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A theoretical study on gas-phase reactions of propadiene with NO_3: mechanism, kinetics and insights

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SHEME 1

$$\mathrm{R} \underset{1}{\overset{a}{\rightleftharpoons}} \mathrm{IM1} \underset{3}{\overset{2}{\rightleftharpoons}} \mathrm{IM3} \underset{5}{\overset{4}{\rightleftharpoons}} \mathrm{IM4} \xrightarrow{6} \mathrm{P3}$$

SHEME2

$$\mathrm{R} \underset{1}{\overset{a}{\rightleftharpoons}} \mathrm{IM2} \underset{3}{\overset{2}{\rightleftharpoons}} \mathrm{IM3} \underset{5}{\overset{4}{\rightleftharpoons}} \mathrm{IM4} \xrightarrow{6} \mathrm{P3}$$

For SCHEME 1:

$$k_{\mathrm{IM1}}(T,P) = \frac{\alpha_a}{h} \frac{Q_t^{\neq} Q_r^{\neq}}{Q_{\mathrm{CH_2=CH=CH_2}} Q_{\mathrm{NO_3}}} e^{-E_a/RT} \times \int_0^{\infty} \frac{\omega}{\mathrm{X}_3} N_a(E^{\neq}) e^{-E^{\neq}/RT} dE^{\neq} \quad (1)$$

$$k_{\mathrm{IM3}}(T,P) = \frac{\alpha_a}{h} \frac{Q_t^{\neq} Q_r^{\neq}}{Q_{\mathrm{CH_2=CH=CH_2}} Q_{\mathrm{NO_3}}} e^{-E_a/RT} \times \int_0^{\infty} \frac{\omega \mathrm{X}_2}{\mathrm{X}_3} N_a(E^{\neq}) e^{-E^{\neq}/RT} dE^{\neq} \quad (2)$$

$$k_{\mathrm{IM4}}(T,P) = \frac{\alpha_a}{h} \frac{Q_t^{\neq} Q_r^{\neq}}{Q_{\mathrm{CH_2=CH=CH_2}} Q_{\mathrm{NO_3}}} e^{-E_a/RT} \times \int_0^{\infty} \frac{\omega \mathrm{X}_2}{\mathrm{X}_3} N_a(E^{\neq}) e^{-E^{\neq}/RT} dE^{\neq} \quad (3)$$

$$k_{\mathrm{P3}}(T,P) = \frac{\alpha_a}{h} \frac{Q_t^{\neq} Q_r^{\neq}}{Q_{\mathrm{CH_2CH=CH_2}} Q_{\mathrm{NO_3}}} e^{-E_a/RT} \times \int_0^{\infty} \frac{k_6(E) \mathrm{X}_1 \mathrm{X}_2}{\mathrm{X}_3} N_a(E^{\neq}) e^{-E^{\neq}/RT} dE^{\neq} \quad (4)$$

Where

$\mathrm{X}_1 = k_4(E)/(k_5(E) + k_6(E) + \omega)$

$\mathrm{X}_2 = k_2(E)/(k_3(E) + k_4(E) + \omega - k_5(E)*\mathrm{X}_1)$

$\mathrm{X}_3 = k_1(E) + k_2(E) - k_3(E)*\mathrm{X}_2 + \omega$

The microcanonical rate constant is calculated using the RRKM theory as follows:

$$k_i(E) = \alpha_i C_i N_i(E_i^{\neq}) / h\rho_j(E_j) \quad (5)$$

In the above equations, α_a is the statistical factor for the reaction path a, and α_i is the statistical factor (degeneracy) for the *i*th reaction path; E_a is the energy barrier for the reaction step a. $Q_{\mathrm{NO_3}}$ and $Q_{\mathrm{CH_2=CH=CH_2}}$ are the total partition function of NO_3 and CH_2=CH=CH_2, respectively; $Q_t^{\neq}$ and $Q_r^{\neq}$ are the translational and rotational partition

functions of entrance transition state, respectively; $N_a(E^{\neq})$ is the number of state for the association transition state with excess energy $E^{\neq}$ above the association barrier. $k_i(E)$ is the energy-specific rate constant for the *i*th channel and C_i is the ratio of the overall rotational partition function of the TS_i and IM_j; $N_i(E_i^{\neq})$ is the number of states at the energy above the barrier height for transition state *i*; $\rho_j(E_j)$ is the density of states at energy E_j of the intermediate. The density of states and the number of states are calculated using the extended Beyer-Swinehart algorithm.

The calculation process for SCHEME 2 is similar to that of SCHEME 1.

The total rate constants k_{tot} is equal to k_{IM1} + k_{IM2} + k_{IM3}(SCHEME 1) + k_{IM3}(SCHEME 2) + k_{IM4}(SCHEME 1) + k_{IM4}(SCHEME 2) + k_{P3}(SCHEME 1) + k_{P3}(SCHEME 2)

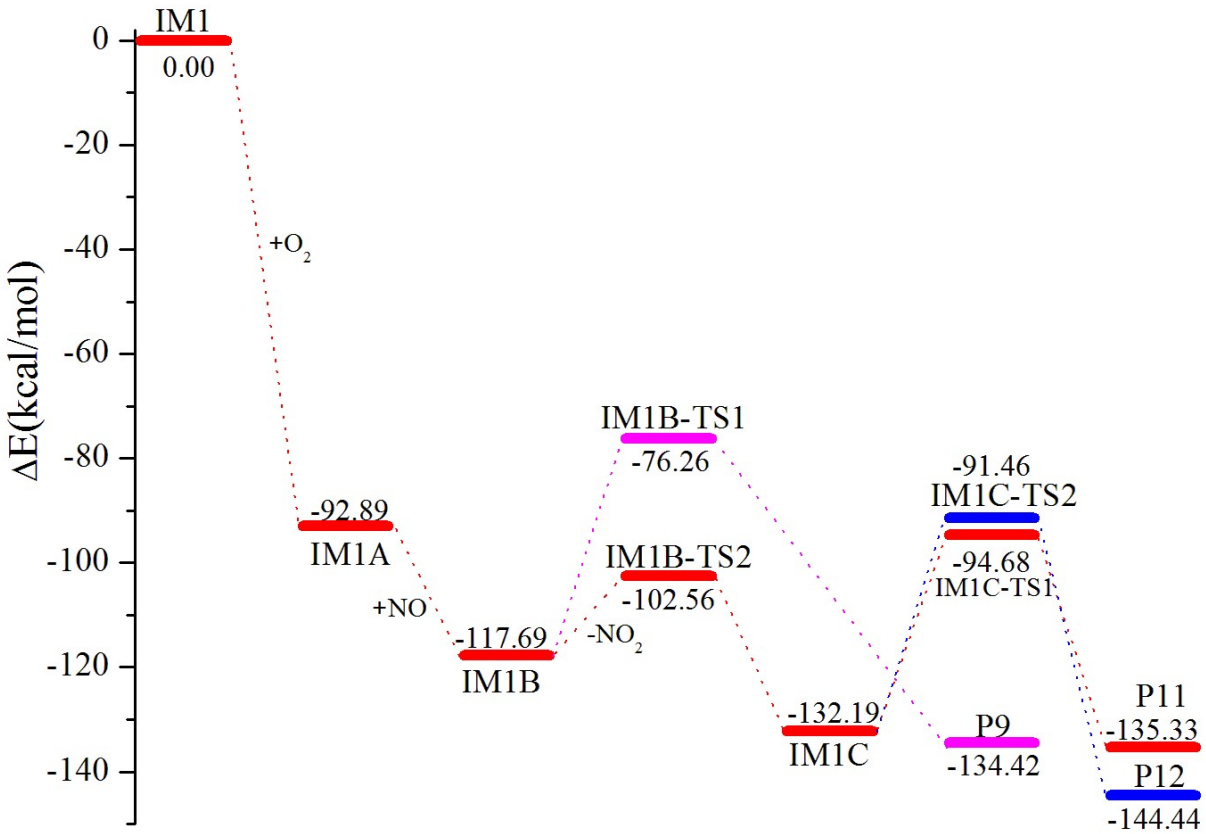

Figure S1. Schematic diagram of the subsequent pathways for IM1 in the presence of O2 and NO_2.

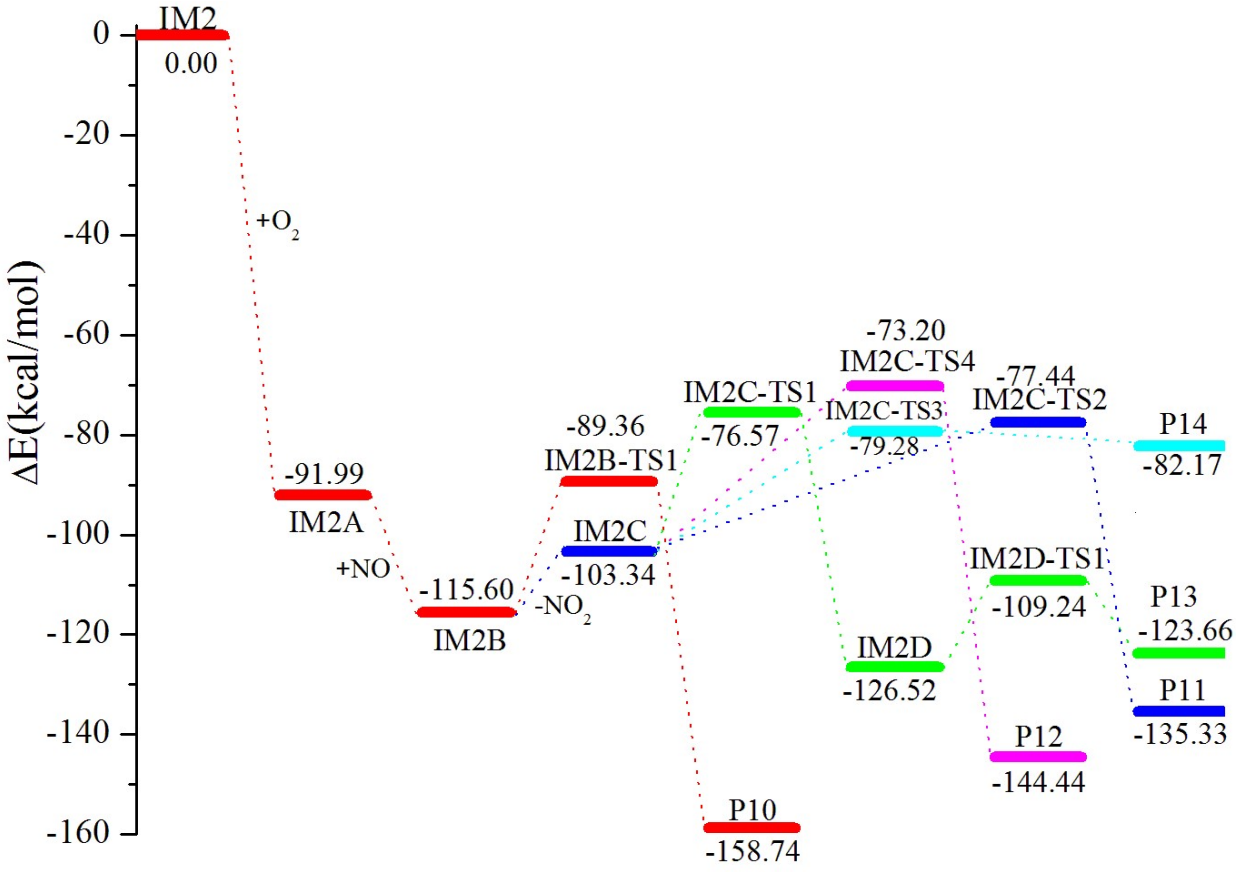

Figure S2. Schematic diagram of the subsequent pathways for IM2 in the presence of O_2 and NO_2.

Table S1. The harmonic vibrational frequencies (imaginary frequency is suffixed with *i*) and the moment of inertia (I_a, I_b and I_c) of all the species in the CH_2=C=CH_2 + NO_3 reaction.

Species	Frequencies (cm^{-1})	I_a, I_b, I_c (amu $bohr^2$)
IM1	58, 71, 145, 191, 341, 426, 475, 604, 633, 760, 844, 895, 897, 915, 981, 1013, 1278, 1315, 1372, 1407, 1451, 1719, 1767, 3052, 3069, 3114, 3151	339.76624, 1026.36185, 1062.89707
IM2	42, 79, 200, 373, 470, 488, 519, 532, 545, 725, 750, 780, 805, 824, 938, 955, 1026, 1265,1329, 1366, 1480, 1505, 1740, 3160, 3166, 3266, 3268	325.63100, 957.44707, 985.45143
IM3	81, 127, 209, 402, 478, 511, 592, 610, 649, 704, 778, 833, 882, 965, 1019, 1050, 1228, 1270, 1336, 1429, 1494, 1622, 1706, 3037, 3131, 3162, 3255	283.38746, 796.24919, 1050.77532
IM4	78, 97, 172, 218, 283, 352, 455, 547, 641, 736, 781, 818, 884, 890, 999, 1090, 1161, 1284, 1347, 1386, 1451, 1724, 1814, 2900, 2999, 3191, 3278	454.96650, 819.44000, 1200.33737
IM5	49, 59, 170, 271, 337, 399, 409, 493, 503, 628, 776, 799, 844, 995, 1007, 1084, 1272, 1286, 1362, 1454, 1460, 1546, 1780, 3048, 3099, 3155, 3273	235.44318, 1328.74025, 1479.83823
IM6	73, 88, 172, 203, 346, 418, 446, 519, 611, 712, 742, 769, 814,887, 1019, 1065, 1112, 1340, 1409, 1472, 1482, 1694, 1741, 3035, 3094, 3127, 3281	338.64696, 934.69133, 1000.58633
TS1	221*i*, 39, 59, 135, 193, 336, 348, 365, 623, 678, 786, 834, 874, 909, 942, 1003, 1044, 1049, 1294, 1399, 1455, 1591, 1955, 3099, 3139, 3173, 3228	303.83023, 1310.46446, 1327.80125
TS2	314*i*, 63, 71, 123,160, 253, 312, 385, 609, 680, 720, 793, 870, 894, 912, 977, 1031, 1056, 1290, 1404, 1449, 1576, 1885, 3128, 3135, 3227, 3228	343.49154, 1050.82503, 1182.19355
TS3	351*i*, 41, 59, 259, 271, 333, 393, 512, 696, 712, 721, 793, 892, 897, 940, 1027, 1037, 1045, 1133, 1401, 1455, 1522, 1903, 3122, 3142, 3211, 3235	311.71580, 927.62244, 1212.84791
TS4	652*i*, 65, 95, 163, 246, 295, 388, 426, 470, 497, 615, 731, 774,812, 889, 917, 968, 998, 1151, 1308, 1367, 1453, 1760, 1995, 3101, 3176, 3183	293.30251, 1039.01431, 1217.19420
TS5	1803*i*, 63, 99, 142, 270, 302, 355, 546, 598, 668, 719, 793, 843, 881, 975, 1081, 1089, 1161, 1282, 1350, 1435, 1613, 1765, 2130, 3067, 3080, 3194	174.63328, 1425.91991, 1551.37502

TS6	612*i*, 105, 126, 219, 302, 473, 494, 567, 578, 714, 794, 860, 902, 933, 978, 1022, 1128, 1189, 1328, 1410, 1470, 1560, 1789, 3045, 3061, 3104, 3156	330.29858, 829.92243, 1034.18617
TS7	764*i*, 123, 157, 332, 421, 493, 538, 580, 631, 683, 730, 756, 875, 900, 917, 958, 1021, 1053, 1251, 1417, 1464, 1542, 1697, 3149, 3163, 3259, 3260	293.36798, 810.19633, 996.14673
TS8	235*i*, 85, 180, 278, 449, 460, 475, 528, 613, 713, 737, 859, 863, 962, 991, 1077, 1183, 1259, 1334, 1422, 1468, 1698, 1774, 2982, 3028, 3161, 3253	354.96814, 762.21606, 1084.92023
TS9	353*i*, 78, 93, 119, 147, 257, 343, 451, 503, 576, 672, 748, 830, 919, 943, 947, 1053, 1180, 1305, 1468, 1482, 1515, 1607, 3146, 3157, 3257,3271	343.15150, 1087.44677, 1243.65003
TS10	775*i*, 76, 144, 155, 228, 257, 298, 319, 419, 482, 581, 655, 703, 740, 887, 905, 991, 1008, 1304, 1349, 1426, 1633, 1683, 1887, 2922, 3157,3254	441.11643, 814.53663, 1186.33033
TS11	666*i*, 51, 68, 180, 245, 254, 273, 300, 351, 472, 558, 641, 657, 689, 881, 1026, 1122, 1198, 1255, 1436, 1479, 1875, 1935, 3021, 3142, 3170,3260	314.38491, 1077.88079, 1330.37076
TS12	2114*i*, 75, 108, 131, 186, 236, 333, 399, 444, 526, 638, 702, 846, 877, 884, 989.9788 1099, 1176, 1271, 1365, 1399, 1690, 1819, 1879, 3043, 3098, 3199	223.52896, 1462.90196, 1623.85459
TS13	1862*i*, 83, 105, 133, 228, 333, 376, 399, 563, 608, 690, 775, 827, 895, 937, 966, 1133, 1162, 1237, 1325, 1424, 1665, 1865, 1911, 3111, 3156, 3247	351.47486, 1098.76665, 1192.01586
TS14	2172*i*, 68, 87, 189, 388, 429, 456, 462, 601, 665, 735, 753, 810, 893, 940, 976, 1054, 1076, 1223, 1347, 1432, 1665, 1755, 1829, 3083, 3184, 3189,	294.08221, 968.43179, 1096.99999
TS15	313*i*, 49, 69, 110, 125, 286, 364, 391, 465, 529, 708, 744, 808, 955, 1000, 1047, 1223, 1358, 1395, 1433, 1474, 1496, 1791, 3031, 3091, 3122, 3221	366.39285, 1096.61258, 1130.54421
TS16	443*i*, 40, 70, 104, 125, 200, 325, 363,408, 494, 497,541, 547, 571, 651, 781, 835, 1078, 1353, 1410, 1412, 1841, 2003, 3097, 3269, 3269, 3462	365.59125, 1058.90116, 1412.10029
TS17	353*i*, 78, 93, 119, 147, 257, 343, 451, 503, 576, 672, 748, 830, 919, 943, 947, 1053, 1180, 1305, 1468, 1482, 1515, 1607, 3146, 3157, 3257, 3271	343.15150, 1087.44677, 1243.65003

Table S2. Zero Point Energies (ZPE) without scaling factor, T_1 diagnostic values, relative Energies (ΔE), relative enthalpies (ΔH) and Gibbs free energy (ΔG) for the species involved in the subsequent reaction of IM1 and IM2 (energies in kcal/mol).

Species	ZPE	T_1	ΔE	ΔH	ΔG
IM1A	51.86	0.026	-92.89	-94.93	-55.74
IM1B	57.01	0.020	-117.69	-120.46	-81.27
IM1C	48.88	0.024	-132.19	-134.49	-95.30
IM2A	51.74	0.024	-91.99	-93.92	-54.73
IM2B	56.72	0.020	-115.60	-118.29	-79.10
IM2C	48.26	0.022	-103.34	-105.63	-66.44
IM2D	48.44	0.024	-126.52	-128.60	-89.42
IM1B-TS1	52.46	0.044	-76.26	-78.99	-39.80
IM1B-TS2	56.44	0.022	-102.56	-105.69	-66.40
IM1C-TS1	46.16	0.024	-94.68	-96.52	-57.33
IM1C-TS2	44.41	0.032	-91.46	-93.73	-54.54
IM2B-TS1	54.78	0.025	-89.36	-92.34	-53.15
IM2C-TS1	45.52	0.032	-76.57	-78.96	-39.78
IM2C-TS2	45.44	0.036	-77.44	-79.03	-39.84
IM2C-TS3	43.14	0.026	-79.28	-81.31	-42.12
IM2C-TS4	44.81	0.033	-73.20	-75.92	-36.74
IM2D-TS1	45.65	0.036	-109.24	-110.56	-71.37
P9: ($CH_2COONOCHO$ + HONO)	51.28	0.020 0.021	-134.42	-136.86	-100.29
P10: (CH_2CONO_2CHO + HONO)	54.84	0.018 0.021	-158.74	-160.84	-124.27
P11: (CH_2CO + CH_2O + NO_2)	41.92	0.017 0.015 0.024	-135.33	-135.42	-166.20
P12: (CH_2COCHO + HONO)	45.23	0.034 0.021	-144.44	-145.64	-126.17
P13: (cy-$CH_2COCHOH$ + NO_2)	46.35	0.014 0.024	-123.66	-125.01	-122.71
P14: (CH_2CONO_2CHO + H)	42.19	0.018	-82.17	-82.98	-71.66

Table S3. Calculated total rate constants and tropospheric lifetime (τ) at different temperatures (in K) and heights (in km) in the Earth atmosphere (in cm^3 $molecule^{-1}$ s^{-1})

T	Altitude	k_{tot}	τ (days)
200	12	1.56×10^{-16}	130.16
217	10	3.10×10^{-16}	65.5
223	9	3.87×10^{-16}	52.47
230	8	4.96×10^{-16}	40.94
236	7	6.08×10^{-16}	33.4
243	6	7.62×10^{-16}	26.65
249	5	9.18×10^{-16}	22.12
256	4	1.13×10^{-15}	17.97
262	3	1.34×10^{-15}	15.15
269	2	1.63×10^{-15}	12.46
275	1	1.90×10^{-15}	10.69
282	0	2.27×10^{-15}	8.95
288	0	2.65×10^{-15}	7.66
296	0	3.19×10^{-15}	6.36
298	0	3.34×10^{-15}	6.08

Table S4 The Cartesian coordinates, thermal correction to Enthalpy, thermal

correction to Gibbs Free Energy and the energy at the CCSD(T)/cc-pVTZ level of all the intermediates and transition states in the CH_2=C=CH_2 + NO_3 and subsequent reactions.

Species		Coordinates(Atom, X, Y, Z)	Thermal correction to Enthalpy	Thermal correction to Gibbs Free Energy	E
IM1	C	-0.83162 1.14757 -0.04294	0.081052	0.039759	-396.3101771
	N	1.23898 -0.11207 0.06937			
	O	1.06826 -0.07222 1.26906			
	O	0.30302 0.57073 -0.76294			
	O	2.10911 -0.6471 -0.57142			
	H	-1.14903 1.95102 -0.71546			
	H	-0.4748 1.58909 0.89083			
	C	-1.91071 0.17636 0.18522			
	C	-2.26626 -1.05297 -0.09286			
	H	-1.64274 -1.71003 -0.70775			
	H	-3.19785 -1.48258 0.27251			
IM2	C	-1.16261 -0.00012 -0.20102	0.072012	0.079990	-396.34657
	C	-1.72771 -1.24002 0.03308			
	H	-1.19029 -2.14998 -0.20387			
	C	-1.72731 1.24023 0.03176			
	H	-2.72462 -1.31873 0.45147			
	H	-2.72413 1.3198 0.4502			
	H	-1.18957 2.14972 -0.20627			
	N	1.22933 0.00002 0.09474			
	O	0.98088 0.00094 1.27614			
	O	2.28177 -0.00046 -0.48775			
	O	0.10349 -0.00067 -0.8306			
IM3	C	-0.56159 1.2499 0.1179	0.081683	0.042807	-396.3531703
	H	-0.66558 1.64887 1.13531			
	H	-1.01086 1.94126 -0.59787			
	O	0.81527 1.12602 -0.2303			
	C	-1.1207 -0.16026 0.00856			
	O	-0.09263 -1.04755 -0.00118			
	N	1.1976 -0.18201 0.27817			
	O	2.23696 -0.63198 -0.09919			
	C	-2.40244 -0.51779 -0.06501			
	H	-2.69864 -1.55937 -0.09907			
	H	-3.1765 0.24019 -0.10893			
IM4	C	-0.71354 1.26044 0.1524	0.080275	0.039313	-396.3405625

	H	-0.88032 1.59645 1.1852			
	H	-1.36914 1.83802 -0.51184			
	O	0.59582 1.4738 -0.26095			
	C	-1.05853 -0.22369 0.01063			
	O	0.05643 -1.01861 -0.07367			
	N	1.1758 -0.27161 0.27434			
	O	2.17525 -0.71438 -0.10286			
	C	-2.27333 -0.75927 -0.04924			
	H	-2.41724 -1.82932 -0.11143			
	H	-3.1452 -0.11855 -0.04879			
IM5	C	-0.49693 1.07934 0.35421	0.080386	0.038607	-396.3985285
	H	-0.4109 1.2712 1.42934			
	H	-0.956 1.94503 -0.12984			
	O	0.81407 1.004 -0.23805			
	C	-1.32663 -0.20031 0.15744			
	O	-1.0805 -1.19932 0.85438			
	N	1.48173 -0.24037 0.09182			
	O	2.54628 -0.26363 -0.40617			
	C	-2.37616 -0.22127 -0.80851			
	H	-2.96528 -1.12653 -0.91119			
	H	-2.61049 0.63354 -1.4354			
IM6	C	1.25114 -0.21521 0.05231	0.080491	0.039633	-396.3089064
	C	2.09168 -1.00207 -0.58242			
	H	2.17223 -1.97771 -1.03658			
	C	1.71785 1.11751 0.57658			
	H	2.77604 1.2188 0.33185			
	H	1.17476 1.95335 0.12437			
	H	1.60464 1.17833 1.6664			
	N	-1.19402 0.05098 -0.06791			
	O	-0.9687 1.01043 -0.76557			
	O	-2.23549 -0.39521 0.33656			
	O	-0.03462 -0.73451 0.38532			
TS1	C	-1.16954 1.15794 0.22294	0.078099	0.035767	-396.2742434
	N	1.4322 -0.11728 0.04071			
	O	1.15045 -0.32641 1.21077			
	O	0.55558 0.50274 -0.76299			
	O	2.47194 -0.41199 -0.5356			
	H	-1.21359 2.02546 -0.42992			
	H	-0.65209 1.26974 1.17007			
	C	-2.00133 0.12288 0.02802			
	C	-2.73994 -0.91947 -0.20316			
	H	-2.34567 -1.77834 -0.74644			
	H	-3.77291 -0.97872 0.13706			

TS2	C	1.6355 -0.03361 -0.01582	0.077557	0.035330	-396.2724481
	C	1.68977 1.26471 -0.35638			
	H	1.03231 1.98265 0.12393			
	C	1.93473 -1.23447 0.40563			
	H	2.3129 1.60119 -1.18204			
	H	2.81931 -1.3893 1.02007			
	H	1.30847 -2.09101 0.18122			
	N	-1.29444 0.02354 0.03818			
	O	-1.03582 0.76453 0.97552			
	O	-2.38957 -0.43785 -0.25866			
	O	-0.3211 -0.35769 -0.79323			
TS3	C	1.53497 0.09767 0.00213	0.078074	0.037166	-396.2672579
	C	1.03983 1.37723 0.05933			
	N	-1.22013 -0.17429 0.00618			
	O	-0.97186 1.09505 -0.06595			
	O	-0.25077 -0.98794 0.16008			
	O	-2.37351 -0.5617 -0.07079			
	H	0.94407 1.88434 1.01446			
	H	1.02979 2.00164 -0.82897			
	C	2.39255 -0.88098 -0.08895			
	H	3.461 -0.67485 -0.13038			
	H	2.07102 -1.91788 -0.12013			
TS4	C	-0.75297 1.06355 0.24587	0.072047	0.030666	-396.2315166
	N	1.28297 -0.25391 -0.00782			
	O	0.67661 -1.17891 0.46769			
	O	0.56999 1.0122 -0.19807			
	O	2.41886 -0.16367 -0.39102			
	H	-0.96318 2.04348 0.66332			
	H	-0.45981 0.62609 2.17964			
	C	-1.70804 0.21951 -0.11312			
	C	-2.66131 -0.64721 -0.30561			
	H	-2.87573 -1.42531 0.42753			
	H	-3.27181 -0.63892 -1.20748			
TS5	C	0.77523 0.13988 0.3659	0.075384	0.034597	-396.2357106
	N	-1.58367 0.03331 -0.03685			
	O	-1.5179 1.23913 -0.06108			
	O	-0.29529 -0.69839 0.11486			
	O	-2.51811 -0.71586 -0.09651			
	H	0.6863 0.77685 1.2505			
	H	1.09838 0.70142 -0.79134			
	C	1.98088 -0.14589 -0.31684			
	C	3.28696 -0.03578 -0.04835			
	H	4.02508 0.14018 -0.82576			

	H	3.66788 -0.19988 0.96214			
TS6	C	1.31265 -0.05448 -0.0354	0.078802	0.039989	-396.2761473
	C	0.66855 1.24937 0.109			
	H	0.95793 1.9601 -0.67123			
	C	2.4128 -0.70206 -0.31769			
	H	3.32893 -0.19054 -0.62841			
	H	2.4666 -1.78809 -0.25704			
	N	-1.18498 -0.21938 0.13266			
	O	-0.78814 1.12495 -0.05514			
	O	-2.10791 -0.61222 -0.56249			
	O	-0.31375 -0.89864 0.74201			
	H	0.85582 1.68452 1.09758			
TS7	C	0.82211 0.27257 -0.42543	0.078620	0.040795	-396.2951493
	C	0.27611 1.36768 0.41159			
	N	-1.42648 -0.28429 -0.19848			
	O	-0.20371 -0.77113 -0.59799			
	O	-1.50018 0.95932 -0.30549			
	O	-2.12937 -1.01936 0.46284			
	H	0.4171 2.3939 0.10199			
	H	0.12044 1.18311 1.4708			
	C	2.02376 0.07415 -0.90789			
	H	2.38584 0.89188 -1.56228			
	H	2.59333 -0.80918 -0.70737			
TS8	C	-0.73413 1.25775 0.16131	0.079738	0.041468	-396.3424561
	H	-0.89893 1.58522 1.20116			
	H	-1.41642 1.83091 -0.4849			
	O	0.56065 1.50796 -0.27326			
	C	-1.04988 -0.23242 0.01096			
	O	0.08117 -1.00922 -0.08961			
	N	1.25428 -0.20607 0.29917			
	O	2.26884 -0.66054 -0.06453			
	C	-2.25424 -0.79685 -0.0458			
	H	-2.37533 -1.87153 -0.11781			
	H	-3.14506 -0.17856 -0.03226			
TS9	C	-0.92876 1.17927 0.49531	0.077183	0.035247	-396.2973738
	H	-0.50117 1.39647 1.46455			
	H	-1.22103 2.01776 -0.12533			
	O	1.13923 1.02586 -0.22929			
	C	-1.28824 -0.18321 0.17598			
	O	-0.68657 -1.1279 0.73753			
	N	1.48807 -0.13775 -0.05587			
	O	2.56506 -0.61 -0.27144			
	C	-2.3352 -0.32577 -0.77176			

	H	-2.77297 -1.30217 -0.94365			
	H	-2.74999 0.52671 -1.29598			
TS10	C	-1.12212 1.03553 0.0228	0.071509	0.029749	-396.3153421
	H	-1.03661 0.97598 1.82664			
	H	-2.18944 1.30671 0.15755			
	O	-0.27677 1.87604 -0.26817			
	C	-0.87147 -0.44174 -0.06007			
	O	0.38653 -0.83543 -0.39116			
	N	1.45064 -0.07091 0.42912			
	O	2.49796 -0.292 -0.013			
	C	-1.87319 -1.32687 0.06709			
	H	-1.70204 -2.39266 -0.03269			
	H	-2.88751 -0.98423 0.24442			
TS11	C	0.26692 1.26463 0.22211	0.076504	0.033582	-396.3383862
	H	0.85144 2.05835 -0.2357			
	H	0.2816 1.16685 1.31139			
	O	-0.84368 0.97456 -0.41005			
	C	1.45318 -0.47695 0.02061			
	O	0.63767 -1.35469 0.04703			
	N	-1.70041 -0.14744 0.43706			
	O	-2.56605 -0.53281 -0.21678			
	C	2.70194 -0.00001 -0.09325			
	H	3.44346 -0.62118 -0.58903			
	H	2.97062 1.0055 0.19545			
TS12	C	0.2237 -0.47652 0.16369	0.073512	0.031556	-396.3164866
	H	0.02396 -1.00154 1.10721			
	H	1.05684 -1.41253 -0.45844			
	O	-0.8819 0.08807 -0.39743			
	C	1.54883 0.26446 0.1187			
	O	1.7876 1.44488 0.10101			
	N	-2.12966 -0.25664 0.38295			
	O	-3.07312 0.14777 -0.17003			
	C	2.43498 -0.93103 -0.16238			
	H	2.80063 -1.50838 0.68842			
	H	3.12054 -0.86819 -1.00635			
TS13	C	-0.34736 -0.85061 0.60192	0.074758	0.033785	-396.3099948
	H	-0.88275 -1.52765 -0.45933			
	H	-0.66194 -1.44059 1.46562			
	O	1.00793 -0.64897 0.64603			
	C	-1.31045 0.13771 0.05595			
	O	-1.79689 -0.69104 -0.92286			
	N	1.4829 0.28335 -0.46215			
	O	2.62018 0.47886 -0.33097			

	C	-1.65855 1.3879 0.36169			
	H	-2.42539 1.91326 -0.19713			
	H	-1.16182 1.91077 1.17093			
TS14	C	1.07314 -0.25313 0.07173	0.074565	0.034633	-396.2409157
	C	2.10791 -0.84957 -0.50489			
	H	2.34281 -1.80684 -0.9627			
	C	1.67096 1.04542 0.51508			
	H	2.73533 0.36539 -0.1118			
	H	1.43283 1.94518 -0.05097			
	H	1.85116 1.19462 1.5816			
	N	-1.29824 0.03259 -0.06992			
	O	-1.04184 1.01671 -0.72082			
	O	-2.34493 -0.4196 0.30455			
	O	-0.16154 -0.79497 0.359			
TS15	C	1.27592 0.093 -0.23924	0.077835	0.035011	-396.2870604
	C	1.75497 1.35751 -0.0002			
	H	1.42731 2.32645 -0.36274			
	C	1.87152 -1.14738 0.37638			
	H	2.79947 -0.92678 0.91089			
	H	1.15765 -1.58664 1.08425			
	H	2.06763 -1.89359 -0.40093			
	N	-1.42194 -0.00399 0.08866			
	O	-1.22041 0.40115 1.19894			
	O	-2.39258 -0.35525 -0.51059			
	O	0.24888 -0.00968 -1.02257			
TS16	C	0.90654 0.48483 0.00002	0.075304	0.030649	-396.2319537
	C	1.21047 1.67712 -0.00016			
	H	1.72125 2.61268 -0.00103			
	C	2.76445 -1.01194 0.00024			
	H	3.57309 -0.29061 -0.0022			
	H	2.53648 -1.51957 0.93056			
	H	2.5335 -1.52249 -0.92774			
	N	-1.44922 -0.14008 0.00004			
	O	-1.68041 1.02864 0.00044			
	O	-2.11839 -1.1278 -0.0002			
	O	0.11023 -0.55077 -0.0003			
TS17	C	1.35084 0.70845 -0.00037	0.072182	0.028186	-396.2594586
	N	-1.825 -0.04687 0.00006			
	O	-0.72012 -0.81871 -0.00034			
	O	-1.70226 1.16863 0.00034			
	O	-2.86123 -0.69037 0.00007			
	H	0.97755 1.72751 -0.00097			
	H	0.35704 -0.05637 -0.00002			

	C	2.51132	0.18713	-0.0001			
	C	3.69118	-0.43528	0.00031			
	H	4.19429	-0.69061	0.93005			
	H	4.19496	-0.69052	-0.92908			
IM1A	C	-0.04302	-0.33023	1.10281	0.092460	0.046322	-546.5095261
	N	1.95252	-0.16673	-0.23344			
	O	1.47206	-1.08334	-0.86079			
	O	1.22966	0.30165	0.92046			
	O	2.97452	0.44544	-0.40069			
	H	-0.254	-0.15612	2.16301			
	H	0.02793	-1.40739	0.93273			
	C	-1.10956	0.27372	0.2223			
	C	-1.10526	1.46962	-0.35983			
	H	-0.25914	2.13195	-0.22477			
	H	-1.9387	1.78755	-0.97275			
	O	-2.15871	-0.64951	0.11884			
	O	-3.22962	-0.22268	-0.5348			
IM1B	C	0.96909	-1.12285	-0.64745	0.102883	0.051516	-676.266867
	N	2.57775	0.57088	-0.07028			
	O	1.91659	1.28781	-0.7865			
	O	2.18764	-0.81087	0.035			
	O	3.55392	0.81194	0.59068			
	H	1.03545	-2.20508	-0.7975			
	H	0.9358	-0.63445	-1.62453			
	C	-0.2533	-0.76084	0.16923			
	C	-0.28808	-0.52792	1.47728			
	H	0.63076	-0.58175	2.04729			
	H	-1.20752	-0.29704	1.9973			
	O	-1.32212	-0.75777	-0.71127			
	O	-2.55668	-0.57272	-0.02877			
	N	-2.92382	0.86754	-0.24864			
	O	-3.97163	1.0565	0.22779			
IM1C	C	0.54995	-0.86848	-0.63914	0.086758	0.043486	-471.4841158
	N	-1.55274	-0.03981	0.17515			
	O	-1.1418	-0.41195	1.25362			
	O	-0.70628	-0.24649	-0.9599			
	O	-2.58944	0.49737	-0.12027			
	H	0.90152	-1.22204	-1.61356			
	H	0.40672	-1.72705	0.01927			
	C	1.60029	0.06699	-0.02888			
	C	1.4132	1.48325	-0.06877			
	H	0.5506	1.94376	-0.53746			
	H	2.17875	2.11254	0.37125			

	O	2.61889 -0.45382 0.44595			
IM2A	C	-0.32656 0.69078 0.01974	0.092440	0.045989	-546.5079965
	C	-1.10661 -0.2958 0.83062			
	H	-0.46414 -1.01913 1.33572			
	C	-0.62946 1.97945 -0.12211			
	H	-1.75243 0.20704 1.55193			
	H	-1.49404 2.40182 0.37745			
	H	-0.03562 2.62673 -0.75852			
	N	1.89499 -0.2228 -0.02165			
	O	1.88559 -0.00817 1.16889			
	O	2.73319 -0.70771 -0.72884			
	O	0.69702 0.16282 -0.7753			
	O	-1.96549 -1.12748 -0.02634			
	O	-2.99319 -0.4324 -0.47898			
IM2B	C	0.33496 -0.62784 0.59809	0.102547	0.050954	-676.2633032
	C	-0.18506 -1.24748 -0.66863			
	H	0.6202 -1.40624 -1.39233			
	C	0.09167 -1.0639 1.83246			
	H	-0.66539 -2.2076 -0.45463			
	H	-0.53618 -1.93287 1.99845			
	H	0.49996 -0.5539 2.69837			
	N	2.3604 0.46016 -0.10398			
	O	2.76564 -0.66134 -0.30979			
	O	2.88021 1.52786 -0.27212			
	O	1.01364 0.58817 0.45541			
	O	-1.08678 -0.39278 -1.38571			
	O	-2.32457 -0.36002 -0.67124			
	N	-2.37265 0.94272 0.03057			
	O	-3.40842 1.03759 0.57			
IM2C	C	-0.88943 0.57797 -0.0747	0.085773	0.042457	-471.4402272
	C	-1.5387 -0.71674 0.37489			
	H	-1.00612 -1.1071 1.26947			
	C	-1.45087 1.78247 -0.00737			
	H	-2.57073 -0.52629 0.7196			
	H	-2.46003 1.90101 0.37332			
	H	-0.92669 2.66778 -0.35042			
	N	1.43669 -0.00456 0.08704			
	O	1.22081 -0.13768 1.27146			
	O	2.43555 -0.1841 -0.55246			
	O	0.33234 0.46579 -0.74102			
	O	-1.46612 -1.73972 -0.52524			
IM2D	C	-1.07937 0.52341 -0.10958	0.086369	0.043335	-471.4749801
	C	-1.61867 -0.75249 0.02901			

	H	-0.63213 -2.36133 0.42906			
	C	-1.74753 1.69522 0.16171			
	H	-2.6327 -0.87236 0.4002			
	H	-2.78247 1.67122 0.4758			
	H	-1.26028 2.6505 0.03148			
	N	1.30482 0.13391 0.12213			
	O	1.0587 -0.22108 1.24413			
	O	2.33324 0.14843 -0.48257			
	O	0.19835 0.6607 -0.6738			
	O	-0.937 -1.87417 -0.33946			
IM1B-TS1	C	0.96562 -1.07968 -0.71162	0.095704	0.044570	-676.19802
	N	3.06637 0.32693 -1.04881			
	O	2.4009 0.55074 -2.02503			
	O	2.19079 -0.80543 -0.02474			
	O	4.12529 0.62392 -0.58082			
	H	1.03583 -2.14682 -0.93412			
	H	1.42806 -0.26104 -1.60938			
	C	-0.24804 -0.78607 0.14135			
	C	-0.27614 -0.65434 1.46084			
	H	0.64507 -0.75275 2.01705			
	H	-1.19237 -0.46628 1.99905			
	O	-1.3241 -0.7157 -0.72641			
	O	-2.55193 -0.56774 -0.039			
	N	-2.9549 0.89437 -0.21191			
	O	-3.99459 1.05074 0.2556			
IM1B-TS2	C	0.53526000 0.32618800 -0.86743100	0.101595	0.051313	-676.2434689
	N	2.76428200 -0.12679200 -0.07300400			
	O	2.74124300 1.02429400 0.30296400			
	O	1.60239500 -0.62635800 -0.75870100			
	O	3.62162600 -0.96481500 0.02834100			
	H	-0.04800600 -0.03677300 -1.72054200			
	H	0.92078800 1.31962700 -1.10537000			
	C	-0.34619100 0.38872000 0.36496200			
	C	-0.31585200 -0.50097100 1.39583200			
	H	0.41715500 -1.30010200 1.44284800			
	H	-1.01576800 -0.38559700 2.21367800			
	O	-1.25722100 1.33326700 0.36116400			
	O	-2.67879500 0.69013400 -0.48304800			
	N	-2.88677900 -0.44689400 0.11161400			
	O	-3.86124800 -1.06464500 -0.25835300			
IM1C-TS1	C	0.38553 -0.99037 -0.55247	0.083092	0.038338	-471.423992
	N	-1.68658 -0.02061 0.16736			
	O	-1.4196 -0.46575 1.25237			

	O	-0.75264 -0.35394 -0.94098			
	O	-2.59316 0.6563 -0.22852			
	H	0.87307 -1.42449 -1.42015			
	H	0.34616 -1.5504 0.37526			
	C	2.02295 0.28212 0.05316			
	C	1.49673 1.5065 -0.04376			
	H	0.63216 1.71747 -0.65479			
	H	1.92098 2.28981 0.57772			
	O	2.8407 -0.54631 0.31824			
IM1C-TS2	C	0.55711 -0.83371 -0.65327	0.079668	0.037052	-471.4164221
	N	-1.89929 -1.10403 -0.15952			
	O	-1.25581 -2.03472 0.37317			
	O	-0.63274 -0.21265 -0.94395			
	O	-2.97503 -0.61028 -0.33316			
	H	0.90837 -1.16558 -1.63283			
	H	-0.05165 -1.6843 0.02122			
	C	1.62253 0.06592 -0.01901			
	C	1.44273 1.48165 0.02686			
	H	0.57432 1.96896 -0.39736			
	H	2.2212 2.07729 0.48612			
	O	2.6446 -0.4813 0.40352			
IM2B-TS1	C	0.68400200 -1.13687200 -0.09470700	0.099023	0.048414	-676.2211926
	C	-0.42087100 -0.79840200 0.87895100			
	H	-0.13223900 -0.96984300 1.92972300			
	C	0.57421800 -1.90461800 -1.17076200			
	H	-0.60729900 0.31824100 0.86381600			
	H	-0.37600900 -2.36028400 -1.41587900			
	H	1.43196900 -2.09897700 -1.80110600			
	N	2.18755300 0.77079600 -0.00345700			
	O	1.30902200 1.35977300 -0.56763300			
	O	3.25783800 1.11972400 0.38077400			
	O	1.93977000 -0.67247300 0.29424000			
	O	-1.61032300 -1.39393700 0.64304600			
	O	-2.69952100 -0.24352300 -0.16853900			
	N	-2.25033600 0.89533800 0.08041800			
	O	-2.80941400 1.89134600 -0.30641100			
IM2C-TS1	C	-0.87535 0.58494 -0.06944	0.081271	0.039121	-471.3960668
	C	-1.54712 -0.69431 0.38597			
	H	-0.98057 -1.84617 0.64738			
	C	-1.41856 1.79475 -0.00018			
	H	-2.54918 -0.47361 0.78876			
	H	-2.4227 1.92559 0.383			
	H	-0.88225 2.66828 -0.34772			

	N	1.45806 -0.02675 0.08345			
	O	1.24842 -0.15944 1.26103			
	O	2.44108 -0.21217 -0.56233			
	O	0.34107 0.45716 -0.73954			
	O	-1.57005 -1.70103 -0.52844			
IM2C-TS2	C	-0.72243 0.18722 -0.49881	0.082330	0.036811	-471.3972296
	C	-2.31101 -0.7573 -0.14038			
	H	-2.88146 -0.40405 -1.02084			
	C	-0.90305 1.52148 -0.52044			
	H	-1.94828 -1.79501 -0.237			
	H	-1.87181 1.93765 -0.28226			
	H	-0.0832 2.18187 -0.78049			
	N	1.86621 -0.08681 0.12403			
	O	1.8326 0.9801 0.65809			
	O	2.68522 -0.93667 -0.0276			
	O	0.20875 -0.64441 -0.5865			
	O	-2.55903 -0.27667 1.00728			
IM2C-TS3	C	-0.87535 0.58494 -0.06944	0.078008	0.034896	-471.3956386
	C	-1.54712 -0.69431 0.38597			
	H	-0.99024 -1.12142 1.24793			
	C	-1.41856 1.79475 -0.00018			
	H	-3.02199 -0.7544 1.02881			
	H	-2.4227 1.92559 0.383			
	H	-0.88225 2.66828 -0.34772			
	N	1.45806 -0.02675 0.08345			
	O	1.24842 -0.15944 1.26103			
	O	2.44108 -0.21217 -0.56233			
	O	0.34107 0.45716 -0.73954			
	O	-1.57005 -1.70103 -0.52844			
IM2C-TS4	C	-0.87621 0.51406 -0.23442	0.079639	0.038977	-471.3899143
	C	-1.54712 -0.69431 0.38597			
	H	-0.62012 -0.61119 1.35001			
	C	-1.43666 1.71087 -0.36499			
	H	-2.56514 -0.43351 0.71866			
	H	-2.45495 1.87987 -0.03826			
	H	-0.89972 2.5319 -0.82226			
	N	1.24517 -0.00307 0.29547			
	O	0.68349 -0.48998 1.43434			
	O	2.38561 0.13084 -0.01951			
	O	0.36405 0.30891 -0.83831			
	O	-1.52654 -1.79324 -0.345			
IM2D-TS1	C	-1.05389 0.4908 -0.11174	0.083067	0.036095	-471.4448463
	C	-1.54797 -0.79003 0.10519			

	H	-1.23235	-2.67801	0.06223	
	C	-1.71152	1.67266	0.14222	
	H	-2.52408	-0.94835	0.54578	
	H	-2.72454	1.67199	0.5218	
	H	-1.22938	2.61729	-0.0624	
	N	1.55792	0.22171	0.32287	
	O	1.32099	0.03374	1.48251	
	O	2.58935	0.22157	-0.27811	
	O	0.20164	0.58343	-0.72738	
	O	-0.79125	-1.8682	-0.21153	