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HO_2 radical, a crucial sink of Furfural in the atmosphere

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Table S1: A list of T1 diagnostic values for the species involved in Furfural + $HO_2^\bullet$ reaction.

Species	T1-diagnostic
t-Furfural	0.015
c-Furfural	0.016
$HO_2^\bullet$	0.028
t-RC	0.035
t-TS	0.021
t-PC	0.027
c-RC	0.034
c-TS	0.029
c-PC	0.026

Table S2: Relative energies (in kcal mol^{-1}) of all species, obtained at different levels of theory. Zero-point energy (ZPE) values are given at M062X/jun-cc-pVTZ level of theory. Here, HAT-AA refers to hydrogen atom transfer assisted addition by $HO_2^\bullet$, while H-Abs denotes hydrogen abstraction by $HO_2^\bullet$.

Reaction Type	Species	M062X/ jun-cc-pVTZ	CCSD(T)/ cc-pVDZ-F12	CCSD(T)/ cc-pVTZ-F12	ZPE
HAT-AA	*c*-Furfural+$HO_2^\bullet$	0.00	0.00	0.00	0.00
	c-RC	-10.69	-10.83	-10.32	1.63
	c-TS	-2.01	-1.01	-1.07	0.14
	c-PC	-14.25	-13.07	-13.09	3.40
HAT-AA	*t*-Furfural+$HO_2^\bullet$	0.00	0.00	0.00	0.00
	t-RC	-9.88	-10.00	-9.46	1.47
	t-TS	-2.29	-1.27	-1.32	0.20
	t-PC	-14.66	-13.39	-13.39	3.45
H-Abs	*c*-Furfural+$HO_2^\bullet$	0.00	0.00		0.00
	RC_{Abs1}	-11.19	-11.85		1.58
	TS_{Abs1}	12.34	12.74		-1.98
	PC_{Abs1}	-2.02	-2.29		1.21
H-Abs	*c*-Furfural+$HO_2^\bullet$	0.00	0.00		0.00
	RC_{Abs2}	-1.85	-2.76		0.47
	TS_{Abs2}	34.11	34.69		-2.69
	PC_{Abs2}	28.56	30.34		0.91

Figure S1: The potential energy surface for the H-abstraction reaction of Furfural from the carbonyl carbon (in kcal mol^{-1}) obtained at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/jun-cc-pVTZ level of theory. All energies are zero-point corrected.

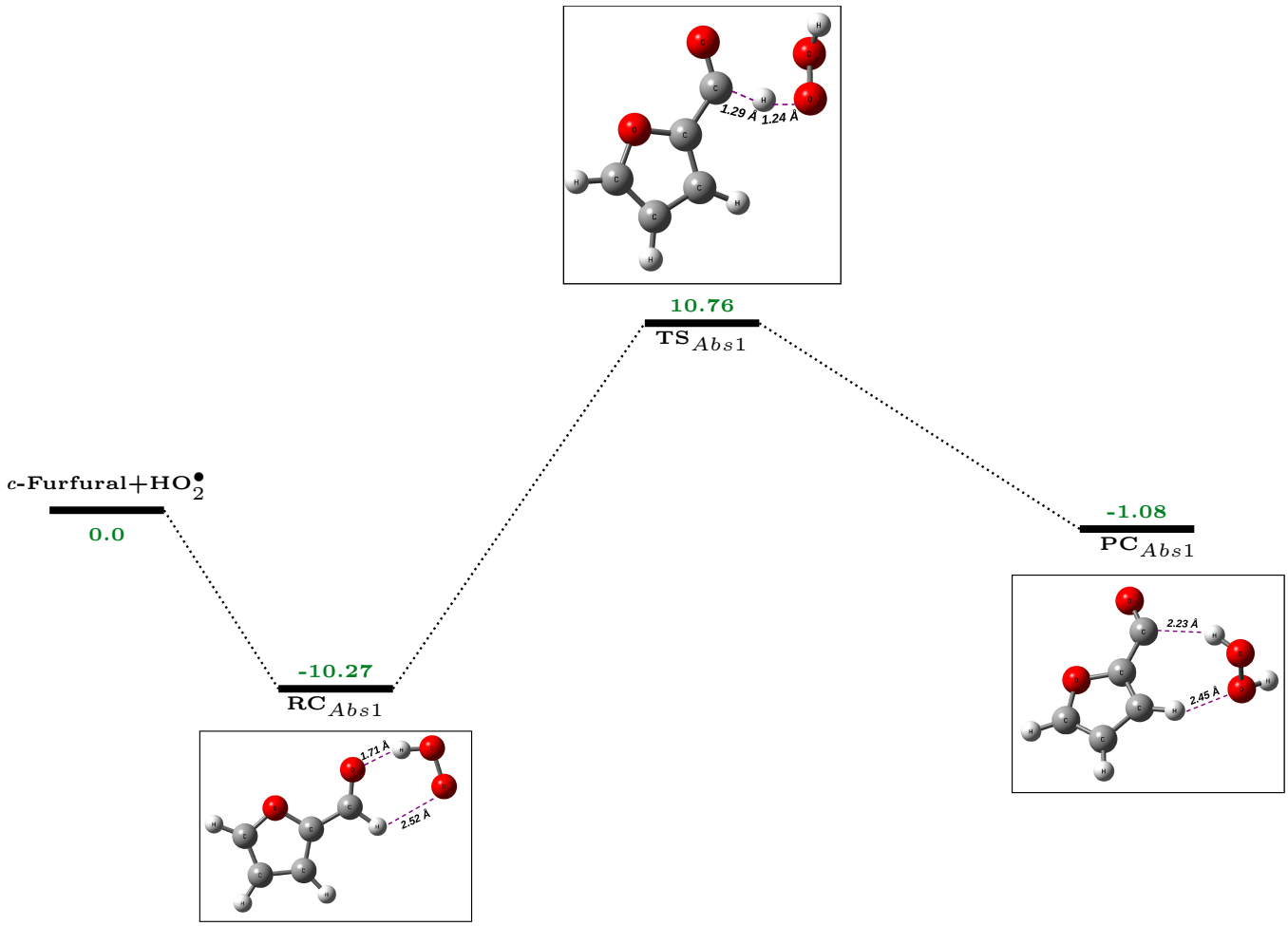


Figure S2: The potential energy surface for the H-abstraction reaction of Furfural from the furan ring (in kcal mol^{-1}) obtained at the CCSD(T)-F12/cc-pVDZ-F12//M06-2X/jun-cc-pVTZ level of theory. All energies are zero-point corrected.

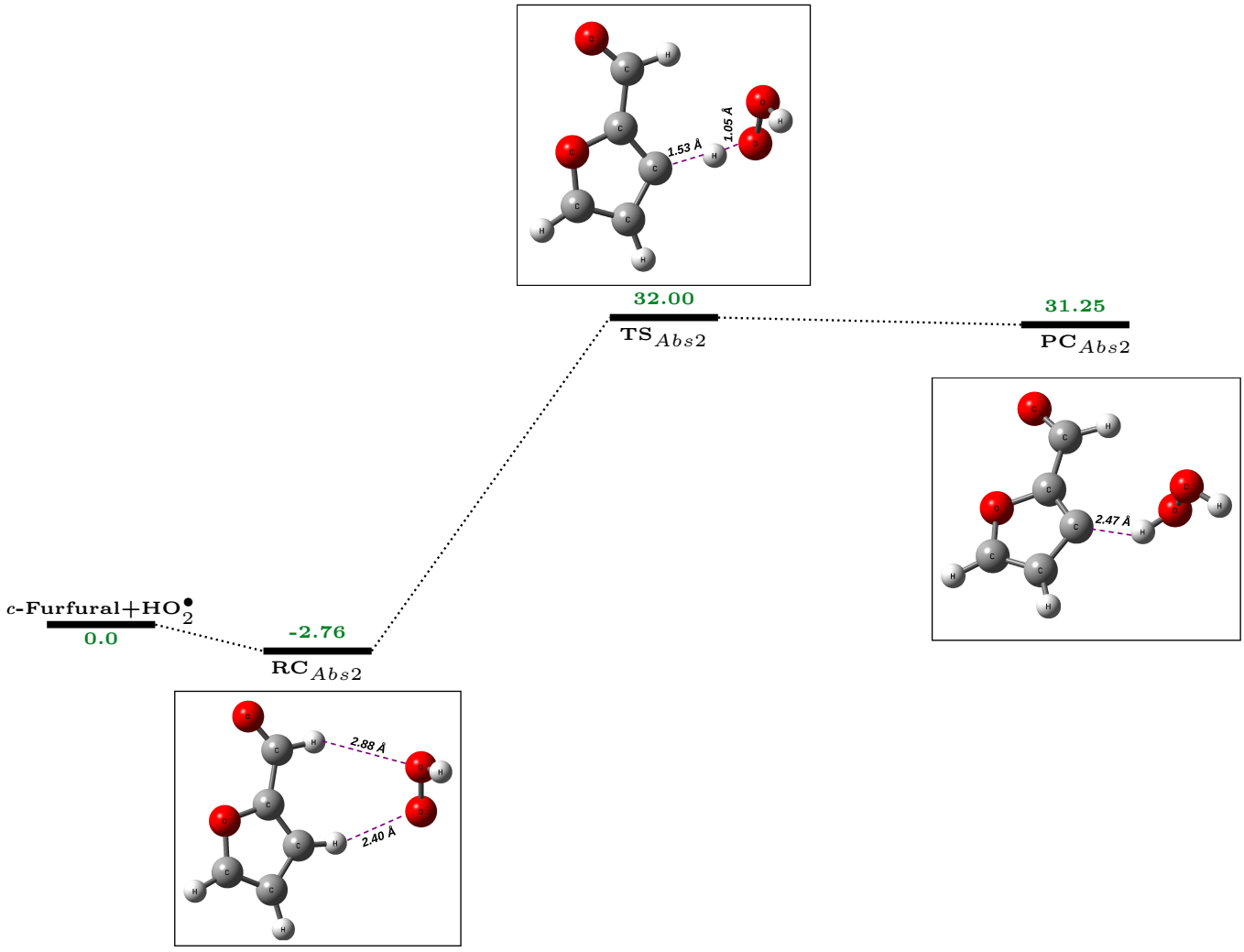
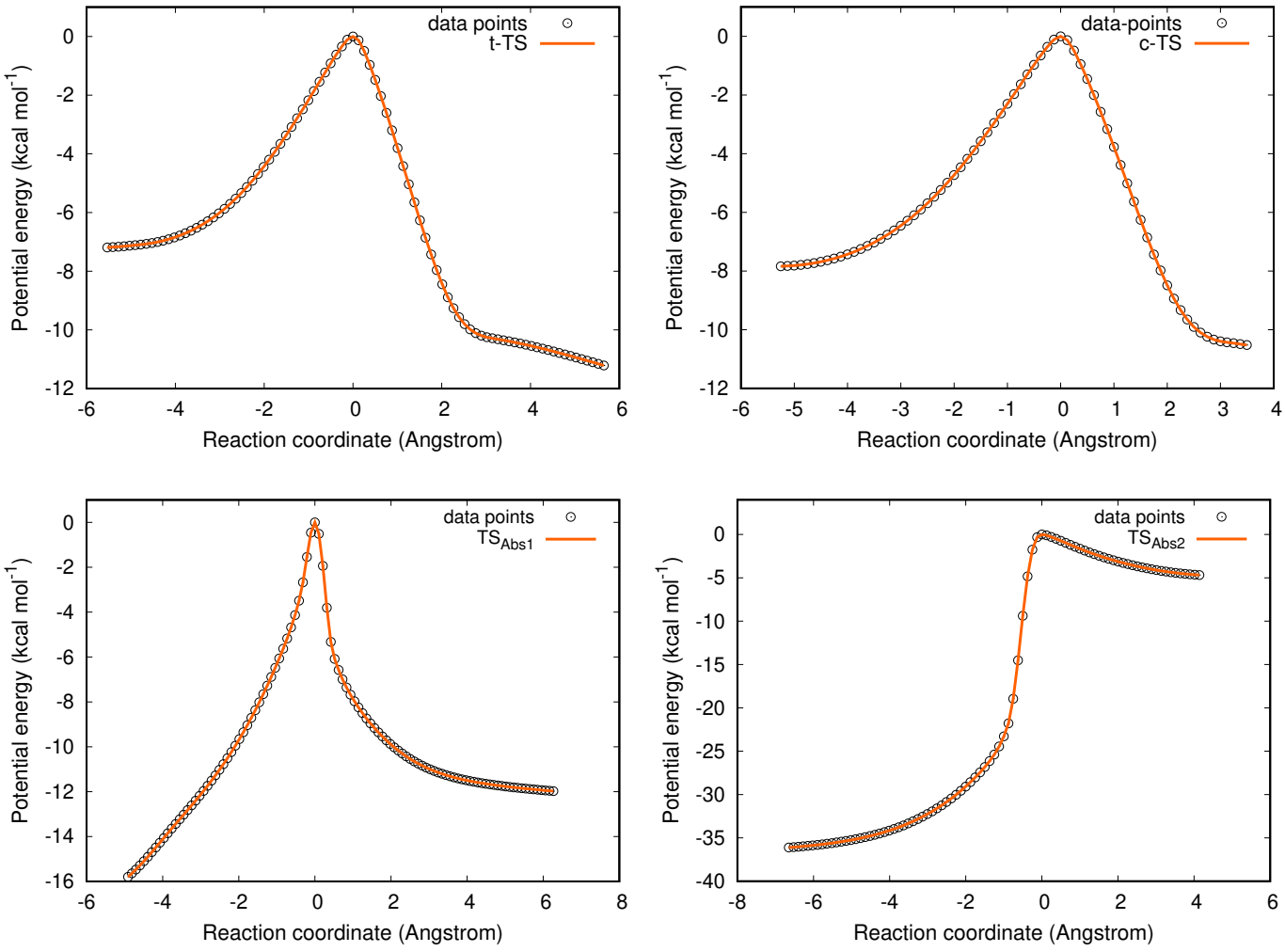


Figure S3: IRC for all the transition states obtained at M062X/jun-cc-pVTZ level of theory.



Details of Pre-equilibrium Approximation

Furfural + $HO_2^\bullet$ is a bimolecular reaction, whose mechanism can be represented by following reaction scheme:

$$\text{Furfural} + HO_2^\bullet \underset{k_r}{\overset{k_f}{\rightleftharpoons}} RC \xrightarrow[TS]{k_{uni}} PC \qquad (with \ \frac{k_f}{k_r} = K_{eq})$$

A straightforward approach to estimate k_{cis} and k_{trans} for the above reaction is to apply the pre-equilibrium approximation, which assumes that the formation of reactant-complex (RC) is much faster than its conversion to product-complex (PC). As a result, equilibrium is established between the reactants and RC, and hence k_{cis} and k_{trans} can be estimated using following expressions:

$$k_{cis} = P_{cis} \cdot K_{eq}^{cis} \cdot k_{uni}^{cis}$$
$$k_{trans} = P_{cis} \cdot K_{eq}^{trans} \cdot k_{uni}^{trans}$$

K_{eq} values are the equilibrium constants associated with the formation of RC along the respective pathways, and they have been estimated using THERMO module implemented in MultiWell suite of programs.[1] THERMO calculates equilibrium constants using following equation:

$$K_{eq} = \frac{Q_{RC}}{Q_{Furfural} Q_{HO_2}} \exp\left[\frac{-(E_{RC} - E_{Furfural} - E_{HO_2})}{RT}\right]$$

Here, Q symbolizes the total partition function of the subscripted species (multiplication of translational, vibrational, rotational, and electronic partition functions), and E indicates the zero-point corrected energy of the subscripted species. Similarly, k_{uni} refers to the unimolecular rate constant for the transformation of reactant-complex (RC) into products via a transition state (TS). These rate constants have been estimated using transition state theory (TST), augmented with Eckart tunneling correction, as implemented in THERMO module of MultiWell program suite. TST employs following expression:

$$k = \tau \frac{k_B T}{h} \frac{Q_{TS}}{Q_{RC}} \exp\left[\frac{-(E_{TS} - E_{RC})}{RT}\right]$$

Here, τ represents the tunneling correction. k_B, T, R and h represent the Boltzmann con-

stant, temperature, ideal gas constant and Planck constant, respectively. Q symbolizes the overall partition functions for the subscripted species, and E_{TS} and E_{RC} are the zero-point corrected electronic energies of the transition state and RC, respectively.

Table S3: Overall bimolecular rate constants (k_{bi}^{tst}, in cm^3 molecule^{-1} s^{-1}) estimated using the pre-equilibrium approximation over the temperature range 190–350 K. The rate constant is calculated as $k_{bi}^{tst} = P_{cis} \cdot K_{eq}^{cis} \cdot k_{uni}^{cis} + P_{trans} \cdot K_{eq}^{trans} \cdot k_{uni}^{trans}$, where P_{cis} and P_{trans} are the Boltzmann populations of the cis and trans conformers, K_{eq}^{cis} and K_{eq}^{trans} are the equilibrium constants, and k_{uni}^{cis} and k_{uni}^{trans} are the unimolecular rate constants calculated using transition state theory (TST) with Eckart tunneling corrections.

T (K)	P_{cis}	K_{eq}^{cis}	k_{uni}^{cis}	P_{trans}	K_{eq}^{trans}	k_{uni}^{trans}	k_{bi}^{tst}
190	0.17	1.09×10^{-16}	1.33×10^{3}	0.83	2.78×10^{-17}	8.20×10^{3}	2.14×10^{-13}
200	0.18	3.24×10^{-17}	3.01×10^{3}	0.82	9.89×10^{-18}	1.54×10^{4}	1.42×10^{-13}
220	0.20	4.06×10^{-18}	1.29×10^{4}	0.80	1.69×10^{-18}	4.75×10^{4}	7.44×10^{-14}
240	0.22	7.30×10^{-19}	4.52×10^{4}	0.78	3.91×10^{-19}	1.25×10^{5}	4.55×10^{-14}
260	0.24	1.73×10^{-19}	1.34×10^{5}	0.76	1.15×10^{-19}	2.90×10^{5}	3.10×10^{-14}
280	0.25	5.10×10^{-20}	3.43×10^{5}	0.75	4.09×10^{-20}	6.03×10^{5}	2.29×10^{-14}
298	0.27	1.97×10^{-20}	7.24×10^{5}	0.73	1.83×10^{-20}	1.08×10^{6}	1.83×10^{-14}
300	0.27	1.79×10^{-20}	7.83×10^{5}	0.73	1.69×10^{-20}	1.14×10^{6}	1.79×10^{-14}
320	0.28	7.22×10^{-21}	1.62×10^{6}	0.72	7.83×10^{-21}	2.01×10^{6}	1.46×10^{-14}
340	0.29	3.27×10^{-21}	3.10×10^{6}	0.71	4.02×10^{-21}	3.32×10^{6}	1.24×10^{-14}
350	0.30	2.28×10^{-21}	4.16×10^{6}	0.70	2.97×10^{-21}	4.17×10^{6}	1.15×10^{-14}

Figure S4: Potential energy scan of reactant-complex t-RC and c-RC along the reaction coordinate describing their dissociation into respective Furfural + $HO_2^{\bullet}$.

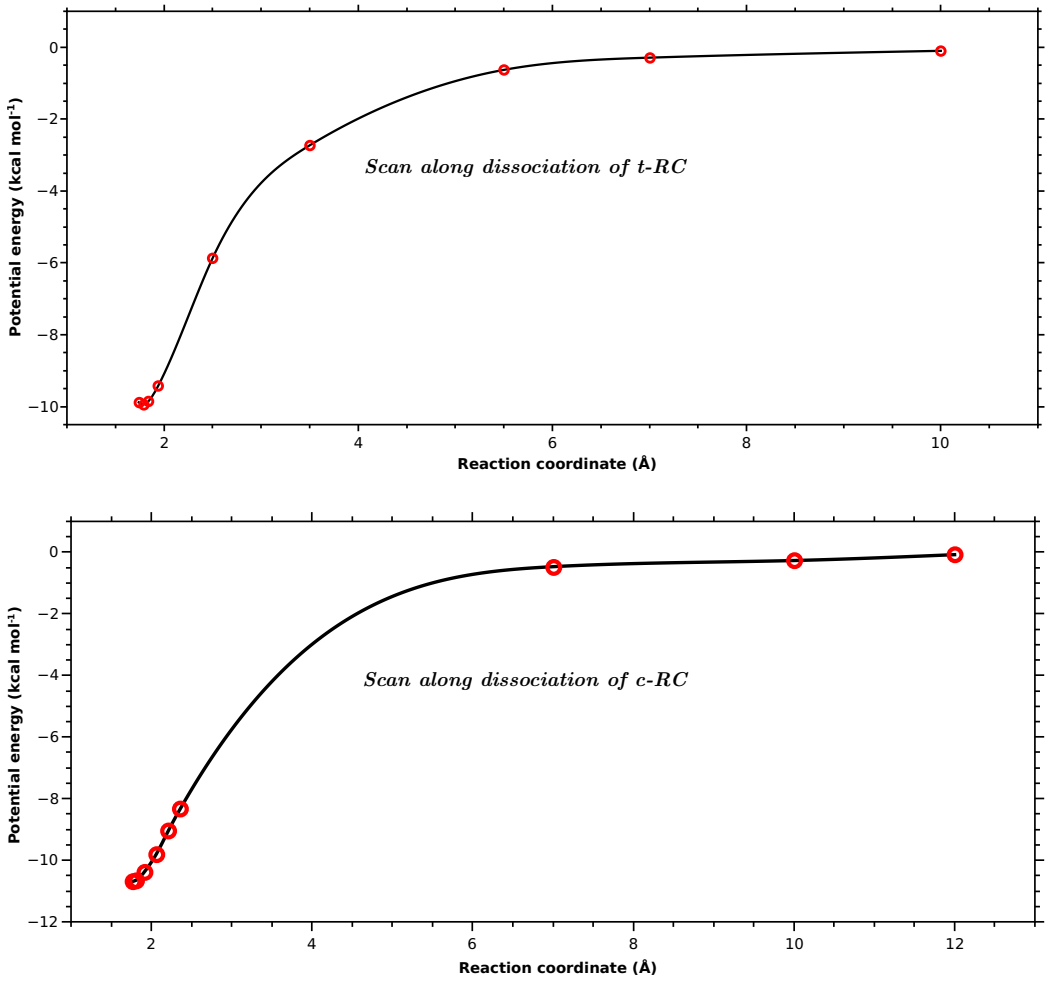


Figure S5: The concentration profiles of Furfural at the highest temperature up to which Furfural decays for a given concentration of $HO_2^\bullet$ as well as $NO^\bullet$.

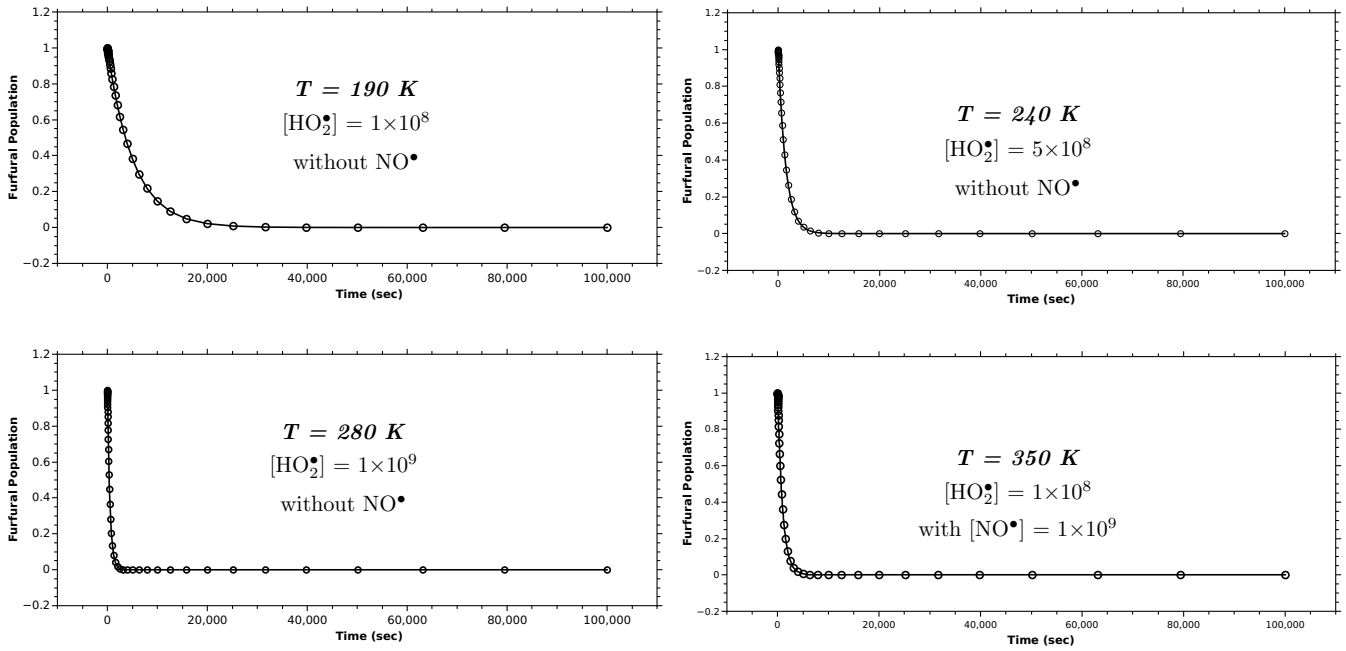


Figure S6: Gibbs free energy profile for t-PC + NO$^\bullet$ reaction (in kcal mol^{-1}) at 298 K, with potential energy values at 0 K given in parentheses. CCSD(T)-F12/cc-pVDZ-F12//MP2/6-311+G(2df,2p) level of theory was used for TS_{NO}, while all other species were computed at CCSD(T)-F12/cc-pVDZ-F12//M06-2X/jun-cc-pVTZ level of theory. All energies include zero-point energy (ZPE) corrections.

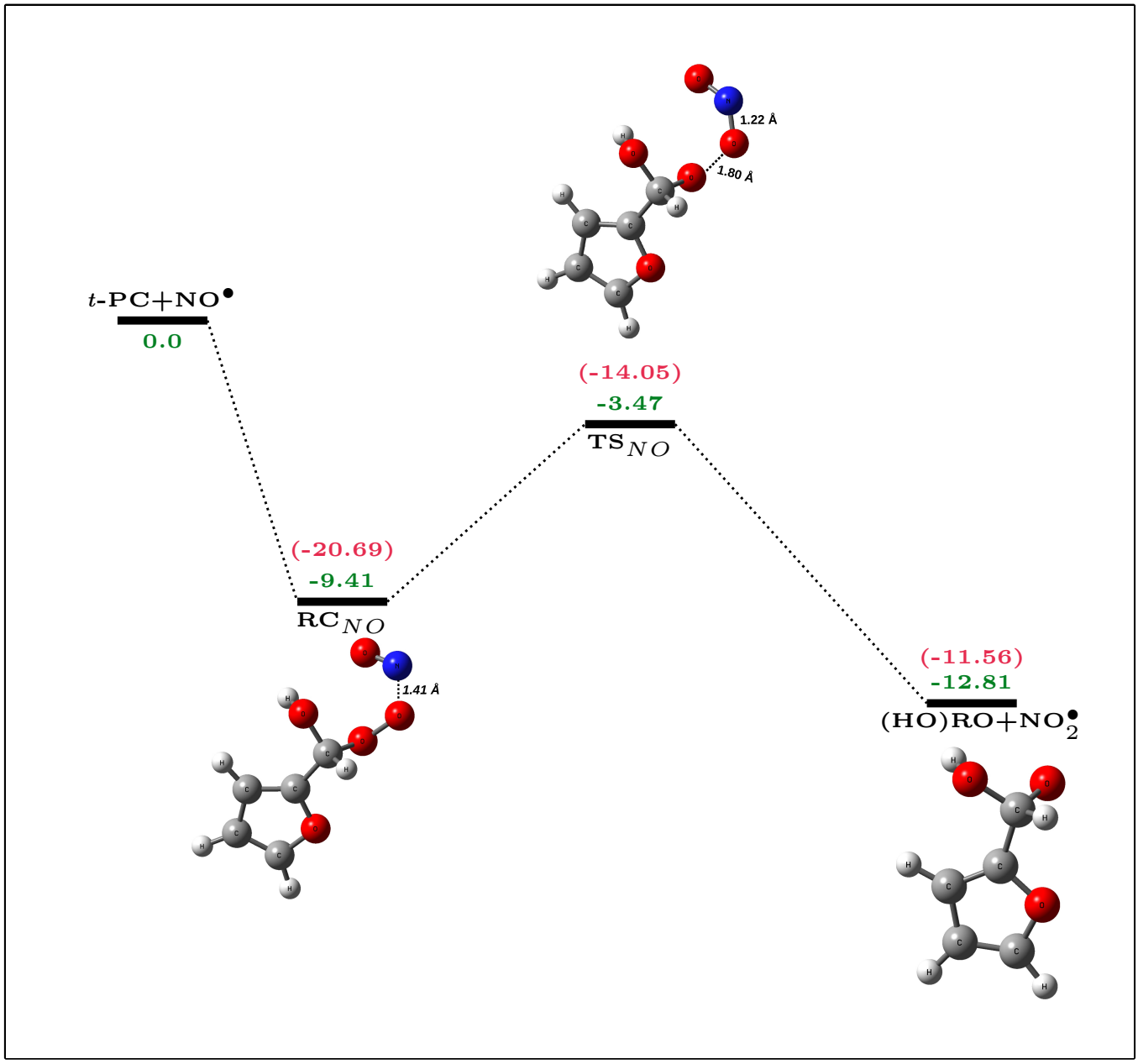


Figure S7: IRC for the transition state (TS_{NO}) of *t*-PC + $NO^{\bullet}$ reaction obtained at MP2/6-311+G(2df,2p) level of theory.

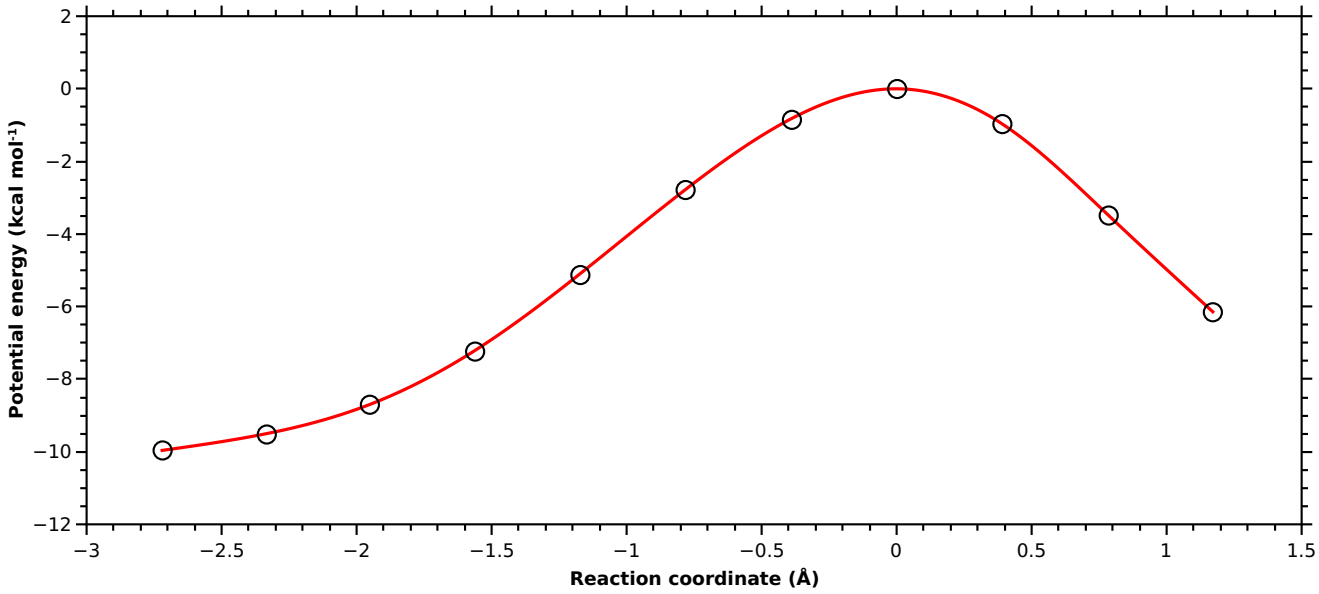


Table S4: Cartesian coordinates and all normal mode frequencies of the optimized geometries calculated at M062X/jun-cc-pVTZ level of theory. The geometry and frequency of TS_{NO} is obtained at MP2/6-311+G(2df,2p) level of theory.

Species	Cartesian coordinate (Å)				Frequencies (cm^{-1})		
	C	-0.270294	-0.082199	0.000001			
	C	0.377098	1.113651	-0.000013	153.6	205.5	248.2
	C	1.765843	0.811358	0.000011	502.7	618.6	656.3
	C	1.852146	-0.544211	-0.000010	761.7	801.0	884.3
t-Furfural	O	0.630783	-1.101645	-0.000005	905.3	938.6	982.7
	H	-0.099801	2.078111	-0.000016	1032.7	1033.3	1133.0
	H	2.590422	1.501762	0.000024	1199.7	1270.7	1273.3
	H	2.684665	-1.224985	-0.000012	1408.0	1462.8	1525.9
	C	-1.681846	-0.447435	0.000008	1651.0	1826.9	2990.0
	H	-1.876598	-1.533791	0.000017	3280.7	3292.1	3304.8
	O	-2.575329	0.360635	0.000006			
	C	-0.249314	0.262623	0.000465			
	C	1.587534	-0.886695	-0.000075	134.2	203.0	293.9
	C	1.972757	0.415012	-0.000426	504.0	616.9	666.8
	H	2.136993	-1.811334	0.000259	774.9	797.7	875.0
c-Furfural	H	2.983336	0.782300	-0.001091	905.2	932.2	969.4
	C	-1.692501	0.464748	0.000180	1027.8	1037.1	1126.4
	H	-1.982912	1.530353	0.001036	1214.7	1255.2	1329.0
	O	-2.512493	-0.415629	-0.000592	1407.9	1452.5	1536.2
	O	0.249295	-0.995872	0.000408	1643.1	1831.3	2974.9
	C	0.767003	1.169371	0.000072	3276.9	3288.0	3307.0
	H	0.655293	2.240332	-0.000025			
	O	0.055057	-0.599920	0.000000			

$HO_2^\bullet$	H	-0.880905	-0.865306	0.000000	1253.9	1458.4	3692.0
	O	0.055057	0.708084	0.000000			
	C	-0.254293	0.129453	0.172444			
	C	0.601460	1.166892	0.039003	-190.1	157.2	251.3
	C	1.898347	0.582706	-0.136130	453.4	614.9	632.2
	C	1.716920	-0.753921	-0.085663	776.8	802.4	866.4
	O	0.407907	-1.048406	0.105115	904.0	915.3	964.9
TS_D	H	0.346701	2.211915	0.052208	995.7	1036.3	1125.1
	H	2.831796	1.096495	-0.282025	1189.5	1249.4	1287.1
	H	2.380454	-1.595397	-0.165976	1416.3	1430.4	1558.2
	C	-1.733818	0.048895	0.385851	1654.7	1861.8	2985.6
	H	-2.081819	0.096447	1.431605	3282.1	3292.3	3312.8
	O	-2.514011	-0.058296	-0.516221			
	C	0.333253	1.555969	0.022598			
	O	1.452027	1.521254	-0.448060	11.8	54.3	66.9
	O	2.786134	-0.802510	-0.186822	111.8	184.8	193.6
	O	2.143183	-1.092944	0.913390	253.2	262.5	509.2
	H	2.431282	0.080092	-0.459351	602.1	612.0	654.6
t-RC	H	-0.023470	2.445257	0.565280	771.6	804.1	890.9
	C	-0.646056	0.503501	-0.092382	906.5	945.2	982.9
	C	-2.609070	-0.333749	0.280596	1042.3	1050.6	1141.0
	C	-1.916571	-1.288234	-0.397412	1204.6	1269.3	1281.0
	H	-3.608687	-0.310875	0.675048	1293.3	1423.0	1472.4
	H	-2.273315	-2.264171	-0.674215	1517.8	1545.8	1654.2
	O	-1.861389	0.756811	0.476735	1791.3	3020.3	3285.1
	C	-0.640479	-0.740328	-0.644901	3295.2	3310.3	3361.2
	H	0.188081	-1.194134	-1.159709			

	C	0.865429	0.062860	0.848593			
	O	1.632282	1.073873	0.752031	-814.1	75.1	79.7
	O	2.667039	-0.209483	-0.857729	150.0	224.6	298.2
	O	1.745981	-1.008820	-0.506153	461.6	592.6	622.2
	H	2.399612	0.682532	-0.105001	669.9	692.3	730.5
t-TS	H	1.036793	-0.687134	1.624136	776.3	794.3	880.6
	C	-0.488476	0.129901	0.323227	905.2	932.3	987.9
	C	-2.479179	-0.660005	-0.029014	1029.9	1056.1	1110.4
	C	-2.450967	0.558046	-0.624528	1131.8	1197.7	1267.7
	H	-3.239510	-1.414449	0.064405	1276.3	1373.0	1387.9
	H	-3.260190	1.026114	-1.156054	1442.7	1537.2	1638.6
	O	-1.297017	-0.935175	0.553546	1663.5	1922.4	3095.1
	C	-1.144816	1.077088	-0.394527	3283.1	3294.7	3307.0
	H	-0.734931	2.022433	-0.703556			
	C	0.975956	0.130583	0.466151			
	O	1.465854	1.407898	0.392559	47.9	97.5	118.4
	O	2.912010	-0.696974	-0.366692	213.9	321.2	400.3
	O	1.631656	-0.710392	-0.557039	429.0	452.7	621.6
	H	2.419791	1.364983	0.529382	631.7	681.0	786.6
	H	1.208098	-0.371324	1.408765	791.3	865.3	905.9
t-PC	C	-0.472010	0.128795	0.168738	916.7	932.1	983.9
	C	-2.434594	-0.796616	0.108153	1029.8	1124.9	1172.1
	C	-2.588529	0.441133	-0.413921	1203.3	1244.0	1260.1
	H	-3.110433	-1.613582	0.284011	1285.8	1298.8	1355.7
	H	-3.504369	0.869497	-0.780256	1424.9	1500.6	1564.6
	O	-1.148952	-1.002752	0.472555	1685.8	3081.6	3284.4

	C	-1.295424	1.051395	-0.374935	3298.7	3310.4	3839.0
	H	-1.010025	2.036462	-0.698084			
	C	0.481834	1.613231	0.032183			
	O	1.541133	1.450503	-0.535876	43.2	65.9	88.2
	O	2.402709	-1.073360	-0.110930	132.5	174.9	213.8
	O	1.768399	-1.091047	1.029947	261.7	306.6	508.1
	H	2.164204	-0.203796	-0.516243	572.7	613.7	668.2
c-RC	H	0.293901	2.519329	0.627551	784.2	802.7	884.0
	C	-0.623637	0.684366	-0.004042	905.8	939.1	974.1
	C	-1.825266	0.705332	0.639982	1032.6	1041.4	1129.8
	O	-0.516834	-0.435976	-0.756290	1218.4	1261.6	1286.3
	C	-2.495717	-0.487863	0.264051	1341.8	1405.7	1456.2
	H	-2.171554	1.478043	1.305054	1532.6	1551.0	1644.0
	C	-1.647991	-1.132584	-0.580689	1790.8	3024.1	3278.9
	H	-3.467601	-0.826092	0.575273	3288.4	3306.5	3392.9
	H	-1.717545	-2.063330	-1.115359			
	C	-0.862868	0.484656	0.752258			
	O	-1.574162	-0.456291	1.226134	-834.0	67.5	80.7
	O	-2.631393	-0.335646	-0.815206	148.6	231.7	293.1
	O	-1.765611	0.579855	-0.962683	462.3	582.7	617.5
	H	-2.331843	-0.654990	0.304308	669.6	707.6	733.7
c-TS	H	-1.089876	1.523017	1.006061	786.4	793.5	872.5
	C	0.511043	0.264228	0.329939	905.9	928.2	973.2
	C	1.533068	1.135898	0.120209	1036.1	1044.3	1105.7
	O	0.909540	-1.000403	0.062421	1126.3	1215.0	1255.1
	C	2.641761	0.349027	-0.303896	1327.1	1367.9	1390.2
	H	1.492891	2.202999	0.255991	1453.0	1526.4	1605.1

	C	2.197810	-0.932101	-0.319484	1686.6	1917.4	3093.7
	H	3.630366	0.686289	-0.559002	3279.6	3289.8	3308.9
	H	2.666579	-1.867683	-0.566840			
	C	-0.971509	0.230093	0.484963			
	O	-1.412367	-0.908089	1.107795	55.1	96.4	117.3
	O	-2.924564	0.301330	-0.668720	208.4	333.0	401.4
	O	-1.641874	0.364205	-0.826353	420.4	447.0	621.3
	H	-2.374500	-0.855660	1.168274	648.9	713.9	783.2
c-PC	H	-1.233754	1.145888	1.020187	787.6	858.6	901.6
	C	0.482041	0.185691	0.227022	916.1	924.3	971.0
	C	1.462486	1.090706	0.450904	1035.3	1123.1	1171.9
	O	0.983820	-0.925760	-0.354138	1208.4	1239.1	1261.8
	C	2.667987	0.489642	-0.027184	1288.3	1320.6	1347.2
	H	1.341522	2.060577	0.901410	1444.6	1469.4	1566.4
	C	2.310181	-0.725905	-0.500737	1686.6	3085.7	3280.6
	H	3.659269	0.905948	-0.016207	3290.4	3310.6	3825.4
	H	2.860235	-1.531600	-0.952151			
	C	0.928639	-0.143284	-0.000004			
	O	1.648202	1.004626	0.000160	29.1	48.0	65.0
	C	2.941429	0.652856	0.000187	129.5	140.8	198.5
	C	3.084717	-0.698971	0.000091	268.6	308.9	524.7
	C	1.765103	-1.220958	-0.000090	614.6	661.9	679.8
RC_{Abs1}	H	3.650692	1.461734	0.000376	782.5	801.1	888.2
	H	4.011469	-1.243969	0.000100	905.0	938.9	972.0
	H	1.460917	-2.253920	-0.000253	1039.6	1051.2	1127.9
	O	-3.533730	-0.911366	0.000126	1217.2	1259.8	1288.1
	C	-0.515598	-0.087221	-0.000312	1340.1	1405.2	1454.9

	O	-1.156567	0.945023	-0.000504	1530.2	1570.5	1640.4
	H	-1.017611	-1.064178	-0.000313	1781.9	3054.0	3280.0
	O	-3.766618	0.374826	0.000337	3288.9	3298.3	3307.2
	H	-2.861501	0.780928	-0.000092			
	C	0.713206	0.105342	-0.039969			
	O	1.747632	0.982857	0.027495	-1960.0	36.3	48.9
	C	2.868814	0.249344	0.080663	77.3	146.1	159.8
	C	2.591498	-1.080945	0.050143	246.6	358.2	434.3
	C	1.177501	-1.175207	-0.029166	477.9	533.1	614.7
TS_{Abs1}	H	3.790722	0.801029	0.137982	669.6	804.5	840.3
	H	3.306198	-1.883457	0.081598	896.6	905.8	943.5
	H	0.566002	-2.060923	-0.068678	976.0	1039.1	1066.1
	O	-2.550982	-1.057506	-0.242034	1105.7	1126.6	1213.9
	C	-0.648869	0.584577	-0.104159	1264.5	1308.0	1424.5
	O	-1.051901	1.702065	-0.088997	1443.8	1502.8	1538.6
	H	-1.511939	-0.373959	-0.189673	1638.4	1895.2	3278.3
	O	-3.463404	-0.238548	0.382007	3286.9	3305.6	3790.9
	H	-3.814637	0.307706	-0.334074			
	C	0.617097	0.319782	-0.070214			
	O	1.934236	0.615882	0.142473	34.9	61.6	71.0
	C	2.594307	-0.548422	0.113764	92.2	137.4	146.1
	C	1.751899	-1.592159	-0.109456	193.5	208.9	388.6
	C	0.457757	-1.024319	-0.229846	506.1	551.1	612.2
	H	3.658174	-0.491361	0.265908	663.8	730.2	806.7
PC_{Abs1}	H	2.024815	-2.629878	-0.176388	904.0	905.1	949.1
	H	-0.482675	-1.521618	-0.398721	959.1	1041.4	1046.2
	O	-2.813091	-0.471693	-0.625587	1126.3	1210.9	1251.3

	C	-0.361870	1.372564	-0.098084	1273.3	1378.4	1440.4
	O	-0.259507	2.536787	0.057530	1471.1	1510.7	1634.3
	H	-2.265666	0.332232	-0.630134	1945.9	3280.4	3286.7
	O	-2.594379	-0.946908	0.697250	3303.8	3668.6	3839.3
	H	-3.427863	-0.726598	1.129010			
	C	-0.788774	0.287976	-0.111839			
	O	-2.103282	0.199555	0.201483	12.2	14.9	26.2
	C	-2.408852	-1.10777	0.233771	33.8	79.6	133.3
	C	-1.324353	-1.871759	-0.056145	162.1	203.5	294.8
	C	-0.261825	-0.955992	-0.286293	504.6	618.7	667.3
RC_{Abs2}	H	-3.429818	-1.348351	0.472226	774.7	799.4	880.6
	H	-1.294741	-2.945393	-0.104702	905.5	934.2	969.4
	H	0.761593	-1.165045	-0.542057	1032.4	1039.2	1126.3
	O	3.135173	-0.968176	-0.271895	1214.9	1257.0	1261.3
	C	-0.151669	1.593545	-0.220081	1330.7	1408.4	1454.5
	O	-0.702296	2.648402	-0.036435	1457.3	1536.2	1641.7
	H	0.916742	1.530172	-0.490845	1828.4	2986.6	3283.3
	O	3.306	0.161298	0.362041	3293.5	3306.3	3684.5
	H	3.574307	-0.076005	1.26735			
	C	-0.635208	0.302298	-0.078107			
	O	-1.946609	0.020710	0.145628	-1006.8	31.4	63.4
	C	-2.073650	-1.317193	0.166839	76.4	131.6	162.9
	C	-0.883906	-1.945761	-0.035014	208.6	286.0	334.4
	C	0.027140	-0.876486	-0.185608	509.2	564.2	587.8
TS_{Abs2}	H	-3.067612	-1.692569	0.337382	641.7	676.3	774.3
	H	-0.702985	-3.004548	-0.064190	809.9	908.0	911.2
	H	1.543940	-0.908946	-0.357165	1031.2	1032.3	1089.5

	O	2.589587	-0.835606	-0.389430	1137.7	1211.1	1301.2
	C	-0.187386	1.690803	-0.165148	1325.4	1398.1	1407.9
	O	-0.919224	2.637916	-0.045351	1429.2	1468.7	1522.5
	H	0.893418	1.793291	-0.349829	1617.9	1827.9	3021.9
	O	2.869555	0.278096	0.408958	3284.7	3306.7	3815.6
	H	3.104821	-0.118120	1.257591			
	C	-0.550812	0.322737	0.189751			
	O	-1.825148	0.415960	-0.285429	38.5	55.1	76.7
	C	-2.353841	-0.818400	-0.264599	96.3	119.1	135.0
	C	-1.473621	-1.741902	0.209615	171.3	203.7	298.5
	C	-0.320354	-0.978334	0.493364	437.4	509.0	610.0
	H	-3.367733	-0.901222	-0.615729	653.2	758.5	782.3
PC_{Abs2}	H	-1.640342	-2.796456	0.332534	886.8	911.5	962.1
	H	1.600796	-0.811034	-1.054568	1038.4	1043.2	1089.3
	O	2.515268	-0.533158	-0.904283	1185.1	1214.1	1297.1
	C	0.266798	1.532300	0.299119	1363.5	1400.8	1413.6
	O	-0.129090	2.627524	-0.003578	1462.5	1520.9	1604.1
	H	1.280634	1.350113	0.685009	1824.2	3042.8	3283.5
	O	2.626966	-0.673432	0.506354	3304.3	3791.8	3837.2
	H	3.213662	-1.434956	0.584746			
	C	0.249736	0.134670	0.728902			
	O	0.780352	1.411005	0.742201	50.9	59.4	103.2
	O	2.226723	-0.965334	0.410376	131.1	206.5	243.9
	O	0.959629	-0.731373	-0.153088	302.0	390.9	415.8
	H	0.757606	1.758862	-0.157380	445.8	469.1	607.7
	H	0.340841	-0.255316	1.743040	621.8	656.3	686.7
RC_{NO}	C	-1.159477	0.112595	0.237567	783.3	820.1	858.4

	C	-3.033443	-0.854617	-0.283503	894.6	905.6	919.7
	C	-3.234183	0.468130	-0.473036	981.5	1027.1	1030.0
	H	-3.655732	-1.721844	-0.409506	1037.2	1128.6	1149.9
	H	-4.141520	0.935066	-0.812249	1192.9	1255.3	1274.2
	O	-1.774352	-1.087512	0.152118	1319.0	1370.4	1423.5
	C	-2.001241	1.107111	-0.126225	1461.1	1563.8	1670.4
	H	-1.781464	2.160170	-0.124193	1831.1	3110.5	3283.1
	N	3.249726	-0.226728	-0.213662	3292.8	3311.8	3832.5
	O	2.908127	0.486066	-1.057395			
	C	0.206170	-0.032868	0.672671			
	O	0.768374	1.220314	0.957926	-718.9	36.1	56.9
	O	2.426488	-1.069826	0.150154	76.9	105.8	178.5
	O	0.774823	-0.649975	-0.420583	197.5	244.8	347.5
	H	0.839698	1.682488	0.114215	359.6	436.0	537.4
	H	0.301473	-0.619526	1.590581	603.6	612.5	675.2
TS_{NO}	C	-1.219688	0.072520	0.238947	681.7	756.8	783.3
	C	-3.182823	-0.753367	-0.225496	818.4	880.3	893.9
	C	-3.258855	0.581966	-0.504465	955.0	1032.2	1044.1
	H	-3.885707	-1.564118	-0.282981	1058.2	1113.2	1128.0
	H	-4.126164	1.103281	-0.868834	1186.9	1262.5	1263.4
	O	-1.943940	-1.072974	0.225702	1302.9	1341.6	1414.6
	C	-1.980810	1.123530	-0.205314	1438.4	1506.1	1588.6
	H	-1.665394	2.149193	-0.274974	1665.0	3081.6	3294.9
	N	3.305621	-0.278957	-0.164775	3307.5	3324.9	3819.2
	O	3.225853	0.728800	-0.786030			
	C	1.428198	-0.261006	0.301876			
	O	2.157111	0.927024	0.370808	36.2	153.0	209.1

(OH)RO$^{\bullet}$	O	1.727292	-1.036297	-0.771650	253.1	318.7	409.3
	H	2.292918	1.237715	-0.530944	579.0	618.6	666.2
	H	1.607657	-0.809591	1.234536	728.3	783.7	860.9
	C	-0.049641	0.006688	0.129145	903.5	921.1	966.8
	C	-2.145063	-0.555902	0.099519	1026.1	1032.7	1122.2
	C	-2.108210	0.757265	-0.221983	1138.0	1181.7	1221.7
	H	-2.943897	-1.264938	0.219374	1249.4	1263.3	1294.8
	H	-2.953889	1.386213	-0.435944	1399.5	1436.5	1547.1
	O	-0.895886	-1.028784	0.313013	1647.7	3029.9	3281.6
	C	-0.727359	1.129097	-0.207682	3294.9	3310.1	3854.2
	H	-0.298478	2.098211	-0.389652			
$NO_2^{\bullet}$	N	0.000000	0.000000	0.314156	782.8	1466.2	1778.7
	O	0.000000	1.090408	-0.137443			
	O	0.000000	-1.090408	-0.137443			
NO$^{\bullet}$	N	0.000000	0.000000	-0.606438		2067.4	
	O	0.000000	0.000000	0.530633			

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