HONO, a key sink of Isoprene derived Criegee Intermediates (MACR-oxide and MVK-oxide)

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S1 Details of the methodology used for the electronic structure theory

To estimate energies at CCSD(T)/CBS level of theory, first we calculated the single point energies at CCSD(T)/aug-cc-pVDZ, and CCSD(T)/aug-cc-pVTZ level of theory, and then extrapolated these energies to corresponding CBS limit using the method of Varandas and Pansini. Specifically, for the extrapolation of correlation energies, the following equation is used:

$$\mathrm{CBS(Corr)} = \frac{2.71^3\mathrm{E_{ATZ}} - 1.91^3\mathrm{E_{ADZ}}}{2.71^3 - 1.91^3}$$

Where, E_{ADZ} and E_{ATZ} are correlation energies at CCSD(T)/aug-cc-pVDZ and CCSD(T)/aug-cc-pVTZ level of theory, respectively. For the extrapolation of Hartree-Fock energies, the following equation is used:

$$\mathrm{CBS(HF)} = \frac{2.96^5\mathrm{E_{ATZ}} - 2.08^5\mathrm{E_{ADZ}}}{2.96^5 - 2.08^5}$$

Where, E_{ADZ} and E_{ATZ} are Hartree-Fock energies at CCSD(T)/aug-cc-pVDZ and CCSD(T)/aug-cc-pVTZ level of theory, respectively.

S2 Details of master equation kinetic calulation

In MESMER, the stationary points obtained from ab initio calculations are used to provide molecular energies, rotational constants, and vibrational frequencies. In addition, the input specifies the reaction paths, the collision energy transfer model, bath gas properties, and the thermodynamic conditions, including temperature and pressure. To set the master equation, one needs the microcanonical rate constant.

The microcanonical rate coefficients were calculated using Rice-Ramsperger-Kassel-Marcus (RRKM) theory for reactions involving a tight transition state (forward step). For barrierless association steps, the Inverse Laplace Transformation (ILT) method was used. The energy wells along the PES are divided into energy grains, where each grain couples the reactant, intermediate, and product species to one another via the microcanonical rate coefficients, k(E). The individual grains can be populated or depopulated through exchange with other grains via collisional energy transfer with the bath gas. Collisional energy transfer probabilities were described using the exponential-down model. To incorporate quantum mechanical tunneling effects, tunneling corrections were evaluated using the unsymmetrical Eckart barrier.

The set of coupled differential equations that describe each of the energy grains is known as the energy grained master equation (EGME) and can be described by:

$$\frac{d\mathbf{p}}{dt} = \mathbf{M}\mathbf{p} \tag{1}$$

where p is the population density vector containing the populations of each grain from each well, and M is the transition matrix that describes the population evolution due to collision energy transfer and reaction. The solution to eqn (1) is

$$\mathbf{p}(t) = \mathbf{U}\, e^{\Lambda t}\, \mathbf{U}^{-1}\, \mathbf{p}(0) \tag{2}$$

where p(0) contains the initial conditions for each grain, U is the matrix of eigenvectors obtained from the diagonalization of $\mathbf{M}$, and Λ is the diagonal matrix of corresponding eigenvalues. The smallest eigenvalues are the chemically significant eigenvalues (CSE). After obtaining CSE, MESMER used a approach suggested by the Bartis-Widom to estimate the phenomenological rate coefficients. In Bartis-Widom method, the time evolution of a kinetic system is described by coupled differential equations in which each molecular species is represented by a single population variable. For a scheme with n species, this leads to an $n \times n$ rate coefficient matrix K, such that

$$\frac{d}{dt}\, c = Kc \tag{3}$$

where c is the vector of species concentrations and matrix element K_{ab} is the rate coefficient $k_{b\to a}(T, P)$ for all possible reactions. Diagonalization of this rate matrix yields n eigenvalues and n eigenvectors.

Table S1: Cartesian coordinates and all normal mode frequencies of the optimized geometries calculated at M06-2X/aug-cc-pVTZ level of theory.

Species	Cartesian coordinates (Å)				Frequency (cm^{-1})		
anti-cis-mvk	O	-0.401177	1.372666	-0.000084	136.7768	149.8276	288.4149
	C	-0.442365	0.166334	0.000023	312.1805	344.0118	399.7909
	C	0.80142	-0.664775	-0.000049	414.7725	641.5922	730.7638
	H	0.683314	-1.741807	-0.000407	823.8677	983.6701	1030.6182
	C	-1.743066	-0.592901	0.000064	1049.9283	1053.3066	1058.2071
	H	-1.789434	-1.240491	0.877428	1116.2156	1279.7007	1347.3101
	H	-2.580732	0.097225	-0.000061	1413.0621	1459.5697	1472.3051
	H	-1.78934	-1.24068	-0.877206	1477.548	1599.1162	1685.7664
	C	1.999672	-0.100004	0.000083	3068.5807	3126.9993	3170.5758
	H	2.907455	-0.68717	-0.000121	3183.791	3186.4508	3309.9811
	H	2.084188	0.979673	0.000314			
anti-cis-mvk-oo	C	0.564665	0.094168	-0.000002	90.1509	144.9295	275.3031
	O	0.330771	-1.144513	0.000009	419.4229	464.0813	607.3644
	O	-0.946516	-1.596938	-0.000036	691.4923	791.5919	968.9155
	C	-0.42473	1.143459	-0.00005	1031.4935	1033.9557	1053.81
	C	-1.757435	1.017488	0.00005	1084.0237	1210.0057	1331.8985
	H	-2.363279	1.915338	-0.000019	1389.422	1438.666	1467.5447
	H	-2.23099	0.051472	0.000191	1477.7011	1711.0377	1832.4064
	C	2.015047	0.444234	0.000025	3062.3961	3123.431	3168.0467
	H	2.251182	1.044531	-0.879496	3184.8984	3192.2895	3263.4212
	H	2.251141	1.04456	0.879537			
	H	2.621509	-0.456192	0.000055			
	H	0.011112	2.135807	-0.000195			
anti-cis-mvk-pc	O	-0.826321	-1.855089	-0.175738	65.0304	107.5952	209.7607

	O	-0.545853	-0.941667	0.873313	225.9633	232.9621	268.2626
	C	-0.125409	0.272211	0.365452	299.9067	312.9522	352.0695
	N	1.24735	0.058297	-0.345763	408.3242	448.6822	482.5432
	O	1.761961	-1.032969	-0.266474	586.489	657.8597	702.2359
	H	0.043214	-2.271136	-0.282924	768.8375	850.2887	899.1538
	O	1.717005	1.017887	-0.902113	967.8772	1006.9338	1038.9024
	C	-1.056914	0.933653	-0.61027	1059.228	1060.9774	1130.2766
	H	-0.627271	1.752725	-1.17079	1196.8326	1319.0615	1322.357
	C	0.177435	1.1446	1.573198	1400.6203	1440.0536	1449.6404
	H	-0.750008	1.287259	2.122392	1481.1989	1488.9572	1497.3553
	H	0.911441	0.655813	2.211558	1695.9462	1740.4283	3084.2494
	H	0.554643	2.107508	1.239525	3169.7761	3178.6129	3182.3021
	C	-2.327075	0.592442	-0.723959	3218.7599	3268.9398	3756.9926
	H	-2.981994	1.129623	-1.395188			
	H	-2.744029	-0.23259	-0.162665			
anti-cis-mvk-rc	O	0.3488	1.263104	1.308416	39.9134	50.2759	72.9839
	O	0.85378	-0.022575	1.228295	110.2151	141.8116	153.6829
	C	1.266567	-0.446948	0.119029	180.6036	243.6812	313.8555
	N	-1.739786	-0.455485	-0.215656	337.6009	345.2713	405.7246
	O	-2.038025	0.64925	0.482916	420.4348	634.3324	720.8716
	H	-1.150594	0.953681	0.864393	776.65	819.8691	966.2941
	O	-2.680695	-0.935977	-0.735924	1017.6286	1028.453	1033.0715
	C	1.355613	0.294393	-1.119625	1052.6009	1064.3019	1077.1934
	H	1.696792	-0.315779	-1.946784	1121.0392	1279.7234	1354.8269
	C	1.684167	-1.874338	0.134963	1404.8725	1464.6651	1465.5257
	H	1.656492	-2.272415	1.143922	1476.0608	1580.3384	1624.72
	H	0.990587	-2.43316	-0.49741	1695.7245	1786.8802	2872.2175

	H	2.681748	-1.979073	-0.2901	3067.0203	3133.5908	3179.4221
	C	1.098483	1.58907	-1.329142	3192.4964	3196.2326	3312.4704
	H	1.244845	1.992257	-2.323229			
	H	0.758772	2.239412	-0.542173			
anti-cis-mvk-ts	O	0.679771	-1.511346	-0.988523	-893.6304	76.7103	91.9043
	O	0.706708	-0.122392	-1.289819	134.1419	139.045	163.965
	C	0.689848	0.657416	-0.285557	231.8227	284.2962	299.4349
	N	-1.497475	-0.00116	0.256593	309.767	340.5753	399.5101
	O	-1.548971	-1.240239	-0.105002	480.8458	578.8646	619.2287
	H	-0.458854	-1.499834	-0.550813	699.6967	811.0332	895.3581
	O	-2.482179	0.468308	0.729617	958.6429	1027.1077	1039.6399
	C	1.134534	0.333885	1.066448	1045.925	1053.642	1109.6067
	H	0.815164	1.054673	1.807977	1240.855	1274.4464	1287.4457
	C	0.45743	2.084635	-0.628671	1349.311	1403.8116	1453.8841
	H	1.38129	2.643759	-0.474267	1467.8213	1474.4146	1596.4412
	H	0.122478	2.183155	-1.656122	1682.5459	1710.6823	1856.794
	H	-0.297636	2.478687	0.051633	3072.079	3139.646	3185.3306
	C	1.962074	-0.656379	1.382313	3191.6222	3205.5718	3290.4881
	H	2.32671	-0.744152	2.396717			
	H	2.287242	-1.380157	0.65134			
syn-cis-mvk-ts	O	0.505984	1.9218	-0.685516	-835.3098	39.2651	73.2155
	O	-0.600082	1.032974	-0.710262	117.1197	147.2196	169.0775
	C	-0.791241	0.390708	0.372715	206.6555	246.3766	293.1648
	N	1.232044	-0.817541	0.059279	328.1742	372.2611	452.1282
	O	1.996571	0.033406	-0.542844	490.3277	577.8694	609.7882
	H	1.333947	1.070131	-0.658004	692.2243	817.0893	885.1738
	O	1.679576	-1.90257	0.253705	968.9391	1011.1734	1016.7787

	C	-1.803667	-0.660819	0.303392	1046.7181	1053.1879	1114.3233
	H	-2.140066	-1.049781	1.254297	1242.7373	1283.085	1299.6972
	C	-0.302457	0.864188	1.68842	1349.0766	1408.2809	1442.9576
	H	0.636853	1.394558	1.606598	1466.1502	1484.1675	1572.9569
	H	-1.066683	1.552544	2.066625	1679.5182	1718.3534	1858.3149
	H	-0.224231	0.022136	2.369935	3048.7379	3155.7894	3180.3006
	C	-2.257968	-1.137898	-0.849505	3219.7195	3228.1116	3275.0114
	H	-3.001858	-1.921434	-0.869643			
	H	-1.886663	-0.767317	-1.795559			
syn-cis-mvk-rc	O	-0.157772	-1.74336	-0.826131	31.6261	60.354	73.0739
	O	0.711802	-0.657817	-0.854669	107.2055	142.316	176.6083
	C	1.256167	-0.355181	0.236087	190.3185	240.5069	257.818
	N	-1.769688	0.528662	0.349591	336.3148	361.0506	450.2316
	O	-2.257074	-0.281414	-0.595185	503.5207	617.271	668.0803
	H	-1.500174	-0.942402	-0.755225	776.55	814.9285	953.999
	O	-2.521001	1.382546	0.660112	1018.5199	1030.5125	1041.5695
	C	2.092391	0.839592	0.233671	1047.5146	1061.3248	1096.9875
	H	2.766433	0.947418	1.072019	1122.0578	1273.2078	1344.4279
	C	1.030623	-1.176467	1.435073	1380.9681	1447.1139	1450.9384
	H	-0.027197	-1.089715	1.695599	1493.1998	1571.1258	1610.1143
	H	1.191355	-2.224854	1.181377	1717.3809	1779.5843	2804.9895
	H	1.657161	-0.850787	2.258449	3067.2871	3124.6838	3180.3691
	C	1.989321	1.777129	-0.703248	3193.8112	3220.0146	3275.2428
	H	2.602757	2.666077	-0.668148			
	H	1.278824	1.68355	-1.513725			
syn-cis-mvk-pc.gjf	O	-0.788863	-2.07154	0.022127	45.2066	83.273	179.8715
	O	0.29049	-1.249031	-0.382479	213.3941	227.6438	270.8963

	C	0.260839	-0.043924	0.290178	285.0012	330.6161	380.4802
	N	-0.932115	0.79463	-0.278243	398.7247	465.0447	513.7601
	O	-1.647078	0.274613	-1.102834	581.1367	621.9422	686.4071
	H	-1.468989	-1.793088	-0.611251	775.3653	861.7551	902.3009
	O	-1.062547	1.907351	0.165042	959.6475	1010.1137	1036.2025
	C	1.509266	0.717078	-0.059864	1041.2341	1085.6269	1118.1562
	H	1.496572	1.752234	0.2553	1237.6549	1297.1322	1331.4102
	C	0.040427	-0.150787	1.789128	1403.594	1439.3545	1447.939
	H	-0.929787	-0.585906	2.010735	1481.1822	1486.5796	1497.1772
	H	0.823557	-0.792027	2.188151	1694.2355	1737.7331	3094.3991
	H	0.112863	0.835945	2.237178	3177.5161	3183.5218	3189.9566
	C	2.550637	0.179395	-0.669051	3214.3445	3274.5582	3749.74
	H	3.431092	0.773763	-0.86808			
	H	2.556469	-0.855044	-0.981516			
syn-cis-mvk	O	0.401177	1.372666	-0.000084	58.3401	165.9567	232.8428
	C	0.442365	0.166334	0.000023	268.943	352.0724	443.9275
	C	-0.80142	-0.664775	-0.000049	469.817	610.6626	682.8817
	H	-0.683314	-1.741807	-0.000407	815.4471	962.7073	992.3037
	C	1.743066	-0.592901	0.000064	1021.8332	1027.8437	1051.627
	H	2.580732	0.097225	-0.000061	1115.4606	1285.3273	1342.6484
	H	1.789434	-1.240491	0.877428	1390.7434	1439.0935	1467.9767
	H	1.78934	-1.24068	-0.877206	1481.9333	1605.6122	1720.1933
	C	-1.999672	-0.100004	0.000083	3066.675	3121.6742	3180.8786
	H	-2.907455	-0.68717	-0.000121	3204.7411	3212.6627	3274.3929
	H	-2.084188	0.979673	0.000314			
syn-cis-mvk-oo	C	0.068102	0.320108	-0.000001	90.15	144.9308	275.3033
	O	0.513856	-0.852523	-0.000001	419.4232	464.0828	607.3646

	O	1.860855	-1.067201	0.000001	691.4932	791.5924	968.916
	C	-1.385943	0.469895	0	1031.4957	1033.9553	1053.8101
	C	-2.239192	-0.549277	0.000001	1084.0242	1210.0065	1331.8992
	H	-3.3058	-0.377466	0.000001	1389.4217	1438.6663	1467.5444
	H	-1.890857	-1.573339	0	1477.7015	1711.0381	1832.4051
	C	0.964642	1.497023	0	3062.3969	3123.4333	3168.0468
	H	0.748434	2.108148	-0.87815	3184.8938	3192.2843	3263.4204
	H	0.748441	2.108141	0.878157			
	H	1.998379	1.173596	-0.000005			
	H	-1.741937	1.492218	0			
syn-trans-mvk-pc	O	-1.89048	-1.322301	0.109767	49.2854	68.9411	196.9194
	O	-0.67211	-1.209918	-0.605337	224.0239	236.9837	250.1608
	C	0.18903	-0.340704	0.049612	313.6486	347.57	391.3463
	N	-0.457097	1.092068	-0.014491	441.736	465.6039	470.5555
	O	-1.408911	1.242814	-0.745983	539.1793	629.4498	684.7171
	H	-2.417962	-0.639488	-0.332955	778.7663	868.0814	903.0234
	O	0.055875	1.946951	0.658212	958.0614	1008.4357	1032.7087
	C	1.399323	-0.266874	-0.837776	1039.6036	1058.904	1123.7901
	H	1.167169	-0.209487	-1.894605	1231.7888	1309.7136	1336.2574
	C	0.427869	-0.672171	1.503221	1411.1568	1436.2178	1448.3928
	H	-0.51717	-0.696355	2.037493	1478.7648	1494.0042	1501.7082
	H	0.891127	-1.655438	1.550265	1697.9124	1745.1776	3100.2114
	H	1.078272	0.067742	1.958266	3180.5301	3182.2224	3196.9318
	C	2.644689	-0.262613	-0.399844	3198.1945	3267.9252	3761.5296
	H	3.470604	-0.20068	-1.09413			
	H	2.887191	-0.316974	0.652562			
syn-trans-mvk	O	-1.435461	-1.005241	-0.00005	133.8546	134.3219	255.3407

	C	-0.544915	-0.187828	-0.000001	295.6019	362.043	459.4305
	C	0.870687	-0.645451	0.000078	492.0611	595.1894	696.3158
	H	0.987974	-1.722201	0.000106	820.7593	970.7222	1000.2768
	C	-0.833614	1.293299	0.000015	1002.539	1034.784	1055.5738
	H	-1.908822	1.441453	-0.001122	1071.7431	1304.4871	1349.2784
	H	-0.397458	1.765523	0.880634	1415.2987	1444.0819	1474.2648
	H	-0.395459	1.76604	-0.879326	1486.7029	1597.8403	1711.9613
	C	1.918375	0.167406	-0.00003	3073.8938	3132.3976	3179.786
	H	2.929055	-0.2174	-0.000057	3205.4172	3209.2377	3269.4344
	H	1.805198	1.24396	-0.000203			
syn-trans-mvk-rc	O	0.477932	1.907251	-0.101241	37.892	67.8119	81.0427
	O	-0.426585	1.07437	-0.735837	105.541	149.3639	179.2683
	C	-1.170366	0.380694	0.00693	198.4466	247.5222	277.4408
	N	1.836342	-0.786859	0.131967	344.2217	373.0518	472.8811
	O	2.480386	0.299152	-0.309325	495.0476	599.6408	696.9832
	H	1.777018	1.027785	-0.255082	774.8983	813.6487	965.525
	O	2.509621	-1.75416	0.134126	1018.662	1025.2546	1039.7135
	C	-2.075176	-0.48608	-0.729212	1042.4334	1056.3276	1071.472
	H	-2.001061	-0.413883	-1.806375	1090.5015	1316.0616	1344.7098
	C	-1.063992	0.501722	1.468546	1387.2652	1447.2065	1467.9378
	H	-0.058867	0.18073	1.750142	1499.5267	1559.0218	1607.4238
	H	-1.126508	1.559198	1.727497	1719.3998	1780.2255	2859.0692
	H	-1.815975	-0.080923	1.985861	3076.0703	3130.4635	3186.8968
	C	-2.922618	-1.328497	-0.147594	3212.5058	3215.1499	3276.0302
	H	-3.562965	-1.961402	-0.745335			
	H	-3.00396	-1.423435	0.925718			
syn-trans-mvk-ts	O	-1.180667	-1.865215	-0.131422	-888.6615	67.7639	83.1886

	O	-0.006409	-1.34636	-0.730122	110.046	149.3766	178.6754
	C	0.686261	-0.575864	0.013702	218.226	266.5097	294.3621
	N	-1.023208	1.053836	-0.034511	336.5124	390.9053	457.9934
	O	-2.110321	0.358727	-0.119782	487.5346	562.521	598.9614
	H	-1.76267	-0.816975	-0.122977	704.096	812.3363	887.3242
	O	-1.138494	2.235662	0.021143	968.9716	1009.466	1023.1156
	C	1.765251	0.076564	-0.717633	1041.8737	1049.7195	1078.4016
	H	1.737273	-0.051857	-1.791265	1250.7657	1285.6824	1315.4311
	C	0.607732	-0.605848	1.494395	1355.825	1419.7564	1447.6934
	H	-0.373986	-0.922262	1.821741	1472.2599	1489.1707	1571.0285
	H	1.350105	-1.332874	1.836705	1683.1889	1720.7803	1858.4724
	H	0.851381	0.369689	1.90229	3064.1353	3167.9445	3186.7413
	C	2.710594	0.791254	-0.119877	3218.9285	3227.2385	3274.7217
	H	3.490973	1.26463	-0.698426			
	H	2.73748	0.933652	0.951455			
syn-trans-mvk-oo	C	0.043181	-0.006791	0.000001	129.3847	173.2943	296.8614
	O	1.049294	-0.764867	0	439.0077	492.2607	543.1877
	O	2.296901	-0.237083	-0.000001	704.6487	780.2889	954.7069
	C	-1.227207	-0.711434	0.000001	1013.9437	1048.5018	1056.3006
	C	-2.400521	-0.085969	-0.000002	1074.0682	1281.4537	1312.8945
	H	-3.326907	-0.641761	-0.000001	1396.4871	1449.7728	1479.3895
	H	-2.471443	0.993755	-0.000005	1482.9255	1719.7152	1819.1664
	C	0.18121	1.466746	0.000001	3071.937	3136.1085	3171.6341
	H	-0.313072	1.878064	-0.880777	3184.8448	3200.9915	3256.0997
	H	-0.313067	1.878064	0.880781			
	H	1.234068	1.723882	-0.000002			
	H	-1.159119	-1.791722	0.000005			

anti-trans-mvk-oo	C	0.067814	0.348467	0.000002	129.3847	173.2943	296.8614
	O	1.326523	0.332246	0	439.0077	492.2606	543.1877
	O	1.98898	-0.854938	-0.000001	704.6487	780.2889	954.7069
	C	-0.689438	-0.887474	0.000001	1013.9437	1048.5018	1056.3006
	C	-2.020318	-0.89098	-0.000001	1074.0682	1281.4537	1312.8945
	H	-2.572813	-1.819981	-0.000001	1396.4871	1449.7728	1479.3895
	H	-2.600525	0.023121	-0.000003	1482.9255	1719.7152	1819.1664
	C	-0.547266	1.704001	0	3071.937	3136.1085	3171.6341
	H	-1.176085	1.833197	-0.881214	3184.8448	3200.9915	3256.0997
	H	-1.176084	1.8332	0.881214			
	H	0.234016	2.45797	-0.000002			
	H	-0.097294	-1.790056	0.000003			
anti-trans-mvk-rc	O	-0.141844	-1.747155	-0.897989	36.8665	42.6542	74.0235
	O	-1.175013	-1.365958	-0.054154	118.7007	148.6957	169.1404
	C	-1.448531	-0.142372	0.046625	181.0283	237.2225	278.5456
	N	2.275724	0.184735	-0.137708	338.711	366.1769	420.2781
	O	1.717542	-0.806467	0.577288	481.9291	620.9047	734.4723
	H	1.058591	-1.25555	-0.060654	779.0238	800.4644	947.3387
	O	3.062273	0.802471	0.484027	1006.5902	1031.9091	1038.23
	C	-0.755259	0.856439	-0.740853	1055.5953	1058.7062	1081.6313
	H	-0.055612	0.487193	-1.474244	1189.6044	1302.6039	1364.8386
	C	-2.529201	0.169411	1.020095	1429.5407	1460.4333	1469.8248
	H	-3.323197	0.733678	0.533178	1477.8771	1516.6382	1615.7628
	H	-2.926924	-0.751929	1.433528	1706.1056	1778.0999	2739.6627
	H	-2.123414	0.781026	1.826674	3077.622	3143.2518	3176.6013
	C	-0.963812	2.155171	-0.536845	3189.7567	3251.5859	3268.5483

	H	-0.435711	2.895745	-1.120839			
	H	-1.646648	2.521669	0.218793			
anti-trans-mvk-pc	O	1.413579	-1.673244	-0.480003	20.3299	54.5144	208.8367
	O	0.796809	-1.150489	0.684002	227.4264	250.0909	274.8814
	C	-0.179449	-0.221321	0.35555	300.7325	329.0653	375.8419
	N	0.553608	1.054114	-0.207075	444.5433	466.8495	485.864
	O	1.758716	1.010455	-0.315436	520.1608	651.735	707.5712
	H	2.124476	-1.025409	-0.606873	778.0383	847.0513	889.525
	O	-0.141208	1.996915	-0.477489	963.8044	1002.7022	1031.5188
	C	-1.131989	-0.694592	-0.703376	1041.2221	1068.1657	1127.4874
	H	-0.679913	-1.287905	-1.485545	1239.7792	1306.5142	1337.8398
	C	-0.792331	0.209373	1.670944	1406.544	1441.5196	1452.6856
	H	0.000613	0.490405	2.361167	1479.6574	1495.4878	1502.0727
	H	-1.451212	1.05794	1.513987	1697.1917	1740.8676	3092.6739
	H	-1.35242	-0.625815	2.083374	3173.2412	3178.8544	3191.4814
	C	-2.426066	-0.429835	-0.702894	3225.2772	3263.7428	3755.5896
	H	-3.062429	-0.806519	-1.491302			
	H	-2.898528	0.167663	0.064771			
anti-trans-mvk	O	1.435461	-1.005241	-0.00005	100.3215	167.5187	267.4124
	C	0.544915	-0.187828	-0.000001	283.863	339.3361	400.8773
	C	-0.870687	-0.645451	0.000078	479.2229	630.5644	736.2758
	H	-0.987974	-1.722201	0.000106	799.0449	960.9895	1006.064
	C	0.833614	1.293299	0.000015	1018.0087	1049.6846	1058.6179
	H	1.908822	1.441453	-0.001122	1076.3624	1287.8513	1365.1547
	H	0.395459	1.76604	-0.879326	1431.3053	1460.7195	1473.2655
	H	0.397458	1.765523	0.880634	1477.1431	1599.1732	1706.1426
	C	-1.918375	0.167406	-0.00003	3072.3734	3132.5634	3174.2095

	H	-2.929055	-0.2174	-0.000057	3181.9322	3244.5198	3264.732
	H	-1.805198	1.24396	-0.000203			
anti-trans-mvk-ts	O	-0.474178	2.002539	-0.491177	-837.7505	72.4828	87.6984
	O	0.215172	1.450591	0.619249	108.2579	168.8051	177.9345
	C	0.827431	0.359414	0.378592	222.1825	281.0025	288.7526
	N	-1.263133	-0.740105	0.097294	320.9707	355.0842	439.0955
	O	-2.030427	0.161644	-0.415699	477.2214	583.905	618.1889
	H	-1.32901	1.171462	-0.514311	709.5361	794.7238	883.5874
	O	-1.721372	-1.828809	0.243039	964.7901	1016.0768	1029.7344
	C	1.208111	-0.02965	-0.971404	1048.6801	1051.5389	1084.3746
	H	0.824405	0.585325	-1.770062	1255.1124	1290.3758	1310.2134
	C	1.345975	-0.320026	1.593394	1358.6839	1427.3678	1453.9078
	H	0.945884	0.159877	2.480726	1460.5199	1478.0584	1578.7667
	H	1.029652	-1.362464	1.568261	1677.9984	1712.5842	1861.1791
	H	2.43477	-0.28122	1.60497	3080.4899	3150.8047	3180.4881
	C	2.007967	-1.068793	-1.18687	3190.5996	3250.9561	3270.6318
	H	2.309067	-1.331126	-2.191073			
	H	2.376693	-1.694501	-0.385135			
syn-trans-macr-pc	O	0.220339	2.021281	0.509989	48.8962	67.687	164.9376
	O	0.305623	1.452855	-0.787205	181.6873	193.0764	246.014
	C	-0.024506	0.114695	-0.748463	329.9417	360.8039	388.7719
	N	1.160641	-0.688688	-0.182545	456.8586	470.0116	486.6576
	O	2.004197	-0.090789	0.446153	630.2577	690.9277	772.4611
	H	1.107636	1.825276	0.849557	819.9224	892.33	934.8994
	O	1.138997	-1.874556	-0.388948	966.1758	981.1869	1008.4616
	C	-1.274757	-0.271471	0.01119	1060.0913	1082.6149	1175.1847
	C	-2.405289	-0.312489	-0.677776	1295.2747	1318.8472	1357.1931

	H	-3.344307	-0.542	-0.192492	1415.8364	1438.9164	1458.0258
	H	-2.432968	-0.106058	-1.739801	1488.2688	1491.8351	1502.9902
	H	-0.07936	-0.196472	-1.789551	1703.6137	1748.4948	3069.0847
	C	-1.175243	-0.574414	1.47553	3134.6411	3147.6048	3164.1143
	H	-0.796287	0.285233	2.025712	3169.4954	3255.2465	3755.8941
	H	-2.154068	-0.840317	1.867077			
	H	-0.499612	-1.413096	1.654522			
syn-trans-macr	C	0.885316	-0.633499	0.000052	55.1092	266.3643	275.8991
	O	1.881076	0.041661	-0.000026	329.6219	348.0353	439.1964
	C	-0.486938	-0.07406	-0.000161	562.1516	721.7366	728.6337
	H	0.944268	-1.738043	0.000205	854.8526	915.7759	936.428
	C	-0.610749	1.414792	0.000075	991.6102	1004.0087	1069.7212
	H	-0.110229	1.833391	0.873331	1078.2194	1353.8599	1410.4313
	H	-0.109946	1.833501	-0.873005	1426.387	1456.5559	1474.0539
	H	-1.653665	1.72268	-0.000262	1496.0929	1624.7844	1692.8771
	C	-1.499569	-0.935875	-0.000036	3083.734	3165.4989	3166.1798
	H	-2.53114	-0.609192	0.000232	3170.9034	3185.4838	3260.154
	H	-1.316251	-2.003762	0.00013			
syn-trans-macr-oo	C	0.243217	-0.951926	-0.000214	156.1248	186.3949	268.2818
	O	1.471594	-0.722121	-0.000103	403.8609	436.7101	630.6303
	O	1.937477	0.552299	0.000316	717.224	844.0328	979.3957
	C	-0.864138	-0.012073	-0.000032	993.9642	1028.551	1040.0109
	H	0.027478	-2.015513	-0.000515	1085.0866	1340.1793	1396.9247
	C	-0.685128	1.477366	-0.000195	1418.2501	1458.6611	1475.5932
	H	-0.115035	1.79541	0.868787	1494.091	1734.8083	1832.5568
	H	-0.114771	1.795206	-0.869074	2959.3181	3070.9586	3129.3913
	H	-1.662739	1.956489	-0.000381	3160.5925	3161.695	3247.8394

	C	-2.069229	-0.59601	0.000227			
	H	-2.974667	-0.004691	0.00038			
	H	-2.181169	-1.672468	0.000378			
syn-trans-macr-rc	O	0.093157	1.888059	0.367753	47.836	61.6386	76.0228
	O	-0.385092	1.499626	-0.876537	103.1769	157.6082	189.6474
	C	-1.0766	0.464889	-0.957843	250.6445	272.6363	282.8778
	N	1.640266	-0.669427	-0.197415	338.2129	359.5935	444.5106
	O	2.182561	0.390192	0.41647	549.5404	722.9114	723.6496
	H	1.424404	1.067857	0.43599	775.07	849.6112	899.942
	O	2.388245	-1.572077	-0.308432	977.3706	1008.1627	1016.829
	C	-1.546099	-0.428234	0.081862	1045.5998	1072.3787	1079.8565
	C	-2.258878	-1.453817	-0.402902	1081.979	1359.2005	1412.0448
	H	-2.673287	-2.204296	0.256519	1429.3731	1463.4002	1477.2876
	H	-2.438383	-1.575663	-1.463009	1500.2012	1581.4062	1654.9996
	H	-1.36125	0.254212	-1.985029	1692.3062	1786.8442	2814.5077
	C	-1.287025	-0.238362	1.546563	3086.7247	3163.7798	3171.9371
	H	-0.222769	-0.306642	1.759656	3172.5371	3180.2602	3263.0943
	H	-1.612665	0.745163	1.873503			
	H	-1.817263	-1.007895	2.104158			
syn-trans-macr-ts	O	0.323015	-1.974615	-0.169291	-886.5498	62.5621	81.9131
	O	0.026	-1.371686	1.081557	97.9209	187.2229	244.6166
	C	-0.556823	-0.251853	1.011375	265.5938	278.211	287.6849
	N	1.34736	0.754976	0.083976	341.2316	378.4759	452.5161
	O	1.894586	-0.202479	-0.599442	528.0299	587.5212	710.5204
	H	1.186781	-1.158649	-0.461925	731.8033	850.7123	897.3161
	O	1.849724	1.825787	0.00666	930.1468	995.8016	1014.0602
	C	-1.404523	0.302511	-0.034803	1017.2258	1075.5869	1081.7508

	C	-2.151751	1.326204	0.391901	1245.7539	1277.1252	1351.5993
	H	-2.848564	1.818713	-0.272551	1393.5338	1425.1772	1464.6187
	H	-2.088417	1.699983	1.40524	1482.4967	1499.275	1605.3712
	H	-0.590473	0.231586	1.98364	1695.2255	1699.7535	1854.8224
	C	-1.459456	-0.218655	-1.438714	3083.1976	3154.0809	3172.0588
	H	-1.716547	-1.274149	-1.455247	3173.2795	3188.3377	3262.6294
	H	-2.197539	0.349294	-2.00079			
	H	-0.488045	-0.116899	-1.920619			
syn-cis-macr-ts	O	-0.161857	-2.062574	0.256011	-786.1741	67.3508	88.6735
	O	0.033835	-1.435758	-1.005492	115.1329	163.8941	205.0779
	C	0.510979	-0.26571	-0.958149	266.2941	285.0834	301.914
	N	-1.390848	0.611579	-0.008931	346.7113	385.1731	428.2786
	O	-1.829816	-0.373802	0.712159	514.022	622.231	670.7309
	H	-1.079778	-1.253962	0.588285	720.3254	892.0092	925.7481
	O	-2.005236	1.623587	0.038181	942.4385	988.5284	1030.8648
	C	1.372134	0.359388	0.040593	1034.667	1046.0555	1091.8017
	C	2.024052	-0.36838	0.947051	1241.7551	1267.2611	1287.1883
	H	2.747508	0.111534	1.593648	1402.6524	1420.7804	1452.5477
	H	1.855459	-1.428448	1.051411	1486.0307	1500.7728	1607.5169
	H	0.432954	0.227213	-1.925516	1696.7354	1716.4762	1844.7504
	C	1.545997	1.840161	-0.142477	3064.7433	3125.2705	3163.7974
	H	0.592616	2.356344	-0.025149	3165.926	3177.7655	3287.0984
	H	2.247129	2.230837	0.590139			
	H	1.925676	2.071055	-1.139276			
syn-cis-macr-oo	C	-0.240858	-0.873635	-0.000064	103.2477	160.6047	287.0264
	O	-1.49121	-0.739336	0.000046	382.0081	401.3578	602.9567
	O	-2.044858	0.486682	0.000038	702.6865	882.8104	973.3123

	C	0.78915	0.133424	-0.000207	1008.4357	1025.2394	1027.4233
	H	0.039754	-1.922193	-0.000127	1089.4222	1286.8395	1410.3359
	C	2.188665	-0.429838	0.000092	1432.9625	1446.2688	1483.8179
	H	2.362752	-1.050201	0.88019	1493.9719	1728.0555	1846.3918
	H	2.36268	-1.051035	-0.879406	2943.5192	3055.7687	3108.5741
	H	2.921438	0.372877	-0.000255	3155.3651	3168.8679	3260.8992
	C	0.543171	1.452761	-0.000055			
	H	1.382344	2.138522	0.000008			
	H	-0.461189	1.83699	0.000323			
syn-cis-macr-pc	O	0.465941	2.06355	-0.499261	49.7554	62.173	207.6968
	O	0.138958	1.499917	0.763378	220.8801	245.6256	280.0816
	C	0.01651	0.129419	0.695875	330.113	355.6051	405.4836
	N	-1.331142	-0.226915	0.032753	423.1188	433.4315	484.4954
	O	-1.761818	0.527356	-0.811976	627.6528	705.058	747.2876
	H	-0.397846	2.042989	-0.940765	823.0529	928.1894	935.0173
	O	-1.859265	-1.243883	0.400454	964.4923	988.8795	1010.4335
	C	1.136622	-0.651038	0.041626	1039.6074	1085.4154	1177.7235
	C	2.332069	-0.090509	-0.051149	1276.854	1299.3684	1381.4379
	H	3.164711	-0.653719	-0.450491	1424.6611	1453.8225	1455.5078
	H	2.511462	0.929524	0.254102	1489.1677	1492.3087	1504.4436
	H	-0.135783	-0.193999	1.726099	1700.4944	1748.7617	3064.806
	C	0.84695	-2.061058	-0.380162	3117.4438	3121.033	3161.8779
	H	0.117954	-2.092176	-1.191738	3181.2876	3274.8626	3737.0661
	H	1.763354	-2.533607	-0.724139			
	H	0.430714	-2.647024	0.439759			
syn-cis-macr	C	-0.863992	-0.63029	-0.000099	97.3025	141.4409	294.68
	O	-1.95653	-0.130101	0.000095	326.9196	340.6966	431.0913

	C	0.423659	0.126694	-0.000022	550.8693	713.4419	713.9045
	H	-0.756211	-1.732588	-0.000361	917.1895	950.1152	956.0949
	C	1.675183	-0.696991	0.000051	1015.9643	1033.7658	1045.8781
	H	1.71368	-1.34525	0.877676	1079.7297	1290.2239	1412.1928
	H	1.713503	-1.345593	-0.877291	1428.7084	1439.8298	1488.9737
	H	2.561127	-0.06655	-0.000138	1499.3033	1602.1007	1682.5196
	C	0.382723	1.45353	-0.000004	3064.3263	3121.178	3161.3555
	H	1.286111	2.049128	-0.000176	3169.762	3185.3922	3315.8177
	H	-0.571408	1.964002	-0.000035			
syn-cis-macr-rc	O	0.075863	2.025635	0.240873	34.4994	48.8624	66.6255
	O	-0.389677	1.508287	-0.946635	110.8151	149.3778	165.9422
	C	-1.050872	0.445824	-0.933244	182.7197	241.3004	293.7108
	N	1.662668	-0.643669	-0.193917	308.1298	370.2042	423.6233
	O	2.101755	0.379679	0.557919	541.0411	687.5505	712.3891
	H	1.380635	1.075971	0.477653	772.264	900.9817	930.557
	O	2.401061	-1.559377	-0.191592	976.1132	989.6531	1010.5636
	C	-1.485783	-0.374264	0.173727	1039.0215	1047.4629	1052.4134
	C	-1.488312	0.051199	1.443394	1084.9626	1289.3146	1416.4086
	H	-1.88469	-0.599369	2.213378	1434.4329	1443.4346	1488.2193
	H	-1.119235	1.024901	1.7163	1499.2903	1563.7522	1630.8045
	H	-1.308606	0.136424	-1.943214	1697.5654	1789.9796	2987.1184
	C	-1.968172	-1.738938	-0.241432	3063.0428	3122.0017	3164.9701
	H	-2.345595	-2.28623	0.618143	3171.512	3177.5352	3309.4345
	H	-2.764622	-1.671196	-0.983652			
	H	-1.149741	-2.311534	-0.680374			
anti-trans-macr-rc	O	-0.807188	2.027005	-0.465343	37.0533	52.3367	62.409
	O	0.314072	1.387198	0.066348	137.2948	164.157	169.962

	C	0.739883	0.422322	-0.596616	191.6818	202.5174	255.6281
	N	-1.785266	-0.815892	0.012772	327.7476	364.5724	480.5763
	O	-2.507509	0.268782	0.303336	506.6098	575.2536	716.198
	H	-1.91441	1.045896	0.008865	777.2877	883.6483	945.0683
	O	-2.328847	-1.825268	0.284878	1005.4001	1012.8477	1025.8516
	C	1.868104	-0.335883	-0.10836	1060.8203	1068.4786	1079.6896
	C	2.254738	-1.359497	-0.873603	1095.4488	1325.6781	1404.2181
	H	3.081396	-1.994865	-0.585771	1438.0808	1459.1707	1480.3133
	H	1.745923	-1.590863	-1.800257	1498.2625	1585.5477	1639.8768
	H	0.236384	0.194649	-1.530945	1715.4528	1782.8388	2737.7409
	C	2.484382	0.057214	1.197244	3075.0642	3136.7544	3169.3348
	H	1.745413	-0.00203	1.996252	3172.603	3197.8291	3263.882
	H	3.319202	-0.596149	1.435844			
	H	2.836084	1.087939	1.160873			
anti-trans-macr-ts	O	-1.371051	-1.88787	0.350969	-709.1592	53.9227	85.2821
	O	-0.095249	-1.485937	-0.135426	97.7026	182.9716	194.702
	C	0.411618	-0.572459	0.573028	200.7874	241.4841	296.4438
	N	-1.19535	0.983836	-0.037444	351.6317	377.2091	480.0519
	O	-2.260485	0.274266	-0.251678	547.056	569.889	625.699
	H	-1.957329	-0.813779	0.033013	730.4399	883.0433	910.7615
	O	-1.271989	2.147431	-0.245947	985.3091	1005.3641	1014.1008
	C	1.650254	0.04402	0.141412	1048.3933	1065.1798	1080.3475
	C	2.242666	0.849121	1.023191	1262.8057	1294.3558	1323.2751
	H	3.164048	1.362216	0.783353	1396.8621	1430.0668	1458.6725
	H	1.814735	1.023261	2.001869	1481.1701	1495.4181	1589.5969
	H	0.003913	-0.415829	1.564818	1695.5168	1724.4744	1849.616
	C	2.130082	-0.236655	-1.246993	3071.046	3132.3896	3169.9362

	H	1.379547	0.084678	-1.970423	3171.5298	3209.2375	3262.4695
	H	3.060091	0.290214	-1.442256			
	H	2.284919	-1.304891	-1.395438			
anti-trans-macr	O	-1.881076	0.04166	-0.000023	161.2767	188.9903	192.9117
	C	-0.885316	-0.6335	0.000049	229.678	367.7781	481.8375
	C	0.486938	-0.07406	-0.000159	506.0341	576.7823	717.4399
	C	1.49957	-0.935875	-0.000035	881.0742	975.9697	984.0614
	H	2.53114	-0.609192	0.000233	1003.1989	1006.2366	1056.6931
	H	1.316251	-2.003761	0.000129	1077.274	1313.0941	1400.5607
	H	-0.944268	-1.738043	0.000196	1435.13	1455.6097	1480.8029
	C	0.610749	1.414792	0.000073	1498.0162	1613.3836	1713.3617
	H	0.110232	1.833391	0.873332	3073.7481	3134.2148	3166.5507
	H	1.653665	1.72268	-0.000266	3172.8746	3178.6088	3263.2734
	H	0.109942	1.833501	-0.873005			
anti-trans-macr-oo	C	0.381929	-0.542369	0.000012	156.1228	186.3933	268.2813
	O	1.292423	0.310678	0	403.8609	436.7089	630.6301
	O	2.576022	-0.131898	0.00001	717.2236	844.0325	979.3956
	C	-0.998077	-0.110284	-0.000088	993.964	1028.549	1040.0108
	H	0.682982	-1.58647	-0.000003	1085.086	1340.179	1396.9235
	C	-1.277499	1.361055	0.000025	1418.2495	1458.6607	1475.5931
	H	-0.833073	1.833729	0.875649	1494.0908	1734.807	1832.5572
	H	-0.833426	1.833652	-0.875825	2959.3286	3070.9593	3129.3923
	H	-2.348597	1.545236	0.000214	3160.5924	3161.696	3247.8391
	C	-1.933489	-1.0632	-0.000016			
	H	-2.98608	-0.815647	0.000163			
	H	-1.666554	-2.111958	0.000123			
anti-trans-macr-pc	O	1.951447	-1.450774	-0.472659	30.8689	59.5586	157.0986

	O	0.64531	-1.359079	0.071907	173.3786	186.2613	205.3685
	C	0.014083	-0.280672	-0.499894	321.6518	358.7164	394.7404
	N	0.698863	1.025068	-0.00961	454.1717	472.5569	537.3318
	O	1.520288	0.937112	0.874279	572.6674	659.3547	721.6706
	H	2.456159	-0.939242	0.178879	831.741	886.5643	923.6729
	O	0.348849	2.037009	-0.55684	986.3901	1001.2658	1031.094
	C	-1.418372	-0.251973	-0.053168	1065.0399	1083.2731	1205.0462
	C	-2.370542	-0.159268	-0.968312	1299.0047	1322.3227	1347.5161
	H	-3.413384	-0.128059	-0.682352	1419.6944	1433.1561	1458.6565
	H	-2.140642	-0.105918	-2.023761	1480.5823	1485.4435	1496.644
	H	0.137945	-0.242189	-1.580289	1707.0175	1759.6789	3063.2577
	C	-1.650407	-0.319437	1.425379	3123.2149	3141.1392	3163.6944
	H	-1.143261	0.502133	1.935855	3173.2774	3260.2486	3759.6036
	H	-2.713301	-0.261479	1.645498			
	H	-1.251277	-1.246765	1.835911			
anti-cis-macr-oo	C	-0.38574	-0.442862	-0.000207	103.2478	160.6049	287.0264
	O	-1.379585	0.309193	0.000203	382.0081	401.3577	602.9568
	O	-2.610653	-0.259221	0.000014	702.6865	882.8105	973.3123
	C	0.968223	0.096296	-0.00011	1008.4356	1025.2395	1027.4233
	H	-0.591708	-1.510721	-0.000641	1089.4222	1286.8396	1410.336
	C	2.061409	-0.933216	0.000128	1432.9626	1446.2689	1483.8179
	H	1.990262	-1.575374	0.879155	1493.9719	1728.0555	1846.3917
	H	1.990629	-1.575315	-0.878983	2943.5191	3055.7686	3108.574
	H	3.037898	-0.456086	0.000322	3155.3651	3168.8679	3260.8992
	C	1.180795	1.412245	-0.000059			
	H	2.187156	1.807615	0.000105			
	H	0.359543	2.115338	-0.000202			

anti-cis-macr-pc	O	-2.098058	-1.115706	0.755258	44.4907	75.6378	171.2367
	O	-0.826189	-1.312137	0.158923	190.6972	191.1606	218.9279
	C	-0.040284	-0.232192	0.472978	330.3633	355.4225	383.0053
	N	-0.617577	1.034821	-0.203648	451.433	473.6235	527.8573
	O	-1.448367	0.886245	-1.066801	572.5225	676.5683	704.142
	H	-2.58034	-0.698044	0.024712	831.9788	927.8101	931.4456
	O	-0.173133	2.085054	0.186151	993.2797	1009.7317	1016.0419
	C	1.360906	-0.425676	-0.051077	1056.0372	1082.1645	1213.4271
	C	1.559293	-1.190386	-1.114591	1258.9647	1328.5466	1384.2789
	H	2.559112	-1.341413	-1.498817	1415.0832	1434.864	1452.7489
	H	0.743099	-1.686552	-1.619944	1481.3023	1486.556	1499.2287
	H	-0.075199	0.015137	1.533755	1705.8728	1750.351	3061.575
	C	2.438726	0.294959	0.69794	3121.708	3122.227	3160.5141
	H	2.475693	-0.043919	1.735112	3177.8077	3268.1732	3762.8996
	H	3.407216	0.114875	0.237765			
	H	2.247596	1.368291	0.713212			
anti-cis-macr-ts	O	1.414295	-1.896634	-0.410548	-497.4176	50.354	90.7428
	O	0.144325	-1.55806	0.138093	112.8687	179.6591	195.0825
	C	-0.409072	-0.625567	-0.498229	210.1371	241.6869	310.9068
	N	1.16495	0.990452	0.109391	364.0801	379.3066	455.1601
	O	2.251231	0.286377	0.23145	536.839	561.5416	670.4488
	H	1.975179	-0.779967	-0.07627	720.512	915.7192	928.705
	O	1.245102	2.140446	0.382289	999.3096	1015.041	1022.9557
	C	-1.660278	-0.036941	-0.033209	1045.6362	1071.9059	1093.8555
	C	-2.36327	-0.660441	0.90951	1263.3739	1286.7513	1306.1514
	H	-3.305539	-0.255224	1.252341	1405.3528	1418.9088	1453.6167

	H	-2.019757	-1.586789	1.348808	1484.1002	1500.5675	1609.6165
	H	-0.004661	-0.389038	-1.476413	1694.7831	1728.4062	1840.4315
	C	-2.041119	1.250279	-0.699911	3061.8981	3122.4222	3163.9854
	H	-2.110627	1.123326	-1.781274	3177.2575	3197.0691	3270.0392
	H	-3.000988	1.601324	-0.330445			
	H	-1.28545	2.012199	-0.501721			
anti-cis-macr	O	-1.95653	-0.130101	0.000095	64.6736	164.3507	202.2132
	C	-0.863992	-0.63029	-0.000099	205.5932	369.2129	456.2075
	C	0.423659	0.126694	-0.000021	494.0628	562.6167	697.2972
	C	0.382723	1.45353	-0.000004	912.4063	978.8444	998.8477
	H	1.286112	2.049128	-0.000176	1006.7729	1016.9943	1048.0586
	H	-0.571408	1.964002	-0.000035	1078.1906	1281.3875	1400.289
	H	-0.756211	-1.732588	-0.000361	1419.6181	1451.1354	1486.9718
	C	1.675183	-0.696991	0.000051	1498.9485	1608.5451	1720.4817
	H	1.713503	-1.345592	-0.877292	3063.2906	3119.8871	3163.3469
	H	2.561127	-0.06655	-0.000137	3165.2649	3178.0517	3269.9736
	H	1.71368	-1.345251	0.877675			
anti-cis-macr-rc	O	0.91385	2.079698	0.457248	37.5068	46.4395	68.5645
	O	-0.22451	1.503398	-0.119307	139.4406	166.1351	172.436
	C	-0.695953	0.536106	0.504609	197.7753	219.1741	248.3972
	N	1.634774	-0.857301	-0.061092	316.6225	365.477	452.84
	O	2.470381	0.167008	-0.233896	498.3614	563.1079	696.1596
	H	1.933038	0.994975	0.04409	780.9128	908.8231	948.6543
	O	2.106224	-1.900962	-0.338504	1015.8991	1022.4913	1042.167
	C	-1.837627	-0.212092	-0.002502	1046.1007	1074.7662	1088.3256
	C	-2.578855	0.29922	-0.984512	1102.5014	1288.5082	1412.9356
	H	-3.434183	-0.239876	-1.368444	1422.5053	1453.3363	1484.8243

	H	-2.352038	1.264002	-1.417064	1499.5078	1602.5642	1640.949
	H	-0.213209	0.27851	1.442907	1728.2055	1787.0936	2658.5549
	C	-2.073916	-1.535112	0.664143	3063.759	3122.8836	3165.4608
	H	-2.245314	-1.406166	1.733758	3177.518	3190.0986	3270.349
	H	-2.938779	-2.031693	0.232507			
	H	-1.202379	-2.180504	0.545132			
pc-syn	O	1.863849	0.630413	-0.422329	57.9645	175.6722	217.5805
	O	1.242658	0.228429	0.78838	276.3163	316.4318	364.5205
	C	0.151511	-0.567655	0.52194	442.37	471.1778	594.6807
	N	-1.022587	0.30818	0.044321	709.5731	764.4237	889.8529
	O	-0.779629	1.438318	-0.313037	921.928	1000.6897	1080.8386
	H	1.350354	1.426323	-0.63121	1166.4326	1212.5775	1321.8955
	O	-2.107144	-0.2163	0.045498	1380.2598	1410.7671	1442.8413
	C	0.350564	-1.675236	-0.487477	1487.1559	1491.7092	1503.6854
	H	0.570113	-1.265892	-1.469263	1700.4032	3096.3294	3139.8241
	H	1.191834	-2.282965	-0.161943	3178.2909	3189.9634	3757.7043
	H	-0.546084	-2.286764	-0.533835			
	H	-0.17843	-0.937491	1.491126			
rc-syn	O	-1.02244	-1.389816	-0.428953	58.4375	59.0787	94.5051
	O	-1.361403	-0.658104	0.700512	101.6788	155.9702	196.2533
	C	-1.52923	0.565794	0.573519	275.6633	349.7127	450.1443
	N	1.448777	0.299881	0.094664	648.8616	774.6642	843.7651
	O	1.528062	-0.979194	-0.29026	884.9684	929.3508	1048.5608
	H	0.559532	-1.260403	-0.378857	1068.043	1094.6681	1175.0646
	O	2.50235	0.806017	0.23921	1373.1895	1421.7909	1436.9889
	C	-1.438881	1.318669	-0.68171	1468.1497	1569.8182	1690.0844
	H	-0.742472	2.144927	-0.532145	1786.2151	2895.7764	3062.7025

	H	-1.119835	0.678897	-1.494913	3123.1754	3178.703	3219.6481
	H	-2.420961	1.753074	-0.886833			
	H	-1.781586	1.046339	1.515168			
ts-syn	O	-1.341713	-1.26625	-0.338101	-516.541	92.6693	145.6611
	O	-1.26691	-0.440145	0.817266	162.3608	239.8073	299.0913
	C	-0.877415	0.732739	0.579942	338.0542	388.8844	433.4216
	N	1.24414	0.087438	0.123175	627.1315	720.0633	855.959
	O	1.078725	-1.075934	-0.446408	913.2895	964.0664	1021.7464
	H	-0.035093	-1.279398	-0.472552	1100.9334	1168.7636	1255.5878
	O	2.355567	0.476548	0.21486	1318.8358	1375.4179	1412.1201
	C	-1.013025	1.4302	-0.715271	1452.1078	1477.0599	1636.21
	H	-0.339621	2.281799	-0.743687	1715.8991	1841.1601	3055.1188
	H	-0.852064	0.762041	-1.552215	3154.2218	3180.9014	3219.1085
	H	-2.044924	1.795624	-0.754544			
	H	-0.699995	1.296479	1.491809			
syn-CH3CHOO	C	-0.471838	0.672873	-0.00011	165.4624	341.5571	449.3907
	O	0.769424	0.575	-0.000074	655.1313	820.6778	897.0603
	O	1.343717	-0.657592	0.000139	936.6833	1070.1347	1162.8798
	C	-1.392753	-0.47536	0.000003	1362.0898	1418.9707	1441.0216
	H	-2.039879	-0.413405	-0.877006	1477.3317	1660.7167	3064.6172
	H	-0.827002	-1.399901	-0.000842	3118.9006	3186.8582	3208.0139
	H	-2.038482	-0.414327	0.878122			
	H	-0.812225	1.703289	-0.000157			
CH3CHO	O	1.22511	-0.27716	0.000012	157.9301	513.5174	775.8678
	C	0.233225	0.397942	-0.000028	901.0328	1138.4157	1145.8064
	C	-1.162542	-0.14778	0.000016	1380.6171	1430.1835	1464.9655
	H	-1.695786	0.224423	-0.876544	1474.8268	1866.198	2944.5426

	H	-1.148137	-1.23395	-0.000521	3062.9238	3125.0588	3180.0912
	H	-1.695288	0.2238	0.87712			
	H	0.314228	1.502036	-0.000078			
anti-CH3CHOO	C	-0.370064	0.399514	0.000016	167.1516	268.6733	329.13
	O	0.566273	-0.412482	-0.000063	566.0613	883.6993	900.5093
	O	1.839961	0.076479	-0.000032	985.3841	1094.9317	1168.55
	C	-1.762798	-0.093107	0.000051	1362.715	1421.5962	1467.6926
	H	-2.286611	0.288683	-0.877786	1469.4834	1674.106	3064.6667
	H	-1.783663	-1.179059	-0.000432	3121.0833	3165.1277	3183.3032
	H	-2.286246	0.287845	0.878481			
	H	-0.096187	1.452105	0.00009			
pc-anti	O	-2.000912	-0.571552	-0.430183	61.9346	199.8273	207.2796
	O	-1.325936	0.469276	0.256716	257.0469	300.3581	350.961
	C	-0.091552	0.64137	-0.317007	453.4207	496.5867	551.1245
	N	0.803381	-0.574638	0.000179	663.5213	746.9175	893.8077
	O	0.371593	-1.420801	0.747324	927.204	1045.6031	1090.2694
	H	-1.747201	-1.338532	0.1065	1162.7296	1238.93	1343.1053
	O	1.881704	-0.584428	-0.537582	1361.7085	1408.8812	1436.2819
	C	0.550498	1.871005	0.276234	1488.076	1493.0043	1502.87
	H	-0.041674	2.740319	0.00217	1703.8646	3090.455	3126.1502
	H	0.578099	1.784939	1.361008	3172.1857	3188.4772	3761.8362
	H	1.559378	1.979148	-0.111216			
	H	-0.137524	0.642394	-1.40528			
ts-anti	O	0.778955	-1.848154	0.149247	-371.0922	98.9322	139.9856
	O	1.297376	-0.635541	-0.387587	154.747	229.5068	253.5322
	C	1.08662	0.344272	0.364607	312.9463	390.1243	430.1856
	N	-1.196336	0.30085	0.070991	548.3801	733.3975	878.9158

	O	-1.470931	-0.959039	-0.118337	931.3241	999.6774	1038.8174
	H	-0.492087	-1.493193	0.006321	1142.2852	1180.8915	1260.5805
	O	-2.099441	1.05935	-0.018818	1352.3775	1391.8274	1431.044
	C	1.467404	1.69395	-0.089549	1456.3087	1473.7236	1649.3056
	H	0.655176	2.381367	0.145138	1699.4375	1849.6056	3070.5711
	H	2.349947	2.012919	0.468283	3138.2807	3185.9573	3203.0541
	H	1.675609	1.70081	-1.155038			
	H	0.813884	0.129879	1.39197			
rc-anti	O	-0.616573	1.844813	0.16948	66.3729	74.3908	134.8461
	O	-1.299339	0.744665	-0.366819	159.677	182.3262	235.2151
	C	-1.362495	-0.24697	0.371927	257.3711	327.6939	354.4944
	N	1.393025	-0.447478	0.098224	560.0993	780.0325	871.613
	O	1.707352	0.821541	-0.160293	894.6404	982.1408	1075.6564
	H	0.828954	1.333596	-0.035489	1096.1673	1118.3486	1181.8152
	O	2.30411	-1.188217	-0.001157	1367.4602	1417.5148	1460.8133
	C	-1.978633	-1.488604	-0.11993	1466.5485	1603.1244	1697.3997
	H	-1.214565	-2.269108	-0.09241	1787.9841	2685.0592	3064.3657
	H	-2.777369	-1.791845	0.557855	3126.4676	3183.867	3195.7493
	H	-2.355182	-1.367322	-1.130703			
	H	-0.95064	-0.141939	1.371512			
NO2	N	0	0	0.314473	783.5181	1465.1762	1775.3149
	O	0	1.090255	-0.137582			
	O	0	-1.090255	-0.137582			
OH	O	0	0	0.107992	3769.6197		
	H	0	0	-0.863937			
HONO	N	0	0.507841	0	578.2528	700.4221	905.044
	O	0.882551	-0.567177	0	1342.3963	1841.1092	3830.8187

	O	-1.101711	0.141484	0	
	H	1.753278	-0.149345	0	

Table S2: Effective rate constants (in s^{-1}) for the reactions of MVK-OO with HONO and $H_2O/(H_2O)_2/SO_2$ over the temperature range of 213–320 K. a=2.46×10^9 molecule cm^{-3}, b=8.9×10^{10} molecule cm^{-3}, c=2.16×10^9 molecule cm^{-3}, and d=9.0×10^{10} molecule cm^{-3}

Temp.	[HONO]^a	[HONO]^b	[H_2O] (RH=20%)	[H_2O] (RH=100%)	[$(H_2O)_2$] (RH=20%)	[$(H_2O)_2$] (RH=100%)	Unimolecular	[SO_2]^c	[SO_2]^d
213	9.90×10^{-2}	3.58	1.42×10^{-5}	7.10×10^{-5}	1.24×10^{-5}	3.10×10^{-4}	2.25×10^{-1}		
216	9.80×10^{-2}	3.55	2.40×10^{-5}	1.20×10^{-4}	3.26×10^{-5}	8.16×10^{-4}	2.68×10^{-1}		
219	9.70×10^{-2}	3.51	4.00×10^{-5}	2.00×10^{-4}	8.18×10^{-5}	2.05×10^{-3}	3.20×10^{-1}		
224	9.50×10^{-2}	3.44	9.07×10^{-5}	4.53×10^{-4}	1.77×10^{-4}	4.43×10^{-3}	4.29×10^{-1}		
235	9.00×10^{-2}	3.26	4.84×10^{-4}	2.42×10^{-3}	7.13×10^{-4}	1.78×10^{-2}	8.25×10^{-1}		
250	8.24×10^{-2}	2.98	3.72×10^{-3}	1.86×10^{-2}	4.91×10^{-3}	1.23×10^{-1}	2.02		
259	7.75×10^{-2}	2.80	1.12×10^{-2}	5.62×10^{-2}	1.61×10^{-2}	4.03×10^{-1}	3.45		
265	7.42×10^{-2}	2.69	2.25×10^{-2}	1.13×10^{-1}	2.67×10^{-2}	6.69×10^{-1}	4.93		
278	6.72×10^{-2}	2.43	9.11×10^{-2}	4.56×10^{-1}			1.06×10^{1}		
280	6.61×10^{-2}	2.39	1.05×10^{-1}	5.23×10^{-1}	1.05×10^{-1}	2.63	1.19×10^{1}		
290	6.09×10^{-2}	2.20	2.52×10^{-1}	1.26	2.17×10^{-1}	5.42	2.14×10^{1}		
298	5.69×10^{-2}	2.06	4.85×10^{-1}	2.42	3.74×10^{-1}	9.35	3.41×10^{1}	9.0×10^{-2}	3.78
300	5.59×10^{-2}	2.02	5.68×10^{-1}	2.84	4.19×10^{-1}	1.05×10^{1}	3.82×10^{1}		
310	5.12×10^{-2}	1.85	1.21	6.04	7.68×10^{-1}	1.92×10^{1}	6.78×10^{1}		
320	4.68×10^{-2}	1.69	2.44	1.22×10^{1}	1.34	3.36×10^{1}	1.19×10^{2}		

Table S3: Effective rate constants (in s^{-1}) for the reactions of MACR-OO with HONO and $H_2O/(H_2O)_2/SO_2$ over the temperature range of 213–320 K. a=2.46×10^9 molecule cm^{-3}, b=8.9×10^{10} molecule cm^{-3}, c=2.16×10^9 molecule cm^{-3}, and d=9.0×10^{10} molecule cm^{-3}

Temp.	[HONO]^a	[HONO]^b	[H_2O] (RH=20%)	[H_2O] (RH=100%)	[$(H_2O)_2$] (RH=20%)	[$(H_2O)_2$] (RH=100%)	Unimolecular	[SO_2]^c	[SO_2]^d
213	1.21×10^{-1}	4.39	1.06×10^{-1}	5.32×10^{-1}	2.92×10^{-2}	7.30×10^{-1}	6.84×10^{-4}		
216	1.20×10^{-1}	4.35	1.61×10^{-1}	8.03×10^{-1}	7.00×10^{-2}	1.75	1.15×10^{-3}		
219	1.19×10^{-1}	4.31	2.40×10^{-1}	1.20	1.60×10^{-1}	4.00	1.90×10^{-3}		
224	1.17×10^{-1}	4.24	4.55×10^{-1}	2.28	2.99×10^{-1}	7.47	4.28×10^{-3}		
235	1.13×10^{-1}	4.08	1.69	8.45	8.90×10^{-1}	2.22×10^{1}	2.26×10^{-2}		
250	1.07×10^{-1}	3.87	8.29	4.15×10^{1}	4.22	1.06×10^{2}	1.74×10^{-1}		
259	1.03×10^{-1}	3.74	1.96×10^{1}	9.81×10^{1}	1.13×10^{1}	2.83×10^{2}	5.27×10^{-1}		
265	1.01×10^{-1}	3.65	3.37×10^{1}	1.68×10^{2}	1.65×10^{1}	4.13×10^{2}	1.06		
278	9.55×10^{-2}	3.46	9.98×10^{1}	4.99×10^{2}			4.36		
280	9.47×10^{-2}	3.43	1.09×10^{2}	5.47×10^{2}	4.85×10^{1}	1.21×10^{3}	5.35		
290	9.06×10^{-2}	3.28	2.11×10^{2}	1.06×10^{3}	8.32×10^{1}	2.08×10^{3}	1.44×10^{1}		
298	8.74×10^{-2}	3.16	3.45×10^{2}	1.73×10^{3}	1.25×10^{2}	3.13×10^{3}	3.02×10^{1}	3.20×10^{-1}	1.35×10^{1}
300	8.66×10^{-2}	3.13	3.88×10^{2}	1.94×10^{3}	1.36×10^{2}	3.39×10^{3}	3.62×10^{1}		
310	8.25×10^{-2}	2.99	6.81×10^{2}	3.41×10^{3}	2.13×10^{2}	5.31×10^{3}	8.60×10^{1}		
320	7.85×10^{-2}	2.84	1.15×10^{3}	5.74×10^{3}	3.20×10^{2}	8.01×10^{3}	1.94×10^{2}		

Table S4: Effective rate constants (in s^{-1}) for the reactions of anti-CH_3CHOO with HONO and $H_2O/(H_2O)_2/SO_2$ over the temperature range of 213–320 K.

Temp.	Unimolecular	$[H_2O]$ (RH=100%)	$[H_2O]$ (RH=20%)	$[(H_2O)_2]$ (RH=100%)	$[(H_2O)_2]$ (RH=20%)	$[HONO]=8.9\times10^{10}$	$[SO_2]=9.0\times10^{10}$
213	1.55×10^{-3}	8.98	1.80	7.48×10^{-1}	2.99×10^{-2}	8.38	
216	2.57×10^{-3}	1.32×10^{1}	2.64	2.00	8.00×10^{-2}	8.39	
219	4.20×10^{-3}	1.92×10^{1}	3.83	5.08	2.03×10^{-1}	8.39	
224	9.25×10^{-3}	3.49×10^{1}	6.98	1.12×10^{1}	4.49×10^{-1}	8.39	
235	4.68×10^{-2}	1.19×10^{2}	2.38×10^{1}	4.73×10^{1}	1.89	8.32	
250	3.40×10^{-1}	5.31×10^{2}	1.06×10^{2}	3.46×10^{2}	1.38×10^{1}	8.13	
259	1.00	1.19×10^{3}	2.39×10^{2}	1.18×10^{3}	4.71×10^{1}	7.97	
265	1.99	1.99×10^{3}	3.98×10^{2}	2.00×10^{3}	7.99×10^{1}	7.85	
275		4.42×10^{3}	8.84×10^{2}	5.55×10^{3}	2.22×10^{2}		
278	7.88	5.55×10^{3}	1.11×10^{3}			7.55	
280	9.64	6.04×10^{3}	1.21×10^{3}	8.30×10^{3}	3.32×10^{2}	7.50	
290	2.53×10^{1}	1.12×10^{4}	2.24×10^{3}	1.77×10^{4}	7.07×10^{2}	7.23	
295							1.8
298	5.22×10^{1}	1.78×10^{4}	3.56×10^{3}	3.13×10^{4}	1.25×10^{3}	7.01	6.03
300	6.23×10^{1}	1.99×10^{4}	3.98×10^{3}	3.53×10^{4}	1.41×10^{3}	6.95	
310	1.45×10^{2}	3.39×10^{4}	6.77×10^{3}	6.69×10^{4}	2.68×10^{3}	6.65	
320	3.20×10^{2}	5.55×10^{4}	1.11×10^{4}	1.21×10^{5}	4.83×10^{3}	6.35	

Table S5: Effective rate constants (in s^{-1}) for the reactions of syn-CH_3CHOO with HONO and $H_2O/(H_2O)_2/SO_2$ over the temperature range of 213–320 K.

Temp.	Unimolecular	$[H_2O]$ (RH=100%)	$[H_2O]$ (RH=20%)	$[(H_2O)_2]$ (RH=100%)	$[(H_2O)_2]$ (RH=20%)	$[HONO]=8.9\times10^{10}$	$[SO_2]=9.0\times10^{10}$
213	1.15	4.60×10^{-6}	9.21×10^{-7}	1.50×10^{-6}	6.01E-08	8.17×10^{-1}	
216	1.37	8.23×10^{-6}	1.65×10^{-6}	4.79×10^{-6}	1.92E-07	8.12×10^{-1}	
219	1.63	1.45×10^{-5}	2.89×10^{-6}	1.45×10^{-5}	5.78E-07	8.08×10^{-1}	
224	2.17	3.58×10^{-5}	7.16×10^{-6}	4.22×10^{-5}	1.69×10^{-6}	7.98×10^{-1}	
235	4.10	2.29×10^{-4}	4.59×10^{-5}	3.14×10^{-4}	1.26×10^{-5}	7.73×10^{-1}	
250	9.68	2.21×10^{-3}	4.42×10^{-4}	4.61×10^{-3}	1.84×10^{-4}	7.29×10^{-1}	
259	1.61×10^{1}	7.56×10^{-3}	1.51×10^{-3}	2.29×10^{-2}	9.17×10^{-4}	7.01×10^{-1}	
265	2.25×10^{1}	1.64×10^{-2}	3.28×10^{-3}	4.94×10^{-2}	1.98×10^{-3}	6.80×10^{-1}	
275		5.52×10^{-2}	1.10×10^{-2}	2.00×10^{-1}	7.99×10^{-3}		
278	4.64×10^{1}	7.81×10^{-2}	1.56×10^{-2}			6.36×10^{-1}	
280	5.18×10^{1}	9.18×10^{-2}	1.84×10^{-2}	3.57×10^{-1}	1.43×10^{-2}	6.29×10^{-1}	
290	8.92×10^{1}	2.48×10^{-1}	4.96×10^{-2}	1.07	4.27×10^{-2}	5.94×10^{-1}	
293							2.61
298	1.37×10^{2}	5.22×10^{-1}	1.04×10^{-1}	2.44	9.75×10^{-2}	5.66×10^{-1}	2.16
300	1.53×10^{2}	6.24×10^{-1}	1.25×10^{-1}	2.92	1.17×10^{-1}	5.59×10^{-1}	
310	2.59×10^{2}	1.47	2.94×10^{-1}	7.45	2.98×10^{-1}	5.25×10^{-1}	
320	4.37×10^{2}	3.28	6.56×10^{-1}	1.77×10^{1}	7.10×10^{-1}	4.92×10^{-1}	

Table S6: Capture rate constants (k_c) for anti-CH_3CHOO + HONO and syn-CH_3CHOO + HONO reactions within the temperature range of 213–320 K.

T (K)	k_c^{anti}	k_c^{syn}
213	1.78×10^{-10}	1.03×10^{-10}
216	1.82×10^{-10}	1.06×10^{-10}
219	1.86×10^{-10}	1.09×10^{-10}
224	1.92×10^{-10}	1.14×10^{-10}
235	2.06×10^{-10}	1.26×10^{-10}
250	2.24×10^{-10}	1.44×10^{-10}
259	2.35×10^{-10}	1.56×10^{-10}
265	2.41×10^{-10}	1.64×10^{-10}
278	2.54×10^{-10}	1.83×10^{-10}
280	2.56×10^{-10}	1.86×10^{-10}
290	2.65×10^{-10}	2.01×10^{-10}
298	2.72×10^{-10}	2.14×10^{-10}
300	2.73×10^{-10}	2.18×10^{-10}
310	2.81×10^{-10}	2.35×10^{-10}
320	2.88×10^{-10}	2.52×10^{-10}

Table S7: T1 diagnostic values for Criegee intermediates (CIs) and the corresponding stationary points, including reactant complexes (RCs), transition states (TSs), and product complexes (PCs).

Species	T1-Diagnostic
Anti-CH_3CHOO	0.035
RC-anti	0.025
TS-anti	0.023
PC-anti	0.016
Syn-CH_3CHOO	0.034
RC-syn	0.025
TS-syn	0.023
PC-syn	0.016
MACR-OO	0.033
MACR-OO-RC	0.024
MACR-OO-TS	0.022
MACR-OO-PC	0.016
MVK-OO	0.033
MVK-OO-RC	0.026
MVK-OO-TS	0.022
MVK-OO-PC	0.016

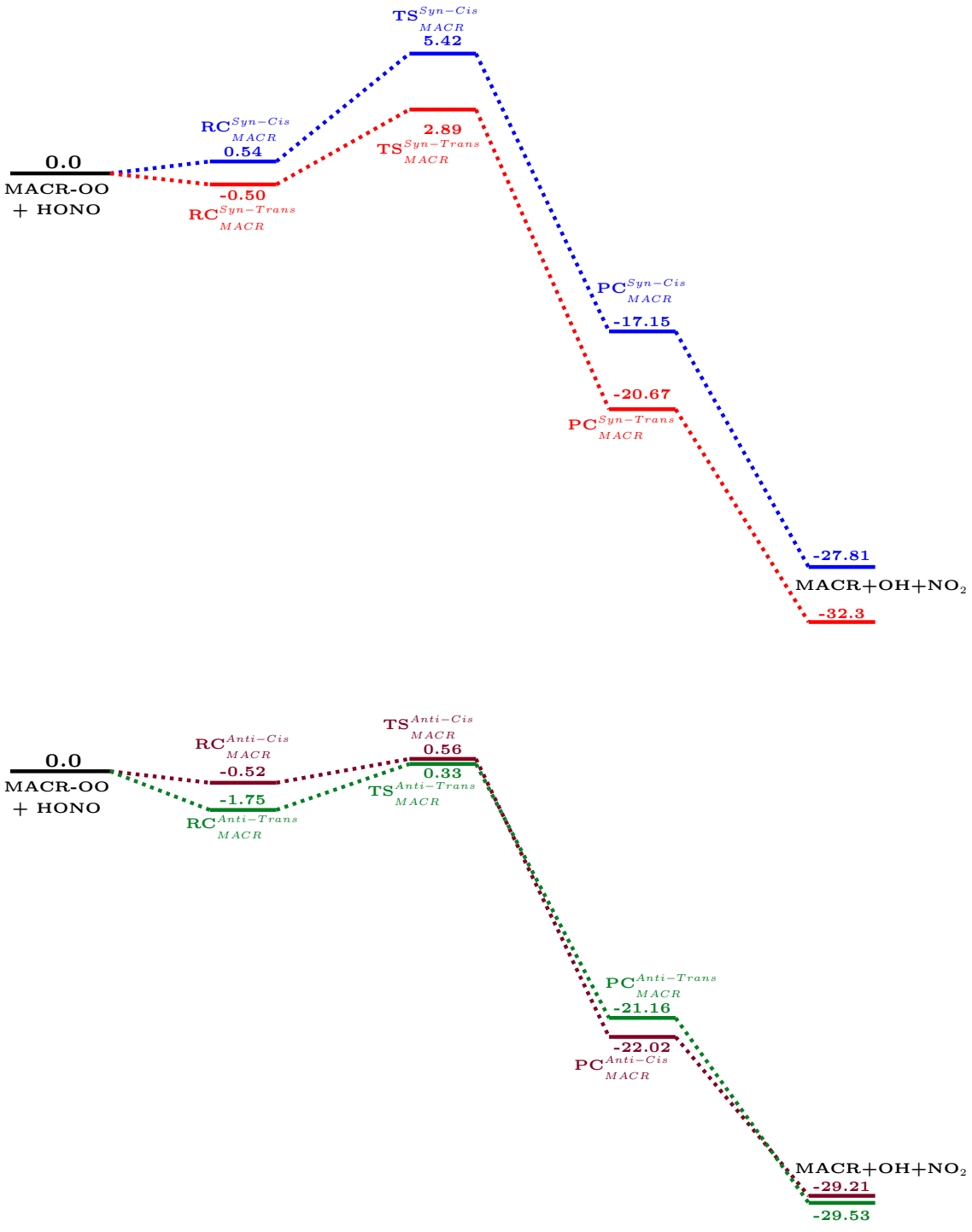

Figure S1: Top panel: Gibbs free energy profile (kcal mol^{-1}) for syn conformer of MACR-OO + HONO reaction obtained at CCSD(T)/CBS level of theory at 298 K. Bottom panel: Gibbs free energy profile (kcal mol^{-1}) for anti conformer of MACR-OO + HONO reaction obtained at same level of theory at 298 K.

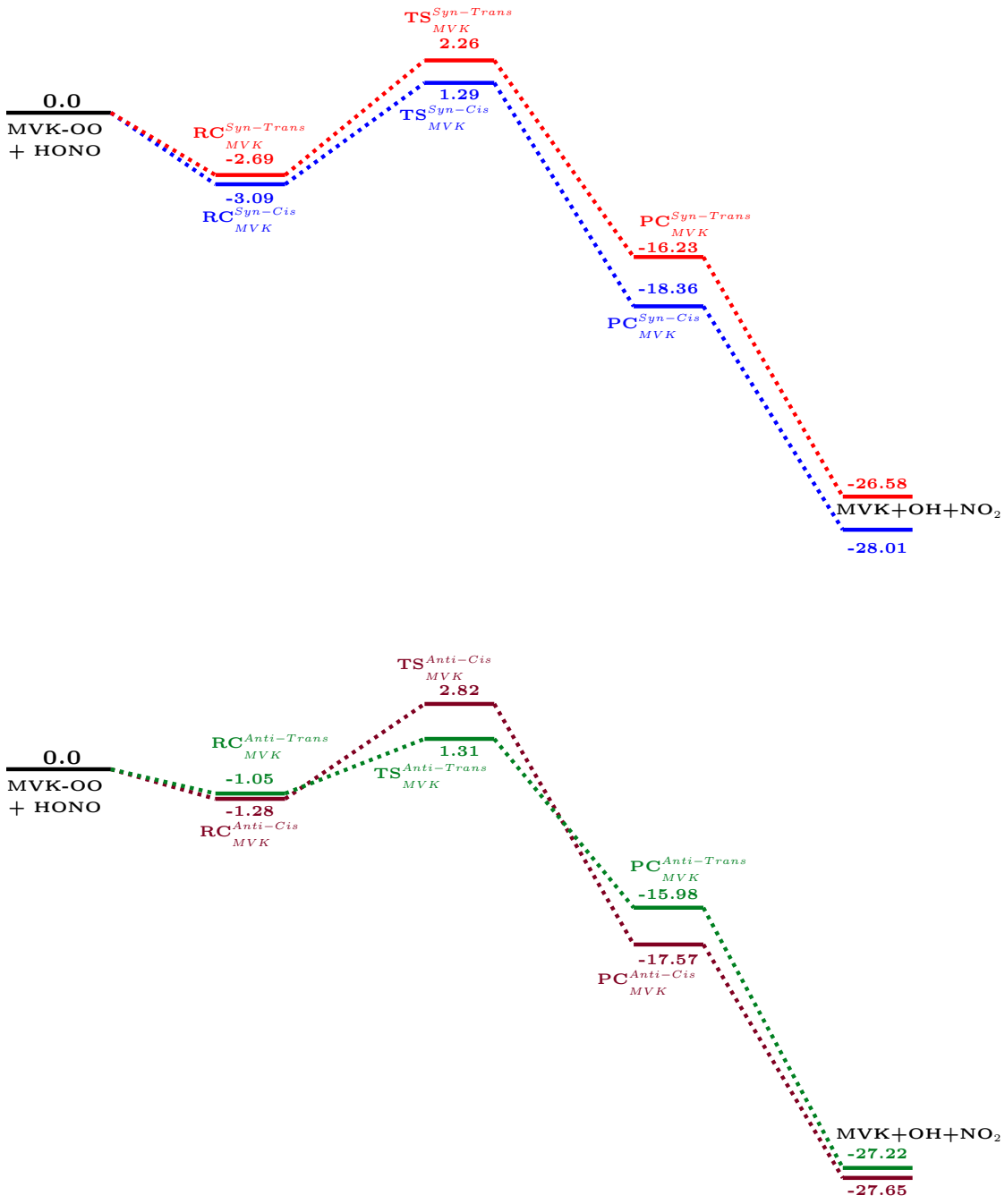

Figure S2: Top panel: Gibbs free energy profile (kcal mol^{-1}) for syn conformer of MVK-OO + HONO reaction obtained at CCSD(T)/CBS level of theory at 298 K. Bottom panel: Gibbs free energy profile (kcal mol^{-1}) for anti conformer of MVK-OO + HONO reaction obtained at same level of theory at 298 K.

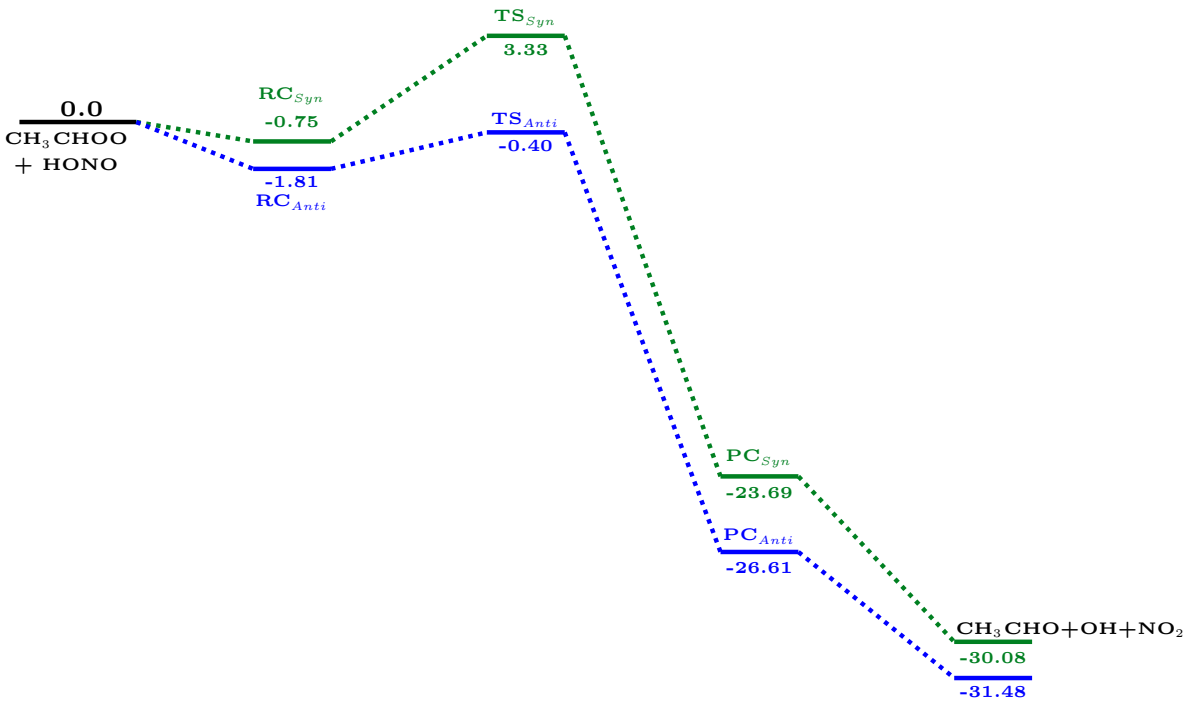

Figure S3: Gibbs free energy profile (kcal mol^{-1}) for syn/anti conformer of CH_3CHOO + HONO reaction obtained at CCSD(T)/CBS level of theory at 298 K.