Supplementary Data

Theoretical Study on the Mechanism of C_2H_{3-5} Oxidation by N_2O

Huanhuan Wang[a], Long Qin[a], Bingzhi Liu[b], Shaohua Zhu[a,c],

Zhandong Wang[b], Ran Sui[a,*]

[a] *Center for Combustion Energy, Department of Energy and Power Engineering, Tsinghua University, Beijing 100084, China*

[b] *National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, 230029, China*

[c] *National Key Laboratory of Solid Propulsion, Northwestern Polytechnical University, Xi'an 710072, China*

TABLE OF CONTENTS

Table S1. Optimized coordinates (Å) and unscaled frequencies (in cm^{-1}) of all stationary points on the initial reaction potential energy surfaces of N_2O + C_2H_3/C_2H_4/C_2H_5 optimized by the G4 method.

Species	Optimized coordinates				Unscaled frequencies (cm^{-1})		
N_2O	N	0.000000	0.000000	-1.200127	624.3321	624.3321	1340.3316
	N	0.000000	0.000000	-0.072438	2361.5840		
	O	0.000000	0.000000	1.113494			
C_2H_3	C	0.707505	-0.142017	-0.000011	707.6188	819.3991	928.4092
	H	1.605040	0.459355	-0.000257	1048.3127	1395.5019	1660.7176
	C	-0.586783	0.029029	0.000215	3055.2051	3152.9496	3256.4587
	H	-1.043106	1.023734	-0.000547			
	H	-1.286261	-0.805163	-0.000420			
TS_a1	N	0.456245	1.130465	-0.000102	-474.7195	71.2174	119.5446
	N	1.204941	0.256188	-0.000008	240.5130	269.3919	517.3038
	O	1.724457	-0.825280	0.000103	604.7417	807.4006	870.6986
	C	-1.749901	-0.792048	0.000052	949.3382	1076.1641	1241.6081
	H	-0.950500	-1.529705	0.000134	1399.6864	1657.7376	2136.1511
	H	-2.766219	-1.192465	0.000077	3078.4349	3173.0162	3267.4193
	C	-1.516648	0.495350	-0.000069			
	H	-2.107936	1.398024	-0.000164			
IM_a1	N	-0.154716	-1.081444	-0.000091	118.7919	243.4836	454.9657
	N	-1.154795	-0.363548	-0.000006	464.8799	669.8232	803.8734
	O	-1.411820	0.826613	0.000097	895.2152	939.6277	1007.5491
	C	1.429573	0.818778	0.000051	1110.8072	1278.7887	1357.2173
	H	0.677038	1.595700	0.000153	1419.6411	1649.1729	1682.1031
	H	2.468523	1.130031	0.000050	3167.1266	3208.0756	3263.8654
	C	1.138439	-0.481866	-0.000073			
	H	1.907507	-1.245167	-0.000173			
TS_a1-1	N	-0.359112	1.132360	0.076803	-547.8874	298.7548	594.5648
	N	-1.212087	0.166098	0.019645	619.9756	704.3184	806.3587
	O	-0.794005	-1.018425	-0.122076	909.1948	972.7941	1001.6977
	C	1.199445	-0.678658	0.075885	1125.2188	1139.8662	1224.2003
	H	1.997624	-1.109849	-0.528428	1253.8195	1408.4231	1506.7158
	H	0.960403	-1.250238	0.966139	3113.7215	3192.1841	3204.8848
	C	0.926354	0.680087	-0.031551			
	H	1.637619	1.409710	-0.402244			
IM_a1-1	N	1.137919	0.449318	-0.000010	293.4523	568.0056	691.1965
	N	0.896031	-0.833540	-0.000002	784.2633	845.9139	928.7649
	O	-0.491732	-1.046541	0.000012	966.1567	975.8207	999.5622
	C	-1.145336	0.222597	-0.000009	1112.3545	1134.8160	1206.3299
	H	-1.786206	0.311992	0.890077	1331.0703	1428.8338	1472.4942
	H	-1.786129	0.311993	-0.890156	2983.8456	3008.4549	3255.6098
	C	0.021059	1.146066	0.000016			
	H	0.014199	2.225924	0.000022			

TS_a1-2	N	-1.161180	0.193214	-0.088726	-1122.5646	103.5207	280.4826
	N	-1.922113	-0.657129	0.056610	348.5220	481.7766	647.3837
	O	1.451783	-0.962014	-0.031354	753.1731	837.8134	1016.7576
	C	1.283290	0.259881	-0.008953	1067.8337	1165.4323	1315.2175
	H	2.068914	0.996545	-0.272021	1365.0199	1453.5562	1667.7218
	H	0.874367	0.759112	1.140431	2092.8690	2909.5499	3242.3766
	C	-0.082390	0.936470	-0.037239			
	H	-0.179894	2.009744	-0.115606			
IM_a1-2	N	0.457898	-1.099088	0.011297	222.0893	444.3496	537.0180
	N	-0.754623	-0.957037	0.013502	585.2394	824.9279	894.4088
	O	-1.116502	0.456070	-0.006543	945.6309	966.3307	1005.2692
	C	1.176597	0.193957	-0.003052	1116.5293	1130.4893	1299.2976
	H	1.862938	0.202445	-0.862688	1307.0128	1460.6096	1654.4151
	H	1.809409	0.258490	0.897251	2966.7351	2994.9267	3239.9340
	C	0.045215	1.158253	-0.073445			
	H	0.005879	2.170113	0.303173			
TS_a1-3	N	-1.200486	-0.004064	-0.060855	-387.6741	311.8205	490.7194
	N	-0.667858	-1.073785	-0.049041	636.0830	763.8989	829.5210
	O	0.924200	-0.833476	0.086811	886.1470	942.6093	1009.4176
	C	-0.269296	1.155146	0.061056	1144.6943	1198.5305	1289.9387
	H	-0.524715	1.645336	1.013051	1319.8874	1459.0168	1768.2848
	H	-0.466347	1.880762	-0.736726	2986.1233	3056.5590	3144.5700
	C	1.066042	0.483013	0.003922			
	H	1.895399	0.857705	-0.591401			
IM_a1-3	N	1.402387	0.310579	-0.328898	78.8587	107.7893	250.0396
	N	1.923449	-0.659734	0.069458	440.6847	534.1971	670.9083
	O	-2.126515	-0.181192	-0.168396	785.9678	1012.9548	1061.1267
	C	0.039628	0.775347	0.193430	1166.3603	1247.4419	1403.9150
	H	-0.284950	1.633743	-0.392599	1446.1755	1828.3180	1888.2539
	H	0.197637	1.071443	1.235563	2918.2653	3069.0586	3164.0759
	C	-0.976355	-0.352169	0.129493			
	H	-0.561067	-1.350636	0.382744			
TS_a1-4	N	1.380407	0.204272	-0.439928	-387.2368	83.4550	113.4418
	N	1.976068	-0.627358	0.086041	253.2604	468.7616	502.0988
	O	-2.058889	-0.273542	-0.314059	848.4115	963.0748	1060.6324
	C	-0.023460	0.839233	0.233200	1121.3532	1159.2889	1415.4408
	H	-0.319562	1.642455	-0.435643	1450.6011	1789.3366	1932.4229
	H	0.322331	1.187542	1.206077	2913.7699	3111.1757	3211.1565
	C	-1.025819	-0.267623	0.308377			
	H	-0.731302	-1.109716	0.969786			
CH_2CHO	O	1.169179	-0.263757	-0.000003	453.3842	497.9835	751.7757
	C	-1.168383	-0.171170	0.000017	975.2938	983.2778	1154.2922
	H	-1.271891	-1.250779	-0.000033	1405.6021	1469.5071	1570.1937

	H	-2.058785	0.448102	-0.000053	2932.0265	3150.7315	3266.9629
	C	0.134613	0.404618	0.000004			
	H	0.179868	1.512041	-0.000011			
N_2	N	0.000000	0.000000	0.549396	2430.7010		
	N	0.000000	0.000000	-0.549396			
TS_a1-5	N	-1.875204	-0.581598	0.071507	-1559.7266	27.7187	37.2691
	N	-2.721849	0.106619	-0.056796	47.2279	49.5003	88.4282
	O	0.668829	1.192041	0.008845	431.3281	637.3745	854.0560
	C	1.838988	-0.958186	-0.042605	1033.7499	1124.0150	1233.1499
	H	2.812418	-1.303733	-0.367474	1450.3501	1853.8908	1916.0482
	H	1.062035	-1.696763	0.175471	2432.3537	3054.2914	3237.8071
	C	1.580855	0.413716	-0.089619			
	H	2.435227	0.055843	0.811609			
CH_3CO	O	-1.261390	0.175764	0.000004	118.5438	458.8332	845.8346
	C	1.169687	0.098554	-0.000018	947.5266	1043.9258	1350.9956
	H	1.688697	-0.290765	0.880497	1455.3763	1456.8129	1937.6285
	H	1.187586	1.193876	-0.000876	3026.8135	3121.4564	3124.7903
	C	-0.248793	-0.434717	-0.000025			
	H	1.689474	-0.292247	-0.879399			
TS_a2	N	0.671380	-1.193778	-0.076910	-516.9693	149.6227	254.1056
	N	1.181353	-0.147959	-0.014881	458.5087	528.3135	649.6801
	O	0.840427	1.031717	0.063783	713.2890	718.4023	890.0185
	C	-1.355277	-0.532331	0.055767	934.5817	1051.1970	1246.8669
	H	-1.479489	-1.076697	0.988658	1360.7784	1489.0635	1978.7895
	H	-1.724724	-1.048271	-0.831170	3093.9987	3172.8577	3264.4388
	C	-1.168026	0.808373	0.049027			
	H	-1.348511	1.607147	-0.653979			
TS_a3	N	1.562810	-0.891258	-0.000051	-654.790700	99.934700	256.084000
	N	0.861641	0.045740	-0.000005	369.184300	418.224800	477.841000
	O	0.720713	1.252876	0.000047	622.098800	792.546600	842.375800
	C	-1.896790	0.176715	0.000022	954.822800	1063.798700	1192.870200
	H	-1.611519	1.226379	0.000063	1358.593800	1677.233400	1883.868400
	H	-2.958918	-0.067288	0.000021	3105.163000	3194.304200	3296.921300
	C	-0.983568	-0.750179	-0.000022			
	H	-0.884275	-1.822684	-0.000066			
IM_a3	N	1.574248	-0.784473	0.000005	131.132500	310.954100	482.020400
	N	0.585158	-0.009338	0.000129	526.486000	599.498600	793.542900
	O	0.667859	1.238487	-0.000280	811.139700	974.469600	998.202100
	C	-1.817431	0.088327	0.000019	1047.744000	1282.077100	1307.828400
	H	-1.735202	1.168217	-0.000113	1396.850200	1496.920400	1699.669900
	H	-2.797626	-0.371289	0.000034	3177.247600	3242.102400	3278.681100
	C	-0.725926	-0.656939	0.000160			
	H	-0.665740	-1.736481	0.000299			
TS_a3-1	N	1.765158	-0.633644	-0.000086	-1211.404500	220.829200	223.651100

	N	0.727667	-0.071007	-0.000041	419.511500	462.403100	579.553900
	O	0.479948	1.215361	-0.000062	672.547800	720.289800	737.813800
	C	-1.773840	0.148629	0.000100	803.380700	959.295900	1089.784600
	H	-0.698675	1.082343	0.000012	1097.304800	1676.501500	1807.589800
	H	-2.809272	0.438359	0.000152	1908.807300	3304.580900	3394.160500
	C	-1.060321	-0.881569	0.000086			
	H	-0.776444	-1.913389	0.000098			
C_2H_2	C	0.000000	0.000000	0.599455	550.670500	550.670500	795.948800
	H	0.000000	0.000000	1.661645	795.948800	2078.984600	3454.916600
	C	0.000000	0.000000	-0.599455	3557.165100		
	H	0.000000	0.000000	-1.661645			
N_2	N	0.000000	0.000000	0.549396	2430.701000		
	N	0.000000	0.000000	-0.549396			
OH	O	0.000000	0.000000	0.108439	3696.511400		
	H	0.000000	0.000000	-0.867515			
IM_a03	N	0.667899	1.312499	0.133993	85.707700	290.199700	433.498400
	N	0.573168	0.067071	0.037859	517.240000	601.427200	780.939600
	O	1.528631	-0.709753	-0.195612	834.743200	977.348300	991.586300
	C	-1.861204	0.044836	-0.159169	1084.275500	1276.125500	1302.224000
	H	-1.864888	1.030501	-0.607705	1416.380500	1506.496300	1698.507500
	H	-2.810985	-0.459770	-0.028897	3173.999100	3238.195200	3268.292700
	C	-0.739622	-0.546901	0.218671			
	H	-0.635688	-1.537302	0.641517			
TS_a3-2	N	-0.299888	1.290344	-0.000242	-1832.656100	275.221700	478.734000
	N	-0.527279	0.037238	-0.000033	578.723700	674.658300	746.066800
	O	-1.644282	-0.478612	0.000003	771.304500	809.503200	877.894500
	C	1.739473	0.010597	0.000085	970.548400	983.660600	1188.764700
	H	0.921630	1.201499	-0.000166	1352.708900	1575.092800	1652.079600
	H	2.812454	-0.101535	0.000158	1876.764000	3235.602500	3281.374800
	C	0.703355	-0.793875	0.000175			
	H	0.553371	-1.864471	0.000356			
IM_a3-1	N	-0.696583	1.290611	0.019210	34.800800	298.906500	529.245200
	N	-0.535075	0.032436	0.010978	562.532100	580.213000	736.978100
	O	-1.460751	-0.783259	-0.059494	753.822100	800.517400	841.772900
	C	1.913208	0.087937	-0.072729	929.415300	1203.424400	1263.110700
	H	0.239796	1.700988	0.092342	1444.978400	1650.675200	1671.328300
	H	2.982781	-0.025393	-0.102289	3164.974000	3315.224900	3406.910200
	C	0.813722	-0.589546	0.079459			
	H	0.723454	-1.661203	0.234206			
TS_a3-3	N	-0.790578	1.291739	-0.000002	-499.574500	44.301300	247.960400
	N	-0.654785	0.051559	0.000001	404.866600	451.920300	466.757000
	O	-1.511647	-0.803813	0.000004	671.382800	681.940400	807.295800
	C	2.055330	0.048880	-0.000002	822.830100	1003.113500	1267.541500
	H	0.154854	1.685578	-0.000004	1382.914200	1736.549300	1774.848400

	H	2.664102	0.924951	-0.000005	3308.164900	3423.695700	3447.839100
	C	1.050934	-0.691869	0.000000			
	H	0.754178	-1.725187	0.000002			
C_2H_2	C	0.000000	0.000000	0.599455	550.670500	550.670500	795.948800
	H	0.000000	0.000000	1.661645	795.948800	2078.984600	3454.916600
	C	0.000000	0.000000	-0.599455	3557.165100		
	H	0.000000	0.000000	-1.661645			
HN_2O	N	-1.083299	-0.248793	0.000000	662.952200	779.925500	1276.011100
	N	0.027121	0.313399	0.000002	1367.678800	1735.422600	3433.470300
	O	1.149064	-0.117008	-0.000002			
	H	-1.799268	0.483821	0.000005			
IM_a04	N	1.449365	-1.199446	-0.042143	27.195600	56.826900	68.233100
	N	1.388719	-0.074634	0.001366	76.613100	88.025600	618.255800
	O	1.325856	1.108176	0.048175	625.226500	705.996100	820.968700
	C	-2.105857	-0.573405	0.079007	930.430700	1046.557000	1342.695300
	H	-2.121552	-1.353406	-0.680245	1395.750000	1656.935100	2363.678900
	H	-2.250942	-0.917896	1.107581	3055.579600	3153.715900	3261.763800
	C	-1.932016	0.687403	-0.215142			
	H	-1.873704	1.640467	0.289511			
TS_a4	N	2.224298	0.543656	-0.121989	-691.453000	9.890600	120.860800
	N	1.441783	-0.287195	0.000809	234.614600	291.763500	513.360300
	O	0.292090	-0.728910	0.117955	519.241300	784.327100	861.681200
	C	-2.361052	-0.030437	-0.111102	942.532500	1052.214900	1089.697200
	H	-2.446280	-1.097139	-0.305786	1390.493700	1672.192300	2079.695400
	H	-3.293760	0.536933	-0.111696	3084.912100	3172.867200	3277.740200
	C	-1.209296	0.541413	0.110421			
	H	-0.837158	1.530404	0.326183			
TS_a5	N	-0.558822	1.169955	-0.000075	-2025.057800	74.136600	133.057900
	N	-1.029483	0.087937	-0.000053	308.847500	411.677200	434.579400
	O	-1.981031	-0.654184	-0.000060	521.379400	589.376800	652.632300
	C	1.934816	0.311512	0.000080	747.998500	933.903400	989.049100
	H	0.732891	0.940329	-0.000021	1271.467000	1418.070700	1868.124900
	H	2.729371	1.042224	0.000104	2011.714000	3256.833100	3475.471200
	C	1.750330	-0.917084	0.000115			
	H	1.393244	-1.920893	0.000129			
IM_a5	N	-0.754408	-0.000828	0.831333	17.045500	41.739400	55.271600
	N	-1.455707	0.000245	-0.194288	103.232200	143.507000	567.613700
	O	-2.647370	0.000356	-0.364060	586.955600	669.553300	796.121500
	C	2.599799	-0.599994	-0.149023	809.334600	838.676800	1282.552000
	H	0.230479	-0.000375	0.538225	1378.527300	1734.888400	2071.713900
	H	2.609926	-1.663080	-0.152096	3386.779600	3446.473500	3548.813800
	C	2.600032	0.600226	-0.148132			
	H	2.610373	1.663296	-0.150038			
TS_a6	N	-1.486516	1.235921	-0.000007	-1782.932400	99.954500	100.999700

	N	-1.028160	0.134138	0.000012	253.508800	346.715900	398.003900
	O	-1.338935	-1.067454	0.000033	641.808400	665.360800	707.232200
	C	1.496539	-0.449400	-0.000008	770.200400	931.383000	1010.846900
	H	0.262571	0.196126	0.000013	1244.197300	1445.989300	1764.539300
	H	1.071726	-1.443331	0.000011	1930.501600	3255.623600	3476.400300
	C	2.470072	0.299775	-0.000036			
	H	3.180251	1.094174	-0.000061			
IM_a6	N	1.983257	-0.967522	0.000008	70.160300	80.676800	129.381200
	N	1.047280	-0.147252	0.000003	166.039900	175.765700	570.552700
	O	1.086470	1.102543	-0.000153	616.265700	651.380000	807.702400
	C	-1.880769	0.509638	0.000019	822.773100	1002.897400	1264.859300
	H	0.087449	-0.577225	0.000115	1440.904700	1556.635700	2062.717800
	H	-1.332619	1.423961	-0.000064	3029.497000	3429.259700	3536.113600
	C	-2.408529	-0.570271	0.000130			
	H	-2.924560	-1.499860	0.000196			
TS_a6-1	N	-2.028935	-0.860697	0.000002	-1680.476200	44.585300	94.279500
	N	-1.119180	-0.136893	0.000001	116.316000	166.696200	201.321700
	O	-0.845283	1.227603	-0.000002	544.051900	586.932200	604.168900
	C	2.128146	0.379596	-0.000001	634.207200	786.631600	800.788500
	H	0.044746	0.197769	0.000000	815.080300	1760.743100	1962.519700
	H	2.268715	1.433898	-0.000004	2068.551900	3442.640300	3544.570600
	C	1.977956	-0.813006	0.000001			
	H	1.848997	-1.868899	0.000004			
TS_a6-2	N	0.867721	1.255336	0.000002	-2140.414000	46.154500	82.510500
	N	1.093581	0.035563	0.000000	118.103500	159.575600	211.625800
	O	2.005047	-0.775199	-0.000002	580.076300	588.386800	624.450100
	C	-1.987367	-0.811500	-0.000001	687.331100	800.488800	814.383200
	H	-0.124330	0.311611	0.000001	1271.418600	1696.137800	1982.159600
	H	-1.761728	-1.851223	-0.000003	2069.786900	3440.730500	3542.686600
	C	-2.245521	0.362530	0.000002			
	H	-2.486106	1.398737	0.000004			

Species	**Optimized coordinates**				**Unscaled frequencies (cm^{-1})**		
N_2O	N	0.000000	0.000000	-1.200127	624.3321	624.3321	1340.3316
	N	0.000000	0.000000	-0.072438	2361.5840		
	O	0.000000	0.000000	1.113494			
C_2H_4	C	-0.663728	0.000000	0.000036	824.3008	968.9275	982.4504
	H	-1.237813	0.921589	0.000083	1072.6221	1237.3287	1385.7144
	H	-1.237813	-0.921589	0.000083	1471.9864	1697.7796	3137.3423
	C	0.663730	0.000000	-0.000043	3153.8613	3209.3728	3237.0544
	H	1.237808	-0.921593	-0.000061			
	H	1.237807	0.921593	-0.000061			
TS_b1	N	-0.693215	1.177060	0.000098	-489.1048	176.1013	304.3848
	N	-1.220728	0.130090	0.000005	473.4553	544.7732	682.3671

	O	-0.868599	-1.046943	-0.000097	731.6852	839.6965	1002.9162
	C	1.248730	0.647806	0.000071	1012.9399	1038.7483	1238.4080
	H	1.476904	1.180607	0.916053	1243.3945	1309.4824	1473.2041
	H	1.476923	1.180785	-0.915802	1559.0400	1945.7299	3155.8880
	C	1.207263	-0.737317	-0.000064	3172.4379	3235.1125	3265.6487
	H	1.328307	-1.299329	-0.917719			
	H	1.328297	-1.299508	0.917483			
IM_b1	N	0.994615	0.733025	-0.000073	83.4372	522.6045	724.2524
	N	1.141248	-0.482223	0.000023	778.1332	829.1786	899.8487
	O	-0.071992	-1.194926	0.000042	948.9004	963.4195	1027.3941
	C	-0.438864	1.109446	-0.000071	1114.2054	1184.7547	1243.7764
	H	-0.632753	1.722226	-0.884162	1311.9473	1347.9739	1485.8598
	H	-0.632732	1.722416	0.883891	1525.8395	1665.5054	3057.7115
	C	-1.157396	-0.245341	0.000073	3072.3041	3098.0723	3119.6983
	H	-1.765954	-0.412682	0.892551			
	H	-1.766104	-0.412795	-0.892280			
TS_b1-1	N	-1.193919	0.009251	-0.000025	-442.8946	101.9270	277.9796
	N	-1.063163	-1.116946	-0.000028	382.2890	546.2120	608.1302
	O	1.150937	-0.874558	0.000026	612.2361	945.8636	971.2207
	C	-0.501089	1.192725	-0.000001	1081.8414	1163.7246	1192.2908
	H	-0.692961	1.764307	0.907619	1245.3028	1418.5876	1461.7355
	H	-0.692929	1.764328	-0.907615	1584.5019	2173.8519	2880.0175
	C	1.286472	0.379940	0.000021	2903.6879	3108.2467	3189.2164
	H	1.632847	0.892847	-0.919511			
	H	1.632825	0.892857	0.919555			
CH_2N_2	N	0.152511	-0.000493	0.000017	426.7226	428.0232	587.5586
	N	1.291635	0.000234	0.000008	1121.8410	1224.0908	1447.7119
	C	-1.136997	0.000165	-0.000052	2217.3658	3197.6402	3321.5409
	H	-1.643983	-0.951389	0.000070			
	H	-1.643059	0.952209	0.000069			
CH_2O	O	-0.674615	-0.000059	-0.000001	1201.6412	1272.4564	1544.0488
	C	0.525601	-0.000017	0.000023	1844.9165	2882.7707	2930.8556
	H	1.121168	0.937611	-0.000039			
	H	1.122145	-0.937033	-0.000084			
TS_b1-2	N	-1.369814	0.441905	0.090404	-623.9829	251.2267	305.2577
	N	-1.374500	-0.683739	0.046697	365.3411	511.8497	523.0966
	O	0.783357	-1.151962	-0.231802	572.3619	853.4215	949.5451
	C	0.374736	1.178554	-0.181480	1020.1175	1081.2403	1156.3015
	H	0.458090	2.118458	0.362893	1298.1605	1338.0495	1438.6799
	H	0.229267	1.268066	-1.255338	1472.9898	2157.8976	2460.2155
	C	1.108631	-0.015932	0.288790	2893.0390	3119.2934	3228.8200
	H	2.015482	0.504493	-0.229414			
	H	1.340306	0.041785	1.372706			
CH_3CH	O	1.234377	-0.276125	-0.000024	168.7185	501.7874	773.0604

O							
	C	-1.169213	-0.148398	0.000004	884.2760	1125.1063	1138.4421
	H	-1.708943	0.223604	0.879292	1373.3407	1431.0152	1459.8837
	H	-1.158492	-1.239568	-0.000034	1471.3912	1840.1633	2862.9807
	C	0.236306	0.396932	0.000028	3029.4659	3089.0678	3149.4503
	H	-1.708950	0.223671	-0.879250			
	H	0.298817	1.510086	-0.000015			
N_2	N	0.000000	0.000000	0.549396	2430.7010		
	N	0.000000	0.000000	-0.549396			
TS_b1-3	N	0.050580	-1.196732	-0.121790	-2727.9425	284.7022	402.0978
	N	1.105119	-0.536691	0.000455	539.3461	695.3604	769.7886
	O	0.882492	0.807888	0.122843	832.4841	873.9614	945.1814
	C	-1.071734	-0.279410	-0.098996	977.4389	1022.5635	1064.9704
	H	-1.696786	-0.602755	1.316405	1171.2296	1242.1228	1296.8985
	H	-1.990221	-0.555195	-0.603009	1328.7086	1374.7660	1547.4333
	C	-0.503531	1.042832	-0.084177	2036.8234	3193.0297	3243.0236
	H	-0.759378	1.852883	-0.749784			
	H	-1.251850	0.395391	1.002031			
$C_2H_2N_2O$	N	-1.035158	0.551536	-0.000281	590.9791	628.7320	702.7522
	N	-0.959811	-0.700797	-0.000035	815.8277	873.6759	950.4527
	O	0.434883	-1.055150	0.000233	982.6635	1108.9592	1146.8994
	C	0.218772	1.119493	0.000145	1159.7164	1372.7851	1451.6193
	H	0.368587	2.184894	0.000264	1550.3171	3280.9453	3306.3692
	C	1.104020	0.091283	-0.000112			
	H	2.180377	0.036475	-0.000114			
H_2	H	0.000000	0.000000	0.371371	4466.4056		
	H	0.000000	0.000000	-0.371371			
TS_b1-4	N	1.128408	0.291598	-0.103341	-1545.385000	142.558100	534.073800
	N	0.835215	-0.942127	-0.012641	634.498100	723.438900	799.831000
	O	-0.598514	-1.023019	0.016897	904.239300	947.063900	989.966300
	C	0.049535	1.160553	0.026259	1056.430700	1081.136700	1142.857700
	H	0.175538	2.177265	-0.317500	1174.774700	1343.562600	1368.879900
	H	1.318644	0.953485	0.813150	1455.161100	1538.397200	2379.628000
	C	-1.185370	0.297318	0.007404	2945.273900	2997.691000	3243.121000
	H	-1.839889	0.426995	0.880530			
	H	-1.796530	0.432885	-0.901455			
IM_b1-3	N	1.043169	0.356822	0.003856	56.737000	347.925400	571.448500
	N	0.849476	-0.929777	0.022030	775.124200	814.703400	830.791900
	O	-0.565674	-1.036009	-0.034715	885.470000	974.214300	1014.316400
	C	0.002390	1.172431	-0.035703	1073.855300	1133.684200	1154.135300
	H	0.099203	2.241778	-0.000735	1290.478800	1370.238300	1438.390800
	H	2.012084	0.649890	0.016248	1552.299600	1588.142800	2890.743600
	C	-1.194581	0.272218	0.026673	2950.998900	3305.631300	3604.390200
	H	-1.789038	0.366641	0.955981			

	H	-1.892217	0.372557	-0.820788			
TS_b1-5	N	-0.593110	0.905411	0.122837	-701.368400	207.128800	556.810500
	N	-1.217861	-0.226076	-0.070190	577.779100	705.796300	758.672700
	O	-0.363455	-1.197670	-0.066297	900.693200	970.837700	1028.344700
	C	0.780159	0.930487	0.015340	1065.633600	1125.556900	1204.889900
	H	1.153244	1.668303	-0.687482	1245.146300	1334.310900	1385.556800
	H	-1.184894	1.723541	0.073274	1498.534000	1542.671700	3054.205700
	C	1.250490	-0.420107	0.059469	3113.502300	3169.840000	3614.253400
	H	1.999783	-0.711697	-0.684178			
	H	1.432407	-0.916411	1.011385			
IM_b1-4	N	-0.220455	0.945426	-0.000002	156.576000	273.430600	277.379400
	N	-1.375913	0.241827	0.000002	447.036500	616.811100	727.553000
	O	-1.245541	-0.966269	0.000009	859.938100	915.068800	921.020400
	C	1.109633	0.509148	-0.000007	1011.672100	1074.022200	1187.670600
	H	1.790350	1.355493	-0.000019	1359.236600	1422.991800	1462.609200
	H	-0.401350	1.937385	-0.000005	1630.183100	1693.134100	3168.979800
	C	1.581150	-0.739994	-0.000001	3186.365600	3312.961200	3638.826200
	H	2.656303	-0.877156	-0.000007			
	H	0.948898	-1.611271	0.000009			
C_2H_3	C	0.707507	-0.142045	0.000004	707.683600	819.403900	928.377300
	H	1.604986	0.459425	0.000028	1048.384100	1395.473700	1660.668900
	C	-0.586791	0.029033	-0.000005	3055.274500	3153.018100	3256.386300
	H	-1.043001	1.023781	0.000014			
	H	-1.286286	-0.805139	-0.000035			
HN_2O	N	1.083295	-0.248793	0.000006	662.948900	779.914900	1275.997400
	N	-0.027113	0.313396	0.000001	1367.704700	1735.407600	3433.499900
	O	-1.149068	-0.117005	-0.000007			
	H	1.799264	0.483818	0.000012			
TS_b2	N	0.288425	1.005900	-0.020512	-684.979300	157.790000	290.410000
	N	1.333762	0.403455	-0.150798	421.940900	551.102300	652.021300
	O	1.461866	-0.837160	-0.040938	753.104600	883.300000	975.640400
	C	-0.875379	-0.099626	0.478251	1085.182400	1179.409800	1247.770600
	H	-1.029549	0.039959	1.547519	1314.457500	1337.708800	1444.903700
	H	-0.002312	-0.921855	0.266621	1588.244900	1668.978300	1788.718900
	C	-1.981157	-0.200844	-0.310629	3139.553500	3148.188700	3238.401700
	H	-1.891565	-0.294977	-1.388773			
	H	-2.987591	-0.188518	0.095575			
IM_b2	N	-0.198313	-1.000862	-0.160421	93.168900	270.042900	327.057400
	N	-1.278429	-0.409157	-0.250765	541.989200	643.882300	668.673500
	O	-1.358775	0.900811	0.186018	826.651800	870.912100	931.579300
	C	0.977912	-0.399016	0.368651	952.883900	1010.201500	1100.255400
	H	1.288146	-0.849100	1.308821	1313.490300	1406.131600	1436.320700
	H	-0.471241	1.167424	0.499659	1632.996300	1669.553500	3157.334400
	C	1.732428	0.501419	-0.261201	3167.633300	3251.679500	3563.601200

	H	1.449497	0.913305	-1.223765			
	H	2.678957	0.817598	0.160747			
TS_b2-1	N	-0.348488	-1.064092	-0.005578	-1180.344600	199.790300	324.239800
	N	0.779496	-1.192099	0.009990	414.209200	439.722400	575.715200
	O	1.587147	0.758567	-0.112391	589.971900	615.449400	704.391600
	C	-1.398170	-0.096126	0.001856	726.914200	753.610100	970.611000
	H	-2.375006	-0.562712	0.003354	1098.277600	1332.172200	1425.840200
	H	1.997442	0.775537	0.761032	1518.216300	1602.600500	2099.238800
	C	-0.947981	1.165939	0.011545	3118.663300	3209.044400	3806.151000
	H	0.474111	1.168505	-0.014191			
	H	-1.733871	1.924591	0.037637			
IM_b2-1	N	0.667018	0.810288	0.004022	101.950800	120.674700	153.316700
	N	0.041254	1.726588	-0.000651	218.450700	262.501400	381.146100
	O	-2.086334	-0.308041	-0.090181	443.633200	610.850000	694.963100
	C	1.381947	-0.385968	0.014584	730.521500	811.517200	975.628100
	H	2.449648	-0.168424	0.040815	1107.195300	1301.177700	1392.298800
	H	-2.528747	-0.516989	0.737636	1701.199500	2322.732600	3046.612400
	C	0.599836	-1.495534	-0.009596	3115.420700	3404.563200	3857.980900
	H	-1.327966	-0.935560	-0.113773			
	H	1.249131	-2.383829	0.003244			
TS_b2-2	N	-0.627292	0.967372	0.004571	-540.840500	96.793200	129.605400
	N	0.245978	1.646590	-0.013265	189.773100	227.962000	262.226200
	O	2.060578	-0.492138	0.103052	276.038200	413.437800	587.077600
	C	-1.520937	-0.342063	-0.003037	684.832000	780.434000	864.963300
	H	-2.531699	0.037463	0.002376	930.183200	1287.178300	1516.815900
	H	2.408196	-0.645749	-0.780606	1694.314400	2317.459400	3140.870500
	C	-0.751223	-1.391830	-0.009294	3238.656600	3406.467300	3855.715100
	H	1.217816	-1.000427	0.109673			
	H	-1.276774	-2.348563	-0.021024			
H_2O	O	0.000000	0.000000	0.118836	1671.434500	3804.119200	3908.087200
	H	0.000000	0.756672	-0.475345			
	H	0.000000	-0.756672	-0.475345			
N_2	N	0.000000	0.000000	0.549396	2430.701000		
	N	0.000000	0.000000	-0.549396			
C_2H_2	C	0.000000	0.000000	0.599455	550.670500	550.670500	795.948800
	H	0.000000	0.000000	1.661645	795.948800	2078.984600	3454.916600
	C	0.000000	0.000000	-0.599455	3557.165100		
	H	0.000000	0.000000	-1.661645			

Species	**Optimized coordinates**				**Unscaled frequencies (cm^{-1})**		
N_2O	N	0.000000	0.000000	-1.200127	624.3321	624.3321	1340.3316
	N	0.000000	0.000000	-0.072438	2361.5840		
	O	0.000000	0.000000	1.113494			
C_2H_5	C	0.011053	-0.693289	0.000000	122.2807	464.0920	806.9699

	H	-1.011955	-1.108025	0.000000	980.0395	1065.5688	1193.9756
	H	0.508262	-1.101685	0.886824	1398.2912	1465.1586	1480.2087
	H	0.508262	-1.101685	-0.886824	1482.6738	2955.4929	3046.4488
	C	0.011053	0.794719	0.000000	3091.7784	3152.6996	3254.3828
	H	-0.068602	1.351407	0.926594			
	H	-0.068602	1.351407	-0.926594			
IM_c0	N	-1.913068	0.998814	-0.339298	21.6055	35.7998	57.6713
	N	-1.569173	-0.031209	-0.037242	70.4960	74.0030	159.1379
	O	-1.211799	-1.116872	0.280749	495.3051	616.3009	623.9067
	C	1.729606	0.644557	0.560069	807.2879	981.8057	1065.3110
	H	1.918274	1.707144	0.458534	1196.1474	1338.8076	1396.5685
	H	1.345359	0.294324	1.511618	1465.0831	1479.3099	1484.5035
	C	2.222098	-0.322634	-0.457795	2361.9286	2957.0409	3049.3750
	H	1.596615	-1.221415	-0.496089	3095.7724	3150.2900	3251.9274
	H	2.252336	0.117750	-1.460121			
	H	3.247267	-0.667602	-0.237797			
TS_c1	N	0.512681	1.067760	-0.311979	-498.9645	37.8168	129.1614
	N	1.295254	0.232907	-0.136305	182.3025	218.9104	522.0321
	O	1.769179	-0.816718	0.217929	586.9626	653.5039	825.8356
	C	-1.363674	0.551463	0.403467	852.2411	1025.3835	1075.5340
	H	-1.865971	1.443619	0.045432	1217.1190	1234.5866	1399.1383
	H	-1.118340	0.562954	1.461768	1471.2558	1479.6179	1489.8256
	C	-1.703788	-0.759466	-0.227775	2074.5866	2989.5225	3071.6036
	H	-0.978657	-1.535543	0.035513	3114.1842	3138.1105	3233.9021
	H	-2.689212	-1.111331	0.115730			
	H	-1.752031	-0.682604	-1.318039			
IM_c1	N	-0.202435	0.188016	0.528390	61.6028	221.1554	290.8546
	N	-1.171732	0.050157	-0.228887	355.6275	429.2726	638.5403
	O	-2.318586	-0.280673	-0.038546	804.2027	918.8580	1034.7306
	C	1.048371	0.603309	-0.129933	1107.5778	1159.2734	1285.4796
	H	1.398520	1.491808	0.405998	1366.4151	1390.5490	1409.6299
	H	0.862223	0.884526	-1.171762	1485.4598	1489.4870	1505.9016
	C	2.091713	-0.509346	-0.034682	1696.3925	3039.1881	3045.3146
	H	1.770994	-1.393016	-0.593802	3084.6471	3120.9817	3126.4110
	H	3.044824	-0.166173	-0.447443			
	H	2.250785	-0.802746	1.006550			
TS_c1-1	N	0.231802	0.911705	0.051175	-1739.1106	102.4194	176.0906
	N	1.380641	0.508192	-0.137095	312.1864	501.2007	593.2012
	O	1.544455	-0.792809	-0.103781	778.5536	835.7369	988.0902
	C	-0.677787	-0.147622	0.428186	1051.9607	1057.1703	1113.2430
	H	-0.703622	-0.293309	1.513430	1144.0810	1228.4242	1353.4671
	H	0.335977	-1.031779	0.073278	1401.4220	1478.0904	1481.8787
	C	-2.016855	-0.154144	-0.247161	1592.2942	1809.3875	3020.7116
	H	-1.917518	-0.092291	-1.333850	3074.5012	3089.4974	3127.4715

	H	-2.563959	-1.066440	0.008334			
	H	-2.625771	0.697604	0.084345			
IM_c1-1	N	-0.053887	-0.737327	-0.051692	150.3091	192.9937	251.2143
	N	-1.349287	-0.661151	0.071439	348.1315	429.4787	530.0223
	O	-1.884290	0.611434	-0.055880	709.7834	810.8541	910.0420
	C	0.761399	0.258144	0.177775	949.4373	1032.0280	1117.3842
	H	0.402586	1.181389	0.642485	1153.7646	1298.8385	1378.4742
	H	-1.226520	1.172404	-0.507331	1406.3920	1454.4497	1472.9585
	C	2.223004	0.118968	-0.078174	1521.1918	3020.3254	3065.9817
	H	2.444981	-0.863077	-0.498933	3074.4199	3142.7964	3609.4901
	H	2.572808	0.893081	-0.773101			
	H	2.796267	0.251402	0.848080			
TS_c1-2	N	0.347596	-1.131600	0.000041	-203.2427	98.8157	110.1726
	N	1.293275	-0.356916	0.000025	163.7390	211.8489	293.3902
	O	1.172576	0.974470	-0.000042	507.6816	551.8487	575.6951
	C	-1.099266	-0.642735	-0.000045	756.1745	907.6515	1038.2818
	H	-1.520337	-1.134757	0.881998	1111.6117	1210.1071	1410.9936
	H	-1.520143	-1.134556	-0.882294	1429.3358	1471.9012	1505.1165
	C	-1.329342	0.829538	0.000048	2054.5559	3022.7172	3072.0421
	H	0.091553	1.179913	-0.000124	3130.5342	3187.9623	3767.0235
	H	-1.673248	1.296254	-0.919128			
	H	-1.672879	1.296184	0.919400			
N_2CHCH_3							
	N	-0.785207	0.110564	0.000113	91.0221	244.7778	449.2987
	N	-1.845949	-0.316509	-0.000227	551.2972	592.4024	912.6987
	C	0.415318	0.580999	0.000095	1047.7244	1108.6784	1226.0593
	H	0.491373	1.659868	0.000123	1415.2132	1435.5615	1474.9738
	C	1.610329	-0.330814	0.000025	1511.7392	2189.1249	3017.6691
	H	1.294601	-1.377043	-0.000719	3063.7535	3119.6513	3217.4171
	H	2.239416	-0.170623	-0.883998			
	H	2.238822	-0.171694	0.884673			
OH	O	0.000000	0.000000	0.108437	3696.7470		
	H	0.000000	0.000000	-0.867498			
TS_c1-3	N	0.347596	-1.131600	0.000041	-929.6884	44.4281	406.8057
	N	1.293275	-0.356916	0.000025	496.7027	508.3414	598.8340
	O	1.172576	0.974470	-0.000042	708.3275	794.3110	863.4285
	C	-1.099266	-0.642735	-0.000045	960.6095	1022.1074	1051.5349
	H	-1.520337	-1.134757	0.881998	1112.4721	1202.5897	1274.1287
	H	-1.520143	-1.134556	-0.882294	1278.2722	1448.1545	1476.2693
	C	-1.329342	0.829538	0.000048	1634.6613	1659.8305	3052.5784
	H	0.091553	1.179913	-0.000124	3097.4704	3123.0596	3220.3929
	H	-1.673248	1.296254	-0.919128			
	H	-1.672879	1.296184	0.919400			
IM_c1-2	N	0.302786	-1.075939	-0.185387	75.1437	215.0718	265.4867

	N	1.302195	-0.362264	-0.205103	360.4360	520.4490	574.7617
	O	1.224789	0.964522	0.199248	638.7935	709.3289	821.4257
	C	-1.009805	-0.571380	0.328201	874.3252	927.3518	1041.0415
	H	-0.924002	-0.487481	1.419289	1104.7800	1248.2416	1305.3950
	H	-1.703901	-1.397160	0.122920	1393.4915	1449.7779	1461.0830
	C	-1.505041	0.701688	-0.266118	1645.8823	3007.7683	3053.1234
	H	0.273033	1.223479	0.227775	3147.3150	3257.1260	3330.0006
	H	-1.529968	0.821188	-1.343676			
	H	-2.059262	1.409371	0.340647			
TS_c1-4	N	0.524768	-1.129063	-0.000069	-509.4148	73.3394	261.3589
	N	1.418474	-0.336908	-0.000083	293.1806	353.8701	541.7278
	O	1.235553	1.038636	0.000079	663.5174	704.7749	733.5409
	C	-1.288497	-0.632062	0.000137	793.6957	820.3049	1043.1975
	H	-1.482339	-1.198137	0.906878	1062.5308	1213.4069	1247.4386
	H	-1.482593	-1.198517	-0.906311	1428.3280	1456.2395	1510.5066
	C	-1.593365	0.737217	-0.000117	1700.2291	3128.9907	3147.3164
	H	0.251025	1.159015	0.000170	3204.2383	3246.8289	3247.8022
	H	-1.741051	1.279531	-0.927808			
	H	-1.740990	1.279887	0.927379			
C_2H_4	C	0.000009	-0.663714	0.000000	824.2861	968.9381	982.4653
	H	-0.000025	-1.237841	0.921565	1072.6239	1237.3155	1385.7369
	H	-0.000025	-1.237841	-0.921565	1472.0015	1697.8410	3137.3563
	C	0.000009	0.663726	0.000000	3153.8785	3209.3673	3237.0500
	H	-0.000026	1.237805	-0.921589			
	H	-0.000026	1.237805	0.921589			
N_2	N	0.000000	0.000000	0.549396	2430.7010		
	N	0.000000	0.000000	-0.549396			
TS_c1-5	N	-0.066889	-0.161270	-0.489426	-2111.8231	121.0483	278.3645
	N	-1.193133	-0.364447	0.164280	321.8594	454.5335	603.6337
	O	-2.113140	0.417685	0.062809	701.7953	799.2340	876.0824
	C	1.186106	-0.696700	0.119669	944.9806	1028.6423	1121.5947
	H	1.654655	-1.436472	-0.532006	1156.2703	1205.9892	1215.2161
	H	1.002153	-1.129035	1.105043	1291.5954	1443.5662	1500.8333
	C	1.826097	0.670701	0.101472	1563.1993	1865.4724	3076.9400
	H	1.808328	1.245925	1.022409	3130.5587	3133.5045	3237.4781
	H	2.651539	0.867270	-0.576378			
	H	0.535389	0.946841	-0.572365			
IM_c1-3	N	0.114857	0.668104	0.202470	54.9485	162.8184	233.5673
	N	1.410445	0.511241	-0.072632	280.5925	401.6157	506.8099
	O	1.781362	-0.645931	-0.167632	601.7319	793.7972	811.4967
	C	-0.855008	-0.428152	0.298515	1015.0999	1071.2459	1112.7669
	H	-0.954266	-0.750019	1.342448	1140.8810	1244.9628	1355.5698
	H	-0.374489	-1.262040	-0.237299	1417.7877	1462.0556	1483.3861
	C	-2.164142	-0.041309	-0.278163	1604.8206	2989.9792	3044.2666

	H	-0.181116	1.631647	0.245538	3160.8271	3272.7985	3632.9016
	H	-2.214810	0.380085	-1.275674			
	H	-3.088434	-0.270869	0.235068			
TS_c1-6	N	-0.564643	1.050620	-0.105451	-517.8487	111.4143	162.8285
	N	-1.355042	0.075699	0.153381	323.8372	399.7413	544.7008
	O	-1.025657	-1.068548	-0.123683	707.2751	779.6644	807.6475
	C	1.308071	0.610084	-0.066723	825.6862	1038.7574	1058.3059
	H	1.519274	1.264575	0.774988	1233.3597	1239.9851	1260.5874
	H	1.539733	1.042106	-1.034258	1340.4250	1467.1050	1542.1444
	C	1.440372	-0.760397	0.101422	1557.0164	3131.3055	3176.5146
	H	-0.893164	1.895226	0.366386	3212.0604	3274.0092	3457.5515
	H	1.544048	-1.423646	-0.746519			
	H	1.442505	-1.212230	1.085161			
ON_2H	N	1.083310	-0.248791	-0.000002	662.9579	779.9467	1275.9708
	N	-0.027120	0.313398	-0.000005	1367.6376	1735.3326	3433.4172
	O	-1.149079	-0.117007	0.000003			
	H	1.799304	0.483805	0.000022			
$TS_{c\text{-}roaming}$	N	1.153605	0.379823	-0.371787	-552.3348	138.7935	226.5708
	N	0.906479	-0.872579	-0.145917	266.1498	455.3132	576.1763
	O	-0.223234	-1.145835	0.343862	708.4002	756.4505	818.5379
	C	0.391010	1.216272	0.325114	840.5143	955.7168	1115.8087
	H	0.391440	2.259323	0.025073	1153.1173	1174.5183	1262.3284
	H	0.082424	0.976321	1.338969	1302.5777	1431.8668	1462.1828
	C	-1.632991	0.216033	-0.238068	1506.8615	3097.7617	3122.8425
	H	-2.276048	-0.428856	0.348620	3224.5370	3228.9834	3264.6461
	H	-1.841249	1.270413	-0.078520			
	H	-1.539402	-0.055061	-1.283396			
IM_c1-4	N	-1.322244	-0.605631	-0.026780	68.7211	144.7962	218.0974
	N	-0.038037	-0.793607	0.043674	268.4557	425.6508	603.6635
	O	0.671041	0.394731	-0.105737	676.3728	886.8434	924.9602
	C	-1.872114	0.581902	0.032726	1063.5092	1100.1325	1172.7312
	H	-2.948250	0.628470	-0.091164	1211.0866	1233.5058	1297.8933
	H	-1.313139	1.491177	0.234341	1462.9843	1478.8910	1500.2470
	C	2.065397	0.130624	0.032932	1508.7047	3036.8176	3111.6129
	H	2.569093	1.080248	-0.155632	3129.4760	3144.7317	3241.6772
	H	2.296338	-0.221435	1.043089			
	H	2.389889	-0.616796	-0.696940			
TS_c1-7	N	1.276063	-0.383723	0.021267	-419.9403	74.4371	120.4996
	N	0.208793	-0.824760	-0.132077	134.9144	295.6674	386.7157
	O	-0.994877	0.571084	-0.052401	477.0606	540.8605	630.5262
	C	2.280618	0.424427	0.050074	1040.8851	1114.0766	1143.3112
	H	3.157185	0.146434	0.616900	1171.9390	1208.8684	1423.3486
	H	2.226578	1.336180	-0.532828	1452.4409	1465.0559	1507.0462
	C	-2.264653	0.026030	0.082048	1949.3910	2954.0612	3006.6438

	H	-2.407535	-0.877166	-0.529484	3025.5689	3155.7080	3281.2407
	H	-2.530418	-0.204153	1.126241			
	H	-2.976581	0.786674	-0.278677			
CH_3O	O	-0.790890	0.000016	-0.007904	717.8772	965.2920	1120.2456
	C	0.571158	0.000044	-0.013546	1365.5238	1368.4630	1521.4194
	H	1.014060	-0.907990	-0.456860	2895.7005	2960.8048	3000.3126
	H	1.014193	0.909168	-0.454443			
	H	0.871921	-0.001567	1.055812			
CH_2NN	N	0.152627	-0.000027	-0.000189	425.2474	427.9712	587.3308
	N	1.291635	0.000013	0.000072	1122.2249	1223.1743	1447.1476
	C	-1.137272	0.000010	-0.000065	2217.5235	3197.5271	3321.9341
	H	-1.643118	-0.952145	0.000604			
	H	-1.643080	0.952182	0.000606			
TS_c2	N	1.600515	-0.874796	-0.269548	-655.2301	58.6985	168.9674
	N	0.910906	0.041374	-0.009648	246.0807	326.2506	481.1008
	O	0.825043	1.252670	0.141434	582.5876	752.2623	852.4670
	C	-0.877769	-0.723937	0.380833	905.7908	1057.8653	1108.2930
	H	-0.769284	-1.728849	-0.013991	1183.4252	1222.5086	1386.3676
	H	-0.772601	-0.655982	1.460799	1465.9586	1473.6338	1491.7701
	C	-1.842938	0.202932	-0.271629	1826.7547	3007.5767	3088.1191
	H	-1.601797	1.239122	-0.019951	3132.2827	3134.3757	3231.1133
	H	-1.854869	0.089046	-1.358585			
	H	-2.857497	-0.004708	0.099406			
IM_c2	N	1.509734	-0.865096	-0.334679	82.4453	217.7098	283.5669
	N	0.676975	-0.016011	0.041759	430.1076	526.8379	669.9611
	O	0.861510	1.218445	0.093440	772.0407	810.8187	988.3157
	C	-0.668273	-0.547145	0.475683	1100.6871	1136.9015	1271.4299
	H	-0.641390	-1.630217	0.341578	1294.7222	1363.0900	1405.3806
	H	-0.725072	-0.311749	1.541318	1470.1218	1484.8893	1505.0439
	C	-1.776328	0.128080	-0.317882	1548.3480	3056.3163	3077.1017
	H	-1.701871	1.211537	-0.215174	3125.1991	3136.7431	3156.9509
	H	-1.717555	-0.133842	-1.377689			
	H	-2.745550	-0.201153	0.066076			
TS_c2-1	N	1.898525	-0.611052	-0.000171	-1279.0731	153.8423	250.0014
	N	0.864703	-0.040141	-0.000051	391.7427	411.0871	501.0156
	O	0.570555	1.220701	-0.000024	554.2339	662.3818	815.9369
	C	-1.036123	-0.948626	0.000092	909.4474	989.2639	1041.2720
	H	-0.844236	-1.498567	-0.914543	1119.5648	1221.6955	1288.0586
	H	-0.844168	-1.498527	0.914738	1318.4847	1462.8776	1545.2282
	C	-1.783496	0.236774	0.000103	1612.4249	1794.8699	3110.3104
	H	-0.707824	1.026681	0.000195	3160.8815	3191.7944	3250.0273
	H	-2.296511	0.517161	-0.917729			
	H	-2.296587	0.517109	0.917910			
TS_c3	N	-2.157755	0.649071	0.215255	-676.2840	15.3850	131.8743

	N	-1.493367	-0.283607	0.095035	180.0655	200.9977	485.4484
	O	-0.399039	-0.817620	-0.159981	519.8286	655.7254	824.7626
	C	1.131331	0.397324	-0.596603	857.0999	1013.6073	1067.1721
	H	0.592273	1.336237	-0.516564	1093.8088	1215.3781	1398.3613
	H	1.280428	0.032937	-1.606828	1473.6051	1475.7177	1487.0657
	C	2.139204	0.053526	0.444059	2043.6029	2988.8263	3073.4403
	H	2.401560	-1.008256	0.414509	3117.8237	3145.6096	3242.7275
	H	3.069870	0.620328	0.283033			
	H	1.782821	0.296365	1.448937			
CH_3CH_2O							
	C	-1.189329	-0.194956	-0.000095	198.2244	356.2026	434.5181
	C	0.183551	0.478267	-0.003477	863.2109	890.7287	1079.9452
	O	1.254796	-0.364996	-0.004793	1090.3405	1235.1021	1343.5187
	H	-1.989917	0.551150	0.039246	1380.9671	1401.7968	1485.7818
	H	-1.287377	-0.858520	0.863659	1495.8867	2876.7410	2911.0163
	H	-1.322000	-0.792619	-0.906718	3039.3340	3112.0558	3121.9508
	H	0.284192	1.204295	-0.835309			
	H	0.311404	1.115794	0.898898			
TS_c4	N	-0.688237	-1.050081	0.085436	-1899.518800	10.685700	80.840000
	N	-1.634905	-0.355209	-0.042541	187.068000	304.003400	421.787100
	O	-2.099664	0.760118	-0.124609	517.749500	673.053500	772.631700
	C	2.580864	-0.050471	-0.263462	827.840500	855.829500	1061.947500
	H	2.793128	0.068804	-1.320351	1196.512800	1241.753500	1272.111900
	H	3.217779	-0.733038	0.288477	1309.594700	1340.281200	1463.810300
	C	1.456432	0.523892	0.319713	1555.451900	1966.139300	3095.128600
	H	1.412532	0.575927	1.407849	3156.291400	3175.117300	3250.766100
	H	0.989296	1.369797	-0.184057			
	H	0.422803	-0.365928	0.167189			
TS_c5	N	-1.927428	0.984578	0.154889	-1917.971900	37.118300	84.208200
	N	-1.711732	-0.110530	-0.147604	159.449400	332.969900	387.062000
	O	-0.785517	-0.989352	-0.232106	445.517000	661.766900	786.612200
	C	2.295774	0.456661	-0.410232	815.586600	883.411900	968.217100
	H	2.209020	1.524293	-0.581375	1099.066700	1220.594700	1232.593600
	H	2.877940	-0.106809	-1.131584	1333.015300	1396.771800	1462.094200
	C	1.567331	-0.180859	0.595514	1551.991900	1955.385700	3085.645400
	H	1.884338	-1.182917	0.889023	3155.322800	3165.101100	3250.049800
	H	1.220377	0.430104	1.429423			
	H	0.387957	-0.522998	0.088667			
TS_c6	N	1.374615	1.317330	-0.000042	-1841.251800	29.115300	91.435000
	N	1.118380	0.151544	-0.000014	223.592800	255.406700	383.833700
	O	1.631591	-0.979055	0.000073	491.642600	702.150700	809.024800
	C	-2.337191	0.367547	0.000087	901.479800	932.223800	1078.251300
	H	-2.686559	0.817415	-0.923301	1191.210200	1231.297000	1240.247800
	H	-2.686352	0.817251	0.923635	1345.476300	1367.220600	1466.932500

	C	-1.422633	-0.651065	-0.000106	1594.289300	1765.564100	3114.007700
	H	-1.212860	-1.198641	0.917258	3156.434300	3196.497400	3250.736800
	H	-1.213004	-1.198425	-0.917630			
	H	-0.145973	0.013828	-0.000038			
IM_c6	N	2.123378	-0.882549	-0.000332	49.565700	88.338700	107.559600
	N	1.138722	-0.121261	-0.000132	129.973600	155.182800	244.229700
	O	1.092770	1.126112	0.000033	569.963000	823.657600	976.633900
	C	-2.076011	-0.747071	0.000129	1002.865300	1025.985800	1068.909600
	H	-2.175519	-1.312212	0.922520	1236.767200	1263.886600	1380.850600
	H	-2.175823	-1.311993	-0.922363	1435.659300	1474.238300	1548.071800
	C	-1.892045	0.573835	0.000257	1676.641100	2975.748100	3138.895000
	H	-1.809733	1.143609	-0.919188	3163.543800	3214.289100	3249.106300
	H	-1.809425	1.143389	0.919810			
	H	0.201979	-0.605598	-0.000110			
TS_c6-1	N	2.132173	-0.868607	-0.000003	-1679.545200	25.272400	88.463600
	N	1.232706	-0.131609	0.000000	108.777300	139.525800	152.338500
	O	0.978154	1.233631	0.000003	266.054900	547.930100	684.484600
	C	-1.868445	-0.852900	0.000004	793.201300	826.496000	991.662700
	H	-1.791637	-1.420812	0.922151	1012.928700	1068.257300	1238.556000
	H	-1.791632	-1.420824	-0.922136	1382.953300	1475.031200	1668.430100
	C	-2.059935	0.467681	-0.000005	1756.890700	1924.811100	3145.428100
	H	-2.146449	1.034395	-0.921538	3159.136600	3221.202900	3248.695100
	H	-2.146454	1.034406	0.921520			
	H	0.067068	0.216611	0.000002			
TS_c6-2	N	-0.996792	1.261053	-0.000112	-2132.520000	28.242200	83.479600
	N	-1.210961	0.039689	-0.000038	108.757000	139.284200	161.580600
	O	-2.115422	-0.778890	-0.000007	264.227300	663.222400	682.620700
	C	2.165279	0.451958	0.000013	826.170900	991.001800	1013.130800
	H	2.295309	1.010335	0.921743	1070.015500	1238.105100	1270.223700
	H	2.295195	1.010171	-0.921832	1382.131600	1474.634800	1658.340700
	C	1.877616	-0.851192	0.000114	1701.752200	1940.794400	3144.982800
	H	1.759448	-1.412230	-0.921839	3157.866000	3220.530300	3247.479400
	H	1.759571	-1.412106	0.922158			
	H	0.010747	0.325162	0.000107			

Table S2. Optimized coordinates (Å) and unscaled frequencies (in cm^{-1}) of all stationary points on the initial reaction potential energy surfaces of N_2O + C_2H_4/C_2H_5 optimized by the M06-2X(D3)/def2-TZVP method.

Species	Optimized coordinates				Unscaled frequencies (cm^{-1})		
N_2O	N	0.000000	0.000000	-1.185951	652.5039	652.5039	1367.2434
	N	0.000000	0.000000	-0.075216	2427.8862		
	O	0.000000	0.000000	1.103521			
C_2H_4	C	0.661052	0.000000	0.000076	829.7317	990.6504	1004.5407
	H	1.228323	0.922395	-0.000144	1068.3138	1243.3910	1388.0368
	H	1.228325	-0.922394	-0.000144	1473.8825	1718.1155	3164.2760
	C	-0.661066	0.000000	-0.000045	3179.6615	3240.4573	3266.4821
	H	-1.228285	-0.922428	0.000052			
	H	-1.228283	0.922429	0.000052			
TS_b1	N	0.732040	1.155256	0.000120	-577.3305	176.2383	331.7060
	N	1.205598	0.103691	-0.000070	496.2169	560.8513	705.1026
	O	0.817107	-1.054176	-0.000032	730.6647	845.0825	1012.1628
	C	-1.227904	0.668557	-0.000102	1054.9342	1055.3726	1243.5921
	H	-1.440919	1.201471	-0.916430	1258.4943	1326.8106	1476.8227
	H	-1.440972	1.201741	0.916072	1577.5731	2019.3616	3180.6210
	C	-1.195634	-0.710700	0.000093	3190.8799	3259.8326	3283.9504
	H	-1.338576	-1.264680	0.916909			
	H	-1.338627	-1.264889	-0.916598			
IM_b1	N	0.969611	0.747901	0.012252	8.4800	525.8594	772.4883
	N	1.144976	-0.450708	0.005226	800.2628	837.5387	932.9778
	O	-0.040481	-1.183666	-0.017961	979.6605	1003.2195	1058.6361
	C	-0.465070	1.091517	-0.013995	1120.6824	1202.3247	1255.5504
	H	-0.654057	1.667757	-0.918486	1324.6501	1363.9970	1495.8423
	H	-0.681155	1.721633	0.846504	1537.9036	1738.7604	3098.3207
	C	-1.144380	-0.273477	0.016429	3111.4862	3142.6062	3162.4619
	H	-1.711738	-0.448106	0.929556			
	H	-1.774607	-0.460551	-0.850842			
TS_b1-1	N	1.173966	0.060914	0.000024	-446.3951	94.3639	298.8911
	N	1.122360	-1.052680	-0.000027	388.4906	573.7836	631.2685
	O	-1.084440	-0.925495	0.000026	649.6019	986.9860	999.2373
	C	0.398197	1.202938	0.000001	1086.9608	1179.6698	1238.6192
	H	0.571208	1.776769	-0.905737	1252.3443	1407.8517	1468.9882
	H	0.571148	1.776752	0.905761	1568.0113	2274.9685	2938.4886
	C	-1.267885	0.329038	-0.000021	2978.8573	3138.1139	3220.8611
	H	-1.661510	0.800503	0.915661			
	H	-1.661481	0.800438	-0.915749			
IM_b1-1	N	-1.249033	-0.170194	0.000139	32.4701	109.7392	131.3898
	N	-1.216260	-1.288811	0.001319	172.6623	182.7614	299.2763
	O	1.721962	-0.658831	-0.002743	443.4826	475.8262	612.8952
	C	-1.226754	1.128579	-0.001298	1132.5416	1189.0639	1219.0156

	H	-1.339676	1.618488	0.949505	1271.7730	1444.8620	1538.2923
	H	-1.337058	1.616311	-0.953504	1852.8915	2278.9640	2948.8456
	C	1.691111	0.538501	0.002314	3017.7394	3224.3512	3352.5328
	H	1.687004	1.127215	-0.931452			
	H	1.684952	1.119191	0.941096			
CH_2N_2	N	-0.157188	-0.000071	0.000406	445.6071	474.3419	612.1916
	N	-1.281125	0.000026	-0.000219	1127.8903	1234.2511	1450.3269
	C	1.134231	0.000015	-0.000203	2252.9214	3231.5798	3360.9446
	H	1.631565	-0.952856	-0.000043			
	H	1.631239	0.953079	-0.000042			
CH_2O	O	-0.670163	0.000167	-0.000013	1214.9755	1277.0377	1542.1913
	C	0.524888	0.000040	0.000055	1873.3674	2944.2384	3017.1535
	H	1.104654	-0.939930	-0.000110			
	H	1.107328	0.938353	-0.000110			
TS_b1-2	N	1.334687	0.423666	-0.088409	-668.6470	260.4831	315.0517
	N	1.353529	-0.687889	-0.052404	374.2706	526.6490	538.7373
	O	-0.781521	-1.134537	0.232558	620.7269	891.8796	979.4213
	C	-0.334678	1.163603	0.182235	1033.9110	1121.9565	1186.3294
	H	-0.381297	2.104341	-0.359901	1309.4406	1340.2410	1446.9840
	H	-0.203940	1.244520	1.256934	1477.2376	2245.8540	2536.3732
	C	-1.107525	0.003217	-0.287189	2969.8727	3138.0056	3243.4792
	H	-2.006207	0.523735	0.226400			
	H	-1.320684	0.052341	-1.368485			
IM_b1-2	N	-1.816651	0.479246	0.286594	28.3223	33.2582	44.5649
	N	-2.576881	-0.147100	-0.170391	69.8656	82.5535	164.2570
	O	0.801452	-1.241643	-0.223589	514.7816	774.1134	901.5812
	C	1.511342	1.041209	-0.192778	1138.8767	1145.5790	1379.9048
	H	1.121150	1.709783	0.578040	1432.5100	1460.8094	1473.9019
	H	0.938139	1.154626	-1.109621	1867.6851	2529.2590	2945.7933
	C	1.439277	-0.371937	0.301052	3064.0483	3130.0363	3181.1073
	H	2.554922	1.316633	-0.359160			
	H	2.025182	-0.588558	1.216378			
CH_3CHO	O	1.224557	-0.277407	-0.000001	159.2397	513.9652	775.7094
	C	-1.162720	-0.147439	-0.000003	901.0397	1138.4973	1146.1890
	H	-1.696342	0.223876	0.877679	1379.6791	1431.6955	1463.6708
	H	-1.147248	-1.234454	-0.000028	1473.1026	1871.1278	2946.0780
	C	0.234145	0.397872	0.000000	3064.7813	3129.2585	3183.1445
	H	-1.696381	0.223937	-0.877631			
	H	0.314971	1.503299	0.000004			
N_2	N	0.000000	0.000000	0.543023	2529.4964		
	N	0.000000	0.000000	-0.543023			
TS_b1-3	N	0.125578	-1.185277	-0.135213	-2696.4303	275.2340	345.0182
	N	1.122559	-0.466263	-0.013051	552.1051	730.1613	776.2755

	O	0.822500	0.844326	0.141047	882.0866	907.4843	966.6505
	C	-1.049120	-0.330432	-0.079115	992.0468	1048.2908	1084.2403
	H	-1.541761	-0.703707	1.291074	1147.3523	1255.5514	1316.9063
	H	-1.962211	-0.650357	-0.561395	1392.2274	1506.1819	1646.9819
	C	-0.568615	1.019917	-0.090273	2051.2103	3222.5106	3255.8176
	H	-0.833154	1.738114	-0.849407			
	H	-1.273418	0.285220	1.045532			
$C_2H_2N_2O$	N	0.893842	0.745491	0.000125	641.2999	719.7001	773.3360
	N	1.062632	-0.489852	-0.000097	828.8941	914.4080	962.3937
	O	-0.185430	-1.105419	0.000001	1010.5567	1111.8319	1161.1243
	C	-0.449742	1.044073	-0.000083	1177.3401	1396.6693	1486.9810
	H	-0.814599	2.053907	-0.000206	1599.5662	3312.5935	3336.4375
	C	-1.094790	-0.139008	0.000099			
	H	-2.130090	-0.430418	-0.000093			
H_2	H	0.000000	0.000000	0.370096	4476.4205		
	H	0.000000	0.000000	-0.370096			
TS_b1-4	N	1.117544	0.263552	-0.107079	-1536.875600	121.198100	535.332600
	N	0.805686	-0.954053	-0.033938	653.393300	776.290500	812.220700
	O	-0.616179	-0.998678	0.053696	940.079000	968.424100	1029.982400
	C	0.078559	1.147748	0.033782	1061.882700	1114.424300	1158.001100
	H	0.239531	2.178784	-0.232898	1195.048300	1369.554600	1396.544300
	H	1.368067	0.911516	0.807898	1504.944400	1543.506100	2381.776800
	C	-1.171848	0.319001	-0.014988	2993.832200	3074.979000	3287.437500
	H	-1.852514	0.481631	0.823374			
	H	-1.728525	0.450507	-0.953581			
IM_b1-3	N	1.044949	0.315582	0.010267	138.445800	451.497700	594.611600
	N	0.800834	-0.949125	0.060124	778.304500	872.698600	877.254600
	O	-0.596808	-1.000431	-0.101790	931.699000	990.223500	1047.265800
	C	0.044413	1.163477	-0.077983	1085.550700	1155.436800	1190.044500
	H	0.183109	2.227085	-0.071421	1313.083600	1374.132000	1461.311400
	H	2.023618	0.573014	0.039107	1547.861200	1596.234500	2938.310400
	C	-1.172101	0.303618	0.074737	3074.670400	3333.039200	3606.271200
	H	-1.650030	0.389902	1.065265			
	H	-1.936587	0.445672	-0.691887			
TS_b1-5	N	-0.595879	0.892461	0.131974	-758.705000	184.730500	551.309300
	N	-1.192130	-0.231341	-0.050644	608.770700	700.979000	783.642000
	O	-0.347173	-1.187638	-0.105475	925.146600	1002.892800	1040.000700
	C	0.782548	0.935864	-0.020538	1075.094500	1177.731900	1224.241400
	H	1.107778	1.596955	-0.812897	1275.740100	1375.494200	1394.394400
	H	-1.208226	1.696192	0.132195	1510.225300	1552.552600	3107.003900
	C	1.227525	-0.405979	0.099200	3167.793600	3205.378100	3614.358600
	H	1.990768	-0.745236	-0.598456			
	H	1.342685	-0.853961	1.081672			
IM_b1-4	N	0.241679	0.941873	-0.000006	162.730200	274.524100	289.523400

	N	1.365157	0.222869	-0.000003	465.148500	622.682200	732.434200
	O	1.211005	-0.968903	0.000009	871.401700	950.670300	955.001000
	C	-1.089703	0.514412	0.000008	1017.901300	1098.226900	1217.920200
	H	-1.763932	1.362027	0.000026	1369.045000	1443.261600	1485.005400
	H	0.432678	1.930075	-0.000011	1686.626500	1721.342700	3198.081200
	C	-1.575377	-0.723410	-0.000007	3212.844800	3329.438400	3665.577700
	H	-2.650917	-0.833159	0.000017			
	H	-0.963238	-1.606932	-0.000037			
C_2H_3	C	0.704782	-0.147233	0.000004	732.538500	868.948300	949.279100
	H	1.584762	0.477067	0.000029	1065.746800	1399.554100	1679.582700
	C	-0.584953	0.030824	-0.000006	3099.348300	3187.632300	3262.775100
	H	-1.026481	1.026853	0.000015			
	H	-1.277258	-0.805470	-0.000034			
HN_2O	N	1.074429	-0.243892	0.000006	671.791800	799.249700	1297.000500
	N	-0.026564	0.301839	0.000001	1414.919200	1784.301600	3473.532000
	O	-1.140208	-0.111688	-0.000007			
	H	1.786612	0.487882	0.000012			
TS_b2	N	-0.365980	-1.033016	-0.048888	-1109.906500	144.652100	252.002500
	N	-1.336012	-0.366346	-0.171325	368.201600	551.249500	646.633600
	O	-1.404515	0.866899	-0.007526	696.958800	909.021100	1012.495100
	C	0.923537	0.067955	0.515192	1076.213100	1155.705100	1239.594900
	H	1.121016	-0.175129	1.552909	1329.182600	1363.177900	1426.705500
	H	-0.016624	0.864822	0.346535	1599.855200	1690.096700	1772.585200
	C	1.955186	0.205538	-0.332985	3159.997000	3195.102000	3249.963900
	H	1.788439	0.409584	-1.384372			
	H	2.984896	0.120102	-0.006624			
IM_b2	N	-0.198547	-0.989394	-0.150531	82.895000	284.307600	327.876600
	N	-1.268562	-0.408856	-0.253031	550.496900	630.891000	666.973700
	O	-1.355662	0.891102	0.170741	836.219200	904.624000	964.753200
	C	0.961113	-0.367760	0.395941	991.895300	1018.857100	1102.942400
	H	1.216195	-0.736012	1.383741	1313.059000	1407.186800	1437.059600
	H	-0.476662	1.191519	0.464257	1701.546500	1713.718600	3180.201800
	C	1.741611	0.467093	-0.274392	3196.573600	3277.219600	3673.659300
	H	1.493017	0.787843	-1.278274			
	H	2.666164	0.819594	0.159985			
TS_b2-1	N	-0.308268	-1.054731	-0.008164	-1394.261500	193.547500	288.201600
	N	0.792249	-1.206465	0.023894	313.456300	417.778700	493.449400
	O	1.554005	0.780091	-0.113272	514.786000	546.451700	708.254300
	C	-1.395984	-0.113576	-0.004023	729.928900	764.188400	981.571400
	H	-2.359139	-0.598206	-0.018038	1098.096000	1325.621700	1392.603200
	H	2.133784	0.898373	0.644384	1490.289300	1673.309300	2255.498800
	C	-0.969105	1.143752	0.021458	3178.422100	3262.287800	3890.683400
	H	0.341696	1.202723	0.021684			
	H	-1.745720	1.903689	0.043416			

IM_b2-1	N	-0.578028	0.844647	-0.000215	29.719400	87.856600	141.287400
	N	0.068599	1.724700	-0.000162	172.344600	281.433300	398.970500
	O	1.974812	-0.367004	0.001270	473.492100	595.316600	684.997000
	C	-1.383535	-0.328152	0.000029	693.373500	718.389800	994.864200
	H	-2.426556	-0.027887	0.000186	1083.904000	1310.240900	1434.689900
	H	2.781290	-0.885488	-0.007752	1639.708200	2447.819100	3099.496500
	C	-0.687239	-1.474321	-0.000261	3172.100900	3363.946100	3934.547700
	H	1.225651	-1.006648	0.000885			
	H	-1.388235	-2.314539	0.000548			
TS_b2-2	N	-0.500470	0.962725	0.000011	-518.543700	79.274100	121.735600
	N	0.276229	1.724251	-0.000194	134.680800	150.910900	245.860300
	O	1.947097	-0.530732	0.000211	280.674700	461.407700	622.431000
	C	-1.484483	-0.293013	0.000210	659.540400	696.184700	907.382600
	H	-2.458401	0.172442	0.000690	957.381200	1293.077600	1520.096300
	H	2.682547	-1.145788	-0.000467	1643.147600	2476.753400	3150.607000
	C	-0.827033	-1.413071	-0.000304	3244.214300	3410.818600	3935.782400
	H	1.129044	-1.075697	0.000136			
	H	-1.491185	-2.277433	-0.000198			
H_2O	O	0.000000	0.116193	0.000000	1608.047700	3864.884200	3971.639600
	H	0.764312	-0.464773	0.000000			
	H	-0.764312	-0.464773	0.000000			
N_2	N	0.000000	0.000000	0.543020	2529.542400		
	N	0.000000	0.000000	-0.543020			
C_2H_2	C	0.000000	0.000000	0.597251	694.648000	694.648000	790.108300
	H	0.000000	0.000000	1.661158	790.108300	2106.322100	3433.974300
	C	0.000000	0.000000	-0.597251	3537.816900		
	H	0.000000	0.000000	-1.661158			

Species	**Optimized coordinates**				**Unscaled frequencies (cm^{-1})**		
N_2O	N	0.000000	0.000000	-1.185951	652.5039	652.5039	1367.2434
	N	0.000000	0.000000	-0.075216	2427.8862		
	O	0.000000	0.000000	1.103521			
C_2H_5	C	-0.011744	-0.691900	0.000000	121.9472	440.8499	810.2145
	H	1.007719	-1.100672	0.000000	982.2761	1082.6746	1195.9859
	H	-0.508640	-1.094241	-0.883967	1403.3421	1470.9709	1486.7657
	H	-0.508640	-1.094241	0.883967	1487.3542	3005.4429	3087.3251
	C	-0.011744	0.792156	0.000000	3131.1890	3177.1009	3278.6589
	H	0.075243	1.343810	-0.923922			
	H	0.075243	1.343810	0.923922			
IM_c0	N	1.409573	-1.176328	-0.039453	20.0774	70.2882	79.4778
	N	1.366206	-0.066823	-0.028742	110.0071	116.8756	192.1898
	O	1.318030	1.110961	-0.018601	500.9722	641.0203	651.4218
	C	-1.603926	-0.024983	0.813619	811.2109	984.7202	1079.0347
	H	-1.734898	-0.934285	1.381823	1198.9301	1366.4329	1402.9451

	H	-1.488757	0.897478	1.363290	1471.8216	1487.5896	1490.7315
	C	-1.875188	-0.002616	-0.646531	2428.2553	3010.6761	3085.4935
	H	-1.342827	0.812382	-1.140266	3129.6484	3174.3601	3276.3577
	H	-1.591462	-0.942406	-1.123268			
	H	-2.942066	0.146794	-0.857934			
TS_c1	N	0.478425	1.019850	-0.376214	-680.4879	43.9876	134.0671
	N	1.268065	0.218391	-0.182330	191.9928	222.1825	542.4402
	O	1.757336	-0.785062	0.247666	619.6929	663.7878	830.9916
	C	-1.264432	0.477614	0.534268	866.2200	1038.3069	1087.0934
	H	-1.775344	1.425297	0.434541	1220.1411	1270.1296	1405.2460
	H	-0.877381	0.267771	1.524506	1477.8703	1487.8571	1491.7347
	C	-1.738060	-0.670396	-0.289232	2088.7964	3034.8207	3104.4588
	H	-1.032585	-1.501562	-0.257292	3143.0448	3152.9935	3251.8449
	H	-2.697289	-1.045246	0.085085			
	H	-1.886561	-0.376766	-1.328572			
IM_c1	N	0.190294	-0.084802	-0.524625	54.3094	226.2024	302.0381
	N	1.123165	0.039049	0.252978	366.1066	439.7685	647.7061
	O	2.232266	-0.407744	0.293185	808.1597	933.5367	1063.7134
	C	-1.026845	0.655597	-0.165125	1119.7666	1172.0398	1298.1774
	H	-1.276978	1.271705	-1.029296	1373.2972	1413.0228	1437.6925
	H	-0.836094	1.311927	0.685580	1491.7921	1493.6024	1509.7996
	C	-2.152548	-0.321376	0.128643	1756.5013	3074.7403	3077.6560
	H	-1.916963	-0.926819	1.003634	3124.9099	3155.2355	3157.8154
	H	-3.078315	0.220420	0.320582			
	H	-2.308587	-0.988265	-0.718593			
TS_c1-1	N	0.237489	0.908981	0.050581	-1851.6019	89.2444	187.8627
	N	1.365222	0.498626	-0.145836	316.8713	501.0463	596.6095
	O	1.527934	-0.789867	-0.101295	786.0994	849.4540	1008.3880
	C	-0.673441	-0.143600	0.441307	1064.0456	1066.7623	1133.8763
	H	-0.714107	-0.250964	1.526107	1157.2315	1237.5415	1357.7028
	H	0.299830	-1.028811	0.104966	1407.9151	1483.3585	1486.4760
	C	-1.995300	-0.155199	-0.254395	1667.1844	1821.2167	3056.5733
	H	-1.871038	-0.136642	-1.336022	3115.1660	3127.8374	3162.0127
	H	-2.559706	-1.044262	0.025358			
	H	-2.584978	0.719156	0.035256			
IM_c1-1	N	-0.051178	-0.730940	-0.068977	148.3671	200.5724	263.6414
	N	-1.349142	-0.650161	0.085005	310.7505	442.7169	532.6794
	O	-1.859709	0.606920	-0.054876	731.0913	840.1225	920.6322
	C	0.751702	0.250589	0.181193	1017.4971	1044.9513	1109.5789
	H	0.389172	1.160836	0.662271	1168.8193	1325.7355	1384.9226
	H	-1.228818	1.150628	-0.558141	1411.6398	1466.4929	1476.8665
	C	2.209536	0.118818	-0.075568	1563.5825	3059.0433	3102.4902
	H	2.426152	-0.849872	-0.519279	3113.0553	3175.2200	3688.3386
	H	2.554126	0.908922	-0.746784			

	H	2.771852	0.225387	0.854987			
TS_c1-2	N	-0.034415	-0.377972	0.193429	-396.5038	93.5263	115.2005
	N	-1.075904	-0.836484	0.060575	168.9978	227.6897	311.8864
	O	-2.235761	0.598381	-0.184370	537.7995	574.0646	608.6349
	C	1.017355	0.332010	0.410170	829.4401	924.3877	1041.7386
	H	0.911410	1.091182	1.173895	1125.0331	1216.9818	1411.6639
	H	-2.995827	0.076018	-0.474795	1444.7285	1475.8614	1511.7390
	C	2.294037	0.081706	-0.321900	2029.6226	3061.4200	3117.0561
	H	2.171530	-0.726188	-1.040173	3165.2007	3212.0389	3835.2221
	H	2.607222	0.977484	-0.860882			
	H	3.095621	-0.186652	0.369262			
N_2CHCH_3							
	N	-0.173488	-0.619134	0.050911	83.2955	250.4534	460.1559
	N	-1.035139	-1.141773	-0.458669	588.0337	613.3085	924.5463
	C	0.818892	-0.022533	0.616791	1054.8983	1120.5404	1233.1050
	H	0.690066	0.192122	1.665153	1417.1495	1455.3124	1480.0263
	C	2.045435	0.327842	-0.170084	1519.4741	2220.3438	3057.0966
	H	1.933226	0.008604	-1.205221	3110.5359	3151.0046	3261.2628
	H	2.225234	1.404496	-0.169688			
	H	2.932938	-0.160689	0.236356			
OH	O	0.000000	0.000000	0.108105	3767.5913		
	H	0.000000	0.000000	-0.864842			
TS_c1-3	N	0.353922	1.120272	0.057373	-1355.0435	39.0746	407.3417
	N	1.280235	0.341277	0.045262	509.1576	523.1117	577.9199
	O	1.148442	-0.968106	-0.063860	754.1505	802.3438	894.8193
	C	-1.079923	0.643531	-0.079310	982.7035	1057.3666	1084.5603
	H	-1.375171	1.016814	-1.060227	1120.2611	1171.3798	1276.5379
	H	-1.599360	1.235198	0.673721	1288.2770	1453.0732	1486.0326
	C	-1.312177	-0.815049	0.067606	1593.3303	1708.6632	3091.2496
	H	0.040401	-1.180071	-0.024608	3138.2493	3146.9713	3242.9218
	H	-1.595736	-1.183515	1.046792			
	H	-1.744163	-1.345317	-0.773012			
IM_c1-2	N	0.254850	-1.033003	-0.202933	145.5694	191.3435	278.6059
	N	1.276465	-0.374702	-0.277836	333.6031	479.6539	545.9082
	O	1.290332	0.917960	0.213334	611.9326	714.1532	861.5174
	C	-0.958297	-0.485612	0.432896	942.6944	958.1777	1062.6811
	H	-0.727884	-0.188489	1.462436	1111.9638	1234.1998	1336.0703
	H	-1.647347	-1.333022	0.497368	1377.6019	1455.0583	1487.7361
	C	-1.579704	0.632093	-0.329194	1722.9398	3034.8290	3067.5531
	H	0.382435	1.244068	0.335290	3175.9232	3286.7722	3688.4100
	H	-1.500229	0.652180	-1.406427			
	H	-2.320834	1.256633	0.147832			
TS_c1-4	N	0.518494	-1.112920	0.000007	-652.7180	35.2886	236.4061
	N	1.407379	-0.333414	0.000407	298.6499	352.7052	540.9624

	O	1.228777	1.027820	-0.000320	634.3560	716.0073	761.0387
	C	-1.269831	-0.630259	-0.000327	795.2968	866.0698	1031.8609
	H	-1.461186	-1.193862	0.905117	1082.0474	1224.4764	1257.8834
	H	-1.461109	-1.192934	-0.906374	1404.5375	1458.4796	1519.9330
	C	-1.590486	0.728868	0.000352	1750.5940	3151.3531	3166.6996
	H	0.250997	1.163582	-0.000533	3227.4395	3270.1059	3288.1460
	H	-1.739389	1.267112	-0.926219			
	H	-1.738742	1.266230	0.927517			
C_2H_4	C	-0.661040	0.000000	-0.000063	829.5716	990.9576	1004.7202
	H	-1.228789	-0.922162	0.000152	1068.3147	1243.2076	1388.0138
	H	-1.228788	0.922163	0.000151	1474.1014	1717.9881	3164.0906
	C	0.661131	0.000000	-0.000009	3179.4790	3240.0433	3266.0635
	H	1.228514	0.922337	0.000064			
	H	1.228515	-0.922336	0.000063			
N_2	N	0.000000	0.000000	0.543020	2529.5424		
	N	0.000000	0.000000	-0.543020			
TS_c1-5	N	-0.058483	0.264491	0.526225	-2046.5292	123.1138	262.5946
	N	-1.155536	0.375372	-0.200073	352.6374	462.6557	638.4075
	O	-2.025090	-0.439128	-0.047340	702.8709	803.8968	905.9399
	C	1.195114	0.686554	-0.147892	952.1579	1044.1508	1137.6809
	H	1.744757	1.400596	0.458604	1170.1078	1213.8654	1236.3407
	H	1.003291	1.086743	-1.140539	1298.1721	1441.7799	1509.4123
	C	1.700176	-0.727942	-0.093633	1590.6015	1884.4599	3120.3813
	H	1.576896	-1.333938	-0.982535	3154.0455	3182.6933	3264.5537
	H	2.520646	-0.979087	0.567401			
	H	0.481521	-0.892010	0.641876			
IM_c1-4	N	-0.181846	0.060599	0.329903	61.3435	147.6169	189.6929
	N	-1.203521	0.372597	-0.436655	342.9741	434.1592	490.9766
	O	-2.269164	-0.035760	-0.047219	658.4534	663.9769	825.0190
	C	1.160122	0.460553	-0.040584	1038.5493	1110.7944	1129.1078
	H	1.564554	1.145788	0.708721	1200.0565	1294.0685	1390.8192
	H	1.037736	1.037298	-0.965320	1465.2582	1472.7568	1493.0573
	C	2.061745	-0.703941	-0.226234	1642.6387	3035.0423	3082.1507
	H	1.695136	-1.587051	-0.728422	3184.5175	3297.4489	3507.6405
	H	3.118148	-0.614035	-0.026100			
	H	-0.377618	-0.509897	1.149004			
TS_c1-6	N	0.584296	1.044751	0.108386	-667.3035	109.4120	164.5861
	N	1.335896	0.059825	-0.151032	317.9204	403.7661	566.3429
	O	0.989255	-1.067125	0.121211	707.8634	763.2087	817.3431
	C	-1.304417	0.616605	0.060514	880.0804	1037.6554	1061.3060
	H	-1.496452	1.259811	-0.790316	1243.9453	1249.5983	1273.6847
	H	-1.530317	1.051273	1.024425	1358.4155	1471.4714	1564.3369
	C	-1.414626	-0.747590	-0.097531	1584.4636	3159.1412	3194.9946
	H	0.927785	1.882797	-0.359160	3243.6107	3296.1543	3495.9609

	H	-1.527251	-1.401324	0.753420			
	H	-1.414898	-1.201671	-1.077437			
ON_2H	N	0.544046	1.069915	0.095201	671.3524	792.7503	1294.7372
	N	1.205585	0.065070	-0.155994	1413.6010	1783.5307	3468.5639
	O	1.083028	-1.082313	0.126177			
	H	1.004572	1.867576	-0.345979			
$TS_{c\text{-}roaming}$	N	-1.137031	0.390569	0.354316	-697.0710	178.4817	265.7638
	N	-0.909605	-0.844160	0.134743	322.8891	494.7837	594.9403
	O	0.224570	-1.117312	-0.337993	754.6165	808.1199	888.3144
	C	-0.312848	1.197998	-0.317865	906.2334	1016.2311	1144.5406
	H	-0.277274	2.233409	-0.004002	1229.7813	1237.0229	1277.9443
	H	-0.056516	0.971944	-1.347513	1321.2263	1445.6910	1488.5487
	C	1.543687	0.174124	0.242775	1518.9779	3092.7727	3139.3260
	H	2.221817	-0.484786	-0.284775	3198.5499	3249.8700	3256.0093
	H	1.817116	1.212818	0.071042			
	H	1.439707	-0.052481	1.296325			
$IM_c1\text{-}4$	N	-1.317974	-0.607357	-0.016217	66.1211	132.8693	182.8257
	N	-0.028659	-0.782522	0.026819	288.7780	451.6321	635.3218
	O	0.657783	0.392507	-0.052268	695.6892	940.5923	975.8294
	C	-1.854446	0.578859	0.016262	1058.1873	1119.8253	1184.0763
	H	-2.932209	0.620163	-0.055241	1225.6853	1251.5872	1301.8876
	H	-1.286134	1.493665	0.130025	1473.6129	1490.9924	1510.0017
	C	2.052142	0.128438	0.014193	1532.6274	3075.3551	3152.4981
	H	2.544318	1.094113	-0.065157	3157.2410	3184.4301	3271.0016
	H	2.300912	-0.346005	0.963000			
	H	2.351106	-0.516618	-0.811428			
$TS_c1\text{-}7$	N	0.584296	1.044751	0.108386	-556.9649	71.2711	127.9971
	N	1.335896	0.059825	-0.151032	137.6796	299.6392	407.9090
	O	0.989255	-1.067125	0.121211	498.6880	568.5400	658.0444
	C	-1.304417	0.616605	0.060514	1064.5475	1120.6994	1166.4179
	H	-1.496452	1.259811	-0.790316	1178.9537	1228.6873	1437.9651
	H	-1.530317	1.051273	1.024425	1464.5723	1467.3268	1514.4116
	C	-1.414626	-0.747590	-0.097531	1960.3143	3011.8534	3078.0990
	H	0.927785	1.882797	-0.359160	3082.4685	3184.9384	3315.8186
	H	-1.527251	-1.401324	0.753420			
	H	-1.414898	-1.201671	-1.077437			
CH_3O	O	-0.981778	-0.571549	0.061449	636.4744	970.8429	1139.7530
	C	-2.218941	-0.012126	-0.094705	1385.5481	1387.6345	1519.6086
	H	-2.418013	0.783830	0.631099	2964.2001	3038.3128	3080.8672
	H	-2.407024	0.320917	-1.121066			
	H	-2.933314	-0.826089	0.116918			
CH_2NN	N	1.177687	0.281342	0.027177	446.2028	473.0865	612.7519
	N	0.234880	0.890366	0.084006	1128.2736	1234.7295	1450.3573
	C	2.260584	-0.419250	-0.037785	2254.7886	3231.7833	3361.1047

	H	3.041334	-0.068597	-0.687841			
	H	2.314077	-1.308082	0.564127			
TS_c2	N	-1.550599	0.883712	-0.299890	-813.8640	54.4130	174.2102
	N	-0.903637	-0.028265	-0.012641	254.9573	332.4335	502.3201
	O	-0.823516	-1.235942	0.147050	608.0501	765.1005	859.5763
	C	0.863281	0.668541	0.450210	909.6753	1076.7425	1122.2182
	H	0.774922	1.710453	0.169888	1182.2262	1227.1266	1393.3431
	H	0.763533	0.477532	1.512826	1469.3760	1480.1282	1495.7609
	C	1.808562	-0.184580	-0.312883	1866.9415	3042.3537	3120.7938
	H	1.633637	-1.237610	-0.099988	3149.5123	3166.7843	3247.0869
	H	1.731552	-0.012949	-1.386086			
	H	2.833082	0.058210	-0.009284			
IM_c2	N	1.475440	-0.873655	-0.340614	83.0012	224.4225	287.9994
	N	0.672466	-0.020702	0.043755	452.9500	558.8813	689.0445
	O	0.869229	1.205460	0.087992	810.9721	828.3427	1007.4327
	C	-0.667244	-0.524842	0.496566	1115.8348	1146.2011	1279.3008
	H	-0.647789	-1.608362	0.400545	1328.0133	1372.3060	1414.7729
	H	-0.720273	-0.243220	1.547014	1479.9251	1488.9259	1507.4601
	C	-1.755336	0.127450	-0.328456	1568.5006	3083.8259	3111.5556
	H	-1.696889	1.209441	-0.237765	3156.7031	3169.2356	3185.7642
	H	-1.662526	-0.148524	-1.378281			
	H	-2.726217	-0.208159	0.033906			
TS_c2-1	N	1.839400	-0.598563	0.000041	-1345.5832	147.3123	317.2318
	N	0.819805	-0.029338	-0.000118	410.1743	425.5503	548.0431
	O	0.544589	1.228978	0.000043	571.2521	689.0192	815.3251
	C	-0.926509	-0.927242	0.000033	978.5074	986.4718	1089.7999
	H	-0.747017	-1.485021	-0.910465	1147.5817	1223.6713	1286.0432
	H	-0.746468	-1.485134	0.910341	1320.1307	1462.2046	1548.6916
	C	-1.766610	0.197019	0.000040	1659.0959	1832.5026	3149.6038
	H	-0.735360	1.044433	-0.000300	3171.3302	3232.7368	3259.1223
	H	-2.291897	0.435271	-0.917324			
	H	-2.291699	0.435276	0.917508			
TS_c3	N	-2.266882	0.494939	-0.000070	-966.1578	32.6724	128.1171
	N	-1.496680	-0.336138	-0.000001	159.9173	223.8879	480.2198
	O	-0.333078	-0.737771	0.000069	522.5347	669.3365	824.7709
	C	1.033195	0.704060	0.000080	864.0006	1035.3269	1081.2786
	H	0.747268	1.208342	0.913785	1128.5343	1215.0290	1403.2295
	H	0.747118	1.208469	-0.913508	1479.6606	1480.2001	1492.6628
	C	2.258996	-0.134287	-0.000075	2143.8097	3036.8205	3108.9974
	H	2.302186	-0.768939	-0.885046	3148.8304	3159.5900	3254.2114
	H	3.157453	0.493026	-0.000160			
	H	2.302384	-0.768982	0.884855			
CH_3CH_2O	C	1.003894	0.868821	0.964099	158.1386	282.3438	435.0925

	C	1.889567	1.948627	1.558704	873.6798	907.6521	1091.6976
	O	3.188616	1.575883	1.772695	1110.1422	1254.5334	1358.6898
	H	-0.013926	1.235532	0.824534	1401.1620	1421.3643	1487.7209
	H	0.973371	0.001345	1.622845	1498.5232	2964.8790	2982.4725
	H	1.393946	0.551745	-0.002734	3071.5831	3147.7933	3153.7437
	H	1.912885	2.853771	0.929235			
	H	1.500747	2.310976	2.525321			
TS_c4	N	-0.893972	-1.117442	-0.286014	-2296.917100	28.876500	75.293400
	N	-1.527722	-0.152417	-0.143129	160.685600	333.415000	411.367200
	O	-1.584937	1.000668	0.193010	546.891500	654.367100	796.330800
	C	2.077218	0.534407	-0.387561	837.868600	905.804400	980.755100
	H	1.814915	1.582982	-0.385315	1201.097400	1231.869300	1295.550100
	H	2.696085	0.178161	-1.198927	1314.064300	1371.361400	1462.064600
	C	1.530242	-0.340102	0.538789	1570.604600	2019.946700	3124.516700
	H	1.989143	-1.318421	0.653482	3179.182300	3208.389300	3278.123200
	H	1.122299	0.079960	1.453484			
	H	0.364148	-0.804843	0.029827			
TS_c5	N	-1.858059	0.990375	0.136035	-2551.722700	38.756600	83.113300
	N	-1.668580	-0.093381	-0.150128	151.299400	327.805800	405.631200
	O	-0.807298	-1.014006	-0.212465	453.783400	669.384000	788.968700
	C	2.254127	0.406756	-0.443736	816.486100	880.076200	968.722300
	H	2.151703	1.445448	-0.725080	1128.863200	1216.524100	1232.364700
	H	2.847606	-0.223122	-1.091363	1341.213300	1380.184500	1463.506700
	C	1.533701	-0.126986	0.623580	1561.826600	2071.192600	3119.590400
	H	1.864699	-1.082633	1.022666	3177.982800	3201.428200	3275.621000
	H	1.172606	0.565254	1.378452			
	H	0.381271	-0.550484	0.134635			
TS_c6	N	1.182893	1.324929	0.000030	-2031.059400	50.471100	56.628000
	N	1.091932	0.160317	-0.000021	215.189700	222.583700	378.988100
	O	1.713905	-0.911153	-0.000018	492.917500	730.493700	817.114200
	C	-2.209763	0.384863	-0.000033	879.783800	965.200900	1078.273900
	H	-2.497471	0.869759	-0.923190	1168.211700	1225.601900	1236.952700
	H	-2.497470	0.869911	0.923043	1290.631900	1359.163000	1470.833900
	C	-1.442277	-0.740445	0.000051	1621.304600	1873.286300	3142.500200
	H	-1.281244	-1.294011	0.919404	3176.013200	3228.708400	3274.219200
	H	-1.281265	-1.294156	-0.919221			
	H	-0.165320	-0.125516	-0.000054			
IM_c6	N	2.117322	-0.890941	-0.000121	43.859700	86.164800	108.840200
	N	1.146552	-0.134062	-0.000105	127.120100	156.340700	220.779800
	O	1.114273	1.106439	-0.000097	619.146300	827.657400	1006.801200
	C	-2.138959	-0.715541	0.000093	1030.575900	1030.684200	1075.721800
	H	-2.274482	-1.266934	0.923063	1242.506100	1298.970500	1384.788800
	H	-2.274837	-1.266690	-0.922970	1432.156200	1476.748000	1564.264200
	C	-1.855108	0.580703	0.000212	1703.123900	3087.929900	3158.609800

	H	-1.729733	1.137949	-0.919465	3178.506900	3236.614200	3266.416600
	H	-1.729377	1.137697	0.919993			
	H	0.211535	-0.609490	-0.000088			
TS_c6-1	N	-2.085060	-0.813201	-0.000078	-1583.703400	19.933100	108.856000
	N	-1.172239	-0.113012	0.000002	118.425600	179.144000	183.652200
	O	-0.882234	1.216411	0.000183	305.733100	582.353500	751.038400
	C	1.736330	-0.865309	-0.000223	833.772200	835.752100	1031.532300
	H	1.635175	-1.422935	-0.923324	1036.118900	1073.110400	1246.166300
	H	1.635163	-1.423400	0.922595	1384.623700	1479.627200	1615.096900
	C	1.990387	0.441144	0.000105	1720.707600	1895.082900	3163.221500
	H	2.095682	0.998060	0.922421	3177.049800	3244.135900	3270.071600
	H	2.095690	0.998521	-0.921931			
	H	0.036951	0.146945	0.000011			
TS_c6-2	N	0.930029	1.252695	0.000190	-1998.616500	8.874400	96.534100
	N	1.155760	0.055758	-0.000011	119.108400	164.626600	165.118500
	O	2.058318	-0.754236	-0.000162	265.541400	678.041500	702.501700
	C	-2.105395	0.428894	0.000027	830.846800	1026.463100	1031.229500
	H	-2.253570	0.976274	-0.922575	1073.199100	1244.501500	1297.944400
	H	-2.253603	0.976186	0.922676	1384.032900	1477.757200	1649.715300
	C	-1.766150	-0.857008	-0.000029	1724.132600	1899.582600	3163.410200
	H	-1.625482	-1.406996	0.922553	3175.730000	3243.269900	3268.065300
	H	-1.625447	-1.406906	-0.922659			
	H	-0.079695	0.304840	0.000059			

Table S3. T_1 diagnostic values of all species on the potential energy surfaces (PESs) of the N_2O + C_2H_3/C_2H_4/C_2H_5 reactions calculated at the CCSD(T)/cc-pVQZ//M06-2X(D3)/def2-TZVP level of theory.

Species	T1 diagnostic	Species	T1 diagnostic	Species	T1 diagnostic
N_2O	0.01915618	**TS_a5**	**0.04933516**	IM_c0	0.01614929
C_2H_3	0.04182453	IM_a5	0.04040237	TS_c1	0.03599627
TS_a1	0.04420484	**TS_a6**	**0.05193176**	IM_c1	0.03687513
IM_a1	**0.05061335**	IM_a6	0.03571127	TS_c1-1	0.03906944
TS_a1-1	**0.04704206**	TS_a6-1	0.03990875	IM_c1-1	0.03155941
IM_a1-1	0.03358879	TS_a6-2	0.04096391	TS_c1-2	0.03564824
TS_a1-2	0.03752522	C_2H_4	0.01091695	N_2CHCH_3	0.01745049
IM_a1-2	0.03127204	TS_b1	0.02119123	TS_c1-3	0.03289613
TS_a1-3	0.0342138	IM_b1	0.01632388	IM_c1-2	0.0167666
IM_a1-3	0.02808948	TS_b1-1	0.01876754	TS_c1-4	0.03530324
TS_a1-4	0.03003087	CH_2N_2	0.01689557	TS_c1-5	0.03679771
CH_2CHO	0.03104509	CH_2O	0.01892862	IM_c1-3	0.01807354
TS_a1-5	0.02177712	TS_b1-2	0.03220549	TS_c1-6	0.03977851
CH_3CO	0.01858745	CH_3CHO	0.01388086	**$TS_{c\text{-roaming}}$**	**0.06110507**
TS_a2	**0.05443636**	TS_b1-3	0.02329083	IM_c1-4	0.03102494
TS_a3	**0.04908823**	$C_2H_2N_2O$	0.01678368	TS_c1-7	0.0357528
trans-IM_a3	0.03547668	H_2	0.00571069	CH_3O	0.01768081
TS_a3-1	0.03990875	TS_b1-4	0.02368553	TS_c2	0.0405248
C_2H_2	0.01317554	IM_b1-3	0.02002277	IM_c2	0.04117226
N_2	0.01278003	TS_b1-5	0.02474235	TS_c2-1	0.03594826
OH	0.00802128	IM_b1-4	0.01658002	TS_c3	0.04073251
cis-IM_a3	0.0344801	TS_b2	0.02818393	CH_3CH_2O	0.0169616
TS_a3-2	0.03674109	IM_b2	0.01585772	TS_c4	0.04356468
IM_a3-1	0.03201844	TS_b2-1	0.02258432	**TS_c5**	**0.04689339**
TS_a3-3	0.04041587	IM_b2-1	0.01511066	**TS_c6**	**0.04827392**
HN_2O	**0.04959993**	TS_b2-2	0.01742973	IM_c6	0.03339764
IM_a04	0.03054269	H_2O	0.0073709	TS_c6-1	0.03756253
TS_a4	**0.04774587**	C_2H_5	0.01091781	TS_c6-2	0.03935072

Table S4. Arrhenius parameters for the rate coefficients of the primary reaction channels of N_2O + $C_2H_3/C_2H_4/C_2H_5$ initial reaction with Ar gas as a bath gas, at 300-3000 K and 1-100 atm, calculated using the G4 method.[a]

Reaction	Channel	P/atm	T/K (300-3000)	*A*	*n*	*E*
$N_2O+C_2H_3$	CH_2CHO+N_2	1	300	6.12E-55	12.264	-2687.1
		10	400	2.93E-26	4.2833	17210
		100	600	2.32E-20	2.6596	21819
	CH_3CO+N_2	1	400	6.65E-19	1.3524	5436.5
		10	400	3.11E-07	-1.7956	16575
		100	400	8.24E-02	-3.2299	22790
	$C_2H_2+N_2+OH$	1	300	2.16E-29	4.7600	31629
		10	300	4.16E-29	4.6811	31829
		100	300	1.03E-27	4.2980	32954
	$C_2H_2+HN_2O$	1	300	1.93E-40	8.0440	26016
		10	300	8.49E-37	7.0314	28570
		100	300	1.48E-34	6.4212	30511
$N_2O+C_2H_4$	$CH_2N_2+CH_2O$	1	300	3.40E-22	2.5256	27012
		10	300	1.36E-21	2.3599	27489
		100	300	4.75E-20	1.9431	28944
Consider IM_b1-2	CH_3CHO+N_2	1	300	9.67E-39	7.2277	25398
		10	300	2.78E-42	8.0241	24753
		100	300	7.01E-42	7.6625	26330
No-Consider IM_b1-2	CH_3CHO+N_2	1	300	6.01E-22	2.4387	26907
		10	300	2.28E-21	2.2797	27360
		100	300	5.19E-20	1.9108	28601
	$C_2H_2N_2O+H_2$	1	300	1.44E-106	25.597	54483
		10	300	2.16E-106	25.548	54604
		100	300	1.85E-105	25.288	55246
	$C_2H_3+HN_2O$	1	700	1.98E-28	3.8585	63410
		10	500	5.21E-29	4.0173	62925
		100	500	6.54E-28	3.7136	63769
	$H_2O+C_2H_2+N_2$	1	300	4.24E-19	1.8341	54948
		10	300	1.16E-18	1.7616	56864
		100	300	5.11E-22	2.7715	57302
$N_2O+C_2H_5$	N_2CHCH_3+OH	1	300	3.33E-20	1.7412	20837
		10	300	2.26E-16	0.6982	24190
		100	300	1.60E-12	-0.3197	28533
	$C_2H_4+N_2+OH$	1	300	9.70E-30	4.7207	23171
		10	300	8.79E-30	4.8813	28431
		100	300	6.11E-27	3.9596	25651
	$C_2H_4+ON_2H$	1	300	7.21E-32	5.7226	28996
		10	400	3.61E-02	4.1041	33500

		100	400	1.46E-26	4.2432	32603
	$CH_2N_2+CH_3O$	1	600	2.50E-27	3.7244	53122
		10	400	2.12E-64	13.9400	24607
		100	500	6.95E-36	6.0768	46392
	$C_2H_5O+N_2$	1	300	3.36E-21	2.5867	22532
		10	300	3.36E-21	2.5867	22532
		100	300	3.36E-21	2.5867	22532

a. $k = AT^n\exp(-E/RT)$. The units of *A, T,* and *E* are cm^3 $molecule^{-1}$ s^{-1}, K and cal mol^{-1}, respectively.

Table S5. The Arrhenius parameters of the rate coefficients for the dominant channels of N_2O + C_2H_4/C_2H_5 initial reaction with Ar gas as a bath gas, at 300-2000 K and 1-100 atm, calculated using the CCSD(T)/cc-pVQZ//M06-2X(D3)/def2-TZVP method.[a]

Reaction	Channel	P/atm	T/K -3000)	*A*	*n*	*E*
$N_2O+C_2H_4$	$CH_2N_2+CH_2O$	1	300	2.93E-21	2.2671	28291
		10	300	8.61E-22	2.4155	27949
		100	300	4.94E-19	1.7042	31772
	CH_3CHO+N_2	1	300	5.55E-37	6.7512	27135
		10	300	2.83E-40	7.5275	27513
		100	300	1.31E-41	7.6912	29100
	$C_2H_2N_2O+H_2$	1	300	1.86E-102	24.483	57686
		10	300	2.93E-26	3.4345	115238
		100	300	7.93E-99	23.474	60231
	$C_2H_3+HN_2O$	1	600	9.79E-30	4.2305	62890
		10	400	7.24E-84	19.120	20421
		100	500	3.34E-65	13.960	34304
	$H_2O+C_2H_2+N_2$	1	300	6.02E-21	2.4135	53740
		10	300	2.59E-19	1.9942	55979
		100	300	3.11E-20	2.3154	57576
$N_2O+C_2H_5$	N_2CHCH_3+OH	1	300	2.21E-19	1.5224	21897
		10	300	1.51E-15	0.48019	25309
		100	300	7.43E-12	-0.48987	29645
	$C_2H_4+N_2+OH$	1	300	1.58E-28	4.3562	22611
		10	300	1.42E-27	4.0941	23363
		100	300	1.43E-25	3.5576	25404
	$C_2H_4+ON_2H$	1	300	5.02E-35	6.4953	26589
		10	400	2.49E-29	4.9073	30461
		100	400	2.49E-29	4.9075	30460
	$CH_2N_2+CH_3O$	1	700	2.37E-26	3.3237	58625
		10	600	2.28E-30	4.4231	55318
		100	500	6.49E-43	7.8717	45419
	$C_2H_5O+N_2$	1	300	3.70E-22	2.7588	22638
		10	300	3.70E-22	2.7588	22638

	100	300	3.70E-22	2.7588	22638

[a.] $k = AT^n \exp(-E/RT)$. The units of *A, T,* and *E* are cm^3 $molecule^{-1}$ s^{-1}, K and cal mol^{-1}, respectively.

Table S6. Arrhenius parameters for the rate coefficients of the primary reaction channels of N_2O + C_2H_3/C_2H_5 initial reaction with Ar gas as a bath gas, at 300-3000 K and 1-100 atm, calculated using the CASPT2/cc-pVQZ//B3LYP/6-31G(2df,p) method.[a]

Reaction	Channel	P (atm)	T/K -3000)	*A*	*n*	*E*
$N_2O+C_2H_3$	CH_2CHO+N_2	1	300	1.110E-19	2.4792	27488
		10	300	1.213E-19	2.4686	24933
		100	300	5.479E-22	3.1172	23164
	CH_3CO+N_2	1	325	4.719E-12	-0.4020	22057
		10	300	1.253E-14	0.2384	15006
		100	300	4.723E-12	-0.4021	19462
	$C_2H_2+N_2+OH$	1	300	1.409E-28	4.5694	40681
		10	300	5.058E-30	4.9652	36899
		100	300	1.421E-28	4.5684	38088
	$C_2H_2+HN_2O$	1	300	4.311E-29	4.9616	18964
		10	300	4.437E-28	4.6804	17093
		100	300	4.437E-28	4.6804	17093
$N_2O+C_2H_5$	$C_2H_4+N_2+OH$	1	300	1.491E-41	8.3314	26189
		10	700	1.146E-24	3.6405	38124
		100	700	1.147E-24	3.6405	38124
	$C_2H_4+ON_2H$	1	300	4.181E-32	5.7871	29149
		10	300	4.180E-32	5.7871	29149
		100	300	4.385E-32	5.7813	29164
	$CH_2N_2+CH_3O$	1	400	2.369E-21	2.1257	68781
		10	700	2.789E-22	2.3552	67068
		100	900	6.375E-23	2.5299	66517

[a] $k = AT^n\exp(-E/RT)$. The units of *A, T,* and *E* are cm^3 $molecule^{-1}$ s^{-1}, K and cal mol^{-1}, respectively.

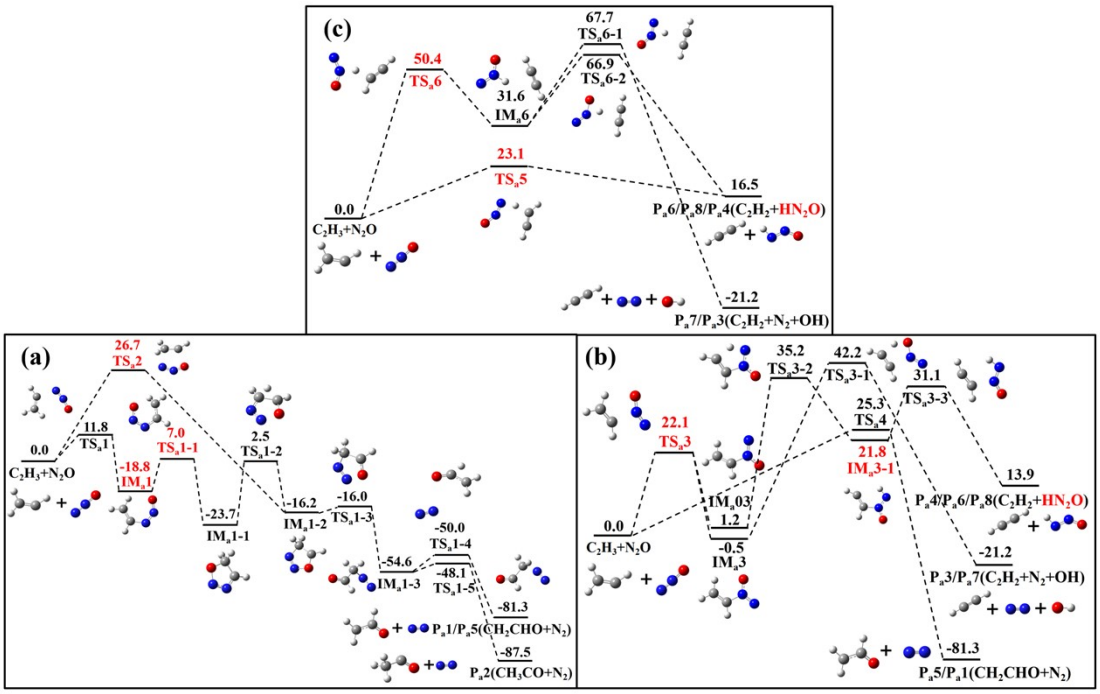

Figure S1. Potential energy surfaces (in kcal mol^{-1}) for the N_2O + C_2H_3 reactions calculated at the CASPT2/cc-pVQZ//B3LYP/6-31G(2df,p) (G4 optimization method) level.

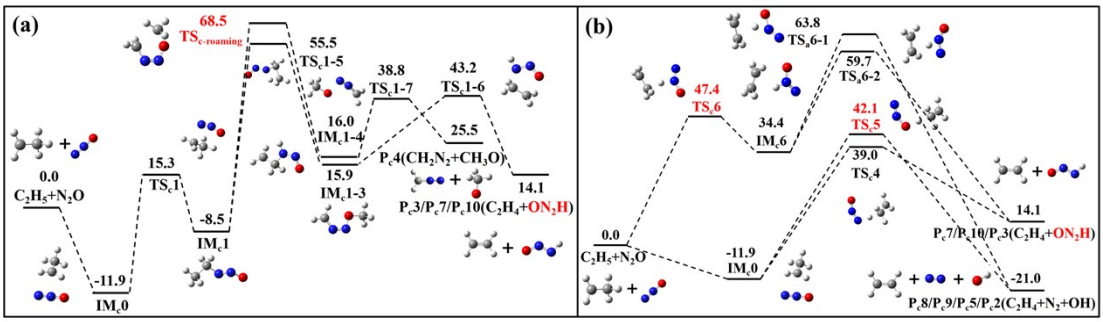

Figure S2. Potential energy surfaces (in kcal mol^{-1}) for the N_2O + C_2H_5 reactions calculated at the CASPT2/cc-pVQZ//B3LYP/6-31G(2df,p) (G4 optimization method) level.

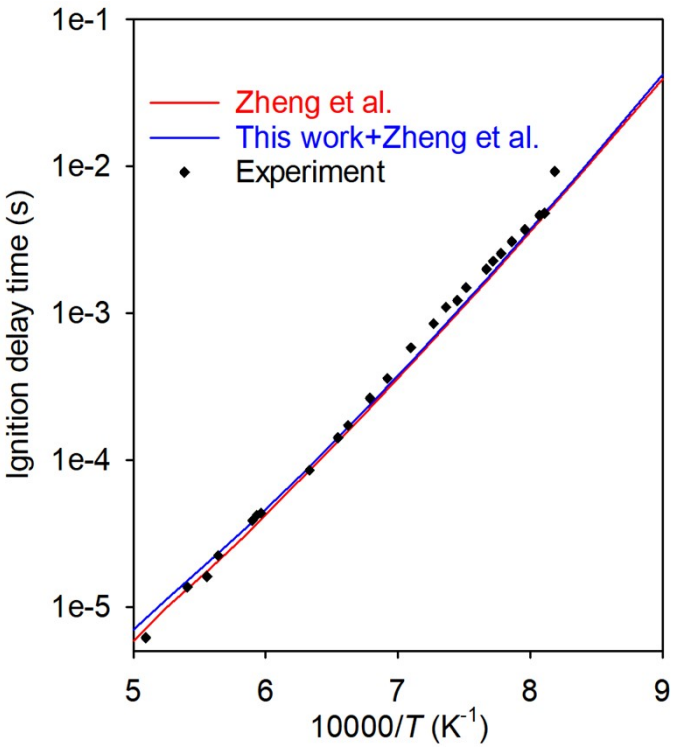

Figure S3. The predicted (lines) [1] and experimental (dots) [2] results for stoichiometric N_2O/C_2H_6 (diluted with N_2) ignition delay times at an equivalence ratio of 0.78 and 4 bar pressure.

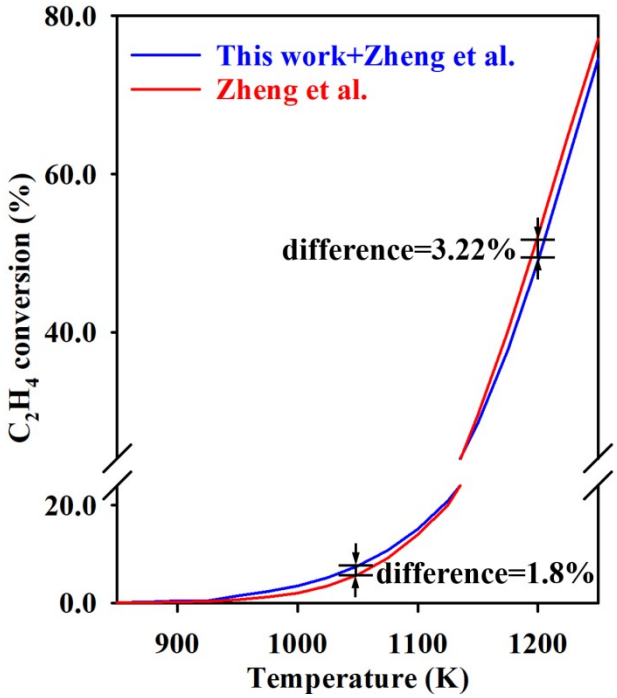

Figure S4. The predicted (lines, using the original model of [1] with and without the $N_2O + C_2H_{3-5}$ reactions of this work) results of fuel conversion rates for a N_2O/C_2H_4/Ar mixture of equivalence ratio 0.5 and at 1 atm pressure**.**

References

[1] D. Zheng, P.-f. Xiong, B.J. Zhong, Chemical Kinetic Model for the Combustion of the Green Propellant of the Nitrous Oxide Fuel Blend, Acta Physico-Chimica Sinica, 35 (2019) 1241-1247

[2] C. Naumann, C. Janzer, U. Riedel. Ethane/Nitrous Oxide Mixtures as a Green Propellant to Substitute Hydrazine : Validation of Reaction Mechanism. (2019) 14-17