Supporting Information for:

Computational Study of the Rate Constants for the reaction of NO_2 with CH_3NHNH, CH_3NNH_2, and CH_2NHNH_2

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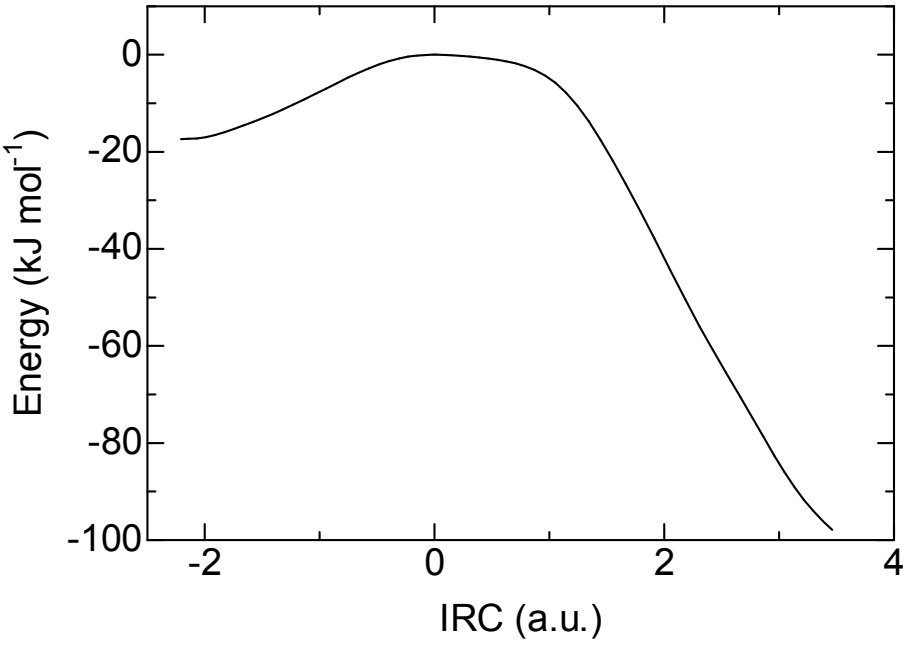

Figure S1. The IRC profile for the roaming transition state TS4 in the CH_3NHNH + NO_2 system, i.e. $CH_3NHNHNO_2 \leftrightarrow CH_3NHNHONO$, calculated at the CASPT2/cc-pVDZ level of theory.

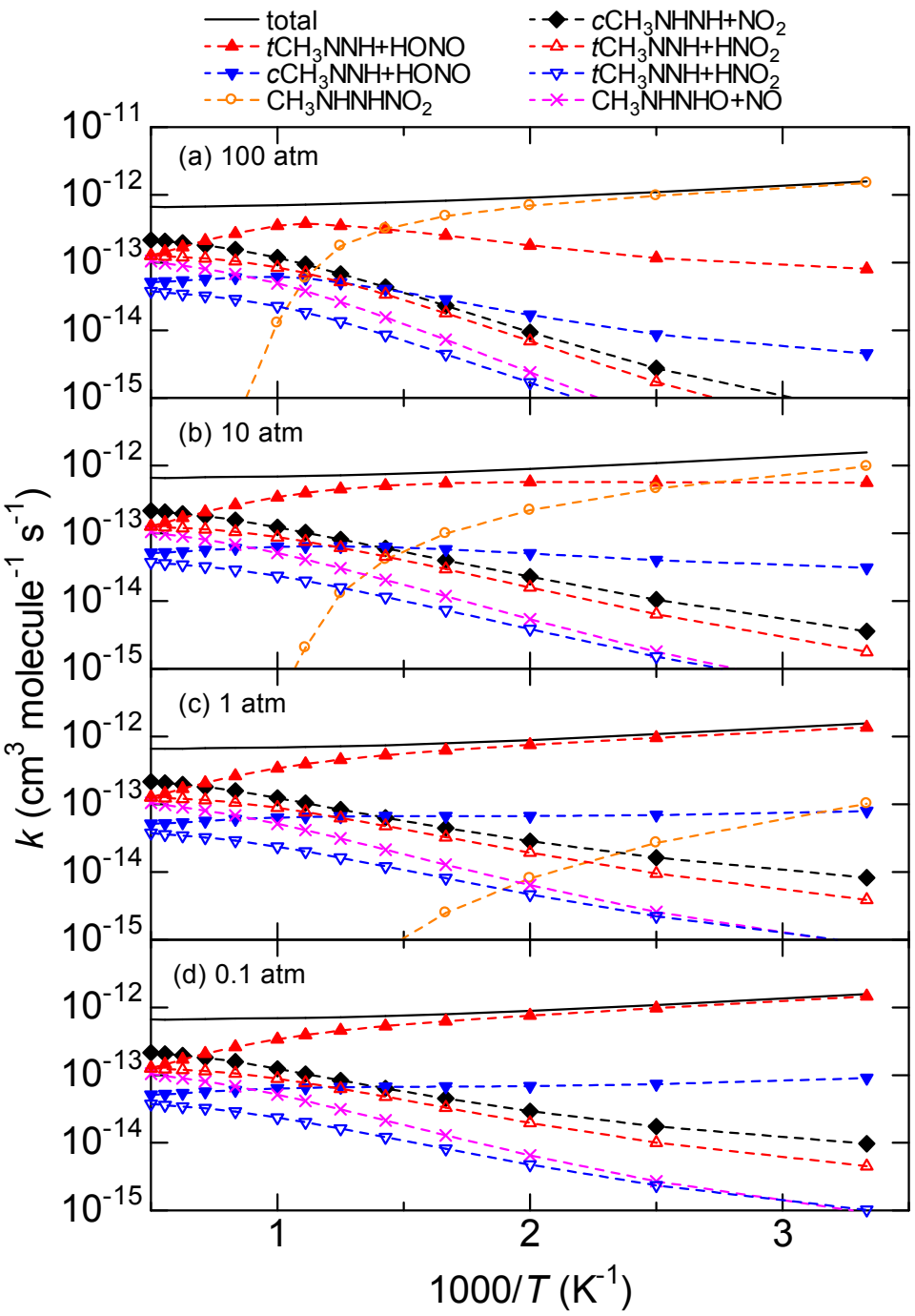

Figure S2. Arrhenius plots of *t*-CH_3NHNH + NO_2 reaction rate coefficients at (a) 100, (b) 10, (c) 1, and (d) 0.1 atm in N_2.

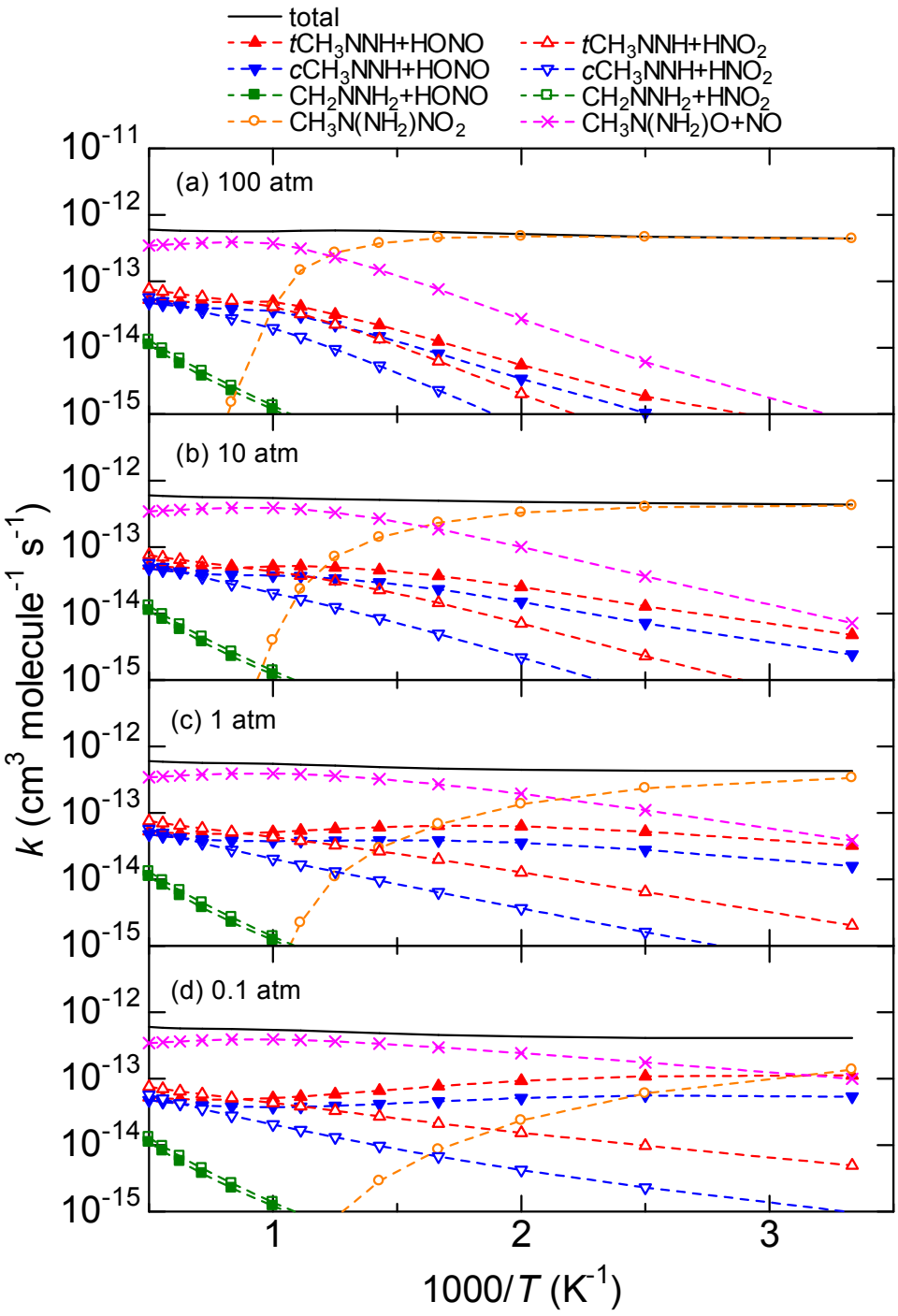

Figure S3. Arrhenius plots of CH_3NNH_2 + NO_2 reaction rate coefficients at (a) 100, (b) 10, (c) 1, and (d) 0.1 atm in N_2.

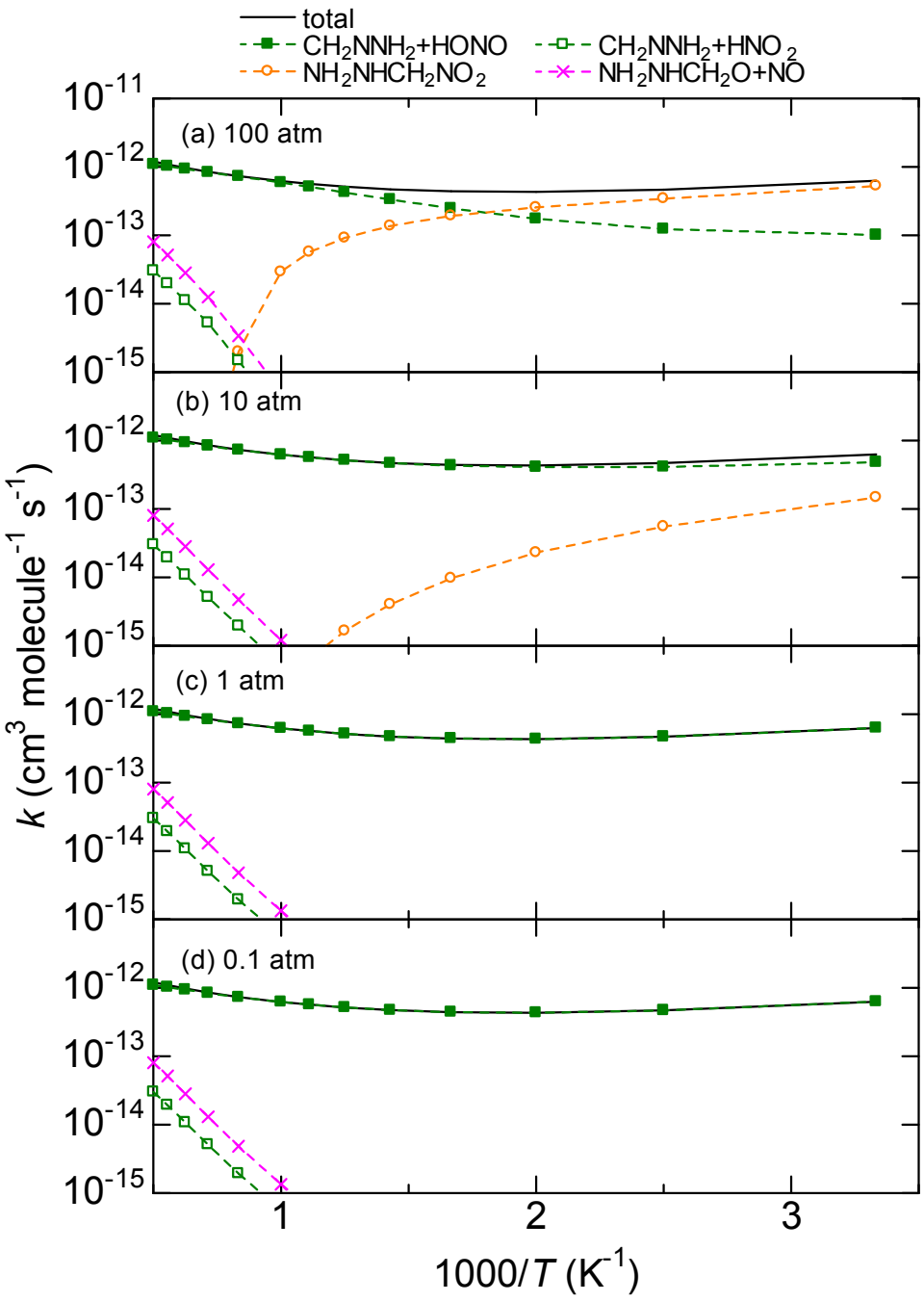

Figure S4. Arrhenius plots of CH_2NHNH_2 + NO_2 reaction rate coefficients at (a) 100, (b) 10, (c) 1, and (d) 0.1 atm in N_2.

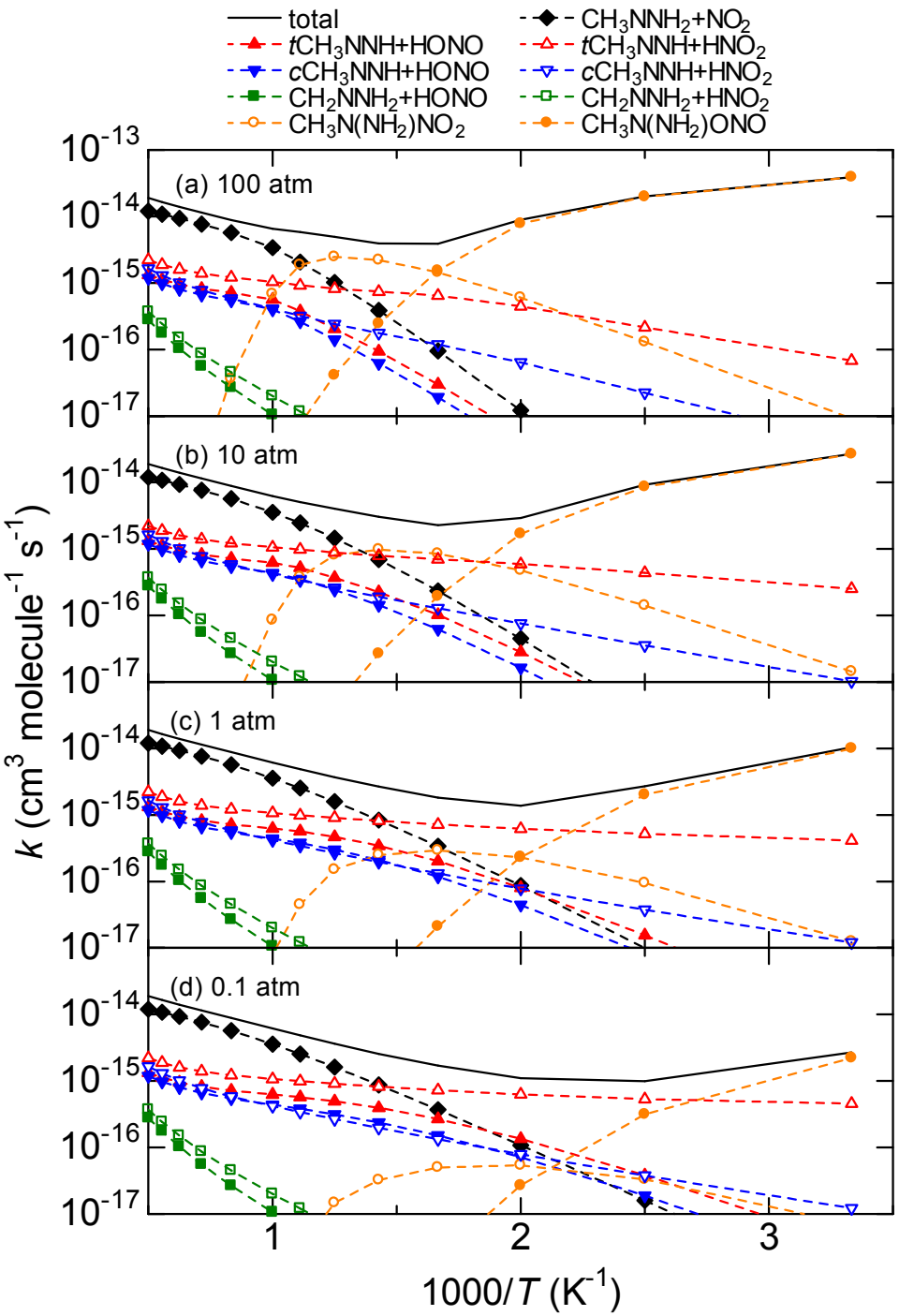

Figure S5. Arrhenius plots of $CH_3N(NH_2)O$ + NO reaction rate coefficients at (a) 100, (b) 10, (c) 1, and (d) 0.1 atm in N_2.

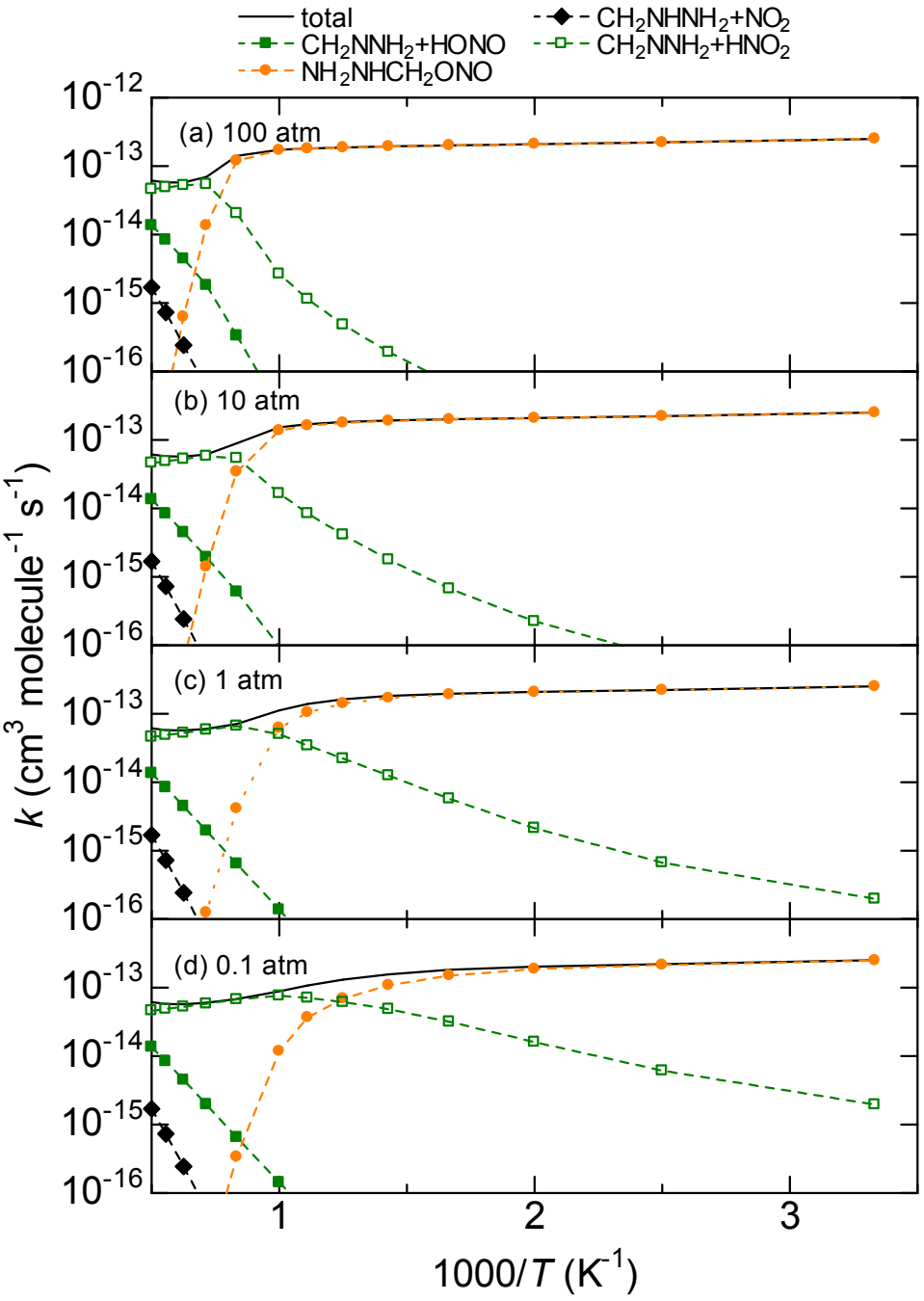

Figure S6. Arrhenius plots of NH_2NHCH_2O + NO reaction rate coefficients at (a) 100, (b) 10, (c) 1, and (d) 0.1 atm in N_2.

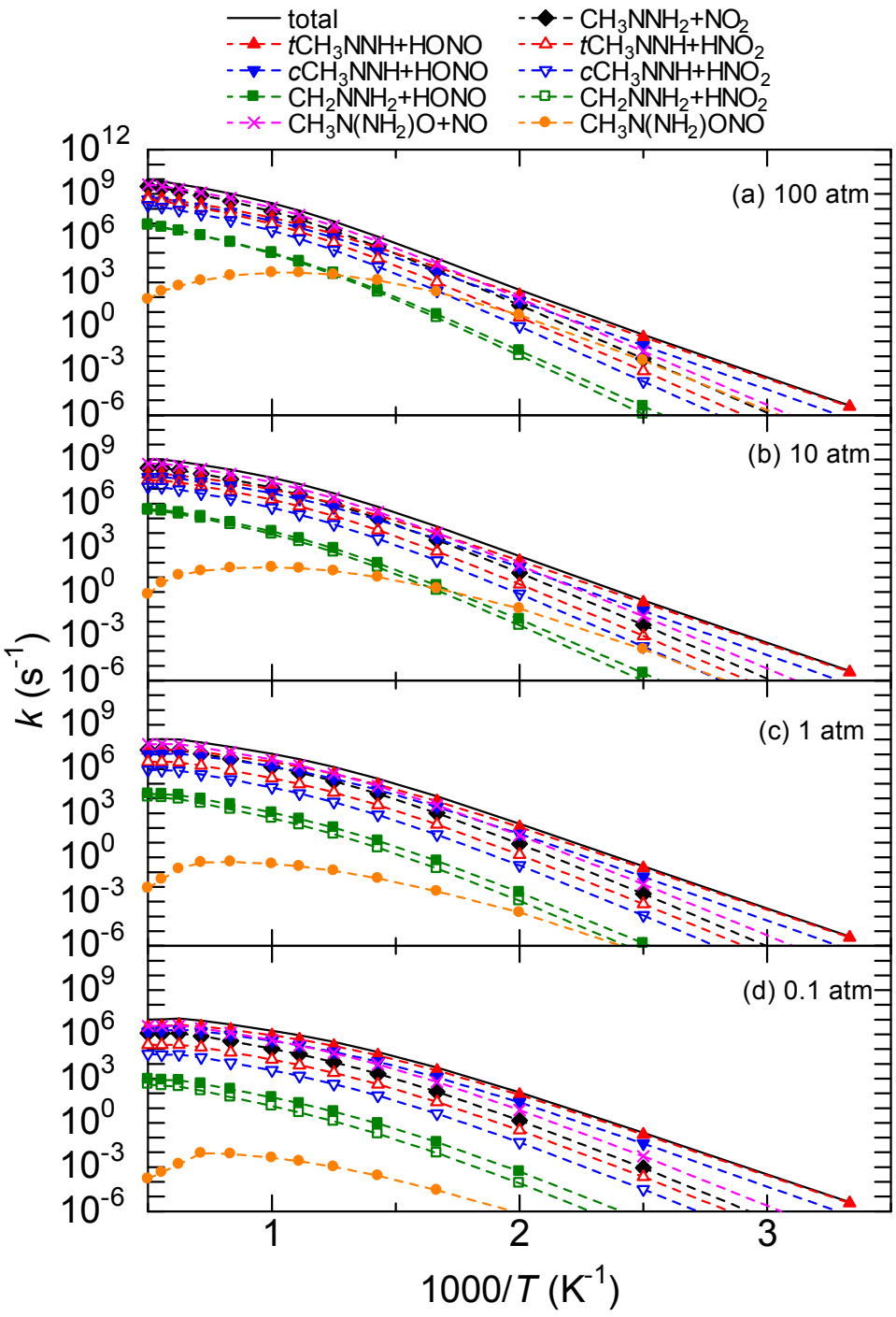

Figure S7. Arrhenius plots of thermal decomposition rate coefficients of $CH_3N(NH_2)NO_2$ at (a) 100, (b) 10, (c) 1, and (d) 0.1 atm in N_2.

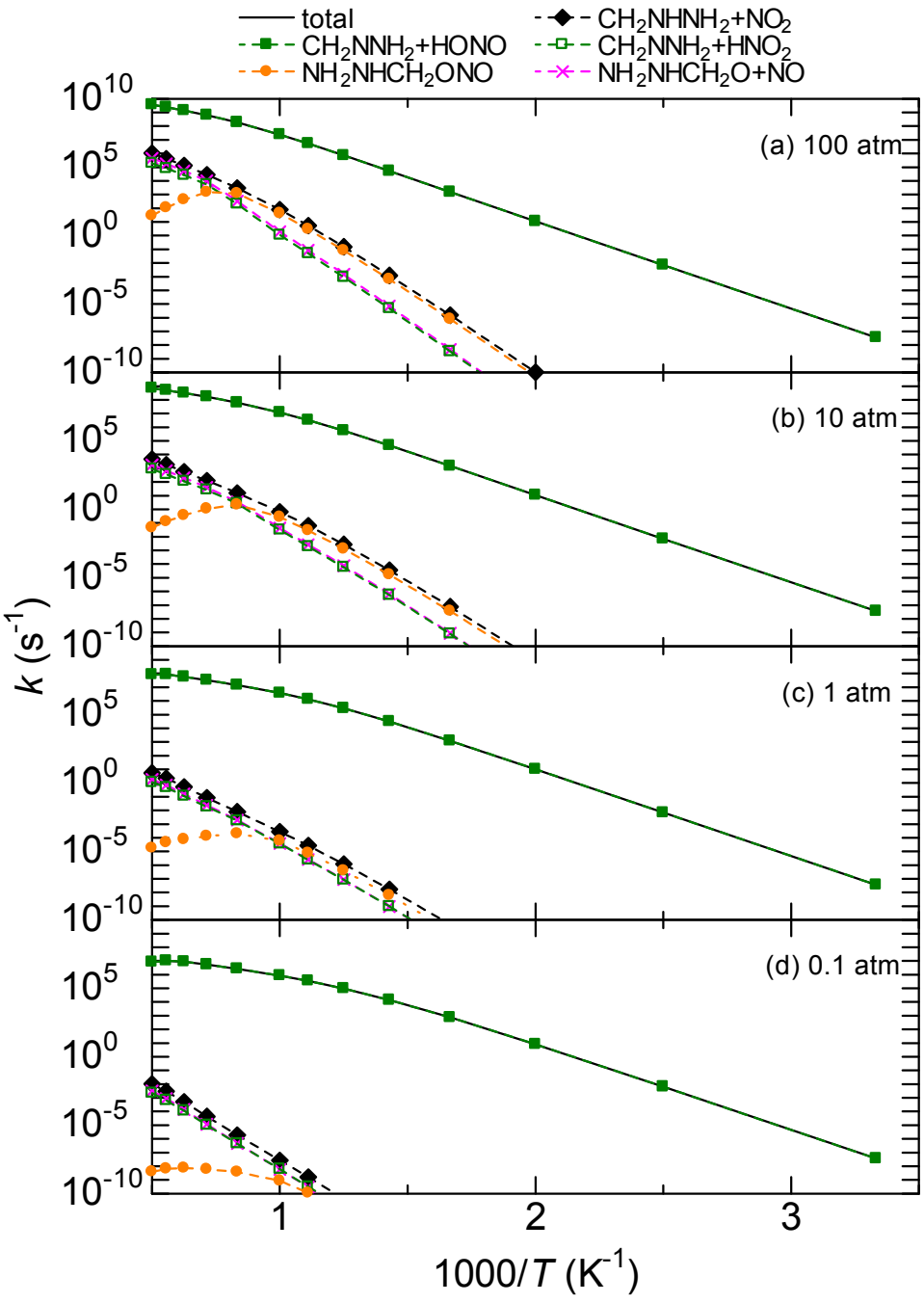

Figure S8. Arrhenius plots of thermal decomposition rate coefficients of $NH_2NHCH_2NO_2$ at (a) 100, (b) 10, (c) 1, and (d) 0.1 atm in N_2.

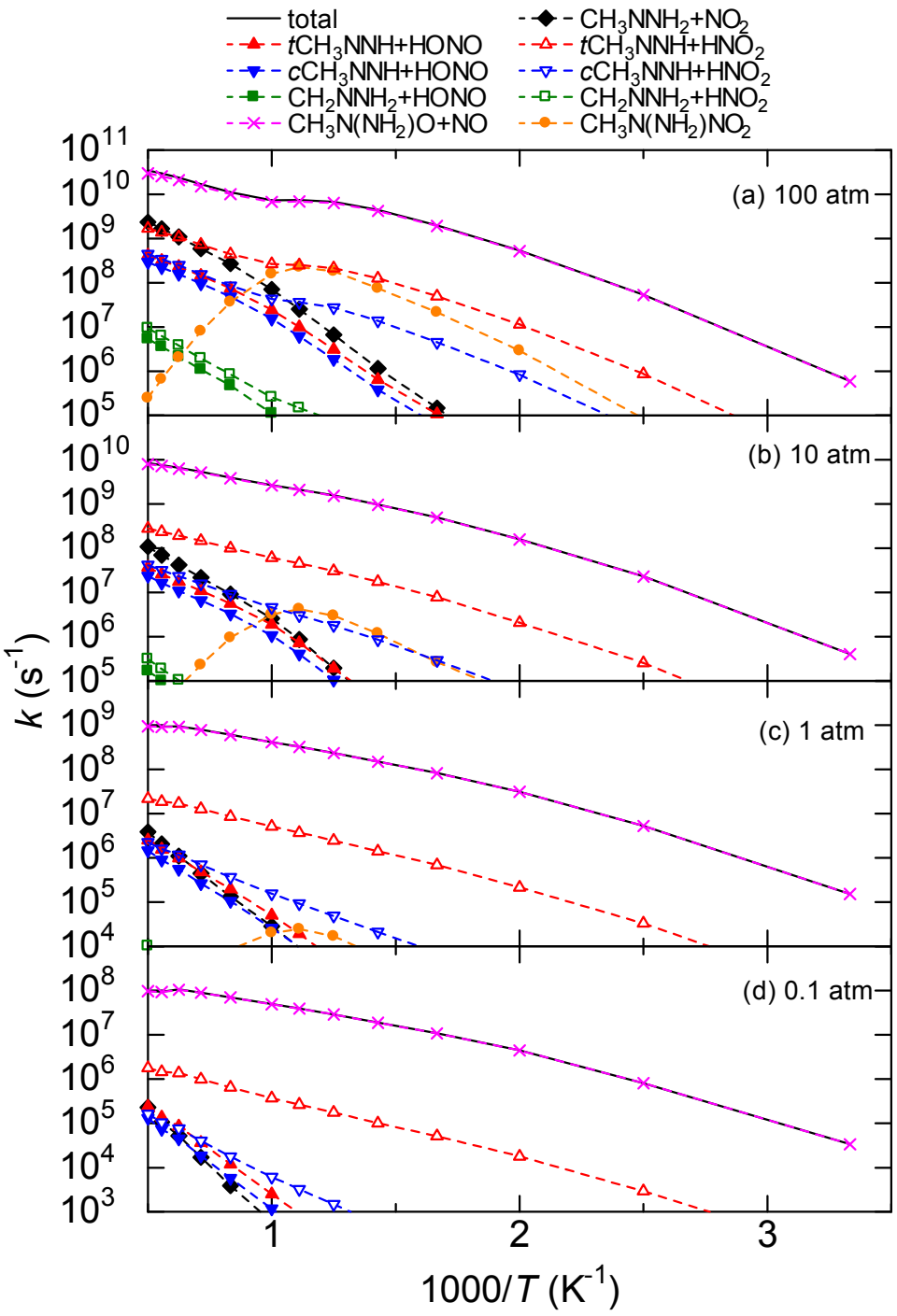

Figure S9 Arrhenius plots of thermal decomposition rate coefficients of $CH_3N(NH_2)ONO$ at (a) 100, (b) 10, (c) 1, and (d) 0.1 atm in N_2.

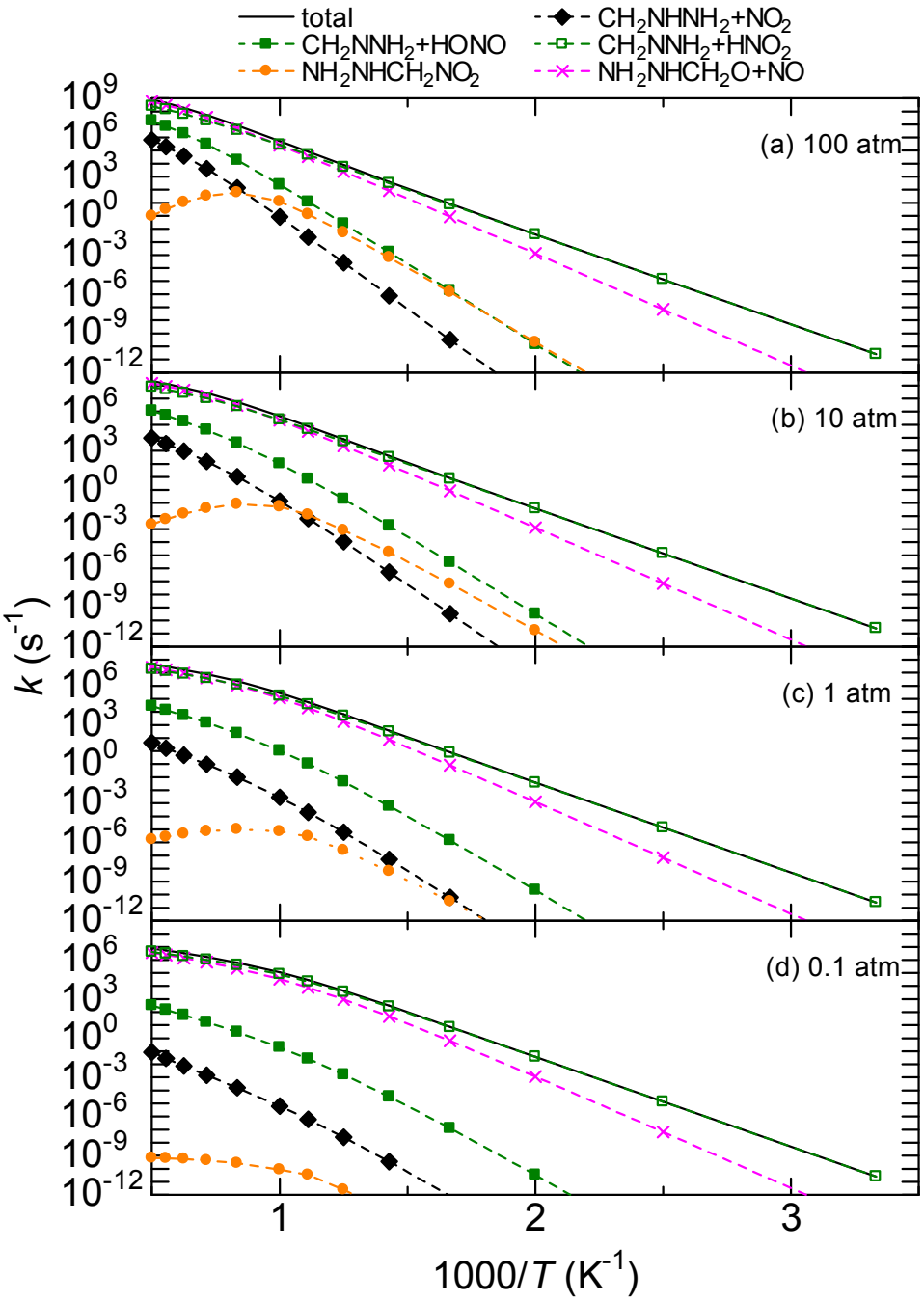

Figure S10. Arrhenius plots of thermal decomposition rate coefficients of NH_2NHCH_2ONO at (a) 100, (b) 10, (c) 1, and (d) 0.1 atm in N_2.

Table S1. The optimized geometries of the most stable isomers for the reactants, products, intermediates, and the transition states calculated at the (U)ωB97X-D/ 6-311++G(d,p) level of theory.

species	atoms	x	y	z
NO_2	O	0.000000	1.092926	-0.139761
	N	0.000000	0.000000	0.319455
	O	0.000000	-1.092926	-0.139761
cCH_3NHNH	N	-1.190245	-0.384199	0.012947
	N	-0.138732	0.437227	-0.089548
	C	1.169542	-0.166700	0.019159
	H	1.927358	0.552675	-0.296743
	H	1.386745	-0.497604	1.042068
	H	1.204354	-1.033777	-0.641580
	H	-0.218192	1.392849	0.236947
	H	-2.014677	0.214858	0.080561
tCH_3NHNH	N	-1.297961	-0.186698	0.053780
	N	-0.139970	0.463748	-0.103111
	C	1.148416	-0.186623	0.024198
	H	1.938766	0.515677	-0.246305
	H	1.328635	-0.553682	1.042969
	H	1.193005	-1.033158	-0.666641
	H	-0.190322	1.423511	0.204204
	H	-1.095062	-1.171956	-0.134098
CH_3NNH_2	N	1.128758	0.197332	0.080877
	N	0.062108	-0.612388	-0.036002
	C	-1.155403	0.156018	0.005209
	H	-1.998714	-0.510568	-0.173831
	H	-1.291135	0.634329	0.986366
	H	-1.170857	0.950770	-0.760218
	H	2.000841	-0.259018	-0.138931
	H	1.052619	1.153773	-0.258760

TABLE S1. (Continued)

species	atoms	x	y	z
CH_2NHNH_2	N	-1.203453	-0.103170	0.063572
	N	0.064195	0.481641	-0.130220
	C	1.200438	-0.278674	0.070003
	H	2.138238	0.261943	0.097050
	H	1.180589	-1.290440	-0.319055
	H	0.087973	1.415159	0.251056
	H	-1.479619	-0.570480	-0.791965
	H	-1.154999	-0.793441	0.809430
*t*HONO	H	1.754544	-0.149774	0.000000
	O	0.887009	-0.571877	0.000000
	N	0.000000	0.508748	0.000000
	O	-1.106327	0.145444	0.000000
HNO_2	H	0.000000	0.000000	1.349427
	N	0.000000	0.000000	0.308696
	O	0.000000	1.086454	-0.219394
	O	0.000000	-1.086454	-0.219394
NO	N	0.000000	0.000000	-0.609410
	O	0.000000	0.000000	0.533234
cCH_3NNH	N	1.192276	0.283026	0.000000
	N	0.000000	0.574594	0.000000
	C	-0.986241	-0.499350	0.000000
	H	-0.520807	-1.497006	0.000000
	H	-1.619618	-0.377939	0.881590
	H	-1.619618	-0.377939	0.881590
	H	1.311561	-0.754358	0.000000
tCH_3NNH	N	1.154779	0.103825	0.000000
	N	0.000000	0.534457	0.000000
	C	-1.005411	-0.520088	0.000000
	H	-0.554901	-1.516899	0.000000
	H	-1.636879	-0.377144	0.880446
	H	-1.636879	-0.377144	-0.880446
	H	1.777671	0.923744	0.000000

TABLE S1. (Continued)

species	atoms	x	y	z
CH_2NNH_2	N	1.107792	0.143766	-0.091195
	N	-0.081571	-0.515702	0.006841
	C	-1.150382	0.168905	0.007666
	H	-1.161405	1.263745	-0.027091
	H	-2.093298	-0.363898	0.036648
	H	1.114085	1.101568	0.248722
	H	1.859366	-0.411290	0.286199
$CH_3NHNHNO_2$	N	-0.048642	-0.841749	0.418424
	N	-1.335200	-0.375258	0.533818
	C	-1.902986	0.277612	-0.642780
	H	-2.930331	0.556598	-0.405327
	H	-1.354357	1.172060	-0.956655
	H	-1.931438	-0.439935	-1.466227
	H	-1.410791	0.178691	1.375151
	H	0.051523	-1.666681	-0.161741
	N	0.967205	0.075354	0.028734
	O	1.928516	-0.415181	-0.518463
	O	0.810206	1.230826	0.344044
$CH_3NHNHONO$	N	0.561134	-0.900095	0.429449
	N	1.665038	-0.372013	-0.207317
	C	1.835703	1.049799	0.047134
	H	2.767310	1.371767	-0.421464
	H	1.013674	1.663937	-0.342170
	H	1.911030	1.204240	1.123649
	H	1.668242	-0.581731	-1.202429
	H	0.618695	-1.910897	0.368693
	O	-0.647648	-0.642834	-0.329969
	N	-1.439431	0.269354	0.399105
	O	-2.414897	0.514479	-0.189748

TABLE S1. (Continued)

species	atoms	x	y	z
CH_3NHNHO	N	0.743104	-0.350083	0.302178
	N	-0.512247	-0.628936	-0.258128
	C	-1.501277	0.380979	0.124802
	H	-2.433019	0.151921	-0.394944
	H	-1.186619	1.400307	-0.124852
	H	-1.681021	0.323329	1.198934
	H	-0.387177	-0.621133	-1.267493
	H	1.165623	-1.127087	0.801758
	O	1.489234	0.556362	-0.158820
$CH_3N(NH_2)NO_2$	N	-1.117473	-1.313896	0.030084
	N	-0.585713	-0.071678	-0.275544
	C	-1.407029	1.077605	0.085744
	H	-1.045547	1.962420	-0.430714
	H	-2.416357	0.841468	-0.241511
	H	-1.401222	1.258980	1.166819
	H	-0.785925	-1.989452	-0.646947
	H	-0.827074	-.1622645	0.955494
	N	0.792388	0.080992	-0.029859
	O	1.442821	-0.938232	0.075289
	O	1.218914	1.215191	0.000916
$CH_3N(NH_2)ONO$	N	-1.415551	-1.228658	0.034148
	N	-0.816056	-0.042917	-0.356665
	C	-1.662711	1.089230	-0.003462
	H	-1.152085	2.008068	-0.287005
	H	-2.585498	0.990030	-0.572849
	H	-1.894056	1.114364	1.070277
	H	-0.920213	-2.007062	-0.380029
	H	-1.448449	-1.329216	1.048299
	O	0.398084	0.159713	0.412281
	N	1.494324	-0.053171	-0.439055
	O	2.494109	0.085495	0.146855

TABLE S1. (Continued)

species	atoms	x	y	z
$CH_3N(NH_2)O$	N	-1.072046	-0.804478	-0.118205
	N	-0.023983	0.103220	0.184120
	C	1.311917	-0.429736	-0.049608
	H	2.025217	0.269628	0.381788
	H	1.401047	-1.406218	0.426792
	H	1.487036	-0.534164	-1.125260
	H	-1.838908	-0.225402	-0.447770
	H	-1.365048	-1.247773	0.748891
	O	-0.238581	1.328894	-0.018524
$NH_2NHCH_2NO_2$	N	1.901852	0.350003	-0.605720
	N	1.382437	-0.429731	0.452937
	C	0.124562	-0.971161	0.151699
	H	-0.230230	-1.633757	0.942497
	H	0.127047	-1.480548	-0.809584
	H	1.393061	0.044425	1.349101
	H	2.910146	0.279548	-0.598985
	H	1.621200	1.322361	-0.521185
	N	-1.002538	0.083458	0.019546
	O	-0.763621	1.214120	0.390985
	O	-2.053985	-0.305517	-0.433406
NH_2NHCH_2ONO	N	2.260562	-0.767435	0.053590
	N	1.407372	0.145517	-0.598747
	C	0.510815	0.893373	0.220767
	H	0.155461	1.760898	-0.341501
	H	0.943736	1.216122	1.177390
	H	1.941233	0.729544	-1.225252
	H	1.752191	-1.628462	0.209574
	H	2.571810	-0.411163	09.55694
	O	-0.608893	0.094060	0.617918
	N	-1.613078	0.156334	-0.351863
	O	-2.492772	-0.565072	-0095588

TABLE S1. (Continued)

species	atoms	x	y	z
NH_2NHCH_2O	N	1.486316	-0.413955	0.079821
	N	0.575197	0.581997	-0.314700
	C	-0.764860	0.460521	0.198163
	H	-1.335768	1.370478	-0.058825
	H	-0.794779	0.407447	1.321525
	H	0.970654	1.491783	-0.118179
	H	1.344636	-1.226060	-0.514068
	H	1.331344	-0.709645	1.045019
	O	-1.419690	-0.654453	-0.152537
TS2*c* (CH_3NHNH)	N	-0.880820	1.283244	-0.282876
$CH_3NHNHNO_2 \leftrightarrow$	N	-1.287395	0.115751	-0.455271
cCH_3NNH + *t*HONO	C	-1.983806	-0.649081	0.572891
	H	-1.229661	-1.029572	1.270360
	H	-2.693392	-0.005944	1.094628
	H	-2.503153	1.483719	0.105437
	H	-0.551923	-0.442572	-1.012664
	H	-1.268155	1.663837	0.592760
	N	1.256943	0.095301	0.134169
	O	2.398939	0.176408	0.498878
	O	0.917063	-0.834860	-0.656381
TS2*t* (CH_3NHNH)	N	0.827666	-1.257624	-0.113295
$CH_3NHNHNO_2 \leftrightarrow$	N	1.295472	-0.137797	-0.412427
tCH_3NNH + *t*HONO	C	2.185308	0.528212	0.522974
	H	2.618937	-0.219161	1.183802
	H	2.958934	1.054655	-0.035639
	H	1.594879	1.247872	1.096715
	H	0.684488	0.479240	-1.000391
	H	0.144242	-1.529883	-0.820695
	N	-1.303395	-0.084061	0.078473
	O	-0.931466	0.930945	-0.563315
	O	-2.424976	-0.161648	0.509453

TABLE S1. (Continued)

Species	atoms	x	y	z
TS4 (CH_3NHNH)	N	-0.808613	-0.843171	-1.078649
$CH_3NHNHNO_2 \leftrightarrow$	N	-0.311599	0.088989	-1.898187
$CH_3NHNHONO$	C	1.059234	0.483205	-1.634845
	H	1.437308	1.086294	-2.474444
CASPT2/cc-pVDZ	H	1.143005	1.057284	-0.692756
	H	1.661693	-0.430656	-1.537020
	H	-0.922546	0.840379	-2.226963
	H	-1.827387	-0.823911	-1.242539
	O	-0.815768	0.780647	1.351454
	N	-0.098337	-0.096081	1.772708
	O	0.991174	-0.507982	1.444939
TS5*c* (CH_3NHNH)	N	-1.238344	1.200072	-0.200493
$CH_3NHNHONO \leftrightarrow$	N	-1.196037	-0.016604	-0.495013
c$CH_3NNH + HNO_2$	C	-1.457302	-1.142692	0.401245
	H	-2.533214	-1.334811	0.429506
	H	-0.918748	-2.014431	0.036419
	H	-1.092077	-0.883381	1.394391
	H	-1.087481	-0.219743	-1.482560
	H	-1.345267	1.296846	0.811433
	O	1.052288	1.018652	0.454276
	N	1.087555	-0.061968	-0.123211
	O	2.091259	-0.748505	-0.187480
TS5*t* (CH_3NHNH)	N	-1.041864	1.177538	-0.098968
t$CH_3NNH + HNO_2$	N	-1.255232	0.009893	-0.488610
	C	-2.042081	-0.892903	0.338768
	H	-2.695642	-1.483921	-0.303054
	H	-1.362866	-1.550884	0.883608
	H	-2.621203	-0.291782	1.035874
	H	-0.597521	-0.417973	-1.153978
	H	-0.408843	1.646606	-0.747544
	O	1.099588	0.843424	0.543118
	N	1.248428	-0.192075	-0.139715
	O	2.310317	-0.782440	-0.125176

TABLE S1. (Continued)

Species	atoms	x	y	z
TS2*c* (CH_3NNH_2)	N	1.041228	1.152423	-0.022056
$CH_3N(NH_2)NO_2 \leftrightarrow$	N	1.151918	0.016169	0.502140
cCH_3NNH + *t*HONO	C	2.036596	-0.915956	-0.156447
	H	2.922450	-1.027633	0.475812
	H	1.526680	-1.878901	-0.186988
	H	2.327436	-0.603478	-1.167391
	H	1.425334	1.291240	-0.965009
	H	0.036396	1.531722	0.144567
	N	-1.159980	-0.248071	-0.032018
	O	-1.385908	0.994839	-0.052478
	O	-2.075347	-1.027446	-0.009868
TS2*t* (CH_3NNH_2)	N	-1.262616	-1.062859	-0.175197
$CH_3N(NH_2)NO_2 \leftrightarrow$	N	-1.334566	0.114151	-0.606631
tCH_3NNH + *t*HONO	C	-1.404471	1.132747	0.423582
	H	-0.885392	2.017729	0.063347
	H	-2.469579	1.373945	0.523371
	H	-1.006925	0.807689	1.388557
	H	-1.248344	-1.760668	-0.915187
	H	-0.557657	-1.231826	0.612948
	N	1.081244	0.069768	-0.165639
	O	1.037091	-0.895158	0.645165
	O	2.113695	0.663812	-0.342948
TS2f (CH_3NNH_2)	N	-1.646470	-1.085716	0.314907
$CH_3N(NH_2)NO_2 \leftrightarrow$	N	-1.269922	-0.207728	-0.532075
CH_2NNH_2 + *t*HONO	C	-1.322137	1.111665	-0.133881
	H	-1.931621	1.319366	0.752720
	H	-1.519463	1.763829	-0.982240
	H	-0.169579	1.334631	0.160709
	H	-1.837675	-0.853842	1.287465
	H	-1.492303	-2.051187	0.064072
	O	1.252423	1.038330	0.381134
	N	1.165131	-0.116389	-0.112447
	O	2.140363	-0.827575	-0.152651

TABLE S1. (Continued)

Species	atoms	x	y	z
TS4 (CH_3NNH_2)	N	-1.177636	-0.087985	1.668457
$CH_3N(NH_2)NO_2 \leftrightarrow$	N	-0.000479	0.294316	1.141042
$CH_3N(NH_2)ONO$	C	1.068905	-0.032448	2.062997
	H	2.032628	0.169414	1.574165
CASPT2/cc-pVDZ	H	1.005139	0.577653	2.986467
	H	1.046219	-1.102231	2.367787
	H	-1.912638	-0.116356	0.965102
	H	-1.178712	-0.901966	2.288834
	O	1.158716	-0.207439	-1.507764
	N	0.079547	0.255989	-1.786137
	O	-1.061950	-0.090100	-1.578339
TS5*c* (CH_3NNH_2)	N	0.787436	1.177980	0.016253
$CH_3N(NH_2)ONO \leftrightarrow$	N	1.327807	0.196378	-0.536649
c$CH_3NNH + HNO_2$	C	2.277277	-0.544828	0.251211
	H	1.915291	-1.576047	0.269085
	H	3.236720	-0.532912	-0.270965
	H	2.387833	-0.166190	1.275268
	H	-0.219708	1.326519	-0.301633
	H	0.932511	1.321310	1.025309
	O	-0.775086	-1.003706	-0.104136
	N	-1.397076	0.058149	-0.043802
	O	-2.592848	0.112299	0.159767
TS5*t* (CH_3NNH_2)	N	0.975408	1.226871	0.076479
$CH_3N(NH_2)ONO \leftrightarrow$	N	1.506735	0.219463	-0.442477
t$CH_3NNH + HNO_2$	C	1.687614	-0.891349	0.462299
	H	1.566673	-1.810435	-0.106466
	H	2.721053	-0.831876	0.822616
	H	0.999746	-0.870872	1.314583
	H	0.824118	2.005221	-0.560403
	H	0.239966	1.095599	0.808147
	O	-0.758209	-0.665953	-0.781902
	N	-1.227952	0.080704	0.077409
	O	-2.398863	0.049852	0.402884

TABLE S1. (Continued)

Species	atoms	x	y	Z
TS5f (CH_3NNH_2)	N	-1.769597	-0.867605	0.397252
$CH_3N(NH_2)ONO \leftrightarrow$	N	-1.436609	0.003239	-0.461872
$CH_2NNH_2 + HNO_2$	C	-1.147257	1.287920	0.033233
	H	-1.513157	1.474528	1.049322
	H	-1.491921	2.035539	-0.678998
	H	-0.009019	1.339886	0.054506
	H	-1.643630	-0.717599	1.397776
	H	-1.863992	-1.816478	0.061248
	N	1.393160	0.209085	-0.051142
	O	0.731484	-0.738881	-0.501063
	O	2.530590	0.056827	0.341948
TS2f (CH_2NHNH_2)	N	2.045969	-0.564830	0.597488
$NH_2NHCH_2NO_2 \leftrightarrow$	N	1.335732	0.085650	-0.429965
CH_2NNH_2 + *t*HONO	C	0.905070	1.273303	-0.175804
	H	0.298963	1.769714	-0.919044
	H	1.255725	1.799320	0.705393
	H	0.551650	-0.498605	-0.911433
	H	2.553759	-1.332833	0.174601
	H	1.364171	-0.961537	1.243151
	N	-1.248014	0.092224	0.100714
	O	-0.921381	-0.874525	-0.652824
	O	-2.377431	0.161128	0.513387
TS4 (CH_2NHNH_2)	N	-0.592799	-0.962020	-1.622398
$NH_2NHCH_2NO_2 \leftrightarrow$	N	-0.148225	0.369069	-1.823360
NH_2NHCH_2ONO	C	0.922278	0.847928	-1.091035
	H	1.098050	1.925981	-1.164793
CASPT2/cc-pVDZ	H	1.786714	0.178623	-1.016030
	H	-0.946218	0.999548	-1.869245
	H	0.089464	-1.566854	-2.087694
	H	-0.496300	-1.175371	-0.617832
	O	0.595389	-0.952387	1.339007
	N	0.167307	0.134138	1.668765
	O	-0.881992	0.694702	1.461315

TABLE S1. (Continued)

species	atoms	x	Y	Z
TS5f (CH_2NHNH_2)	N	-1.925559	-0.949363	0.390808
	N	-1.237202	-0.122603	-0.496759
	C	-1.094858	1.141778	-0.284207
	H	-1.697551	1.657203	0.445849
	H	-0.461566	1.702942	-0.952608
	H	-0.280618	-0.532565	-0.788925
	H	-2.438732	-0.403315	1.073324
	H	-2.559618	-1.538211	-0.135043
	N	1.261048	-0.178325	-0.118458
	O	1.064047	-0.178325	-0.118458
	O	2.350856	0.839424	0.581817

TABLE S2. Rotational constants (GHz) and unscaled harmonic frequencies (cm^{-1}) for the reactants, products, intermediates, and transition states calculated at the (U)ωB97X-D/6-311++G(d,p) level of theory. The energy differences of the rotational-conformer relative to the most stable one, i.e. ΔE_{RCD}, calculated at the RHF-UCCSD(T)-F12/VDZ-F12//(U)ωB97X-D/6-311++G(d,p) level of theory are also listed.

species	ΔE_{RCD}	rotational constant (GHz)	frequencies (cm^{-1})
NO_2	0[a]	246.06, 13.23, 12.55	780, 1446, 1772
cCH_3NHNH	0	48.51, 10.21, 8.96	172, 394, 517, 633, 1005, 1136, 1153, 1334, 1340, 1457, 1484, 1514, 1562, 3022, 3108, 3150, 3480, 3560
tCH_3NHNH	0	46.61, 10.20, 8.91	200, 365, 491, 720, 987, 1129, 1158, 1317, 1429, 1460, 1486, 1514, 1565, 3009, 3089, 3137, 3457, 3632
CH_3NNH_2	0	46.92, 10.55, 9.17	164, 443, 486, 627, 991, 1064, 1109, 1311, 1340, 1435, 1483, 1488, 1664, 2957, 3017, 3141, 3476, 3670
CH_2NHNH_2	0, 461	46.64, 10.32, 8.98	291, 364, 449, 636, 695, 910, 1013, 1241, 1288, 1344, 1465, 1525, 1693, 3145, 3265, 3488, 3595, 3630
*t*HONO	0[b]	96.83, 12.89, 11.38	596, 683, 885, 1334, 1825, 3846
HNO_2	0[a]	108.18, 13.38, 11.91	815, 1091, 1456, 1558, 1719, 3239
NO	0, 119[c]	51.84, 51.84	2040
cCH_3NNH	0[b]	56.05, 11.34, 10.02	198, 587, 877, 945, 1155, 1166, 1421, 1461, 1471, 1500, 1725, 2983, 3103, 3112, 3140
tCH_3NNH	0[b]	61.14, 11.16, 10.02	185, 566, 874, 965, 1157, 1181 1418, 1475, 1476, 1505, 1708, 3035, 3131, 3135, 3351
CH_2NNH_2	0	65.81, 11.51, 9.89	426, 524, 653, 796, 964, 1087, 1194, 1324, 1485, 1674, 1725, 3050, 3222, 3505, 3682
$CH_3NHNHNO_2$	0, 73	7.52, 2.66, 2.39	115, 161, 222 ,323, 465, 532, 600, 723, 796, 817, 988, 1010, 1153, 1196, 1285, 1412, 1431, 1464, 1498, 1518, 1560, 1731, 3038, 3114, 3147, 3597, 3626

TABLE S2. (Continued)

Species	ΔE_{RCD}	rotational constant (GHz)	frequencies (cm^{-1})
$CH_3NHNHONO$	0, 27, 42, 216, 240, 337, 346, 562	8.53, 2.12, 1.83	90, 145, 183, 230, 338, 461, 516, 642, 664, 799, 1000, 1015, 1052, 1165, 1237, 1254, 1455, 1493, 1497, 1519, 1556, 1808, 3020, 3112, 3156, 3512, 3572
CH_3NHNHO	0, 1194	20.87, 5.48, 4.90	96, 216, 378, 402, 650, 819, 992, 1143, 1173, 1225, 1420, 1454, 1481, 1489, 1505, 1532, 3034, 3118, 3148, 3519, 3537
$CH_3N(NH_2)NO_2$	0, 1706	5.45, 4.00, 2.40	107, 159, 237, 318, 356, 436, 613, 646, 802, 893, 899, 1030, 1142, 1200, 1336, 1375, 1396, 1459, 1497, 1506, 1686, 1711, 3040, 3157, 3204, 3500, 3618
$CH_3N(NH_2)ONO$	0, 153, 1036, 1754	8.65, 2.21, 1.90	71, 181, 235, 287, 368, 413, 498, 550, 625, 721, 878, 991, 1005, 1162, 1172, 1280, 1371, 1452, 1490, 1501, 1688, 1802, 3015, 3134, 3180, 3472, 3630
$CH_3N(NH_2)O$	0, 80	10.85, 9.30, 5.33	83, 187, 345, 431, 554, 840, 952, 1097, 1137, 1243, 1302, 1443, 1475, 1482, 1528, 1655, 3045, 3136, 3183, 3503, 3603
$NH_2NHCH_2NO_2$	0, 553, 2377, 2593	7.75, 2.54, 2.21	72, 159, 290, 387, 425, 534, 580, 703, 764, 899, 910, 1016, 1142, 1277, 1301, 1337, 1356, 1451, 1481, 1541, 1676, 1706, 3110, 3190, 3523, 3557, 3638
NH_2NHCH_2ONO	0, 89, 357, 414, 514, 542, 569, 787, 800, 890, 1180	10.25, 1.83, 1.74	71, 124, 190, 303, 324, 443, 540, 633, 719, 860, 904, 1020, 1062, 1182, 1234, 1314, 1353, 1429, 1483, 1511, 1704, 1809, 3017, 3110, 3477, 3610, 3626
NH_2NHCH_2O	0, 214, 358, 562	17.96, 5.78, 4.83	149, 300, 365, 584, 741, 823, 902, 982, 1110, 1194, 1228, 1328, 1335, 1400, 1503, 1705, 2742, 2966, 3462, 3597, 3617

TABLE S2. (Continued)

Species	ΔE_{RCD}	rotational constant (GHz)	frequencies (cm^{-1})
TS2*c* (CH_3NHNH)	0	7.28, 2.03, 1.86	548*i*, 87, 116, 155, 212, 267, 360, 510, 667, 838, 884, 984, 1130, 1168, 1208, 1408, 1439, 1473, 1497, 1599, 1614, 1688, 2705, 3045, 3141, 3181, 3387
TS2*t* (CH_3NHNH)	0	7.81, 1.95, 1.77	306*i*, 94, 128, 132, 254, 290, 364, 518, 686, 831, 860, 995, 1151, 1165, 1248, 1437, 1459, 1481, 1488, 1562, 1607, 1706, 3062, 3085, 3151, 3193, 3520
TS4[d] (CH_3NHNH)	0, 508[e]	5.51, 2.01, 1.79	92*i*, 48, 77, 96, 99, 139, 218, 431, 546, 725, 751, 1016, 1133, 1148, 1356, 1369, 1403, 1449, 1479, 1506, 1561, 1686, 3063, 3171, 3222, 3435, 3525
TS5*c* (CH_3NHNH)	0	5.98, 2.56, 2.01	62*i*, 111, 160, 205, 281, 329, 407, 532, 588, 813, 958, 980, 1137, 1163, 1335, 1392, 1451, 1485, 1488, 1569, 1575, 1642, 3060, 3155, 3192, 3499, 3594
TS5*t* (CH_3NHNH)	0	7.02, 2.07, 1.75	156*i*, 69, 108, 157, 231, 273, 383, 528, 644, 800, 914, 990, 1150, 1161, 1273, 1434, 1437, 1481, 1490, 1538, 1565, 1689, 3073, 3160, 3196, 3380, 3522
TS2*c* (CH_3NNH_2)	0	6.52, 2.23, 1.74	480*i*, 139, 163, 170, 211, 338, 387, 489, 585, 837, 913, 966, 1113, 1156, 1221, 1414, 1432, 1460, 1490, 1551, 1623, 1707, 2568, 3015, 3112, 3156, 3382
TS2*t* (CH_3NNH_2)	0	6.12, 2.46, 2.04	478*i*, 120, 167, 229, 266, 341, 361, 520, 564, 830, 903, 963, 1117, 1154, 1231, 1422, 1431, 1468, 1490, 1566, 1613, 1724, 2772, 3034, 3113, 3185, 3549
TS2f (CH_3NNH_2)	0	6.05, 2.28, 1.79	683*i*, 85, 131, 211, 310, 385, 498, 562, 590, 629, 812, 892, 1092, 1156, 1184, 1353, 1369, 1424, 1468, 1519, 1635, 1687, 1743, 3046, 3174, 3482, 3677

TABLE S2. (Continued)

Species	ΔE_{RCD}	rotational constant (GHz)	frequencies (cm^{-1})
TS4[d] (CH_3NNH_2)	0	5.64, 1.96, 1.50	59*i*, 27, 55, 71, 115, 127, 167, 481, 487, 699, 747, 1007, 1062, 1109, 1321, 1360, 1360, 1421, 1479, 1482, 1642, 1686, 3001, 3080, 3197, 3447, 3653
TS5*c* (CH_3NNH_2)	0	9.29, 1.88, 1.65	335*i*, 84, 152, 182, 224, 297, 312, 411, 550, 813, 897, 980, 1106, 1159, 1342, 1405, 1419, 1456, 1492, 1568, 1588, 1708, 2855, 3014, 3120, 3137, 3369
TS5*t* (CH_3NNH_2)	0	7.26, 2.16, 1.93	280*i*, 79, 186, 219, 231, 254, 300, 490, 544, 808, 854, 978, 1108, 1150, 1335, 1395, 1425, 1460, 1489, 1567, 1575, 1718, 3027, 3102, 3131, 3180, 3562
TS5f (CH_3NNH_2)	0	7.61, 2.01, 1.75	134*i*, 64, 135, 252, 273, 369, 400, 527, 616, 681, 811, 987, 1110, 1152, 1280, 1351, 1429, 1445, 1487, 1517, 1567, 1697, 2486, 3049, 3167, 3465, 3658
TS2f (CH_2NHNH_2)	0, 1031	7.32, 2.00, 1.83	368*i*, 93, 155, 206, 271, 300, 360, 490, 727, 777, 847, 962, 1040, 1071, 1235, 1245, 1357, 1442, 1565, 1620, 1661, 1746, 2525, 3176, 3307, 3494, 3615
TS4[d] (CH_2NHNH_2)	0	5.37, 2.02, 1.91	245*i*, 33, 98, 111, 132, 145, 314, 429, 458, 715, 738, 760, 956, 1056, 1259, 1315, 1340, 1357, 1469, 1524, 1673, 1687, 3173, 3301, 3404, 3559, 3609
TS5f (CH_2NHNH_2)	0	7.00, 2.05, 1.75	290*i*, 105, 149, 207, 276, 308, 419, 492, 742, 781, 834, 858, 996, 1053, 1226, 1318, 1358, 1464, 1539, 1584, 1684, 1712, 2660, 3175, 3309, 3542, 3647

[a] C_{2V} group. [b] C_s group. [c] Spin-orbital splitting for NO ($^2\Pi_{3/2} \leftarrow {}^2\Pi_{1/2}$) [d] Calculated at the CASPT2/cc-pVDZ level of theory. [e] Calculated at the MRCI+Q/aug-cc-pVTZ// CASPT2/cc-pVDZ level of theory.

Table S3. Standard enthalpies of formation (kJ mol^{-1}), entropies (J K^{-1} mol^{-1}) and heat capacities (J K^{-1} mol^{-1}) of CH_3NHNH_2, NO_2 and bimolecular products.

species	$\Delta H_f°_{298}$ [a]	$S°_{298}$	$C_p°$						
			300 K	400 K	500 K	600 K	700 K	800 K	900 K
				1000 K	1200 K	1400 K	1600 K	1800 K	2000 K
NO_2	36.20	239.82	37.11	40.19	43.18	45.78	47.92	49.64	51.01
				52.10	53.70	54.76	55.50	56.03	56.42
CH_3NNH_2	222.47	281.96	63.84	76.70	88.77	99.29	108.34	116.18	123.01
				128.98	138.76	146.25	152.02	156.49	160.00
cCH_3NHNH	231.73	281.91	63.47	76.02	88.03	98.58	107.69	115.59	122.47
				128.49	138.37	145.94	151.77	156.29	159.83
tCH_3NHNH	232.54	281.29	64.50	76.95	88.77	99.16	108.15	115.96	122.77
				128.74	138.54	146.07	151.86	156.36	159.89
CH_2NNH_2	281.26	282.26	72.72	86.57	98.33	108.17	116.49	123.63	129.82
				135.22	144.02	150.71	155.82	159.45	162.81
*t*HONO	-77.40	247.88	45.17	51.16	55.94	59.70	62.69	65.13	67.15
				68.87	71.62	73.71	75.32	76.58	77.58
HONO[b]	-76.84	253.26	45.88	51.58	56.21	59.89	62.83	65.23	67.24
				68.94	71.67	73.74	75.35	76.61	77.60
HNO_2	-40.33	238.18	38.67	44.12	49.54	54.33	58.36	61.72	64.52
				66.85	70.48	73.09	75.02	76.46	77.57
NO	78.93	210.58	29.80	29.85	30.33	31.02	31.77	32.49	33.13
				33.68	34.54	35.17	35.62	35.95	36.20
cCH_3NNH	204.76	261.34	54.85	65.61	76.17	85.61	93.83	100.95	107.12
				112.45	121.05	127.50	132.36	136.07	138.95
tCH_3NNH	188.17	261.63	54.20	64.91	75.51	84.96	93.16	100.26	106.40
				111.72	120.34	126.83	131.76	135.54	138.48
CH_2NNH_2	183.05	261.79	58.02	70.81	81.85	91.08	98.83	105.45	111.18
				116.18	124.41	130.76	135.70	139.58	142.67
$CH_3NHNHNO_2$	121.89	341.04	98.70	119.88	138.50	154.02	166.85	177.54	186.56
				194.23	206.46	215.59	222.49	227.79	231.91
$CH_3NHNHONO$	190.62	363.68	108.75	127.92	144.77	158.94	170.78	180.75	189.24
				196.51	208.19	216.94	223.59	228.69	232.67
CH_3NHNHO	161.34	310.38	79.27	95.76	110.52	122.83	132.98	141.44	148.61
				154.75	164.61	172.05	177.72	182.10	185.52

Table S3. (Continued)

species	$\Delta H_f°_{298}$ [a]	$S°_{298}$	$C_p°$						
			300 K	400 K	500 K	600 K	700 K	800 K	900 K
				1000 K	1200 K	1400 K	1600 K	1800 K	2000 K
$CH_3N(NH_2)NO_2$	115.78	338.35	100.85	122.12	141.29	157.55	171.07	182.30	191.64
				199.44	211.45	219.99	226.14	230.66	234.03
$CH_3N(NH_2)ONO$	176.47	351.80	110.74	132.44	150.39	164.83	176.54	186.19	194.28
				201.13	212.01	220.11	226.23	230.91	234.55
$CH_3N(NH_2)O$	140.50	319.57	79.43	94.07	107.55	119.16	129.05	137.53	144.86
				151.22	161.61	169.54	175.62	180.33	184.01
$NH_2NHCH_2NO_2$	66.55	337.59	102.42	125.01	144.22	160.13	173.31	184.32	193.60
				201.46	213.86	222.94	229.66	234.72	238.59
NH_2NHCH_2ONO	84.50	361.20	113.78	133.37	149.96	163.75	175.23	184.91	193.16
				200.27	211.75	220.44	227.08	232.22	236.25
NH_2NHCH_2O	163.03	310.01	81.39	97.81	112.28	124.36	134.42	142.92	150.19
				156.47	166.65	174.40	180.33	184.94	188.54

[a] Estimated by the enthalpy difference from H_2, N_2, O_2 and C calculated at RHF-USSCD(T)-F12/VDZ-F12//(U)ωB97X-D/6-311++G(d,p) level of theory and $\Delta H_f°_{298}$(C) = 716.67 kJ mol^{-1} taken from [Chase, M. W., Jr. J. Phys. Chem. Ref. Data Monogr. 1998, 9, 1-1951.]. [b] Thermal equilibrium mixture of *trans*- and *cis*-HONO, taken from [Kanno et al. Int. J. Chem. Kinet. 2014, 46, 489-499.].

Table S4. Modified Arrhenius parameters for selected reactions.

P (atm)	A^a	n	E_a/R (K)	A^a	n	E_a/R (K)
	cCH$_3$NHNH + NO$_2$ → tCH$_3$NHNH + NO$_2$			cCH$_3$NHNH + NO$_2$ → tCH$_3$NNH+HONO		
100	1.37×10^{-10}	-0.66	2777.9	1.11×10^{-5}	-2.31	1808.7
50	5.47×10^{-11}	-0.56	2464.7	1.33×10^{-5}	-2.36	1562.9
20	6.09×10^{-12}	-0.30	2014.4	3.45×10^{-6}	-2.22	1141.4
10	9.04×10^{-13}	-0.07	1694.1	6.39×10^{-7}	-2.02	807.3
5	1.57×10^{-13}	0.14	1426.8	1.02×10^{-7}	-1.80	505.1
2	2.80×10^{-14}	0.35	1179.0	1.39×10^{-8}	-1.55	214.5
1	1.23×10^{-14}	0.45	1063.8	5.92×10^{-9}	-1.45	98.9
0.5	7.57×10^{-15}	0.51	997.4	4.01×10^{-9}	-1.40	48.8
0.2	5.44×10^{-15}	0.56	952.1	3.55×10^{-9}	-1.38	34.0
0.1	4.82×10^{-15}	0.57	935.8	3.51×10^{-9}	-1.38	33.2
	cCH$_3$NHNH + NO$_2$ → cCH$_3$NNH + HONO			cCH$_3$NHNH + NO$_2$ → CH$_3$NHNHNO$_2$		
∞				6.35×10^{-16}	0.88	-790.0
100	2.69×10^{-10}	-1.04	1656.5	3.96×10^{69}	-26.35	11611.8
50	2.35×10^{-10}	-1.05	1389.9	2.51×10^{70}	-26.74	11467.6
20	5.15×10^{-10}	-0.88	964.1	2.20×10^{70}	-26.95	11068.9
10	9.20×10^{-12}	-0.68	632.6	2.85×10^{69}	-26.86	10628.2
5	1.51×10^{-12}	-0.46	334.9	6.11×10^{67}	-26.55	10077.5
2	2.23×10^{-13}	-0.22	47.6	2.95×10^{64}	-25.82	9237.2
1	8.94×10^{-14}	-0.11	-81.8	1.56×10^{61}	-25.04	8570.2
0.5	5.48×10^{-14}	-0.05	-149.8	1.96×10^{57}	-24.07	7912.2
0.2	4.24×10^{-14}	-0.02	-185.8	4.56×10^{51}	-22.63	7192.8
0.1	3.93×10^{-14}	-0.01	-196.6	2.83×10^{47}	-21.54	6849.0
	cCH$_3$NHNH + NO$_2$ → tCH$_3$NNH+HNO			cCH$_3$NHNH + NO$_2$ → cCH$_3$NNH + HNO$_2$		
100	1.90×10^{-8}	-1.38	3242.8	1.68×10^{-9}	-1.22	3237.0
50	2.60×10^{-9}	-1.15	2804.0	2.20×10^{-10}	-0.99	2792.7
20	1.85×10^{-10}	-0.83	2306.4	1.42×10^{-11}	-0.66	2284.3
10	2.60×10^{-11}	-0.60	1985.8	2.08×10^{-12}	-0.42	1967.8
5	5.06×10^{-12}	-0.40	1734.1	3.79×10^{-13}	-0.22	1710.4
2	1.04×10^{-12}	-0.20	1504.2	7.49×10^{-14}	-0.02	1447.4
1	4.70×10^{-13}	-0.10	1395.0	3.65×10^{-14}	0.07	1376.0
0.5	3.06×10^{-13}	-0.05	1334.8	2.31×10^{-14}	0.13	1313.2
0.2	2.22×10^{-13}	-0.01	1292.6	1.70×10^{-14}	0.17	1272.3
0.1	1.95×10^{-13}	0.01	1276.2	1.53×10^{-14}	0.18	1258.0

Table S4. (Continued)

P (atm)	A^a	n	E_a/R (K)	A^a	n	E_a/R (K)
	cCH$_3$NHNH + NO$_2$ → CH$_3$NHNHO + NO			cCH$_3$NHNH + NO$_2$ → CH$_3$NHNHONO		
100	1.40×10^{-9}	-1.04	3529.6	1.35×10^{56}	-23.56	9675.6
50	1.53×10^{-10}	-0.78	3064.9	2.58×10^{52}	-22.69	8673.2
20	7.34×10^{-12}	-0.42	2527.1	2.39×10^{47}	-21.51	7518.2
10	8.66×10^{-13}	-0.16	2191.1	2.51×10^{43}	-20.55	6790.7
5	1.55×10^{-13}	0.06	1934.7	1.94×10^{39}	-19.54	6218.6
2	3.09×10^{-14}	0.25	1707.7	1.19×10^{34}	-18.22	5785.0
1	1.46×10^{-14}	0.35	1605.6	6.42×10^{30}	-17.38	5759.4
0.5	9.81×10^{-15}	0.40	1550.3	2.94×10^{28}	-16.80	5985.8
0.2	7.32×10^{-15}	0.43	1511.4	3.61×10^{26}	-16.35	6497.9
0.1	6.60×10^{-15}	0.45	1497.7	4.69×10^{25}	-16.17	6922.1
	tCH$_3$NHNH + NO$_2$ → cCH$_3$NHNH + NO$_2$			tCH$_3$NHNH + NO$_2$ → tCH$_3$NNH+HONO		
100	2.06×10^{-10}	-0.71	2679.8	5.52×10^{-5}	-2.48	1932.5
50	8.01×10^{-11}	-0.61	2365.2	5.14×10^{-5}	-2.50	1667.3
20	8.79×10^{-12}	-0.35	1912.7	1.05×10^{-5}	-2.32	1230.4
10	1.33×10^{-12}	-0.12	1595.1	1.70×10^{-6}	-2.11	890.0
5	2.29×10^{-13}	0.09	1326.8	2.56×10^{-7}	-1.87	587.2
2	4.23×10^{-14}	0.30	1082.0	3.78×10^{-8}	-1.64	311.5
1	1.85×10^{-14}	0.40	966.8	1.67×10^{-8}	-1.54	202.0
0.5	1.11×10^{-14}	0.46	897.4	1.19×10^{-8}	-1.50	159.3
0.2	7.98×10^{-15}	0.51	852.5	1.07×10^{-8}	-1.48	146.6
0.1	7.05×10^{-15}	0.52	836.2	1.06×10^{-8}	-1.48	145.6
	tCH$_3$NHNH + NO$_2$ → cCH$_3$NNH + HONO			tCH$_3$NHNH + NO$_2$ → CH$_3$NHNHNO$_2$		
∞				4.13×10^{-15}	0.68	-614.8
100	2.11×10^{-9}	-1.27	1807.8	5.24×10^{69}	-26.35	11639.3
50	1.55×10^{-9}	-1.26	1528.7	2.69×10^{70}	-26.72	11470.8
20	2.84×10^{-10}	-1.06	1092.3	1.84×10^{70}	-26.90	11042.8
10	4.57×10^{-11}	-0.85	755.3	2.05×10^{69}	-26.80	10581.6
5	7.36×10^{-12}	-0.62	460.9	4.54×10^{67}	-26.50	10030.1
2	1.09×10^{-12}	-0.39	179.7	2.52×10^{64}	-25.79	9209.9
1	4.64×10^{-13}	-0.28	58.1	1.51×10^{61}	-25.03	8570.0
0.5	2.97×10^{-13}	-0.23	-3.8	2.41×10^{57}	-24.09	7965.7
0.2	2.33×10^{-13}	-0.20	-37.1	6.60×10^{51}	-22.67	7318.5
0.1	2.19×10^{-13}	-0.19	-46.2	4.79×10^{47}	-21.59	7036.6

Table S4. (Continued)

P (atm)	A^a	n	E_a/R (K)	A^a	n	E_a/R (K)
	tCH$_3$NHNH + NO$_2$ → tCH$_3$NNH+HNO$_2$			tCH$_3$NHNH + NO$_2$ → cCH$_3$NNH + HNO$_2$		
100	1.97×10^{-7}	-1.65	3382.3	1.82×10^{-8}	-1.49	3377.1
50	2.50×10^{-8}	-1.41	2941.2	2.28×10^{-9}	-1.25	2934.3
20	1.65×10^{-9}	-1.08	2441.7	1.47×10^{-10}	-0.92	2430.8
10	2.48×10^{-10}	-0.85	2131.0	2.05×10^{-11}	-0.68	2112.6
5	4.56×10^{-11}	-0.64	1876.5	3.78×10^{-12}	-0.48	1859.0
2	9.18×10^{-12}	-0.45	1647.2	7.61×10^{-13}	-0.28	1630.8
1	4.40×10^{-12}	-0.35	1544.9	3.65×10^{-13}	-0.19	1528.5
0.5	2.74×10^{-12}	-0.30	1481.6	2.30×10^{-13}	-0.13	1466.3
0.2	2.06×10^{-12}	-0.26	1442.0	1.68×10^{-13}	-0.09	1424.4
0.1	1.79×10^{-12}	-0.24	1424.0	1.45×10^{-13}	-0.07	1406.0
	tCH$_3$NHNH + NO$_2$ → CH$_3$NHNHO+NO			tCH$_3$NHNH + NO$_2$ → CH$_3$NHNHONO		
100	1.79×10^{-8}	-1.34	3675.7	1.91×10^{56}	-23.57	9961.1
50	1.84×10^{-9}	-1.07	3209.7	2.22×10^{52}	-22.64	8619.3
20	9.20×10^{-11}	-0.71	2681.8	1.03×10^{47}	-21.37	7406.0
10	1.12×10^{-11}	-0.45	2352.0	7.83×10^{42}	-20.38	6651.2
5	1.97×10^{-12}	-0.24	2096.8	5.09×10^{38}	-19.35	6606.2
2	3.90×10^{-13}	-0.04	1871.3	2.89×10^{33}	-18.02	5635.9
1	1.97×10^{-13}	0.05	1776.2	1.81×10^{33}	-17.21	5635.4
0.5	1.27×10^{-13}	0.10	1717.9	1.01×10^{28}	-16.64	5892.8
0.2	9.66×10^{-14}	0.14	1680.9	1.62×10^{26}	-16.23	6447.8
0.1	8.71×10^{-14}	0.15	1667.8	2.62×10^{25}	-16.08	6901.9
	CH$_3$NNH$_2$ + NO$_2$ → tCH$_3$NNH + HONO			CH$_3$NNH$_2$ + NO$_2$ → cCH$_3$NNH+HONO		
100	1.84×10^{-8}	-1.49	2736.3	2.79×10^{-9}	-1.26	2774.0
50	4.01×10^{-8}	-1.62	2526.4	4.96×10^{-9}	-1.36	2547.7
20	2.88×10^{-8}	-1.61	2147.2	2.71×10^{-9}	-1.31	2148.9
10	1.02×10^{-8}	-1.50	1809.0	8.81×10^{-10}	-1.19	1807.7
5	2.15×10^{-9}	-1.32	1444.4	1.62×10^{-10}	-0.99	1435.6
2	1.69×10^{-10}	-1.02	950.9	1.10×10^{-11}	-0.67	936.2
1	2.06×10^{-11}	-0.77	589.0	1.29×10^{-12}	-0.41	576.3
0.5	2.57×10^{-12}	-0.51	254.9	1.53×10^{-13}	-0.15	243.0
0.2	2.02×10^{-13}	-0.20	-126.4	1.23×10^{-14}	0.16	-130.5
0.1	4.10×10^{-14}	0.00	-352.0	2.53×10^{-15}	0.35	-351.9

Table S4. (Continued)

P (atm)	A^a	n	E_a/R (K)	A^a	n	E_a/R (K)
	$CH_3NNH_2 + NO_2 \rightarrow CH_2NNH_2 + HONO$			$CH_3NNH_2 + NO_2 \rightarrow CH_3N(NH_2)NO_2$		
∞				5.29×10^{-14}	0.41	96.4
100	2.82×10^{-17}	1.00	3197.4	4.63×10^{68}	-25.78	12297.4
50	9.87×10^{-18}	1.11	2856.1	1.86×10^{70}	-26.38	12357.5
20	9.28×10^{-19}	1.38	2352.1	6.95×10^{71}	-27.02	12331.4
10	9.39×10^{-20}	1.66	1954.6	4.09×10^{72}	-27.37	12234.9
5	8.31×10^{-21}	1.95	1572.0	1.09×10^{73}	-27.62	12079.0
2	3.88×10^{-22}	2.33	1119.7	1.13×10^{73}	-27.80	11783.9
1	4.86×10^{-23}	2.59	828.8	5.27×10^{72}	-27.83	11511.1
0.5	8.70×10^{-24}	2.80	594.2	1.14×10^{72}	-27.76	11194.6
0.2	1.55×10^{-24}	3.02	366.4	5.16×10^{70}	-27.54	10724.4
0.1	6.24×10^{-25}	3.13	248.5	2.20×10^{69}	-27.27	10339.8
	$CH_3NNH_2 + NO_2 \rightarrow t\text{-}CH_3NNH + HNO_2$			$CH_3NNH_2 + NO_2 \rightarrow c\text{-}CH_3NNH + HNO_2$		
100	2.11×10^{-7}	-1.70	3865.8	1.73×10^{-9}	-1.10	3879.0
50	1.04×10^{-7}	-1.63	3522.0	6.27×10^{-10}	-1.00	3510.8
20	1.80×10^{-8}	-1.44	3040.7	6.91×10^{-11}	-0.74	2994.2
10	2.82×10^{-9}	-1.22	2660.0	8.27×10^{-12}	-0.49	2595.9
5	3.31×10^{-10}	-0.96	2279.6	8.25×10^{-13}	-0.21	2209.6
2	1.71×10^{-11}	-0.60	1805.7	3.96×10^{-14}	0.16	1743.1
1	1.91×10^{-12}	-0.33	1482.9	4.62×10^{-15}	0.42	1434.6
0.5	2.84×10^{-13}	-0.10	1210.1	7.23×10^{-16}	0.65	1176.5
0.2	3.56×10^{-14}	0.16	926.1	1.06×10^{-16}	0.89	917.9
0.1	1.12×10^{-14}	0.30	771.8	3.73×10^{-17}	1.02	780.5
	$CH_3NNH_2 + NO_2 \rightarrow CH_2NNH_2 + HNO_2$			$CH_3NNH_2 + NO_2 \rightarrow CH_3N(NH_2)O + NO$		
100	3.08×10^{-15}	0.45	3965.7	2.50×10^{-3}	-2.71	4071.1
50	5.02×10^{-16}	0.66	3544.5	1.79×10^{-3}	-2.70	3759.8
20	2.52×10^{-17}	1.01	2987.2	5.25×10^{-4}	-2.57	3322.7
10	2.14×10^{-18}	1.31	2587.0	1.08×10^{-4}	-2.39	2962.0
5	1.80×10^{-19}	1.62	2216.3	1.56×10^{-5}	-2.16	2593.6
2	1.03×10^{-20}	1.97	1809.7	9.67×10^{-7}	-1.82	2125.9
1	1.62×10^{-21}	2.20	1560.1	1.15×10^{-7}	-1.56	1800.0
0.5	3.85×10^{-22}	2.38	1371.1	1.67×10^{-8}	-1.32	1517.9
0.2	1.04×10^{-22}	2.54	1202.8	1.96×10^{-9}	-1.06	1219.2
0.1	5.69×10^{-23}	2.62	1124.8	5.99×10^{-10}	-0.91	1057.3

Table S4. (Continued)

P (atm)	A^a	n	E_a/R (K)	A^a	n	E_a/R (K)
	$CH_3NNH_2 + NO_2 \rightarrow CH_3N(NH_2)ONO$			$CH_2NHNH_2 + NO_2 \rightarrow CH_2NNH_2 + HONO$		
100	4.65×10^{54}	-22.78	9965.8	6.20×10^{-16}	1.01	252.4
50	5.05×10^{52}	-22.39	9403.1	5.70×10^{-16}	1.00	15.1
20	2.95×10^{50}	-21.98	8873.7	1.04×10^{-16}	1.20	-364.5
10	8.28×10^{48}	-21.71	8614.9	2.30×10^{-17}	1.38	-605.9
5	2.27×10^{47}	-21.42	8451.0	8.44×10^{-18}	1.51	-748.4
2	1.89×10^{45}	-21.01	8362.1	5.32×10^{-18}	1.57	-809.8
1	5.40×10^{43}	-20.70	8361.9	5.09×10^{-18}	1.57	-815.3
0.5	2.18×10^{42}	-20.41	8405.6	5.09×10^{-18}	1.57	-815.3
0.2	3.33×10^{40}	-20.02	8441.5	5.09×10^{-18}	1.57	-815.3
0.1	1.26×10^{39}	-19.71	8427.4	5.09×10^{-18}	1.57	-815.3
	$CH_2NHNH_2 + NO_2 \rightarrow NH_2NHCH_2NO_2$			$CH_2NHNH_2 + NO_2 \rightarrow CH_2NNH_2 + HNO_2$		
∞				6.27×10^{-19}	1.86	-961.8
100	1.07×10^{67}	-25.42	11796.3	1.25×10^{-33}	6.18	3313.1
50	1.75×10^{70}	-26.64	11953.7	3.33×10^{-31}	5.43	3316.6
20	2.09×10^{72}	-27.63	11766.9	2.33×10^{-29}	4.84	3109.2
10	1.19×10^{72}	-27.87	11371.3	8.83×10^{-29}	4.63	2843.0
5	1.70×10^{70}	-27.63	10789.4	7.46×10^{-29}	4.62	2493.0
2	2.63×10^{65}	-26.62	9879.5	1.03×10^{-29}	4.84	1950.6
1	2.07×10^{60}	-25.40	9234.7	8.45×10^{-31}	5.14	1510.1
0.5	3.65×10^{54}	-23.96	8794.0	5.60×10^{-32}	5.48	1102.8
0.2	1.92×10^{47}	-22.09	8743.4	2.68×10^{-33}	5.85	690.5
0.1	4.63×10^{42}	-20.90	9118.3	6.09×10^{-34}	6.04	503.4
	$CH_2NHNH_2 + NO_2 \rightarrow NH_2NHCH_2O + NO$			$CH_2NHNH_2 + NO_2 \rightarrow NH_2NHCH_2ONO$		
100	5.35×10^{-33}	6.13	3625.9	1.68×10^{35}	-15.20	12343.6
50	1.13×10^{-30}	5.41	3617.7	1.09×10^{42}	-17.43	13072.5
20	7.80×10^{-29}	4.83	3420.6	1.75×10^{50}	-20.17	13869.7
10	2.81×10^{-28}	4.63	3153.7	5.97×10^{55}	-22.07	14344.2
5	2.42×10^{-28}	4.62	2810.7	3.27×10^{60}	-23.75	14669.2
2	3.57×10^{-29}	4.83	2278.9	1.66×10^{65}	-25.52	14812.4
1	3.52×10^{-30}	5.11	1856.6	2.49×10^{67}	-26.47	14672.1
0.5	2.71×10^{-31}	5.42	1460.5	1.66×10^{68}	-27.04	14302.9
0.2	1.40×10^{-32}	5.79	1048.5	1.67×10^{67}	-27.17	13504.9
0.1	3.25×10^{-33}	5.97	858.0	8.55×10^{64}	-26.82	12714.5

Table S4. (Continued)

P (atm)	A^a	n	E_a/R (K)	A^a	n	E_a/R (K)
	$CH_3NHNHO + NO \rightarrow cCH_3NHNH + NO_2$			$CH_3NHNHO + NO \rightarrow tCH_3NHNH + NO_2$		
100	1.41×10^{-6}	-2.06	5734.3	1.22×10^{-5}	-2.31	5979.1
50	1.53×10^{-7}	-1.80	5269.0	1.29×10^{-6}	-2.04	5517.3
20	7.40×10^{-9}	-1.44	4731.5	5.92×10^{-8}	-1.67	4979.9
10	8.82×10^{-10}	-1.18	4396.4	7.51×10^{-9}	-1.42	4652.5
5	1.52×10^{-10}	-0.96	4137.3	1.29×10^{-9}	-1.20	4397.2
2	3.03×10^{-11}	-0.76	3909.4	2.61×10^{-10}	-1.00	4172.8
1	1.52×10^{-11}	-0.68	3813.2	1.34×10^{-10}	-0.92	4081.3
0.5	9.44×10^{-12}	-0.62	3750.6	8.66×10^{-11}	-0.87	4021.3
0.2	7.38×10^{-12}	-0.59	3716.6	6.56×10^{-11}	-0.83	3983.7
0.1	6.70×10^{-12}	-0.58	3703.7	5.92×10^{-11}	-0.82	3970.9
	$CH_3NHNHO + NO \rightarrow tCH_3NNH + HONO$			$CH_3NHNHO + NO \rightarrow cCH_3NNH + HONO$		
100	1.48×10^{0}	-3.99	5318.6	5.74×10^{-5}	-2.79	5141.3
50	1.72×10^{-1}	-3.75	4809.0	6.55×10^{-6}	-2.54	4643.9
20	5.76×10^{-3}	-3.34	4179.2	2.65×10^{-7}	-2.15	4047.3
10	4.48×10^{-4}	-3.03	3774.0	2.45×10^{-8}	-1.86	3663.4
5	4.96×10^{-5}	-2.76	3453.6	3.16×10^{-9}	-1.61	3359.5
2	6.47×10^{-6}	-2.51	3180.0	4.72×10^{-10}	-1.38	3093.1
1	3.08×10^{-6}	-2.42	3084.3	2.07×10^{-10}	-1.28	2982.3
0.5	2.16×10^{-6}	-2.37	3041.5	1.35×10^{-10}	-1.22	2926.6
0.2	1.94×10^{-6}	-2.36	3028.4	1.07×10^{-10}	-1.19	2896.0
0.1	1.94×10^{-6}	-2.36	3028.6	1.02×10^{-10}	-1.19	2887.9
	$CH_3NHNHO + NO \rightarrow CH_3NHNHNO_2$			$CH_3NHNHO + NO \rightarrow tCH_3NNH + HNO_2$		
100	1.14×10^{74}	-27.86	15096.6	1.66×10^{-7}	-2.14	1010.8
50	4.42×10^{73}	-27.92	14593.7	9.76×10^{-9}	-1.79	610.7
20	1.74×10^{72}	-27.76	13823.7	4.61×10^{-10}	-1.41	203.3
10	3.10×10^{70}	-27.44	13163.1	9.82×10^{-11}	-1.22	4.4
5	1.19×10^{68}	-26.93	12434.2	3.93×10^{-11}	-1.11	-110.2
2	7.80×10^{63}	-25.97	11403.1	2.41×10^{-11}	-1.04	-170.6
1	1.03×10^{60}	-25.03	10612.5	2.23×10^{-11}	-1.04	-179.5
0.5	3.98×10^{55}	-23.93	9861.2	2.08×10^{-11}	-1.03	-187.7
0.2	2.57×10^{49}	-22.34	9050.0	2.08×10^{-11}	-1.03	-187.5
0.1	8.10×10^{44}	-21.16	8659.2	2.08×10^{-11}	-1.03	-187.5

Table S4. (Continued)

P (atm)	A^a	n	E_a/R (K)	A^a	n	E_a/R (K)
	$CH_3NHNHO + NO \rightarrow cCH_3NNH + HNO_2$			$CH_3NHNHO + NO \rightarrow CH_3NHNHONO$		
100	5.31×10^{-9}	-1.85	971.2	2.50×10^{61}	-25.23	8235.3
50	3.33×10^{-10}	-1.51	577.6	2.66×10^{59}	-24.79	7683.7
20	1.78×10^{-11}	-1.15	181.3	6.46×10^{56}	-24.21	7020.3
10	3.92×10^{-12}	-0.96	-17.1	5.41×10^{54}	-23.75	6571.1
5	1.58×10^{-12}	-0.85	-131.7	3.22×10^{52}	-23.34	6172.3
2	9.63×10^{-13}	-0.78	-196.0	2.21×10^{49}	-22.48	5743.7
1	8.43×10^{-13}	-0.77	-212.6	9.07×10^{46}	-21.90	5536.5
0.5	8.15×10^{-13}	-0.76	-216.6	5.45×10^{44}	-21.36	5452.3
0.2	8.15×10^{-13}	-0.76	-216.6	2.46×10^{42}	-20.80	5544.1
0.1	8.15×10^{-13}	-0.76	-216.6	1.36×10^{41}	-20.52	5733.9
	$CH_3N(NH_2)O + NO \rightarrow CH_3NNH_2 + NO_2$			$CH_3N(NH_2)O + NO \rightarrow tCH_3NNH + HONO$		
100	3.69×10^{-2}	-3.28	7507.7	3.97×10^{-4}	-3.07	6301.6
50	2.58×10^{-2}	-3.26	7195.2	7.03×10^{-4}	-3.17	6032.2
20	7.49×10^{-3}	-3.14	6757.1	8.01×10^{-4}	-3.22	5665.2
10	1.55×10^{-3}	-2.95	6396.1	5.05×10^{-4}	-3.19	5364.8
5	2.25×10^{-4}	-2.72	6028.0	1.89×10^{-4}	-3.09	5038.0
2	1.40×10^{-5}	-2.39	5561.5	2.64×10^{-5}	-2.86	4576.7
1	1.64×10^{-6}	-2.13	5223.8	4.26×10^{-6}	-2.64	4222.2
0.5	2.38×10^{-7}	-1.89	4952.4	5.94×10^{-7}	-2.41	3878.7
0.2	2.90×10^{-8}	-1.63	4656.4	4.24×10^{-8}	-2.08	3458.6
0.1	8.56×10^{-9}	-1.48	4490.7	6.68×10^{-9}	-1.86	3183.5
	$CH_3N(NH_2)O + NO \rightarrow cCH_3NNH + HONO$			$CH_3N(NH_2)O + NO \rightarrow CH_2NNH_2 + HONO$		
100	4.44×10^{-5}	-2.80	6314.0	1.21×10^{-14}	-0.09	6456.5
50	6.35×10^{-5}	-2.87	6030.7	4.72×10^{-15}	0.01	6106.9
20	6.06×10^{-5}	-2.90	5654.3	6.54×10^{-16}	0.23	5623.9
10	3.11×10^{-5}	-2.84	5340.8	8.53×10^{-17}	0.47	5239.3
5	1.01×10^{-5}	-2.71	5005.7	9.22×10^{-18}	0.74	4863.6
2	1.14×10^{-6}	-2.46	4533.2	4.63×10^{-19}	1.11	4404.5
1	1.68×10^{-7}	-2.23	4176.9	5.91×10^{-20}	1.36	4105.8
0.5	2.13×10^{-8}	-1.98	3830.4	9.85×10^{-21}	1.58	3856.9
0.2	1.61×10^{-9}	-1.67	3424.3	1.55×10^{-21}	1.81	3608.5
0.1	2.53×10^{-10}	-1.44	3155.0	5.66×10^{-22}	1.94	3478.3

Table S4. (Continued)

P (atm)	A^a	n	E_a/R (K)	A^a	n	E_a/R (K)
	$CH_3N(NH_2)O + NO \rightarrow CH_3N(NH_2)NO_2$			$CH_3N(NH_2)O + NO \rightarrow t CH_3NNH + HNO_2$		
100	5.55×10^{71}	-26.90	15732.2	1.98×10^{-14}	-0.23	1279.0
50	3.23×10^{72}	-27.24	15587.5	1.66×10^{-15}	0.08	908.1
20	2.58×10^{73}	-27.66	15422.2	9.90×10^{-17}	0.42	506.6
10	9.18×10^{73}	-27.94	15295.9	1.82×10^{-17}	0.64	274.5
5	1.92×10^{74}	-28.15	15138.2	5.03×10^{-18}	0.79	102.0
2	1.95×10^{74}	-28.30	14858.3	1.71×10^{-18}	0.93	-41.9
1	9.69×10^{73}	-28.33	14595.6	1.03×10^{-18}	0.99	-108.7
0.5	2.36×10^{73}	-28.27	14283.2	7.53×10^{-19}	1.03	-148.9
0.2	1.52×10^{72}	-28.08	13822.9	6.23×10^{-19}	1.05	-174.0
0.1	8.81×10^{70}	-27.85	13434.2	5.77×10^{-19}	1.06	-183.9
	$CH_3N(NH_2)O + NO \rightarrow c CH_3NNH + HNO_2$			$CH_3N(NH_2)O + NO \rightarrow CH_2NNH_2 + HNO_2$		
100	9.02×10^{-17}	0.48	1728.6	7.57×10^{-22}	1.91	3016.6
50	1.18×10^{-17}	0.73	1430.6	4.66×10^{-22}	1.97	2925.8
20	1.72×10^{-18}	0.97	1153.8	4.76×10^{-22}	1.97	2901.5
10	6.87×10^{-19}	1.08	1024.4	6.14×10^{-22}	1.93	2916.2
5	4.09×10^{-19}	1.14	951.6	7.38×10^{-22}	1.91	2927.4
2	3.30×10^{-19}	1.17	916.2	8.60×10^{-22}	1.89	2935.4
1	3.42×10^{-19}	1.17	916.2	9.04×10^{-22}	1.88	2936.4
0.5	3.45×10^{-19}	1.16	914.3	8.92×10^{-22}	1.88	2932.8
0.2	3.49×10^{-19}	1.16	914.7	8.86×10^{-22}	1.88	2930.0
0.1	3.51×10^{-19}	1.16	914.9	8.59×10^{-22}	1.89	2925.9
	$CH_3N(NH_2)O + NO \rightarrow CH_3N(NH_2)ONO$			$NH_2NHCH_2O + NO \rightarrow CH_2NHNH_2 + NO_2$		
100	5.40×10^{55}	-23.38	7795.0	4.44×10^{-32}	5.86	11406.2
50	1.22×10^{54}	-23.00	7311.1	9.46×10^{-30}	5.14	11399.4
20	7.84×10^{51}	-22.49	6696.0	6.47×10^{-28}	4.56	11201.0
10	2.07×10^{50}	-22.13	6269.5	2.35×10^{-27}	4.36	10934.7
5	7.40×10^{48}	-21.80	5891.2	2.10×10^{-27}	4.34	10594.4
2	1.37×10^{47}	-21.42	5458.9	3.09×10^{-28}	4.56	10063.0
1	9.83×10^{45}	-21.18	5189.1	3.05×10^{-29}	4.83	9639.7
0.5	8.82×10^{44}	-20.97	4952.7	2.38×10^{-30}	5.14	9245.0
0.2	5.20×10^{43}	-20.73	4693.5	1.24×10^{-31}	5.51	8834.7
0.1	7.96×10^{42}	-20.58	4531.1	2.68×10^{-32}	5.70	8636.0

Table S4. (Continued)

P (atm)	A^a	n	E_a/R (K)	A^a	n	E_a/R (K)
	$NH_2NHCH_2O + NO \rightarrow CH_2NNH_2 + HONO$			$NH_2NHCH_2O + NO \rightarrow NH_2NHCH_2NO_2$		
100	2.90×10^{-25}	3.91	8877.9	1.36×10^{51}	-20.65	19110.6
50	2.95×10^{-22}	2.99	9003.5	1.87×10^{56}	-22.46	19406.2
20	2.23×10^{-19}	2.10	9013.6	3.25×10^{60}	-24.11	19350.9
10	1.06×10^{-17}	1.58	8979.0	6.23×10^{61}	-24.82	19029.3
5	2.14×10^{-16}	1.17	8916.6	2.96×10^{61}	-25.05	18538.3
2	2.16×10^{-15}	0.84	8739.4	6.29×10^{58}	-24.69	17777.1
1	2.77×10^{-15}	0.78	8504.7	2.43×10^{55}	-23.99	17255.5
0.5	1.02×10^{-15}	0.89	8188.0	1.64×10^{51}	-23.04	16910.9
0.2	1.02×10^{-16}	1.16	7741.9	3.67×10^{45}	-21.68	16897.6
0.1	1.50×10^{-17}	1.40	7740.8	4.52×10^{41}	-20.72	17213.7
	$NH_2NHCH_2O + NO \rightarrow CH_2NNH_2 + HNO_2$			$NH_2NHCH_2O + NO \rightarrow NH_2NHCH_2ONO$		
100	1.46×10^{-32}	5.77	236.0	3.81×10^{40}	-16.74	8558.6
50	2.48×10^{-28}	4.51	819.9	5.09×10^{44}	-18.05	9183.3
20	4.85×10^{-23}	2.94	1519.0	1.24×10^{50}	-19.77	9981.9
10	2.46×10^{-19}	1.83	1979.3	1.09×10^{54}	-21.04	10550.3
5	5.99×10^{-16}	0.81	2369.5	7.09×10^{57}	-22.27	11083.9
2	4.49×10^{-12}	-0.36	2759.5	4.36×10^{62}	-23.83	11727.3
1	1.21×10^{-9}	-1.10	2951.7	9.44×10^{65}	-24.93	12148.6
0.5	1.06×10^{-7}	-1.70	3044.4	1.04×10^{69}	-25.95	12504.8
0.2	6.86×10^{-6}	-2.26	3021.2	3.13×10^{72}	-27.14	12858.6
0.1	4.37×10^{-5}	-2.53	2898.3	4.63×10^{74}	-27.90	13028.2
	$CH_3NHNHNO_2 \rightarrow cCH_3NHNH + NO_2$			$CH_3NHNHNO_2 \rightarrow tCH_3NHNH + NO_2$		
100	4.32×10^{42}	-8.90	20131.6	3.93×10^{42}	-8.85	20258.8
50	1.22×10^{43}	-9.15	19995.6	8.80×10^{42}	-9.08	20096.5
20	5.88×10^{42}	-9.24	19639.5	3.28×10^{42}	-9.14	19707.8
10	6.12×10^{41}	-9.10	19241.9	3.18×10^{41}	-9.00	19297.0
5	1.43×10^{40}	-8.77	18752.3	7.94×10^{39}	-8.69	18809.5
2	1.07×10^{37}	-8.07	18010.3	7.33×10^{36}	-8.02	18092.6
1	9.05×10^{33}	-7.33	17417.5	7.19×10^{33}	-7.30	17531.4
0.5	2.07×10^{30}	-6.43	16839.5	1.84×10^{30}	-6.41	16994.5
0.2	8.51×10^{24}	-5.05	16196.8	8.91×10^{24}	-5.05	16423.8
0.1	7.23×10^{20}	-3.99	15894.9	9.31×10^{20}	-4.01	16188.6

Table S4. (Continued)

P (atm)	A^a	n	E_a/R (K)	A^a	n	E_a/R (K)
	$CH_3NHNHNO_2 \rightarrow tCH_3NNH + HONO$			$CH_3NHNHNO_2 \rightarrow cCH_3NNH + HONO$		
100	1.35×10^{30}	-5.30	13119.4	2.74×10^{33}	-6.41	15570.4
50	1.42×10^{31}	-5.66	13190.3	2.77×10^{34}	-6.79	15596.6
20	1.79×10^{32}	-6.08	13219.1	2.12×10^{35}	-7.17	15526.5
10	7.66×10^{32}	-6.34	13189.8	4.30×10^{35}	-7.37	15391.2
5	2.14×10^{33}	-6.56	13116.9	4.17×10^{35}	-7.47	15186.8
2	4.34×10^{33}	-6.76	12957.7	1.31×10^{35}	-7.47	14821.8
1	4.51×10^{33}	-6.85	12794.1	2.46×10^{34}	-7.38	14487.3
0.5	3.10×10^{33}	-6.90	12597.9	2.50×10^{33}	-7.22	14116.3
0.2	1.08×10^{33}	-6.88	12299.5	5.17×10^{31}	-6.89	13590.1
0.1	3.44×10^{32}	-6.83	12054.5	1.50×10^{30}	-6.56	13177.8
	$CH_3NHNHNO_2 \rightarrow CH_3NHNHO + NO$			$CH_3NHNHNO_2 \rightarrow tCH_3NNH + HNO_2$		
100	1.36×10^{44}	-9.40	21417.1	7.12×10^{44}	-9.56	21014.2
50	2.38×10^{43}	-9.33	20922.3	1.12×10^{44}	-9.45	20540.3
20	5.62×10^{41}	-9.06	20198.6	3.66×10^{42}	-9.20	19887.5
10	9.00×10^{39}	-8.70	19588.5	1.01×10^{41}	-8.90	19352.7
5	4.09×10^{37}	-8.19	18924.8	9.13×10^{38}	-8.46	18766.9
2	4.41×10^{33}	-7.27	17992.8	2.56×10^{35}	-7.65	17924.3
1	9.76×10^{29}	-6.38	17281.5	1.15×10^{32}	-6.84	17265.6
0.5	6.78×10^{25}	-5.34	16607.3	1.56×10^{28}	-5.88	16629.3
0.2	7.96×10^{19}	-3.81	15873.8	3.79×10^{22}	-4.44	15922.5
0.1	3.48×10^{15}	-2.67	15528.3	2.40×10^{18}	-3.35	15581.3
	$CH_3NHNHNO_2 \rightarrow cCH_3NNH + HNO_2$			$CH_3NHNHNO_2 \rightarrow CH_3NHNHONO$		
100	1.31×10^{44}	-9.51	21056.9	2.03×10^{85}	-23.95	24160.5
50	2.21×10^{43}	-9.42	20583.4	3.99×10^{79}	-22.44	22936.8
20	7.22×10^{41}	-9.17	19922.8	4.35×10^{71}	-20.34	21378.6
10	1.89×10^{40}	-8.86	19377.9	2.78×10^{65}	-18.71	20300.5
5	1.56×10^{38}	-8.42	18781.1	1.76×10^{59}	-17.08	19357.6
2	3.87×10^{34}	-7.59	17925.6	2.42×10^{51}	-15.04	18402.1
1	1.59×10^{31}	-6.77	17258.7	7.72×10^{45}	-13.62	17935.3
0.5	1.97×10^{27}	-5.80	16615.8	5.94×10^{40}	-12.33	17671.4
0.2	4.35×10^{21}	-4.35	15902.7	2.45×10^{34}	-10.72	17566.5
0.1	2.62×10^{17}	-3.25	15558.9	6.72×10^{29}	-9.58	17652.4

Table S4. (Continued)

P (atm)	A^a	n	E_a/R (K)	A^a	n	E_a/R (K)
	$CH_3N(NH_2)NO_2 \rightarrow CH_3NNH_2 + NO_2$			$CH_3N(NH_2)NO_2 \rightarrow t CH_3NNH + HONO$		
100	6.03×10^{44}	-9.33	20759.7	1.66×10^{34}	-6.64	16113.1
50	1.70×10^{46}	-9.86	20838.2	8.17×10^{35}	-7.21	16300.4
20	6.25×10^{47}	-10.47	20866.4	8.83×10^{37}	-7.91	16505.2
10	4.92×10^{48}	-10.84	20830.6	2.14×10^{39}	-8.39	16628.7
5	2.08×10^{49}	-11.15	20746.2	3.76×10^{40}	-8.83	16724.6
2	4.95×10^{49}	-11.41	20559.9	9.16×10^{41}	-9.34	16802.7
1	4.36×10^{49}	-11.51	20368.3	6.35×10^{42}	-9.66	16823.3
0.5	2.01×10^{49}	-11.53	20140.6	2.93×10^{43}	-9.93	16810.6
0.2	2.76×10^{48}	-11.44	19795.6	1.19×10^{44}	-10.21	16743.0
0.1	2.89×10^{47}	-11.28	19508.5	2.20×10^{44}	-10.37	16653.3
	$CH_3N(NH_2)NO_2 \rightarrow c CH_3NNH + HONO$			$CH_3N(NH_2)NO_2 \rightarrow CH_2NNH_2 + HONO$		
100	9.63×10^{35}	-7.17	16997.5	6.38×10^{41}	-9.19	21312.5
50	4.89×10^{37}	-7.75	17177.1	2.43×10^{43}	-9.78	21378.5
20	5.12×10^{39}	-8.45	17365.3	8.41×10^{44}	-10.41	21358.8
10	1.15×10^{41}	-8.93	17471.6	4.88×10^{45}	-10.76	21270.3
5	1.80×10^{42}	-9.36	17546.5	1.33×10^{46}	-11.02	21126.2
2	3.51×10^{43}	-9.85	17591.5	1.59×10^{46}	-11.22	20859.4
1	1.96×10^{44}	-10.15	17583.3	7.91×10^{45}	-11.27	20609.9
0.5	6.93×10^{44}	-10.39	17538.7	2.00×10^{45}	-11.23	20328.4
0.2	1.86×10^{45}	-10.63	17424.7	1.17×10^{44}	-11.05	19919.8
0.1	2.36×10^{45}	-10.74	17297.2	6.10×10^{42}	-10.81	19591.8
	$CH_3N(NH_2)NO_2 \rightarrow CH_3N(NH_2)O + NO$			$CH_3N(NH_2)NO_2 \rightarrow t CH_3NNH + HNO_2$		
100	6.25×10^{46}	-9.91	20775.0	1.43×10^{45}	-9.70	20971.2
50	2.41×10^{47}	-10.17	20644.1	7.79×10^{45}	-10.03	20847.5
20	1.84×10^{48}	-10.56	20532.0	7.05×10^{45}	-10.45	20718.5
10	8.18×10^{48}	-10.85	20461.9	3.05×10^{47}	-10.74	20622.7
5	2.70×10^{49}	-11.11	20373.9	9.19×10^{47}	-11.00	20506.4
2	6.02×10^{49}	-11.35	20199.2	1.76×10^{48}	-11.23	20297.5
1	5.66×10^{49}	-11.45	20018.2	1.47×10^{48}	-11.32	20094.3
0.5	3.01×10^{49}	-11.48	19799.0	6.87×10^{47}	-11.35	19855.3
0.2	5.63×10^{48}	-11.42	19459.4	1.06×10^{47}	-11.27	19492.2
0.1	8.29×10^{47}	-11.29	19171.2	1.31×10^{46}	-11.13	19187.3

Table S4. (Continued)

P (atm)	A^a	n	E_a/R (K)	A^a	n	E_a/R (K)
	$CH_3N(NH_2)NO_2 \rightarrow cCH_3NNH + HNO_2$			$CH_3N(NH_2)NO_2 \rightarrow CH_2NNH_2 + HNO_2$		
100	5.81×10^{44}	-9.68	21329.6	1.06×10^{44}	-9.78	22417.5
50	3.70×10^{45}	-10.03	21202.7	7.79×10^{44}	-10.18	22276.9
20	3.16×10^{46}	-10.46	21044.4	4.49×10^{45}	-10.60	22048.5
10	1.11×10^{47}	-10.74	20912.6	7.85×10^{45}	-10.81	21830.9
5	2.52×10^{47}	-10.96	20755.3	6.79×10^{45}	-10.94	21571.0
2	3.13×10^{47}	-11.15	20492.3	1.81×10^{45}	-10.97	21163.2
1	1.85×10^{47}	-11.21	20250.5	2.89×10^{44}	-10.89	20813.9
0.5	6.07×10^{46}	-11.20	19975.5	2.31×10^{43}	-10.71	20437.5
0.2	5.74×10^{45}	-11.07	19568.6	2.84×10^{41}	-10.35	19909.5
0.1	4.84×10^{44}	-10.89	19233.2	4.45×10^{39}	-9.97	19495.3
	$CH_3N(NH_2)NO_2 \rightarrow CH_3N(NH_2)ONO$			$NH_2NHCH_2NO_2 \rightarrow CH_2NHNH_2 + NO_2$		
100	1.05×10^{86}	-23.96	23850.3	8.11×10^{46}	-10.16	33735.0
50	4.41×10^{82}	-23.13	23108.7	7.14×10^{48}	-10.96	33731.6
20	4.46×10^{78}	-22.17	22331.1	3.91×10^{49}	-11.51	33395.5
10	9.47×10^{75}	-21.56	21914.7	3.85×10^{48}	-11.49	32912.0
5	3.95×10^{73}	-21.02	21657.2	1.82×10^{46}	-11.09	32297.6
2	1.07×10^{71}	-20.47	21578.4	1.89×10^{41}	-9.99	31421.1
1	4.87×10^{69}	-20.22	21711.9	1.50×10^{36}	-8.75	30822.1
0.5	7.47×10^{68}	-20.12	21962.3	3.37×10^{30}	-7.32	30441.2
0.2	2.00×10^{68}	-20.14	22336.6	3.36×10^{23}	-5.52	30489.7
0.1	8.61×10^{67}	-20.17	22558.3	1.67×10^{19}	-4.41	30956.4
	$NH_2NHCH_2NO_2 \rightarrow CH_2NNH_2 + HONO$			$NH_2NHCH_2NO_2 \rightarrow NH_2NHCH_2O + NO$		
100	1.42×10^{26}	-3.89	16643.5	1.17×10^{30}	-5.12	33264.8
50	2.21×10^{28}	-4.60	16946.0	9.19×10^{33}	-6.51	33403.4
20	1.47×10^{31}	-5.53	17313.7	7.24×10^{36}	-7.72	33189.4
10	1.58×10^{33}	-6.20	17559.6	2.27×10^{37}	-8.16	32785.1
5	1.57×10^{35}	-6.88	17786.8	3.64×10^{36}	-8.22	32262.7
2	6.21×10^{37}	-7.76	18061.6	5.43×10^{33}	-7.79	31538.3
1	3.47×10^{39}	-8.37	18219.3	2.11×10^{30}	-7.07	31062.2
0.5	1.21×10^{41}	-8.92	18331.2	1.84×10^{26}	-6.13	30779.7
0.2	6.78×10^{42}	-9.56	18416.4	7.85×10^{20}	-4.84	30865.6
0.1	7.91×10^{43}	-9.98	18429.0	2.04×10^{17}	-3.96	31273.9

Table S4. (Continued)

P (atm)	A^a	n	E_a/R (K)	A^a	n	E_a/R (K)
	$NH_2NHCH_2NO_2 \rightarrow CH_2NNH_2 + HNO_2$			$NH_2NHCH_2NO_2 \rightarrow NH_2NHCH_2ONO$		
100	2.02×10^{30}	-5.30	33053.0	9.92×10^{94}	-25.31	41681.9
50	3.10×10^{34}	-6.78	33253.5	1.58×10^{99}	-26.84	41994.9
20	5.85×10^{37}	-8.09	33118.3	2.16×10^{102}	-28.18	41973.2
10	3.26×10^{38}	-8.59	32764.8	6.60×10^{102}	-28.65	41668.8
5	8.28×10^{37}	-8.71	32282.9	6.89×10^{101}	-28.71	41203.8
2	1.93×10^{35}	-8.33	31597.7	3.78×10^{98}	-28.20	40505.4
1	9.63×10^{31}	-7.63	31144.0	6.36×10^{94}	-27.43	40031.8
0.5	1.03×10^{28}	-6.71	30880.2	2.84×10^{90}	-26.47	39753.9
0.2	5.49×10^{22}	-5.44	30985.4	7.64×10^{84}	-25.23	39856.1
0.1	1.49×10^{19}	-4.56	31398.5	1.49×10^{81}	-24.42	40259.4
	$CH_3NHNHONO \rightarrow cCH_3NHNH + NO_2$			$CH_3NHNHONO \rightarrow tCH_3NHNH + NO_2$		
100	2.34×10^{18}	-2.20	10223.5	2.16×10^{18}	-2.16	10304.4
50	8.70×10^{14}	-1.35	9396.2	5.03×10^{14}	-1.25	9439.4
20	5.04×10^{9}	-0.04	8317.4	1.58×10^{9}	0.13	8308.1
10	1.61×10^{5}	1.11	7555.2	3.62×10^{4}	1.32	7516.5
5	2.11×10^{0}	2.38	6888.8	3.99×10^{-1}	2.62	6836.9
2	2.01×10^{-6}	3.98	6361.0	3.80×10^{-7}	4.21	6318.0
1	5.34×10^{-10}	4.93	6313.4	1.14×10^{-10}	5.14	6293.8
0.5	9.80×10^{-13}	5.65	6506.3	2.55×10^{-13}	5.84	6518.6
0.2	7.60×10^{-15}	6.19	7034.7	2.63×10^{-15}	6.34	7090.4
0.1	1.15×10^{-15}	6.36	7506.6	4.77×10^{-16}	6.50	7589.4
	$CH_3NHNHONO \rightarrow tCH_3NNH + HONO$			$CH_3NHNHONO \rightarrow cCH_3NNH + HONO$		
100	5.60×10^{21}	-3.07	9527.2	2.27×10^{19}	-2.58	9577.8
50	8.16×10^{18}	-2.35	8783.9	2.26×10^{16}	-1.84	8797.4
20	3.50×10^{14}	-1.25	7792.1	5.68×10^{11}	-0.68	7760.5
10	6.97×10^{10}	-0.31	7089.8	7.35×10^{7}	0.30	7026.8
5	7.11×10^{6}	0.72	6476.4	4.99×10^{3}	1.38	6387.0
2	8.83×10^{1}	2.00	5981.8	4.18×10^{-2}	2.70	5870.5
1	9.04×10^{-2}	2.78	5915.7	3.74×10^{-5}	3.49	5796.6
0.5	3.52×10^{-4}	3.40	6067.7	1.38×10^{-7}	4.13	5940.2
0.2	4.28×10^{-6}	3.88	6549.5	1.55×10^{-9}	4.61	6402.6
0.1	7.28×10^{-7}	4.04	6996.2	2.47×10^{-10}	4.78	6835.2

Table S4. (Continued)

P (atm)	A^a	n	E_a/R (K)	A^a	n	E_a/R (K)
	$CH_3NHNHONO \rightarrow CH_3NHNHNO_2$			$CH_3NHNHONO \rightarrow CH_3NHNHO + NO$		
100	1.57×10^{76}	-20.53	16553.4	2.68×10^{21}	-3.09	6728.1
50	1.41×10^{72}	-19.50	15683.3	5.46×10^{19}	-2.66	6364.4
20	2.11×10^{66}	-18.02	14527.6	1.68×10^{17}	-2.04	5855.1
10	4.66×10^{61}	-16.86	13708.3	1.66×10^{15}	-1.55	5491.1
5	6.53×10^{56}	-15.65	12974.6	1.26×10^{13}	-1.04	5165.7
2	4.43×10^{50}	-14.13	12270.5	2.75×10^{10}	-0.41	4882.1
1	1.73×10^{46}	-13.06	11957.1	3.09×10^{8}	0.06	4784.2
0.5	5.14×10^{41}	-11.95	11764.9	2.65×10^{6}	0.57	4761.0
0.2	7.07×10^{35}	-10.51	11716.3	1.93×10^{4}	1.10	4937.6
0.1	3.82×10^{31}	-9.46	11830.6	1.65×10^{3}	1.34	5196.2
	$CH_3NHNHONO \rightarrow t CH_3NNH + HNO_2$			$CH_3NHNHONO \rightarrow c CH_3NNH + HNO_2$		
100	4.33×10^{18}	-2.21	4512.7	9.79×10^{17}	-2.20	4663.6
50	5.65×10^{17}	-1.99	4293.1	1.14×10^{17}	-1.97	4428.1
20	3.59×10^{16}	-1.71	3972.7	6.14×10^{15}	-1.67	4086.2
10	5.44×10^{15}	-1.53	3737.6	8.09×10^{14}	-1.49	3835.7
5	1.03×10^{15}	-1.40	3523.1	1.32×10^{14}	-1.33	3606.8
2	4.55×10^{14}	-1.41	3358.3	4.57×10^{13}	-1.32	3422.5
1	4.92×10^{14}	-1.51	3296.1	3.89×10^{13}	-1.40	3344.1
0.5	2.91×10^{14}	-1.53	3204.0	1.76×10^{13}	-1.39	3235.7
0.2	1.45×10^{14}	-1.57	3102.6	5.86×10^{12}	-1.38	3112.7
0.1	8.63×10^{13}	-1.59	3040.8	2.47×10^{12}	-1.36	3035.7
	$CH_3N(NH_2)ONO \rightarrow CH_3NNH_2 + NO_2$			$CH_3N(NH_2)ONO \rightarrow t CH_3NNH + HONO$		
100	4.36×10^{20}	-2.68	11028.8	2.65×10^{20}	-2.91	10029.5
50	3.14×10^{18}	-2.17	10574.1	2.24×10^{18}	-2.40	9529.5
20	3.56×10^{15}	-1.47	10065.2	2.10×10^{15}	-1.64	8917.2
10	1.66×10^{13}	-0.91	9747.2	8.20×10^{12}	-1.04	8517.1
5	6.88×10^{10}	-0.34	9496.0	3.76×10^{10}	-0.46	8214.3
2	5.40×10^{7}	0.40	9279.9	7.80×10^{7}	0.20	8018.3
1	3.58×10^{5}	0.93	9203.8	2.31×10^{6}	0.57	8032.3
0.5	4.35×10^{3}	1.39	9286.2	2.27×10^{5}	0.78	8154.5
0.2	2.41×10^{1}	1.93	9174.4	3.96×10^{4}	0.90	8369.7
0.1	9.58×10^{-4}	3.12	8379.5	6.43×10^{3}	1.05	8392.2

Table S4. (Continued)

P (atm)	A^a	n	E_a/R (K)	A^a	n	E_a/R (K)
	$CH_3N(NH_2)ONO \rightarrow cCH_3NNH + HONO$			$CH_3N(NH_2)ONO \rightarrow CH_2NNH_2 + HONO$		
100	9.06×10^{19}	-2.81	10113.1	1.15×10^{17}	-2.38	11317.0
50	7.26×10^{17}	-2.29	9612.0	1.32×10^{15}	-1.94	10899.6
20	6.46×10^{14}	-1.53	9000.5	2.00×10^{12}	-1.30	10416.3
10	2.42×10^{12}	-0.93	8601.1	8.63×10^{9}	-0.75	10091.2
5	1.05×10^{10}	-0.35	8296.7	2.52×10^{7}	-0.15	9807.1
2	1.93×10^{7}	0.32	8092.5	8.44×10^{3}	0.69	9514.5
1	4.99×10^{5}	0.70	8094.6	2.31×10^{1}	1.32	9365.5
0.5	4.10×10^{4}	0.94	8200.7	1.00×10^{-1}	1.90	9270.3
0.2	5.47×10^{3}	1.09	8391.2	1.15×10^{-4}	2.63	9152.8
0.1	6.10×10^{2}	1.28	8375.9	8.70×10^{-11}	4.32	7962.1
	$CH_3N(NH_2)ONO \rightarrow CH_3N(NH_2)NO_2$			$CH_3N(NH_2)ONO \rightarrow CH_3N(NH_2)O + NO$		
100	2.04×10^{75}	-20.09	16463.2	1.67×10^{23}	-3.53	5909.0
50	9.19×10^{71}	-19.22	15827.4	1.46×10^{22}	-3.25	5675.9
20	2.30×10^{67}	-18.02	15039.3	5.86×10^{20}	-2.91	5358.4
10	7.33×10^{63}	-17.13	14519.3	7.08×10^{19}	-2.70	5133.1
5	3.53×10^{60}	-16.30	14117.2	1.47×10^{19}	-2.58	4947.2
2	5.53×10^{56}	-15.36	13829.2	3.25×10^{18}	-2.50	4755.3
1	3.15×10^{54}	-14.83	13805.9	1.13×10^{18}	-2.46	4631.0
0.5	7.81×10^{52}	-14.48	13916.8	4.04×10^{17}	-2.41	4522.1
0.2	3.21×10^{51}	-14.25	14143.3	1.08×10^{17}	-2.37	4398.1
0.1	3.67×10^{50}	-14.11	14245.3	4.07×10^{16}	-2.33	4316.9
	$CH_3N(NH_2)ONO \rightarrow tCH_3NNH + HNO_2$			$CH_3N(NH_2)ONO \rightarrow cCH_3NNH + HNO_2$		
100	3.16×10^{21}	-3.35	6388.8	7.40×10^{20}	-3.29	7026.3
50	1.63×10^{20}	-3.03	6092.6	1.38×10^{19}	-2.86	6834.6
20	2.43×10^{18}	-2.59	5678.0	3.85×10^{16}	-2.23	6324.8
10	1.14×10^{17}	-2.28	5370.9	3.55×10^{14}	-1.74	5948.8
5	7.52×10^{15}	-2.03	5094.7	3.13×10^{12}	-1.25	5606.2
2	2.81×10^{14}	-1.75	4771.6	4.86×10^{9}	-0.57	5216.5
1	2.24×10^{13}	-1.53	4544.7	3.42×10^{7}	-0.04	4986.8
0.5	1.80×10^{12}	-1.32	4336.2	3.85×10^{5}	0.44	4847.9
0.2	7.24×10^{10}	-1.04	4092.6	3.85×10^{3}	0.91	4819.4
0.1	7.45×10^{9}	-0.85	3933.7	3.31×10^{2}	1.14	4887.0

Table S4. (Continued)

P (atm)	A^a	n	E_a/R (K)	A^a	n	E_a/R (K)
	$CH_3N(NH_2)ONO \rightarrow CH_2NNH_2 + HNO_2$			$NH_2NHCH_2ONO \rightarrow CH_2NHNH_2 + NO_2$		
100	6.90×10^{25}	-2.17	8491.2	3.86×10^{21}	-2.52	33028.0
50	1.04×10^{13}	-1.46	8033.8	1.10×10^{26}	-4.00	33405.8
20	7.32×10^{8}	-0.41	7500.5	4.02×10^{31}	-5.89	33820.9
10	4.00×10^{5}	0.43	7210.7	2.59×10^{35}	-7.23	34052.2
5	3.55×10^{2}	1.21	7088.4	4.69×10^{38}	-8.43	34176.2
2	1.81×10^{-1}	2.04	7227.9	5.42×10^{41}	-9.67	34103.8
1	2.79×10^{-3}	2.48	7517.4	7.08×10^{42}	-10.27	33829.8
0.5	1.56×10^{-4}	2.78	7891.4	6.23×10^{42}	-10.54	33357.5
0.2	1.27×10^{-5}	3.00	8376.7	7.12×10^{40}	-10.36	32457.3
0.1	1.84×10^{-10}	4.33	7536.4	9.72×10^{37}	-9.81	31612.3
	$NH_2NHCH_2ONO \rightarrow CH_2NNH_2 + HONO$			$NH_2NHCH_2ONO \rightarrow NH_2NHCH_2NO_2$		
100	8.59×10^{28}	-4.49	30444.4	1.01×10^{102}	-28.05	40514.8
50	2.53×10^{32}	-5.63	30718.7	1.66×10^{105}	-29.28	40655.0
20	4.62×10^{36}	-7.06	31030.9	1.33×10^{107}	-30.23	40420.4
10	6.35×10^{39}	-8.13	31275.3	4.93×10^{106}	-30.42	39959.6
5	8.14×10^{42}	-9.20	31536.8	4.87×10^{104}	-30.16	39320.9
2	4.63×10^{46}	-10.53	31827.1	7.13×10^{99}	-29.17	38356.0
1	7.07×10^{48}	-11.36	31912.9	8.27×10^{94}	-28.03	37687.0
0.5	1.69×10^{50}	-11.96	31838.7	2.87×10^{89}	-26.73	37224.0
0.2	4.52×10^{50}	-12.37	31491.8	3.06×10^{82}	-25.05	37095.7
0.1	7.59×10^{49}	-12.36	31063.8	6.51×10^{77}	-23.94	37343.1
	$NH_2NHCH_2ONO \rightarrow NH_2NHCH_2O + NO$			$NH_2NHCH_2ONO \rightarrow CH_2NNH_2 + HNO_2$		
100	2.39×10^{26}	-3.89	21520.3	3.32×10^{17}	-1.63	16675.8
50	1.65×10^{28}	-4.47	21805.5	1.47×10^{19}	-2.15	16934.6
20	9.53×10^{30}	-5.35	22224.0	4.15×10^{21}	-2.93	17313.2
10	1.75×10^{33}	-6.08	22557.4	4.12×10^{23}	-3.56	17615.1
5	3.85×10^{35}	-6.83	22890.9	4.74×10^{25}	-4.22	17919.9
2	4.78×10^{38}	-7.84	23309.7	2.66×10^{28}	-5.11	18313.3
1	8.52×10^{40}	-8.59	23593.4	2.98×10^{30}	-5.78	18594.6
0.5	1.08×10^{43}	-9.29	23835.7	2.85×10^{32}	-6.42	18855.0
0.2	3.11×10^{45}	-10.14	24074.9	8.33×10^{34}	-7.24	19158.0
0.1	1.11×10^{47}	-10.69	24184.0	4.38×10^{36}	-7.82	19351.2

[a] Units of the rate constants are cm^3 $molecule^{-1}$ s^{-1} or s^{-1}.