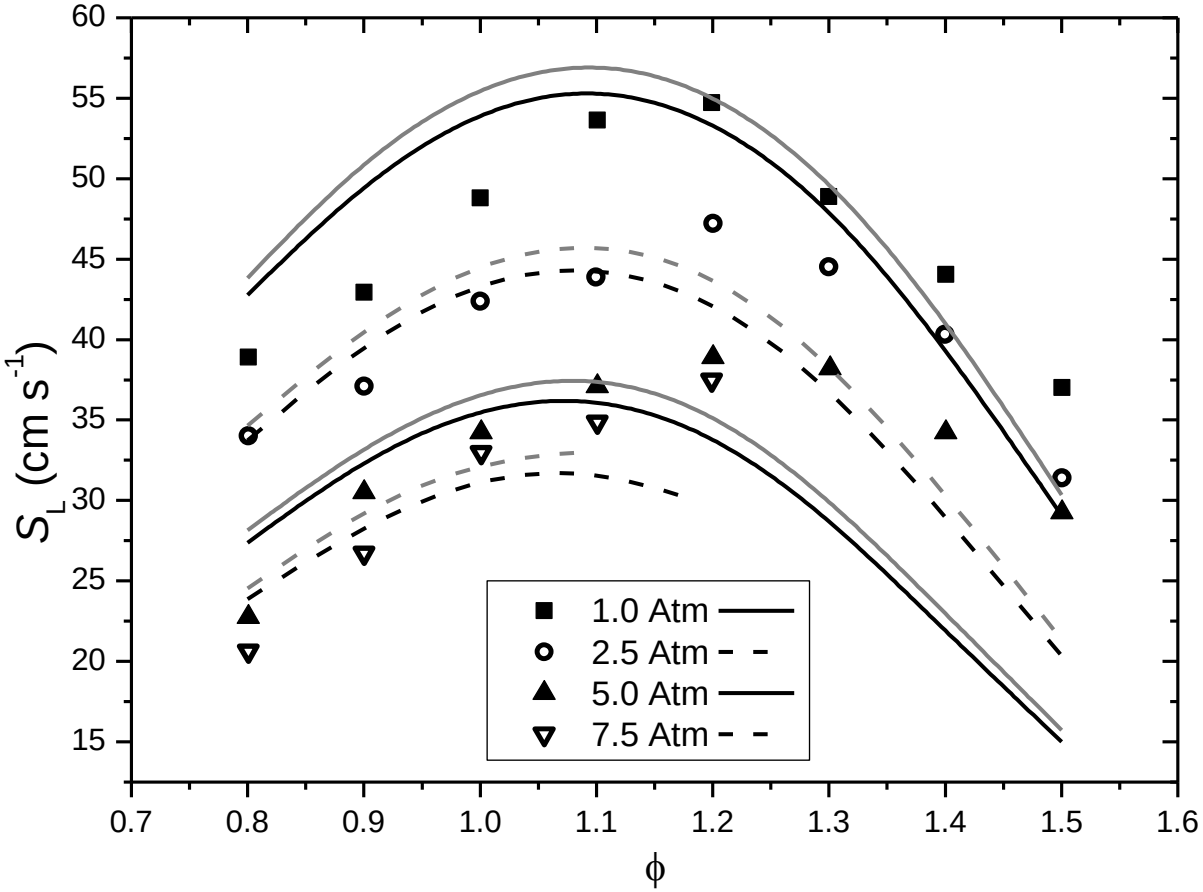


Figure 4: Effect of simultaneously decreasing A-factor for hydrogen atom abstraction by hydrogen and hydroxyl radicals from the alkyl side chain of 2,5-dimethylfuran (Grey lines). Black lines are computations from unmodified mechanism.