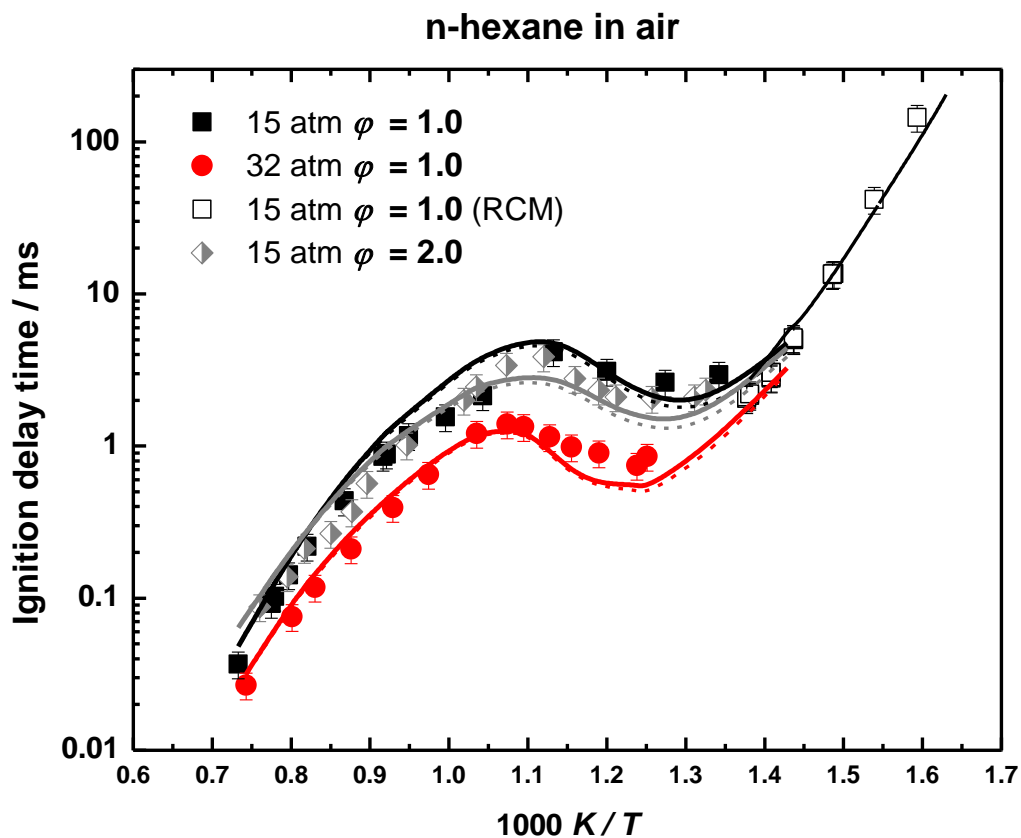


25. Validation for *n*-hexane

Ignition delay time : Shock Tube + RCM

p_c	T_c	φ
15 – 32 atm	625 – 1430 K	1.0 , 2.0



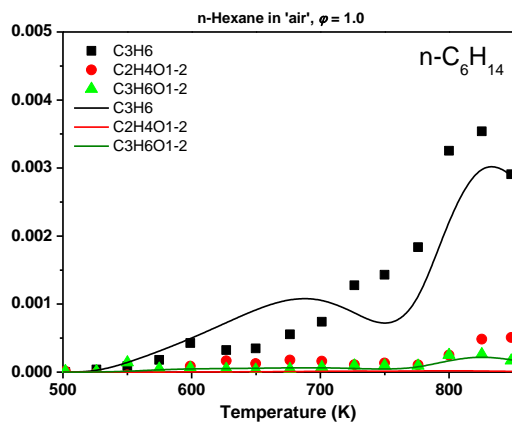
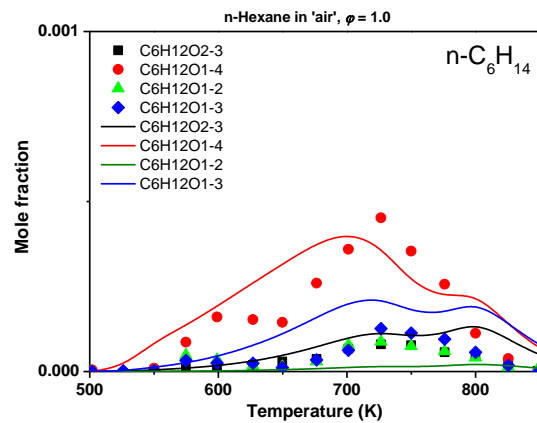
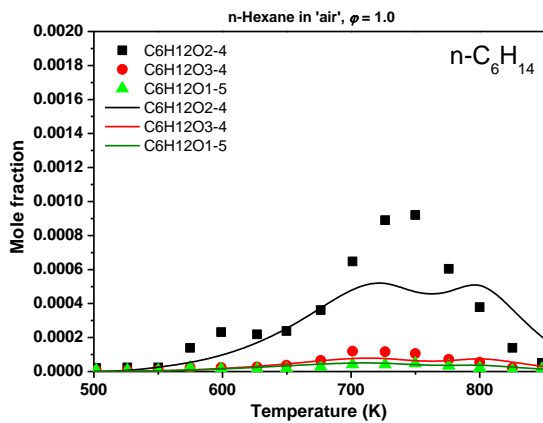
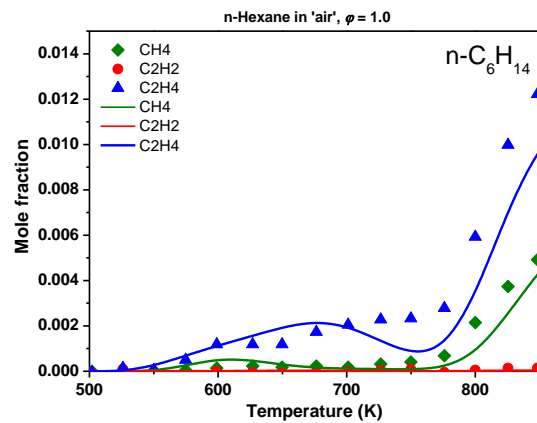
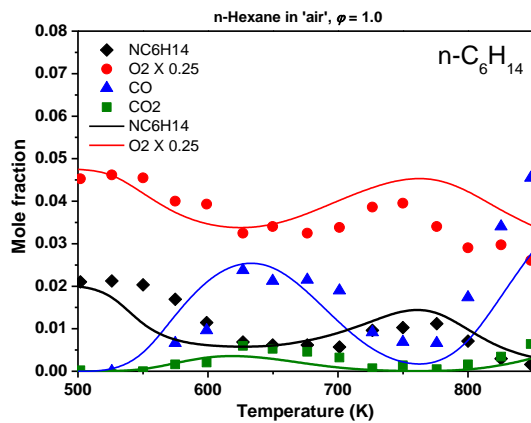
REFERENCES

- [1] Zhang et al., Combustion and Flame 162, 4194 – 4207 (2015)

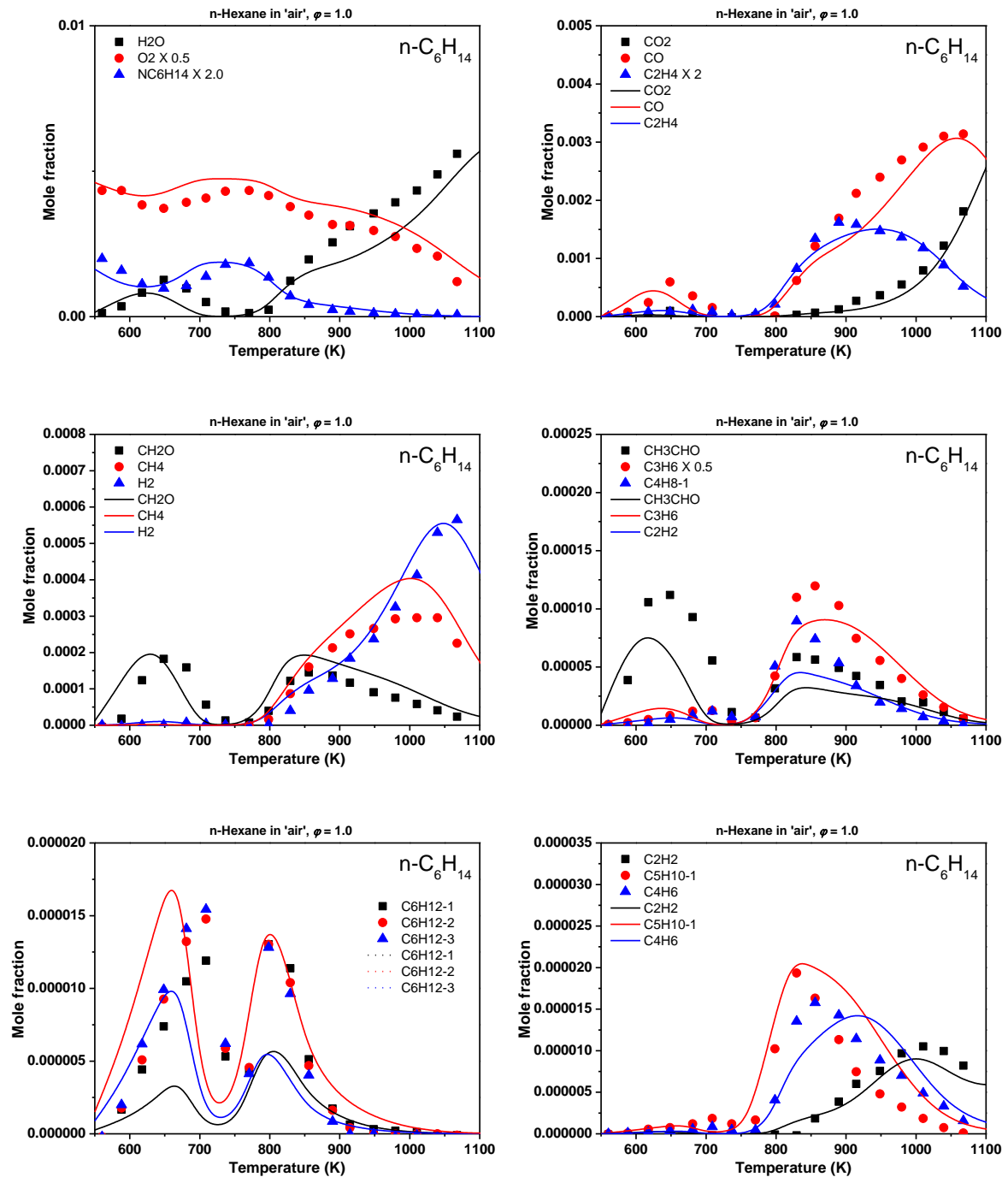
Jet Stirred Reactor

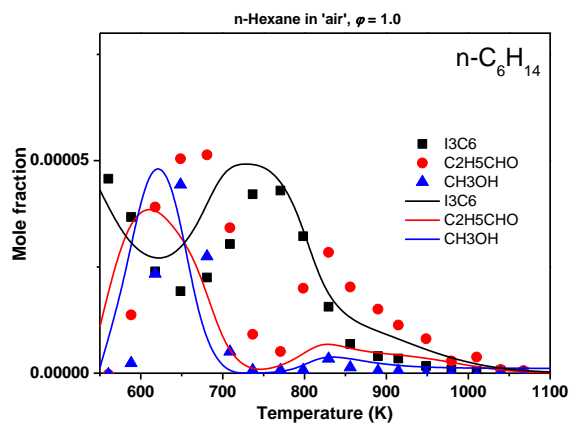
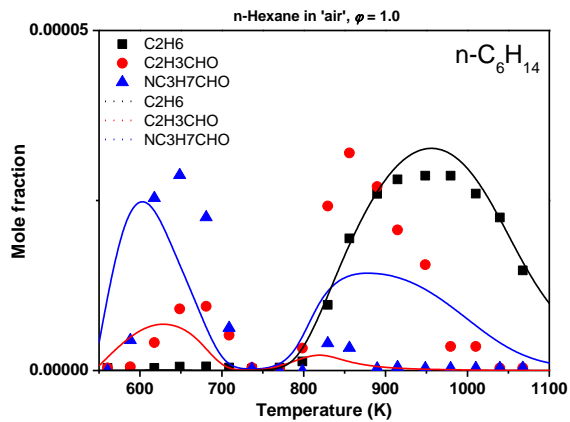
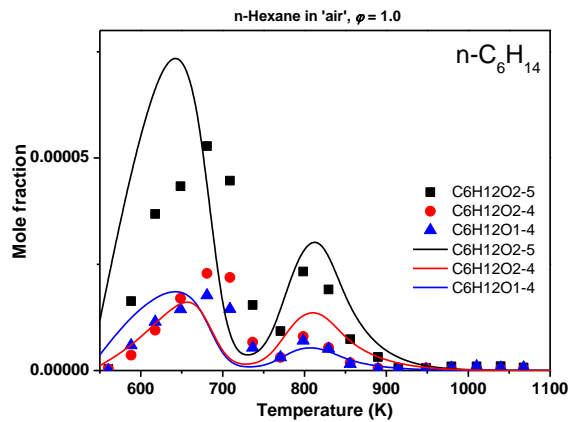
p	T	ϕ
1, 10 atm	500 – 1100 K	0.5 – 2.0

n-hexane JSR : PHI 1.0 _ 1 ATM

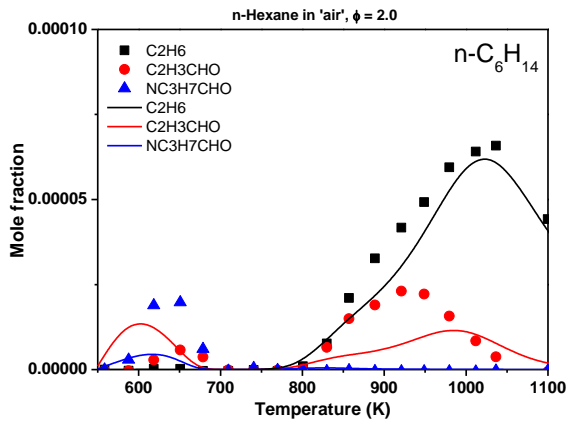
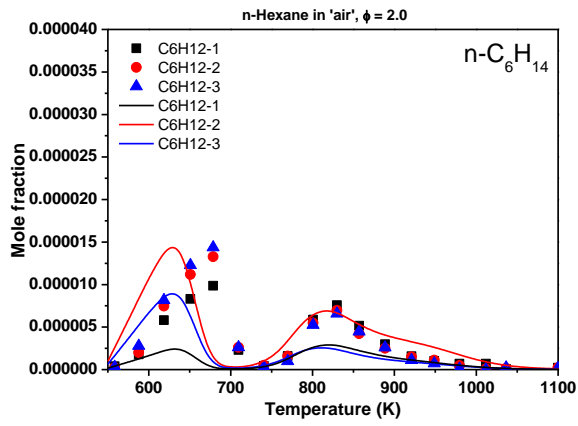
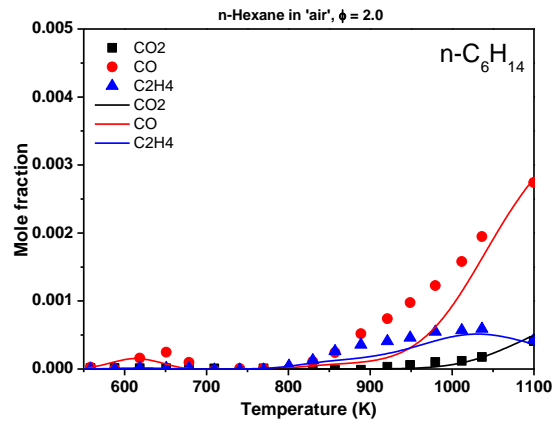
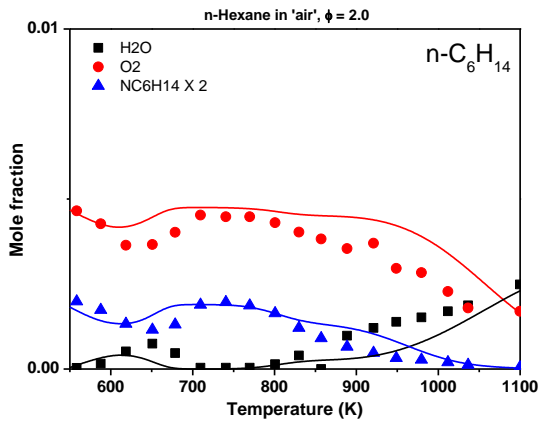


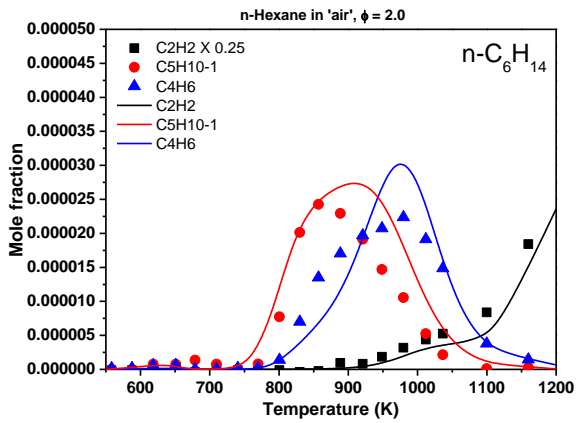
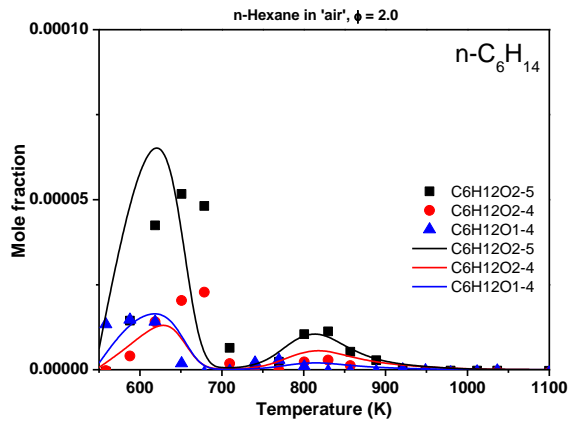
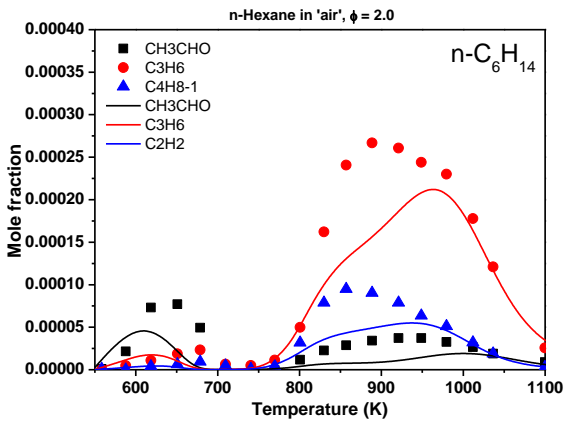
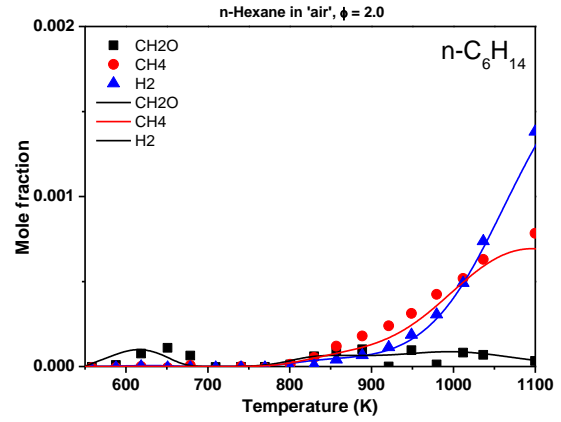
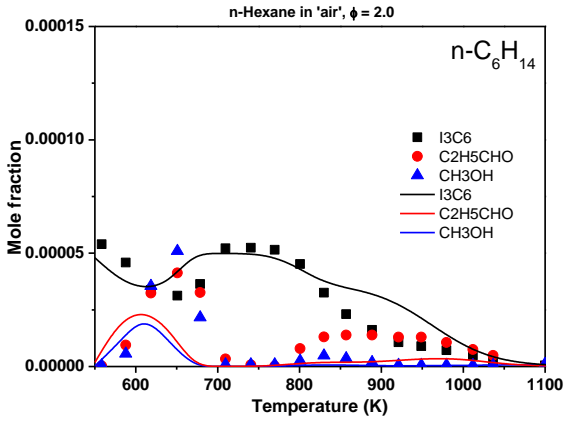
n-hexane ; JSR :PHI 1.0 _ 10 ATM



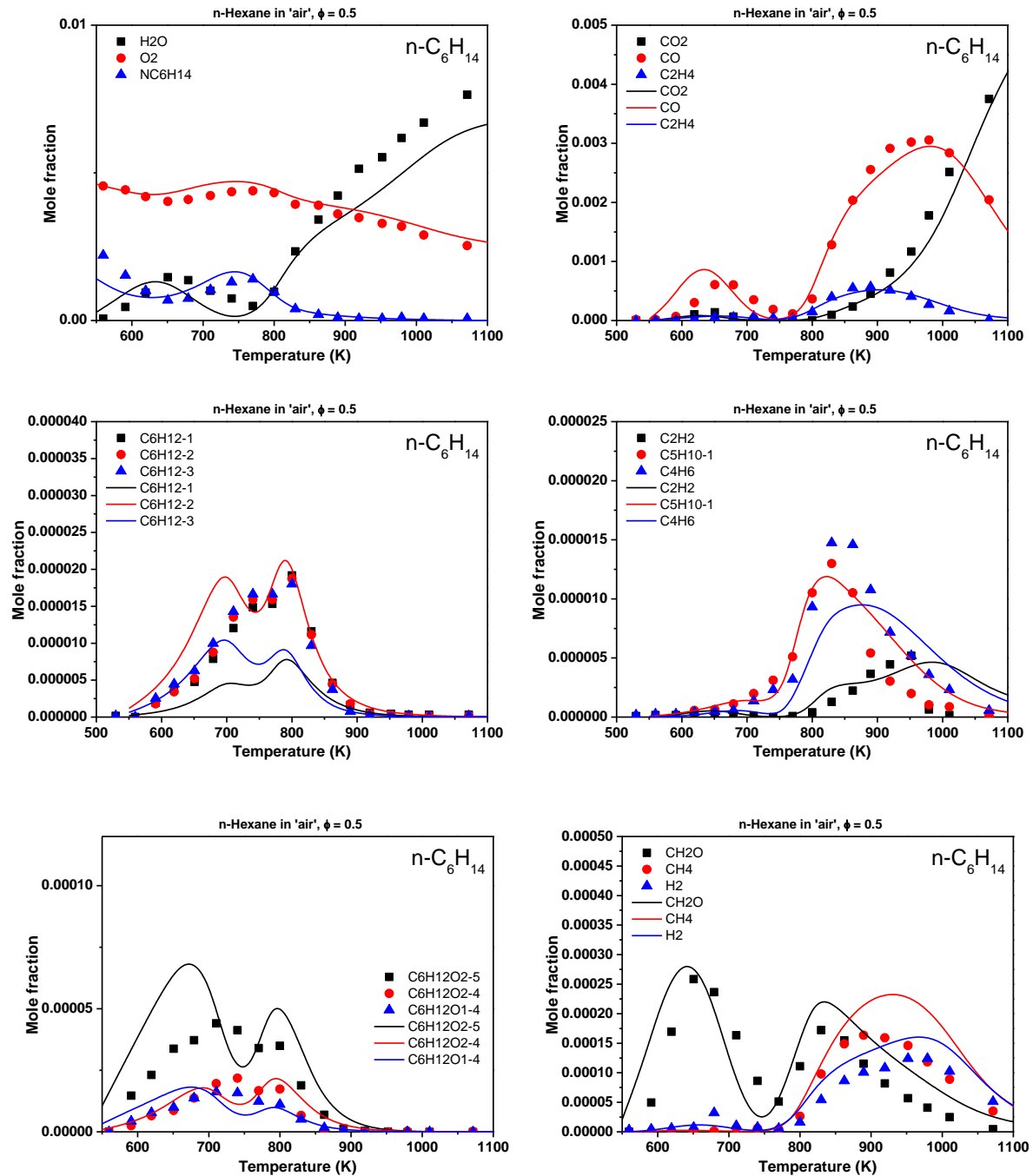


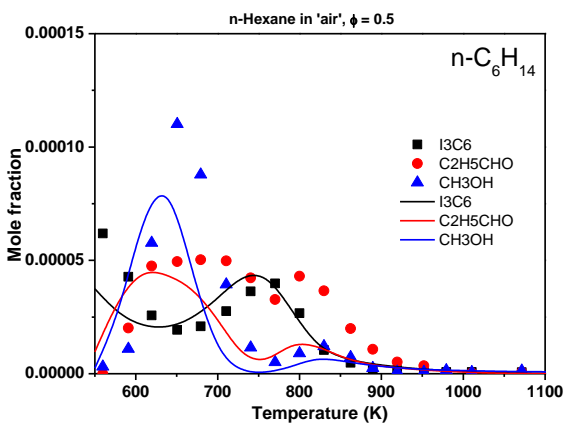
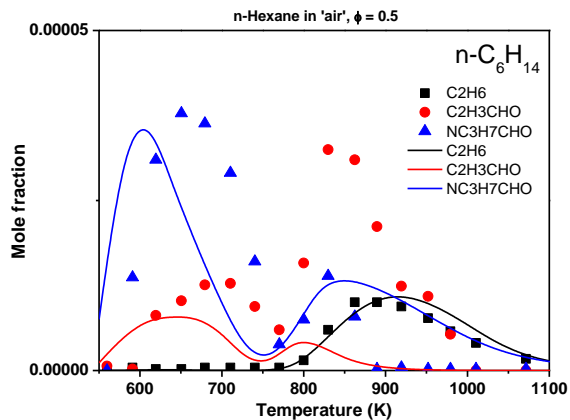
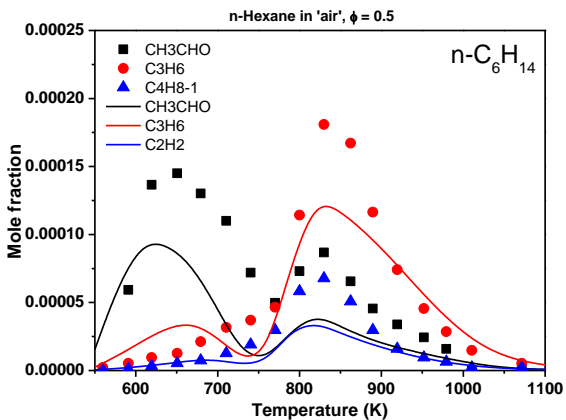
n-hexane ; JSR :PHI 2.0 _ 10 ATM





n-hexane ; JSR :PHI 0.5_ 10 ATM



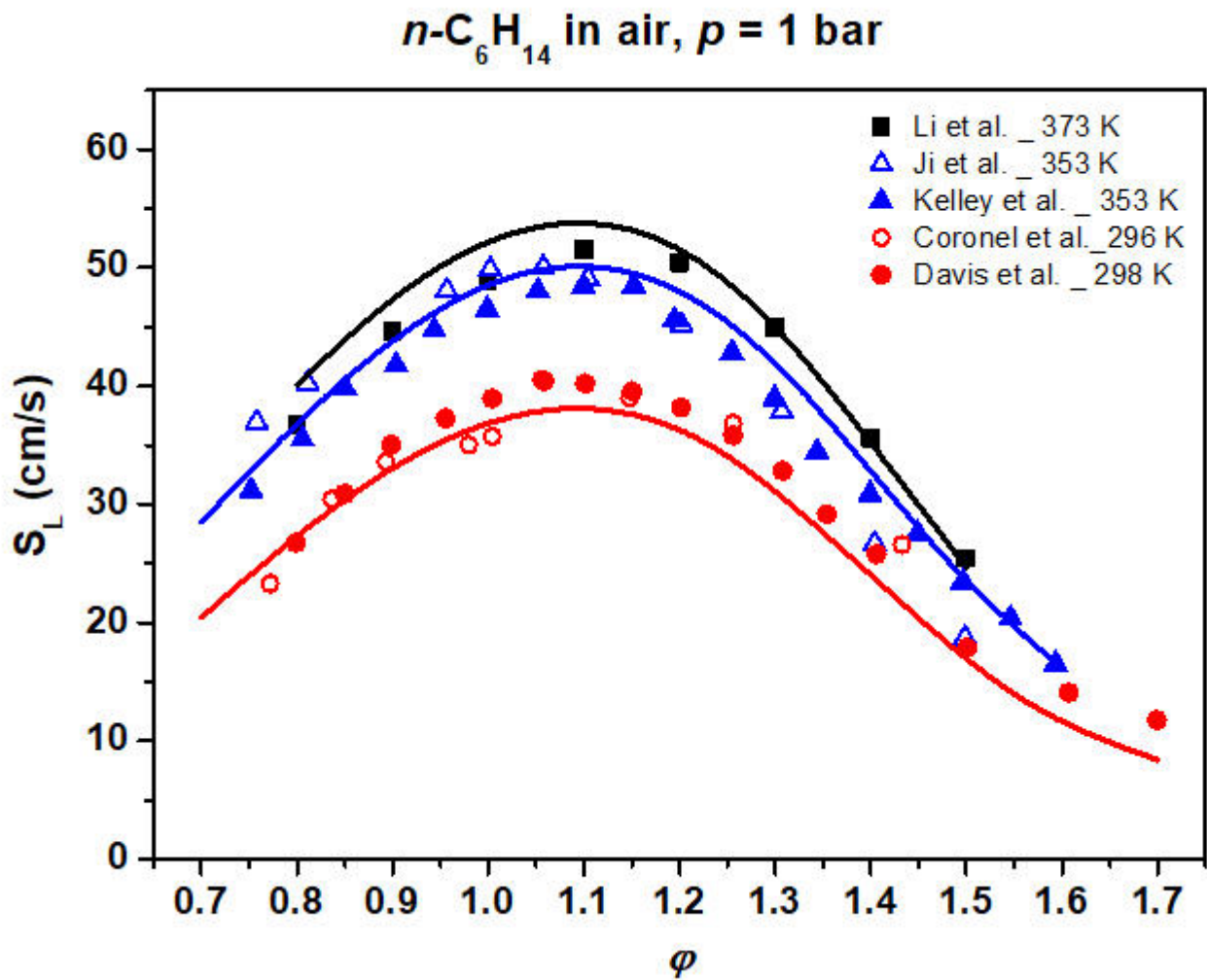


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Laminar flame speed

- [1] Li et al., Fuel 243, 533–540 (2019)
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- [4] Coronel et al., 8th US Nat. Combust. Meeting (2013)
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26. Validation for C₆H₁₂-1

Ignition delay time : Shock Tube

Shijun Dong, et al. A comprehensive experimental and kinetic modeling study of 1-hexene

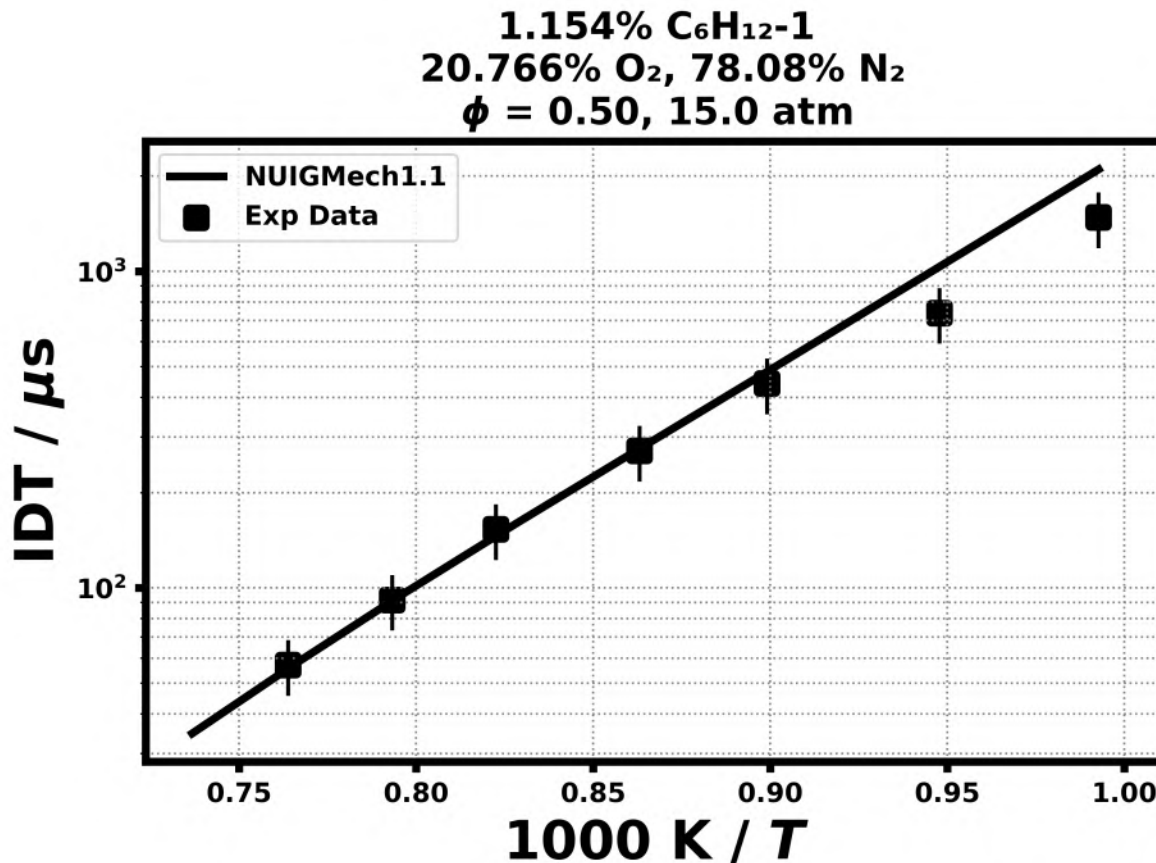


Figure 1: Dataset: 15_ATM.1.15_C6H12-1_PHL0.5

1.1.2 Case: C6H12-1/ST/DONG/15_ATM.2.28_C6H12-1_PHI.1.0

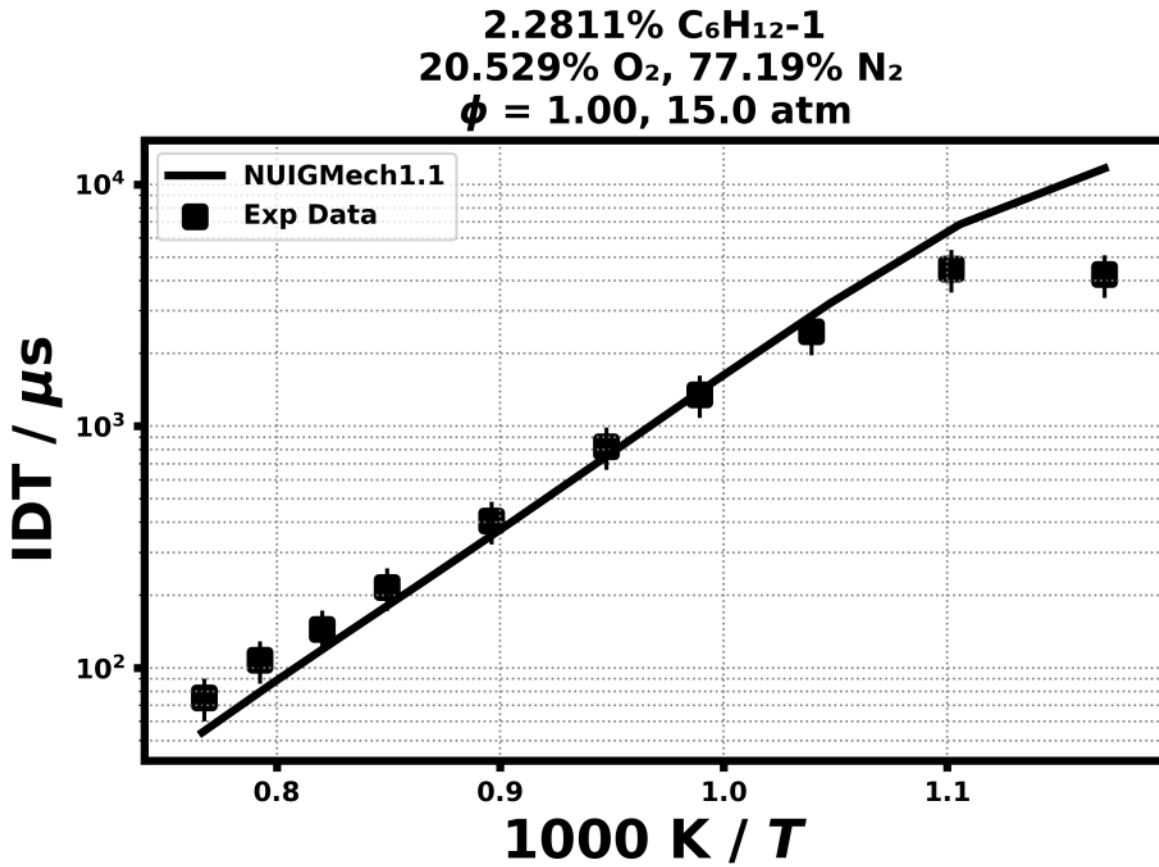


Figure 2: Dataset: 15_ATM.2.28_C6H12-1_PHI.1.0

1.1.3 Case: C6H12-1/ST/DONG/15_ATM_4.46_C6H12-1_PHI.2.0

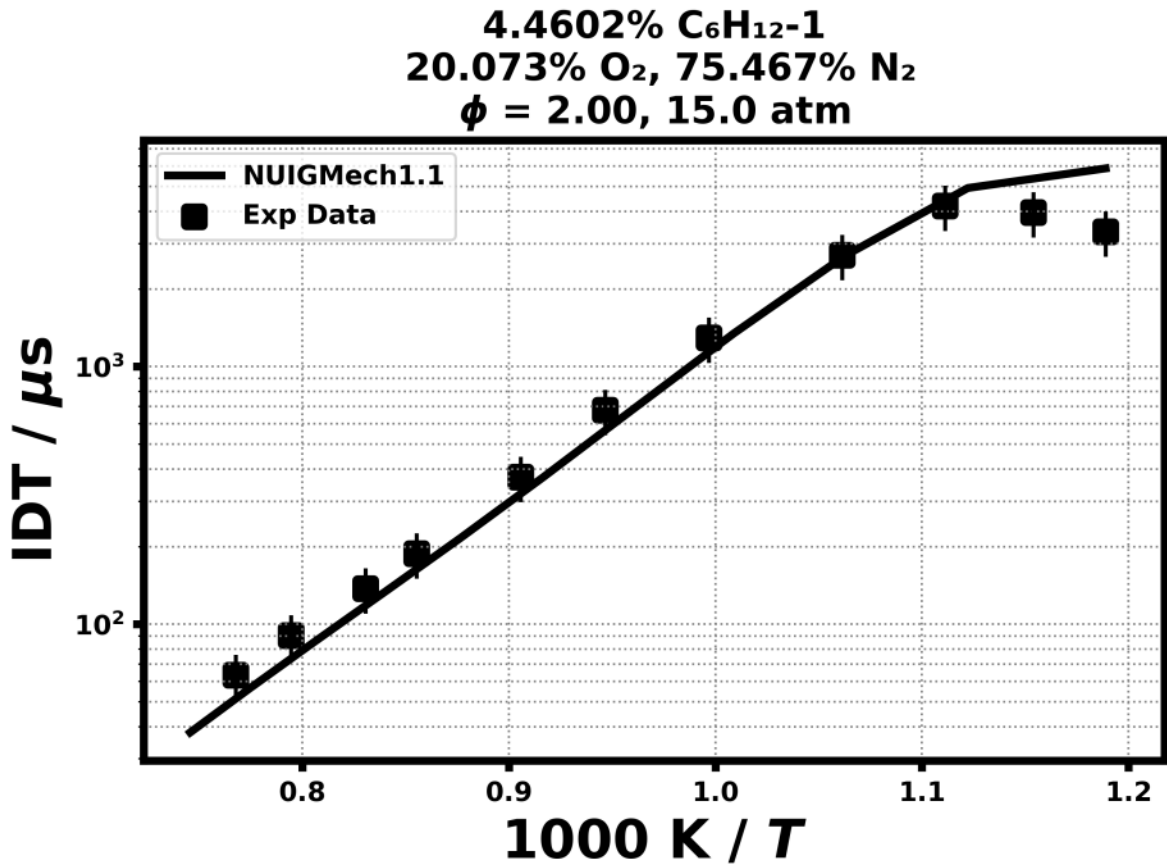


Figure 3: Dataset: 15_ATM_4.46_C6H12-1_PHI.2.0

1.1.4 Case: C6H12-1/ST/DONG/30_ATM_1.15_C6H12-1_PHI.0.5

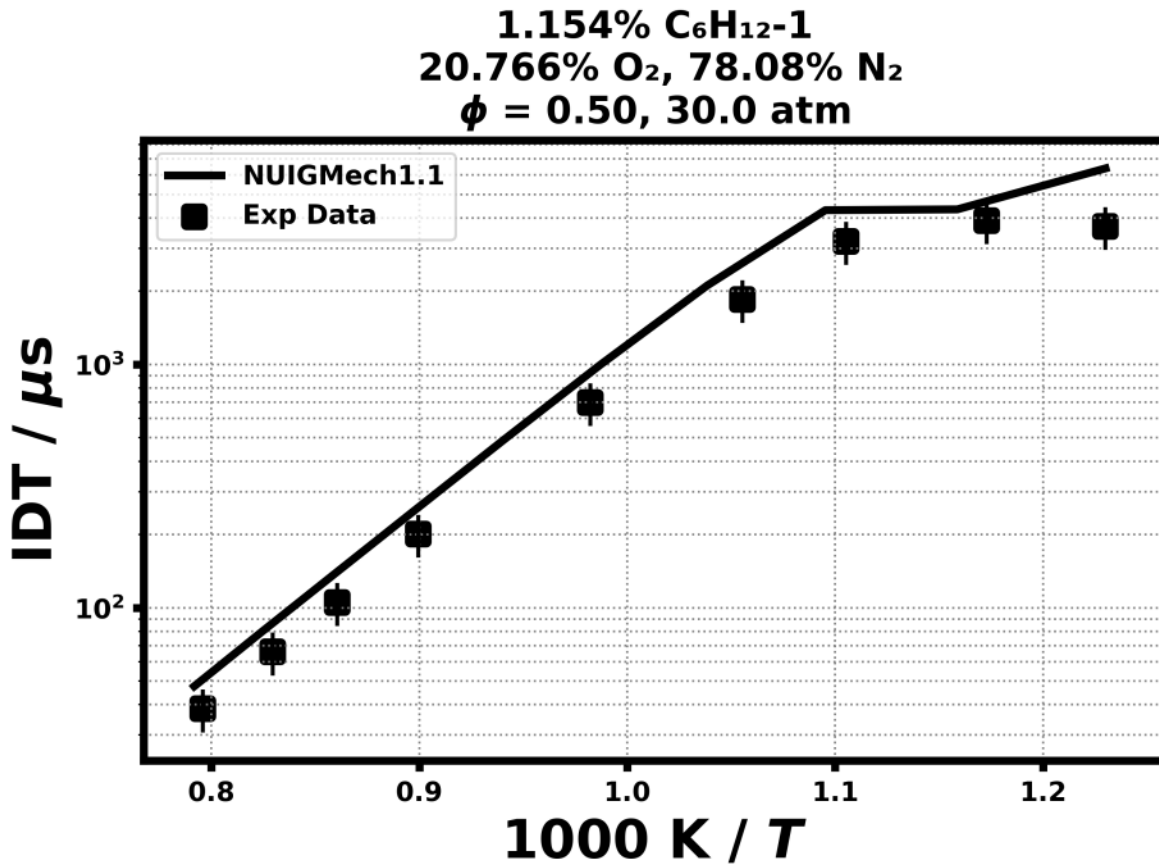


Figure 4: Dataset: 30_ATM_1.15_C6H12-1_PHI.0.5

1.1.5 Case: C6H12-1/ST/DONG/30_ATM_2.28_C6H12-1_PHI.1.0

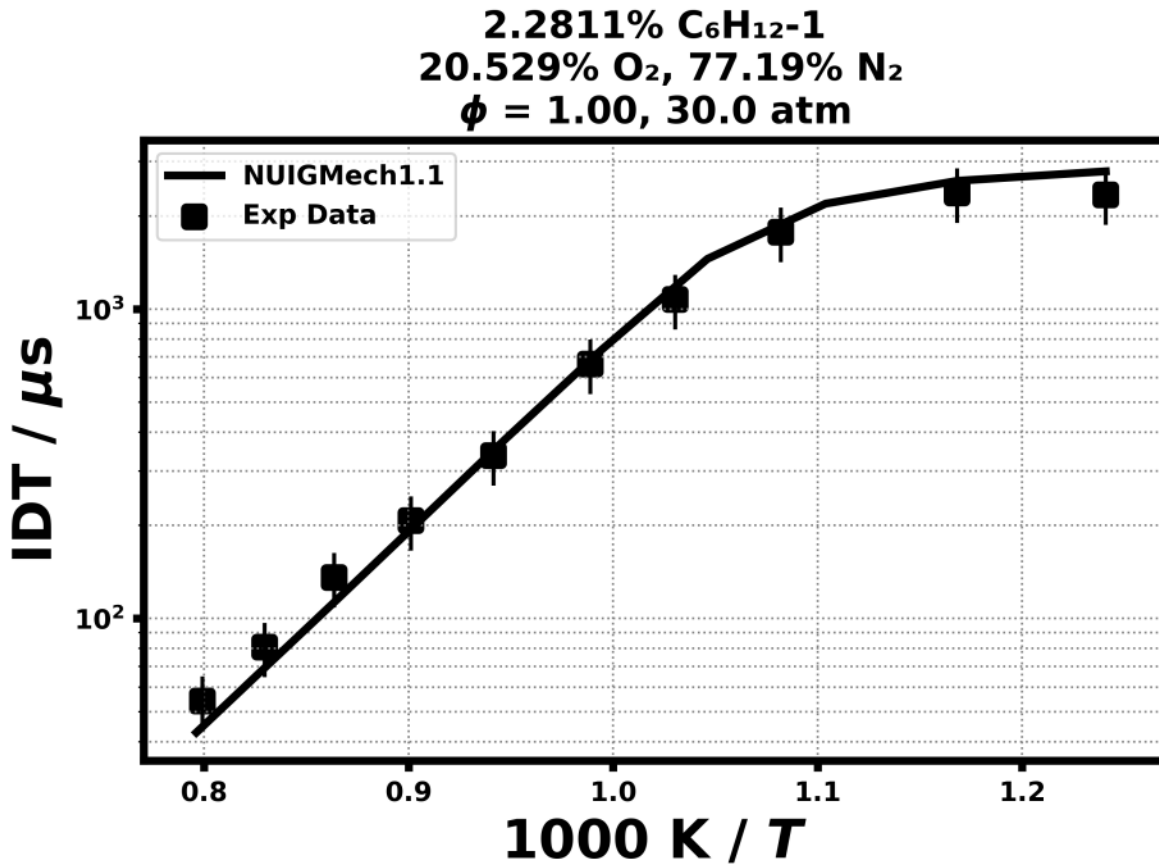


Figure 5: Dataset: 30_ATM_2.28_C6H12-1_PHI.1.0

1.1.6 Case: C6H12-1/ST/DONG/30_ATM_4.46_C6H12-1_PHI.2.0

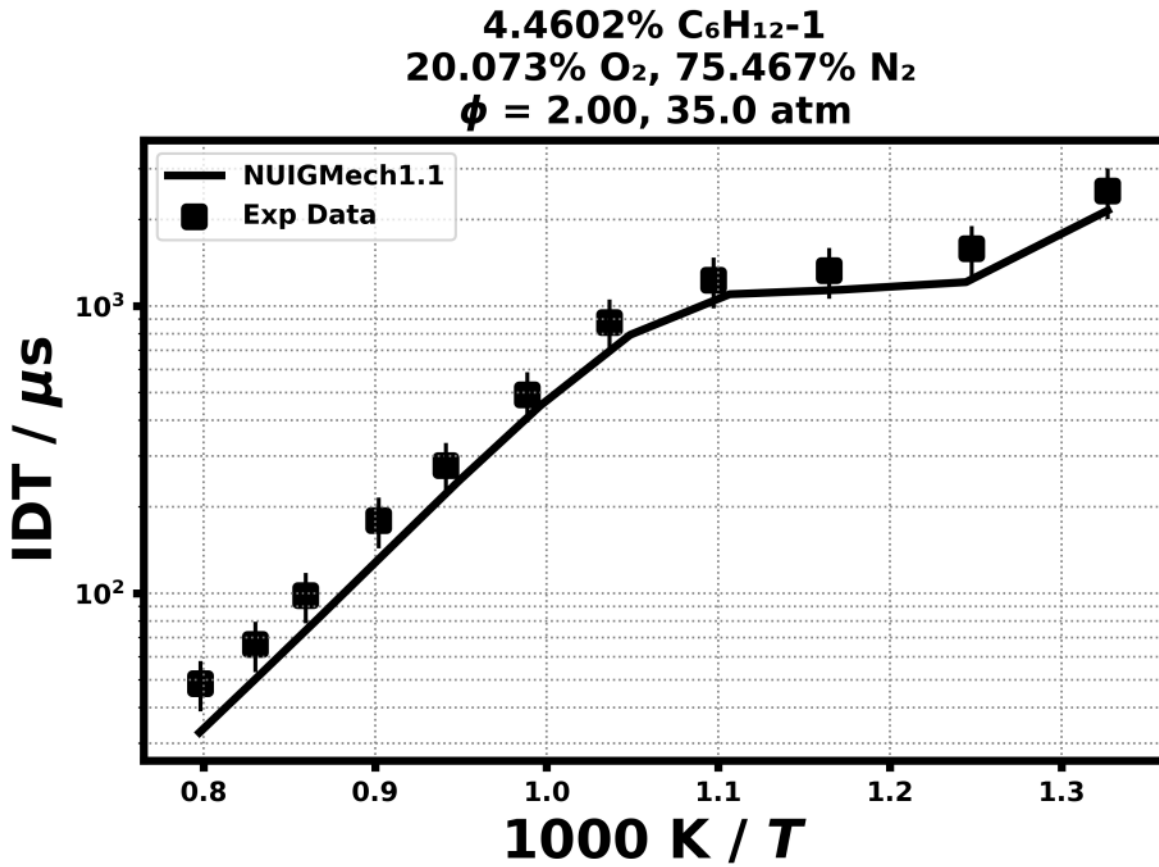


Figure 6: Dataset: 30_ATM_4.46_C6H12-1_PHI.2.0

1.1.7 Case: C6H12-1/ST/Marco/10_ATM.2.3_C6H12-1_PHI_1.0

Mehl, Marco, et al. "Oxidation and combustion of the n-hexene isomers: A wide range kinetic modeling study." *Combustion and Flame* 155.4 (2008): 756-772.

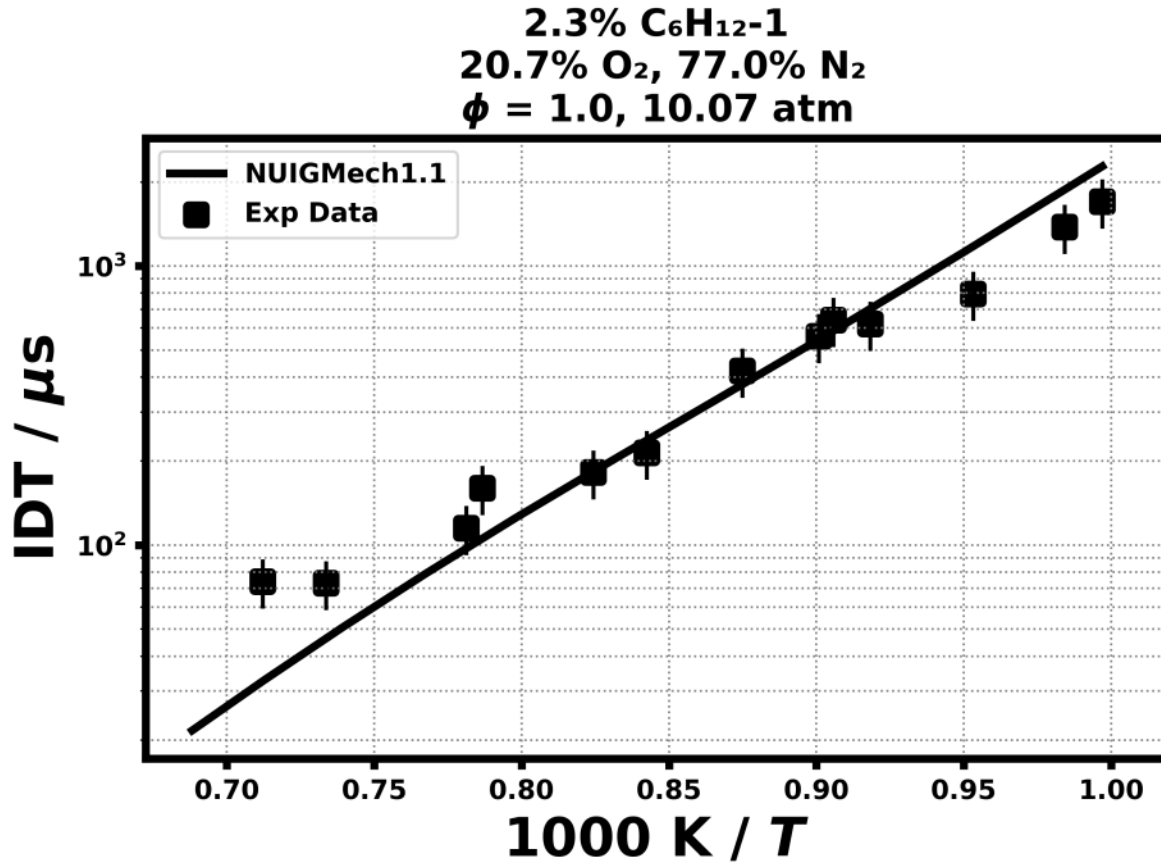


Figure 7: Dataset: 10_ATM.2.3_C6H12-1_PHI_1.0

Validation for C₆H₁₂-1

1.1.8 Case: C6H12-1/ST/Yahyaoui/10_ATM_0.1_C6H12-1_PHL0.5

Yahyaoui, Mohammed, et al. "Experimental and modeling study of 1-hexene oxidation behind reflected shock waves." *Proceedings of the Combustion Institute* 30.1 (2005): 1137-1145.

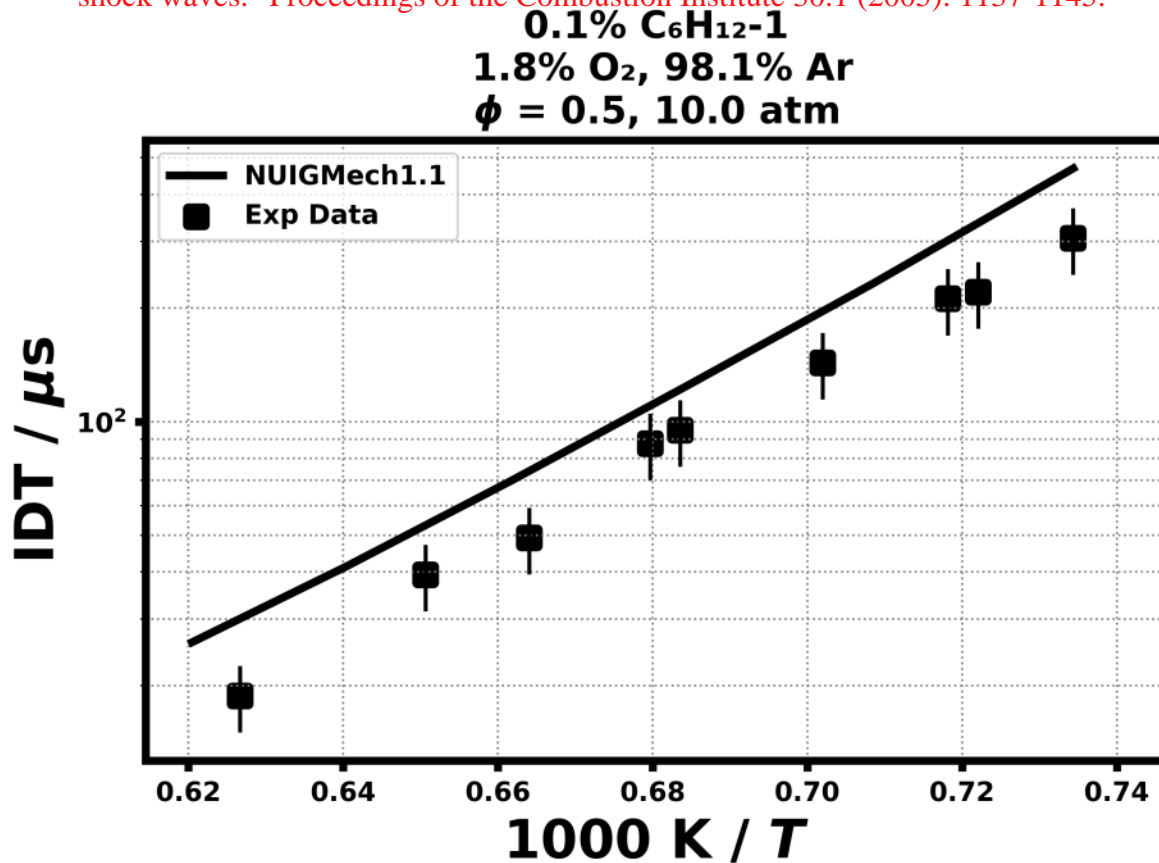


Figure 8: Dataset: 10_ATM_0.1_C6H12-1_PHL0.5

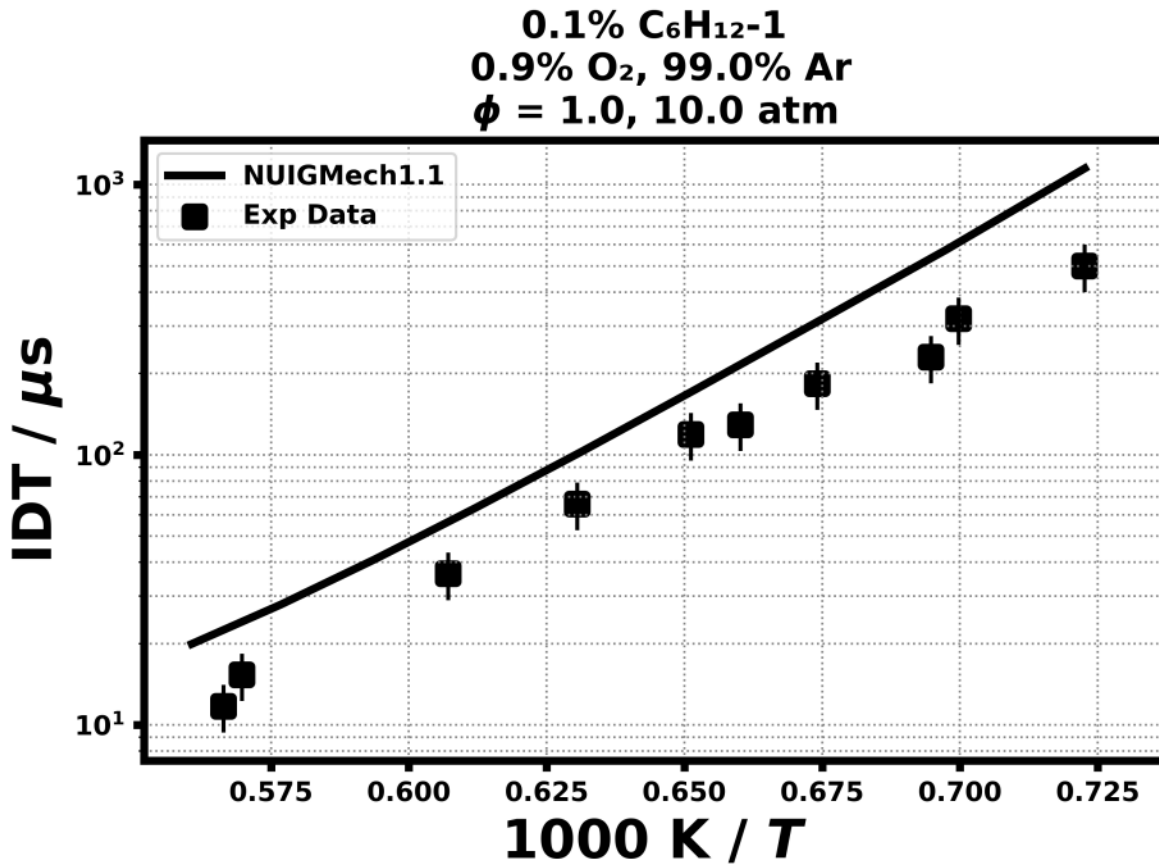


Figure 9: Dataset: 10_ATM_0.1_C6H12-1_PHL1.0

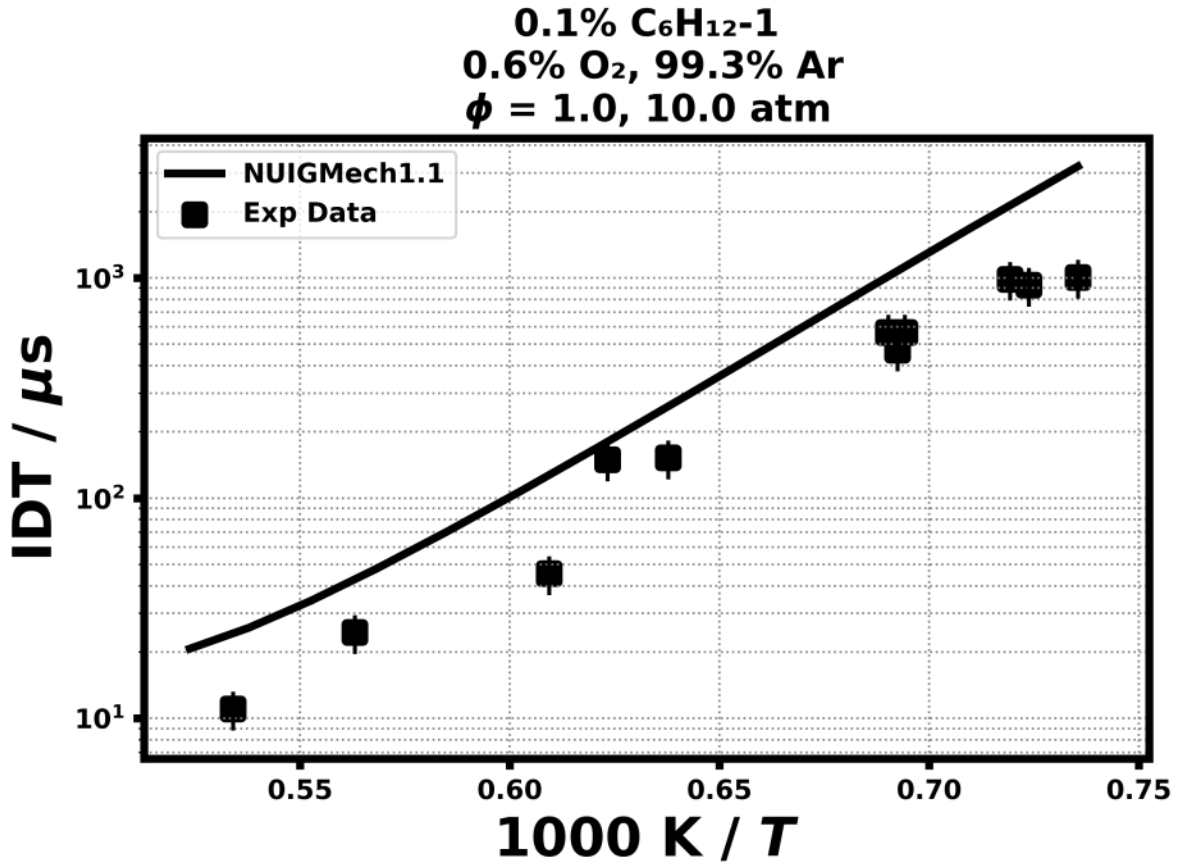


Figure 10: Dataset: 10_ATM.0.1_C6H12-1_PHL1.5

1.1.11 Case: C6H12-1/ST/Yahyaoui/2_ATM_0.1_C6H12-1_PHL0.5

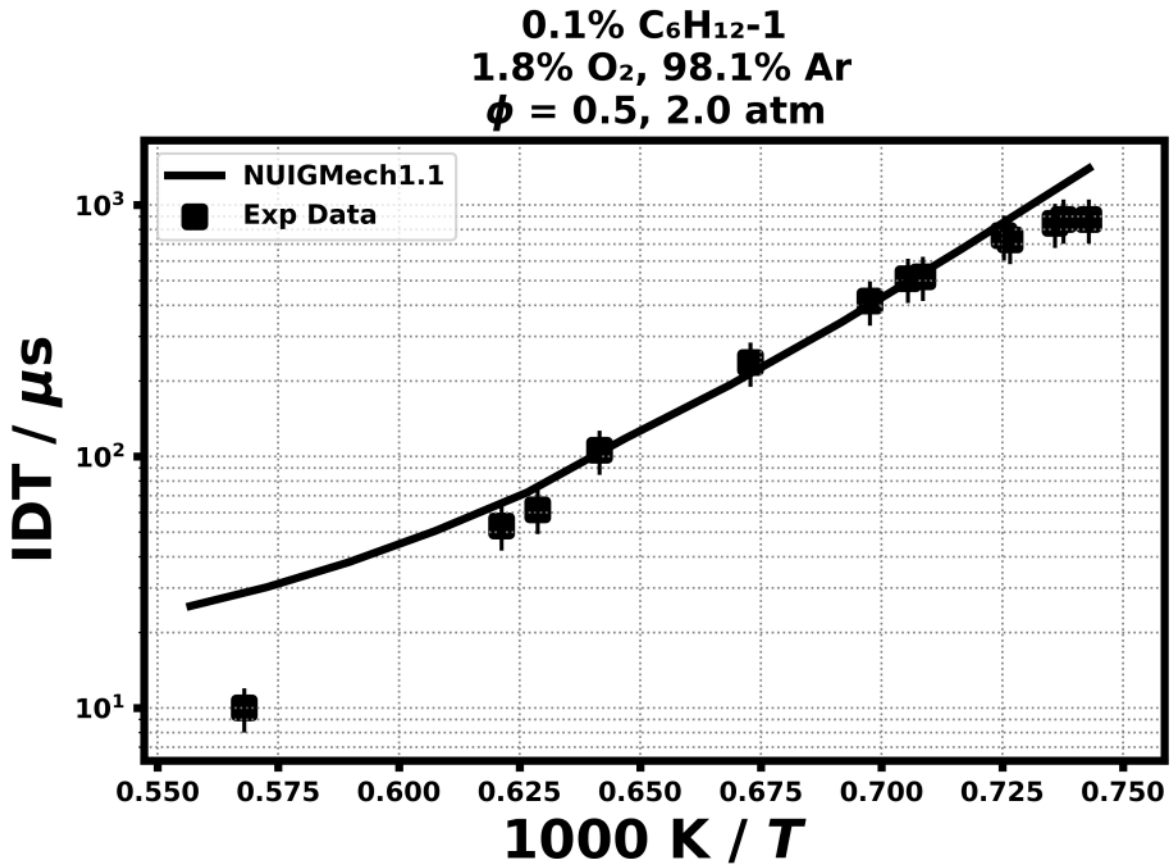


Figure 11: Dataset: 2_ATM_0.1_C6H12-1_PHL0.5

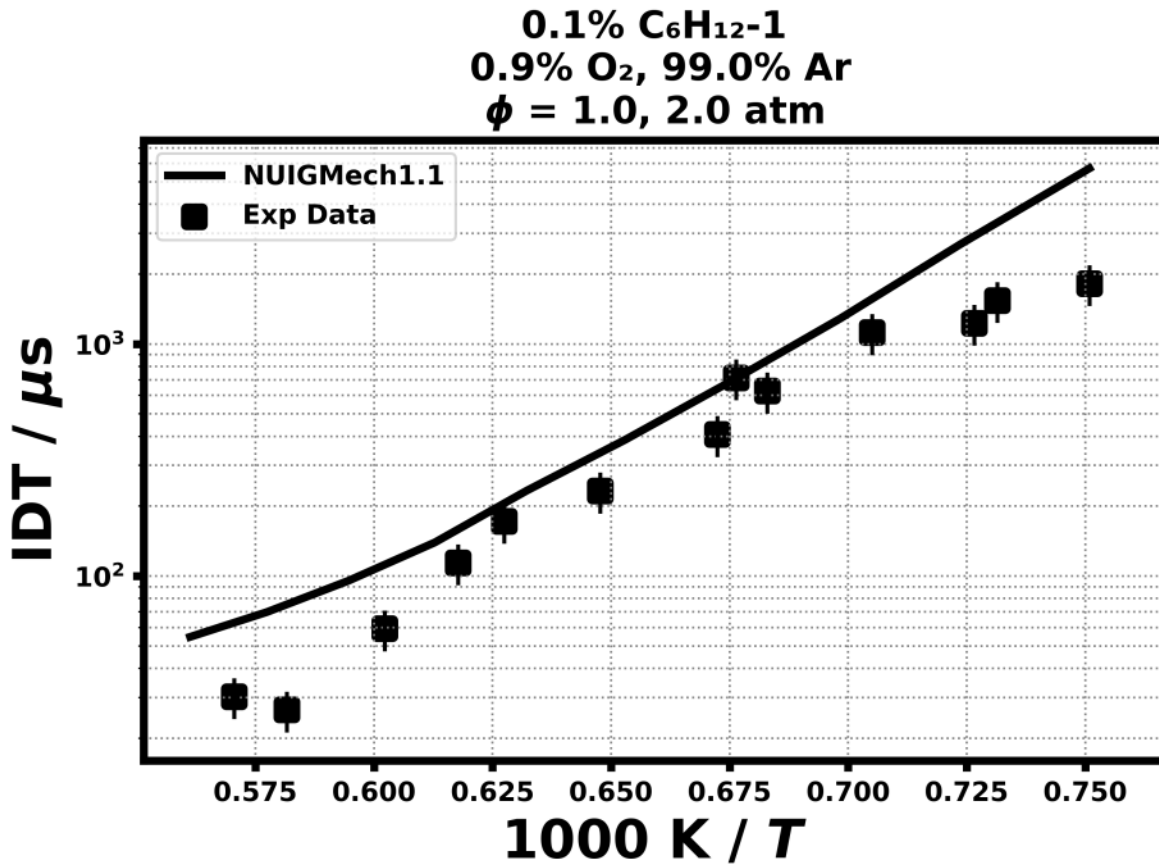


Figure 12: Dataset: 2_ATM_0.1_C6H12-1_PHI1.0

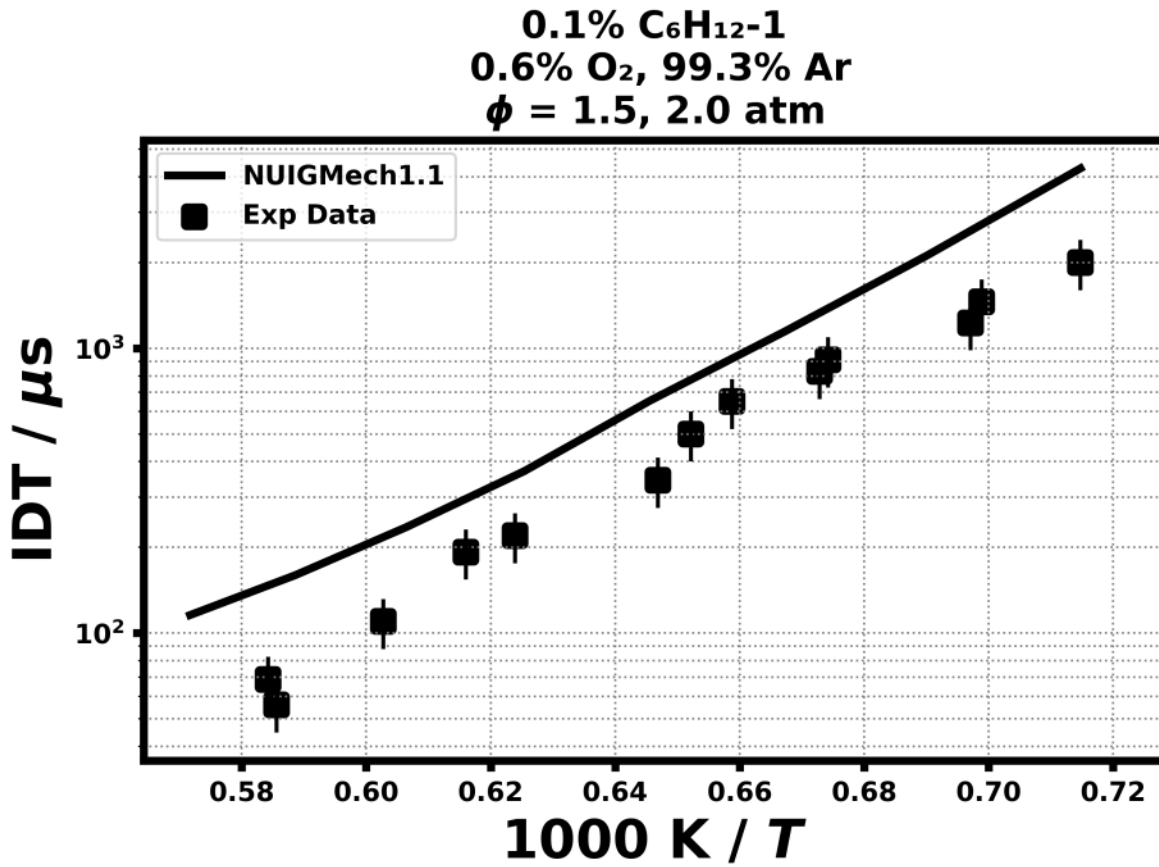


Figure 13: Dataset: 2_ATM_0.1_C6H12-1_PHI1.5

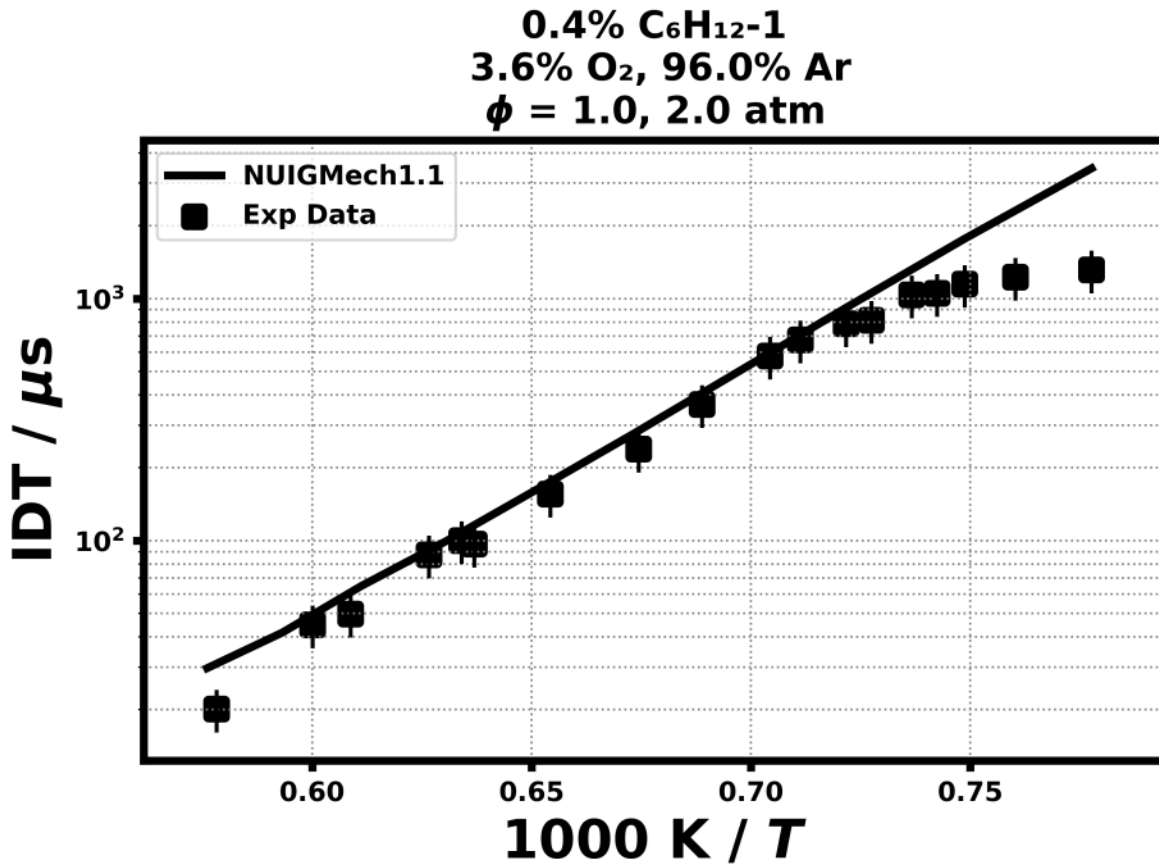


Figure 14: Dataset: 2_ATM_0.4_C6H12-1_PHI1.0

RCM Ignition delay time

1.154% C₆H₁₂-1
20.766% O₂, 78.08% N₂
 $\phi = 0.5, 30.0 \text{ atm}$

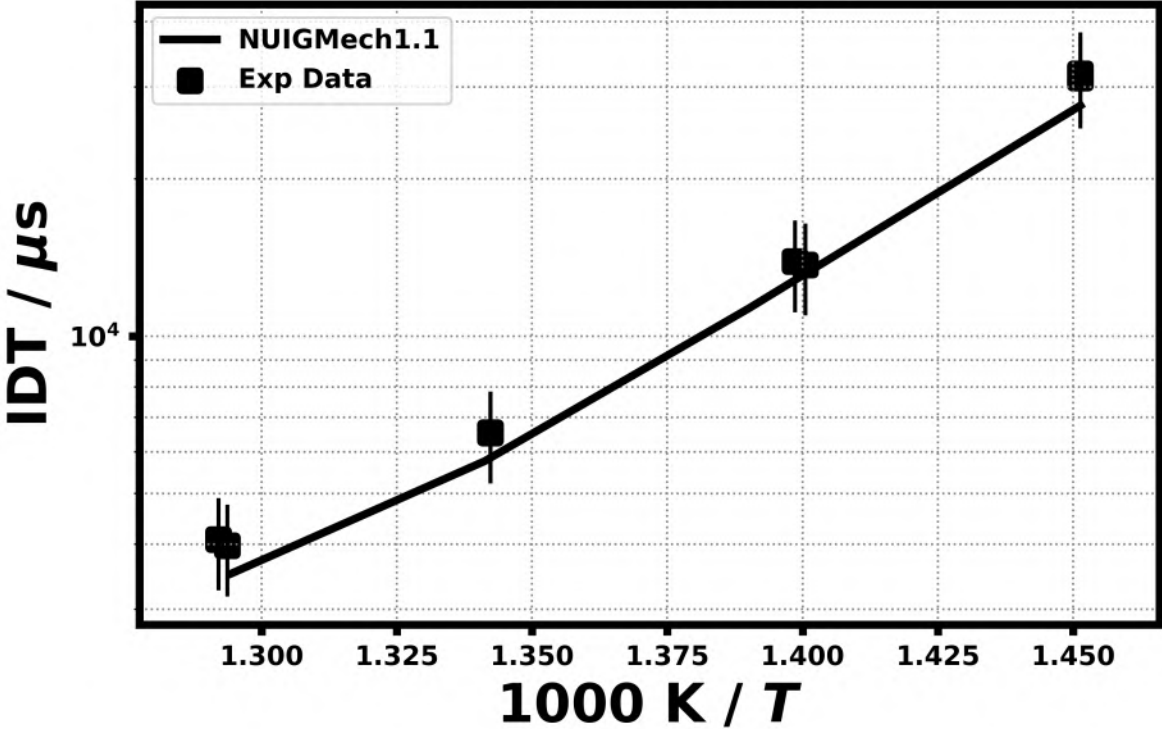


Figure 17: Dataset: F050_30ATM_100_N2

1.2.4 Case: C6H12-1/RCM/DONG/F100_15ATM_100_N2

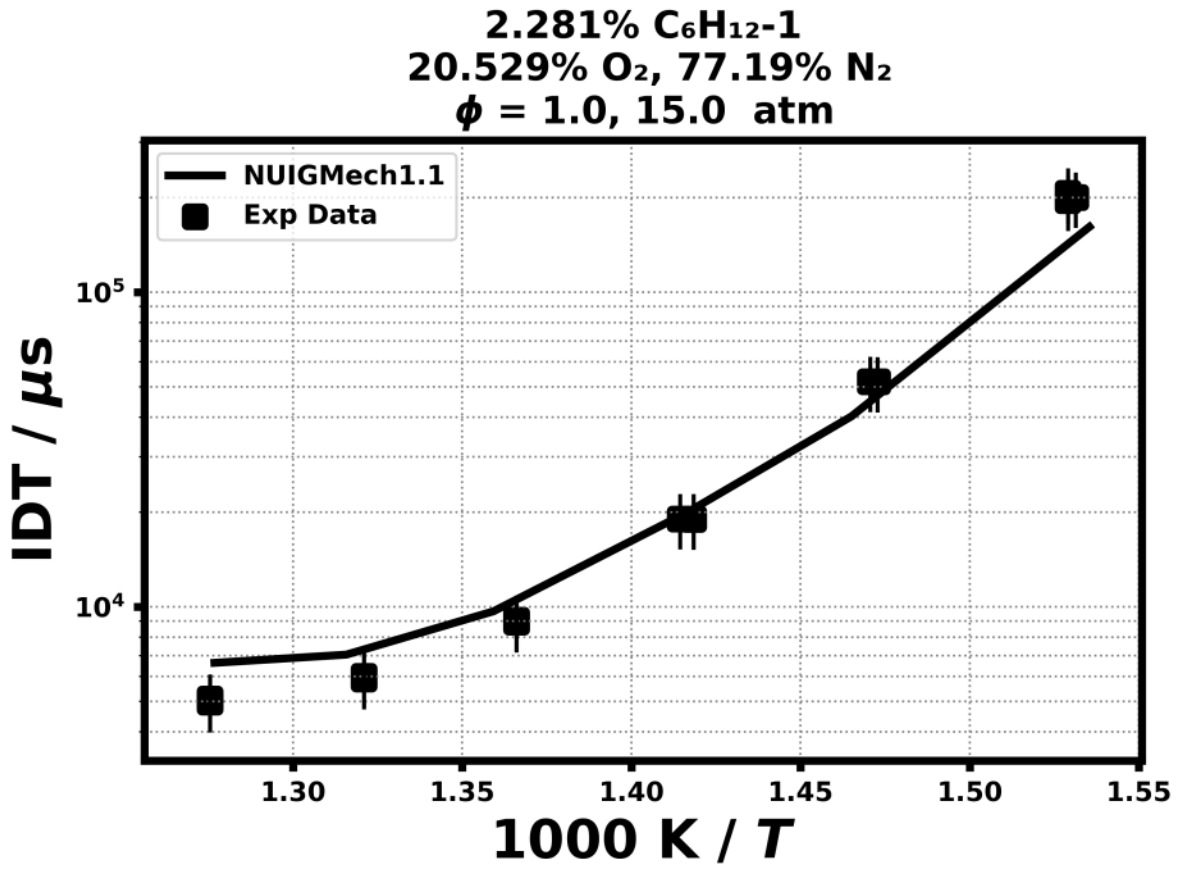


Figure 18: Dataset: F100_15ATM_100_N2

1.2.5 Case: C6H12-1/RCM/DONG/F100_30ATM_100_N2

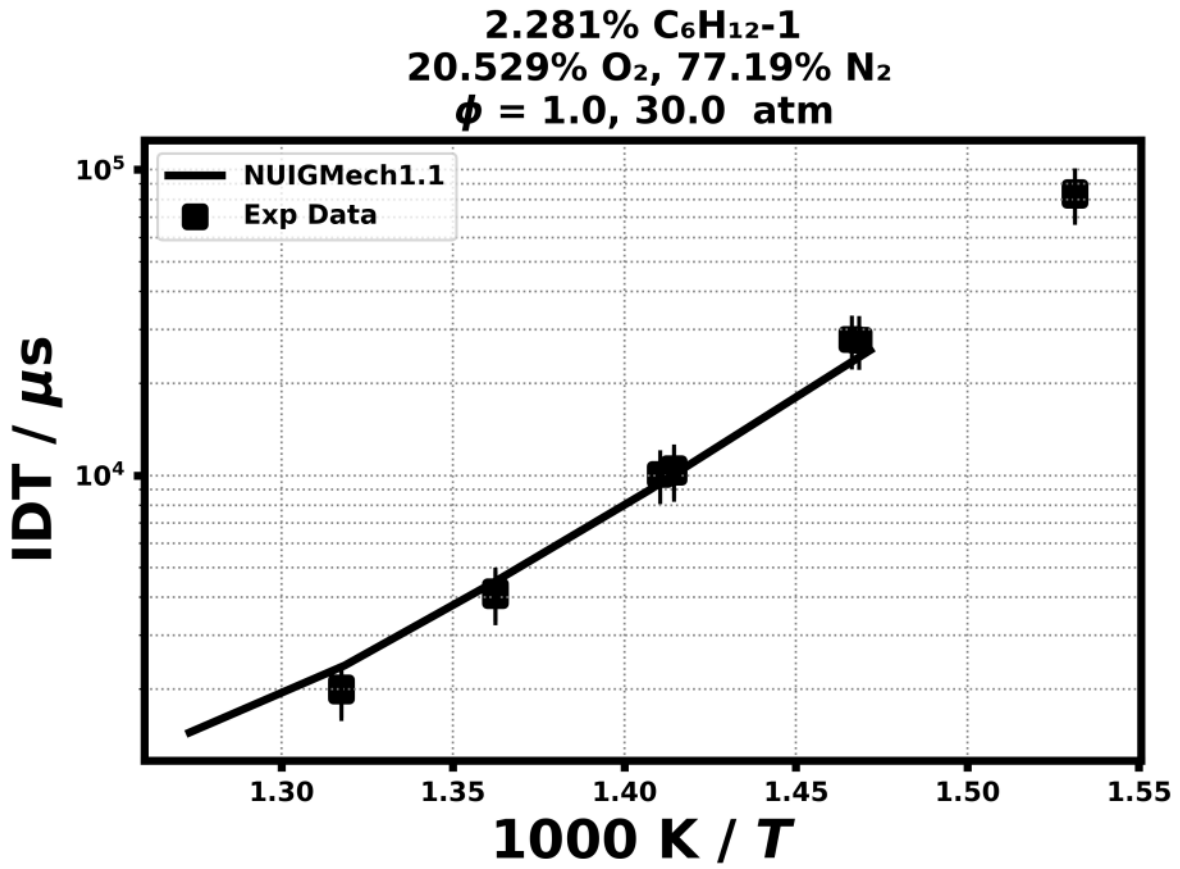


Figure 19: Dataset: F100_30ATM_100_N2

1.2.8 Case: C6H12-1/RCM/DONG/F200_30ATM_100_N2

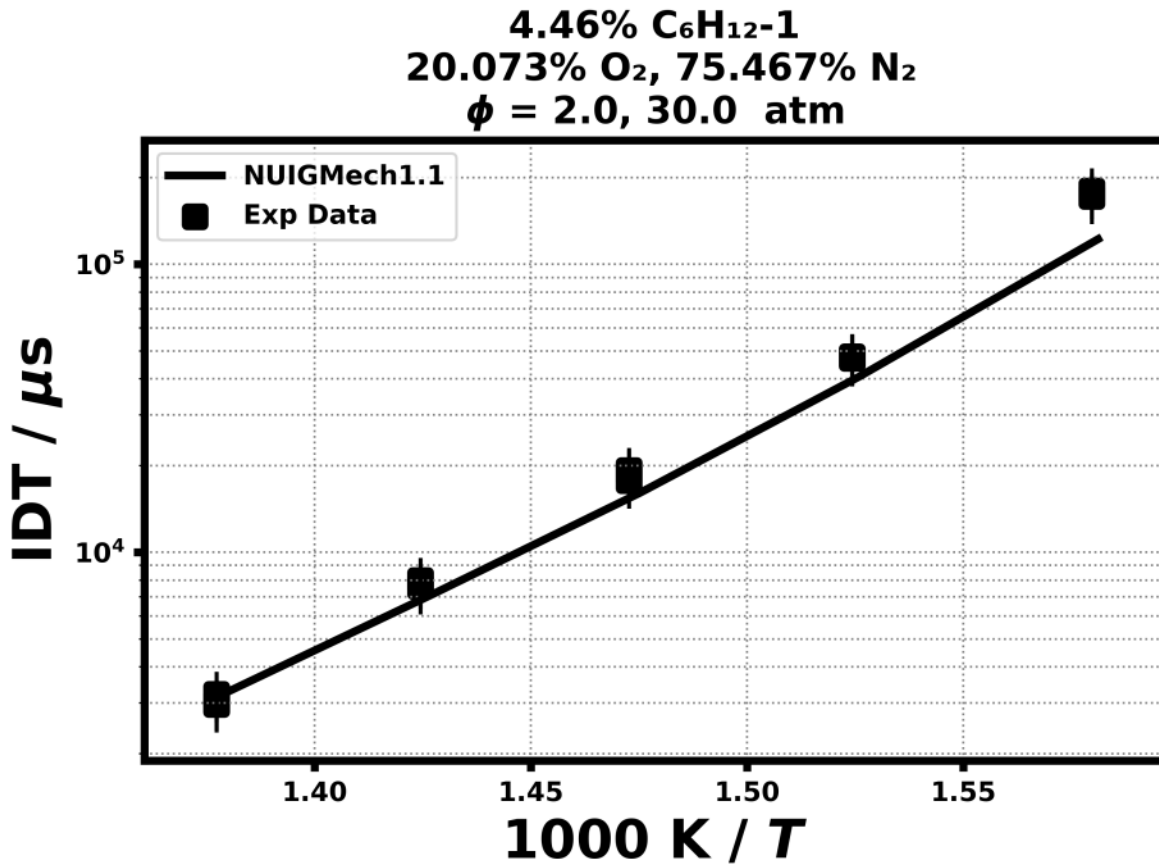


Figure 22: Dataset: F200_30ATM_100_N2

Jet-Stirred Reactor

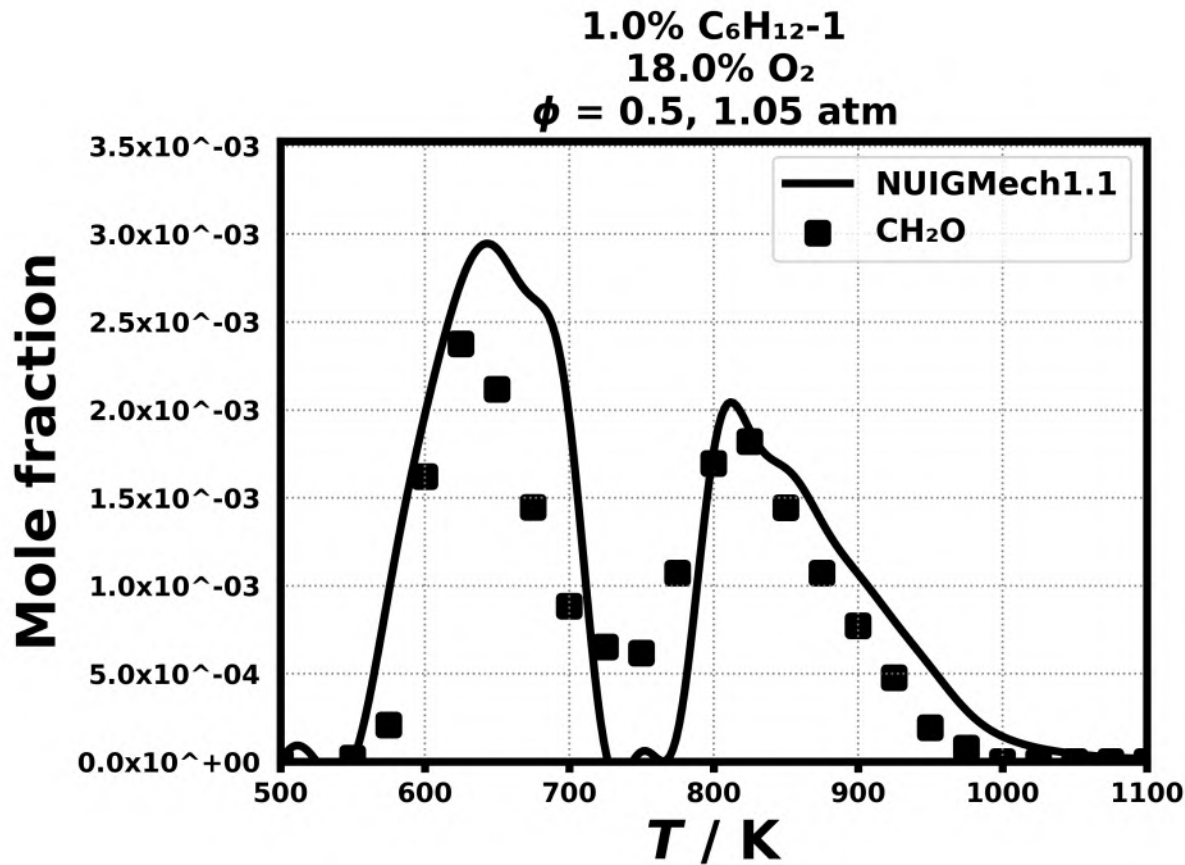


Figure 23: Dataset: 1.05_ATM_PHI.0.5

1.3.2 Case: C6H12-1/JSR/Meng/Meng_CRDS/1.05_ATM_PHI.0.5

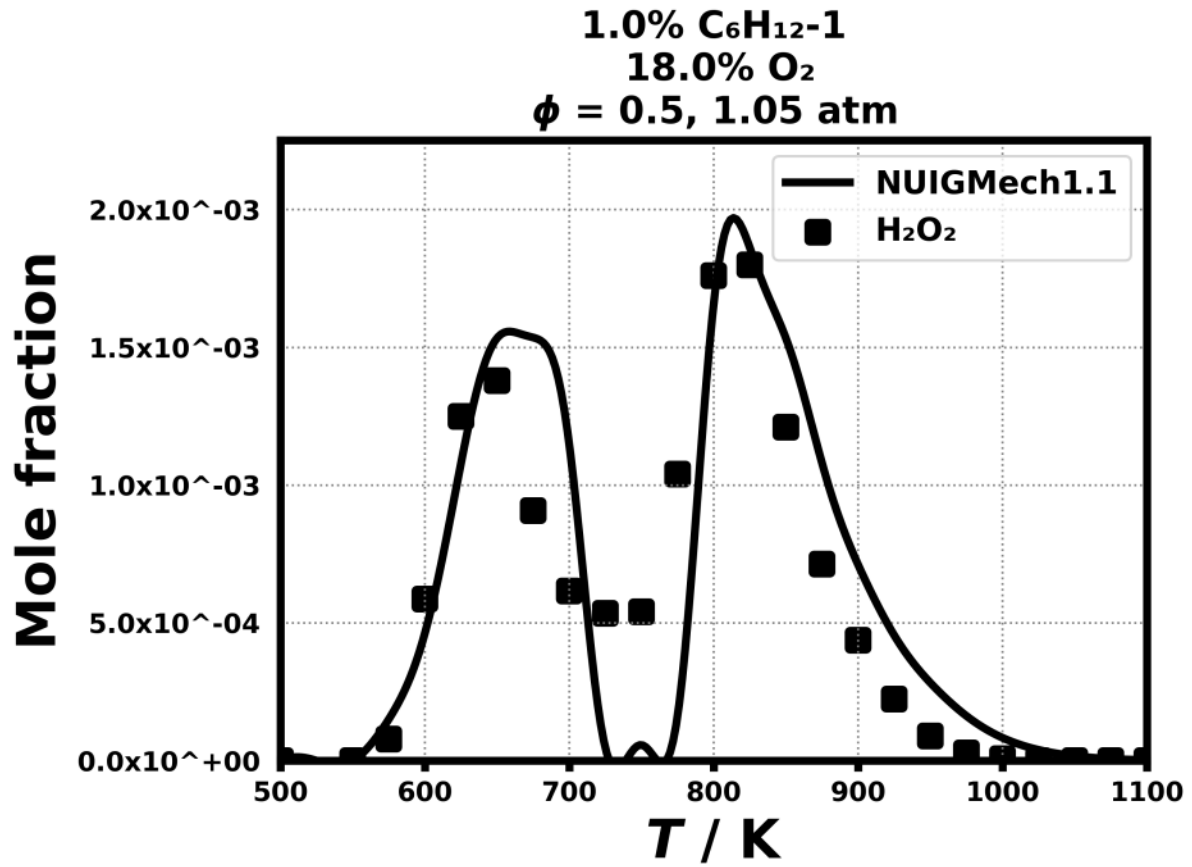


Figure 24: Dataset: 1.05_ATM_PHI.0.5

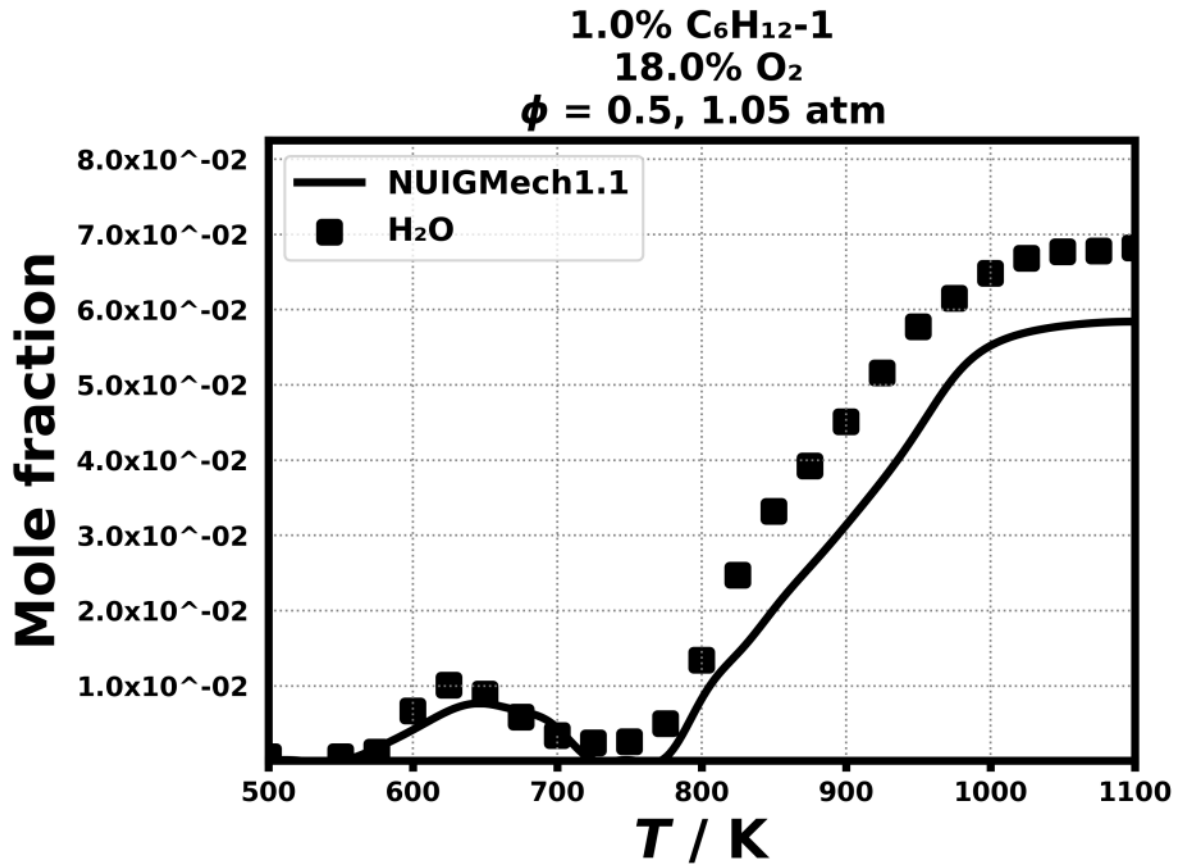


Figure 25: Dataset: 1.05_ATM_PHI.0.5

1.3.4 Case: C6H12-1/JSR/Meng/Meng_CRDS/1.05_ATM_PHI.0.5

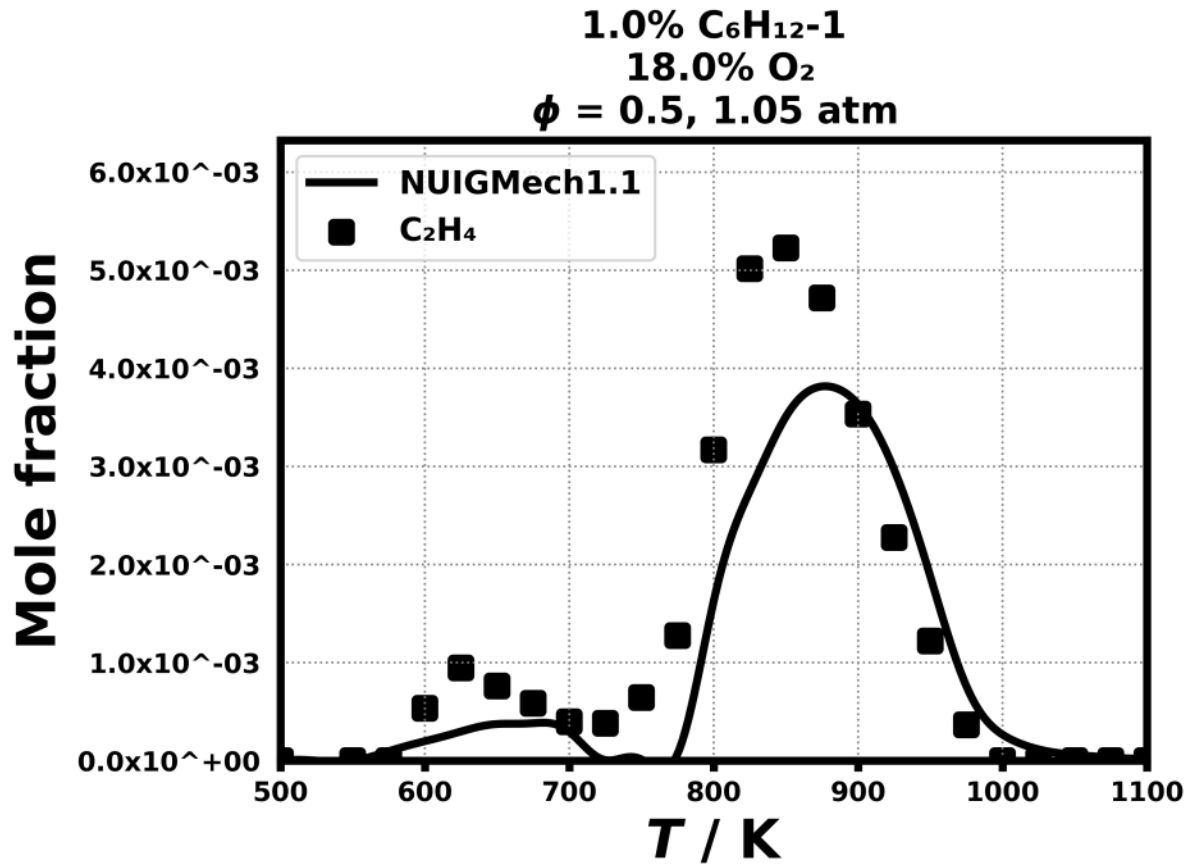


Figure 26: Dataset: 1.05_ATM_PHI.0.5

1.3.5 Case: C6H12-1/JSR/Meng/Meng_CRDS/1.05_ATM_PHI.0.5

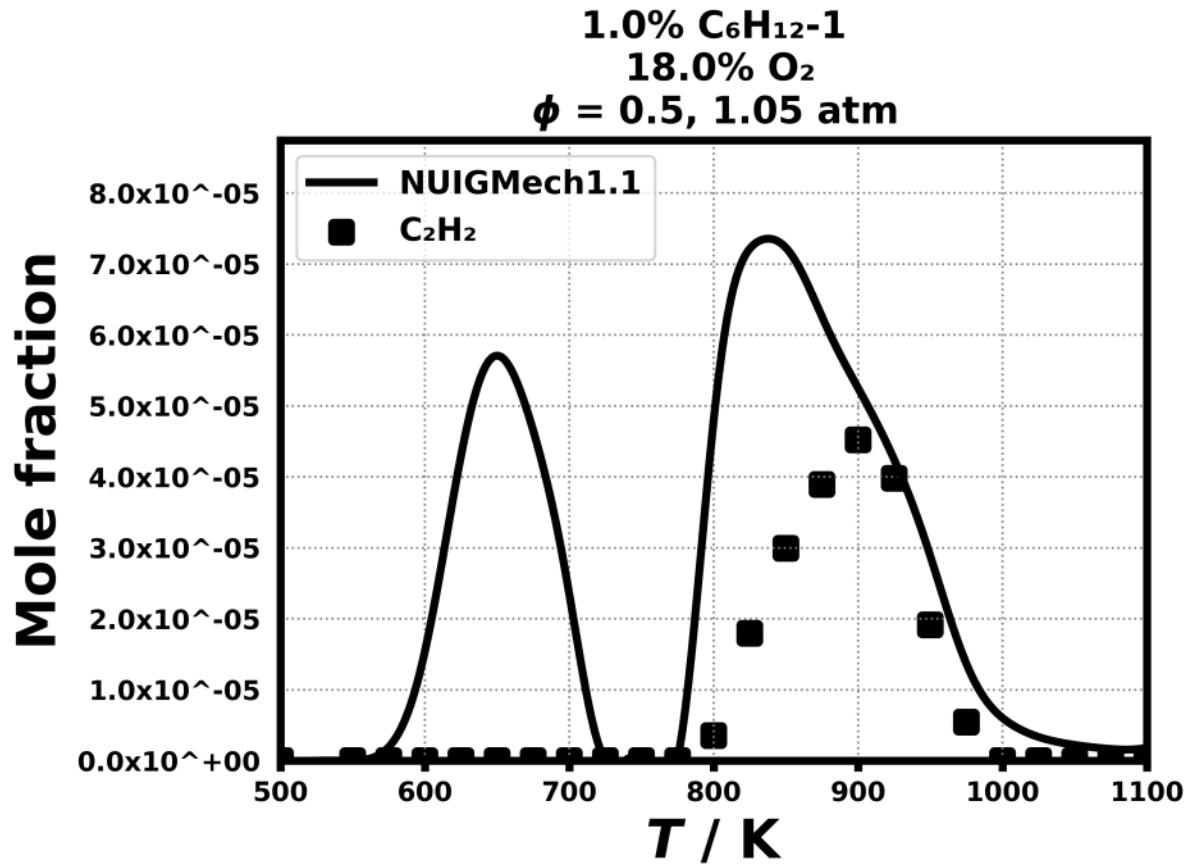


Figure 27: Dataset: 1.05_ATM_PHI.0.5

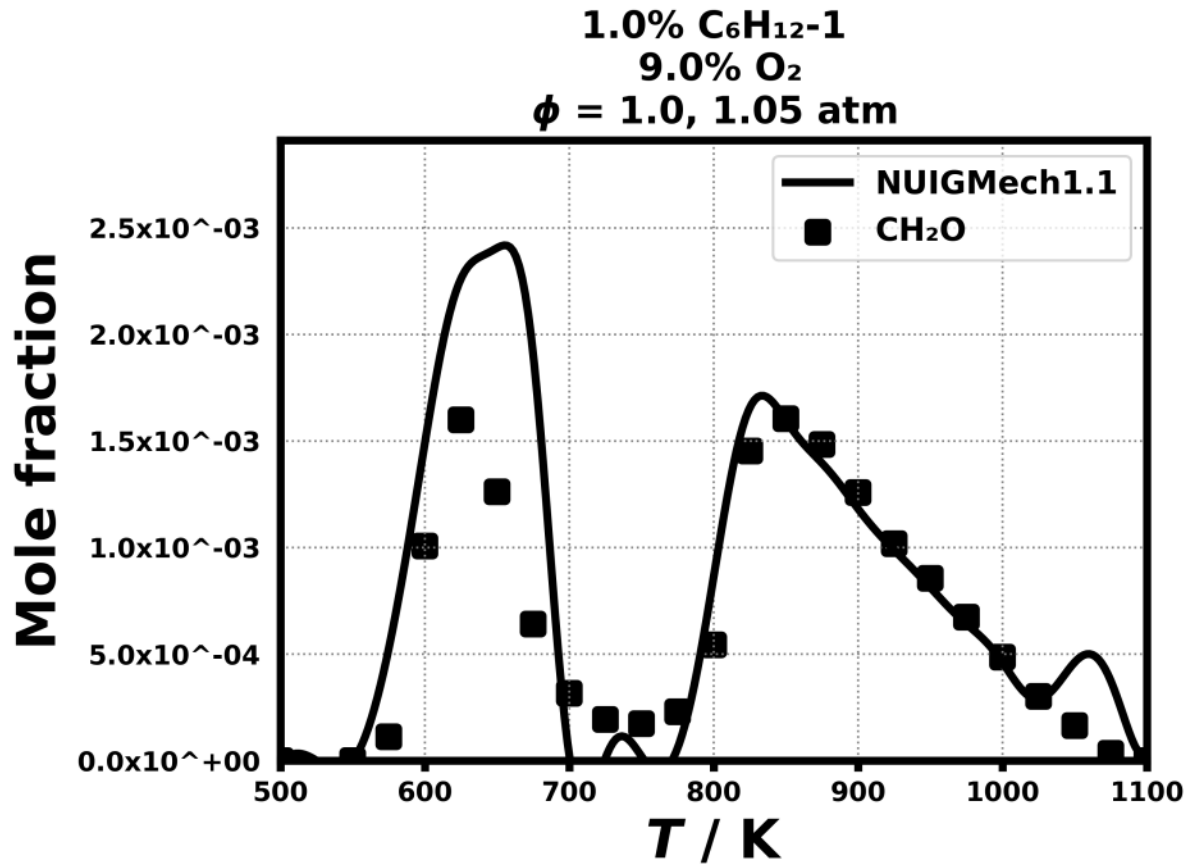


Figure 28: Dataset: 1.05_ATM_PHI.1.0

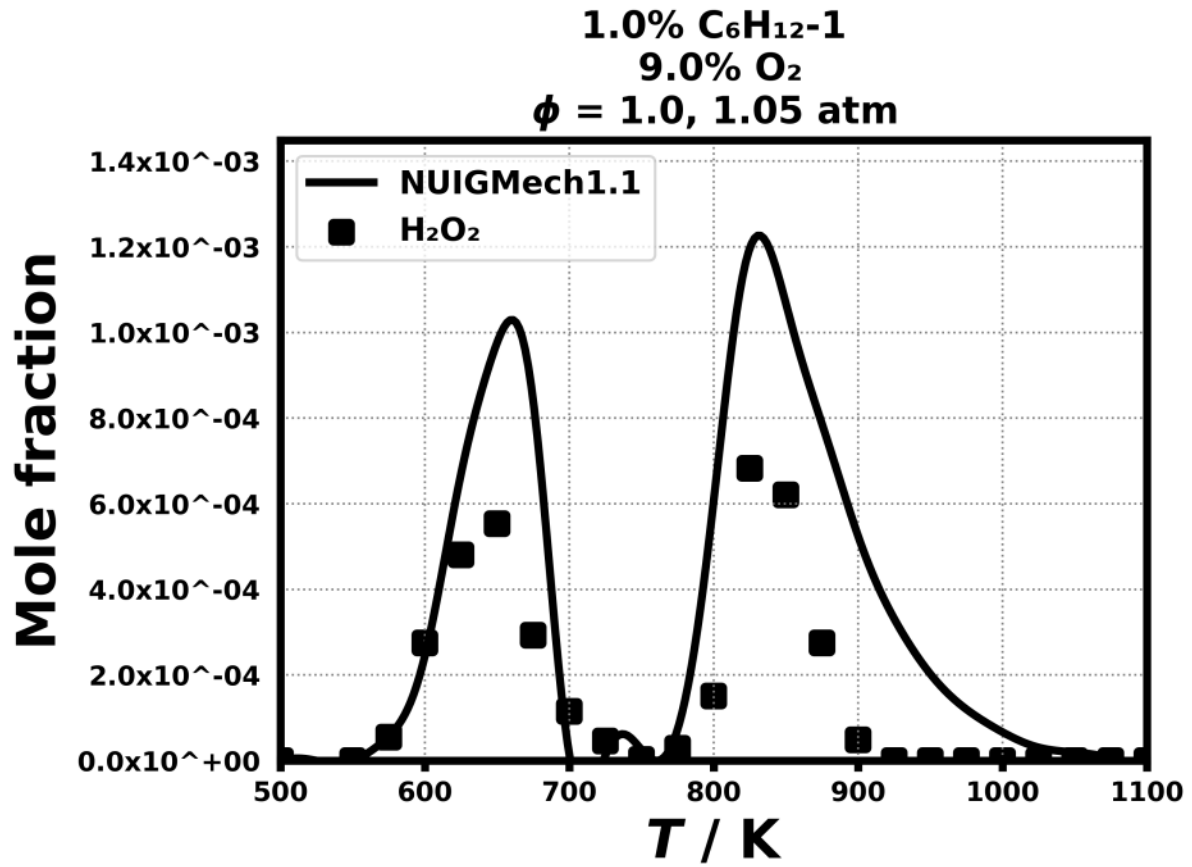


Figure 29: Dataset: 1.05_ATM_PHI.1.0

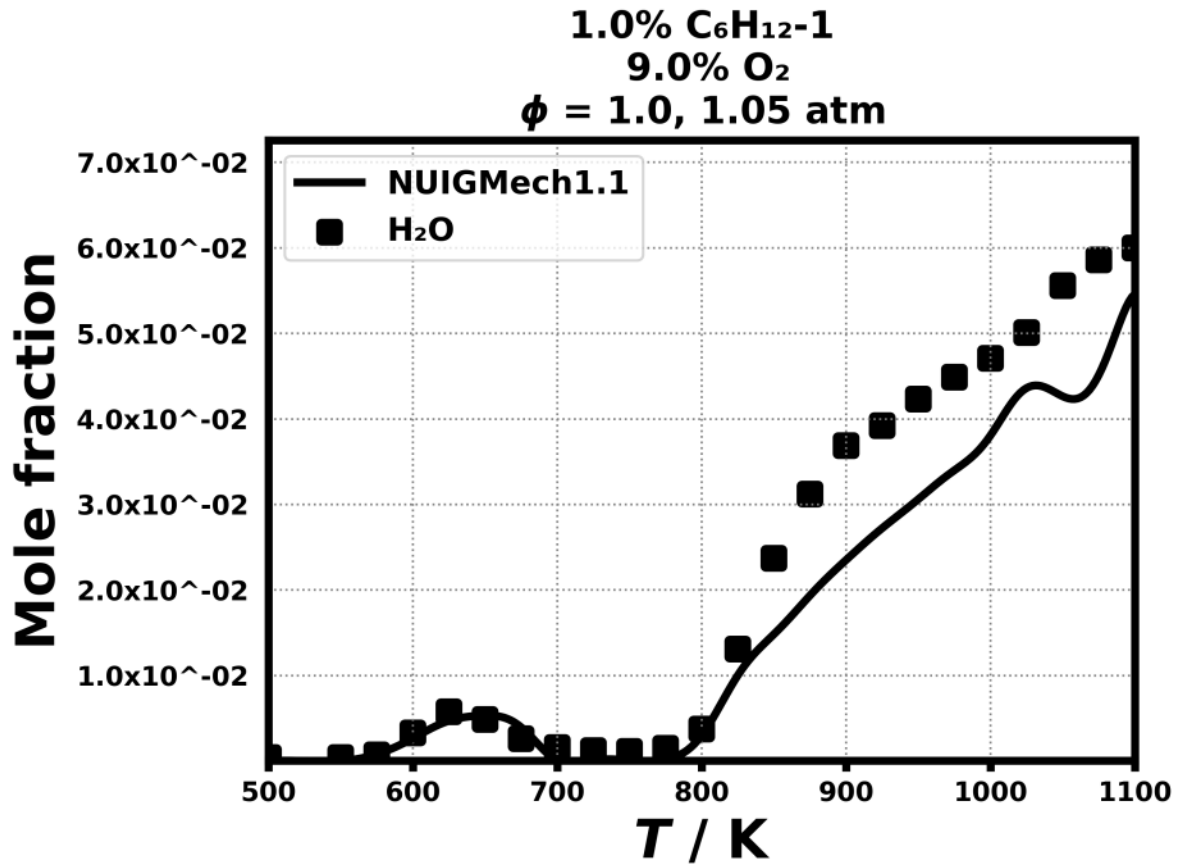


Figure 30: Dataset: 1.05_ATM_PHI.1.0

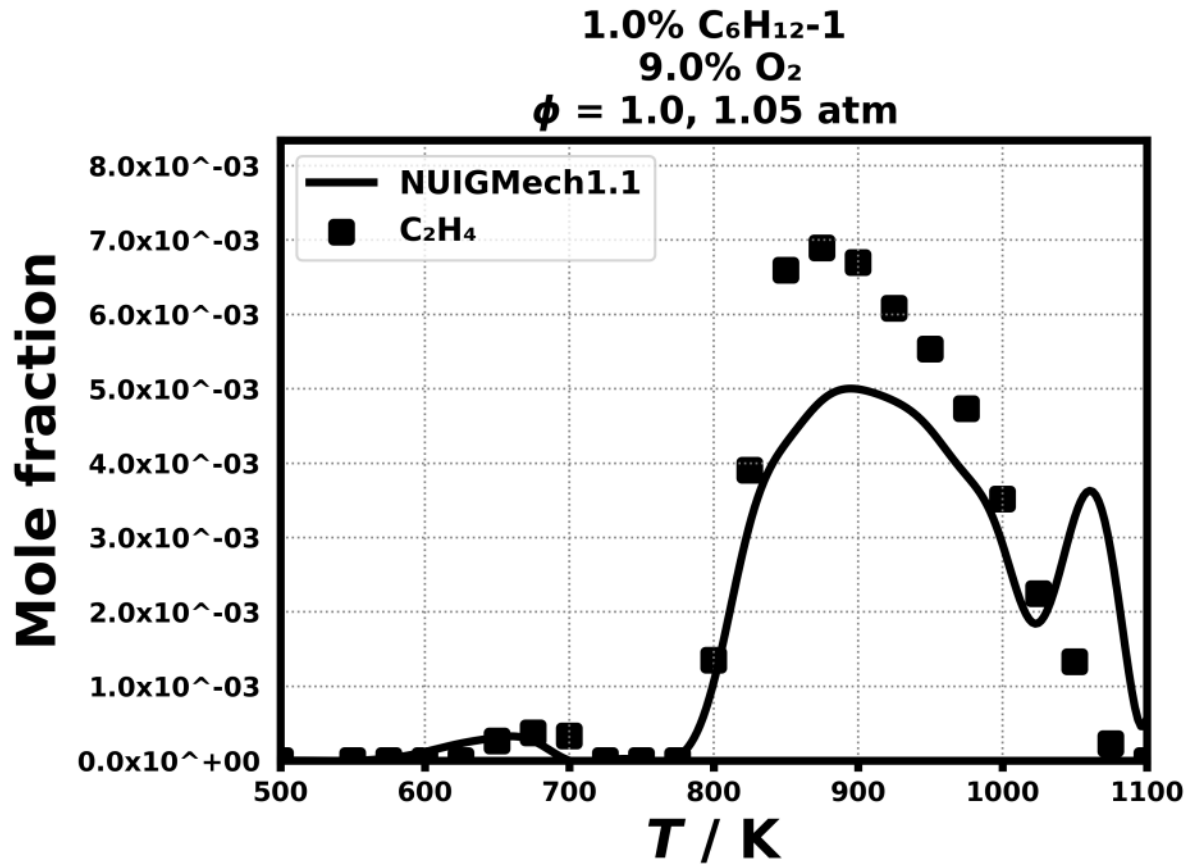


Figure 31: Dataset: 1.05_ATM_PHI.1.0

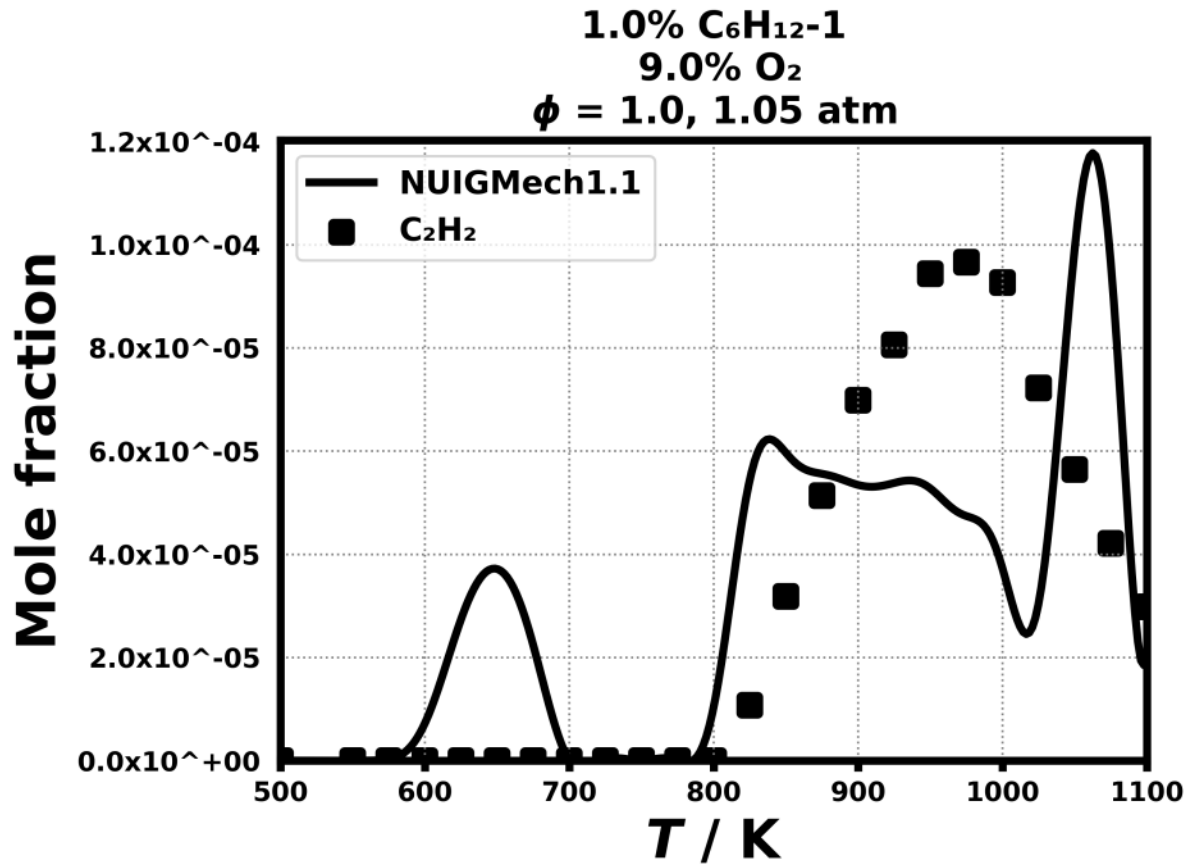


Figure 32: Dataset: 1.05_ATM_PHI.1.0

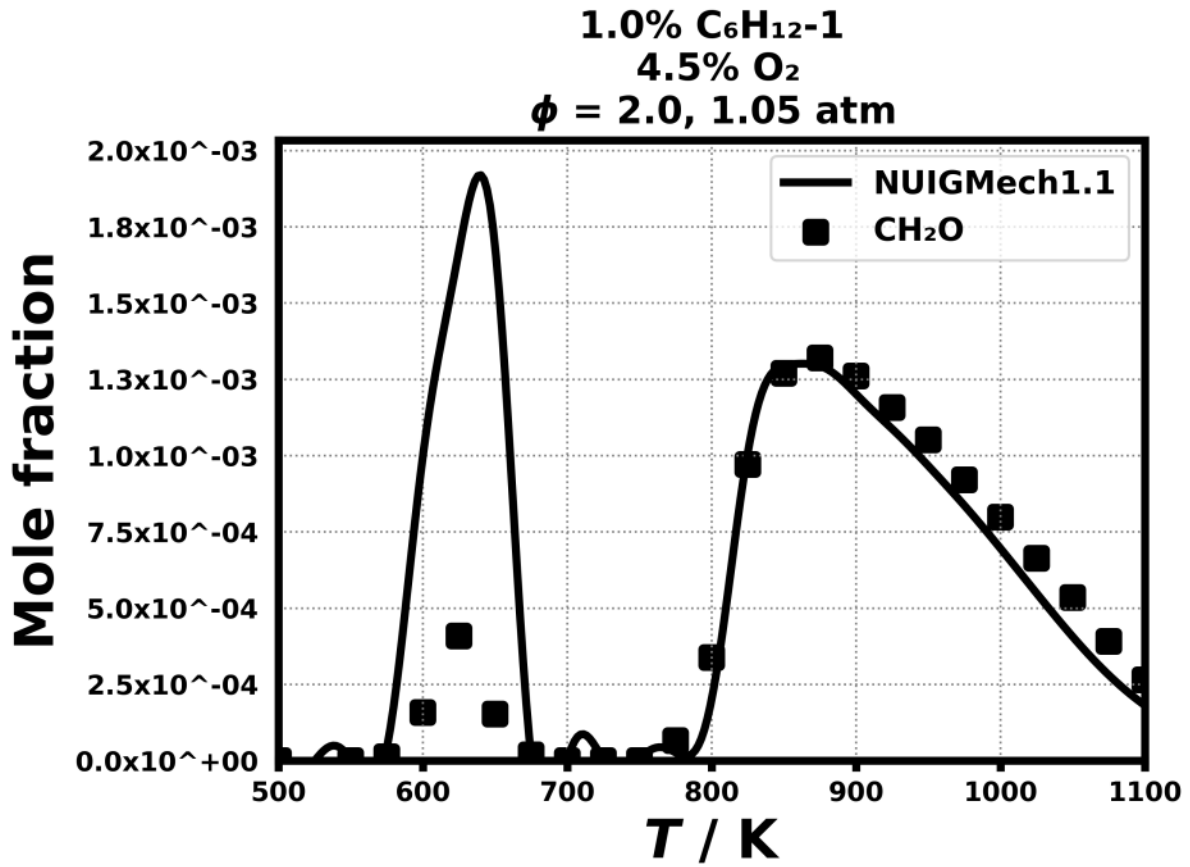


Figure 33: Dataset: 1.05_ATM_PHI.2.0

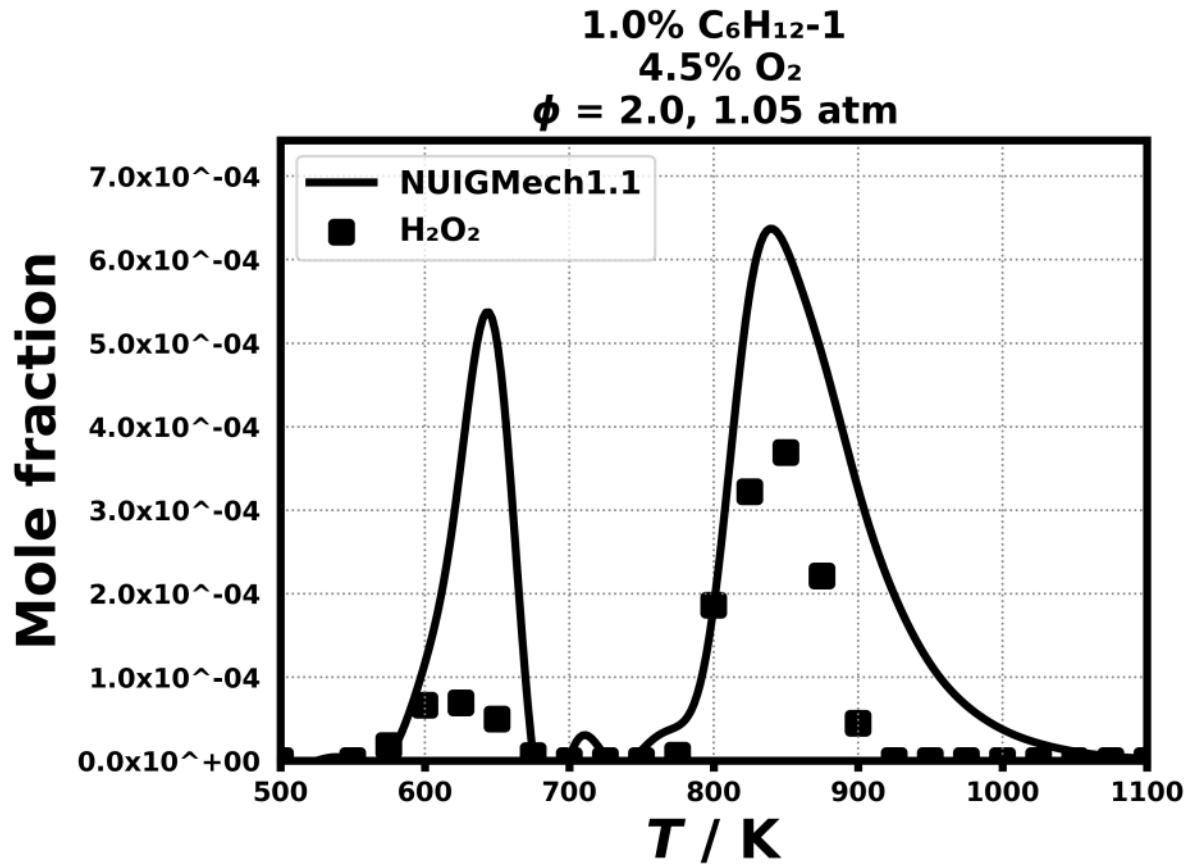


Figure 34: Dataset: 1.05_ATM_PHI.2.0

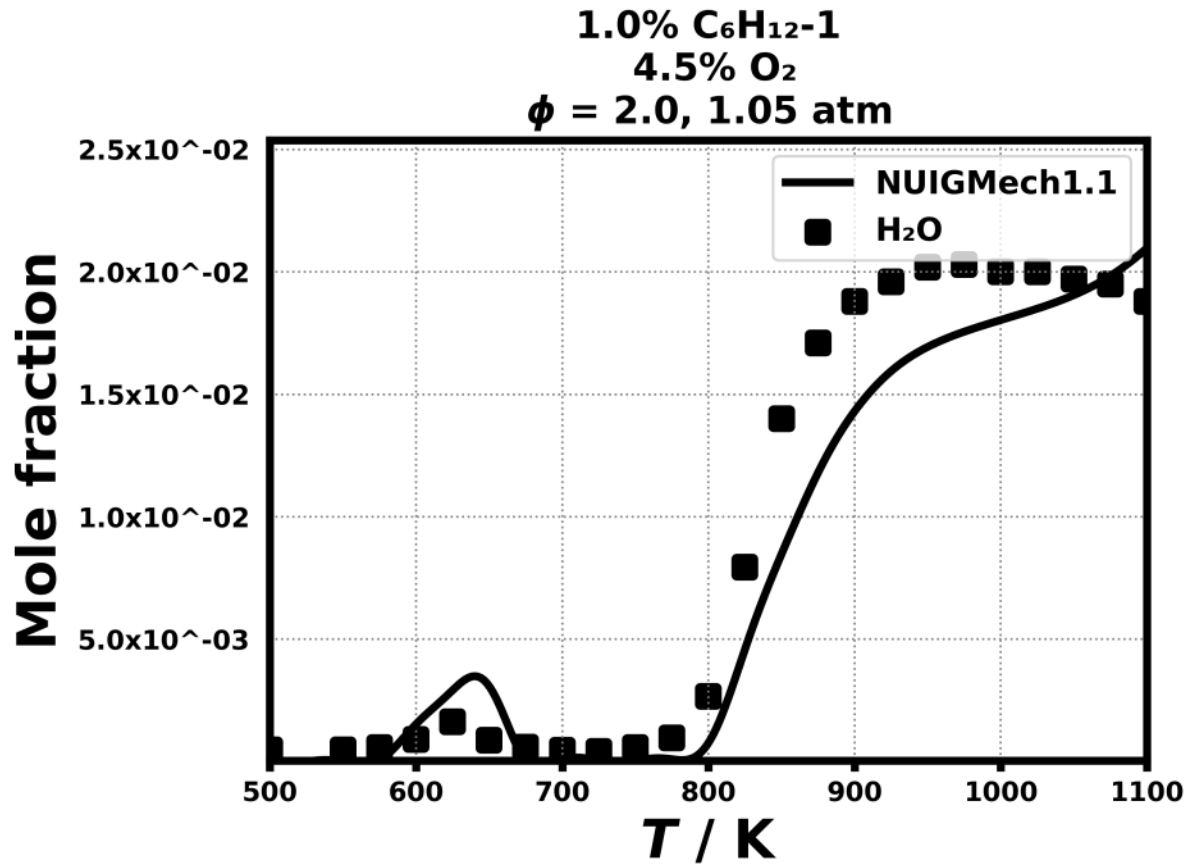


Figure 35: Dataset: 1.05_ATM_PHI.2.0

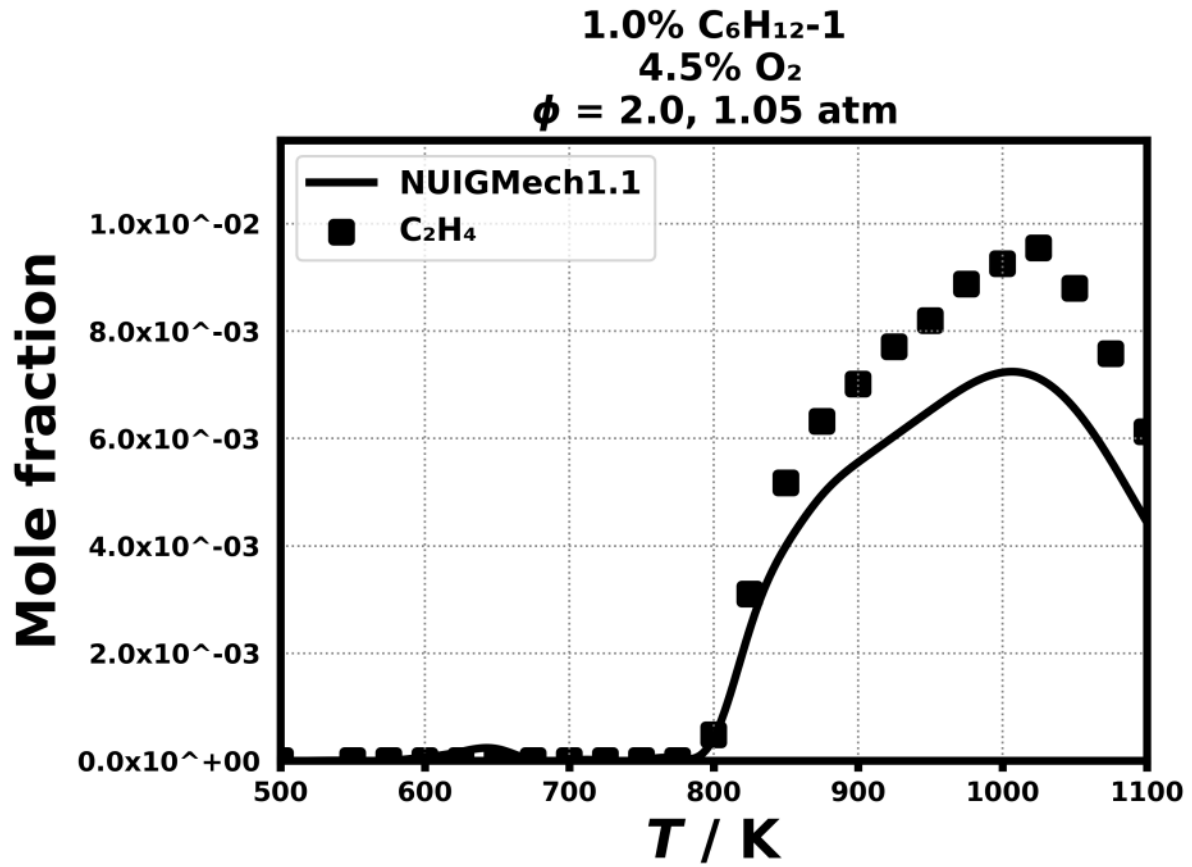


Figure 36: Dataset: 1.05_ATM_PHI.2.0

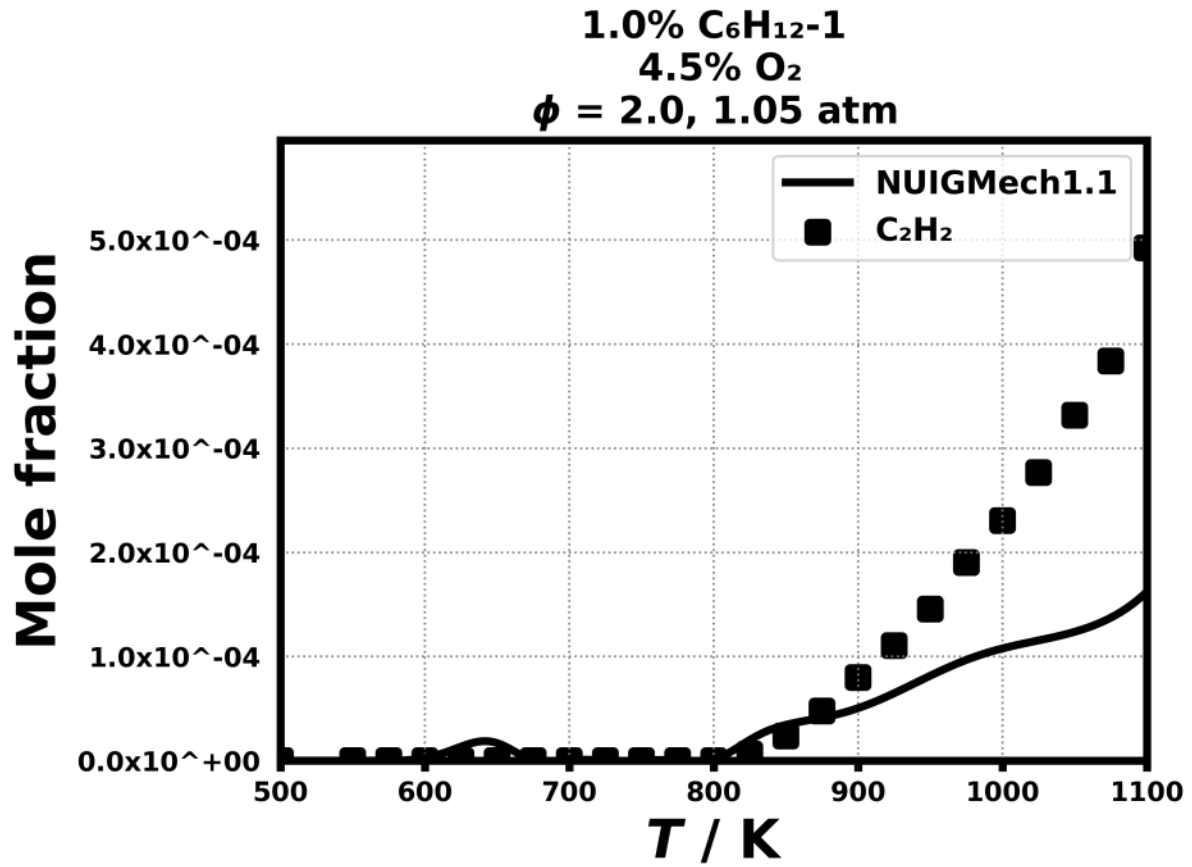


Figure 37: Dataset: 1.05_ATM_PHI.2.0

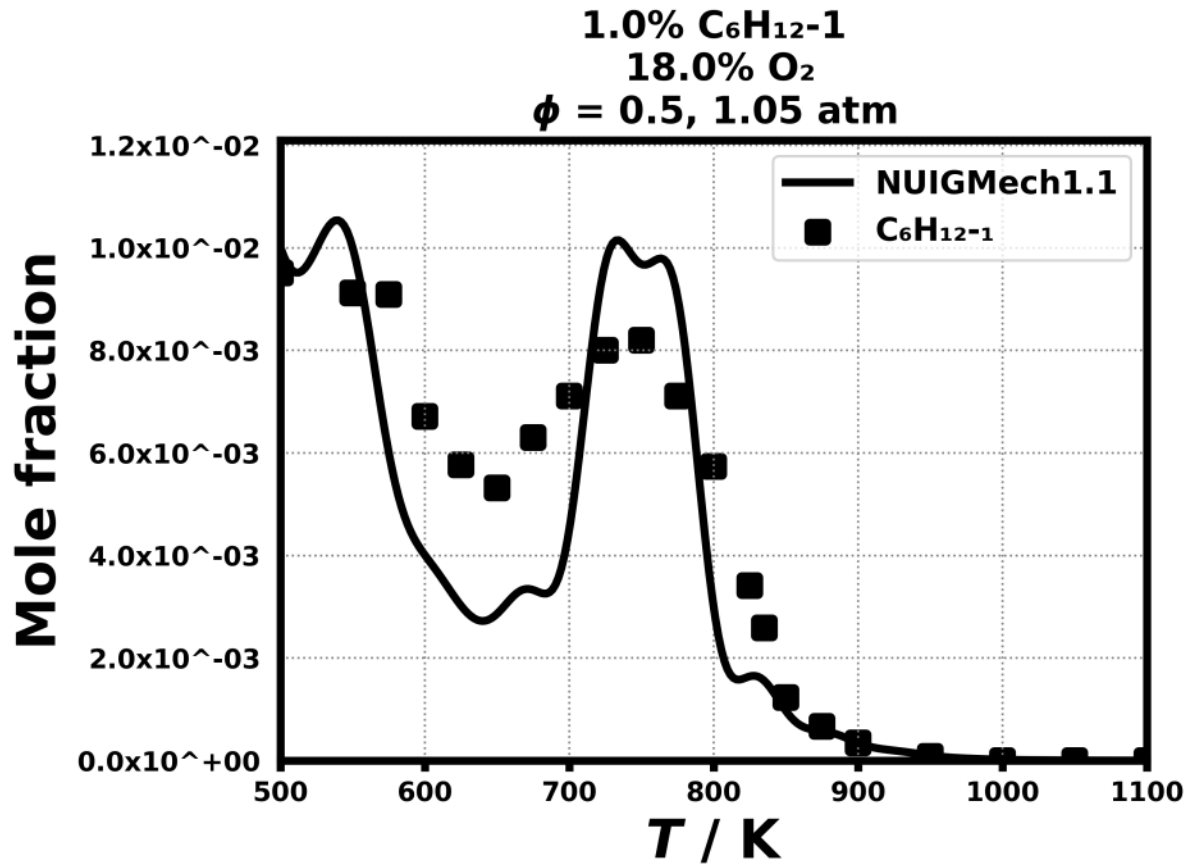


Figure 38: Dataset: 1.05_ATM_PHI_0.5

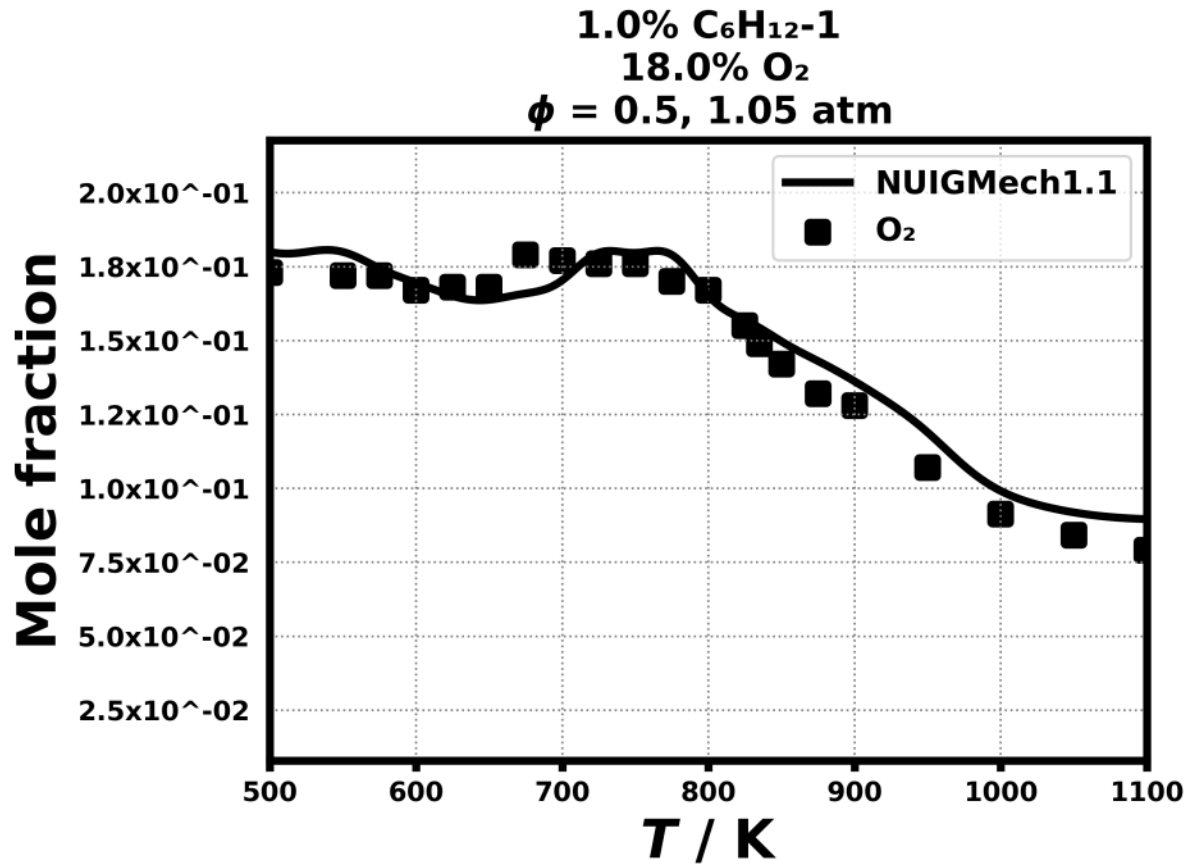


Figure 39: Dataset: 1.05_ATM_PHI_0.5

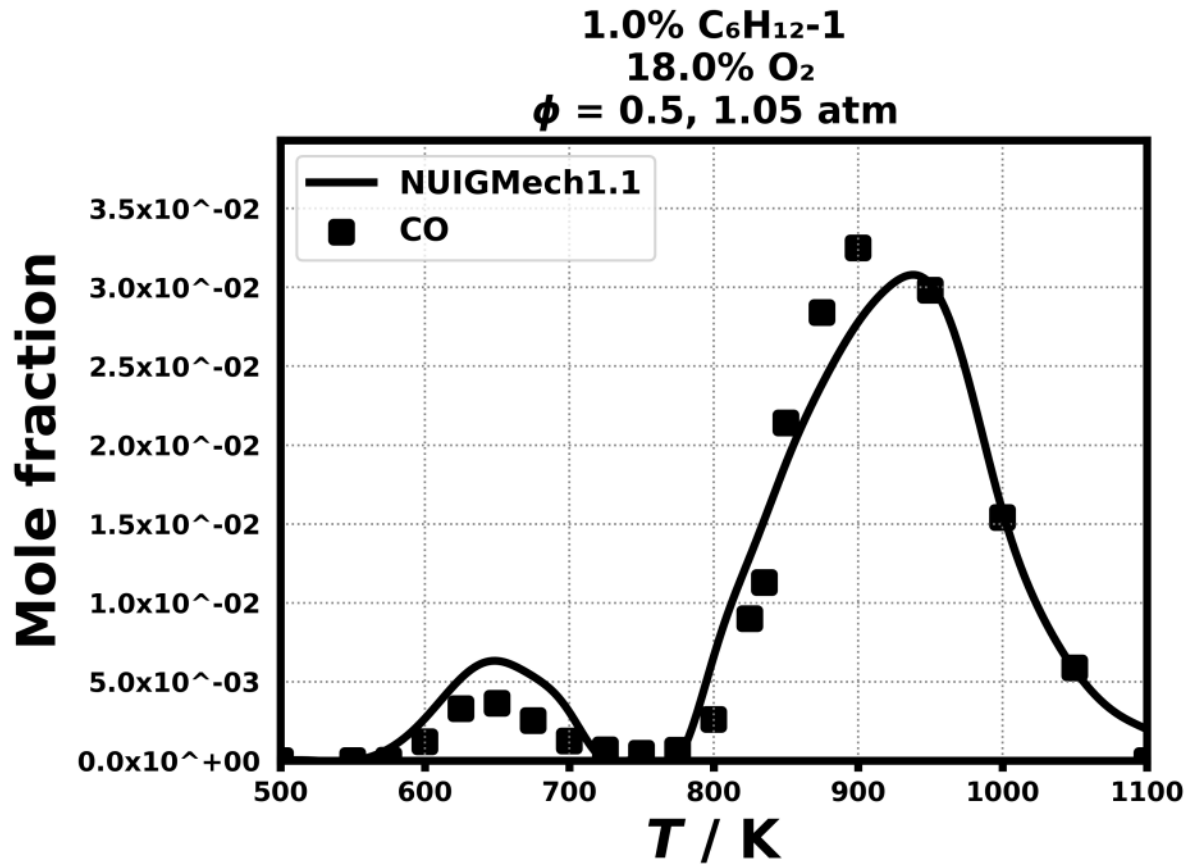


Figure 40: Dataset: 1.05_ATM_PHI.0.5

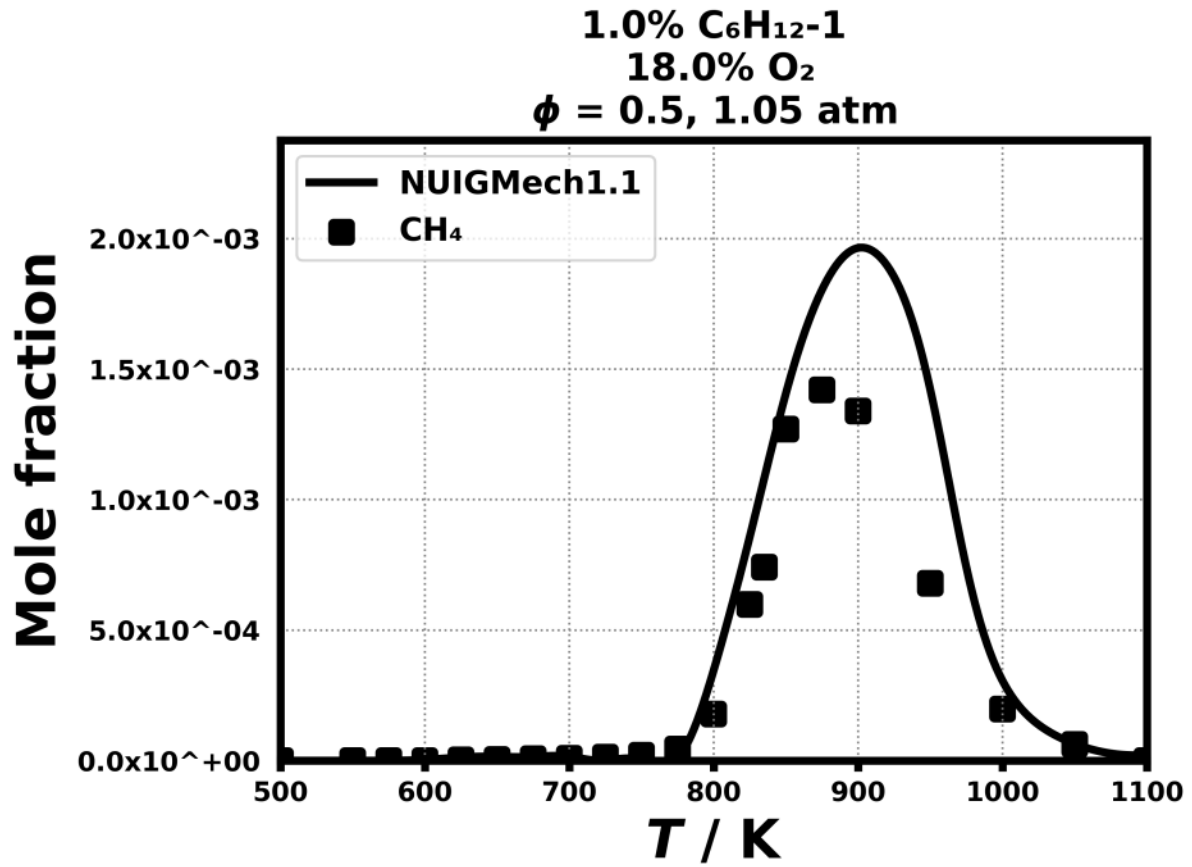


Figure 41: Dataset: 1.05_ATM_PHI_0.5

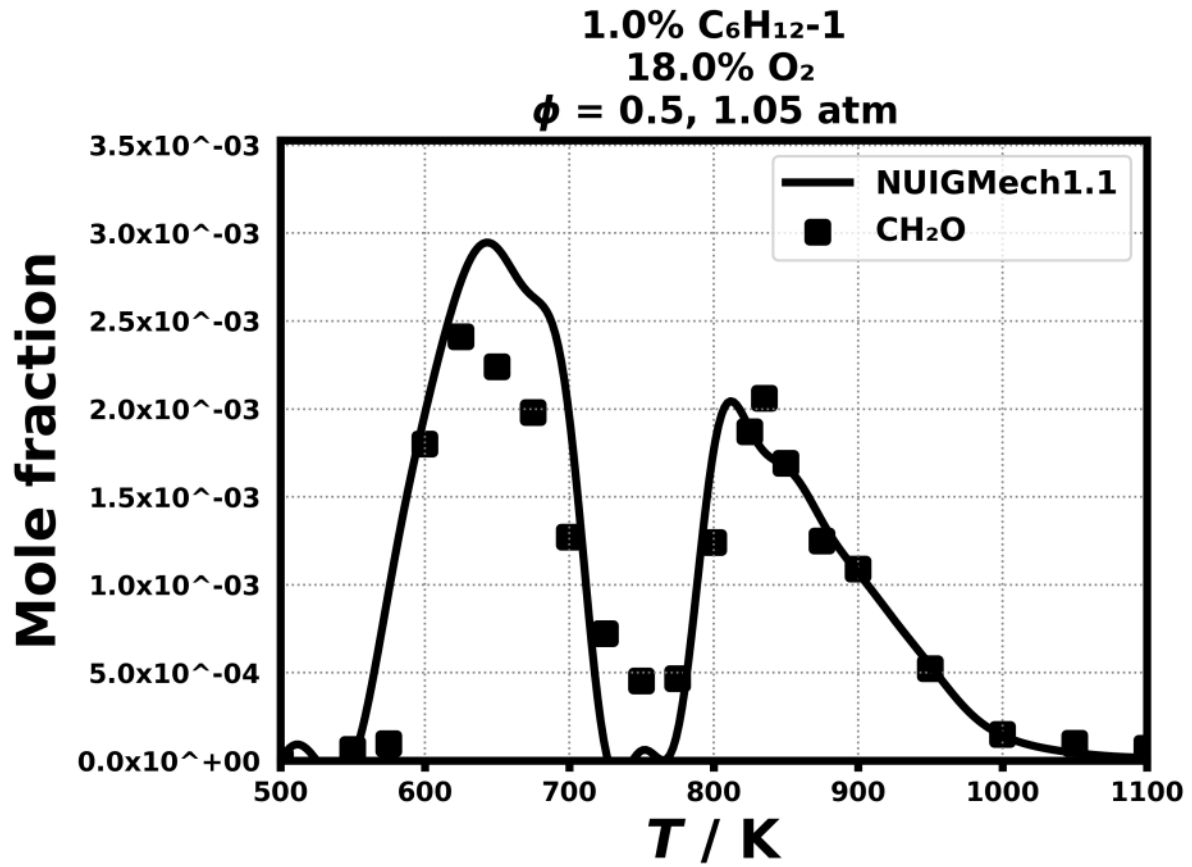


Figure 42: Dataset: 1.05_ATM_PHI_0.5

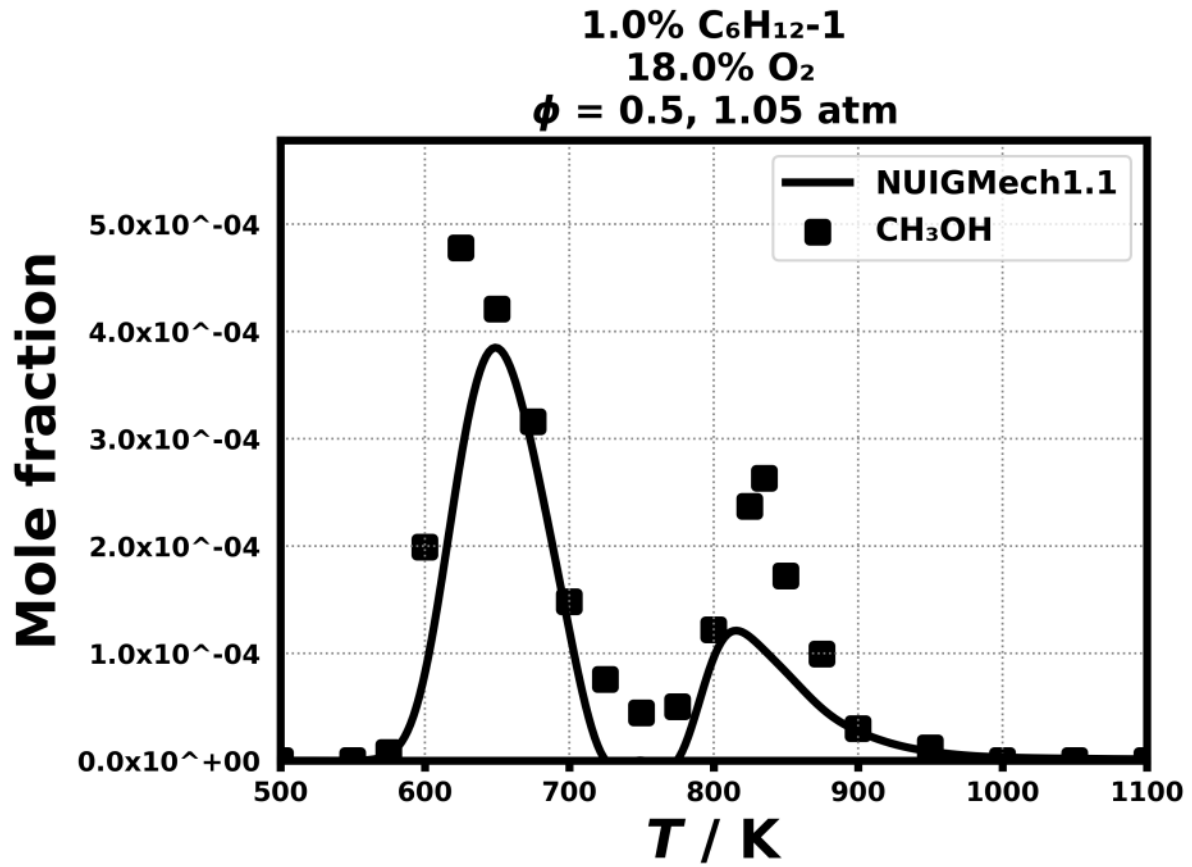


Figure 43: Dataset: 1.05_ATM_PHI0.5

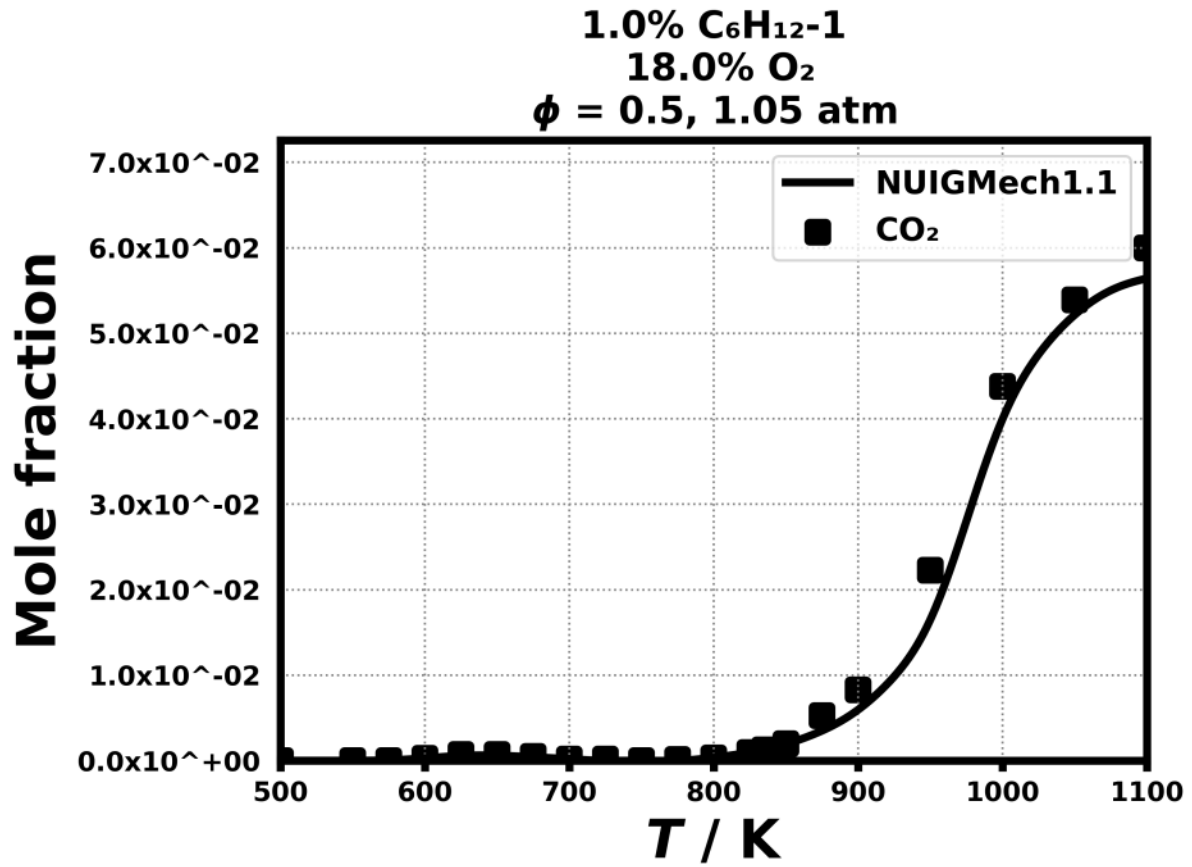


Figure 44: Dataset: 1.05_ATM_PHI.0.5

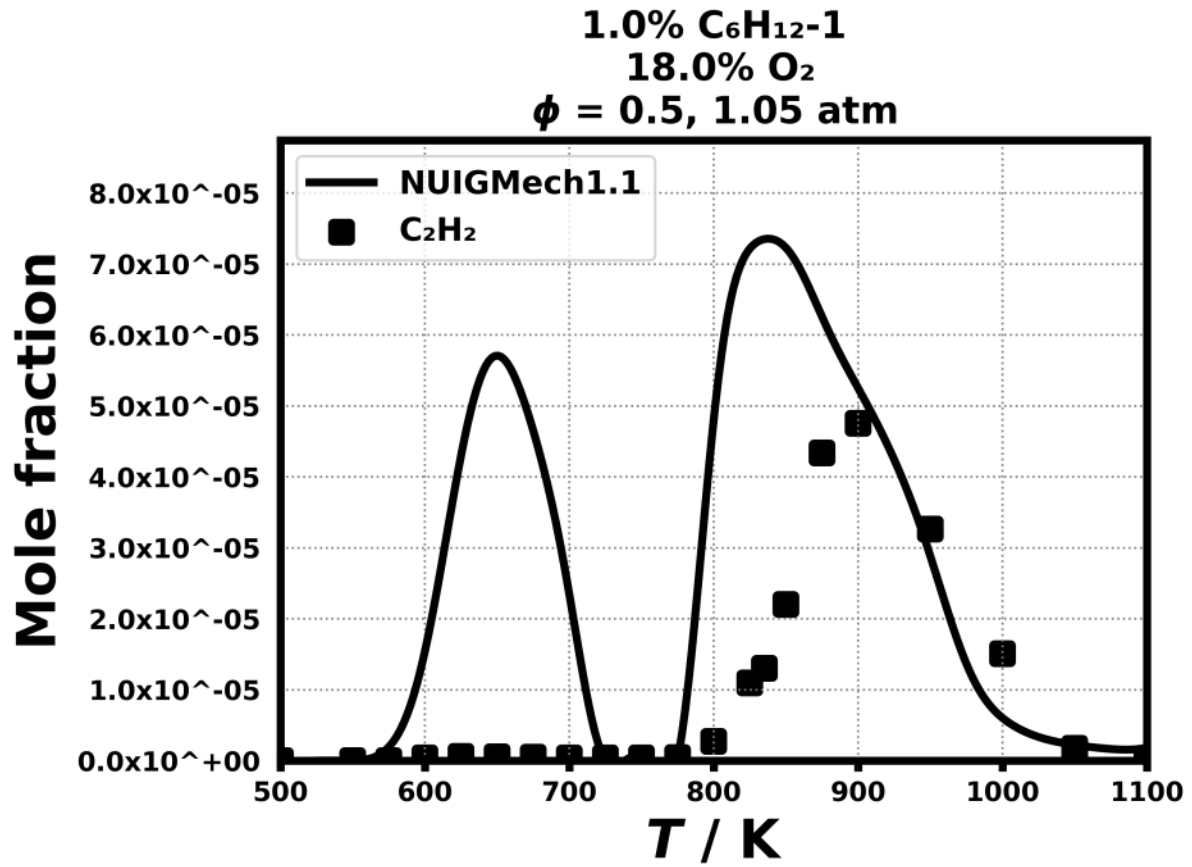


Figure 45: Dataset: 1.05_ATM_PHI.0.5

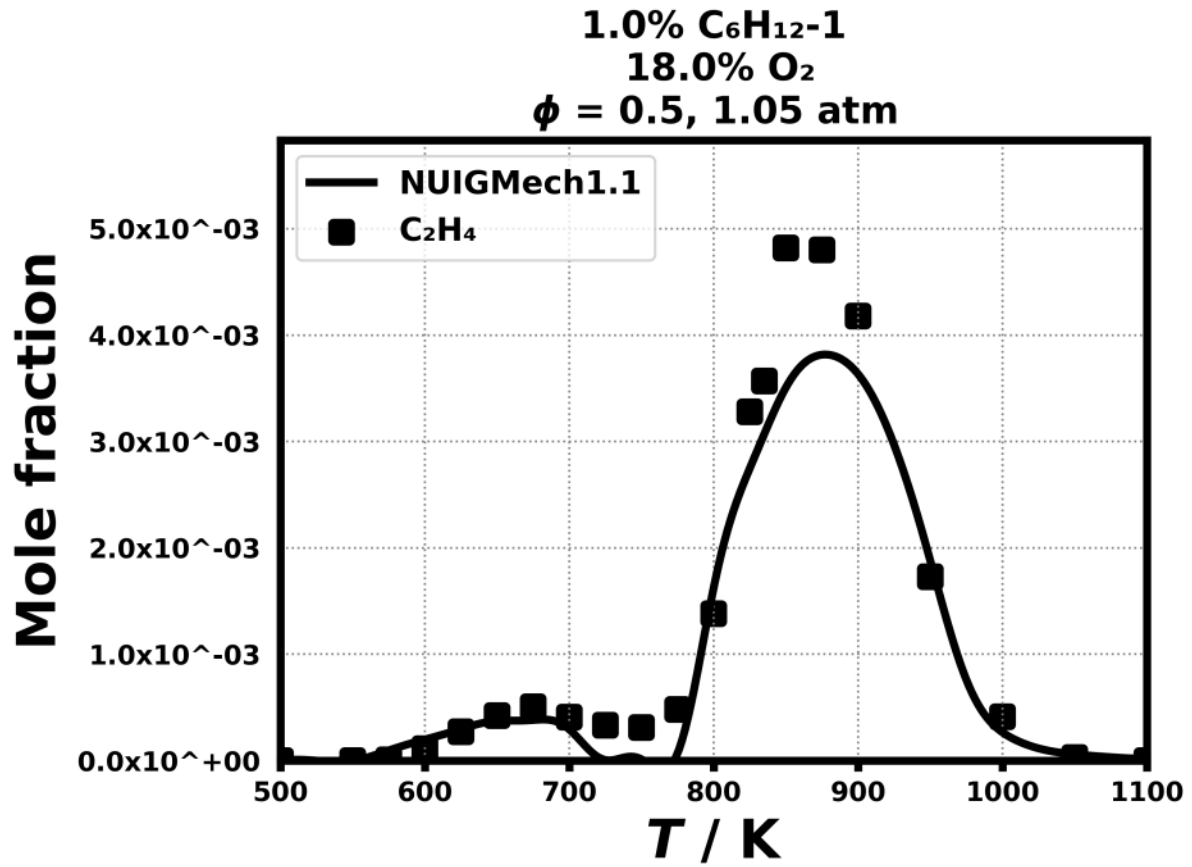


Figure 46: Dataset: 1.05_ATM_PHI0.5

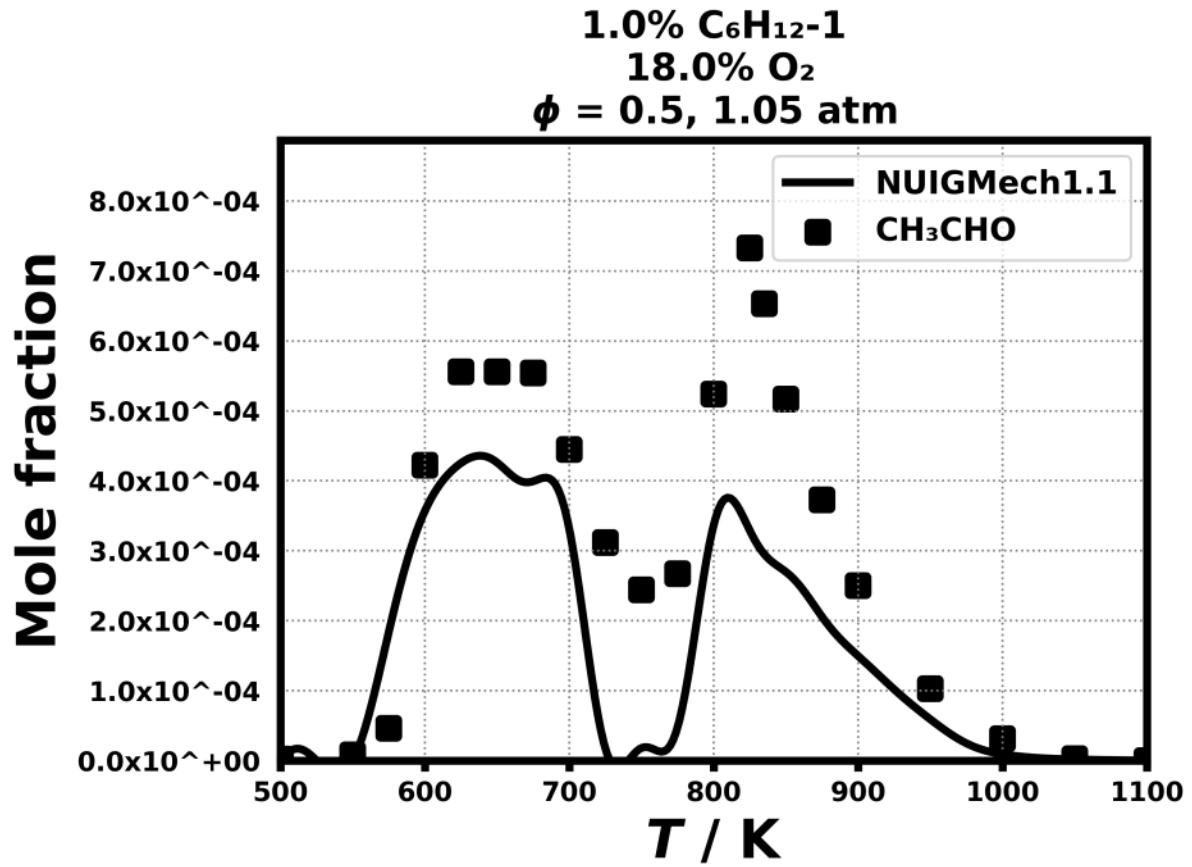


Figure 47: Dataset: 1.05_ATM_PHI_0.5

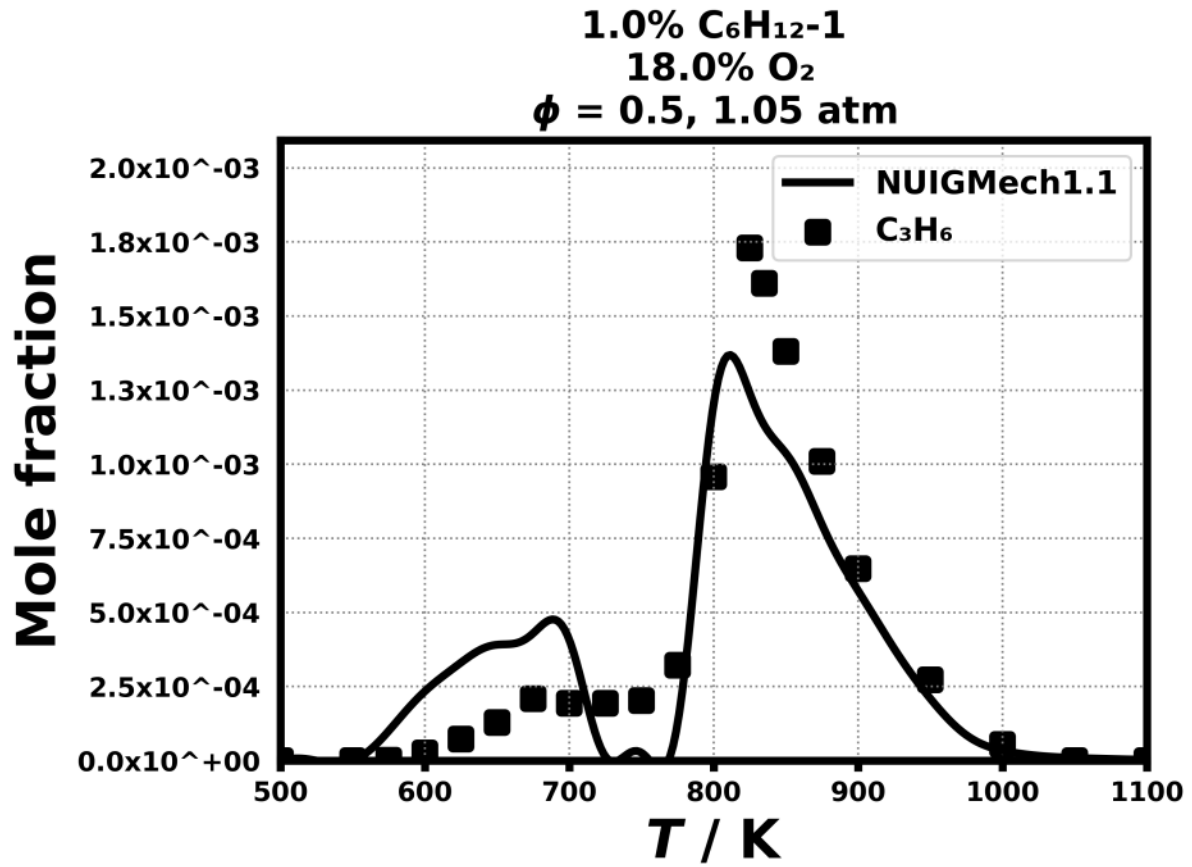


Figure 48: Dataset: 1.05_ATM_PHI.0.5

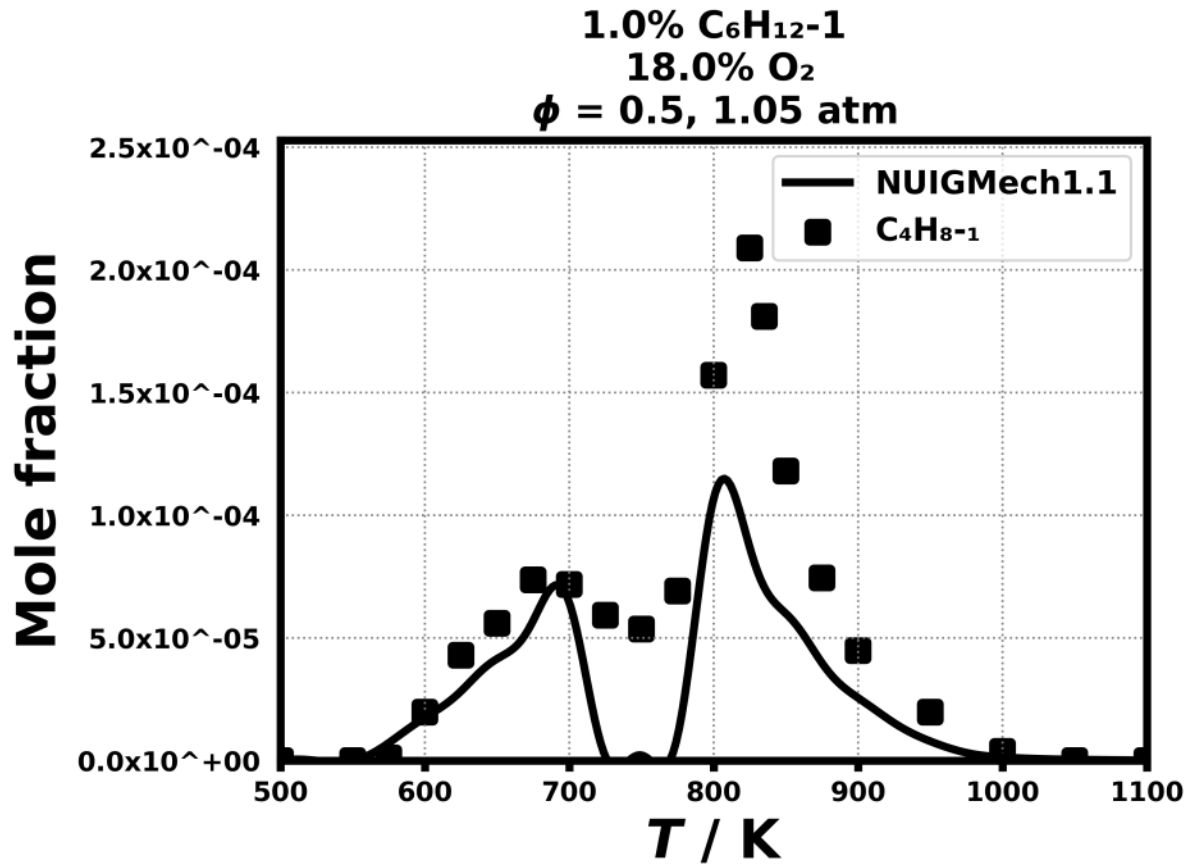


Figure 49: Dataset: 1.05_ATM_PHI_0.5

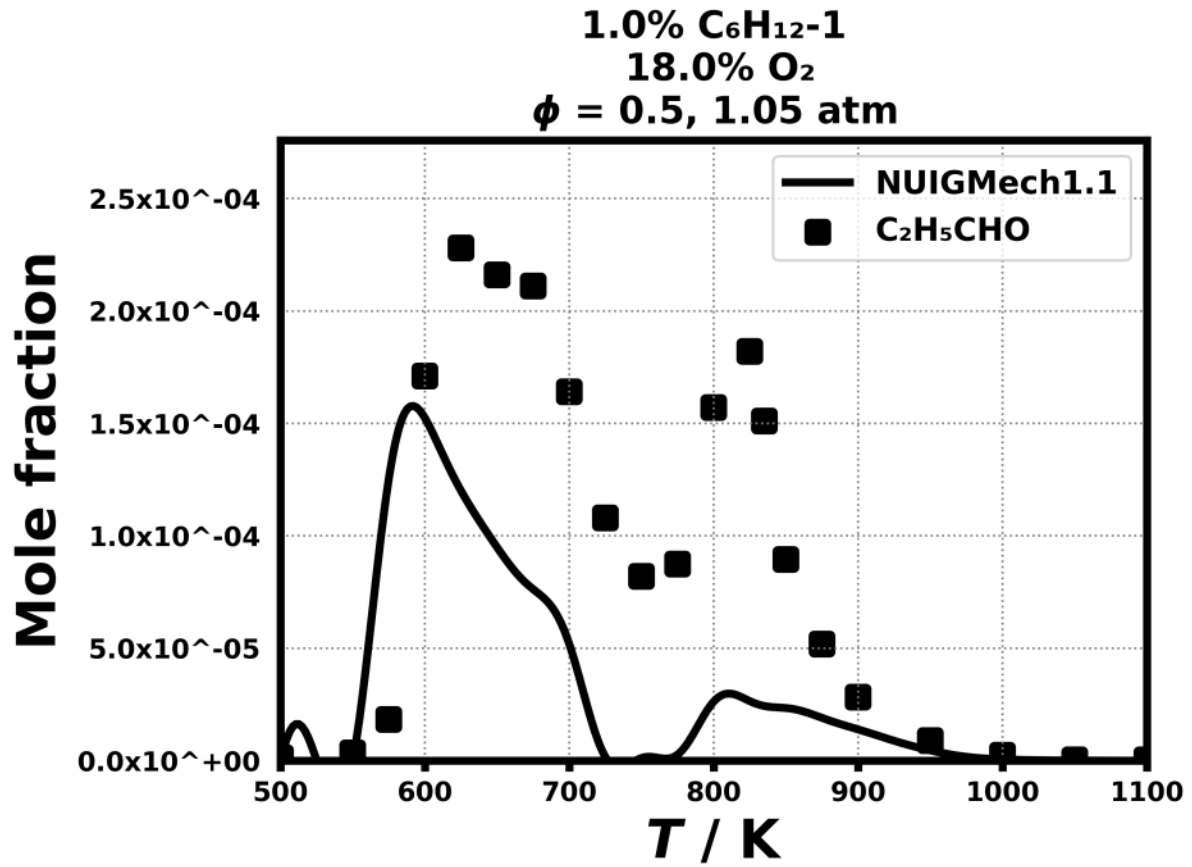


Figure 50: Dataset: 1.05_ATM_PHI.0.5

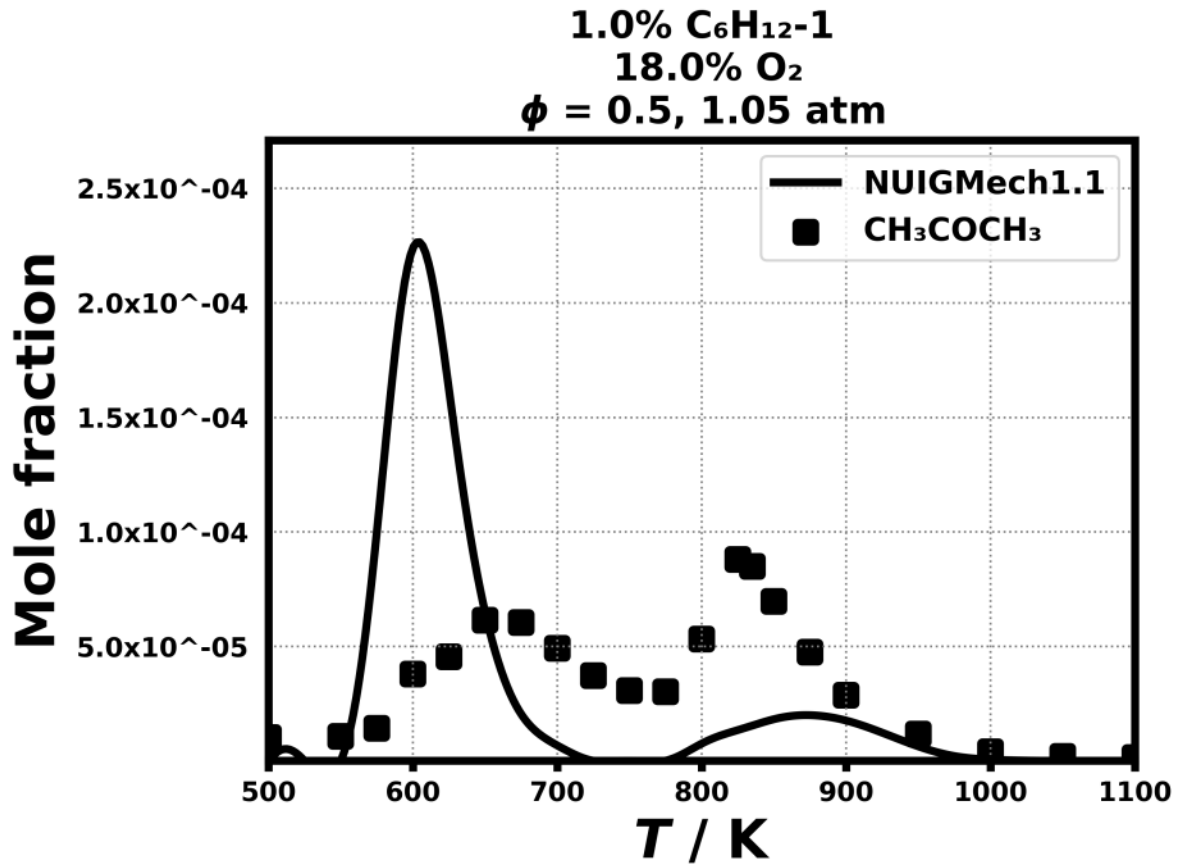


Figure 51: Dataset: 1.05_ATM_PHI.0.5

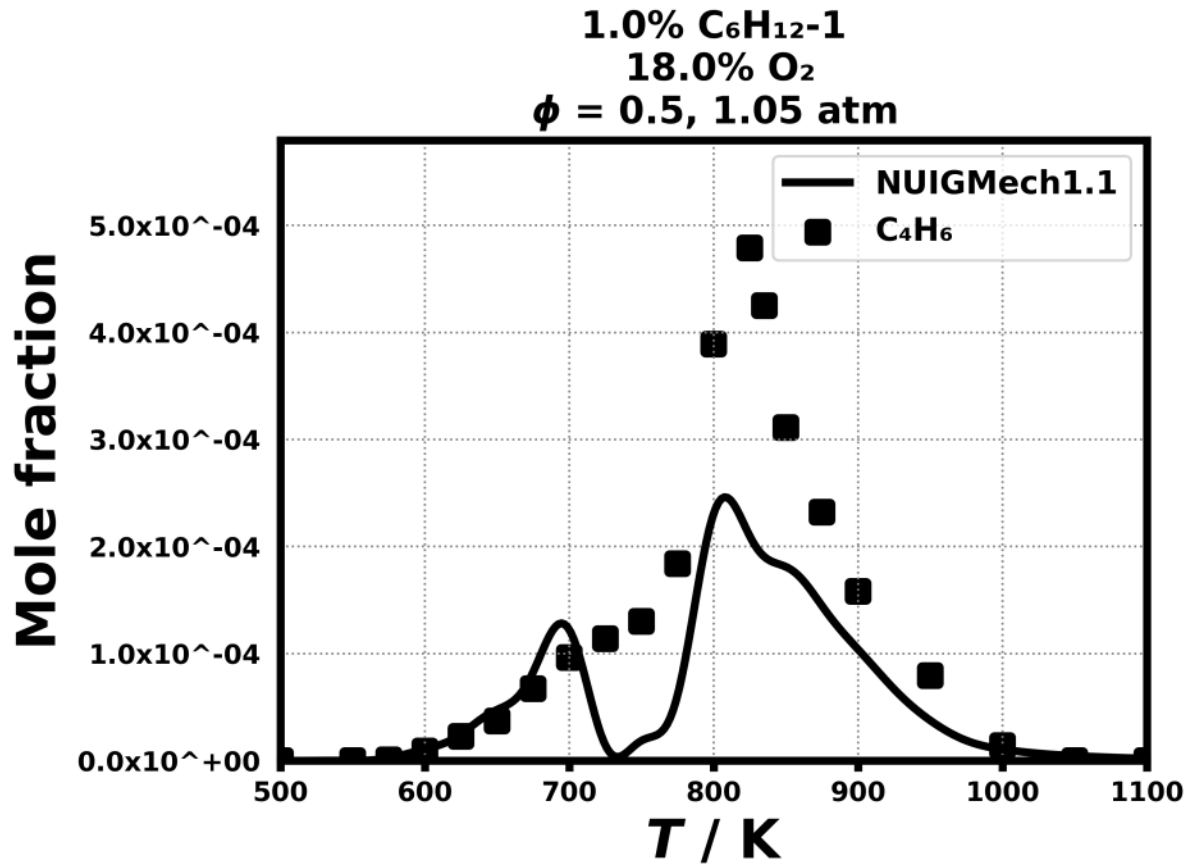


Figure 52: Dataset: 1.05_ATM_PHI_0.5

1.3.31 Case: C6H12-1/JSR/Meng/Meng_GC/1.05_ATM_PHI_0.5

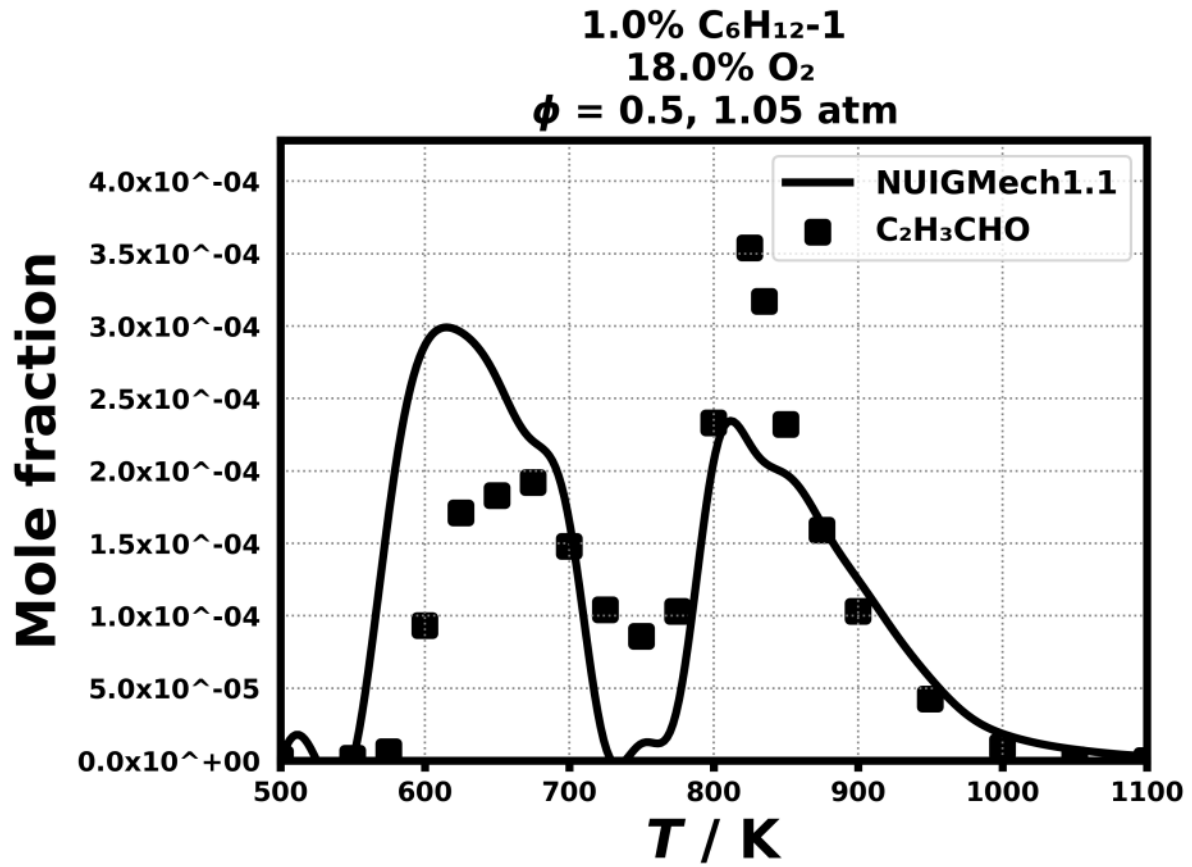


Figure 53: Dataset: 1.05_ATM_PHI_0.5

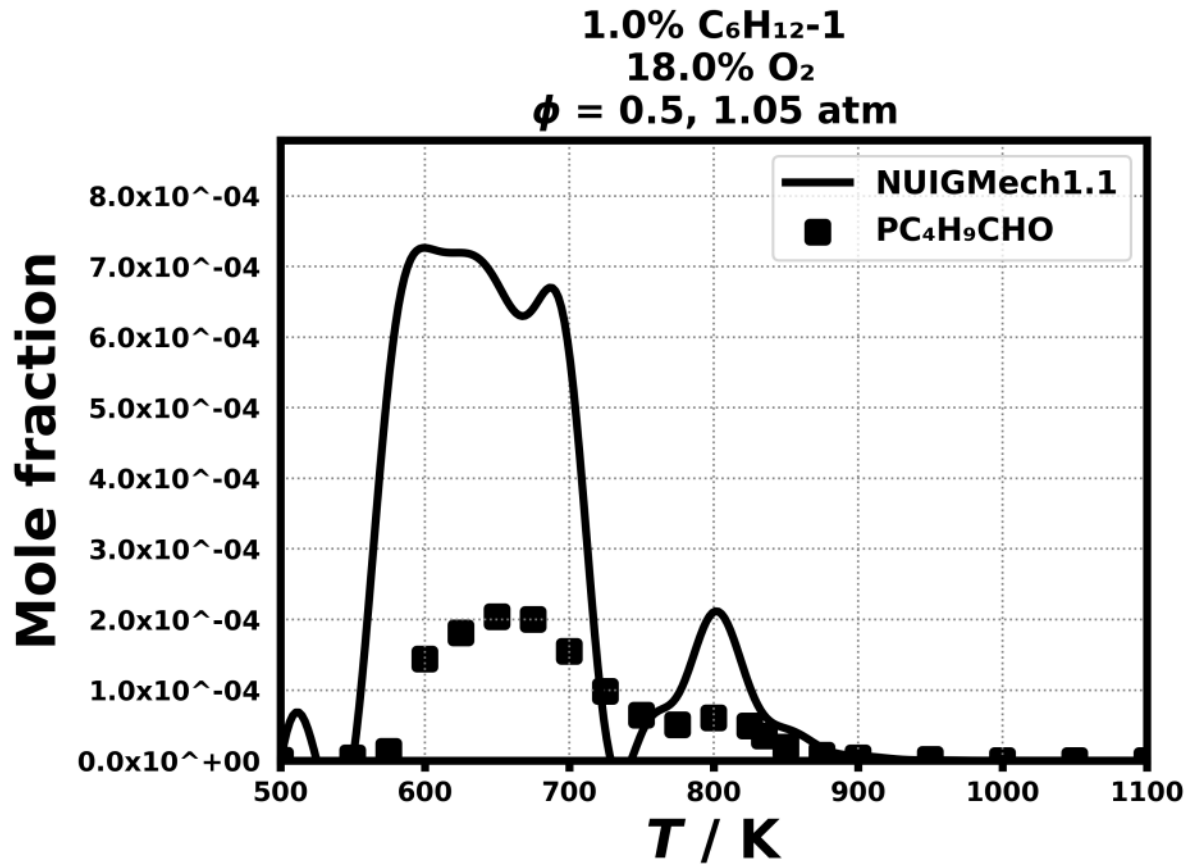


Figure 54: Dataset: 1.05_ATM_PHI_0.5

1.3.33 Case: C6H12-1/JSR/Meng/Meng_GC/1.05_ATM_PHI_0.5

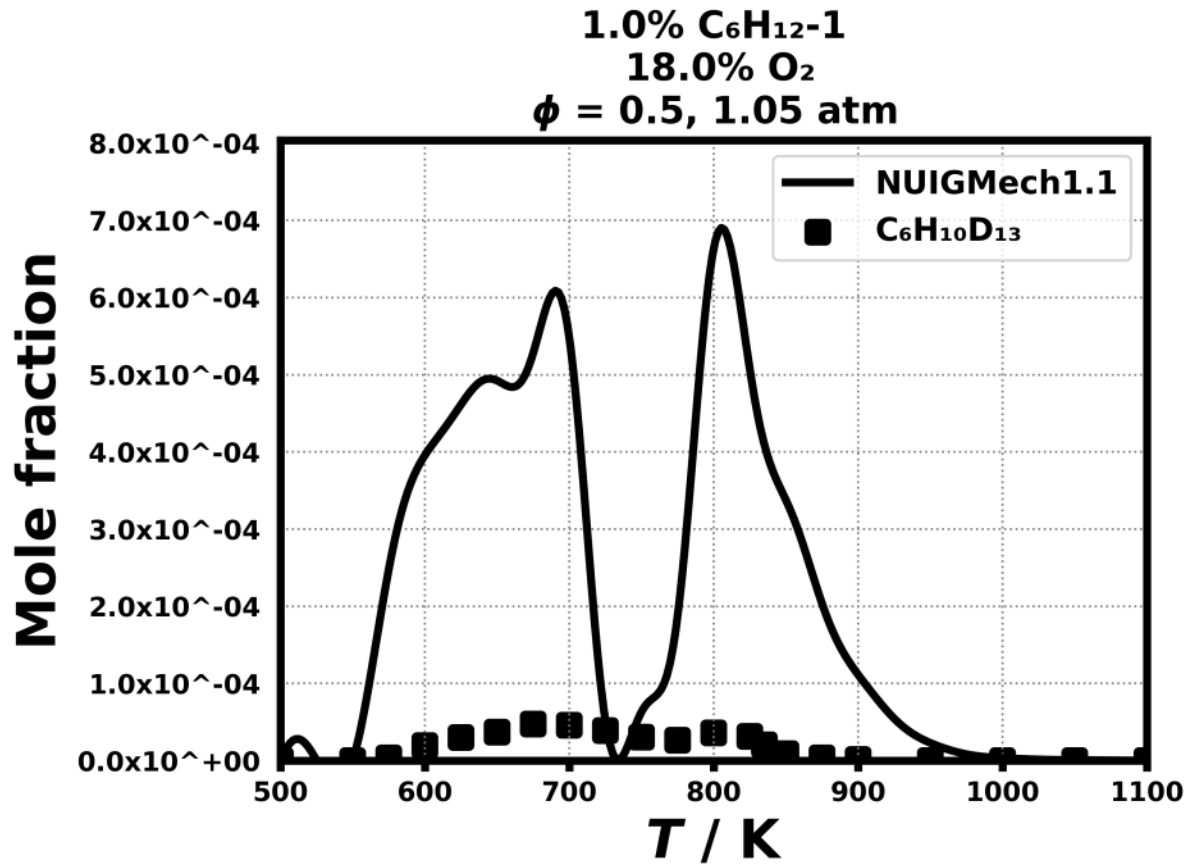


Figure 55: Dataset: 1.05_ATM_PHI_0.5

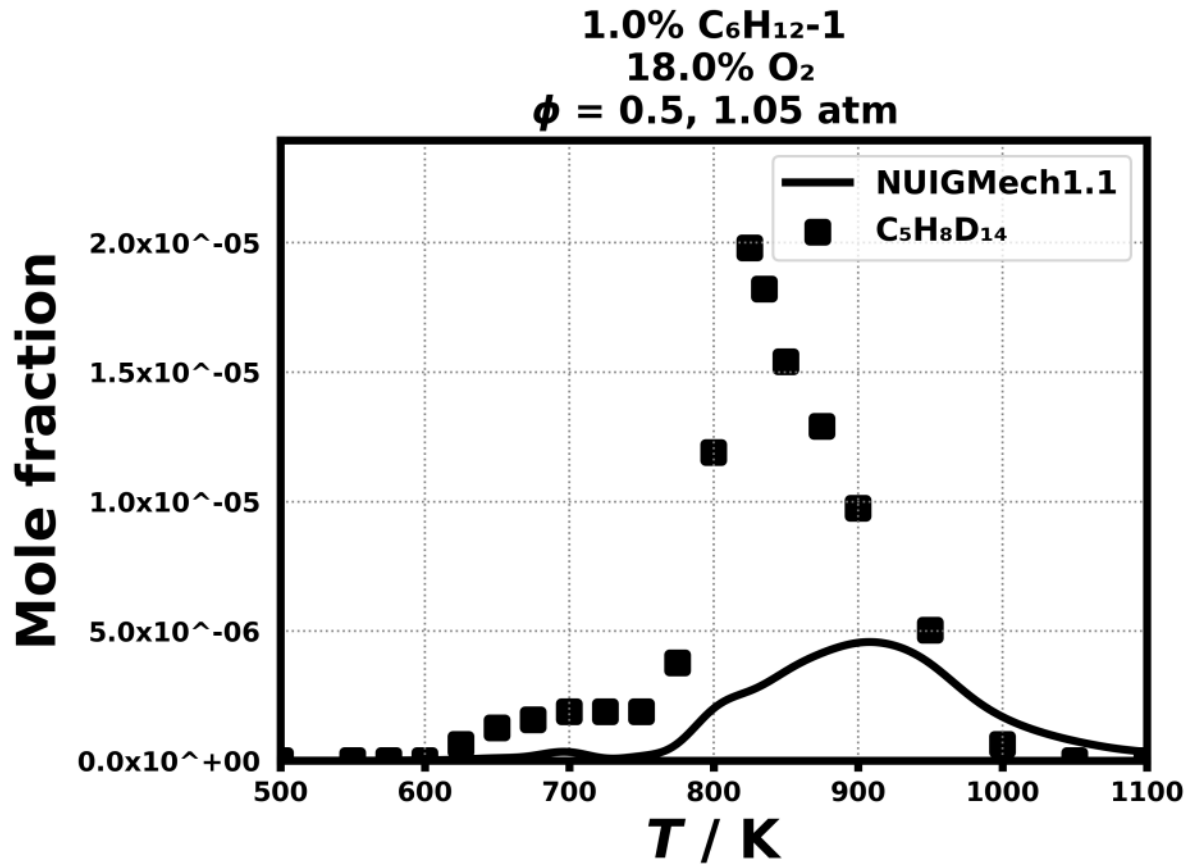


Figure 56: Dataset: 1.05_ATM_PHI_0.5

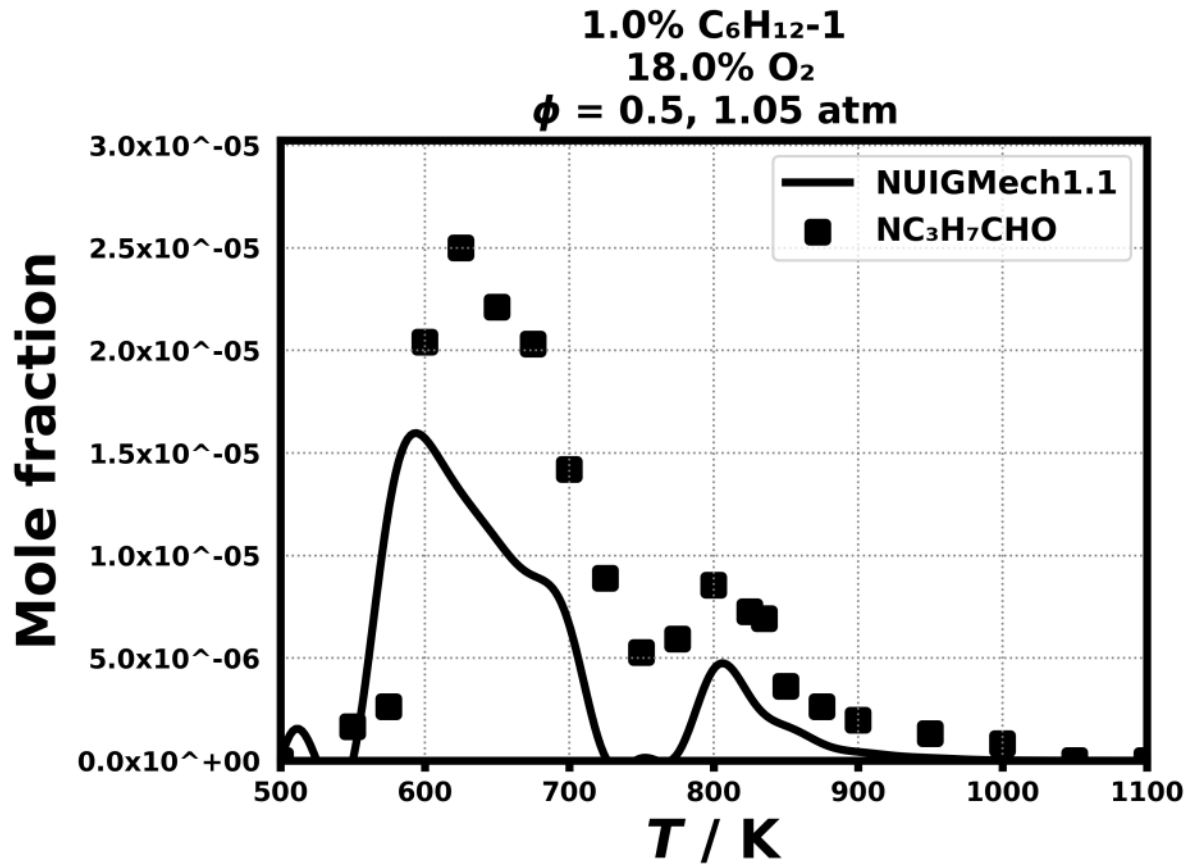


Figure 57: Dataset: 1.05_ATM_PHI_0.5

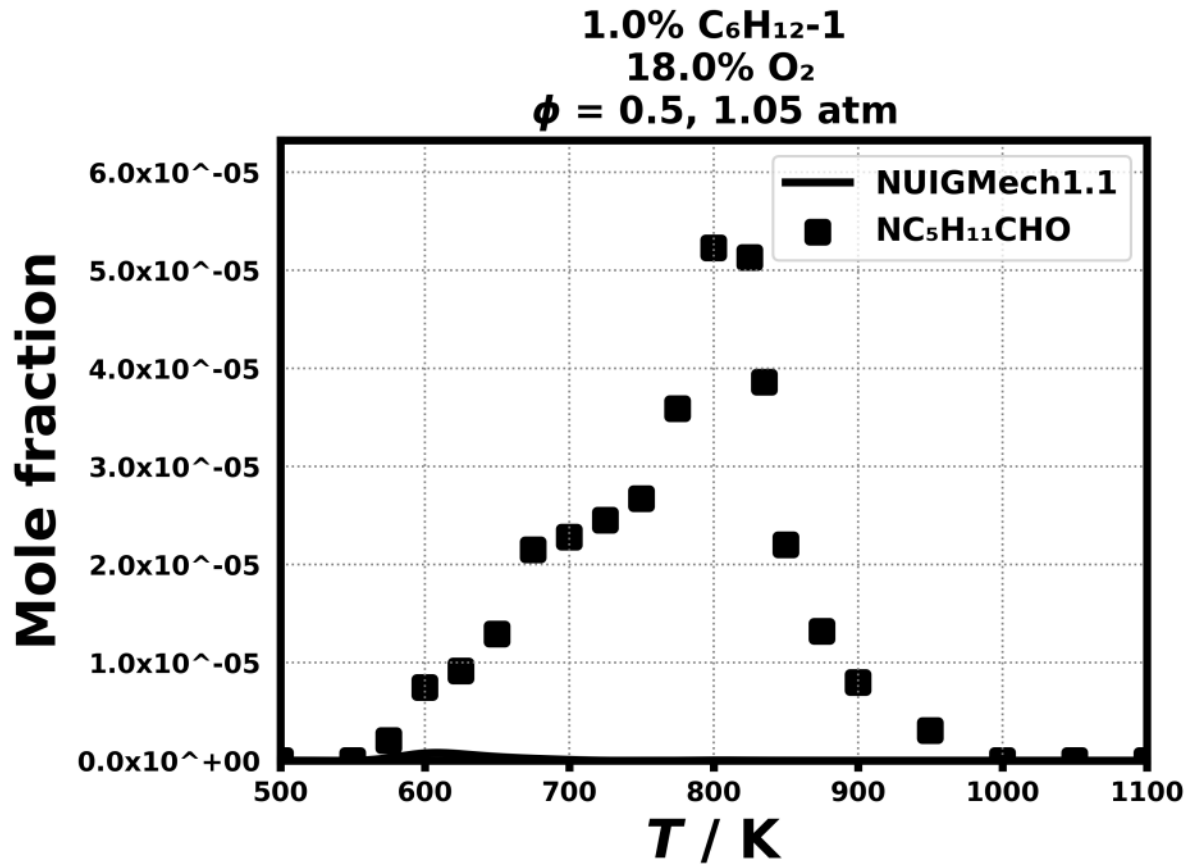


Figure 58: Dataset: 1.05_ATM_PHI_0.5

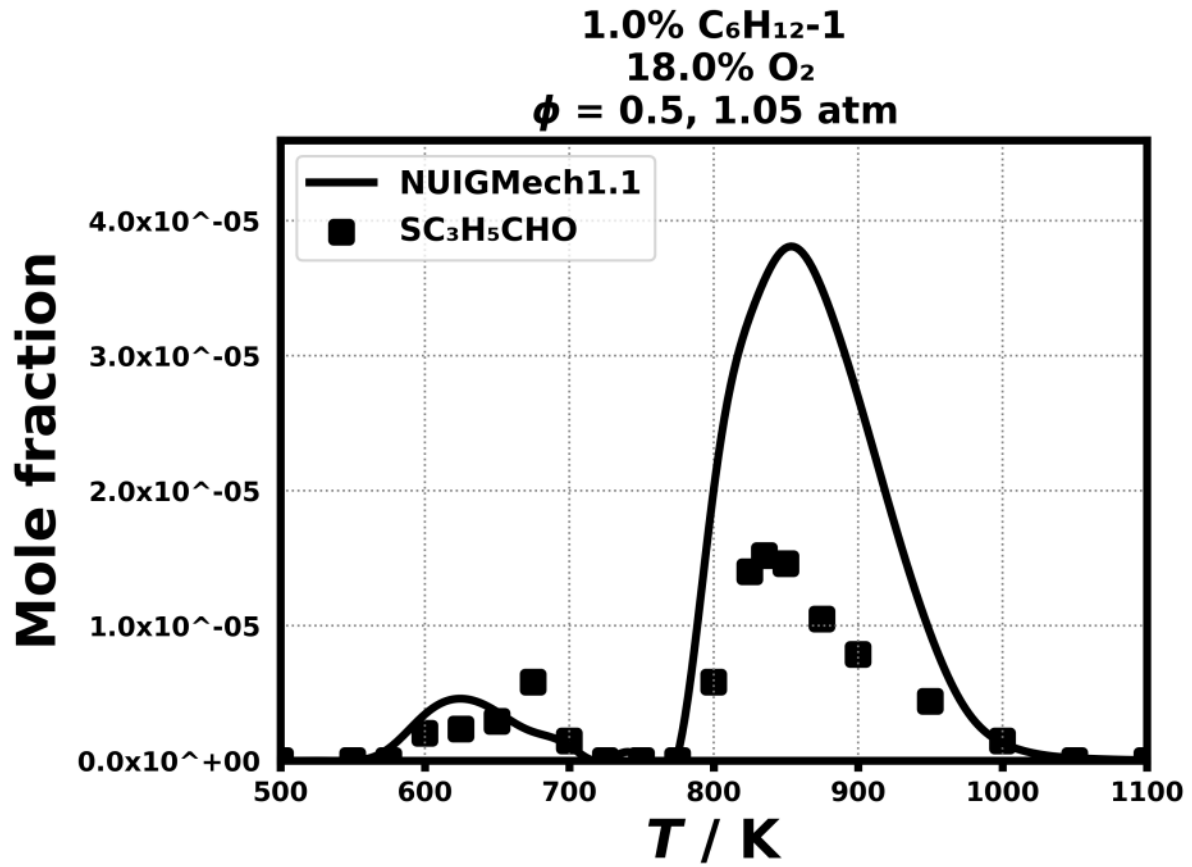


Figure 59: Dataset: 1.05_ATM_PHI_0.5

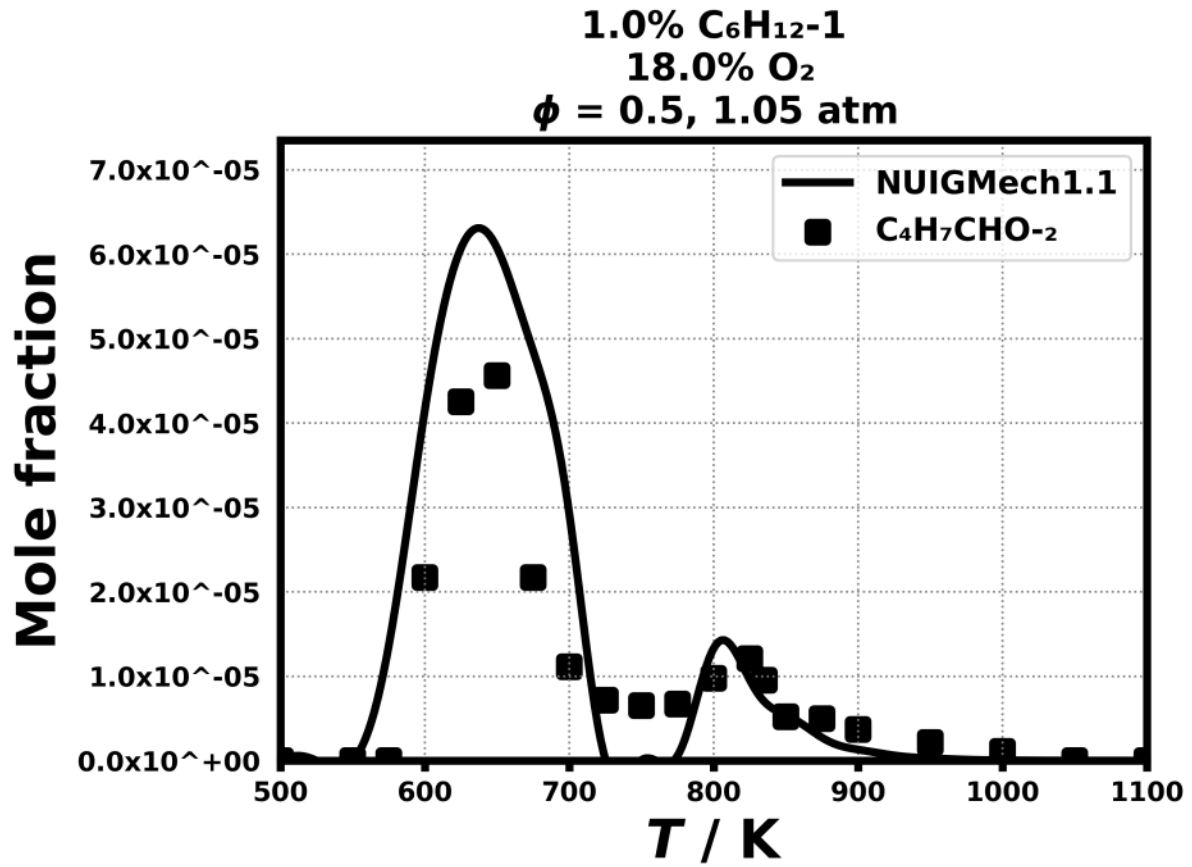


Figure 60: Dataset: 1.05_ATM_PHI_0.5

1.3.39 Case: C6H12-1/JSR/Meng/Meng_GC/1.05_ATM_PHI.0.5

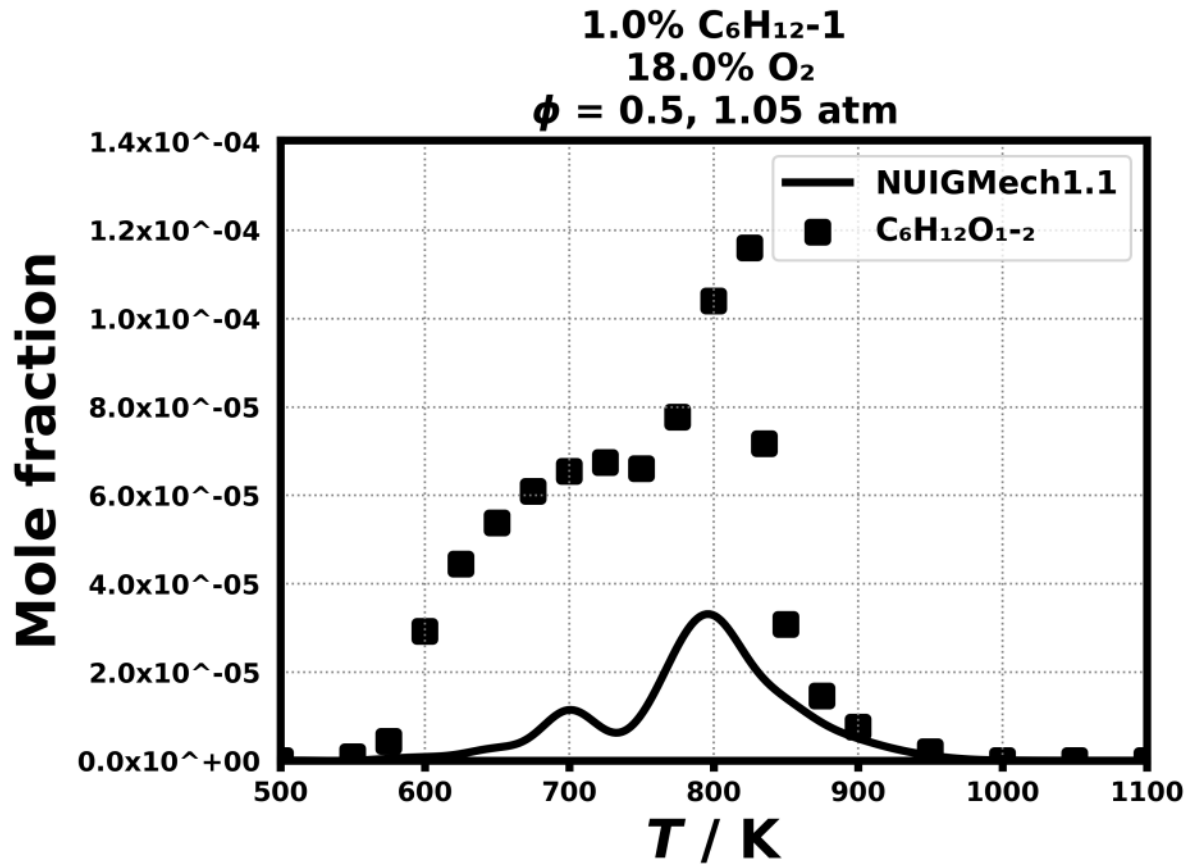


Figure 61: Dataset: 1.05_ATM_PHI.0.5

1.3.40 Case: C6H12-1/JSR/Meng/Meng_GC/1.05_ATM_PHI_0.5

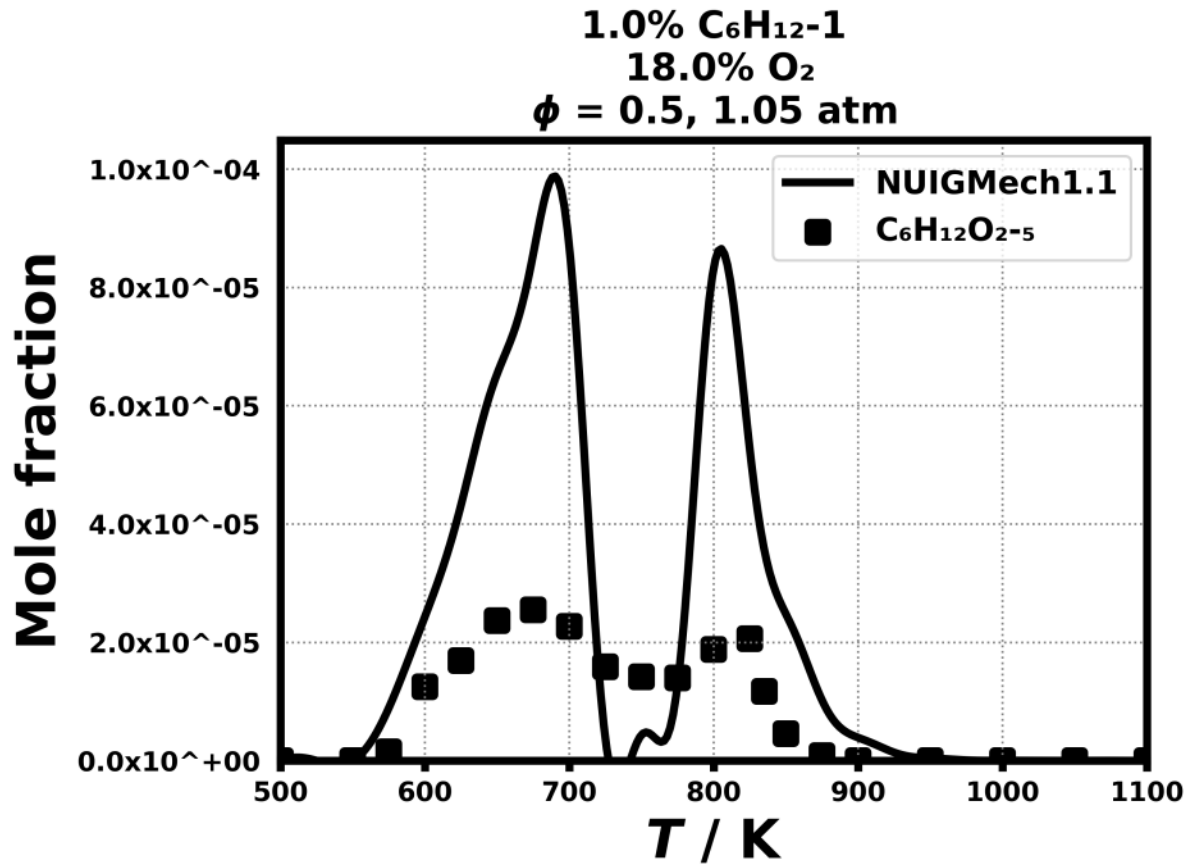


Figure 62: Dataset: 1.05_ATM_PHI_0.5

1.3.41 Case: C6H12-1/JSR/Meng/Meng_GC/1.05_ATM_PHI_1.0

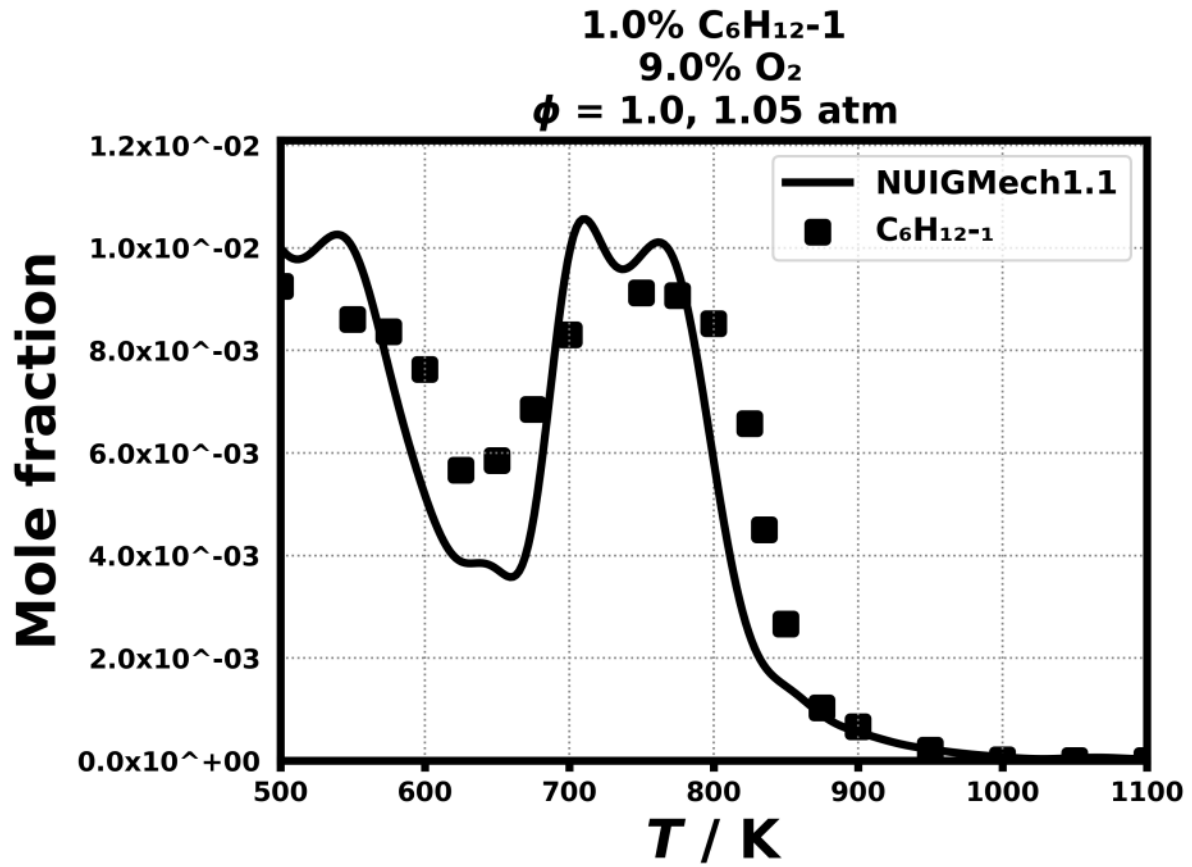


Figure 63: Dataset: 1.05_ATM_PHI_1.0

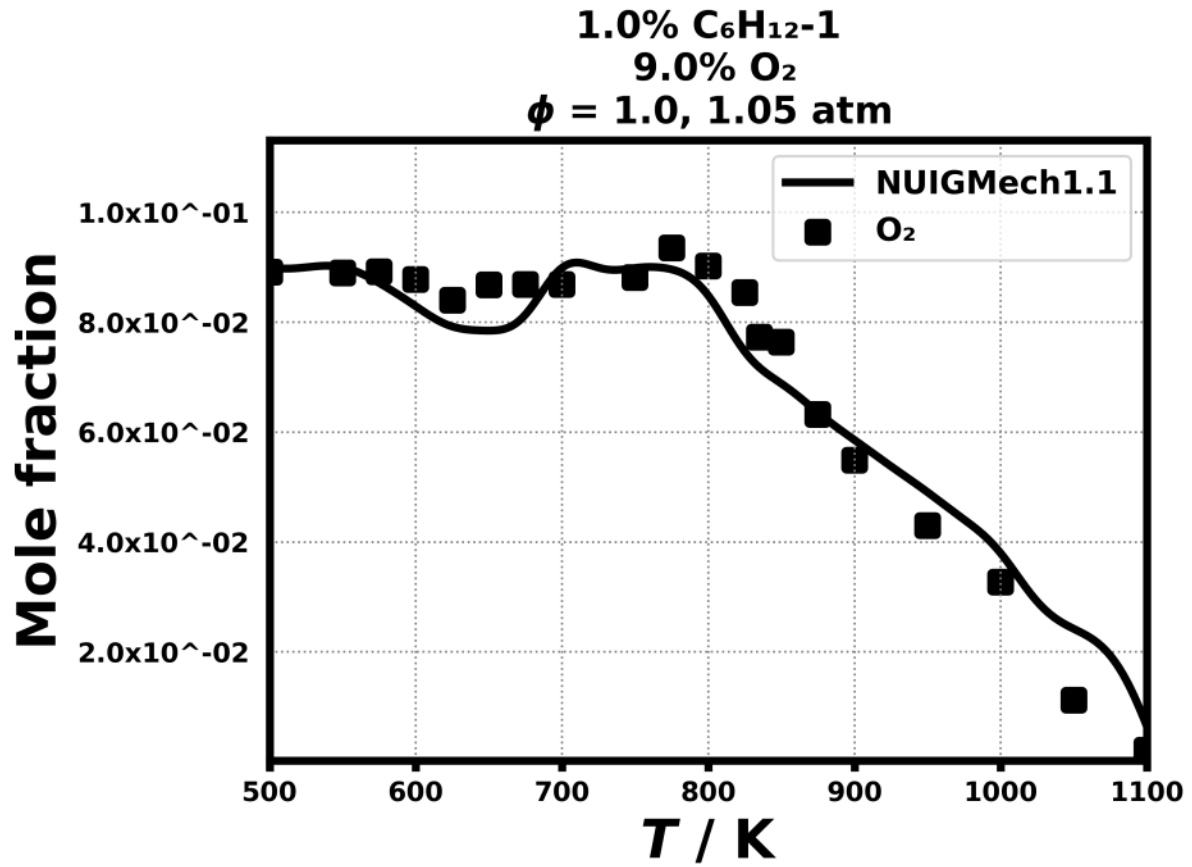


Figure 64: Dataset: 1.05_ATM_PHI_1.0

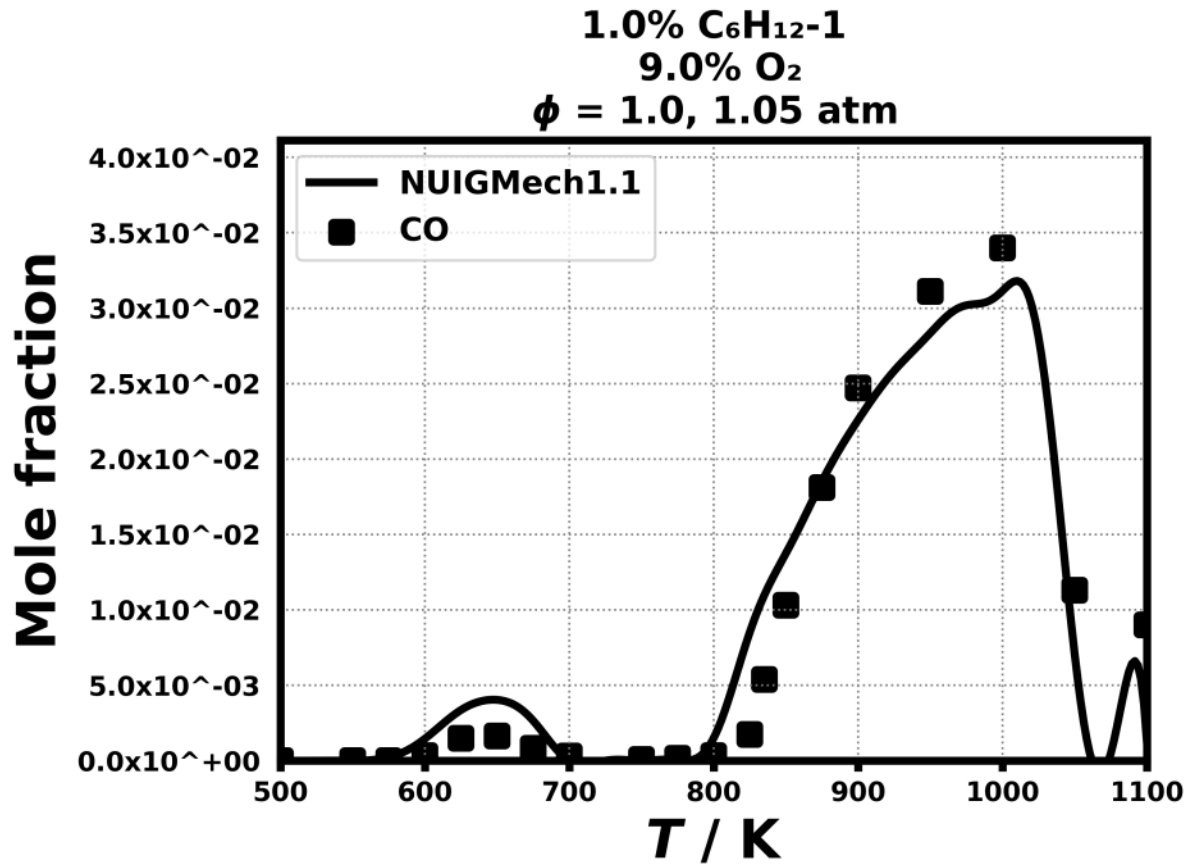


Figure 65: Dataset: 1.05_ATM_PHI_1.0

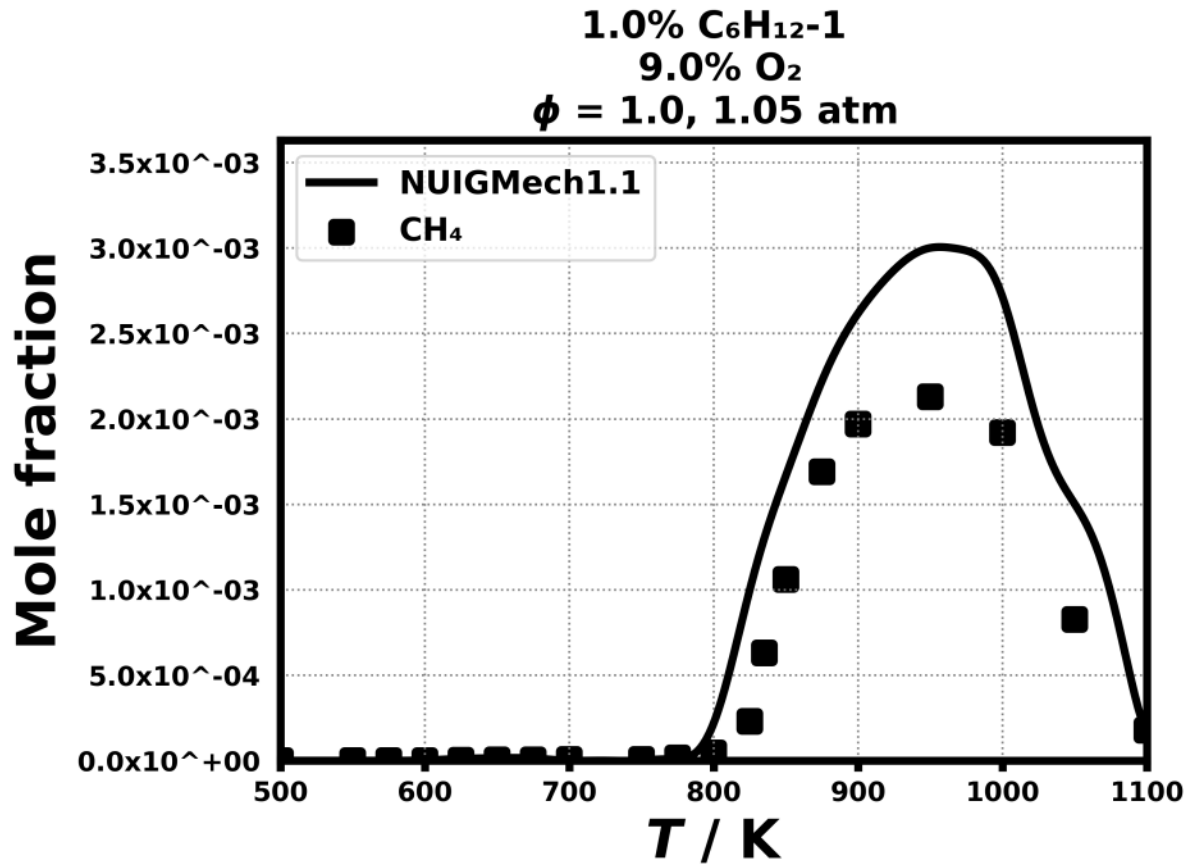


Figure 66: Dataset: 1.05_ATM_PHI_1.0

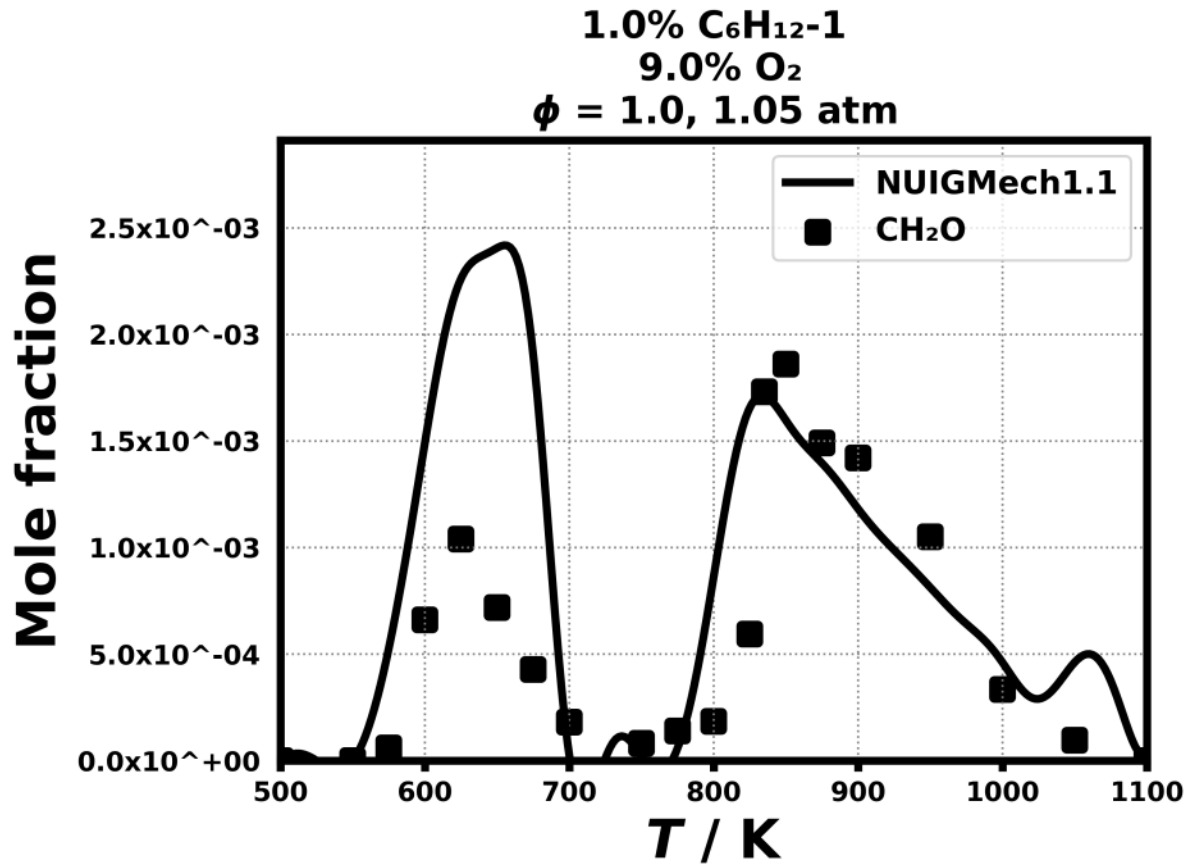


Figure 67: Dataset: 1.05_ATM_PHI_1.0

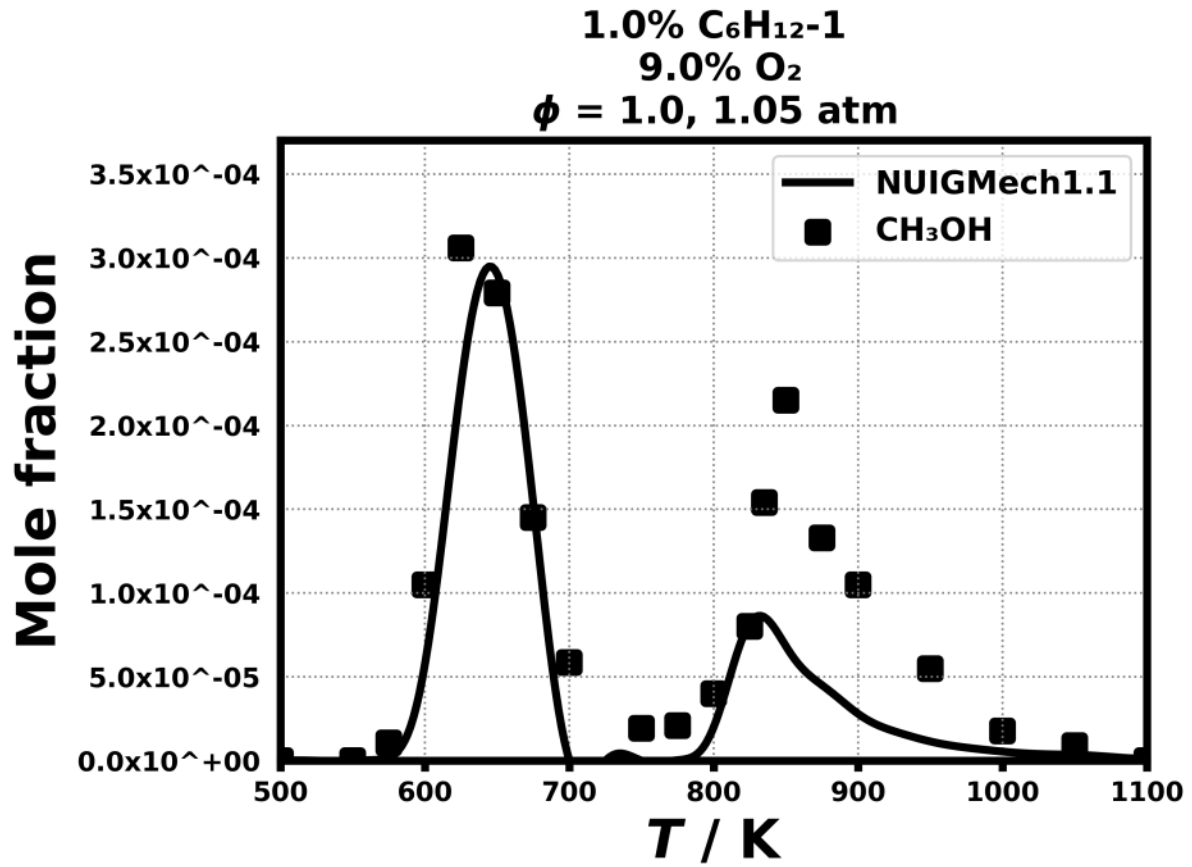


Figure 68: Dataset: 1.05_ATM_PHI_1.0

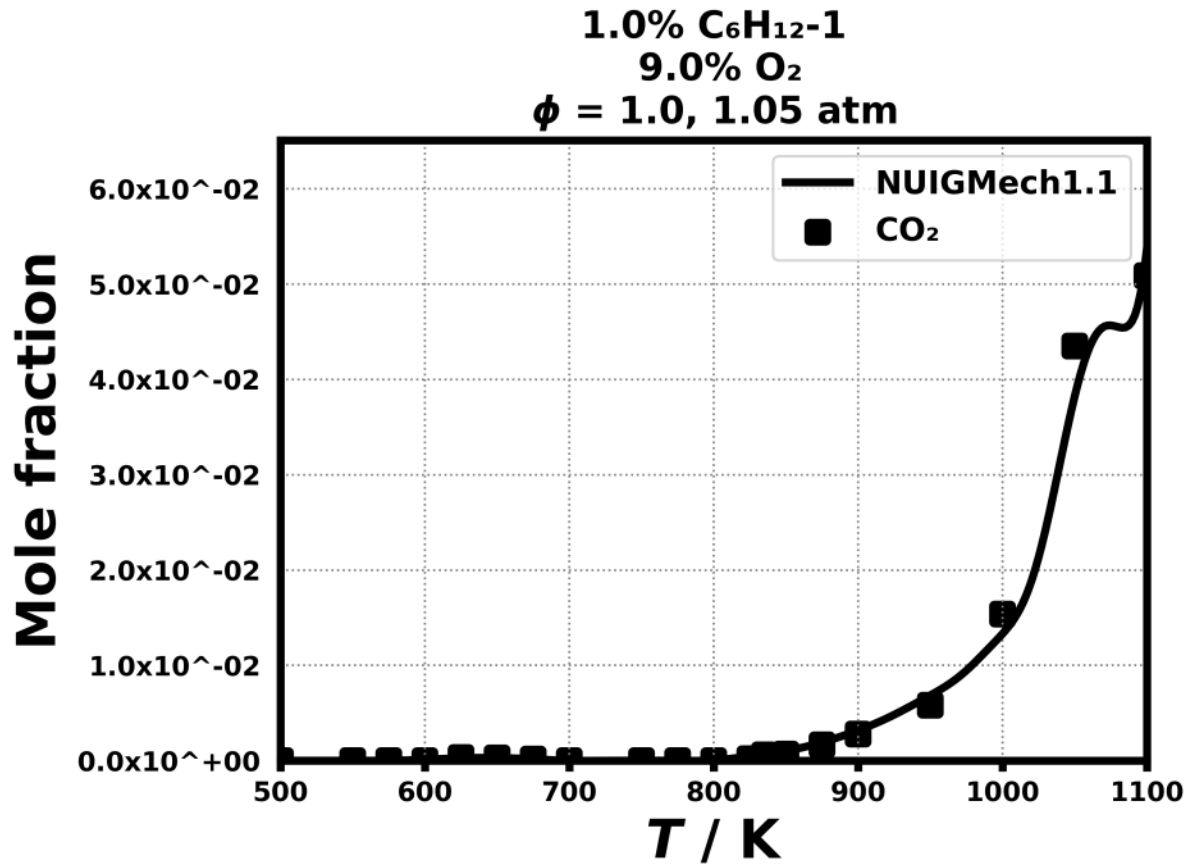


Figure 69: Dataset: 1.05_ATM_PHI_1.0

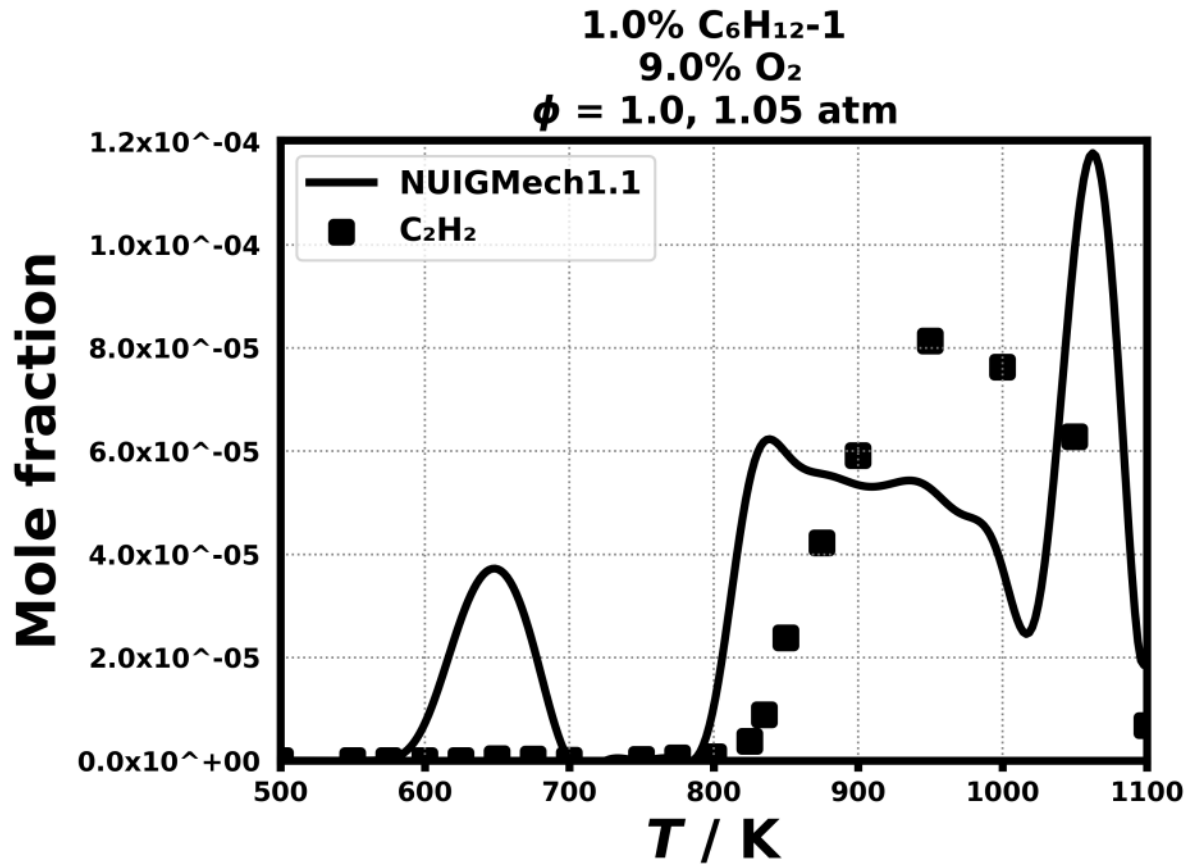


Figure 70: Dataset: 1.05_ATM_PHI_1.0

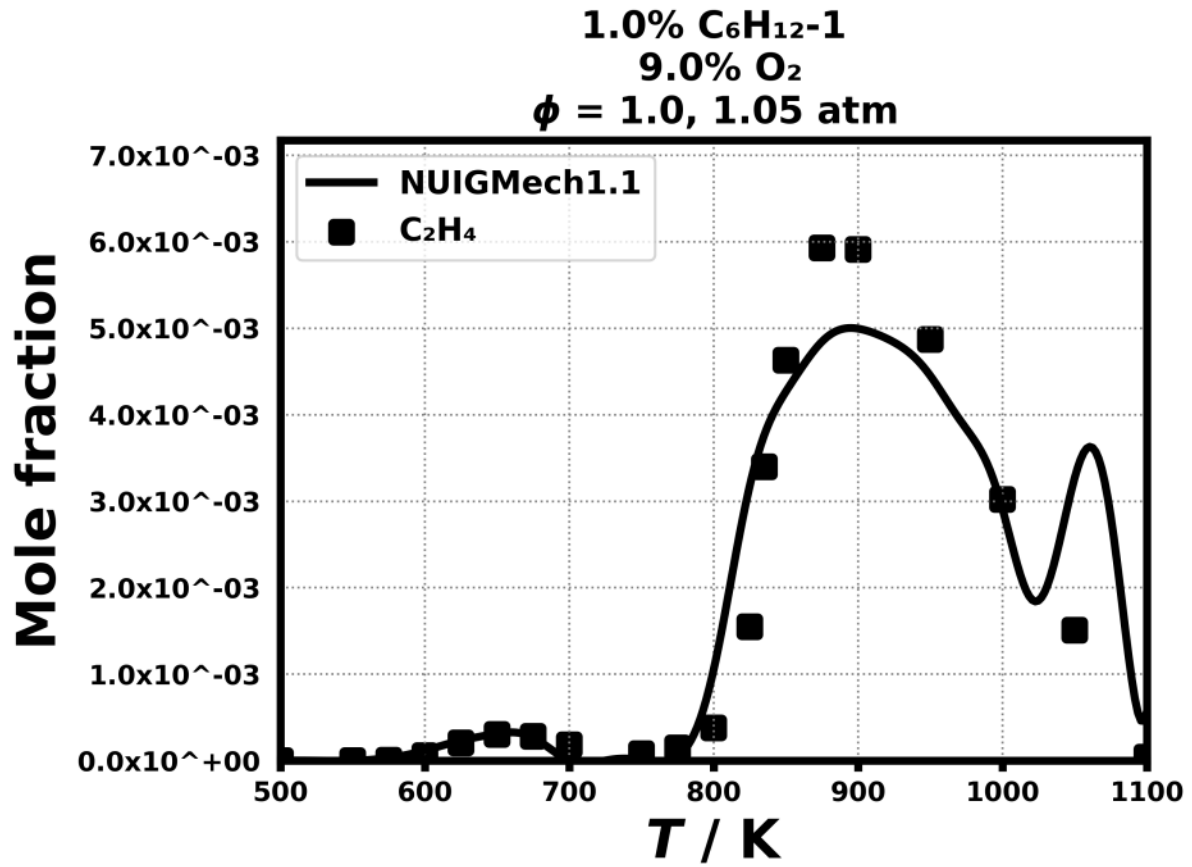


Figure 71: Dataset: 1.05_ATM_PHI_1.0

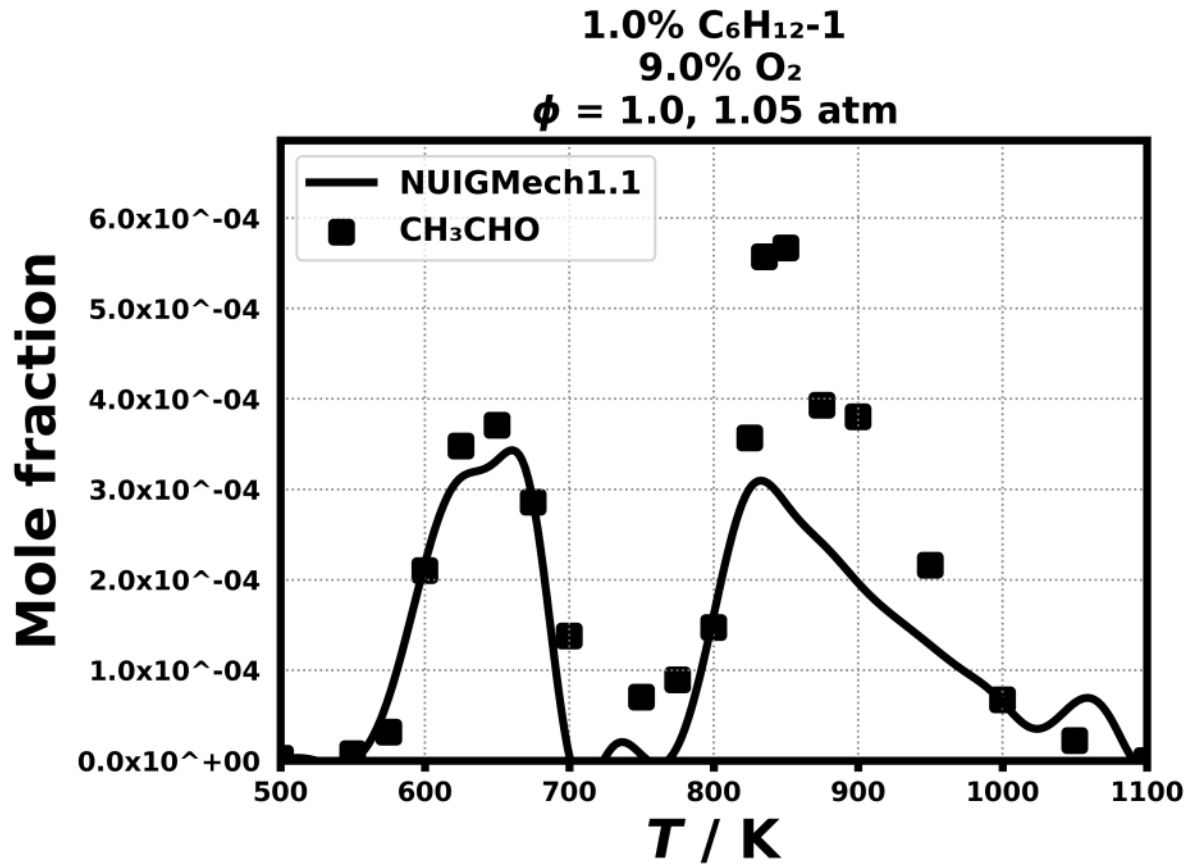


Figure 72: Dataset: 1.05_ATM_PHI_1.0

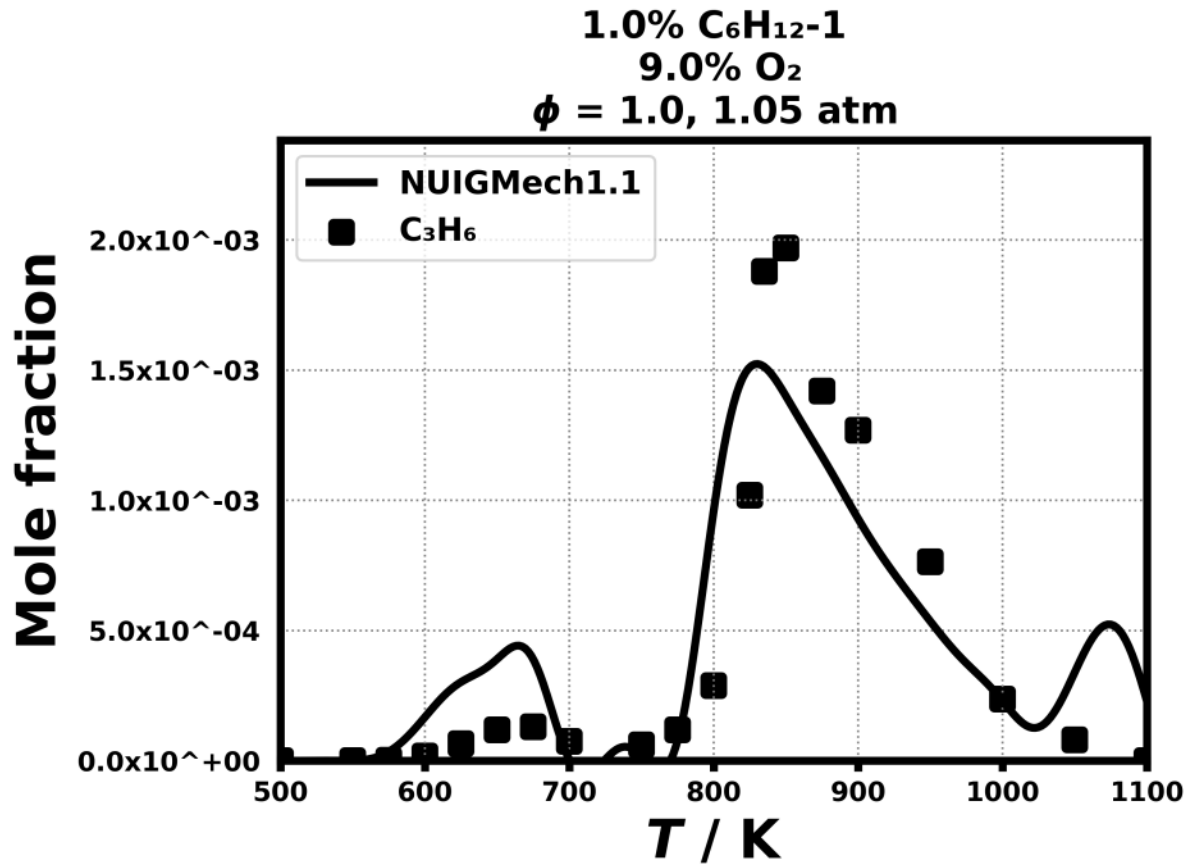


Figure 73: Dataset: 1.05_ATM_PHI_1.0

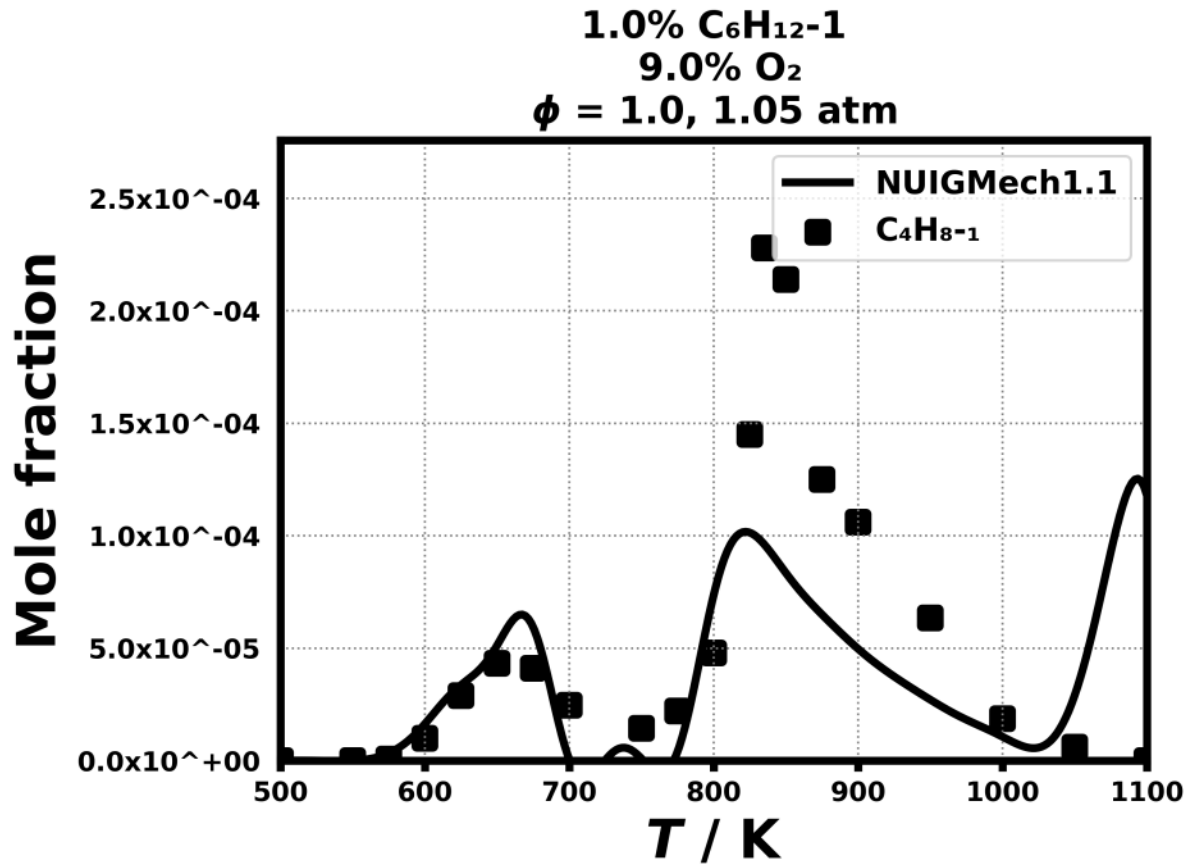


Figure 74: Dataset: 1.05_ATM_PHI_1.0

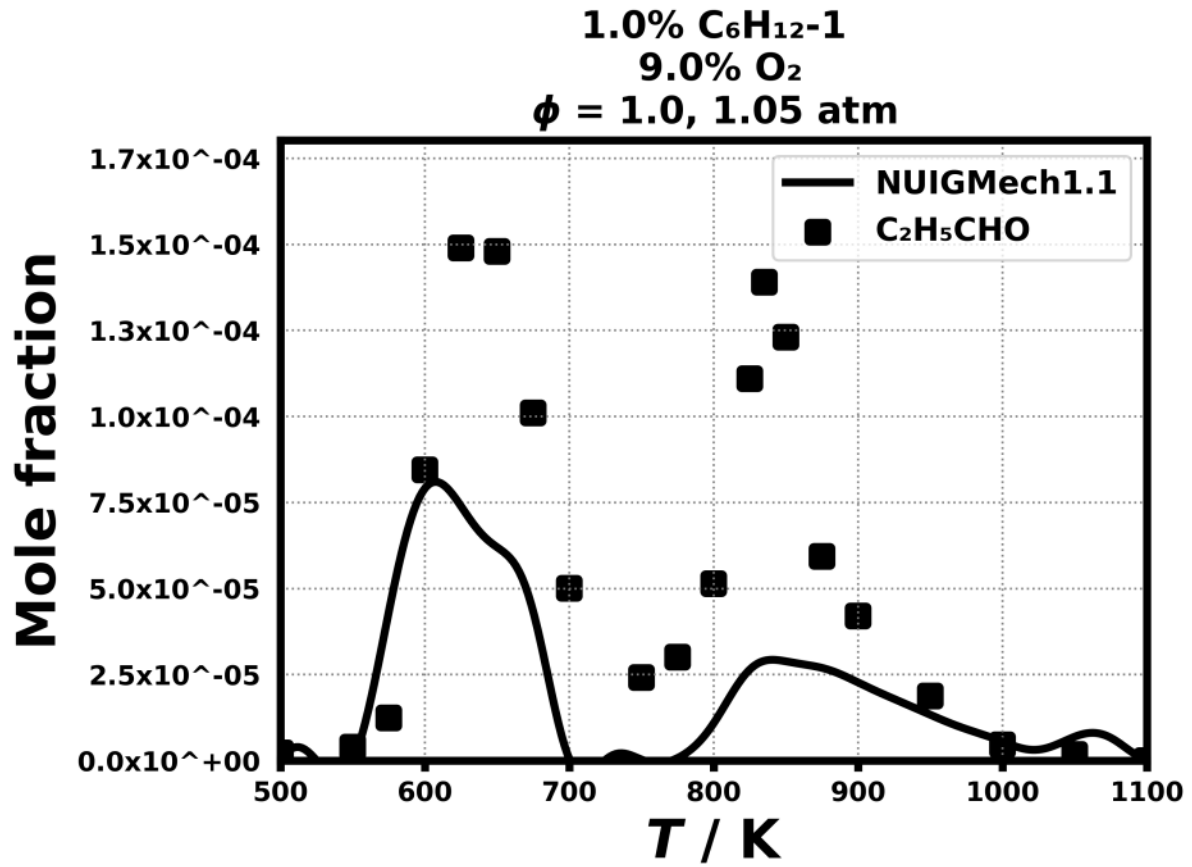


Figure 75: Dataset: 1.05_ATM_PHI_1.0

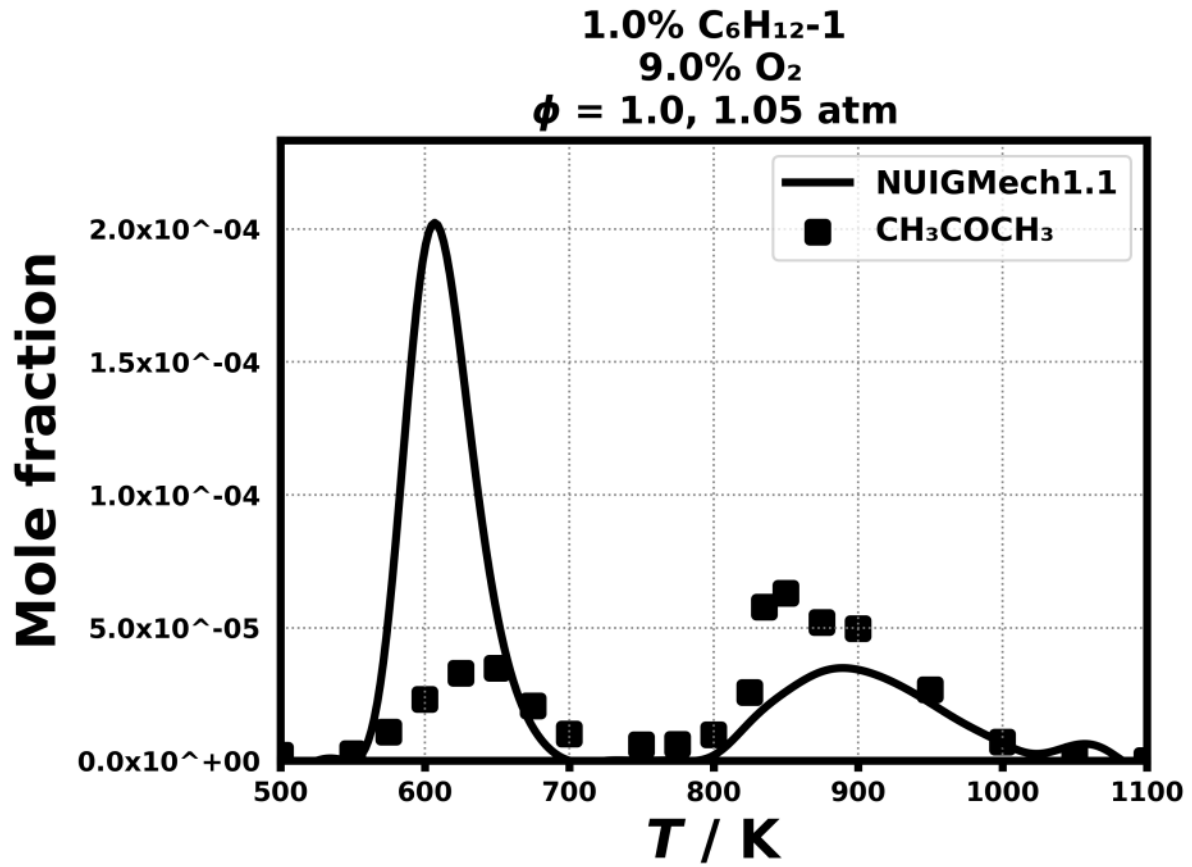


Figure 76: Dataset: 1.05_ATM_PHI_1.0

1.3.55 Case: C6H12-1/JSR/Meng/Meng_GC/1.05_ATM_PHI_1.0

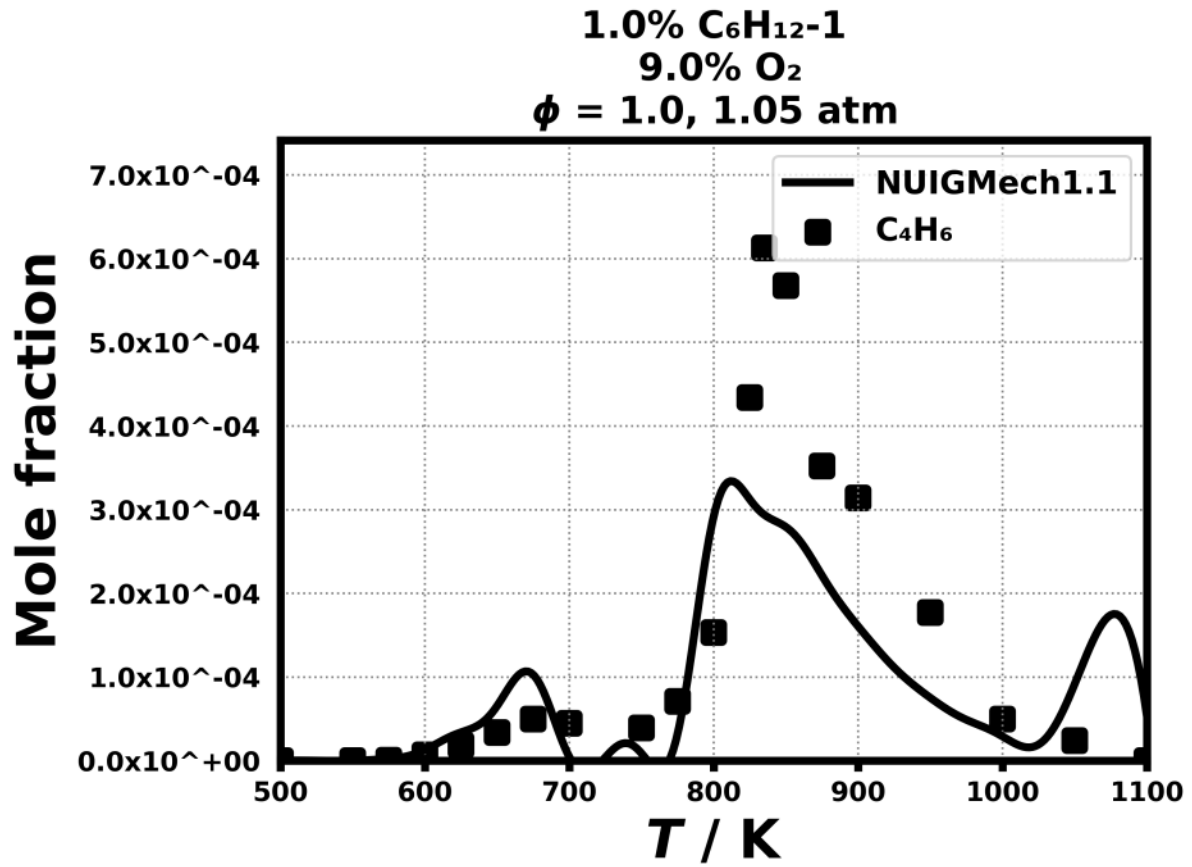


Figure 77: Dataset: 1.05_ATM_PHI_1.0

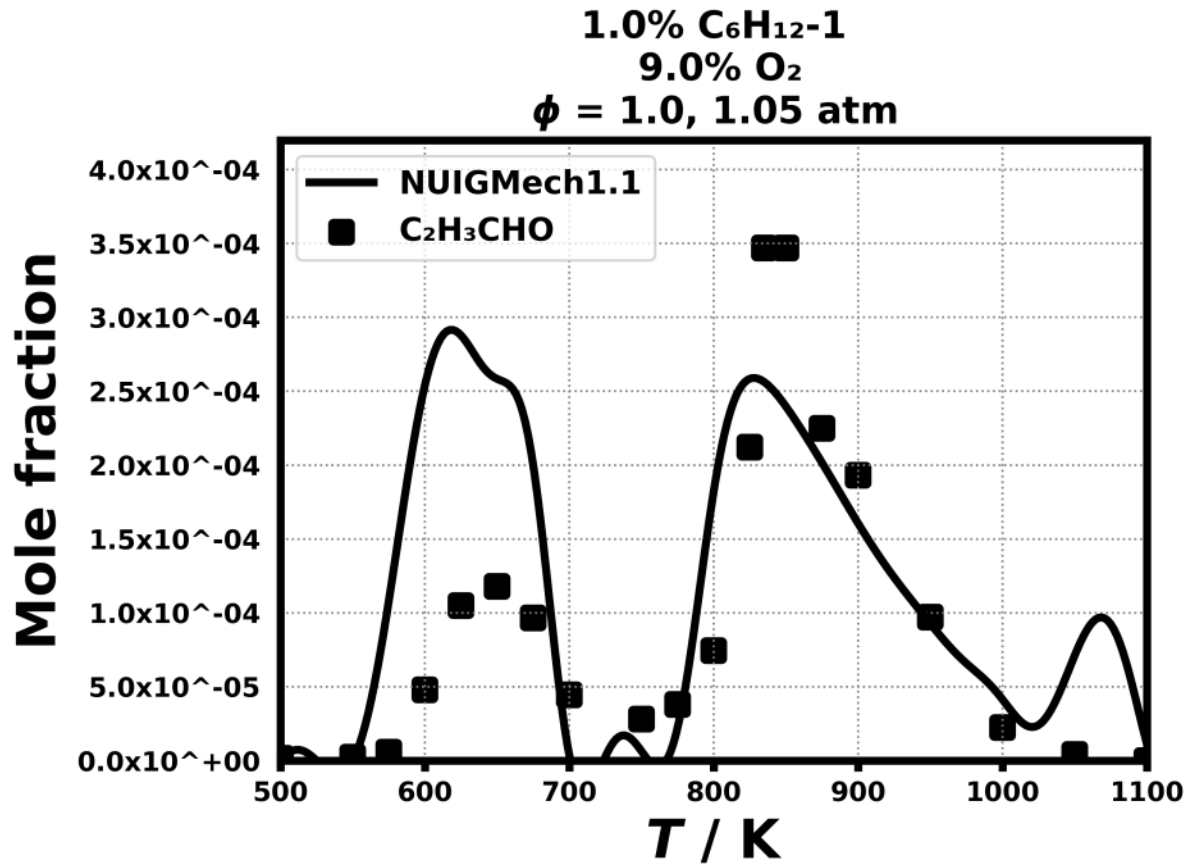


Figure 78: Dataset: 1.05_ATM_PHI_1.0

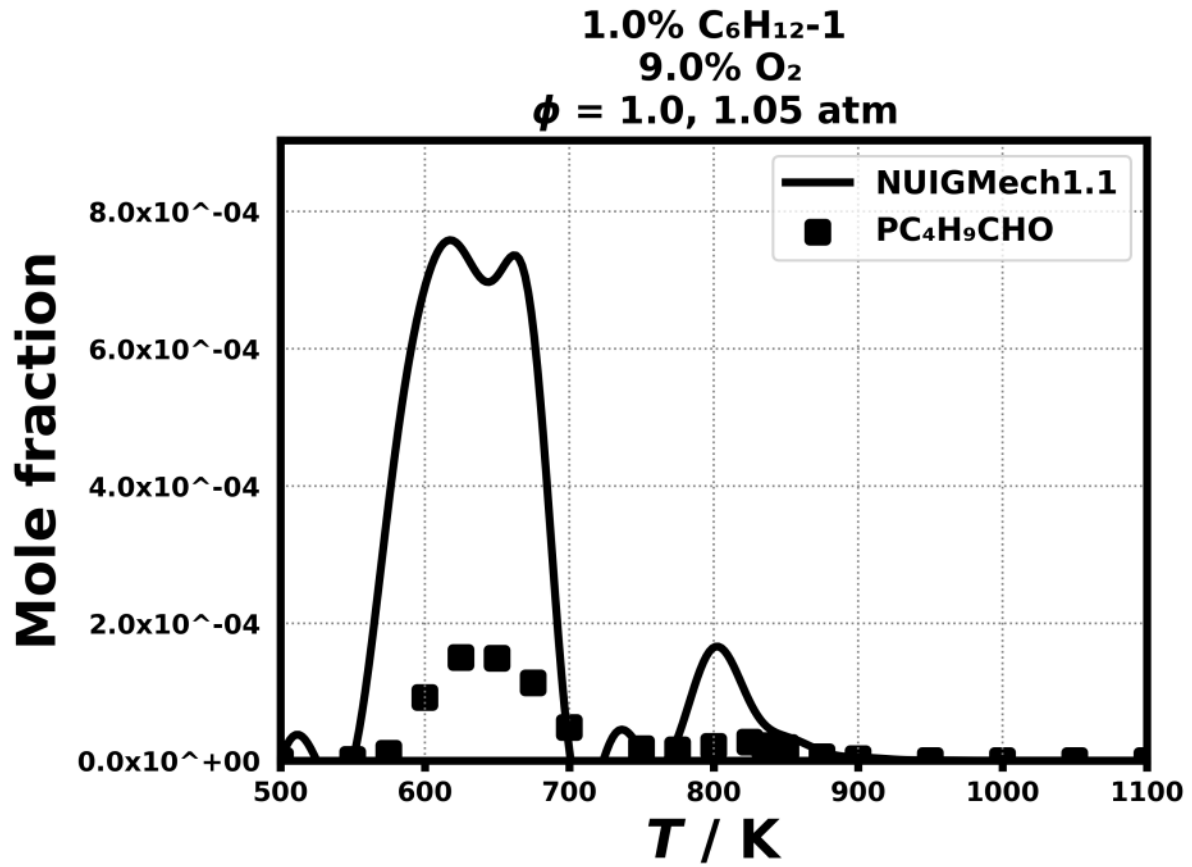


Figure 79: Dataset: 1.05_ATM_PHI_1.0

1.3.58 Case: C6H12-1/JSR/Meng/Meng_GC/1.05_ATM_PHI_1.0

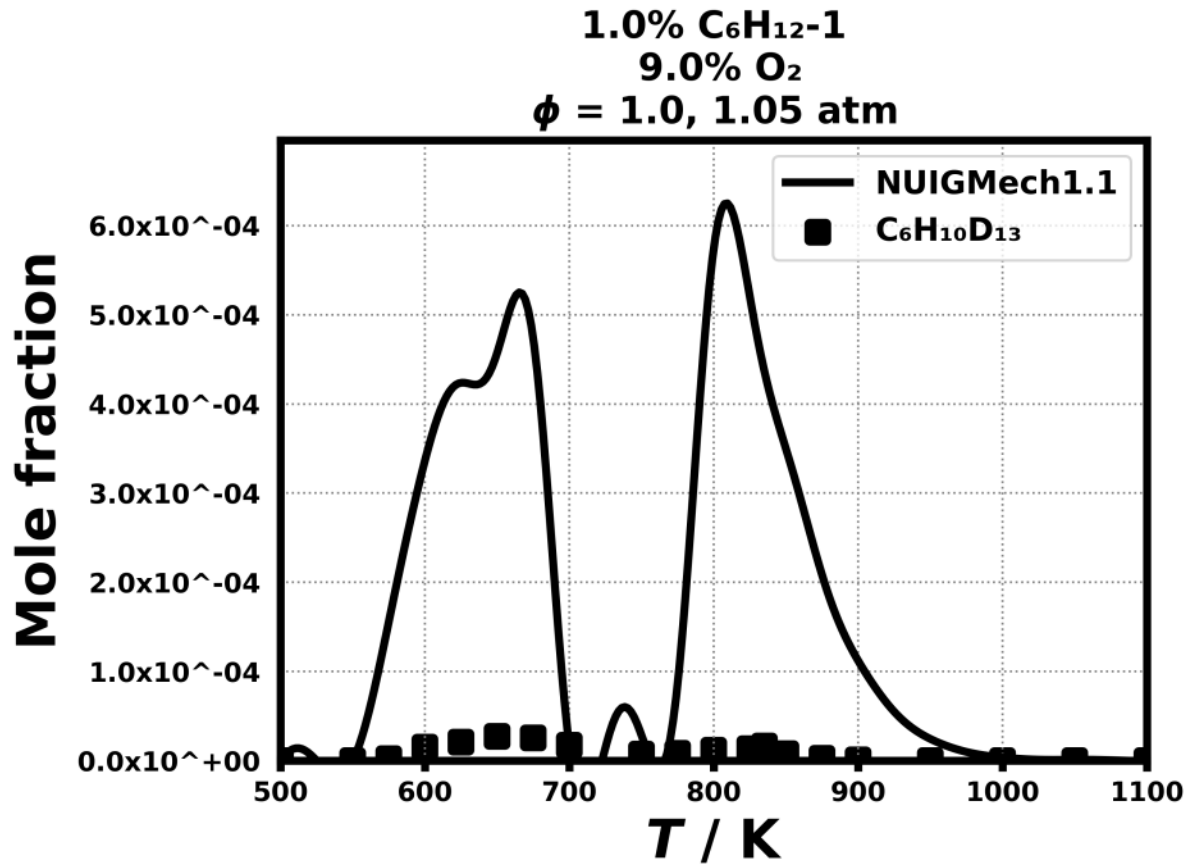


Figure 80: Dataset: 1.05_ATM_PHI_1.0

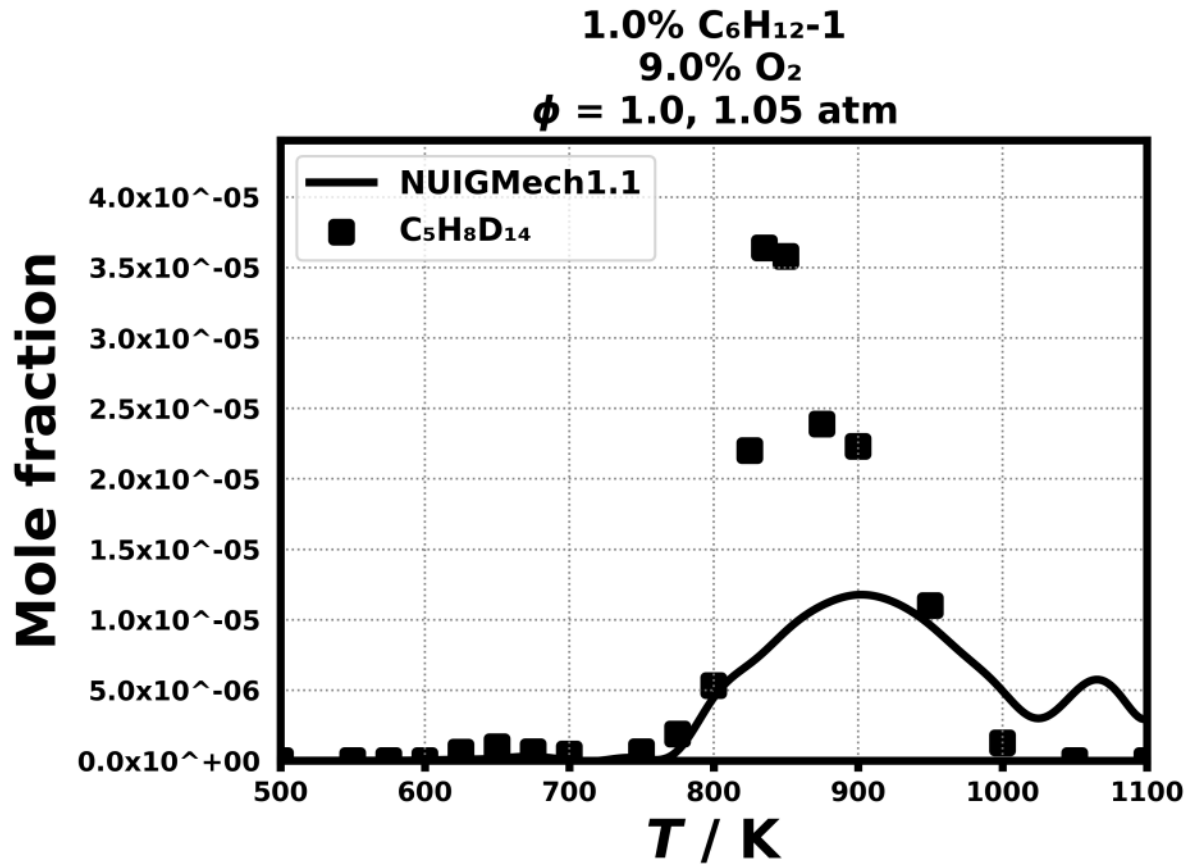


Figure 81: Dataset: 1.05_ATM_PHI_1.0

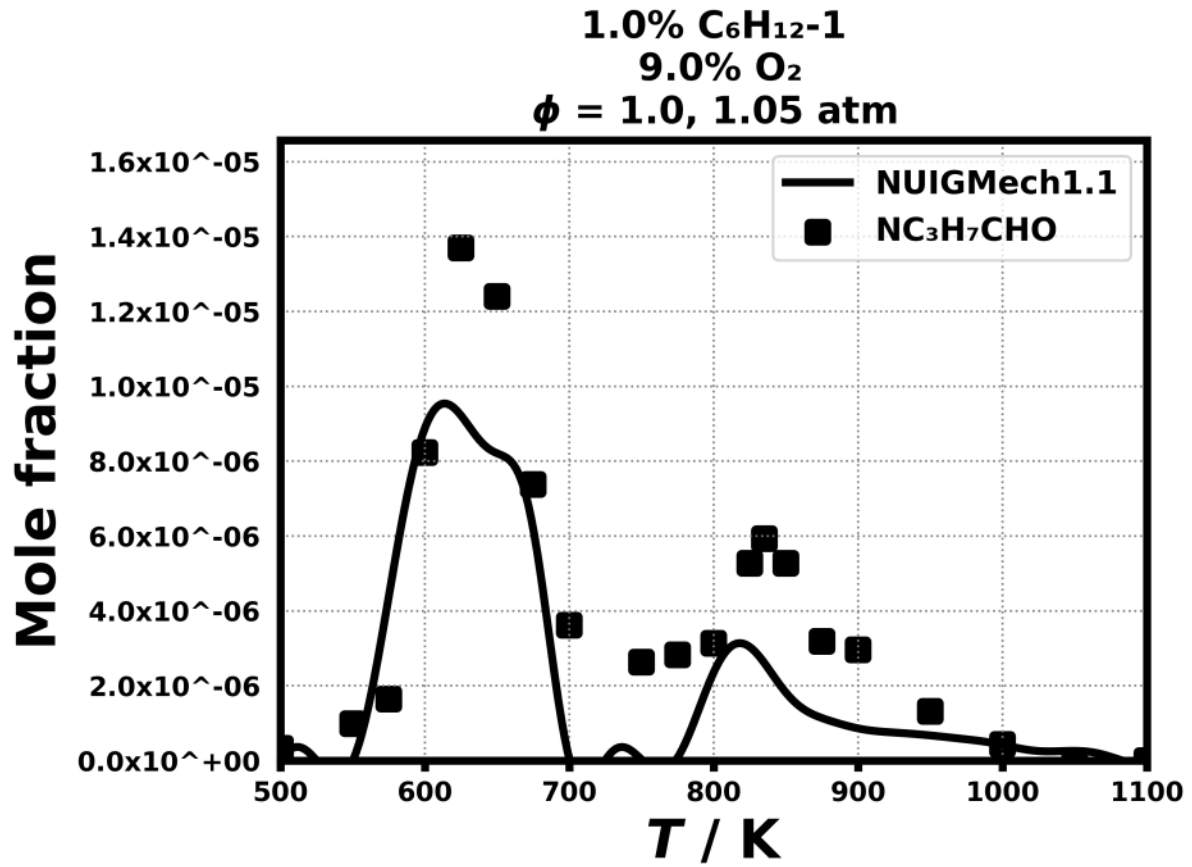


Figure 82: Dataset: 1.05_ATM_PHI_1.0

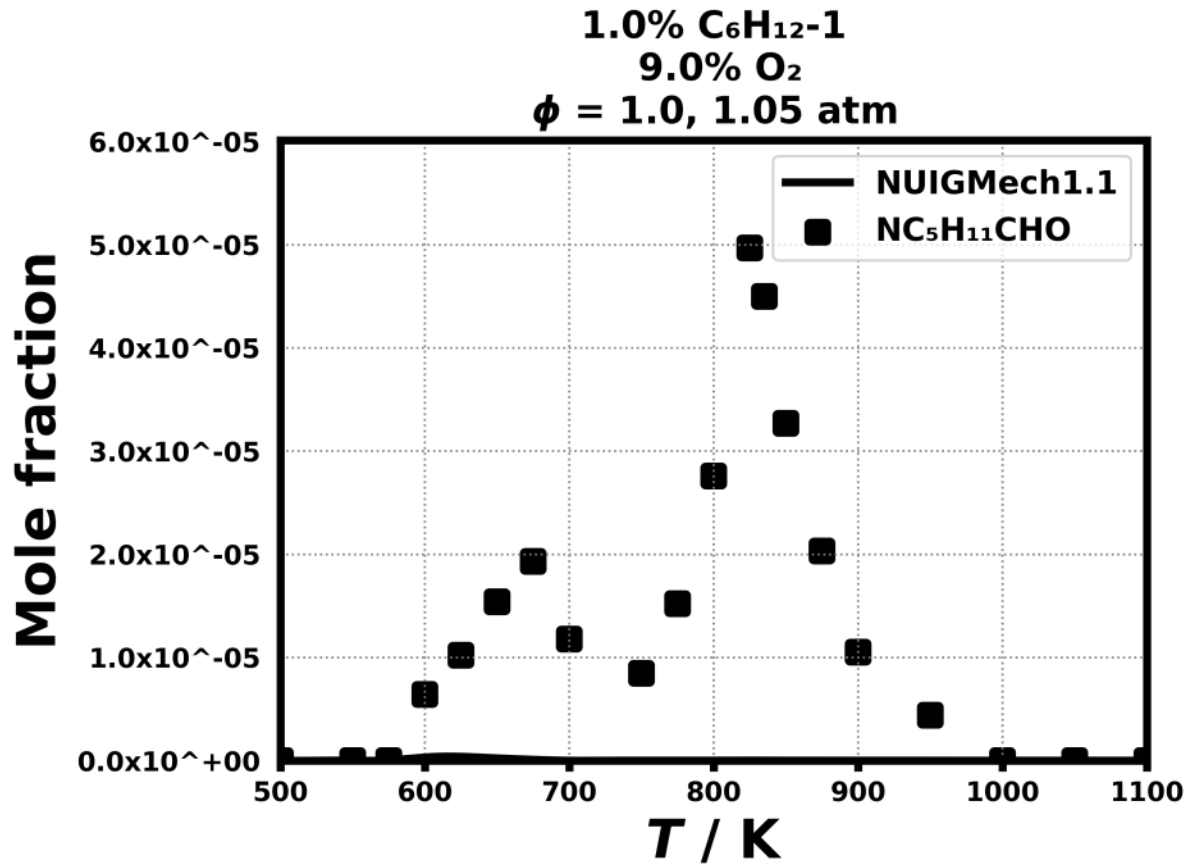


Figure 83: Dataset: 1.05_ATM_PHI_1.0

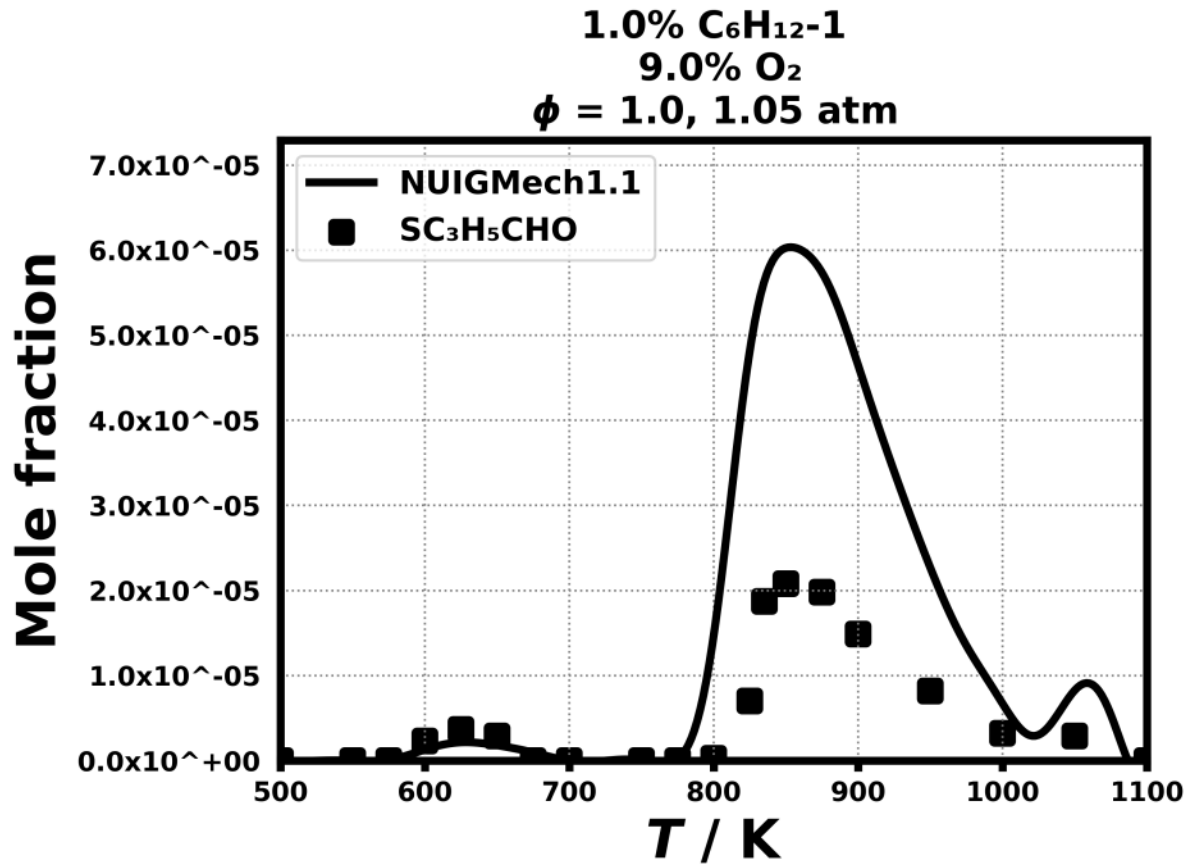


Figure 84: Dataset: 1.05_ATM_PHI_1.0

1.3.63 Case: C6H12-1/JSR/Meng/Meng_GC/1.05_ATM_PHI_1.0

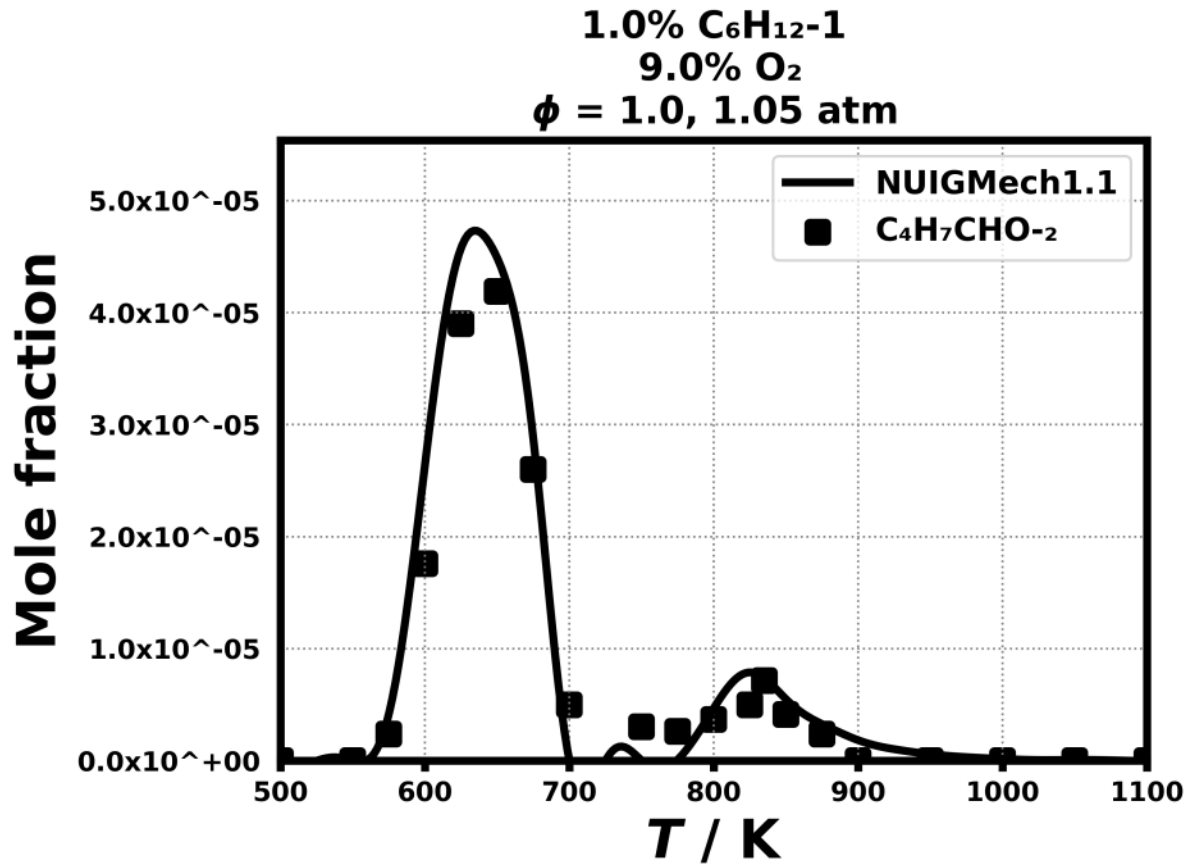


Figure 85: Dataset: 1.05_ATM_PHI_1.0

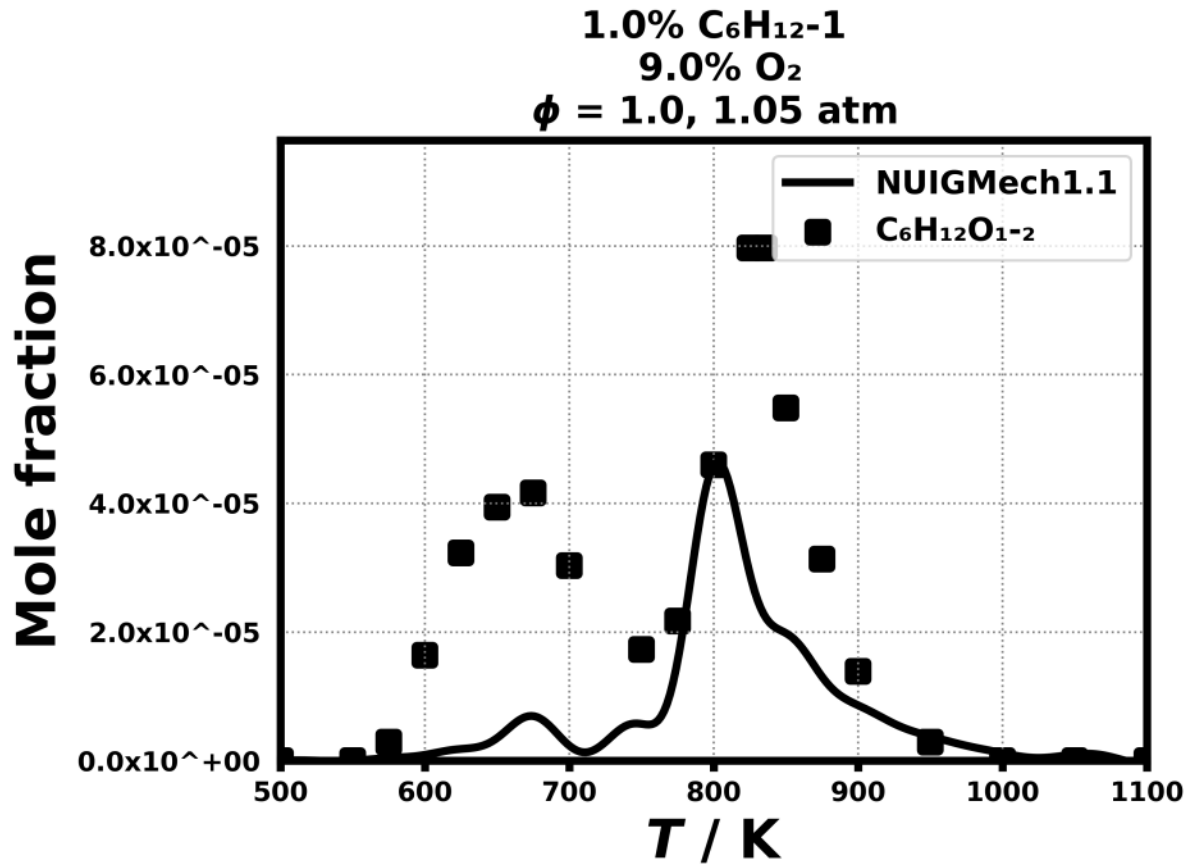


Figure 86: Dataset: 1.05_ATM_PHI_1.0

1.3.65 Case: C6H12-1/JSR/Meng/Meng_GC/1.05_ATM_PHI_1.0

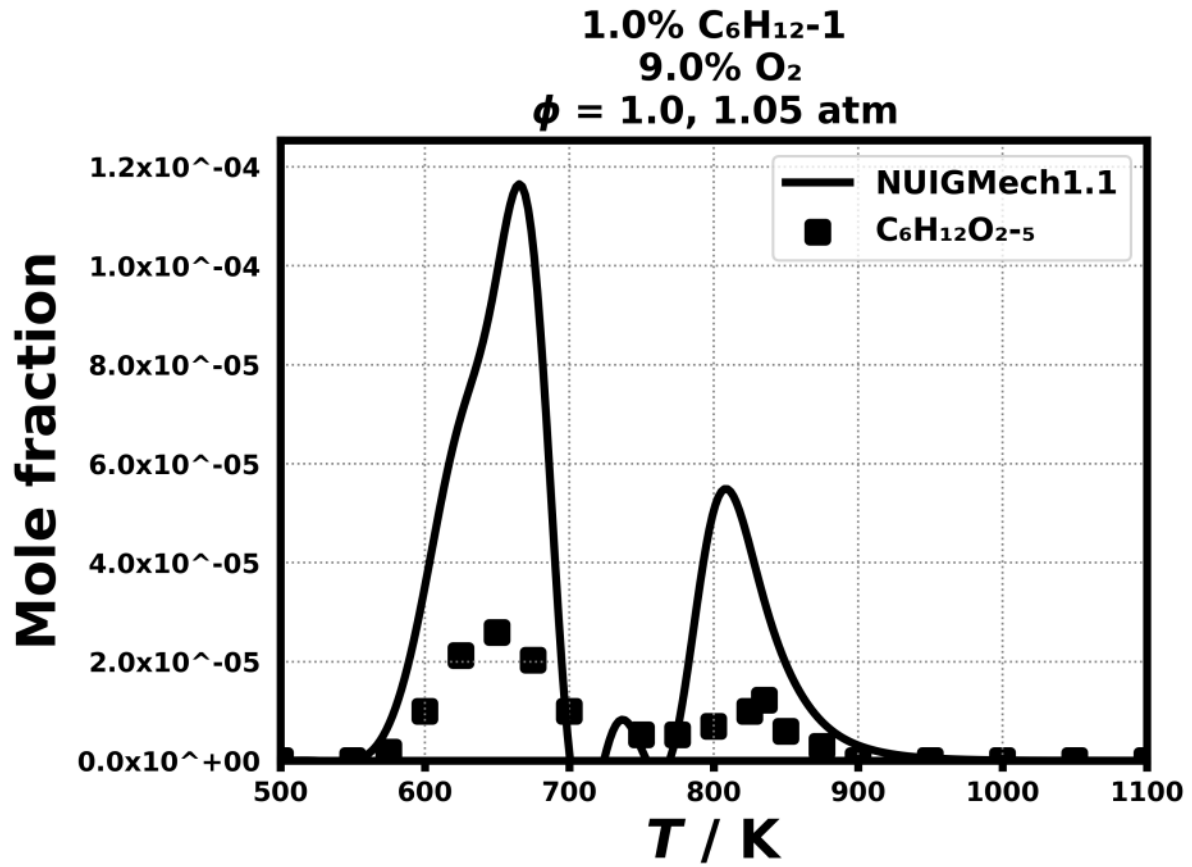


Figure 87: Dataset: 1.05_ATM_PHI_1.0

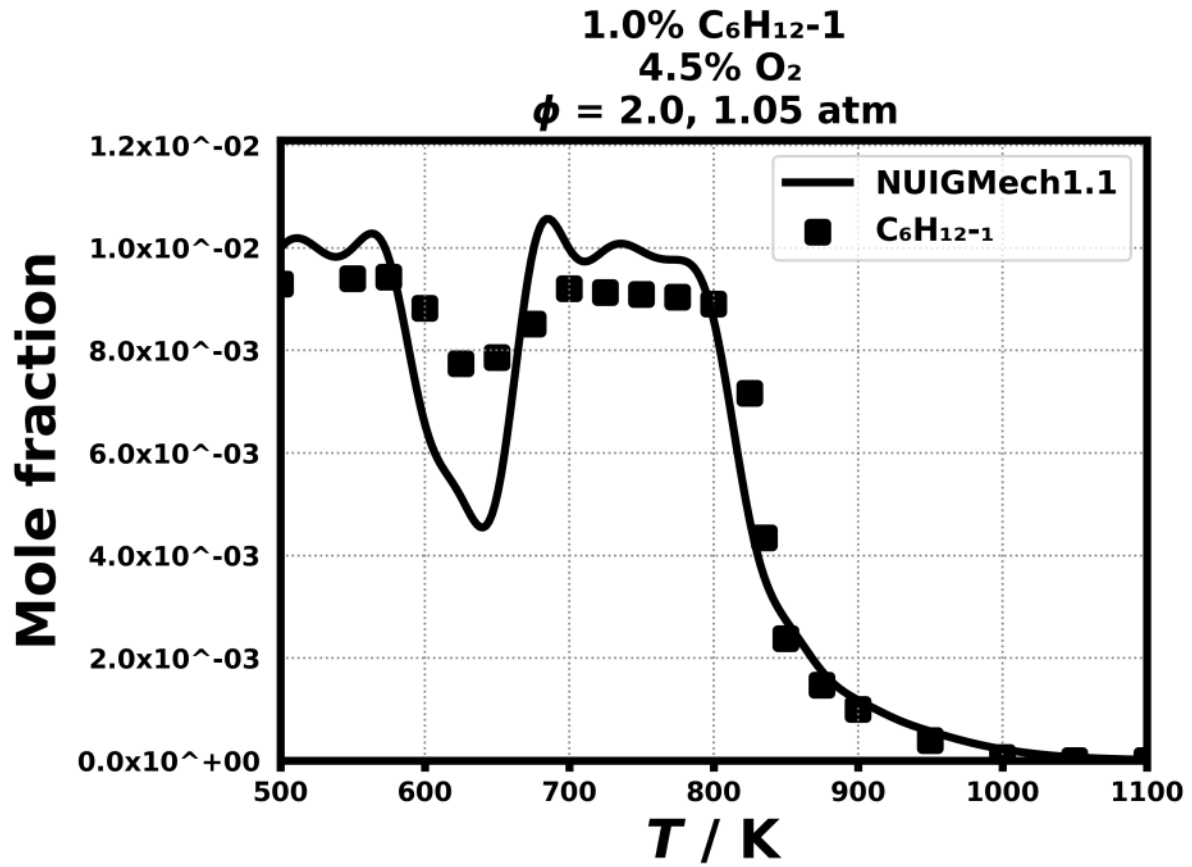


Figure 88: Dataset: 1.05_ATM_PHI_2.0

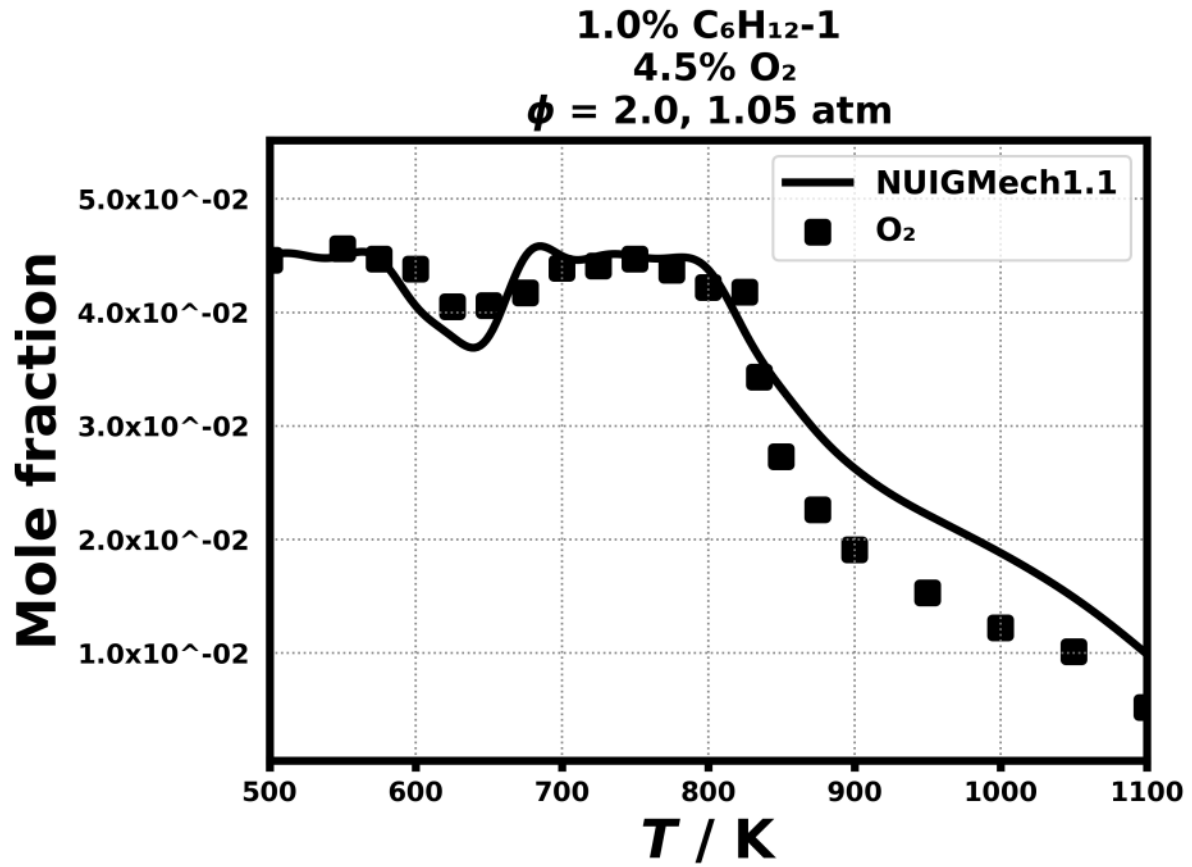


Figure 89: Dataset: 1.05_ATM_PHI_2.0

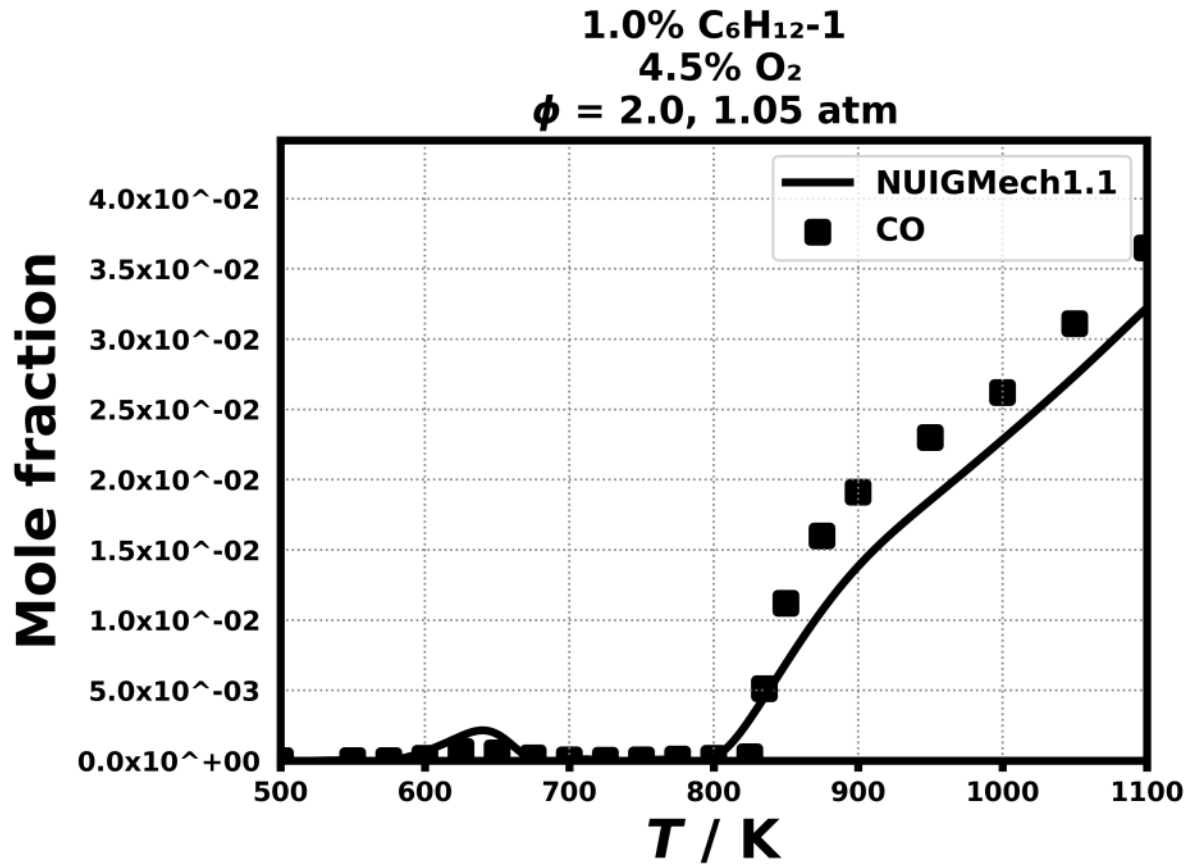


Figure 90: Dataset: 1.05_ATM_PHI_2.0

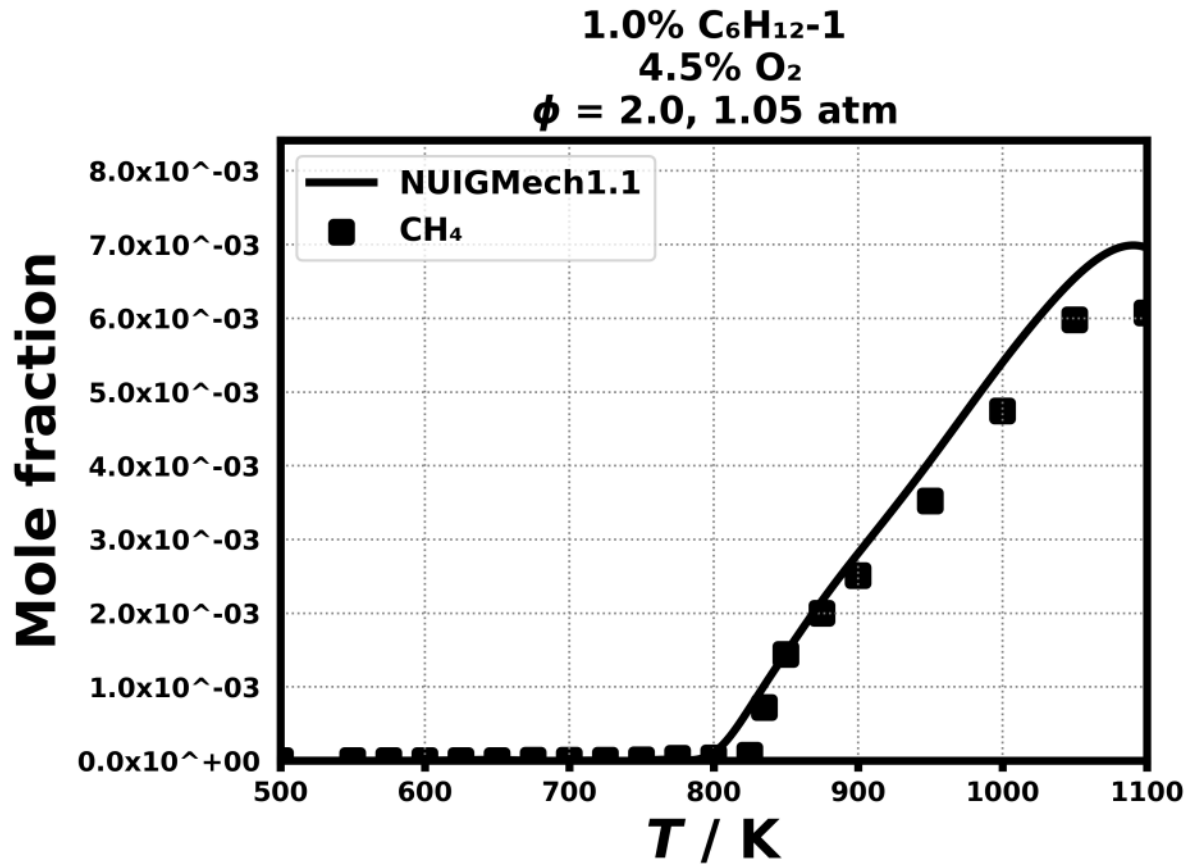


Figure 91: Dataset: 1.05_ATM_PHI_2.0

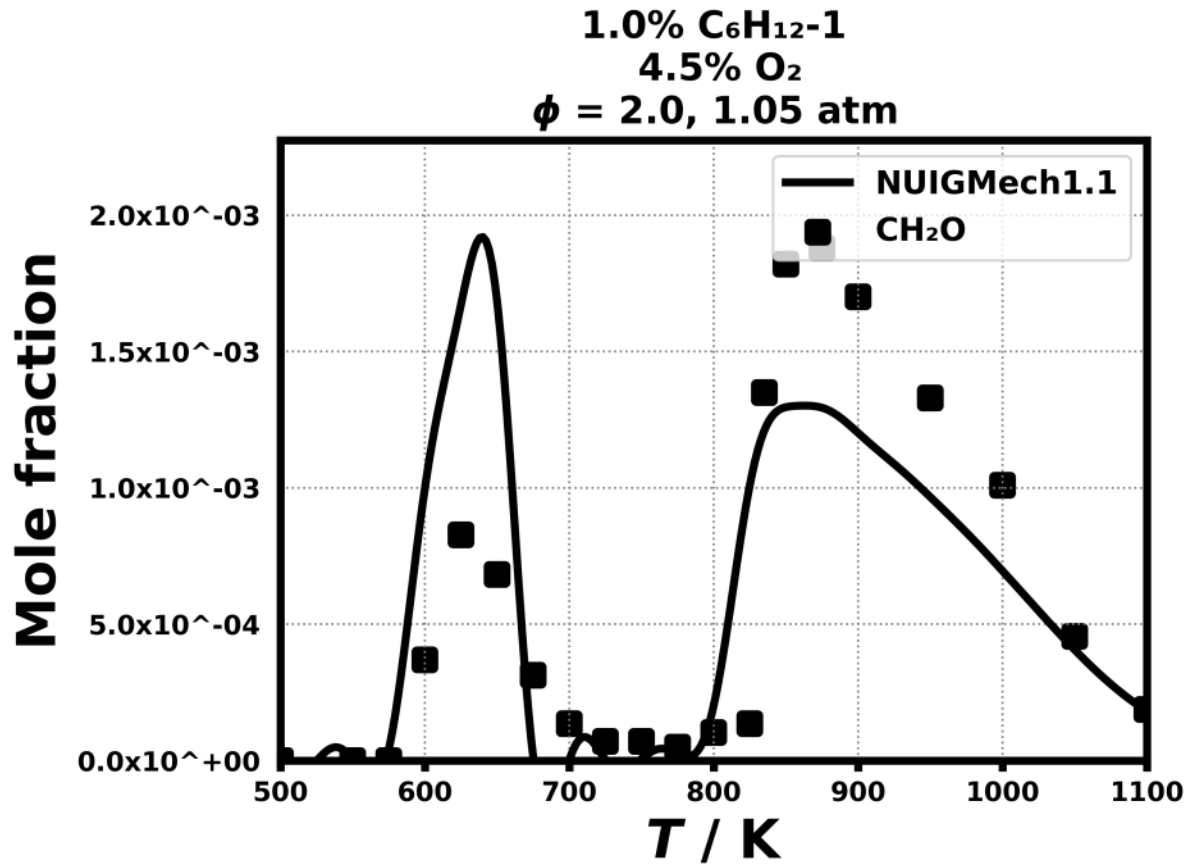


Figure 92: Dataset: 1.05_ATM_PHI_2.0

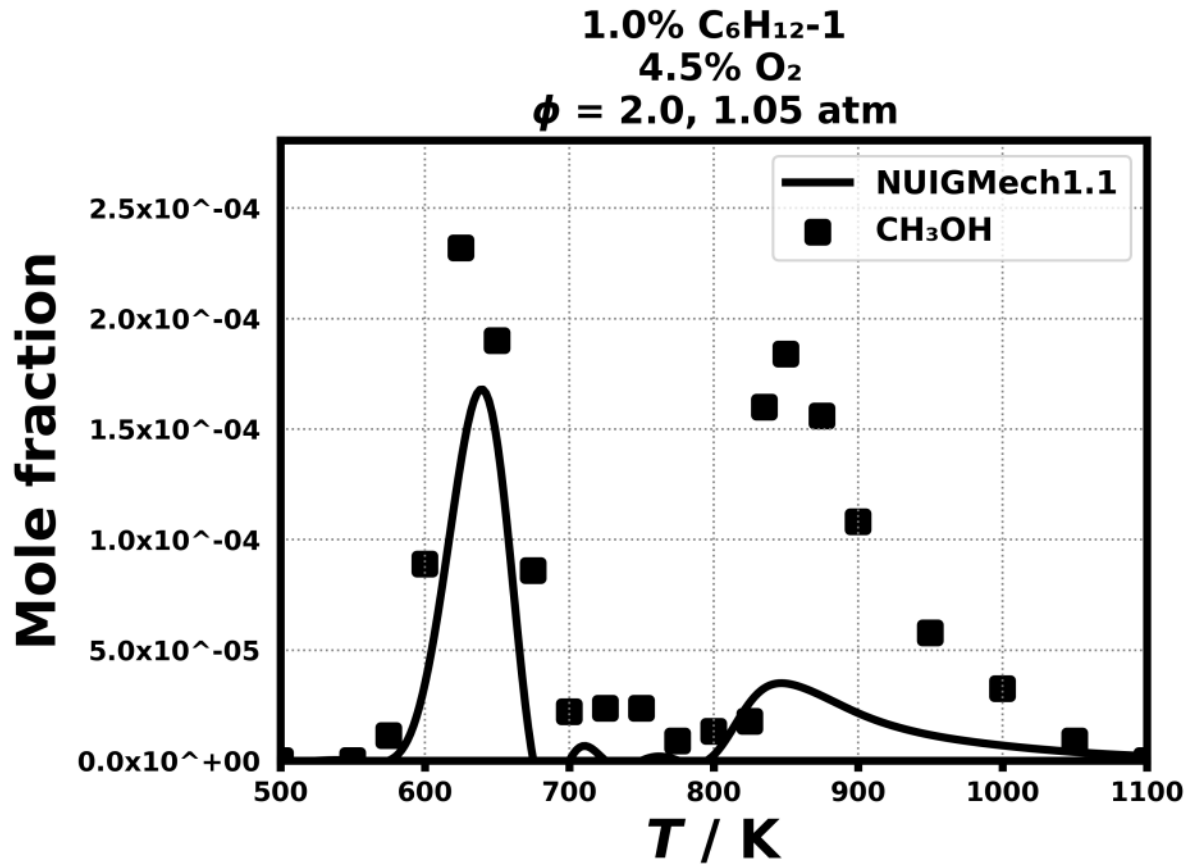


Figure 93: Dataset: 1.05_ATM_PHI_2.0

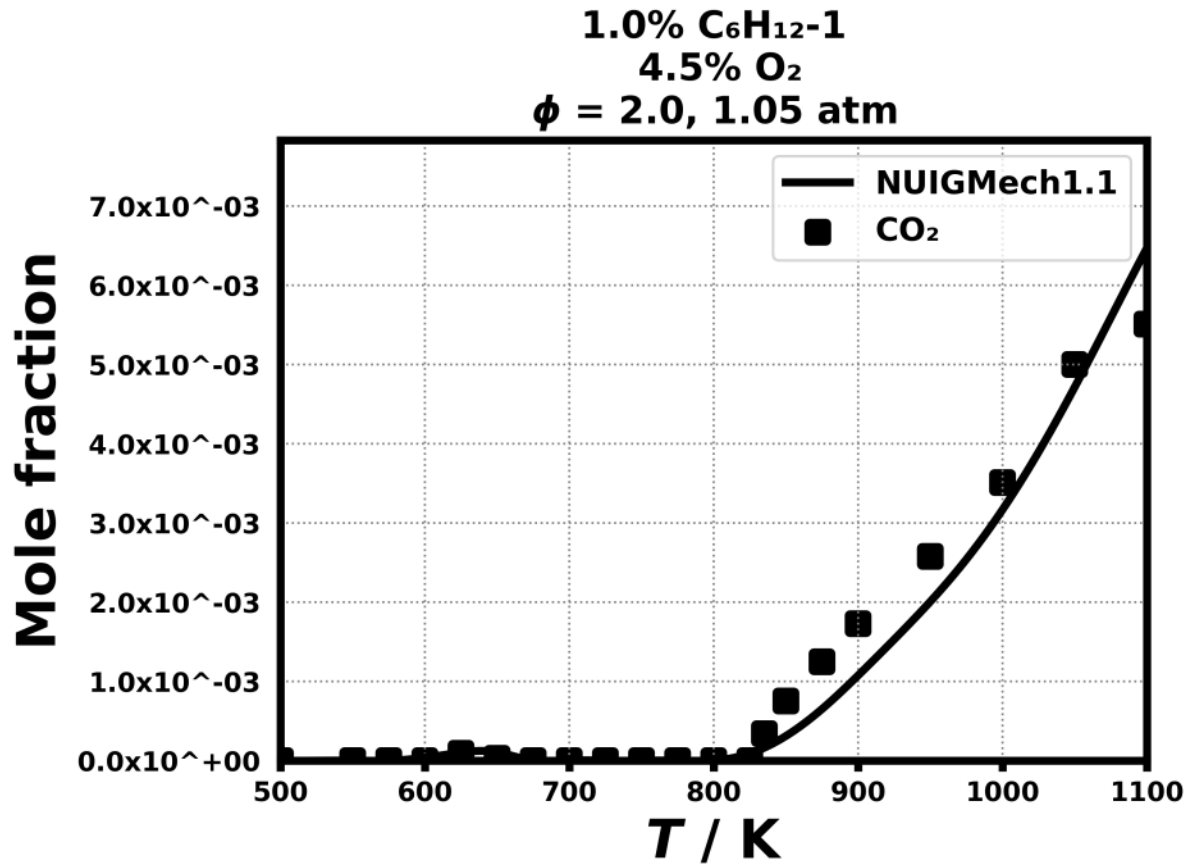


Figure 94: Dataset: 1.05_ATM_PHI_2.0

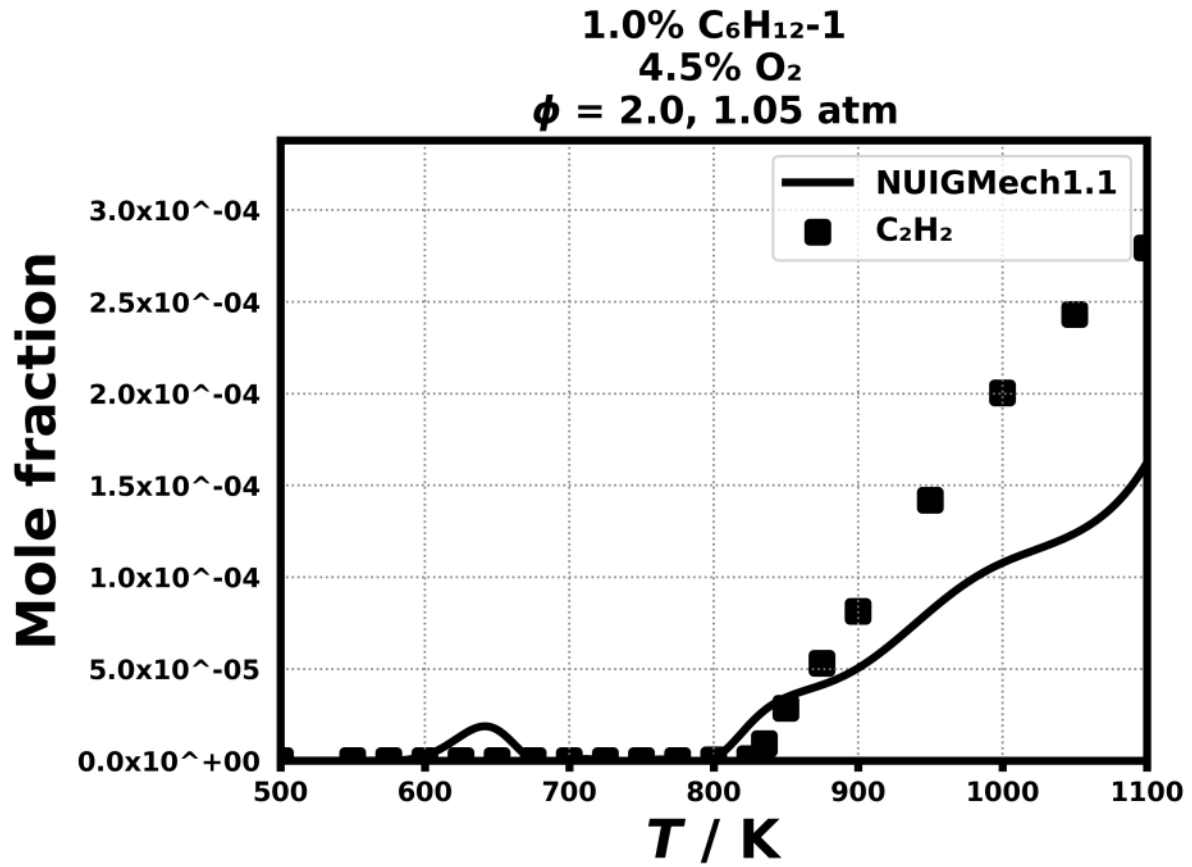


Figure 95: Dataset: 1.05_ATM_PHI_2.0

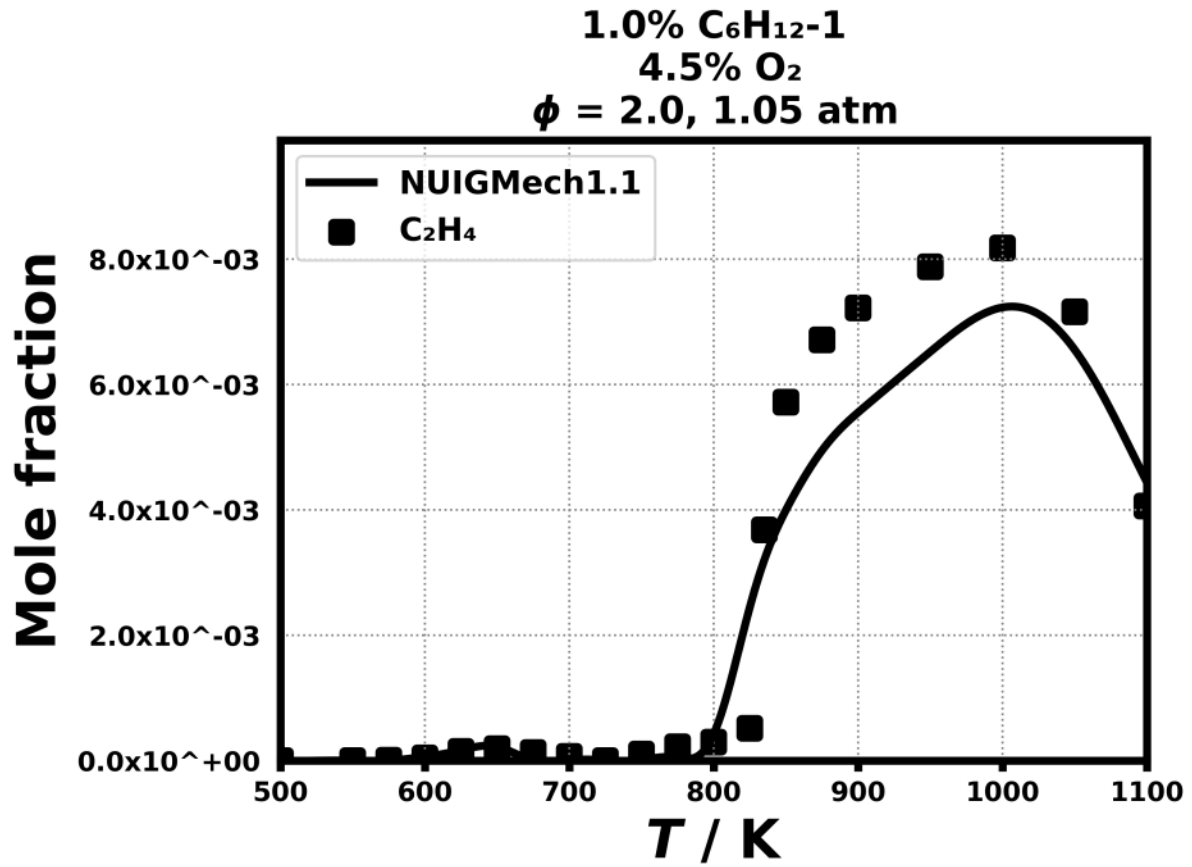


Figure 96: Dataset: 1.05_ATM_PHI_2.0

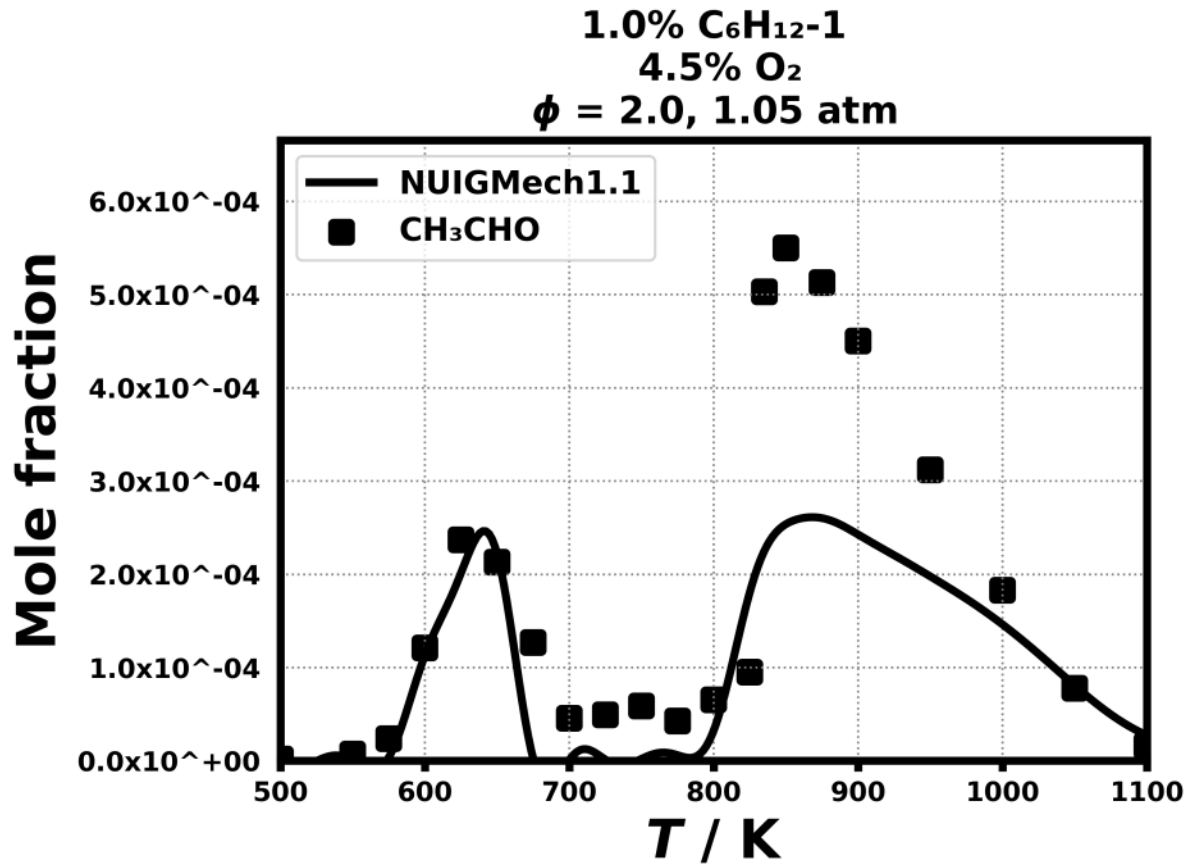


Figure 97: Dataset: 1.05_ATM_PHI_2.0

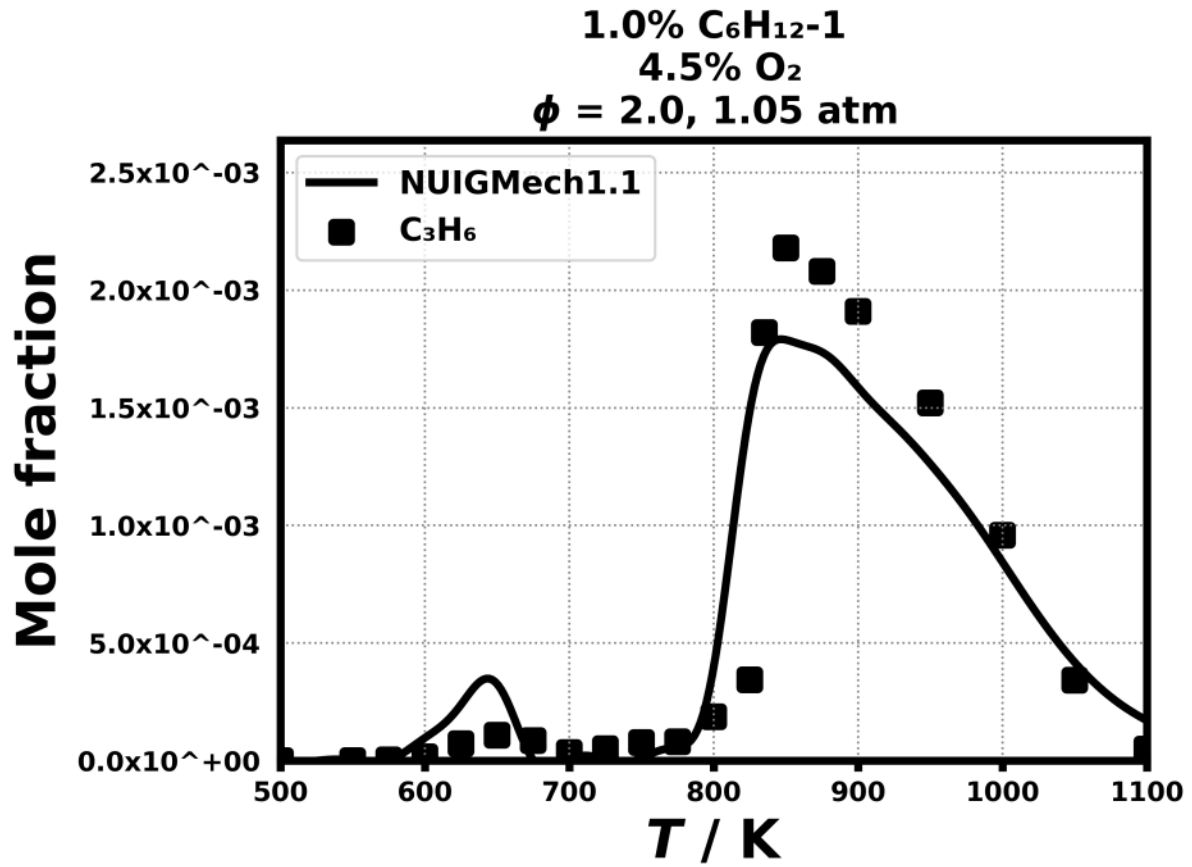


Figure 98: Dataset: 1.05_ATM_PHI_2.0

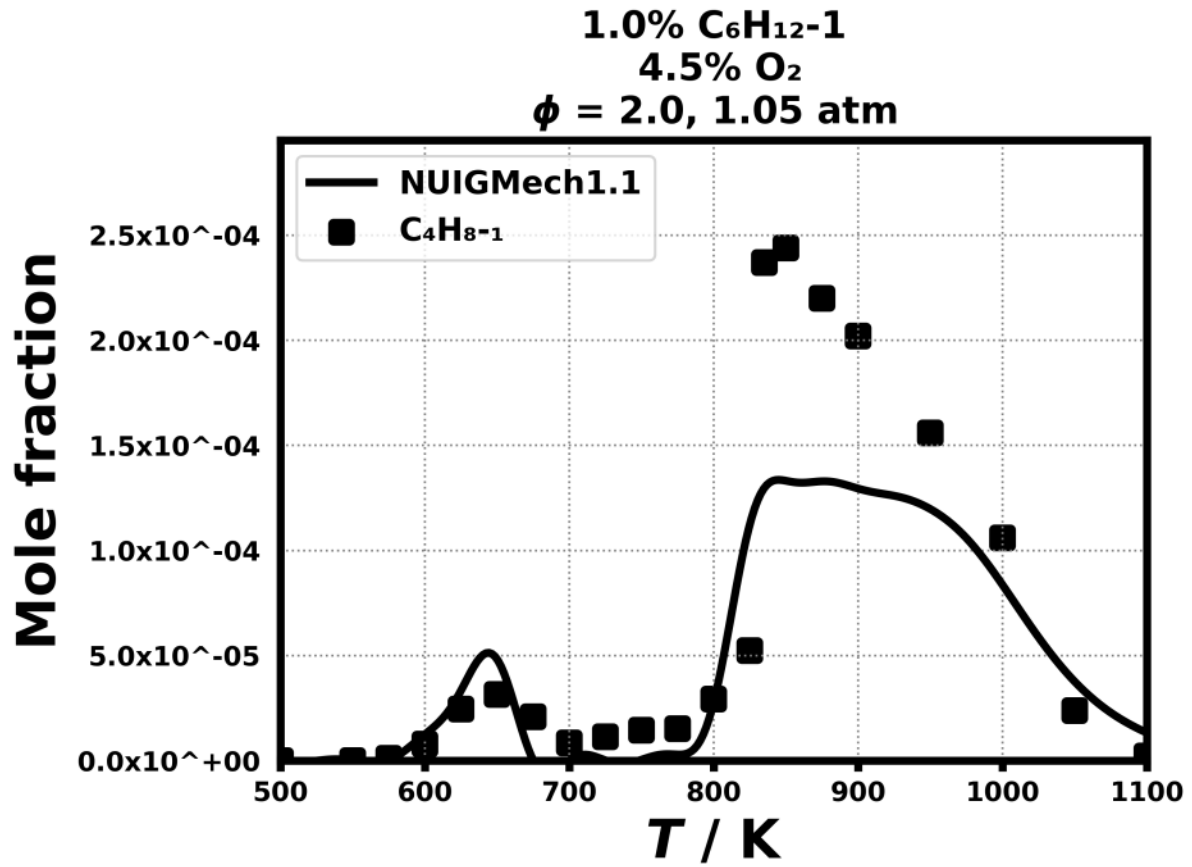


Figure 99: Dataset: 1.05_ATM_PHI_2.0

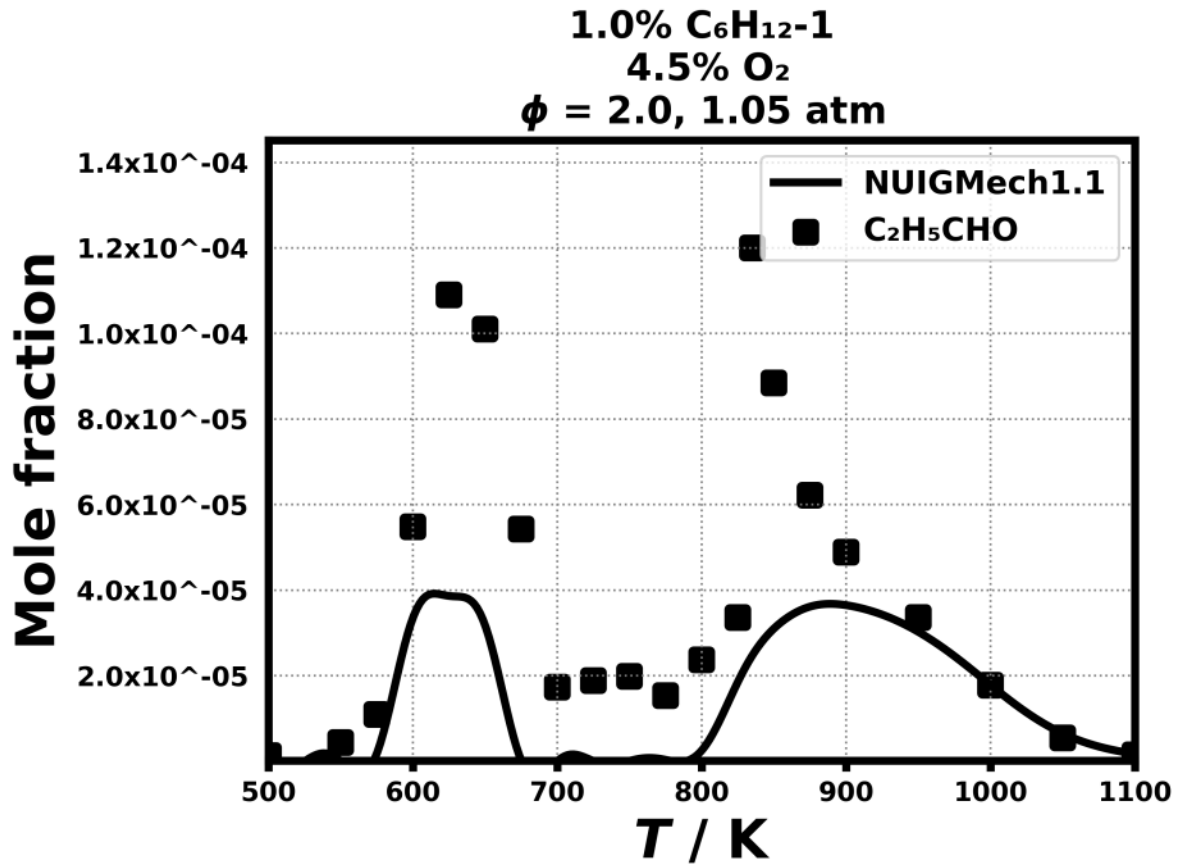


Figure 100: Dataset: 1.05_ATM_PHI_2.0

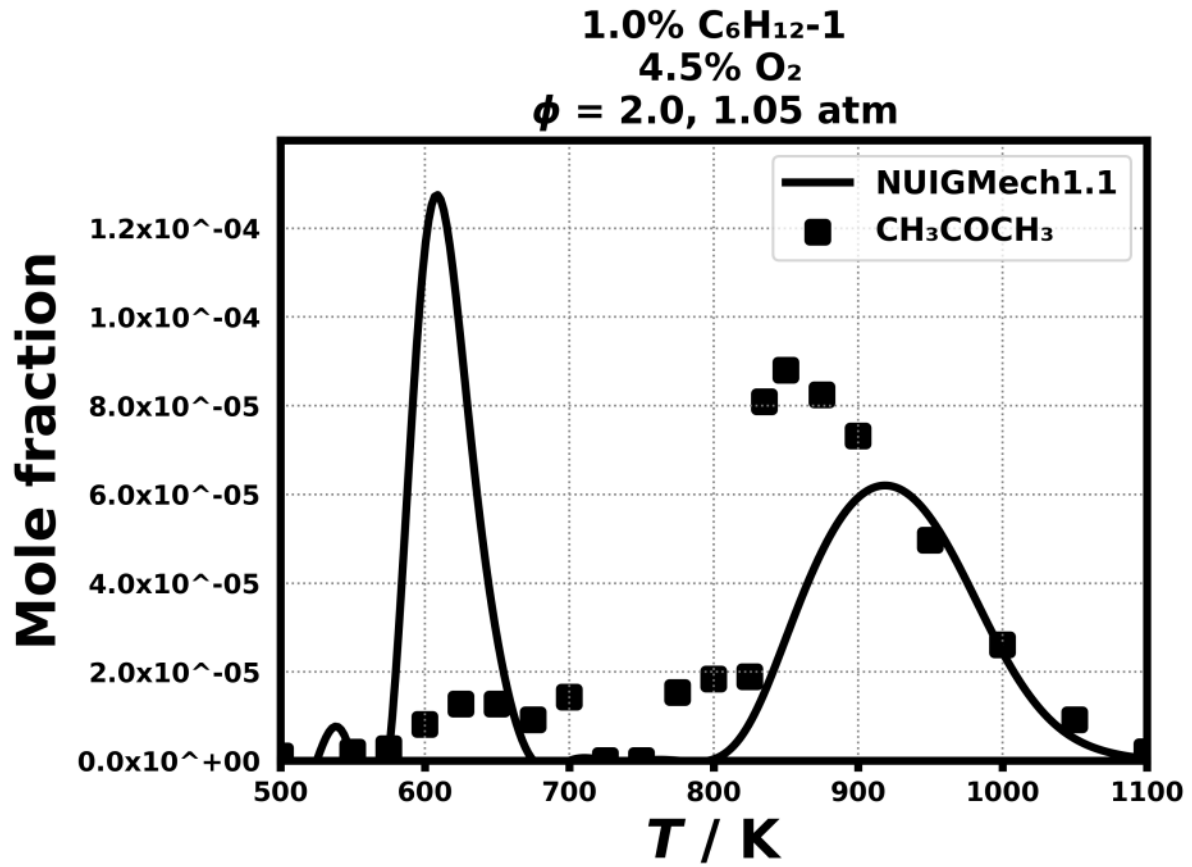


Figure 101: Dataset: 1.05_ATM_PHI_2.0

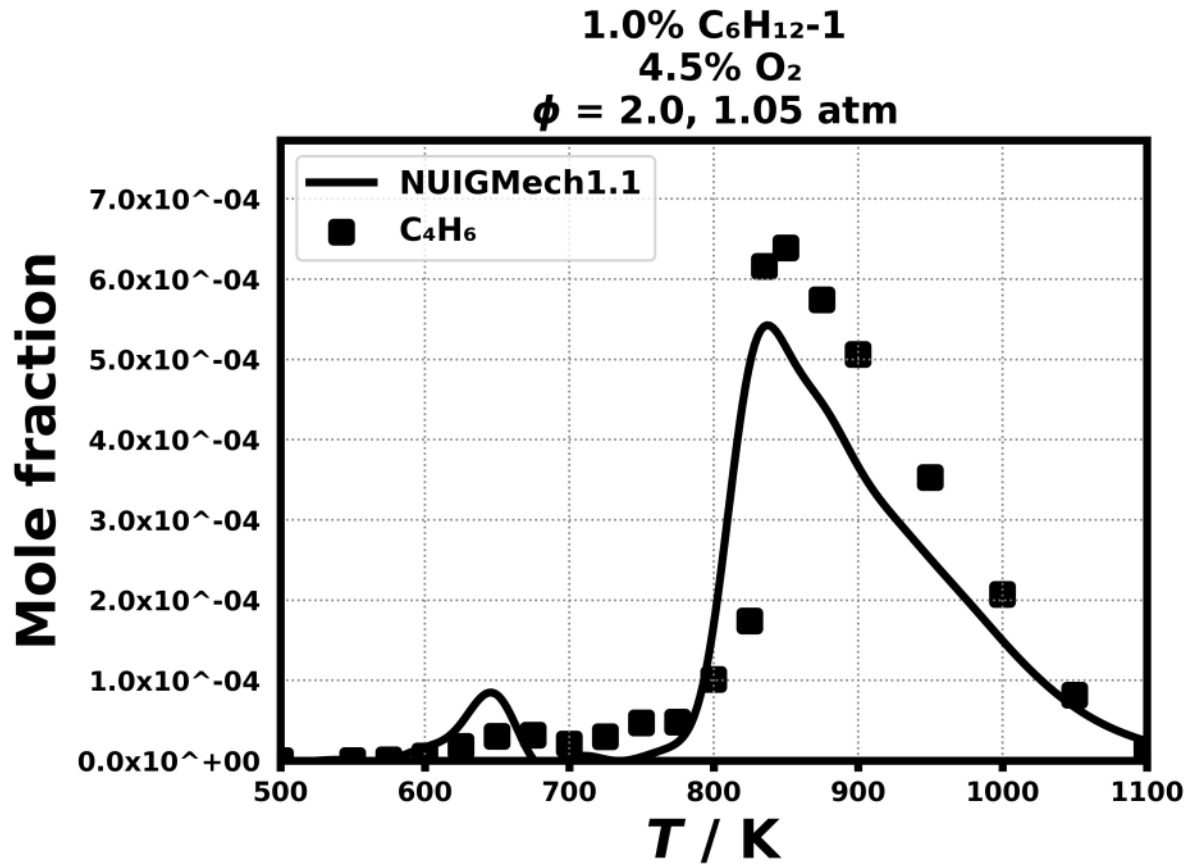


Figure 102: Dataset: 1.05_ATM_PHI_2.0

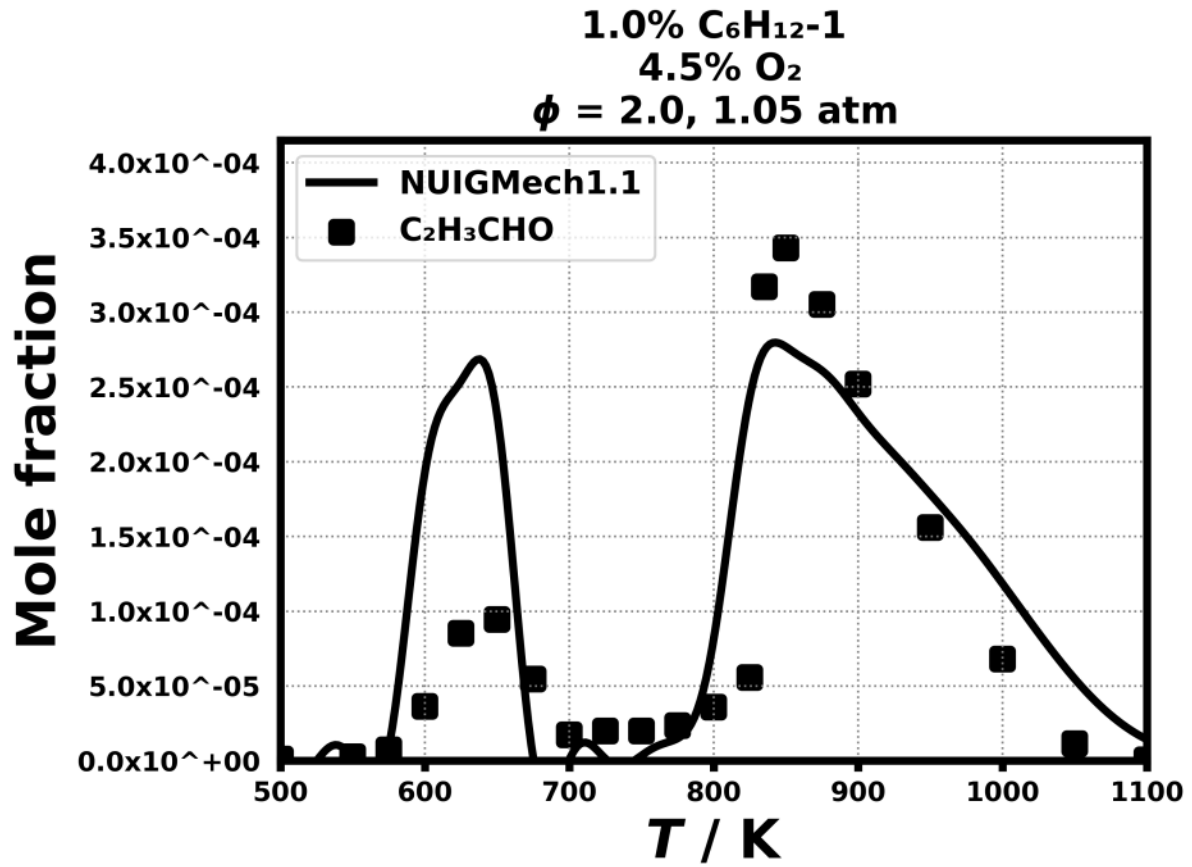


Figure 103: Dataset: 1.05_ATM_PHI_2.0

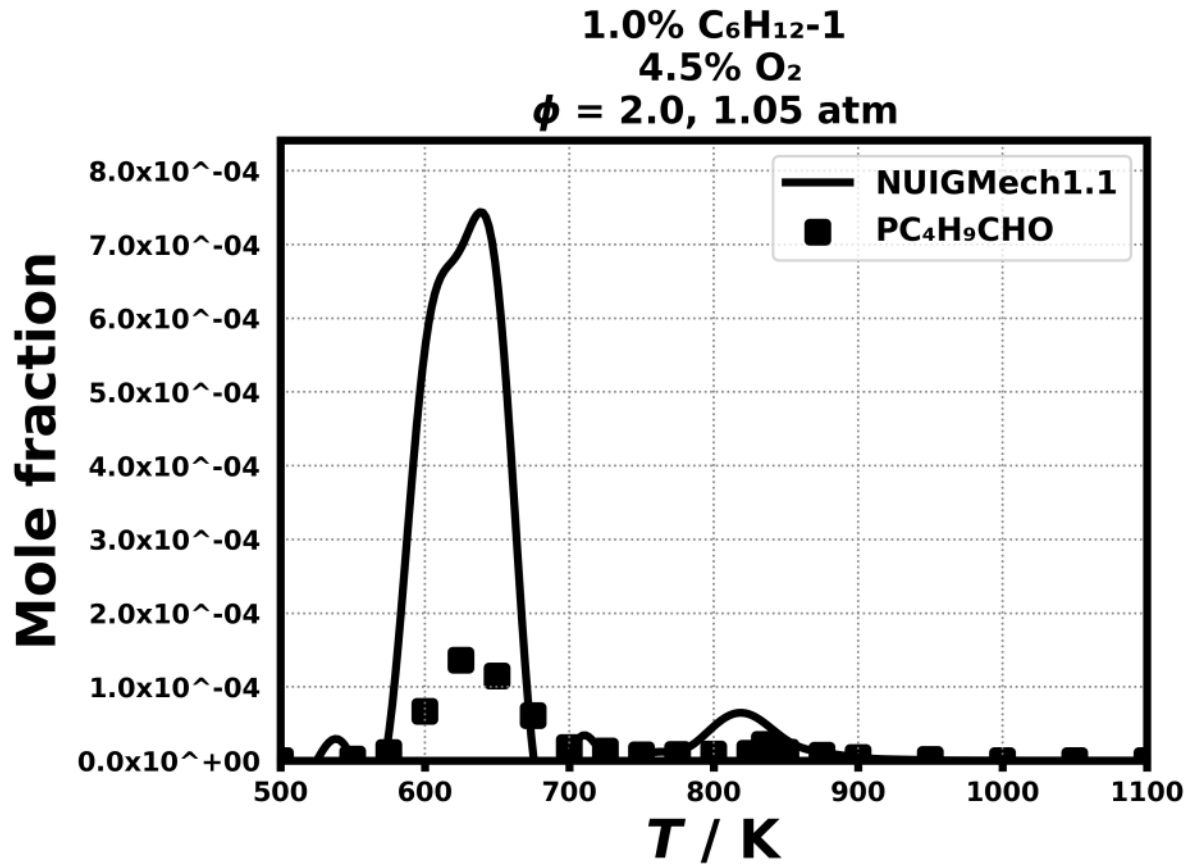


Figure 104: Dataset: 1.05_ATM_PHI_2.0

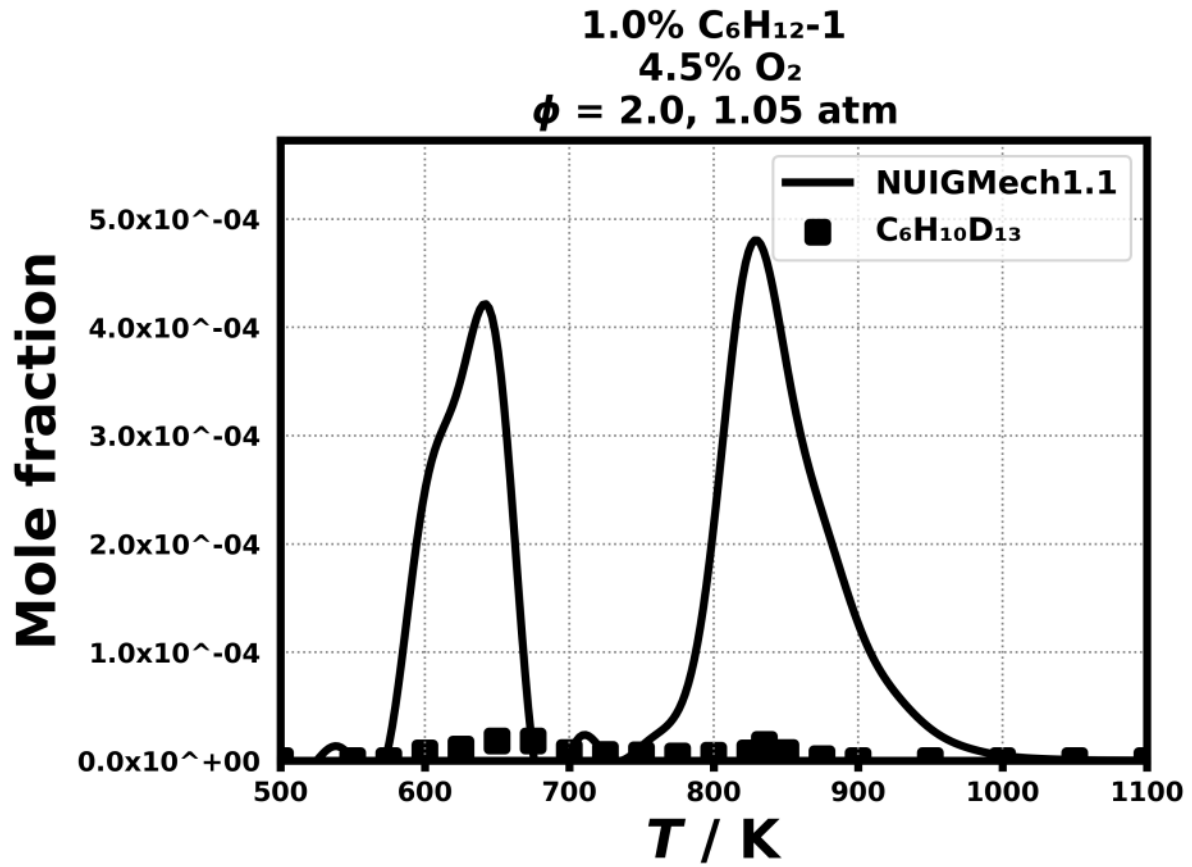


Figure 105: Dataset: 1.05_ATM_PHI_2.0

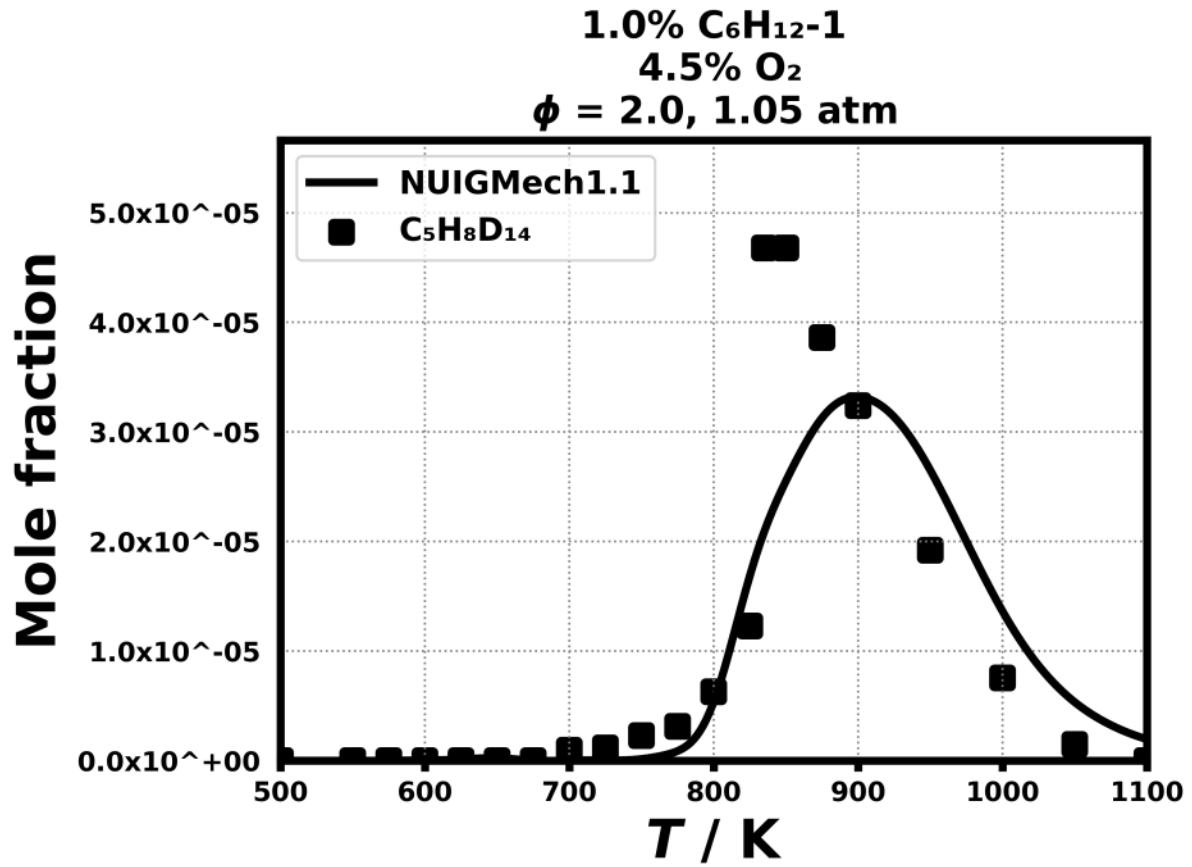


Figure 106: Dataset: 1.05_ATM_PHI_2.0

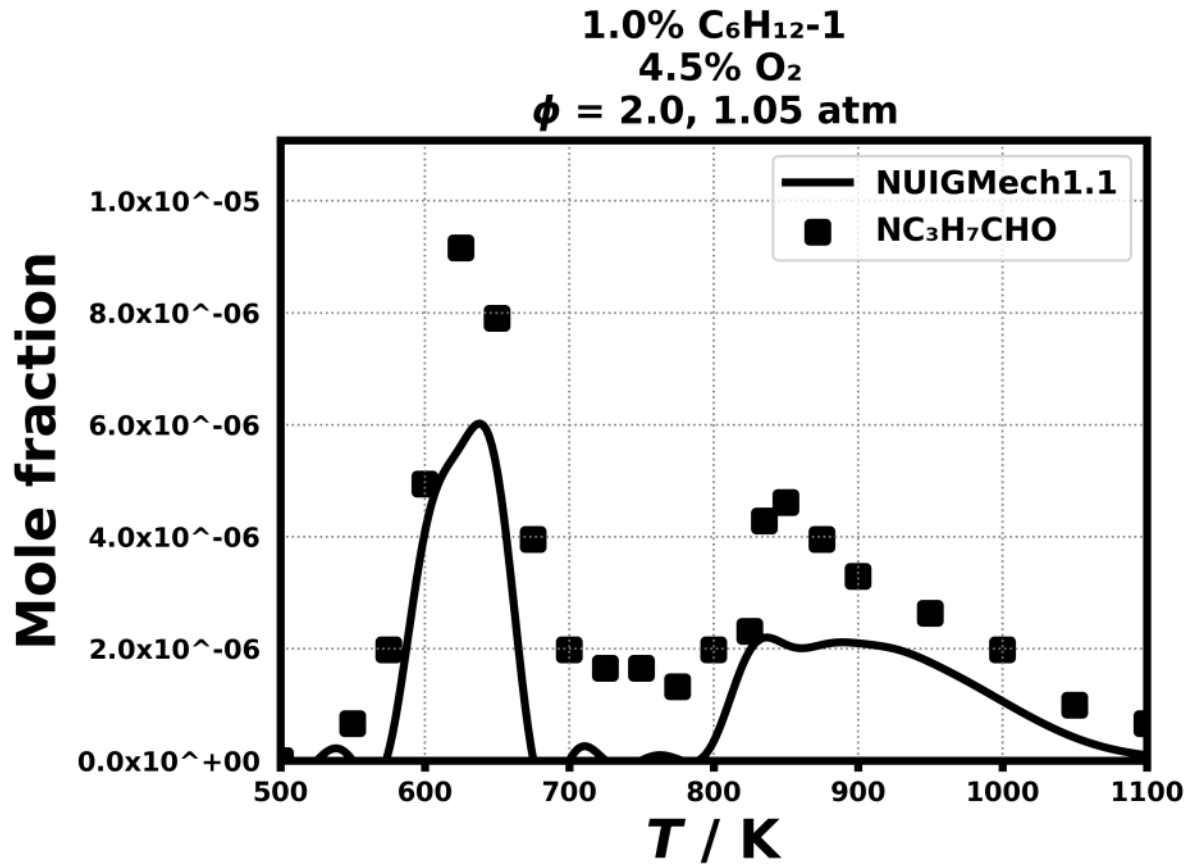


Figure 107: Dataset: 1.05_ATM_PHI_2.0

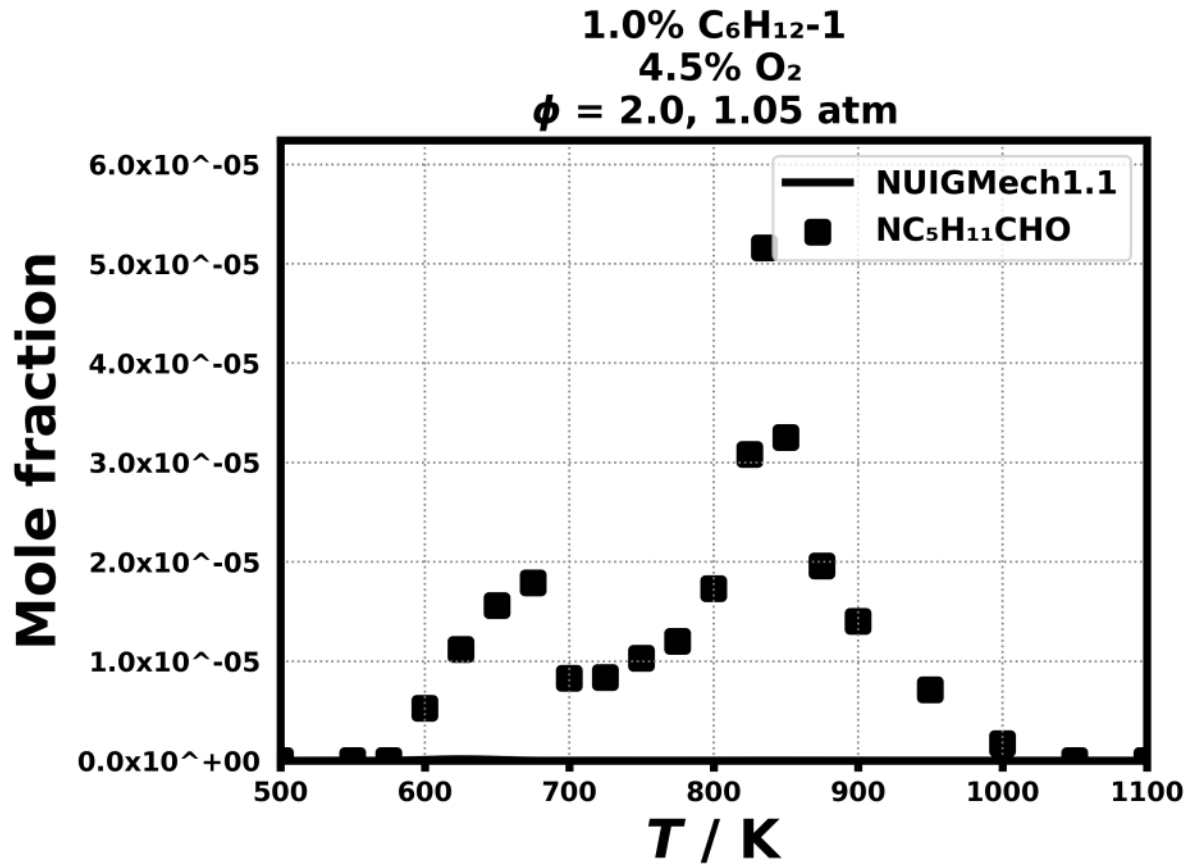


Figure 108: Dataset: 1.05_ATM_PHI_2.0

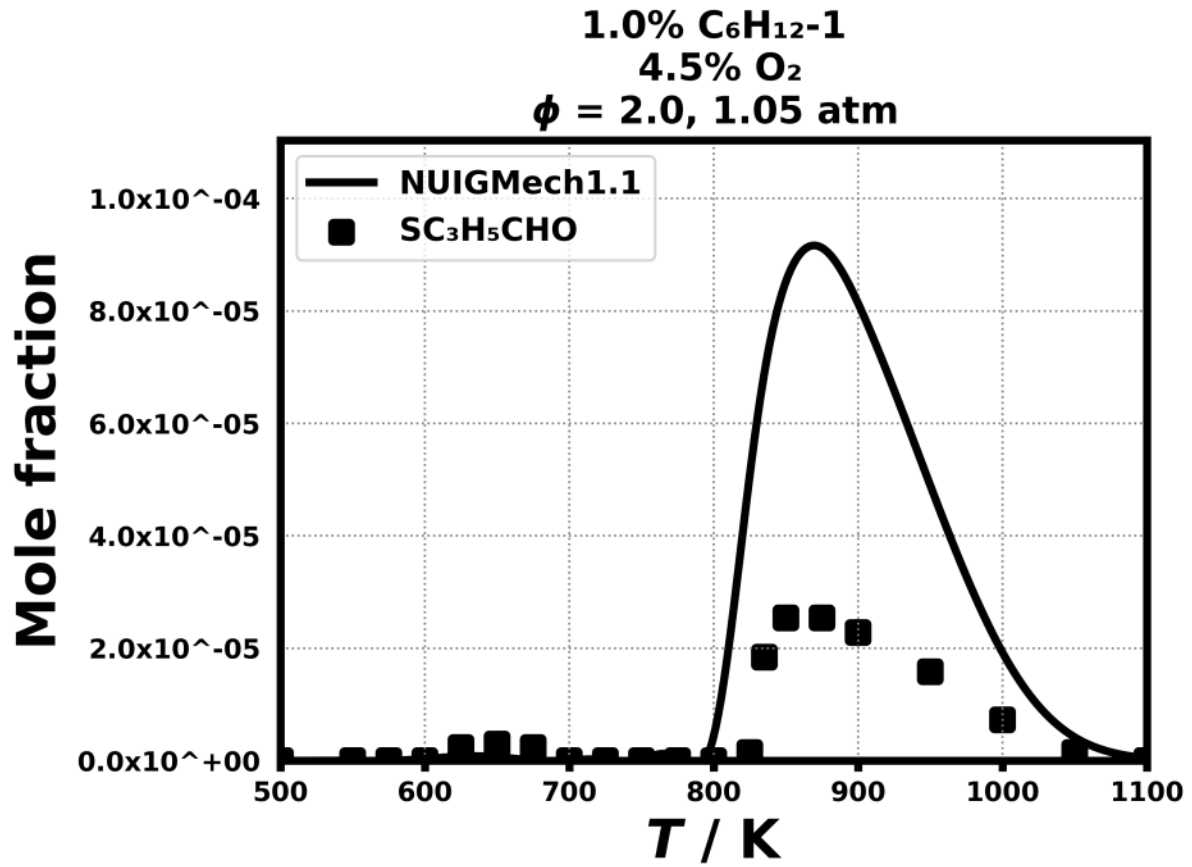


Figure 109: Dataset: 1.05_ATM_PHI_2.0

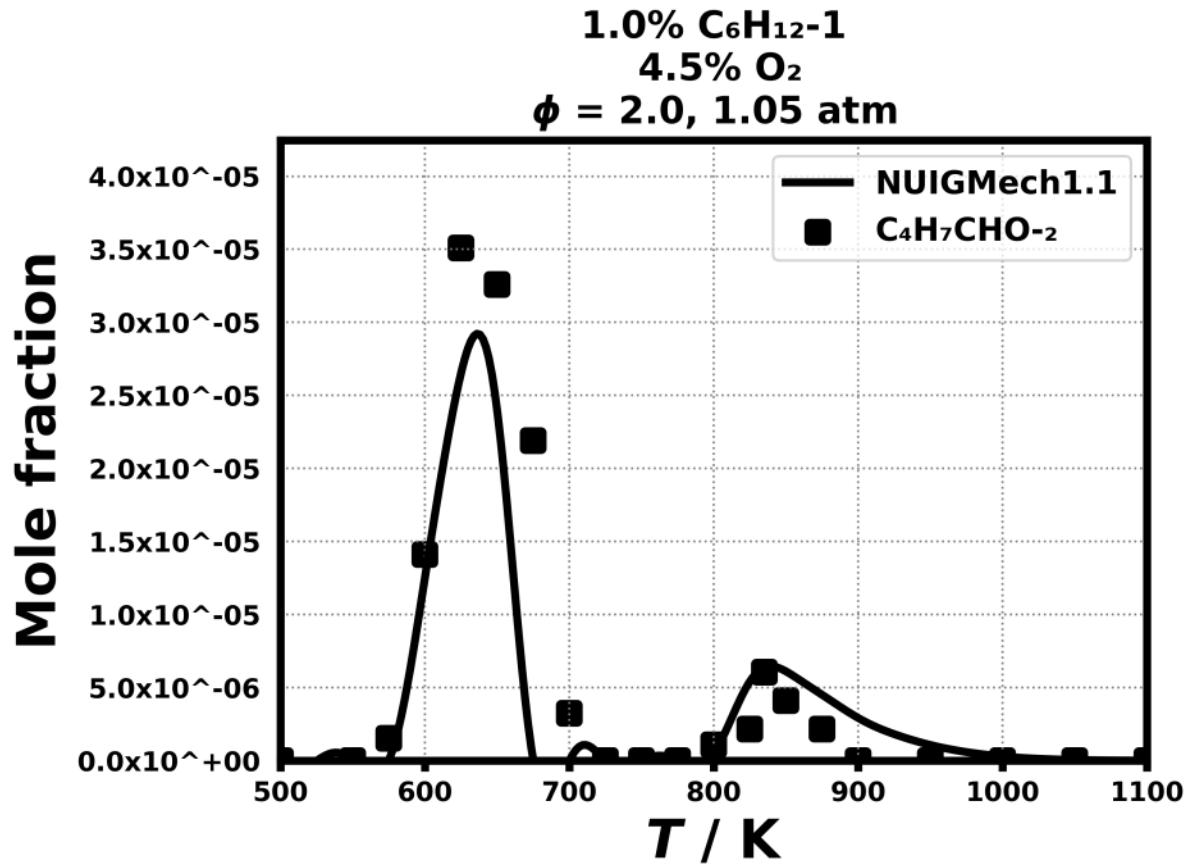


Figure 110: Dataset: 1.05_ATM_PHI_2.0

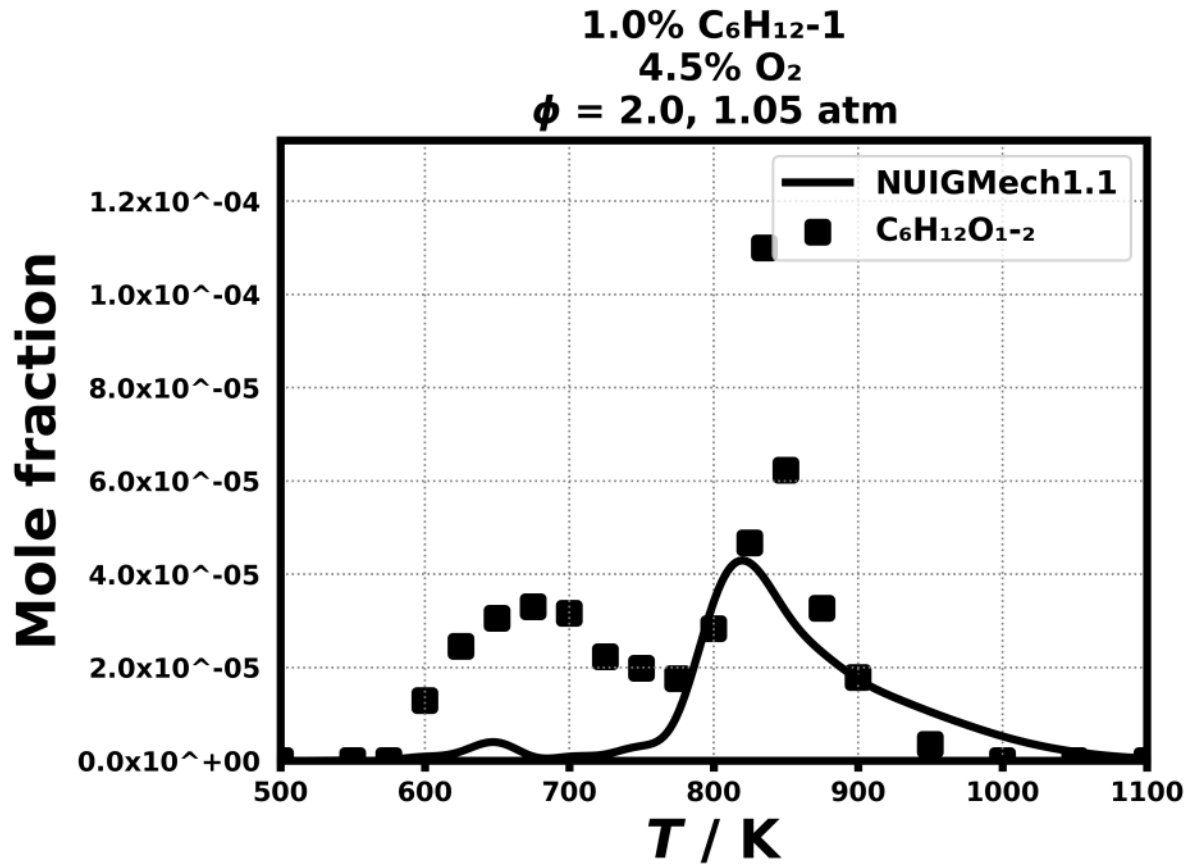


Figure 111: Dataset: 1.05_ATM_PHI_2.0

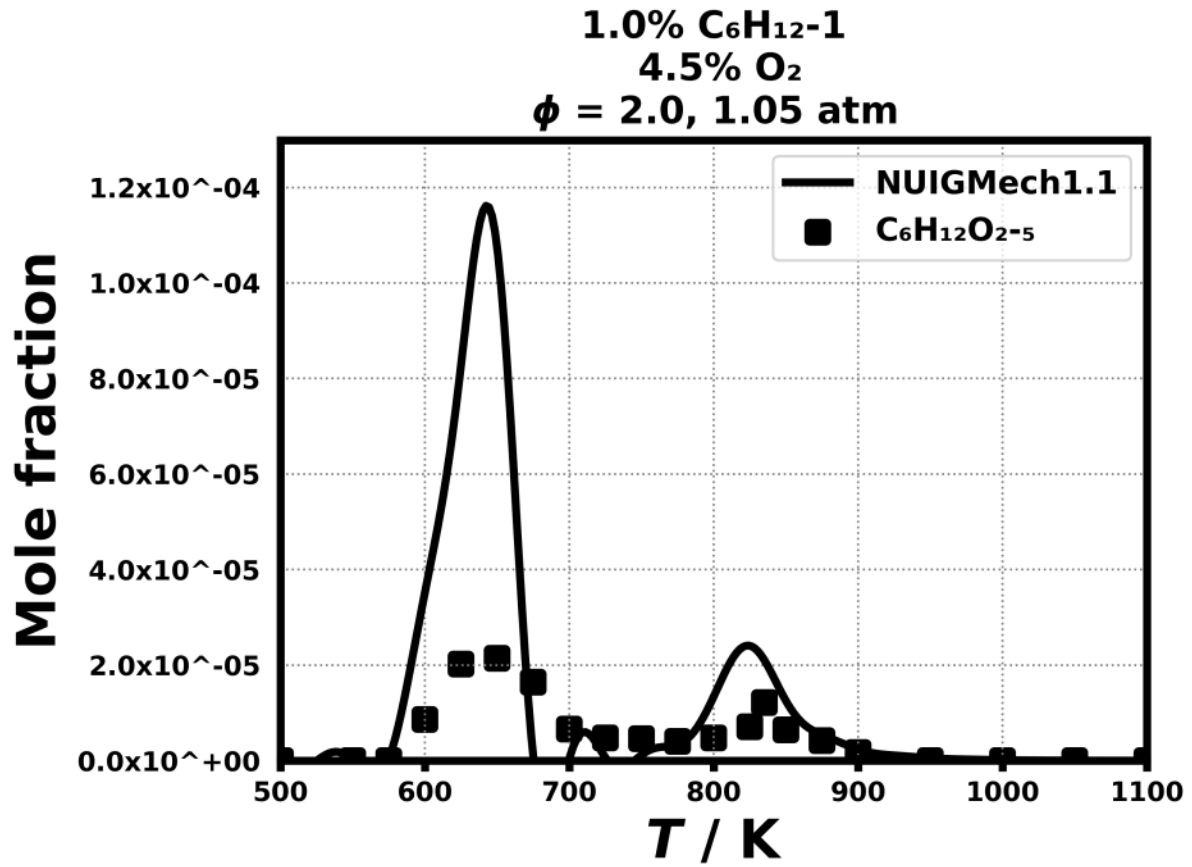


Figure 112: Dataset: 1.05_ATM_PHI_2.0

1.3.91 Case: C6H12-1/JSR/Yahyaoui/10_ATM_PHI.0.5

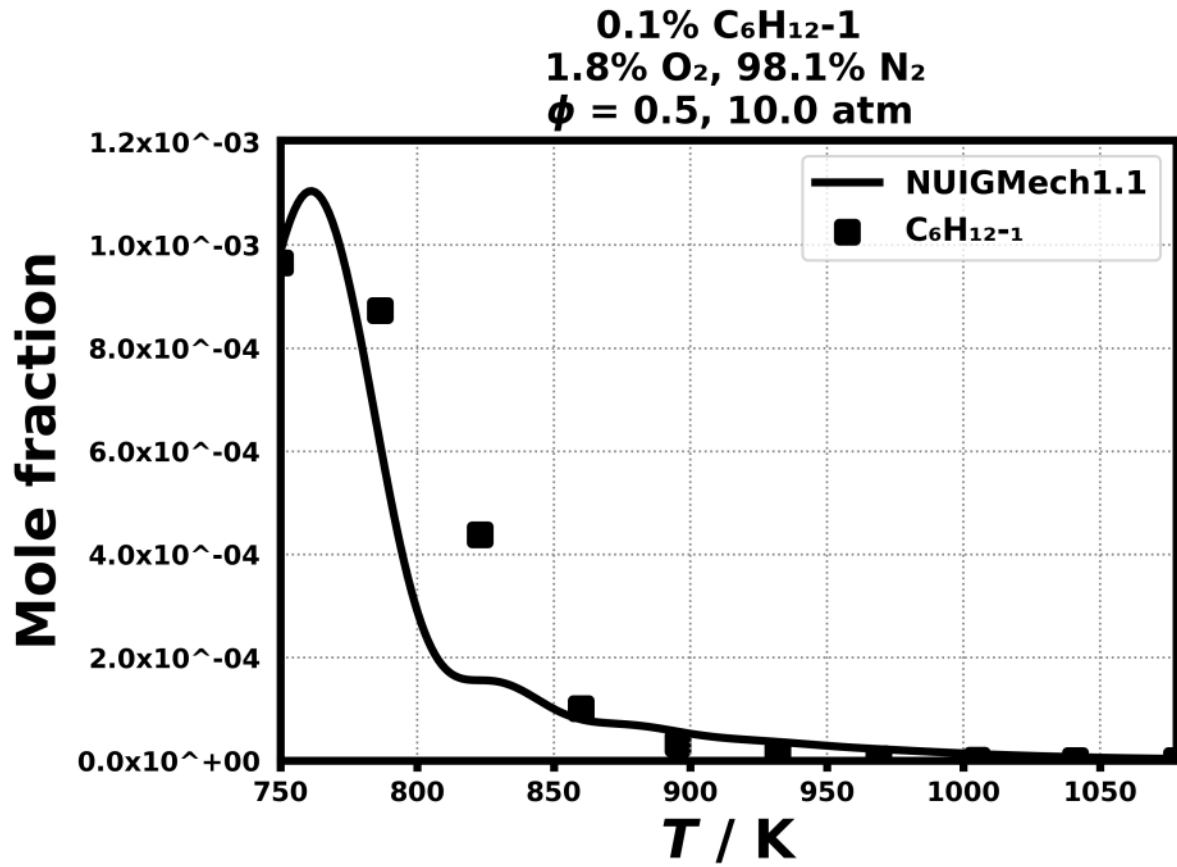


Figure 113: Dataset: 10_ATM_PHI.0.5

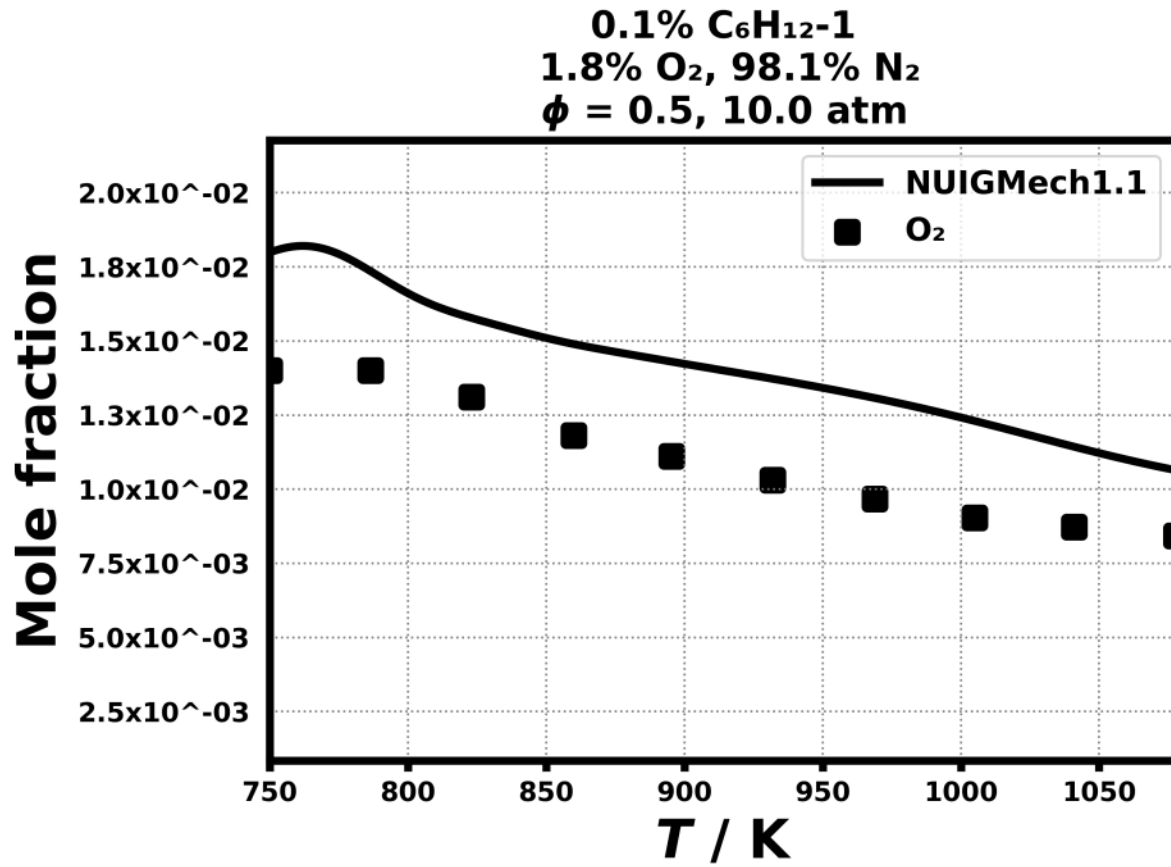


Figure 114: Dataset: 10_ATM_PHI_0.5

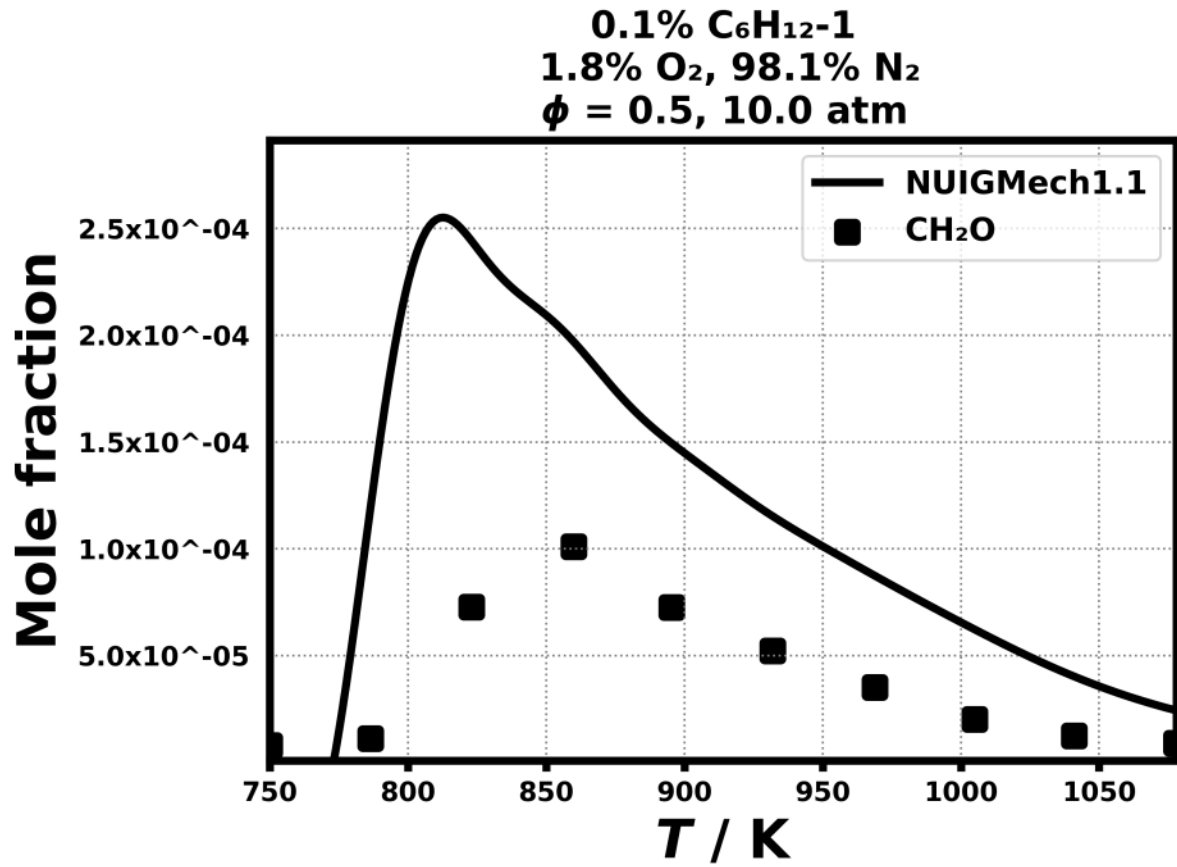


Figure 115: Dataset: 10_ATM_PHI_0.5

1.3.94 Case: C6H12-1/JSR/Yahyaoui/10_ATM_PHI_0.5

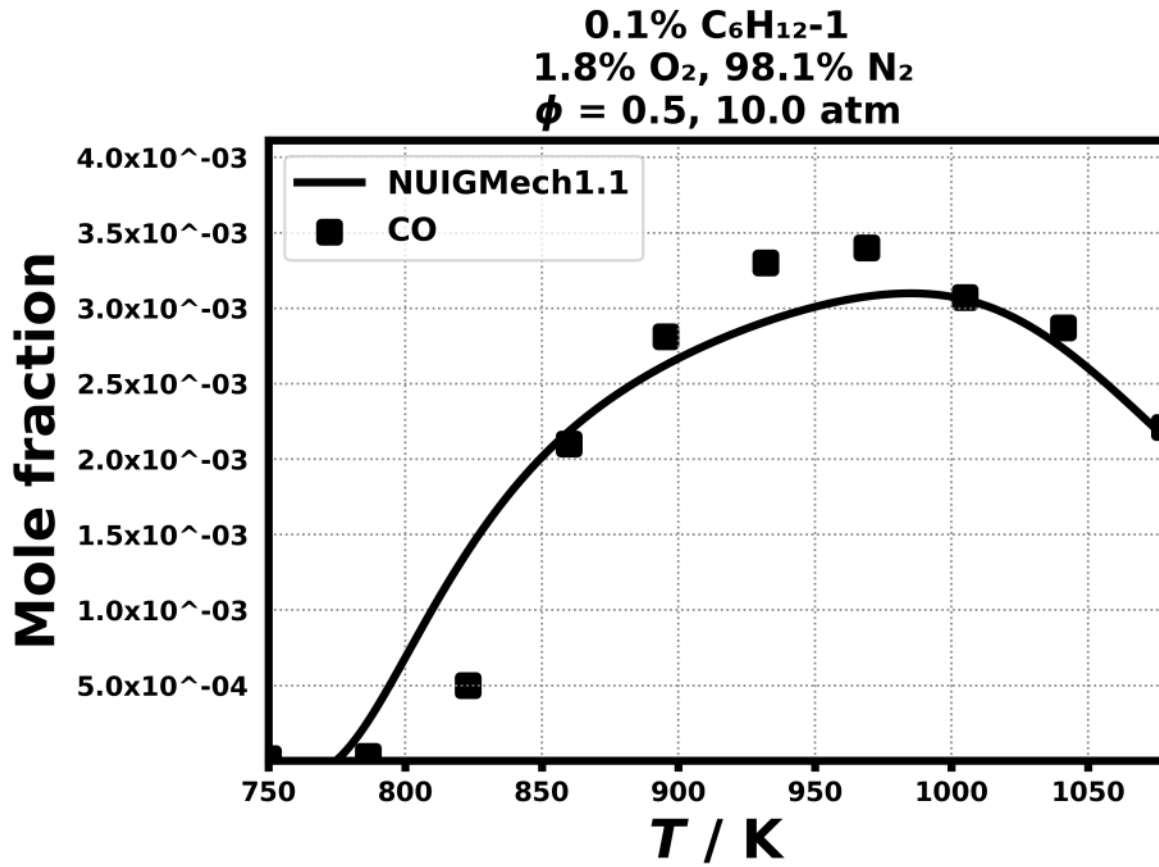


Figure 116: Dataset: 10_ATM_PHI_0.5

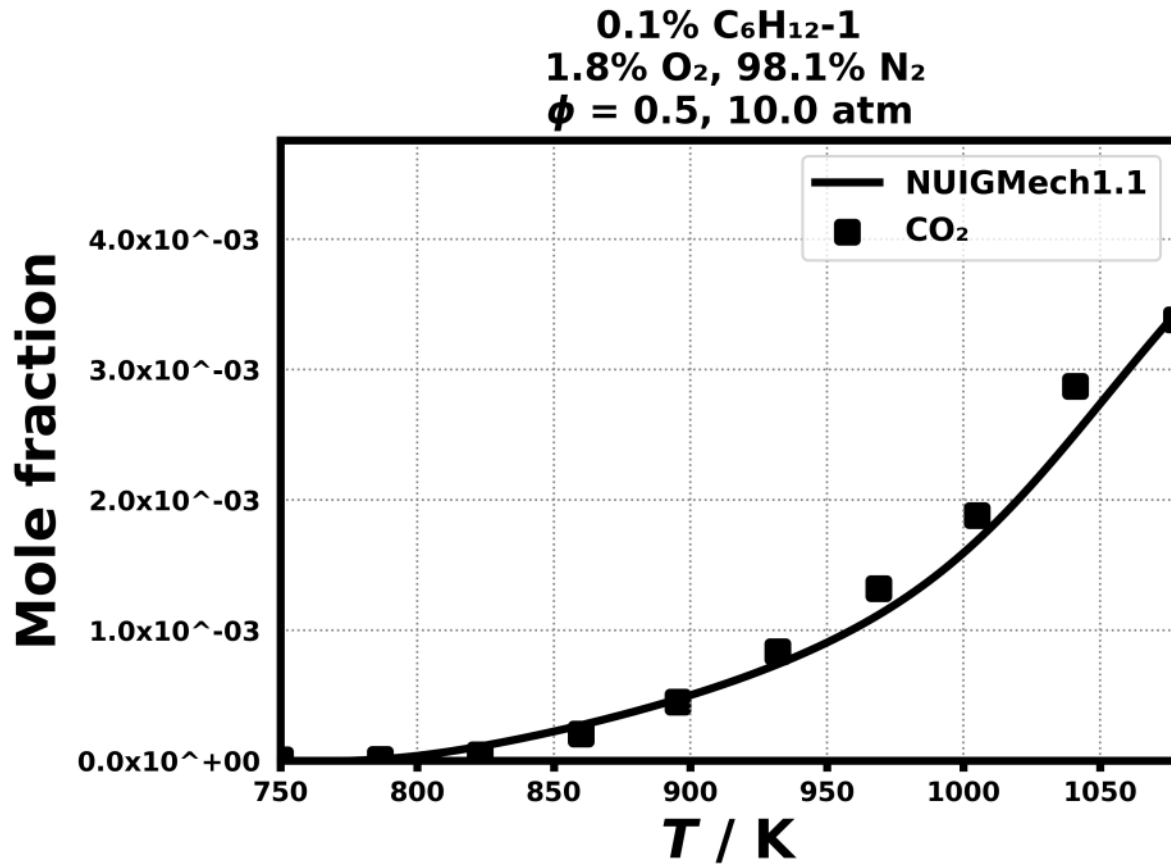


Figure 117: Dataset: 10_ATM_PHI_0.5

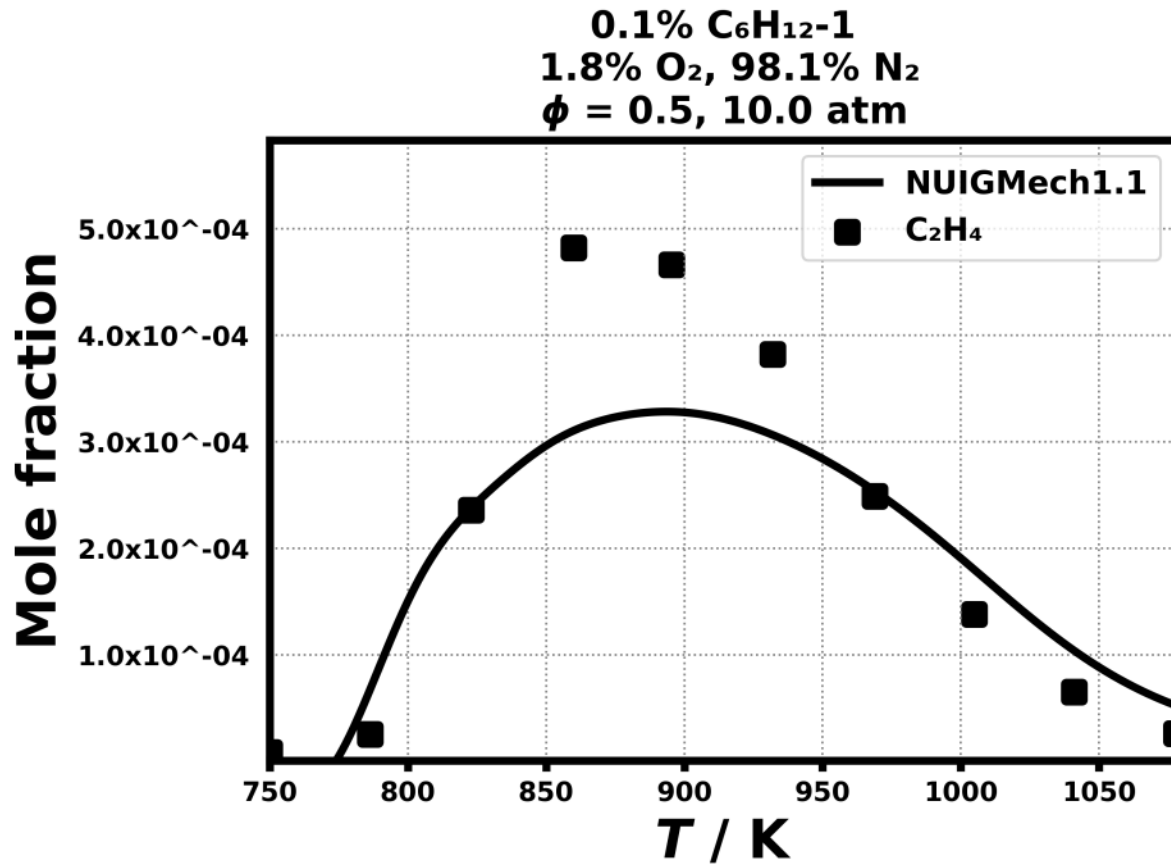


Figure 118: Dataset: 10_ATM_PHI_0.5

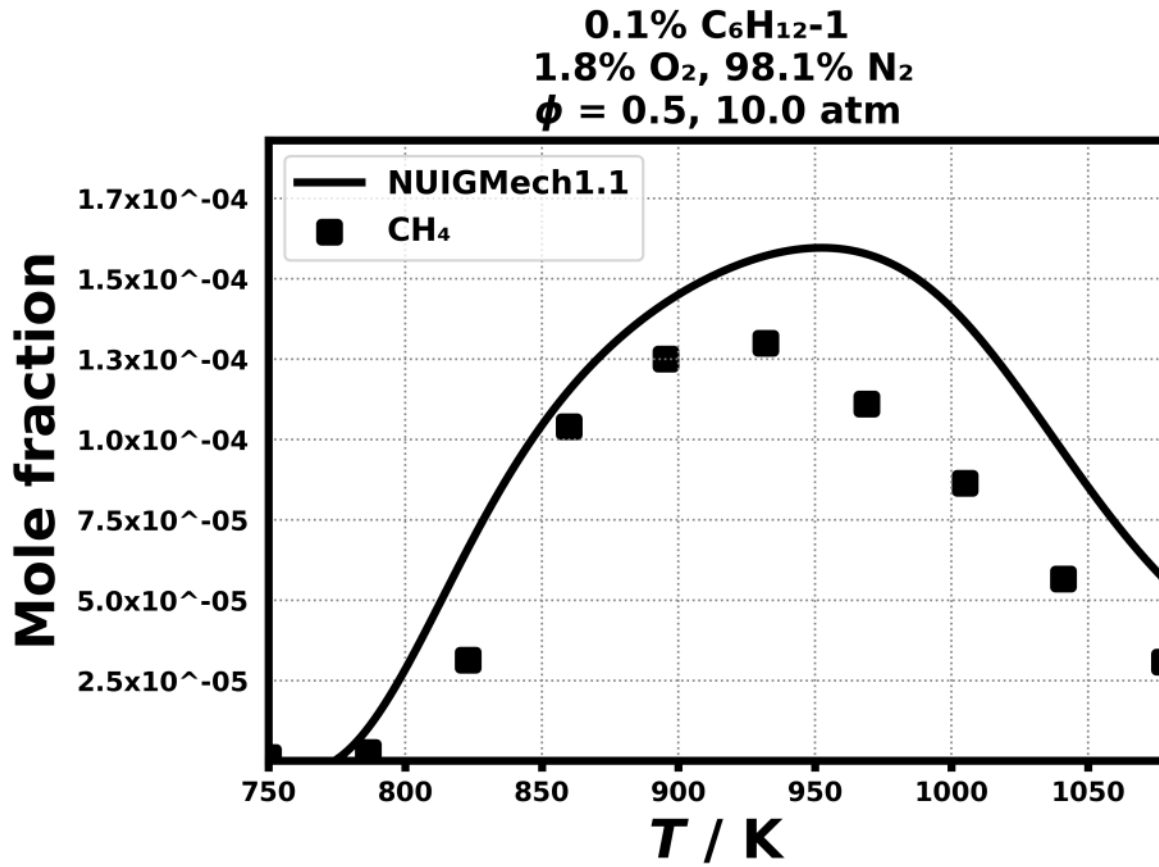


Figure 119: Dataset: 10_ATM_PHI.0.5

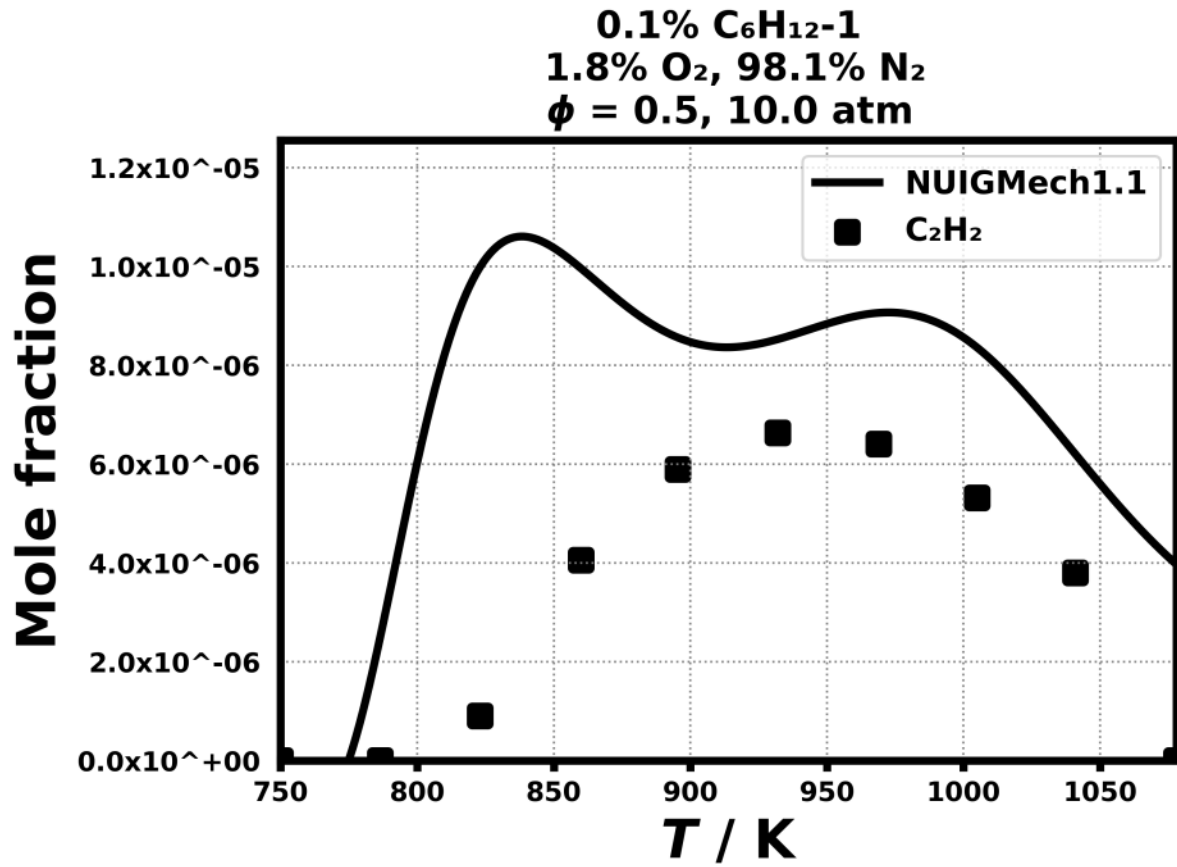


Figure 120: Dataset: 10_ATM_PHI_0.5

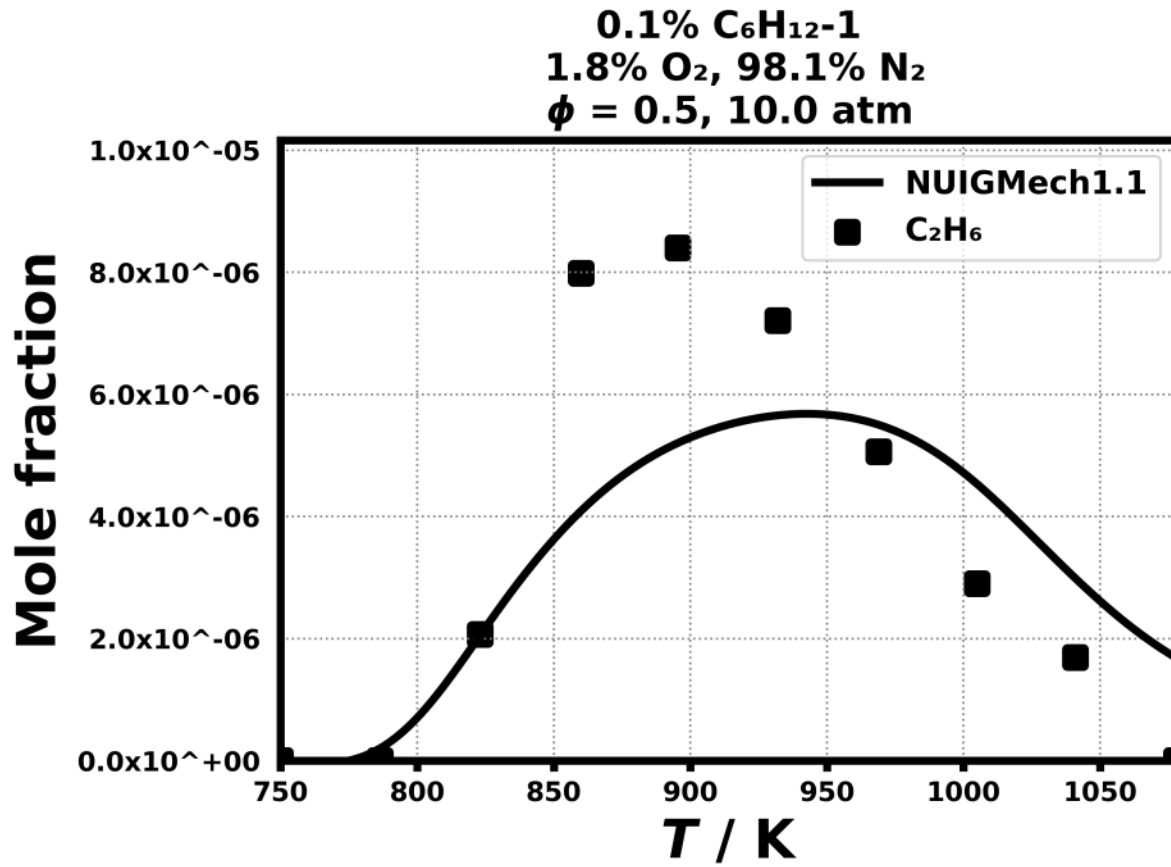


Figure 121: Dataset: 10_ATM_PHI0.5

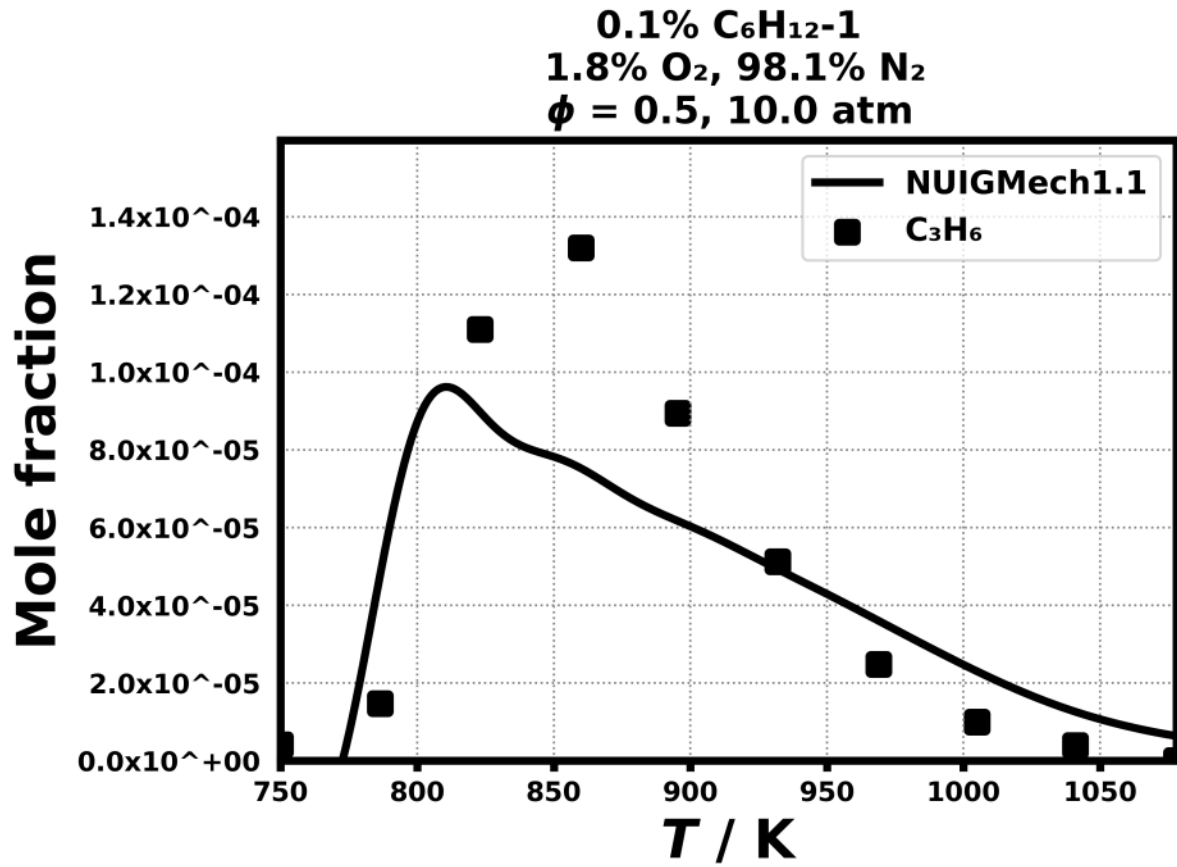


Figure 122: Dataset: 10_ATM_PHI_0.5

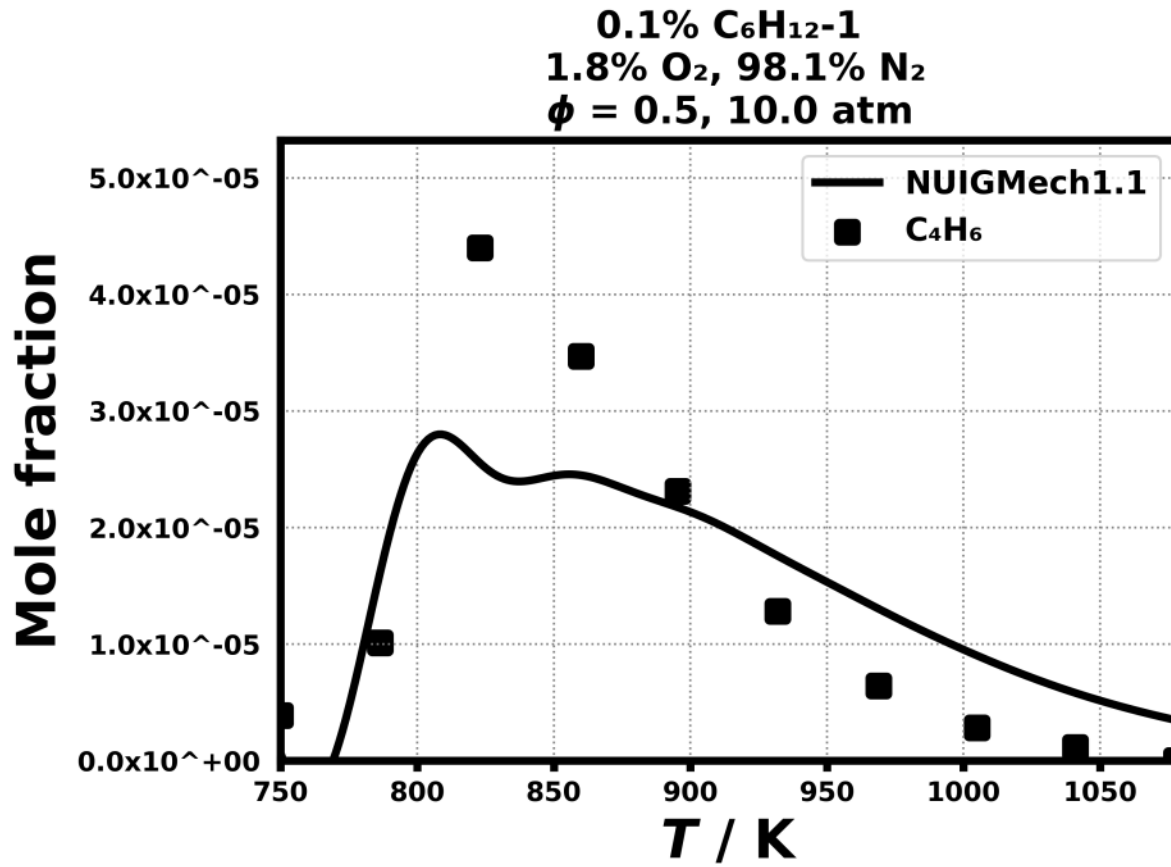


Figure 123: Dataset: 10_ATM_PHI_0.5

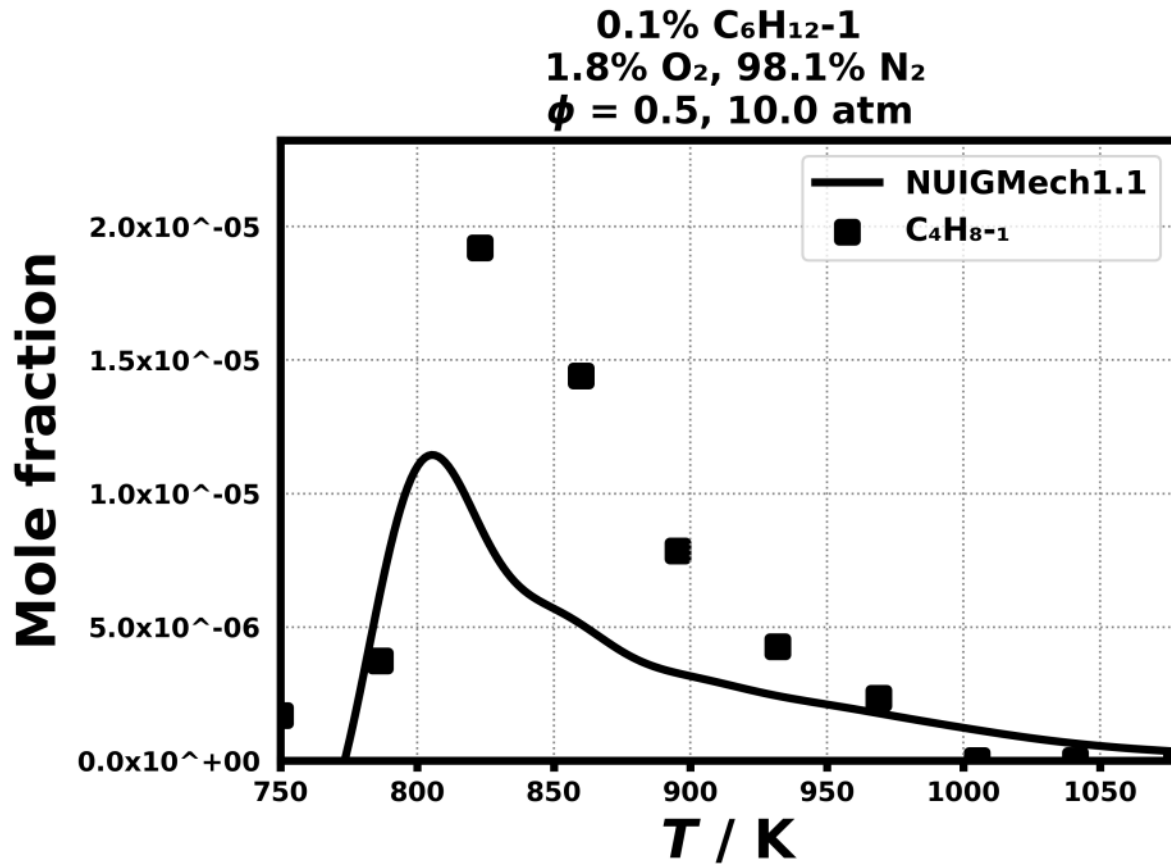


Figure 124: Dataset: 10_ATM_PHI_0.5

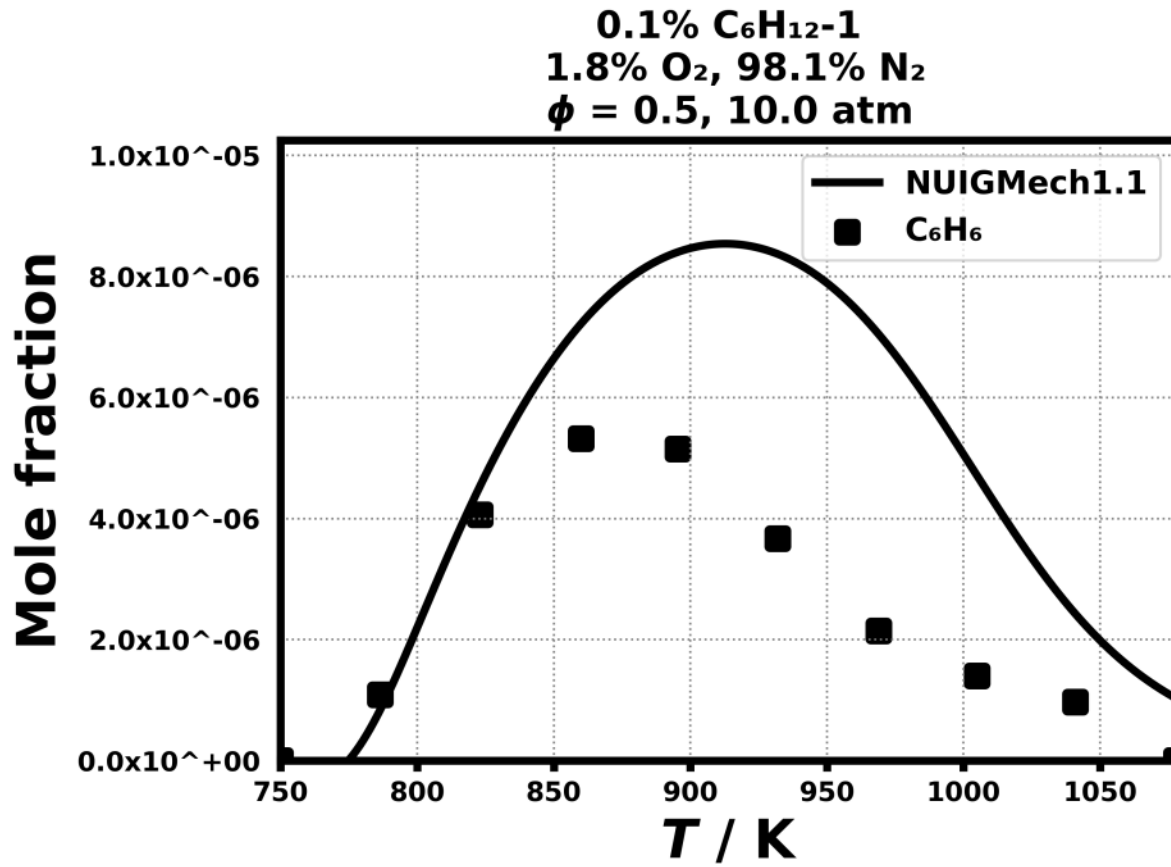


Figure 125: Dataset: 10_ATM_PHI_0.5

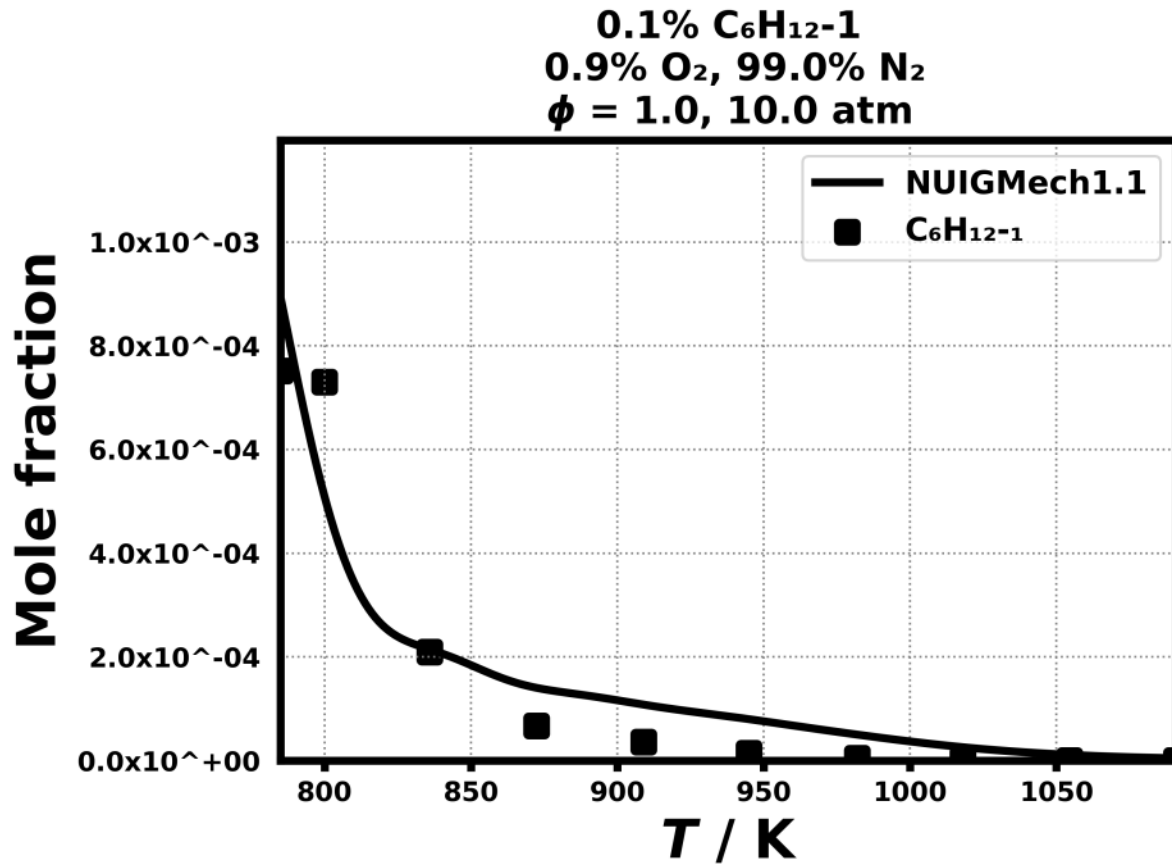


Figure 126: Dataset: 10_ATM_PHI1.0

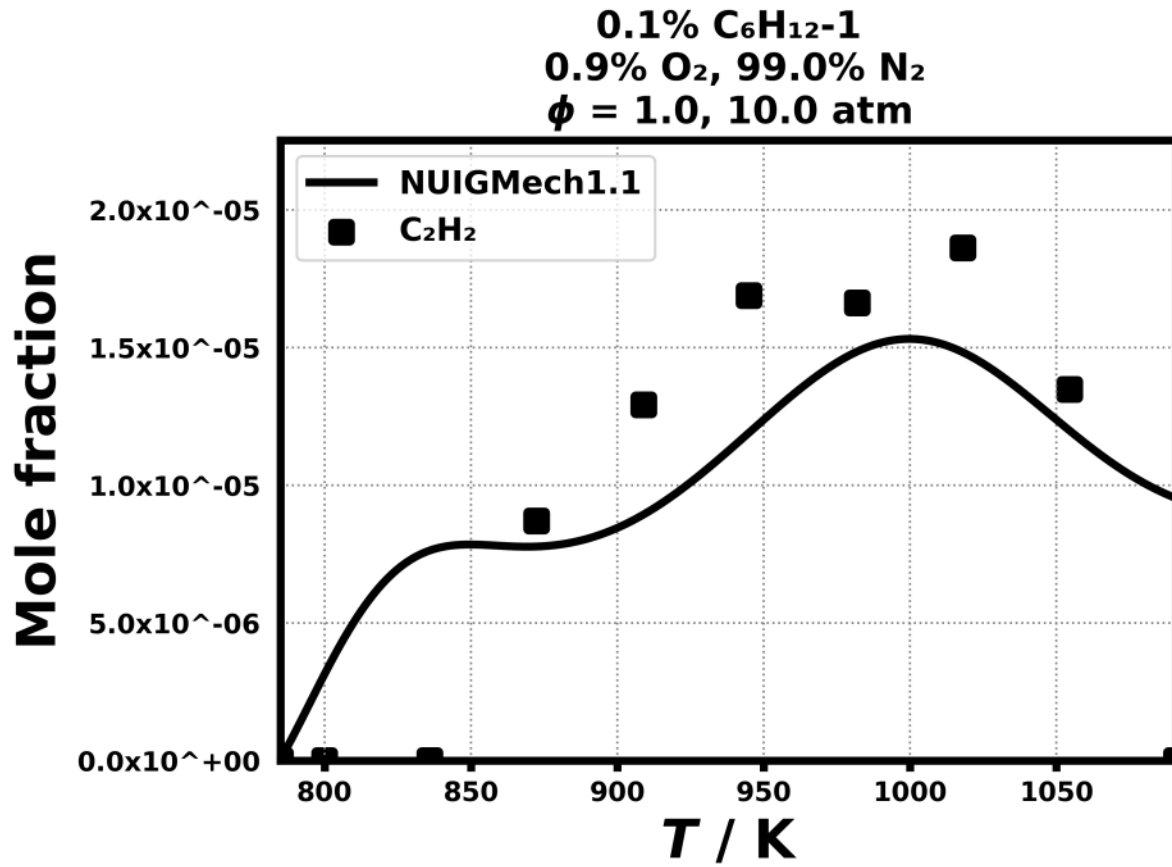


Figure 127: Dataset: 10_ATM_PHI1.0

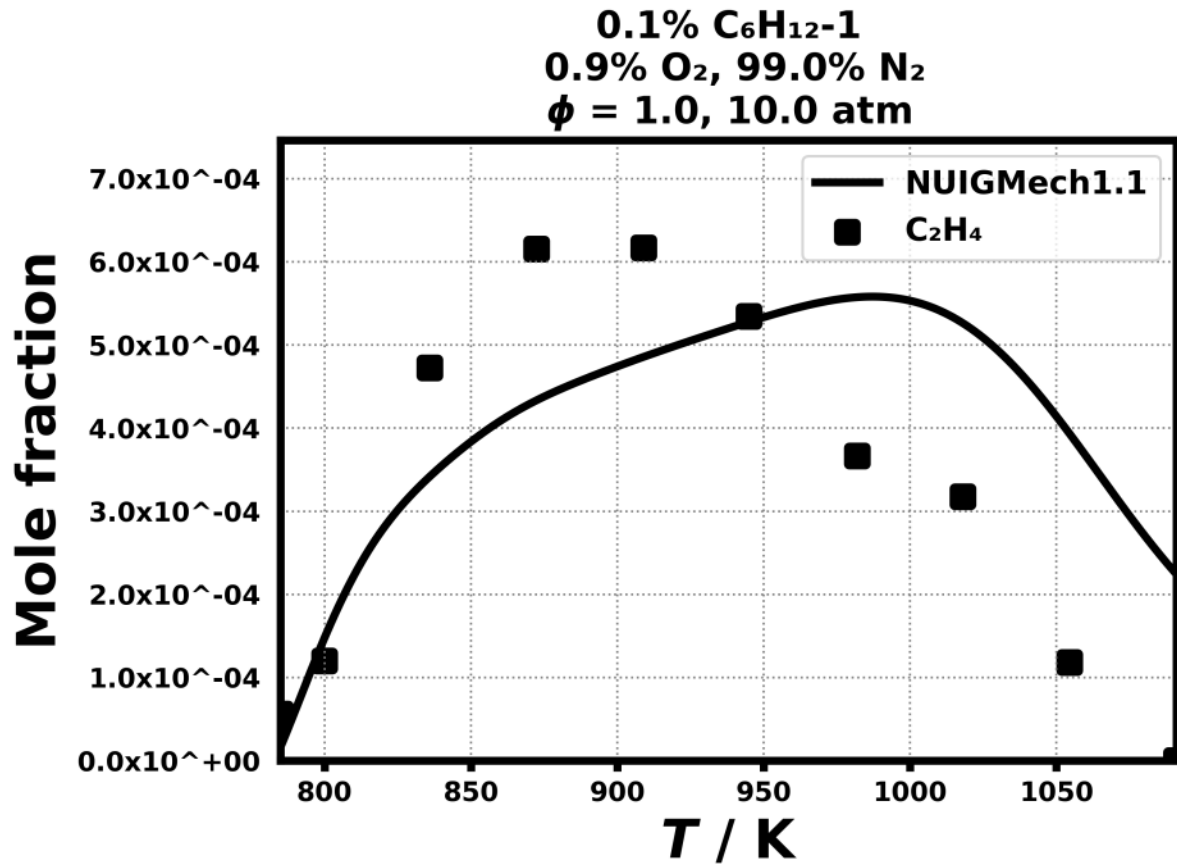


Figure 128: Dataset: 10_ATM_PHI1.0

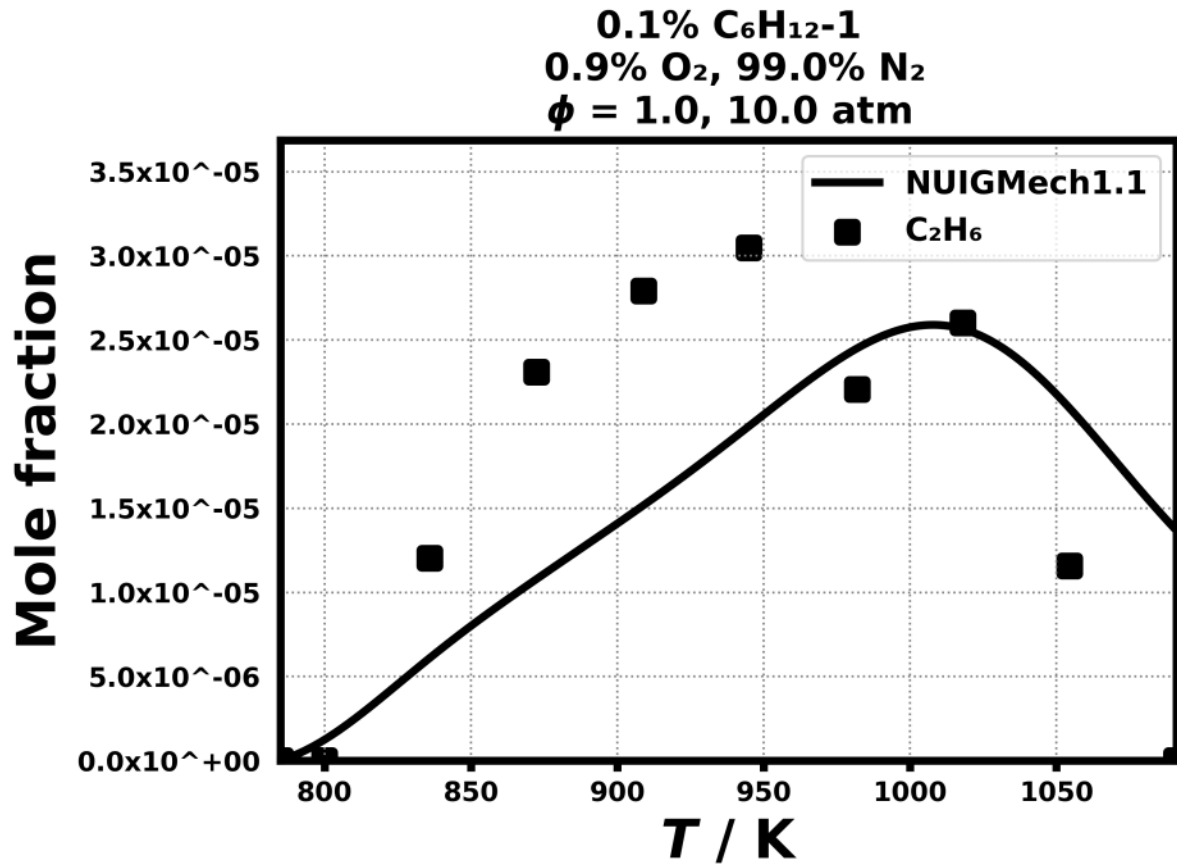


Figure 129: Dataset: 10_ATM_PHI1.0

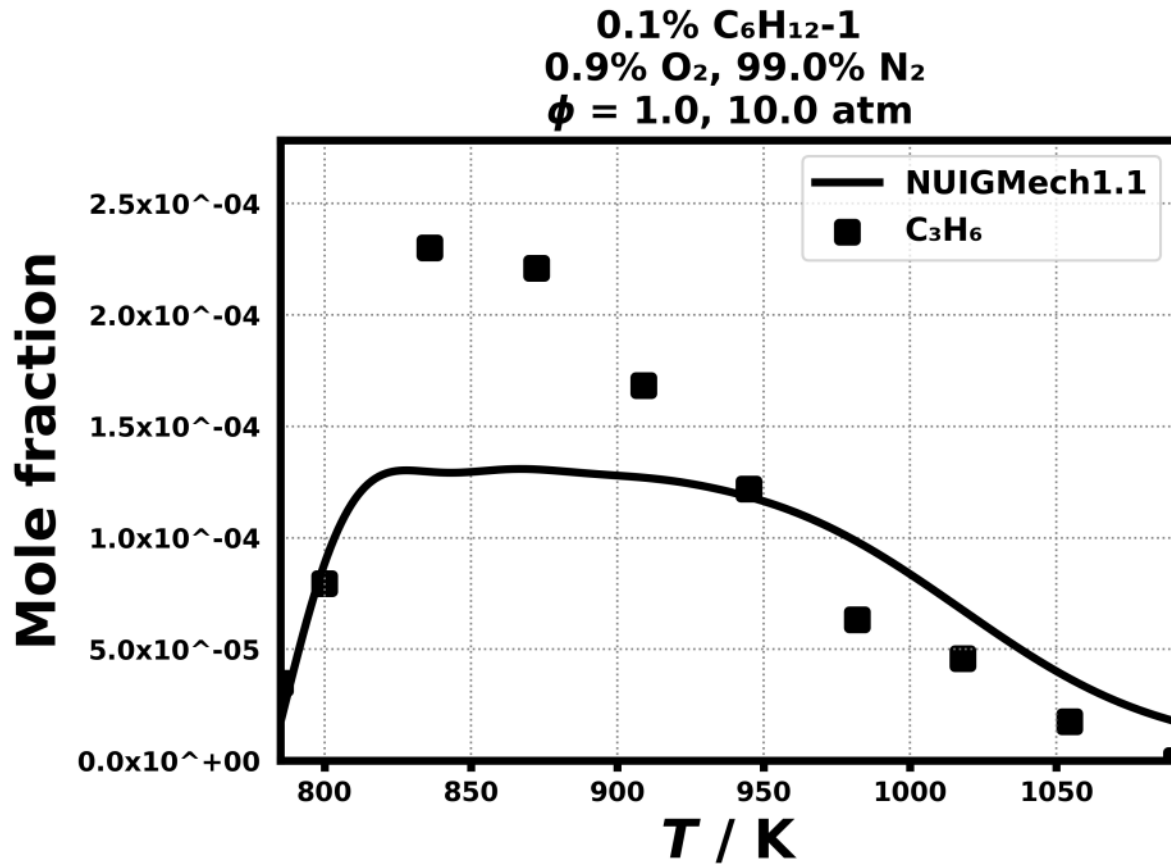


Figure 130: Dataset: 10_ATM_PHI1.0

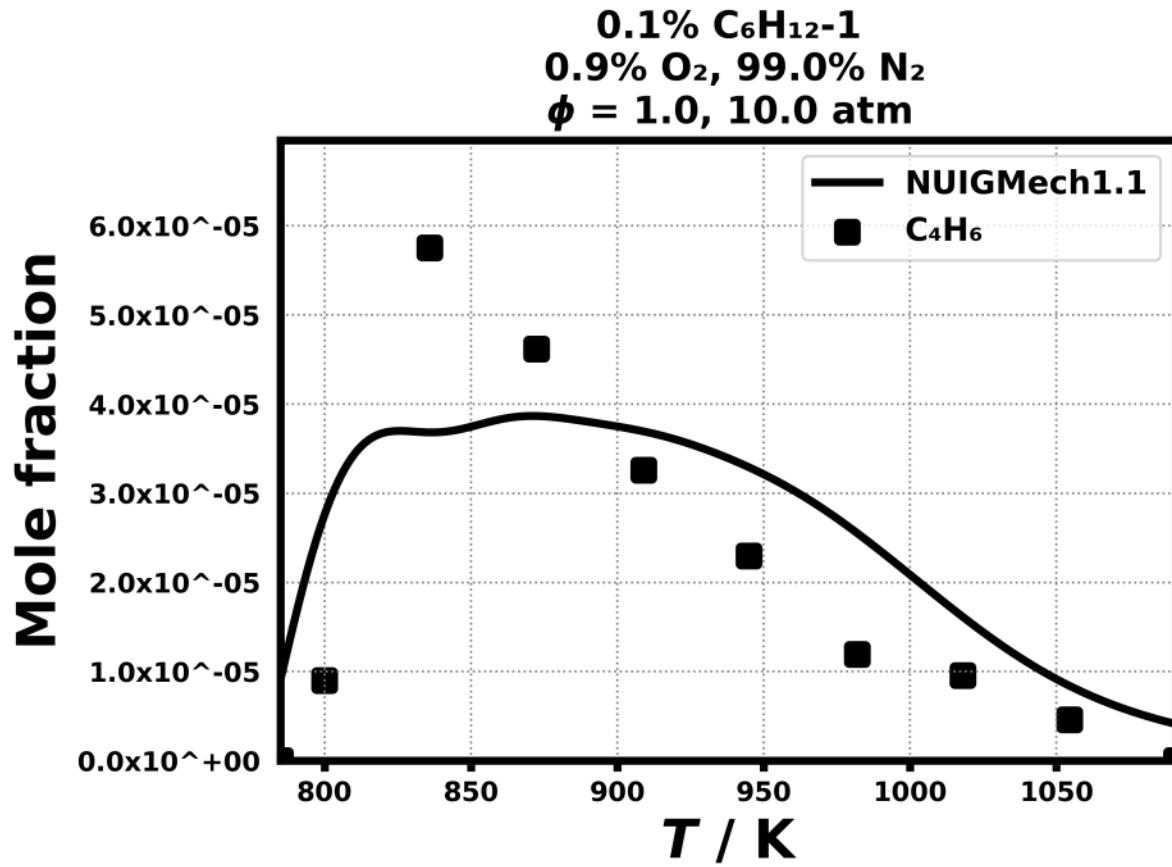


Figure 131: Dataset: 10_ATM_PHI1.0

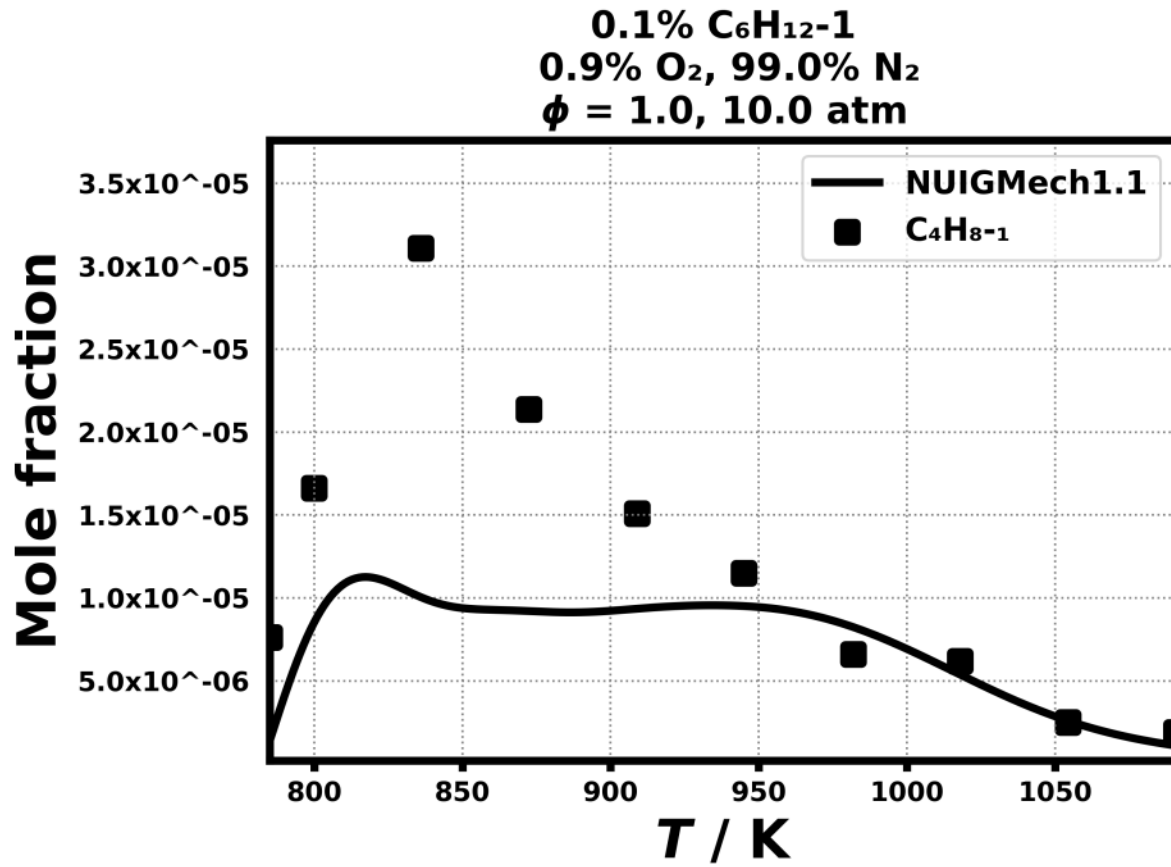


Figure 132: Dataset: 10_ATM_PHI1.0

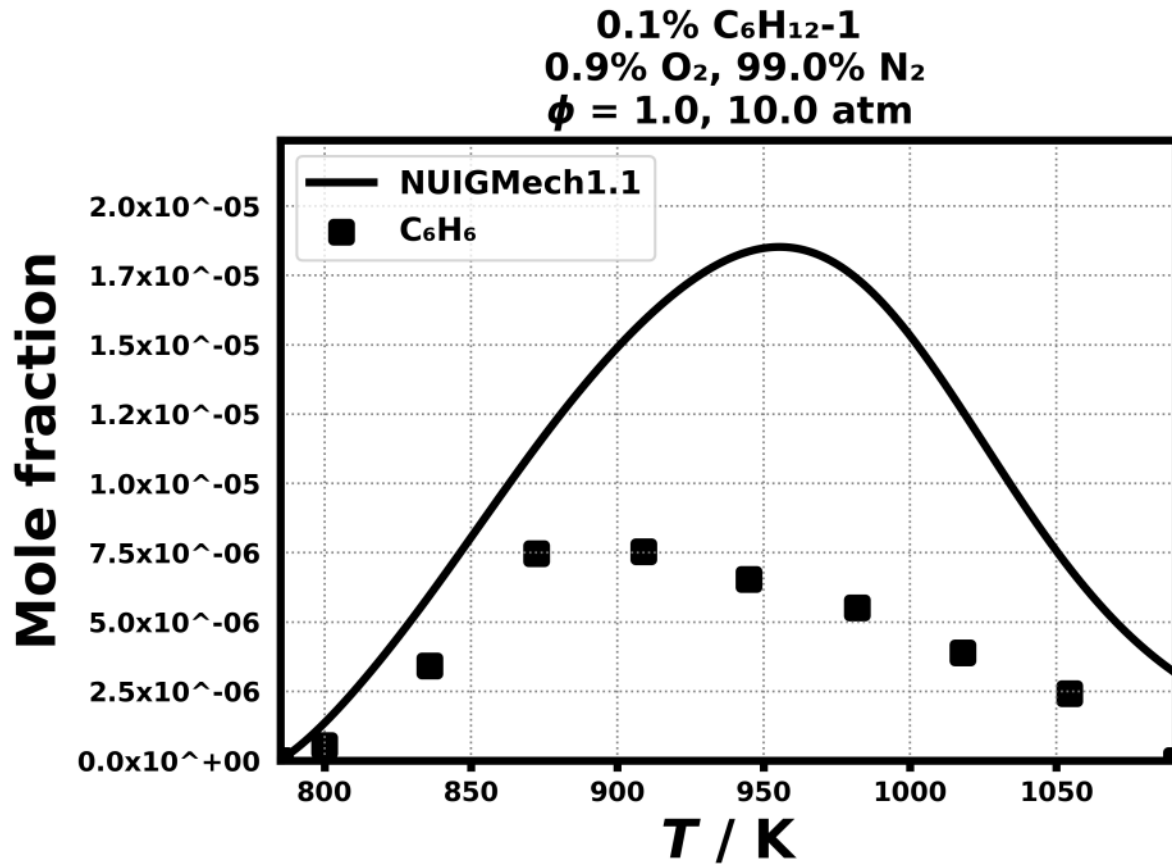


Figure 133: Dataset: 10_ATM_PHI1.0

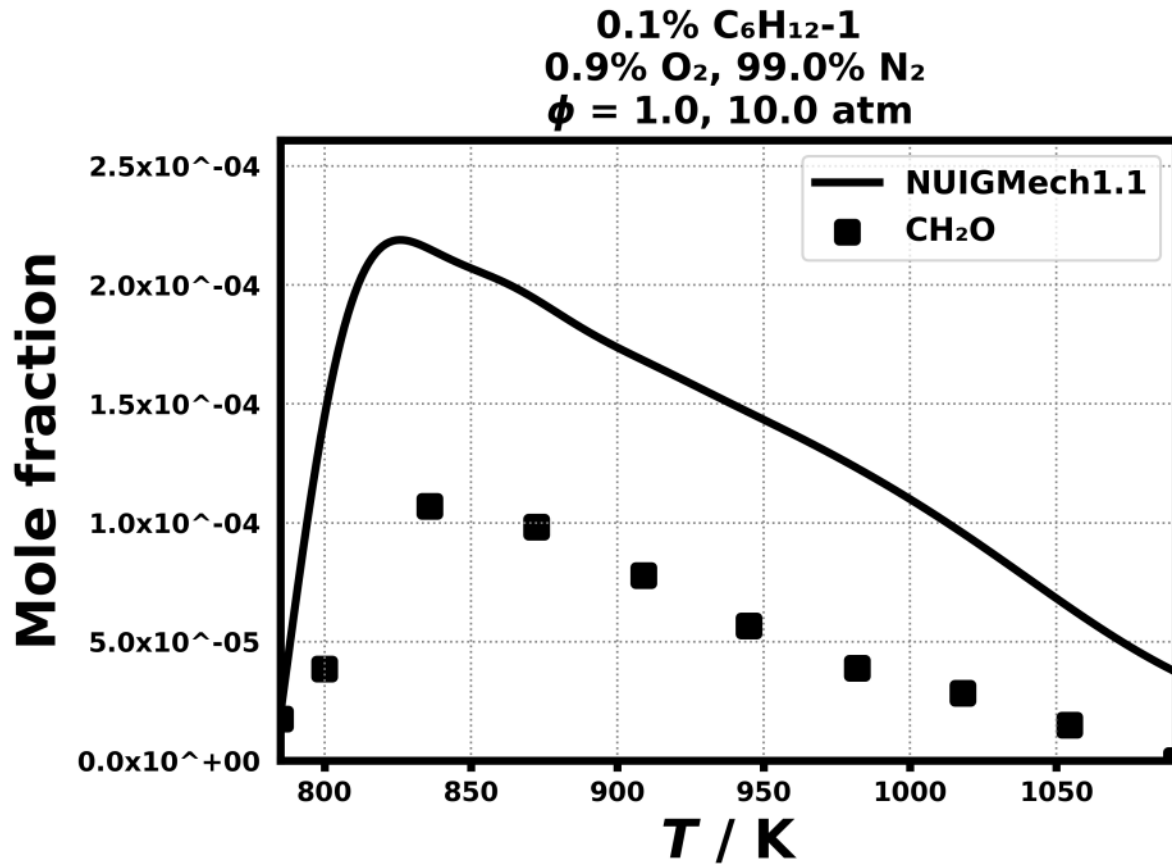


Figure 134: Dataset: 10_ATM_PHI1.0

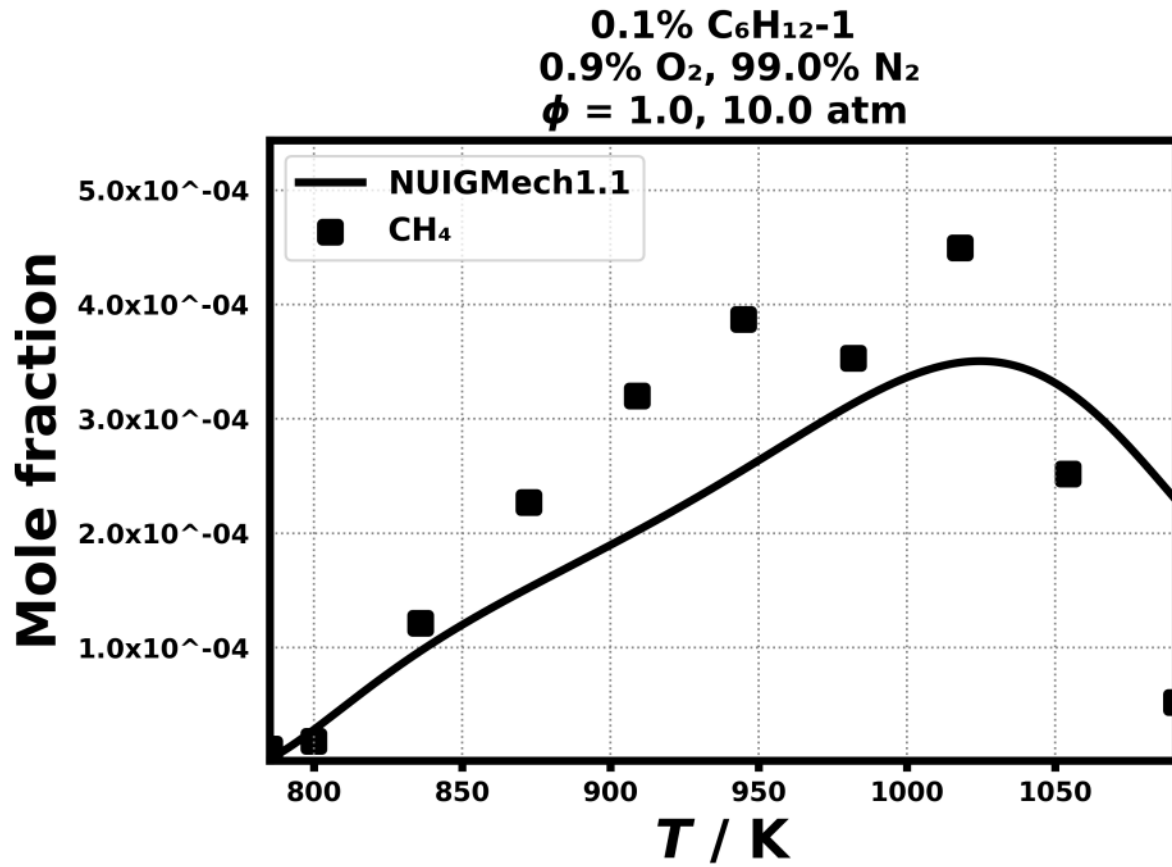


Figure 135: Dataset: 10_ATM_PHI1.0

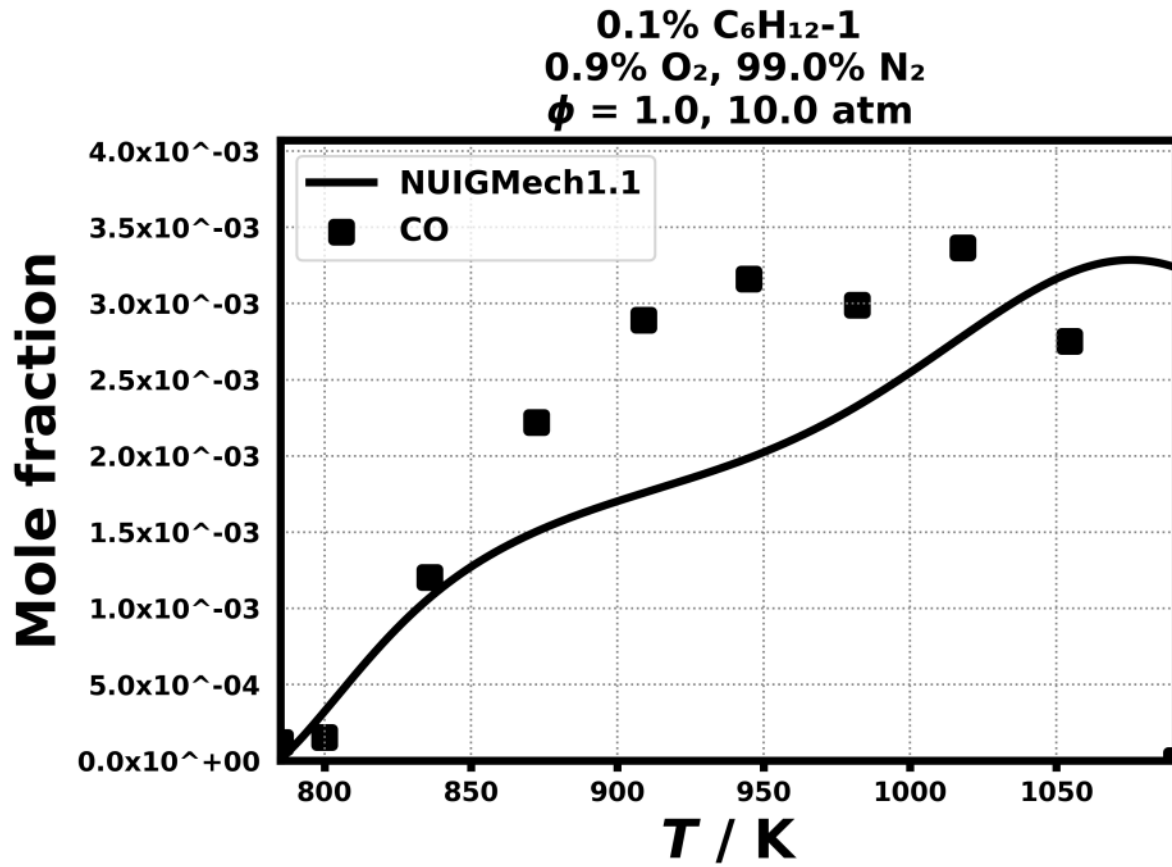


Figure 136: Dataset: 10_ATM_PHI_1.0

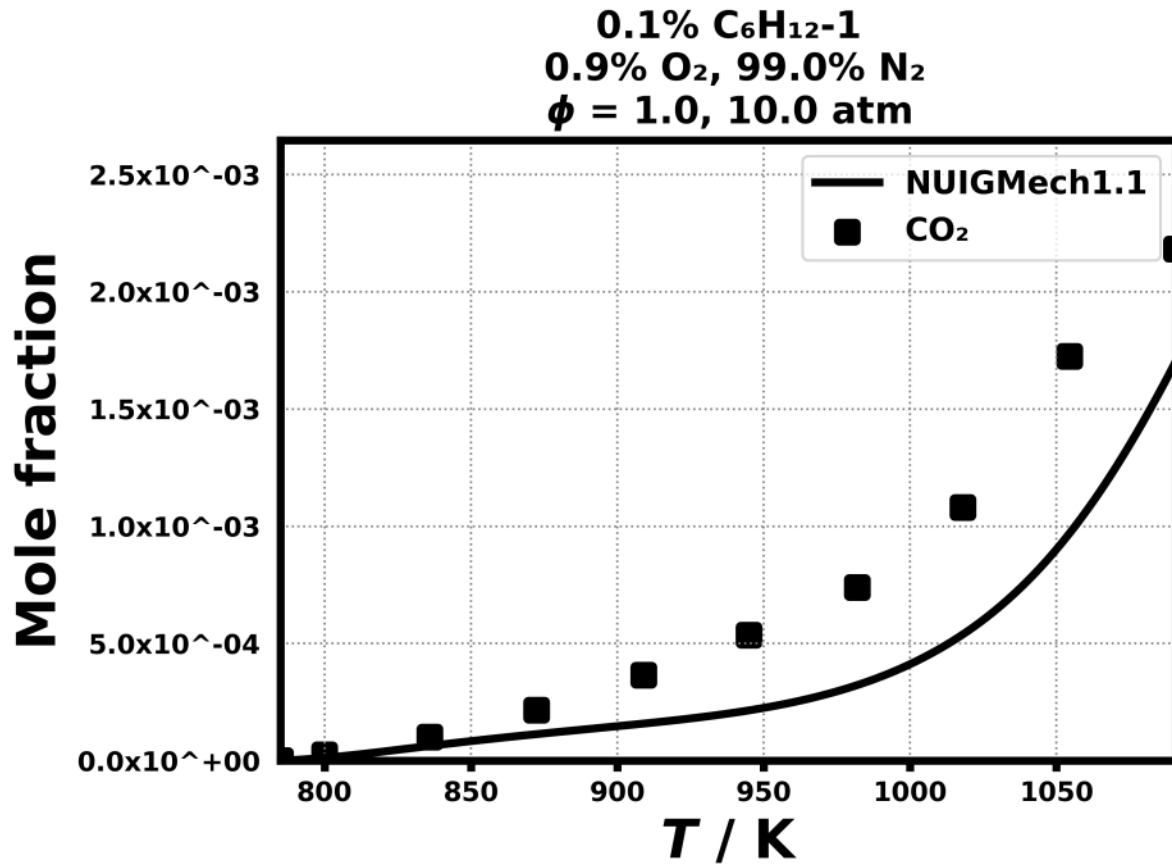


Figure 137: Dataset: 10_ATM_PHI_1.0

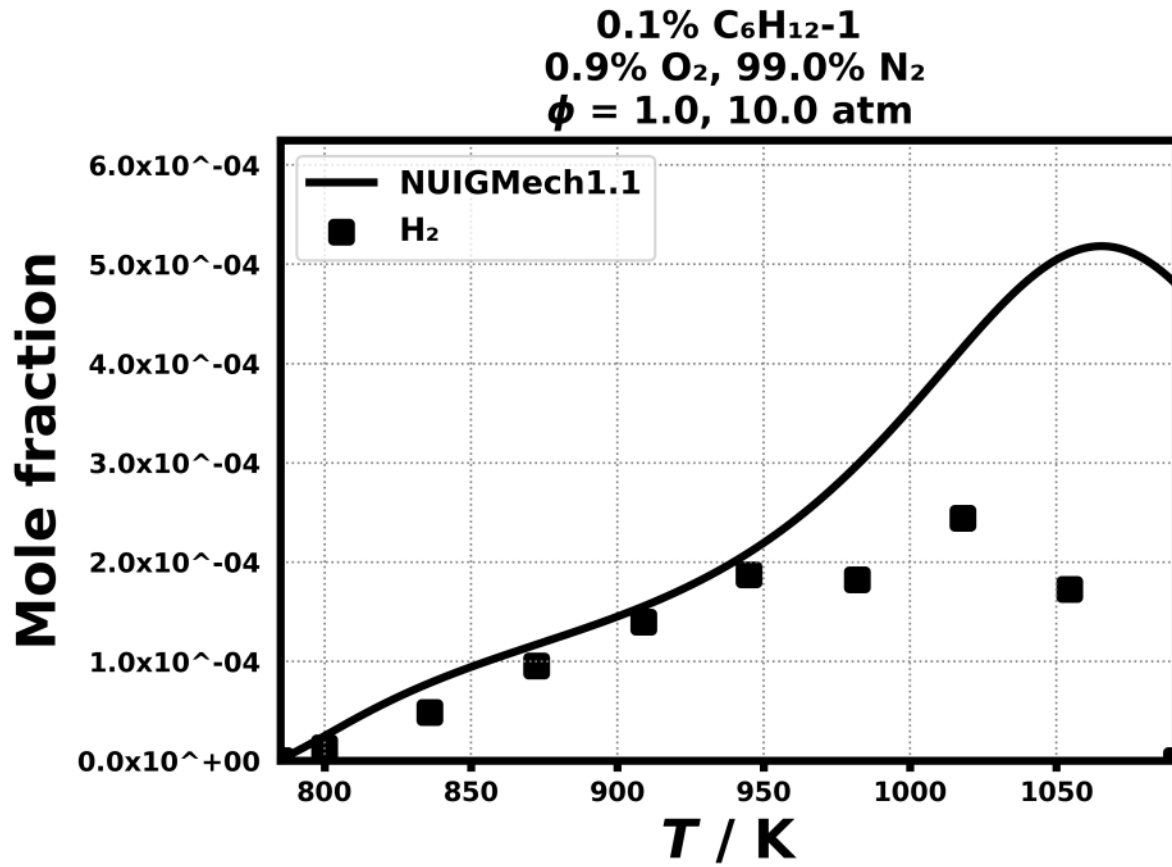


Figure 138: Dataset: 10_ATM_PHI1.0

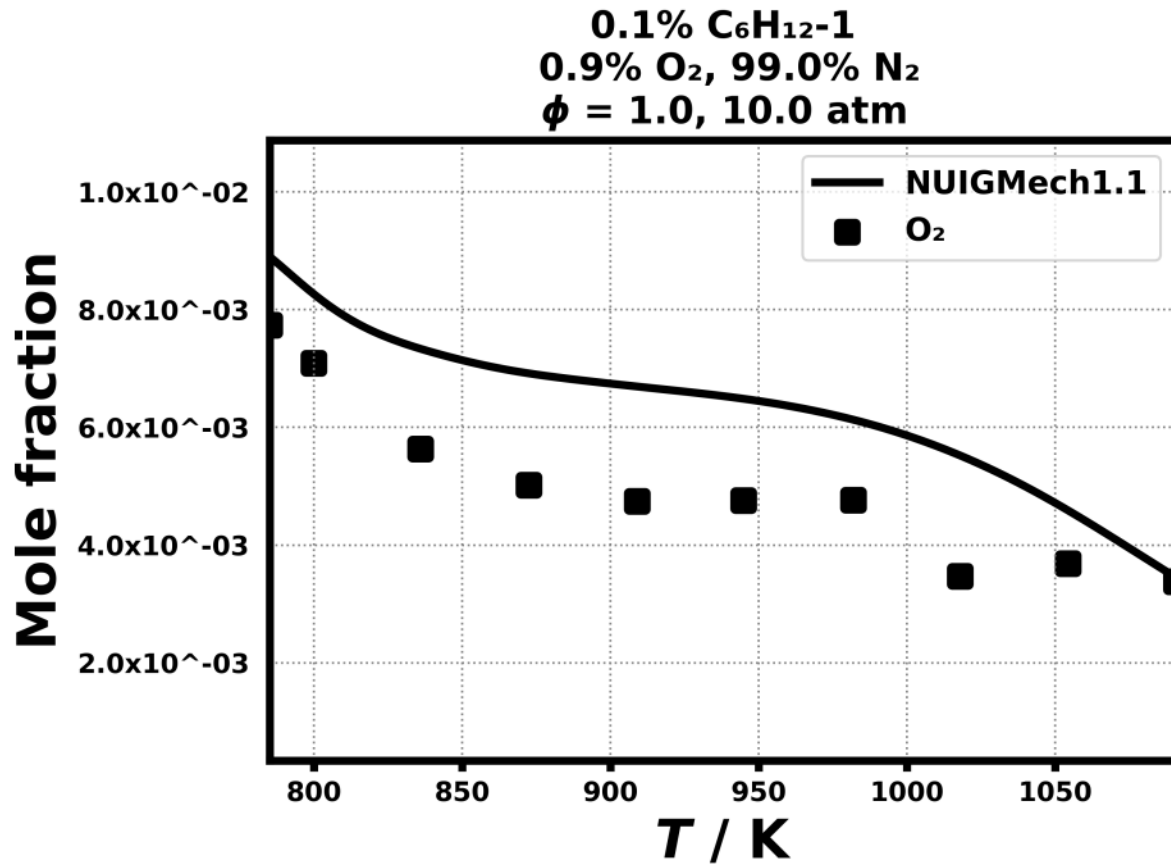
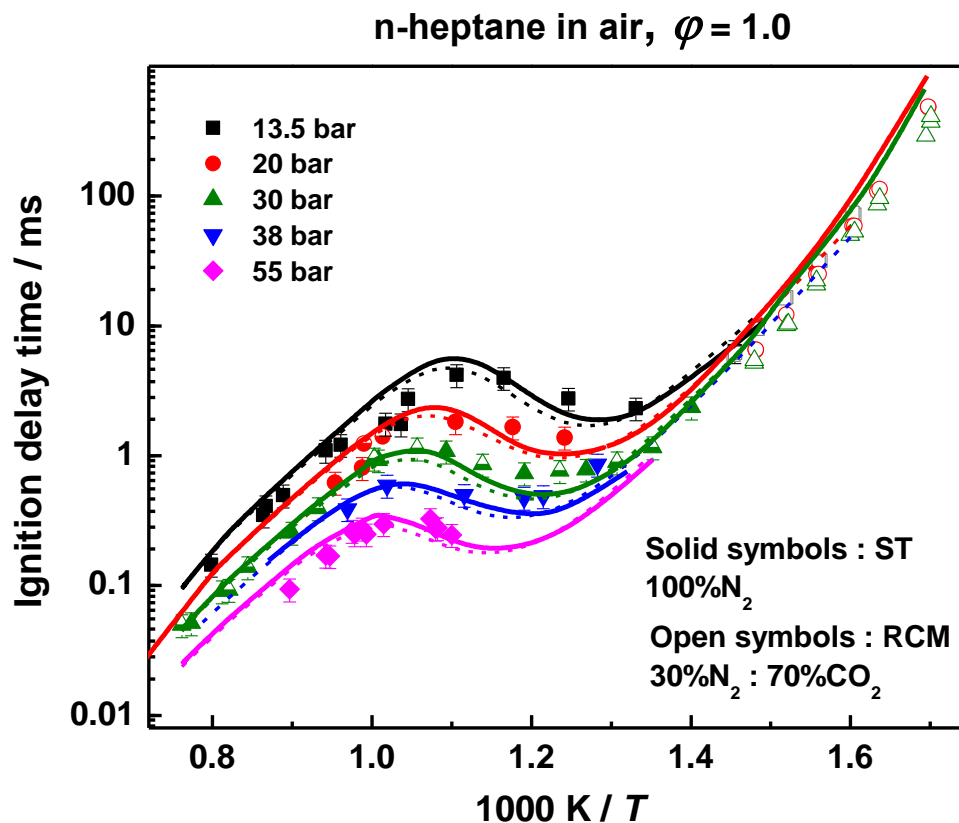


Figure 139: Dataset: 10_ATM_PHI1.0

27. Validation for n-C₇H₁₆

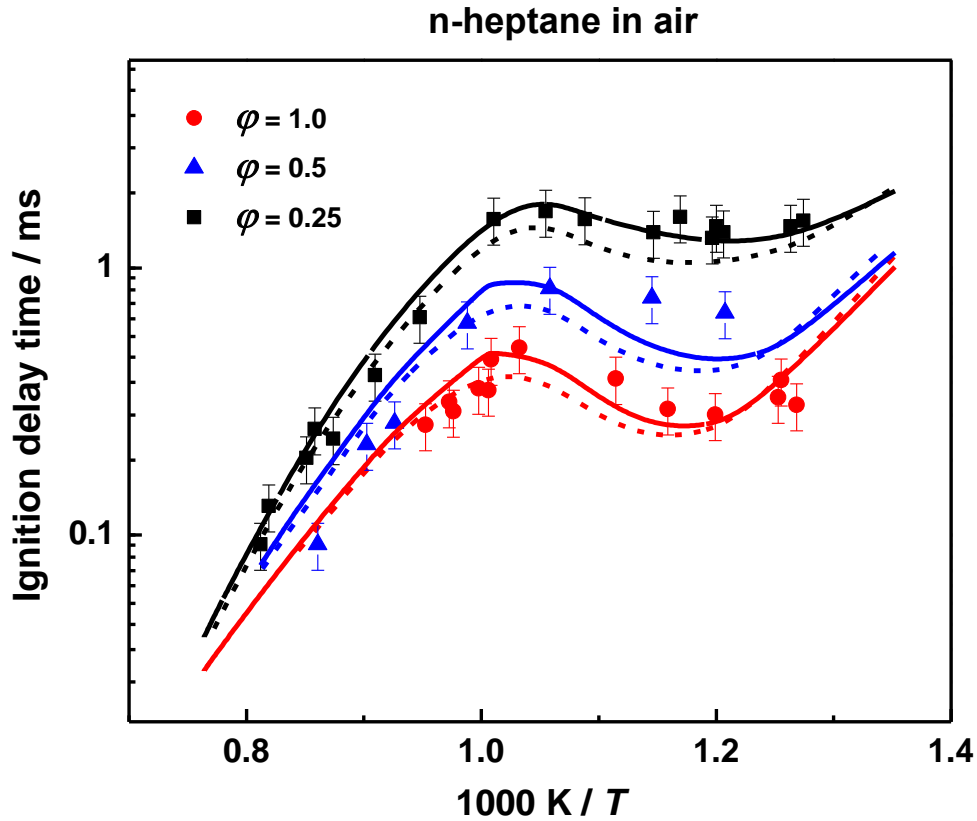
Ignition delay time : Shock Tube + RCM

p_c	T_c	ϕ
13.5 – 55 bar	590 – 1250 K	1.0
45 , 50 atm	800 – 1250 K	0.25 – 1.0



Solid lines : NUIGMech1.1

Short-dashed lines : NUIGMech1.1 without updated rate rules



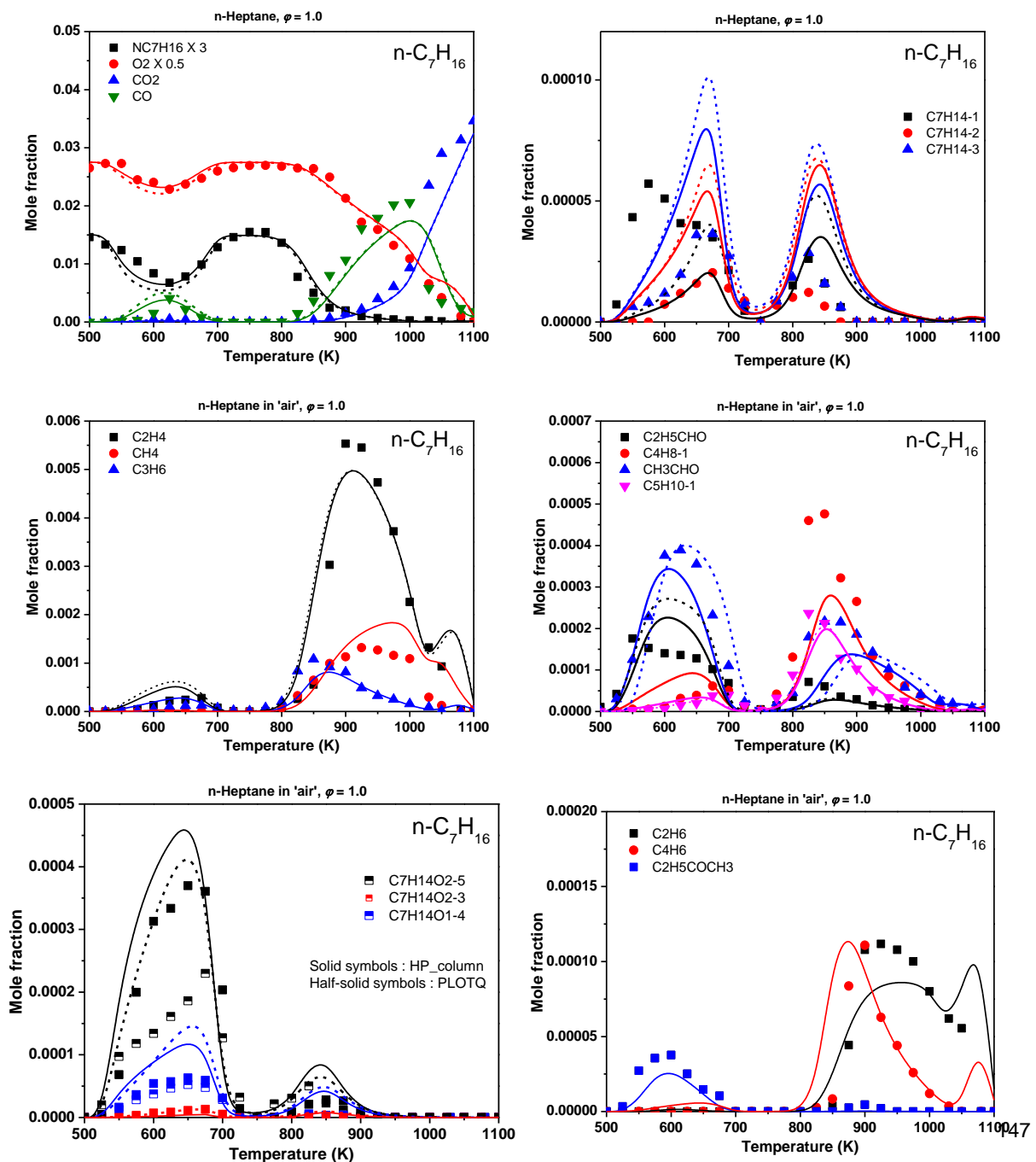
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- [1] Zhang et al., *Combustion and Flame* 172, 116 – 135 (2016).
- [2] Heufer et al., *Shock Waves* 20, 307 – 316 (2010).
- [3] Gauthier et al., *Combustion and Flame* 139 (28), 300 – 311 (2004).
- [4] Wu et al., *submitted to Combustion and Flame (under review)*
- [5] Shen et al., *Energy & Fuels* 23, 2482 – 2489 (2009).

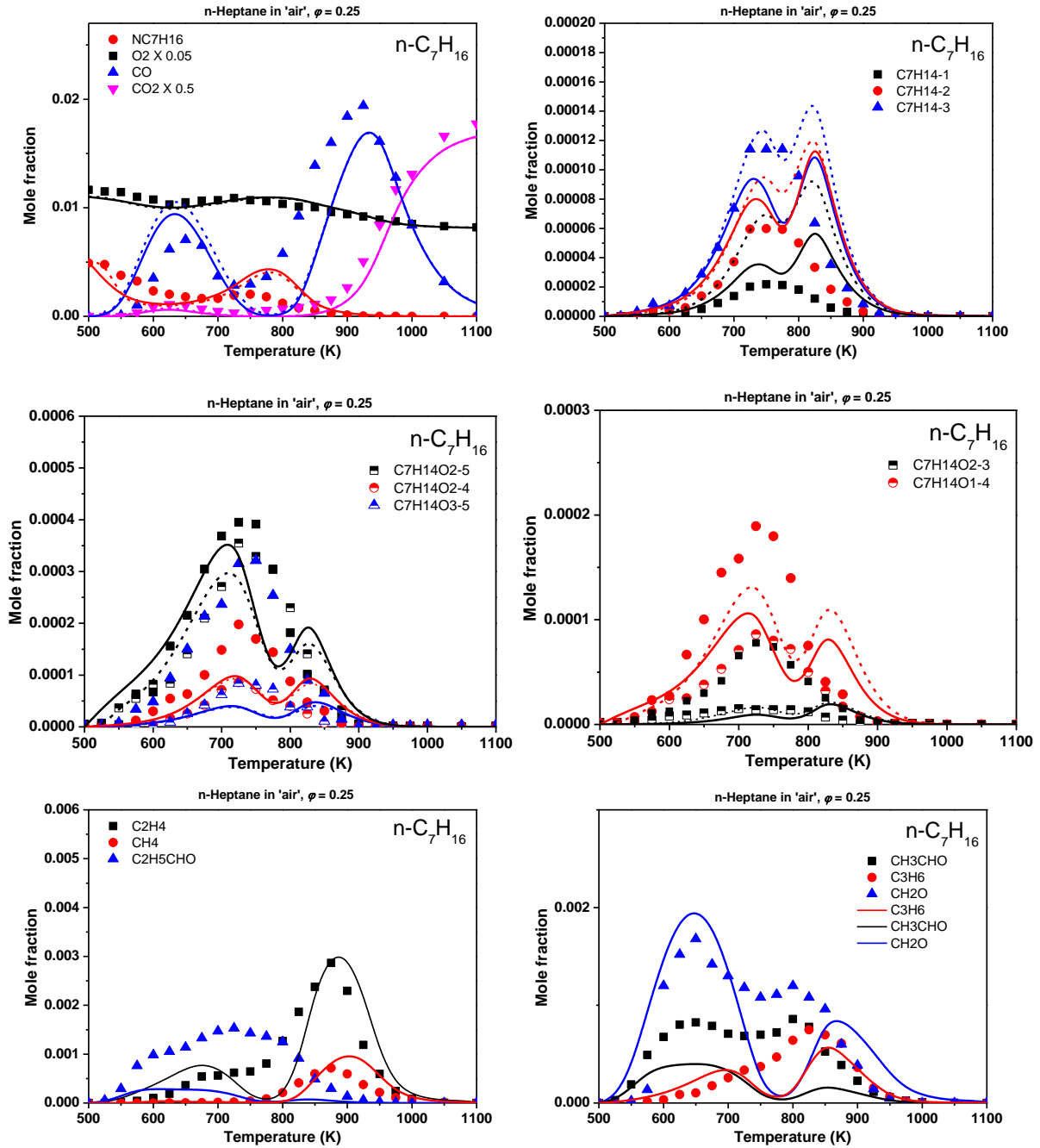
Jet Stirred Reactor

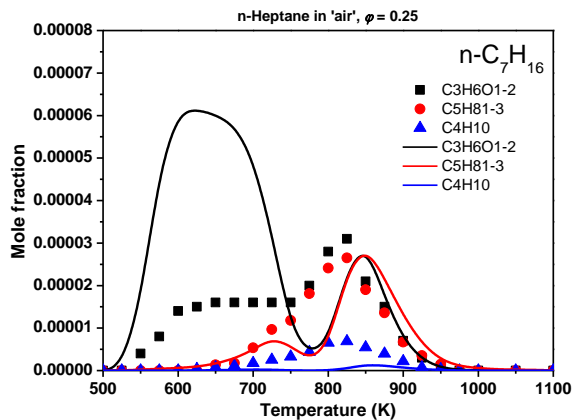
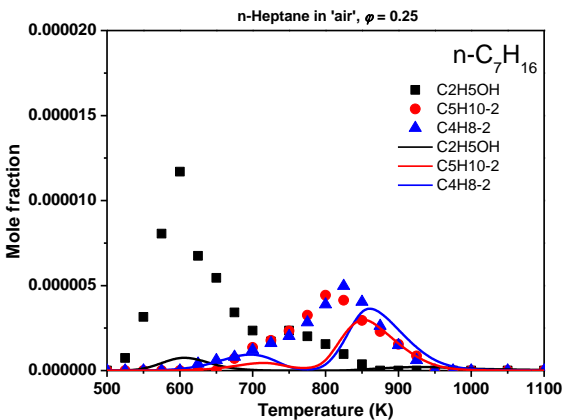
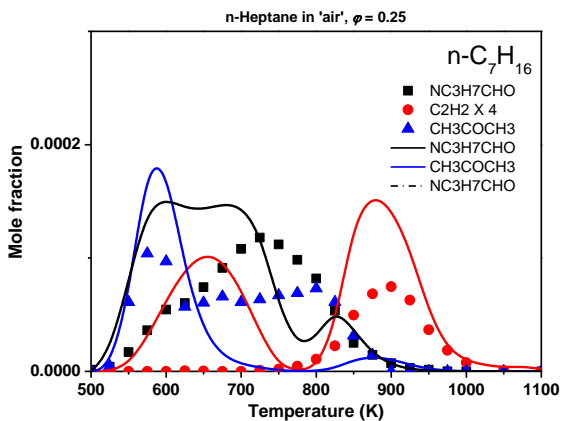
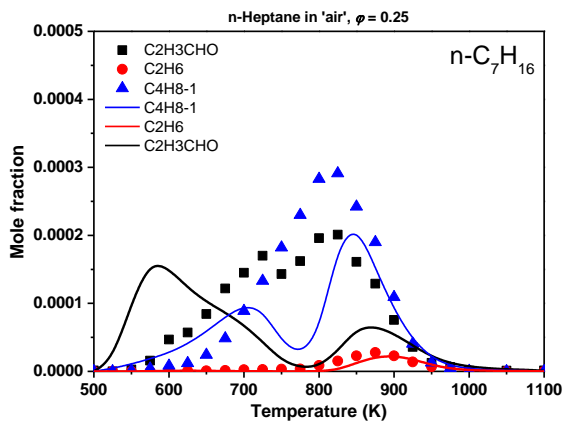
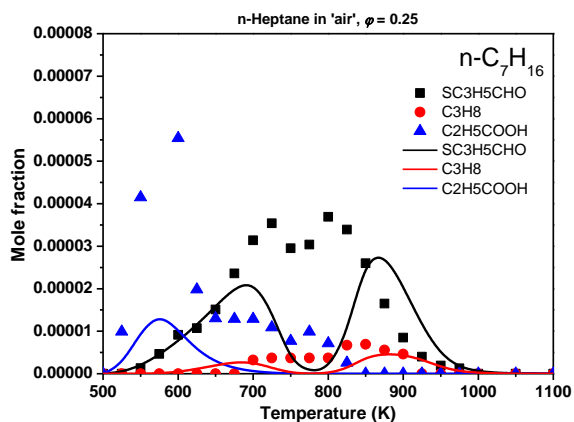
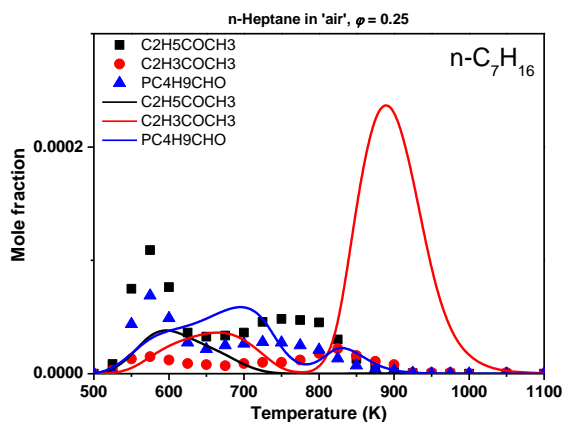
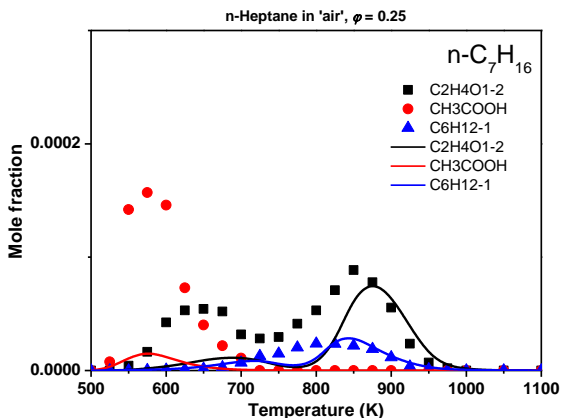
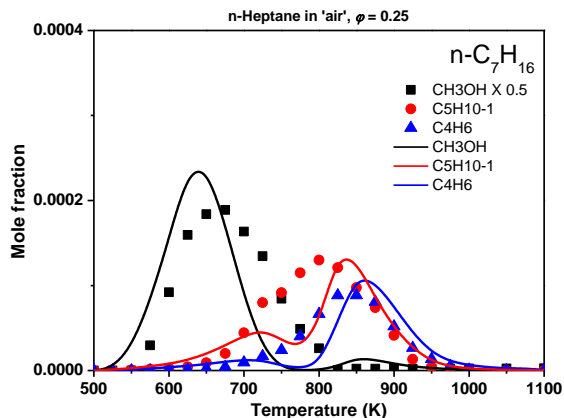
p	T	φ
1, 10 atm	500 – 1100 K	0.25 – 4.0

n-heptane JSR : PHI 1.0, 1 BAR

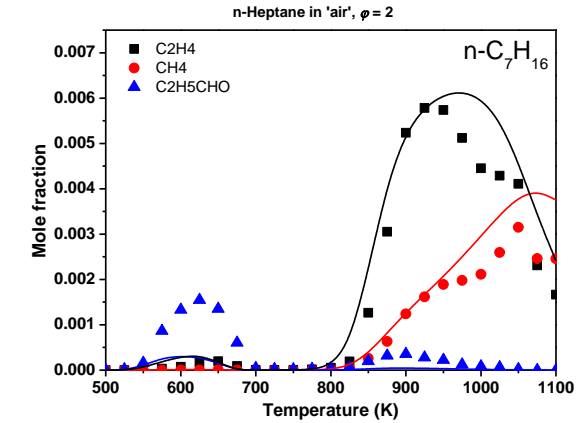
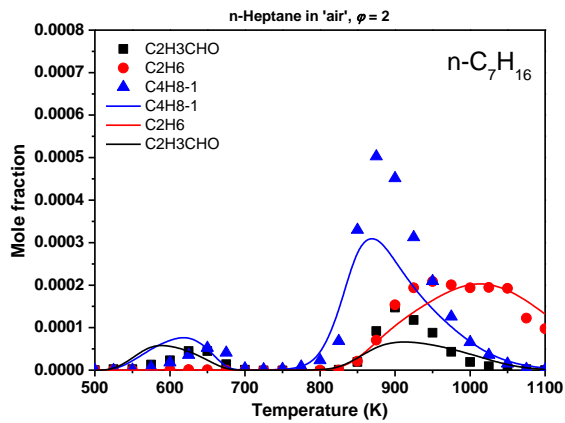
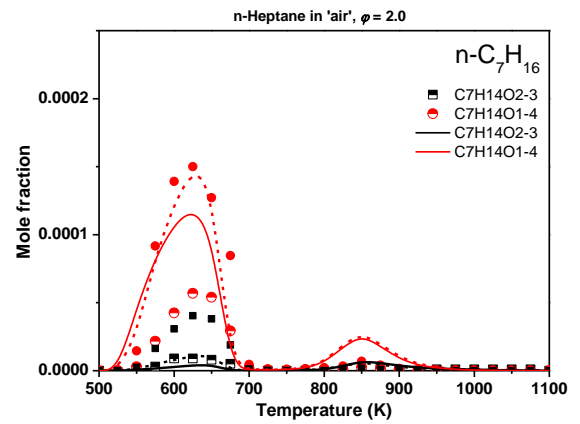
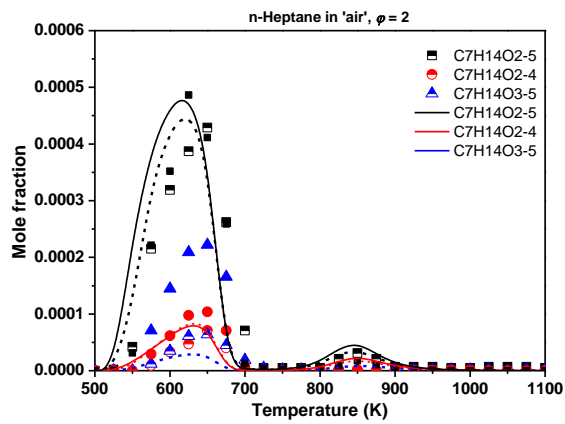
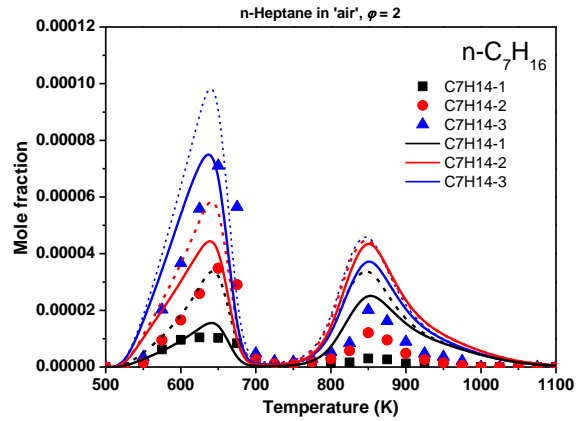
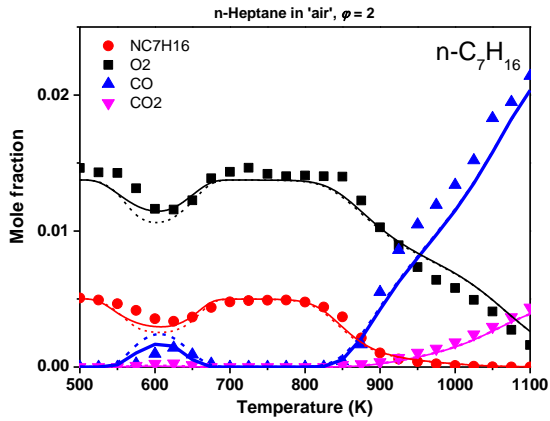


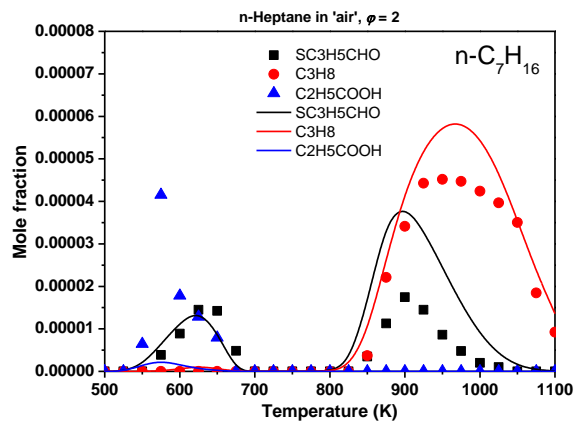
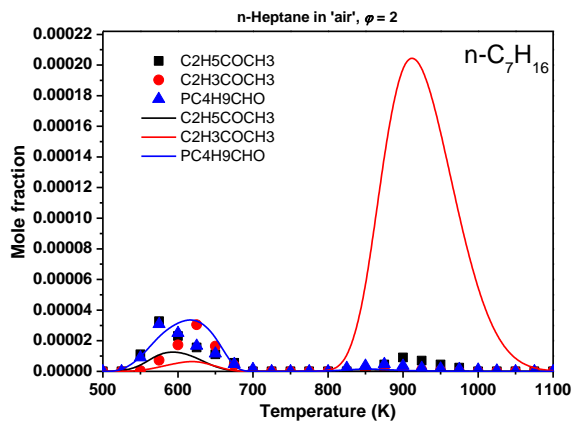
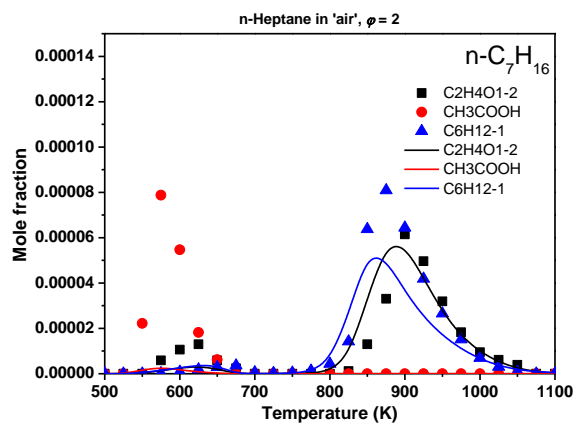
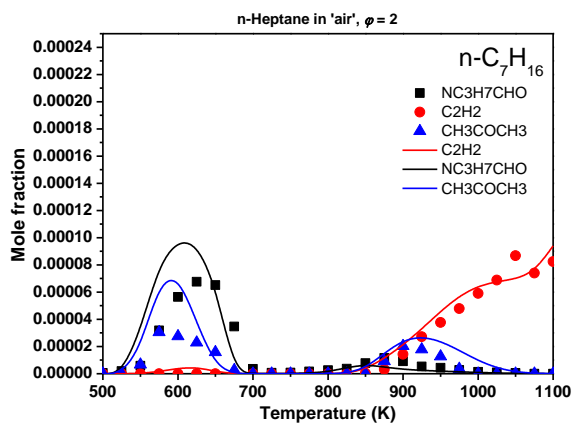
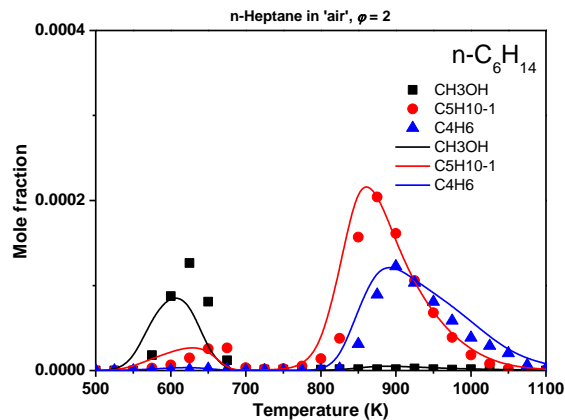
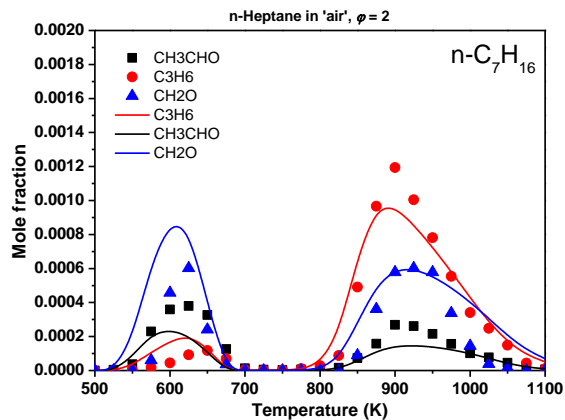
n-heptane JSR : PHI 0.25, 1 BAR

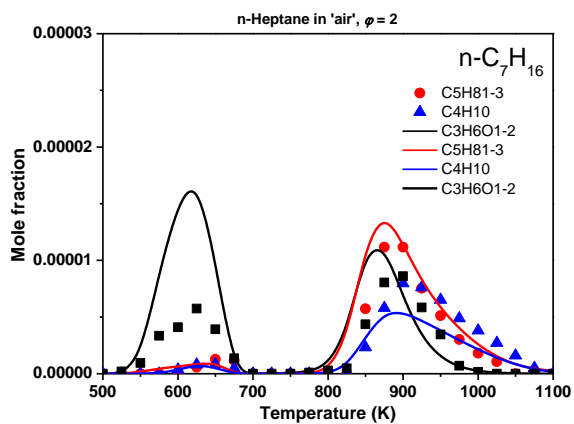
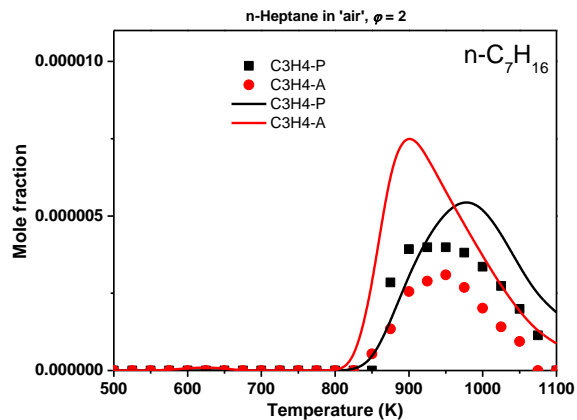
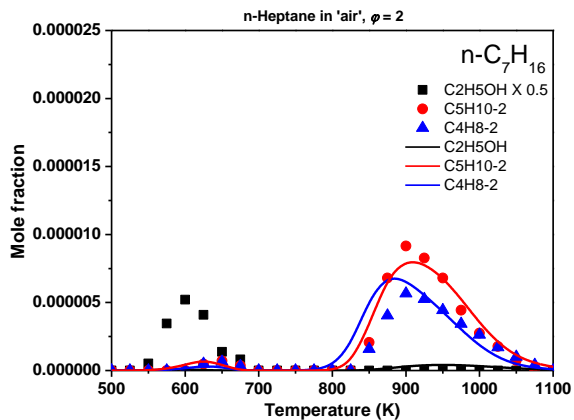




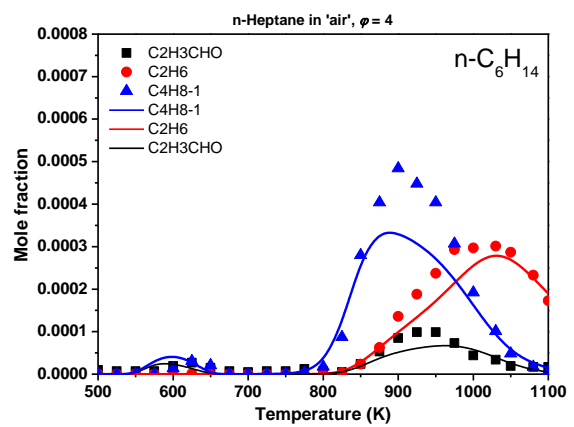
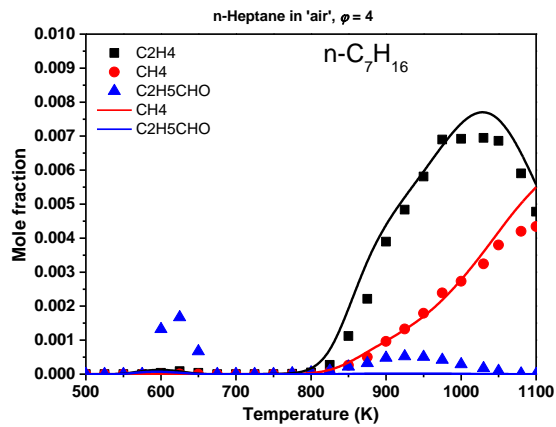
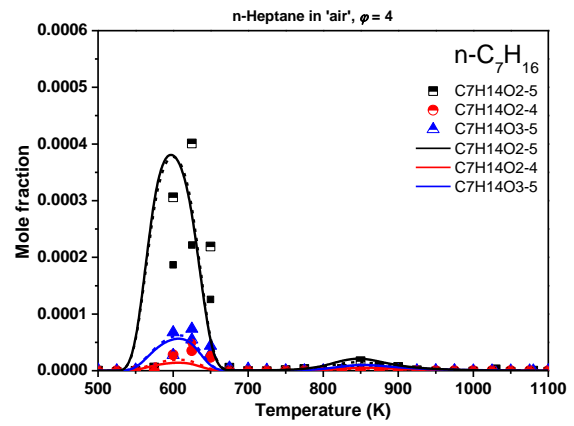
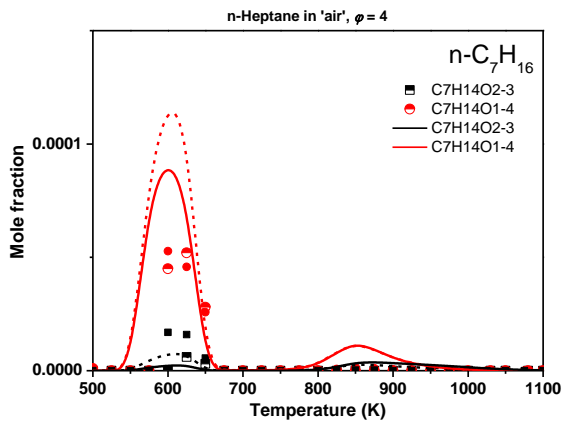
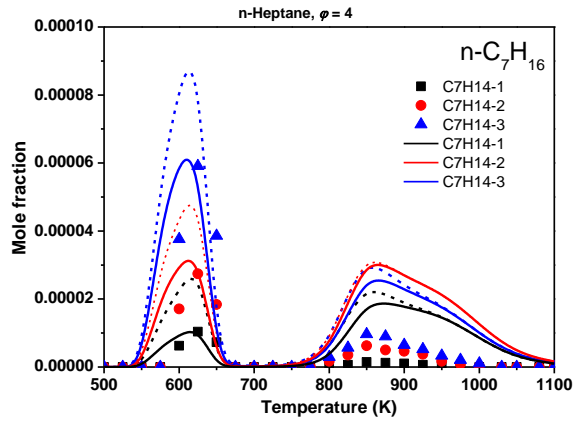
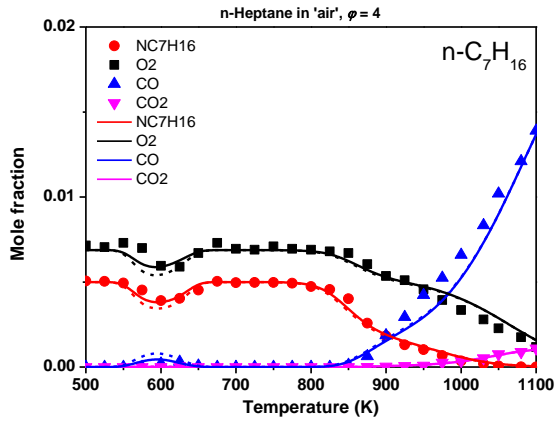
n-heptane JSR : PHI 2.0, 1 BAR

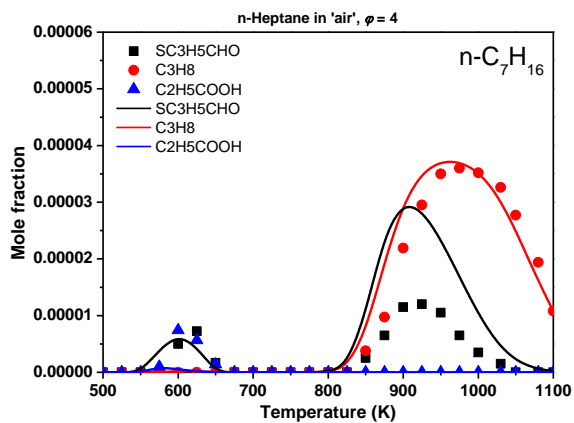
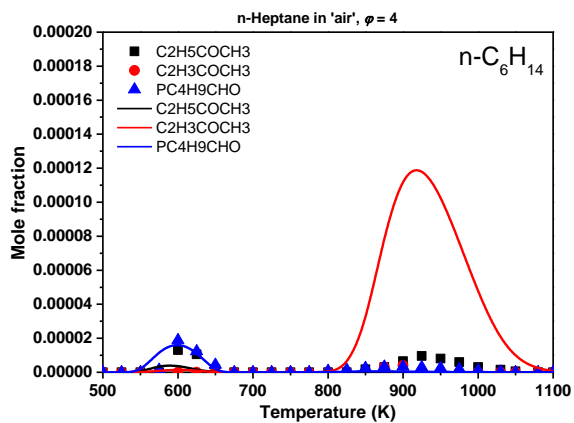
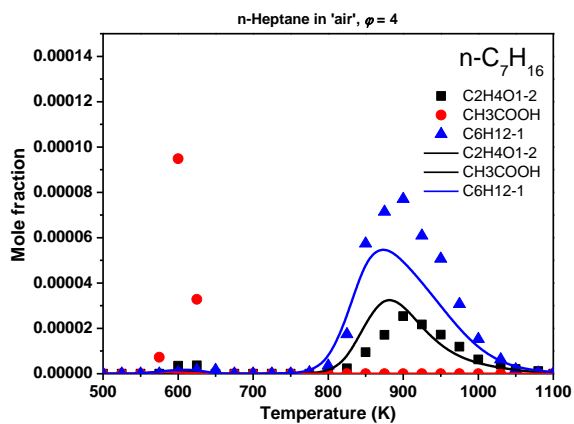
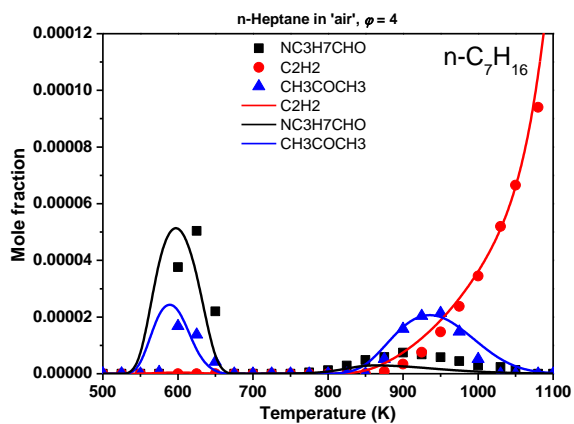
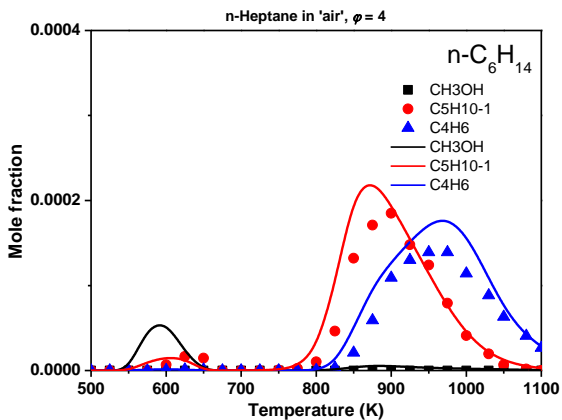
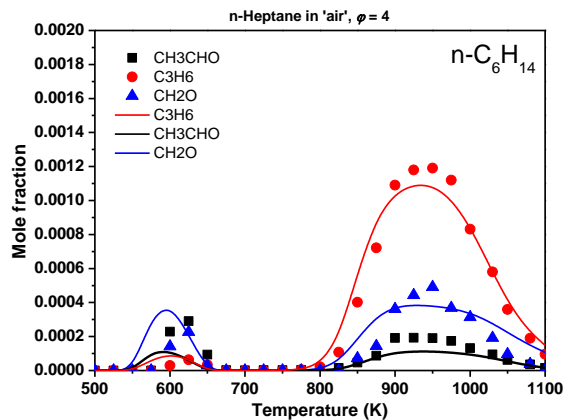


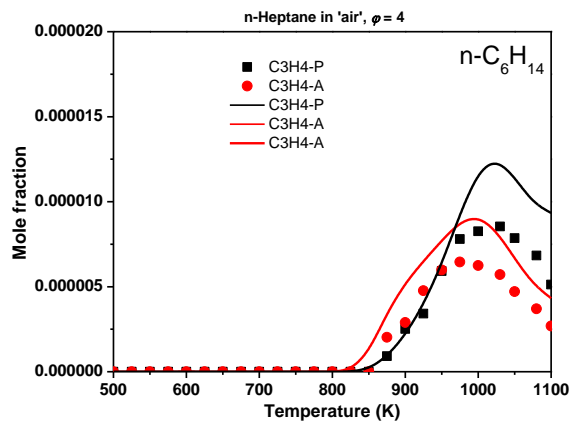
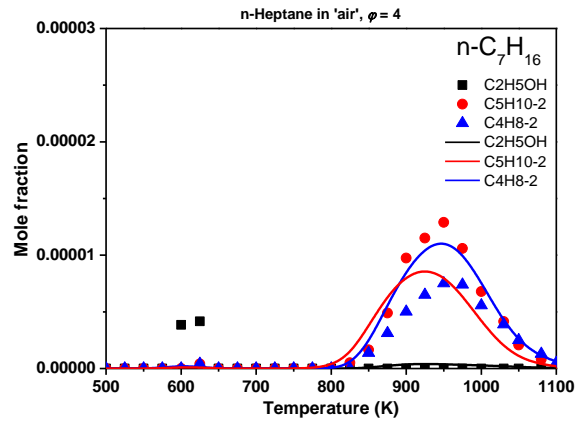
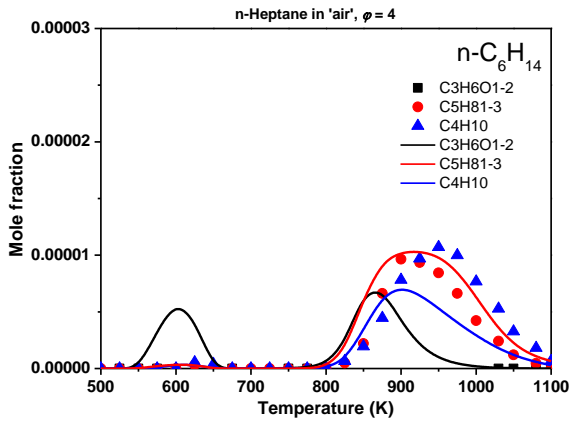




n-heptane JSR : PHI 4.0, 1 BAR





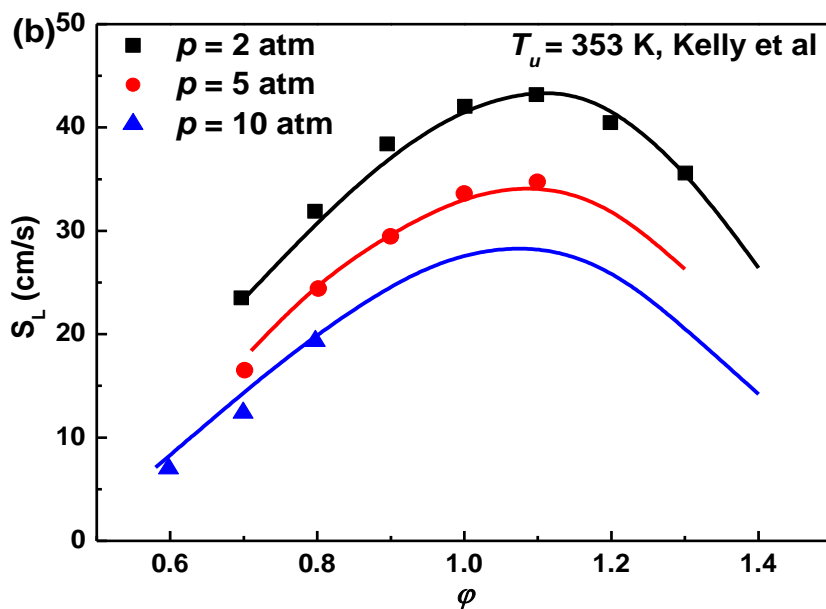
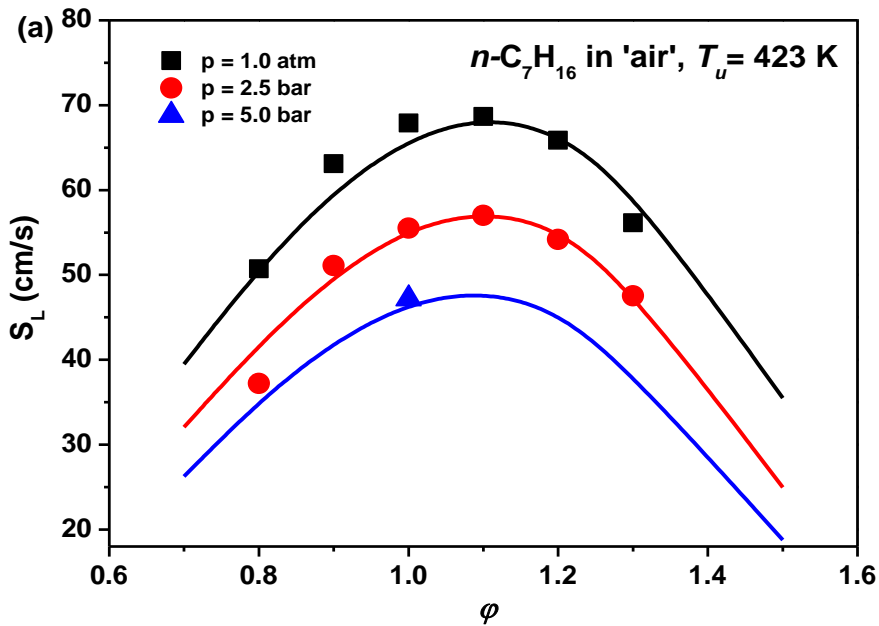


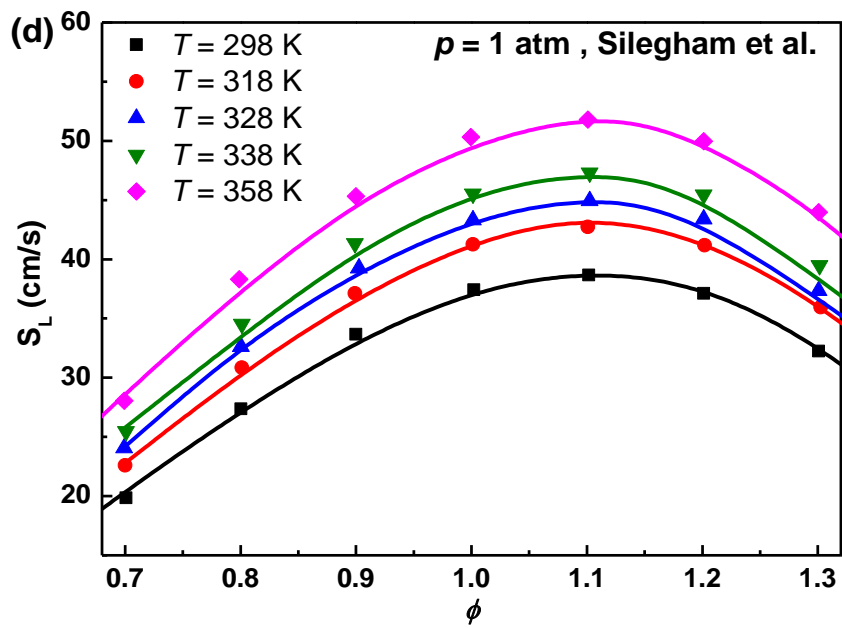
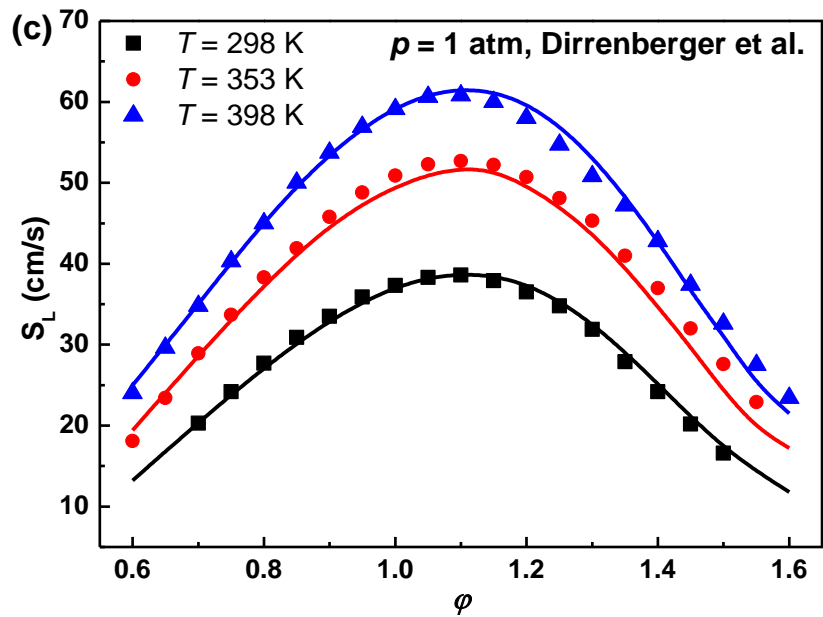
REFERENCES

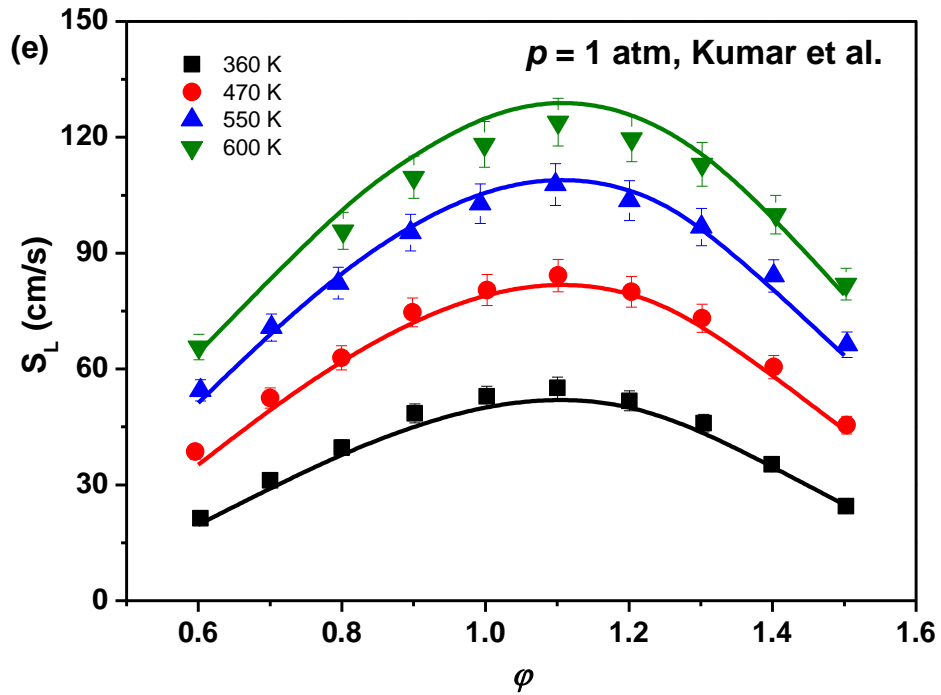
- [1] Zhang et al., Combustion and Flame 172, 116 – 135 (2016).
- [2] Dagaut et al., Combust. Sci. Tech. 95, 233 – 260 (1993).

Flame Speed

p	T	ϕ
1 – 10 atm	298 – 600 K	0.6 – 1.6







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