Electronic Supplementary Information

Molecular geometries.

NH_3, R(N-H): 1.013Å, ∠(H-N-H): 107.29°.

MMA (In the methyl of MMA, two equivalent hydrogen atoms are labeled as H, and the third hydrogen atom is labeled as H'), R(N-H): 1.014 Å, R(N-C): 1.465 Å, R(C-H): 1.092 Å, R(C-H'):1.099 Å, ∠(H-N-H): 106.71°, ∠(H-N-C): 110.37°, ∠(N-C-H): 108.98°, ∠(N-C-H'): 114.95°, ∠(H-C-H): 107.43°, ∠(H-C-H'): 108.13°, ∠(H-N-C-H): 62.66°, ∠(H-N-C-H): 179.61°, ∠(H-N-C-H'): 58.86°.

TMA (In each methyl of TMA, two equivalent hydrogen atoms are labeled as H, and the third hydrogen atom is labeled as H'), R(N-C): 1.455 Å, R(C-H): 1.094 Å, R(C-H'): 1.107 Å, ∠(N-C-H): 109.62°, ∠(N-C-H'): 112.23°, ∠(C-N-C): 110.37°, ∠(H-C-H): 108.52°, ∠(H-C-H'): 108.38°, ∠(C-N-C-H): 59.35°, ∠(C-N-C-H): 178.38°, ∠(C-N-C-H'): 61.13°

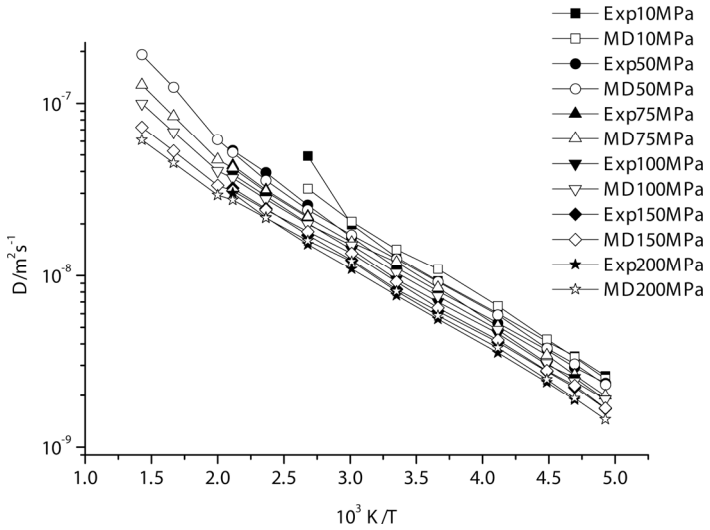

Fig. S1 Self-diffusion coefficients *D* for NH_3.

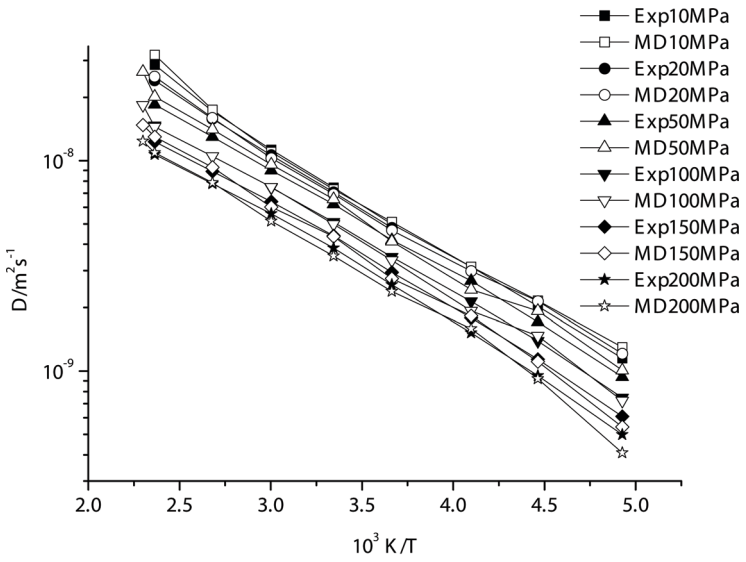

Fig. S2 Self-diffusion coefficients *D* for MMA

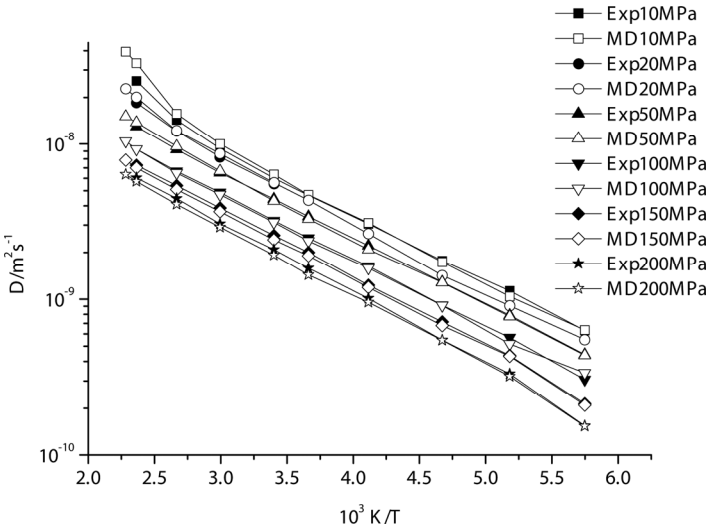

Fig. S3 Self-diffusion coefficients *D* for TMA

Table S1 The average intermolecular potential energies ($kJ \cdot mol^{-1}$) for NH_3 at 10 MPa

T / K	203	213	223	243	273	298.5	332	373
E_{inter}	-24.63	-23.84	-23.10	-21.52	-19.29	-17.91	-15.96	-13.31

Table S2 The average intermolecular potential energies ($kJ \cdot mol^{-1}$) for MMA at 10 MPa

T / K	203	224	244	273	299	333	373	423
E_{inter}	-28.13	-26.48	-25.02	-24.19	-21.96	-19.52	-16.49	-12.46

Table S3 The average intermolecular potential energies ($kJ \cdot mol^{-1}$) for TMA at 10 MPa

T / K	174	193	214	243	273	294	334	375
E_{inter}	-25.56	-24.36	-22.82	-21.07	-19.14	-17.75	-15.58	-12.71

Table S4 The average errors of simulated self-diffusion coefficients compared with the experimental data [a] for NH_3

T / K	10 MPa	50 MPa	75 MPa	100 MPa	150 MPa	200 MPa
203	-3.8	-2.1	-	-0.5	0.6	-
213	-1.2	4.4	-	-4.7	2.7	2.1
223	2.9	2.2	-	2.0	1.1	4.2
243	10.5	11.5	-	4.8	2.9	6.7
273	17.2	13.2	-	8.1	4.5	4.8
298.5	10.9	12.6	-	9.5	10.6	5.8
332	4.0	3.0	-	5.6	9.8	11.0
373	-35.2	-5.9	-1.4	-1.0	4.7	5.3
423	-	-9.9	-2.5	-4.2	-1.6	-0.9
473	-	-2.6	-3.5	-4.9	-3.7	-9.0

[a] The experimental self-diffusion coefficients were taken from the literature (20).

Table S5 The average errors of simulated self-diffusion coefficients compared with the experimental data [a] for MMA

T / K	10 MPa	20 MPa	50 MPa	100 MPa	150 MPa	200 MPa
203	13	-	7.6	-3.5	-10.7	-18.2
224	6.4	-	12.9	5.8	-2.6	-3.2
244	0.0	-	-9.0	-9.8	2.2	4.6
273	2.8	-2.7	-1.4	-3.4	-6.5	-7.0
299	-2.0	-2.1	5.6	-2.4	-0.7	-8.3
333	-2.7	-2.8	6.4	0.5	-5.6	-7.7

373	1.7	1.3	8.5	-2.8	4.7	1.0
423	11.5	4.1	9.2	-1.4	5.7	1.9

[a] The experimental self-diffusion coefficients were taken from the literature (21).

Table S6 The average errors of simulated self-diffusion coefficients compared with the experimental data [a] for TMA

T / K	10 MPa	20 MPa	50 MPa	100 MPa	150 MPa	200 MPa
174	0.8	-	-1.1	10.1	-2.3	-0.6
193	-8.0	-	-1.8	-9.0	-1.1	-3.6
214	-2.3	-	-0.8	-0.4	-5.0	-0.5
243	1.3	-	-5.4	-3.1	-3.3	-5.3
273	0.6	-	-3.5	-4.0	-5.0	-9.5
294	5.3	1.8	-2.7	-2.8	-6.2	-8.1
334	7.0	5.5	2.3	-3.1	-5.4	-4.9
375	9.8	0.8	4.9	-2.6	-5.6	-8.3
423	29.7	8.1	6.2	0.0	-3.8	-5.1

[a] The experimental self-diffusion coefficients were taken from the literature (21).