Supporting Information

Fundamental Reaction Pathways for Cytochrome P450-catalyzed 5′-Hydroxylation and *N*-Demethylation of Nicotine

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Supporting Information Available: Ten tables showing the energies, free energies, Mulliken spin densities, imaginary frequencies, and Cartesian coordinates in the two reaction pathways. This material is available free of charge via the Internet at http://pubs.acs.org.

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	B1		B2//B1		B2//B1 + solv.		B2//B1 + 2NH--S		B2//B1 + 2NH--S + solv.	
	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}
5'-hydroxylation										
^{4}RC	-2084.653464	**0.0**	-2085.085604	**0.0**	-2085.160352	**0.0**	-2198.226500	**0.0**	-2198.307668	**0.0**
^{2}RC	-2084.653882	**-0.3**	-2085.086061	**-0.3**	-2085.160568	**-0.1**	-2198.226726	**-0.1**	-2198.307602	**0.0**
^{4}TS$_H$	-2084.615741	**23.7**	-2085.050248	**22.2**	-2085.125243	**22.0**	-2198.186897	**24.9**	-2198.267327	**25.3**
^{2}TS$_H$	-2084.616421	**23.2**	-2085.048091	**23.5**	-2085.125315	**22.0**	-2198.188016	**24.1**	-2198.270516	**23.3**
^{4}IM	-2084.629813	**14.8**	-2085.064494	**13.2**	-2085.141868	**11.6**	-2198.204631	**13.7**	-2198.286579	**13.2**
^{2}IM	-2084.630306	**14.5**	-2085.065185	**12.8**	-2085.14210	**11.5**	-2198.202519	**15.0**	-2198.284410	**14.6**
^{4}TS$_{reb}$	-2084.619181	**21.5**	-2085.061588	**15.1**	-2085.139177	**13.3**	-2198.203053	**14.7**	-2198.285037	**14.2**
^{2}TS$_{reb}$	-2084.625860	**17.3**	-2085.060916	**15.5**	-2085.140353	**12.5**	-2198.196672	**18.7**	-2198.279707	**17.5**
^{4}PC	-2084.719385	**-41.4**	-2085.155329	**-43.8**	-2085.236512	**-47.8**	-2198.301310	**-46.9**	-2198.386925	**-49.7**
^{2}PC	-2084.719554	**-41.5**	-2085.151152	**-41.1**	-2085.228886	**-43.0**	-2198.291085	**-40.5**	-2198.373690	**-41.4**
***N*-methylhydroxylation**										
^{4}RC	-2084.653638	**0.0**	-2085.085488	**0.0**	-2085.160501	**0.0**	-2198.226654	**0.0**	-2198.307660	**0.0**
^{2}RC	-2084.653973	**-0.2**	-2085.085954	**-0.3**	-2085.160711	**-0.1**	-2198.226838	**-0.1**	-2198.307875	**-0.1**
^{4}TS$_H$	-2084.610639	**27.0**	-2085.045765	**24.9**	-2085.120393	**25.2**	-2198.184672	**26.3**	-2198.265006	**26.8**
^{2}TS$_H$	-2084.610577	**27.0**	-2085.043059	**26.6**	-2085.119253	**25.9**	-2198.184115	**26.7**	-2198.266050	**26.1**
^{4}IM	-2084.622022	**19.8**	-2085.057040	**17.9**	-2085.133874	**16.7**	-2198.197970	**18.0**	-2198.278676	**18.2**
^{2}IM	-2084.622336	**19.6**	-2085.057562	**17.5**	-2085.133459	**17.0**	-2198.196658	**18.8**	-2198.277560	**18.9**
^{4}TS$_{reb}$	-2084.610579	**27.0**	-2085.052677	**20.6**	-2085.129428	**19.5**	-2198.193931	**20.5**	-2198.275743	**20.0**
^{2}TS$_{reb}$	-2084.614711	**24.4**	-2085.050679	**21.8**	-2085.128463	**20.1**	-2198.189957	**23.0**	-2198.271879	**22.5**
^{4}PC	-2084.712711	**-37.1**	-2085.148607	**-39.6**	-2085.231053	**-44.3**	-2198.295390	**-43.1**	-2198.382016	**-46.7**
^{2}PC	-2084.713981	**-37.9**	-2085.145408	**-37.6**	-2085.223606	**-39.6**	-2198.284576	**-36.3**	-2198.367387	**-37.5**

Table S2. Calculated energies with zero-point corrections for *N*-(hydroxymethyl)nornicotine decomposition. All relative values are in kcal/mol relative to the reactant RC.

	B1 (gas-phase)		B2//B1 (gas-phase)		B2//B1 + solv.		B1 (gas-phase).		B2//B1 (gas-phase)		B2//B1 + solv.	
	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}	E (a.u.)	G_{rel}
protonated *N*-(hydroxymethyl)nornicotine							**protonated *N*-(hydroxymethyl)nornicotine (with water assisted)**					
RC	-574.328461	**0.0**	-574.459799	**0.0**	-574.573897	**0.0**	-650.741517	**0.0**	-650.904537	**0.0**	-651.018336	**0.0**
TS	-574.257423	**44.6**	-574.389194	**44.3**	-574.502708	**44.7**	-650.684881	**35.5**	-650.846924	**36.1**	-650.958575	**37.5**
PC	-574.335110	**-4.2**	-574.469677	**-6.2**	-574.575934	**-1.3**	-650.745516	**-2.5**	-650.911611	**-4.4**	-651.013999	**2.7**
deprotonated *N*-(hydroxymethyl)nornicotine							**deprotonated *N*-(hydroxymethyl)nornicotine (with water assisted)**					
RC	-573.963926	**0.0**	-574.103559	**0.0**	-574.127107	**0.0**	-650.367029	**0.0**	-650.535255	**0.0**	-650.566379	**0.0**
TS	-573.902251	**38.7**	-574.040308	**39.7**	-574.080516	**29.2**	-650.337081	**18.8**	-650.506291	**18.2**	-650.550704	**9.8**
PC	-573.947412	**10.4**	-574.088480	**9.5**	-574.114062	**8.2**	-650.350449	**10.4**	-650.521920	**8.4**	-650.552079	**9.0**

Table S3. Calculated energies for the rate-determining step of nicotine hydroxylation by Cpd I with zero-point corrections using different density functionals. All data were calculated at the B2//B1 level. All relative values are in kcal/mol relative to the reactant ^{4}RC.

	BP86		BLYP		B3LYP*		B3LYP		B3PW91	
	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}	E (a.u.)	E_{rel}
5'-hydroxylation										
^{4}RC	-2085.236408	**0.0**	-2084.472060	**0.0**	-2072.593132	**0.0**	-2085.085604	**0.0**	-2084.446659	**0.0**
^{2}RC	-2085.238034	**-1.0**	-2084.473617	**-1.0**	-2072.593913	**-0.5**	-2085.086061	**-0.3**	-2084.447163	**-0.3**
^{4}TS$_H$	-2085.211946	**15.4**	-2084.442044	**18.8**	-2072.559901	**20.9**	-2085.050248	**22.2**	-2084.414850	**20.0**
^{2}TS$_H$	-2085.209354	**17.0**	-2084.439924	**20.2**	-2072.555756	**23.5**	-2085.048091	**23.5**	-2084.410583	**22.6**
***N*-methylhydroxylation**										
^{4}RC	-2085.236307	**0.0**	-2084.471937	**0.0**	-2072.593184	**0.0**	-2085.085488	**0.0**	-2084.446568	**0.0**
^{2}RC	-2085.237823	**-1.0**	-2084.473234	**-0.8**	-2072.593734	**-0.3**	-2085.085954	**-0.3**	-2084.447075	**-0.3**
^{4}TS$_H$	-2085.206243	**18.9**	-2084.437436	**21.6**	-2072.555510	**23.6**	-2085.045765	**24.9**	-2084.409665	**23.2**
^{2}TS$_H$	-2085.202848	**21.0**	-2084.434749	**23.3**	-2072.551003	**26.5**	-2085.043059	**26.6**	-2084.404932	**26.1**

Table S4. Calculated free energies for nicotine hydroxylation by Cpd I with thermal corrections. All relative values are in kcal/mol relative to the reactant ^{4}RC. (B1: LACVP (6-31G*); B2: LACV3P+* (6-311+G*)).

	B1		B2//B1		B2//B1 + solv.		B2//B1 + 2NH--S		B2//B1 + 2NH--S + solv.	
	G (a.u.)	G_{rel}	G (a.u.)	G_{rel}	G (a.u.)	G_{rel}	G (a.u.)	G_{rel}	G (a.u.)	G_{rel}
5'-hydroxylation										
^{4}RC	-2084.723935	**0.0**	-2085.156074	**0.0**	-2085.230822	**0.0**	-2198.29697	**0.0**	-2198.378138	**0.0**
^{2}RC	-2084.723489	**0.3**	-2085.155668	**0.3**	-2085.230175	**0.4**	-2198.296333	**0.4**	-2198.377209	**0.6**
^{4}TS$_H$	-2084.683971	**25.1**	-2085.118478	**23.6**	-2085.193473	**23.4**	-2198.255127	**26.3**	-2198.335557	**26.7**
^{2}TS$_H$	-2084.682903	**25.7**	-2085.114573	**26.0**	-2085.191797	**24.5**	-2198.254498	**26.7**	-2198.336998	**25.8**
^{4}IM	-2084.698274	**16.1**	-2085.132956	**14.5**	-2085.210330	**12.9**	-2198.273093	**15.08**	-2198.355041	**14.5**
^{2}IM	-2084.697842	**16.4**	-2085.132721	**14.7**	-2085.209636	**13.3**	-2198.270055	**16. 9**	-2198.351946	**16.4**
^{4}TS$_{reb}$	-2084.686446	**23.5**	-2085.128853	**17.1**	-2085.206442	**15.3**	-2198.270318	**16.7**	-2198.352302	**16.2**
^{2}TS$_{reb}$	-2084.691415	**20.4**	-2085.126472	**18.6**	-2085.205909	**15.6**	-2198.270318	**21.8**	-2198.345263	**20.6**
^{4}PC	-2084.789788	**-41.3**	-2085.225732	**-43.7**	-2085.306915	**-47.7**	-2198.371713	**-46.9**	-2198.457328	**-49.7**
^{2}PC	-2084.789426	**-41.1**	-2085.221025	**-40.8**	-2085.298759	**-42.6**	-2198.360958	**-40.2**	-2198.443563	**-41.1**
***N*-methylhydroxylation**										
^{4}RC	-2084.723059	**0.0**	-2085.154908	**0.0**	-2085.229921	**0.0**	-2198.296074	**0.0**	-2198.377080	**0.0**
^{2}RC	-2084.722801	**-0.2**	-2085.154783	**0.1**	-2085.229540	**0.2**	-2198.295667	**0.3**	-2198.376704	**0.2**
^{4}TS$_H$	-2084.678800	**31.6**	-2085.113927	**25.7**	-2085.188555	**26.0**	-2198.252834	**27.1**	-2198.333168	**27.6**
^{2}TS$_H$	-2084.677841	**32.0**	-2085.110323	**28.0**	-2085.186517	**27.2**	-2198.251379	**28.0**	-2198.333314	**27.5**
^{4}IM	-2084.691167	**23.0**	-2085.126185	**18.0**	-2085.203019	**16.9**	-2198.267115	**18.2**	-2198.347821	**18.4**
^{2}IM	-2084.690915	**22.6**	-2085.126141	**18.1**	-2085.202038	**17.5**	-2198.265237	**19.4**	-2198.346139	**19.4**
^{4}TS$_{reb}$	-2084.677510	**29.4**	-2085.119608	**22.2**	-2085.196359	**21.1**	-2198.260862	**22.1**	-2198.342674	**21.6**
^{2}TS$_{reb}$	-2084.682733	**28.1**	-2085.118700	**22.7**	-2085.196484	**21.0**	-2198.257978	**23.9**	-2198.339900	**23.3**
^{4}PC	-2084.783049	**-37.6**	-2085.218945	**-40.2**	-2085.301391	**-44.8**	-2198.365728	**-43.7**	-2198.452354	**-47.2**
^{2}PC	-2084.783102	**-39.0**	-2085.214529	**-37.4**	-2085.292727	**-39.4**	-2198.353697	**-36.2**	-2198.436508	**-37.3**

Table S5. Calculated free energies with thermal corrections for *N*-(hydroxymethyl)nornicotine decomposition. All relative values are in kcal/mol relative to the reactant RC.

	B1 (gas-phase)		B2//B1 (gas-phase)		B2//B1 + solv.		B1 (gas-phase).		B2//B1 (gas-phase)		B2//B1 + solv.	
	G (a.u.)	G_{rel}	G (a.u.)	G_{rel}	G (a.u.)	G_{rel}	G (a.u.)	G_{rel}	G (a.u.)	G_{rel}	G (a.u.)	G_{rel}
protonated *N*-(hydroxymethyl)nornicotine							**protonated *N*-(hydroxymethyl)nornicotine (with water assisted)**					
RC	-574.367423	**0.0**	-574.498761	**0.0**	-574.612859	**0.0**	-650.785681	**0.0**	-650.948702	**0.0**	-651.062501	**0.0**
TS	-574.297676	**43.8**	-574.429447	**43.5**	-574.542961	**43.9**	-650.729326	**35.4**	-650.891369	**36.0**	-651.003020	**37.3**
PC	-574.379006	**-7.3**	-574.513572	**-9.3**	-574.619829	**-4.4**	-650.791348	**-3.6**	-650.957443	**-5.5**	-651.059831	**1.7**
deprotonated *N*-(hydroxymethyl)nornicotine							**deprotonated *N*-(hydroxymethyl)nornicotine (with water assisted)**					
RC	-574.00319	**0.0**	-574.142823	**0.0**	-574.166371	**0.0**	-650.408680	**0.0**	-650.576905	**0.0**	-650.608029	**0.0**
TS	-573.940292	**39.5**	-574.078349	**40.5**	-574.118557	**30.0**	-650.377579	**19.5**	-650.546789	**18.9**	-650.591202	**10.6**
PC	-573.991135	**7.6**	-574.132203	**6.7**	-574.157785	**5.4**	-650.396784	**7.5**	-650.568255	**5.4**	-650.598414	**6.0**

Table S6. Mulliken spin densities of key moieties of nicotine hydroxylation by Cpd I. All data were computed at the B1 level.

	5'-hydroxylation						***N*-methylhydroxylaiton**					
	Fe	O	SH	Por	H	nic(rest)	Fe	O	SH	Por	H	nic(rest)
^{4}RC	1.2569	0.7648	0.5732	0.3970	0.0001	0.0087	1.2543	0.7670	0.5772	0.3938	-0.0006	0.0084
^{2}RC	1.3772	0.7274	-0.6248	-0.4861	0.0002	0.0079	1.3744	0.7296	-0.6285	-0.4821	-0.0004	0.0070
$^{4}TS_{H}$	1.2018	0.4444	0.4724	0.3580	-0.0687	0.5920	1.1886	0.3695	0.4604	0.3830	-0.0624	0.6609
$^{2}TS_{H}$	1.0994	0.4156	-0.4821	-0.5652	-0.0794	0.6117	1.1055	0.3399	-0.4968	-0.5443	-0.0715	0.6673
^{4}IM	0.9291	0.1019	0.4290	0.5451	-0.0022	0.9971	0.9423	0.0987	0.4261	0.5362	-0.0034	1.0000
^{2}IM	1.0357	0.0410	-0.4655	-0.6019	-0.0044	0.9951	1.0407	0.0326	-0.4702	-0.5955	-0.0031	0.9954
$^{4}TS_{reb}$	2.0257	-0.0085	0.3019	-0.0879	-0.0001	0.7689	2.0725	-0.0369	0.3291	-0.0707	0.0031	0.7029
$^{2}TS_{reb}$	1.1567	-0.0362	-0.3188	-0.6092	0.0009	0.8066	0.8750	0.0277	0.3634	0.5582	-0.0047	-0.8196
^{4}PC	2.4116	0.0004	0.5316	0.0624	-0.0003	-0.0056	2.4099	0.0004	0.5287	0.0658	-0.0035	-0.0014
^{2}PC	1.1633	0.0003	-0.0432	-0.1195	-0.0003	-0.0007	1.1657	0.0002	-0.0422	-0.1229	-0.0010	0.0001

Table S7. Imaginary frequencies of all transition states.

5´-hydroxylation by Cpd I				*N*-methylhydroxylation by Cpd I			
$^{4}TS_{H}$	i1046.46	$^{2}TS_{H}$	i1192.41	$^{4}TS_{H}$	i532.59	$^{2}TS_{H}$	i678.13
$^{4}TS_{reb}$	i433.95	$^{2}TS_{reb}$	i302.88	$^{4}TS_{reb}$	i498.73	$^{2}TS_{reb}$	i134.49
decomposition of protonated *N*-(hydroxymethyl)nornicotine				decomposition of deprotonated *N*-(hydroxymethyl)nornicotine			
without water	i251.73	with water	i149.69	without water	i1533.37	with water	i1063.27

Table S8. Cartesian coordinates for 5′-hydroxylation by Cpd I. The geometries were optimized at the B3LYP/B1 level.

^{4}RC				^{2}RC			
26	-0.065242	-0.464374	-0.517286	26	-0.093769	-0.504372	-0.513343
7	0.551861	-2.094534	0.492157	7	0.540127	-2.113384	0.505448
7	1.792140	0.320412	-0.373484	7	1.743171	0.326470	-0.337818
7	-0.731156	1.306063	-1.224899	7	-0.787719	1.257995	-1.240130
7	-1.967837	-1.117569	-0.400603	7	-1.981947	-1.194840	-0.429612
6	-0.207163	-3.177850	0.847426	6	-0.200660	-3.213352	0.850951
6	1.829997	-2.386115	0.888448	6	1.817074	-2.373572	0.930170
6	2.910154	-0.298170	0.136452	6	2.865567	-0.265132	0.191274
6	2.221565	1.529588	-0.861537	6	2.153767	1.542141	-0.827077
6	0.033894	2.397201	-1.590984	6	-0.037875	2.358566	-1.605651
6	-2.028482	1.621834	-1.580198	6	-2.082272	1.540480	-1.626515
6	-3.088708	-0.492214	-0.880232	6	-3.107749	-0.592610	-0.929757
6	-2.390134	-2.338812	0.064733	6	-2.386953	-2.424041	0.028981
6	0.612977	-4.181799	1.480601	6	0.629519	-4.194401	1.505956
6	1.880994	-3.688268	1.507744	6	1.884631	-3.671055	1.557212
6	4.068968	0.542423	-0.036960	6	4.008986	0.599144	0.032071
6	3.642351	1.675123	-0.661678	6	3.567945	1.719181	-0.605306
6	-0.803273	3.420440	-2.163038	6	-0.884025	3.357511	-2.207693
6	-2.078189	2.942999	-2.153678	6	-2.148908	2.853479	-2.217701
6	-4.247321	-1.335701	-0.713399	6	-4.251075	-1.459806	-0.780173
6	-3.812886	-2.483224	-0.125287	6	-3.802943	-2.597879	-0.184082
6	-1.577623	-3.298964	0.649720	6	-1.563547	-3.366651	0.627678
6	2.931381	-1.552326	0.729767	6	2.902762	-1.517121	0.789443
6	1.407520	2.494542	-1.444893	6	1.330536	2.485730	-1.431718
6	-3.122413	0.785490	-1.430414	6	-3.160123	0.680739	-1.487573
1	-2.051153	-4.215940	0.986099	1	-2.022229	-4.293810	0.956578
1	3.885885	-1.911894	1.101530	1	3.857610	-1.855266	1.179906
1	1.881379	3.412407	-1.778886	1	1.792032	3.410512	-1.764097
1	-4.086421	1.161130	-1.759133	1	-4.126483	1.031719	-1.836109
1	0.248345	-5.127960	1.858835	1	0.279234	-5.146926	1.881735
1	2.774791	-4.144508	1.913094	1	2.779967	-4.104236	1.983892
1	5.067726	0.292406	0.297135	1	5.007574	0.372080	0.382626
1	4.218766	2.546920	-0.943488	1	4.129993	2.601646	-0.882965
1	-0.447455	4.381067	-2.512495	1	-0.541331	4.321373	-2.561410
1	-2.982302	3.431658	-2.493520	1	-3.056121	3.319103	-2.580892
1	-5.254137	-1.065419	-1.004286	1	-5.258307	-1.210721	-1.088061
1	-4.388825	-3.351544	0.167319	1	-4.365598	-3.477749	0.099697
8	0.190775	-1.140481	-1.988393	8	0.201862	-1.136191	-1.995885
16	-0.398824	0.856031	1.612726	16	-0.496454	0.835034	1.601600
1	-1.747916	0.945857	1.587522	1	-1.846445	0.893299	1.547914
1	2.790651	-3.346541	-4.073263	1	2.844207	-3.291018	-4.063336
6	2.440875	-2.332393	-3.868432	6	2.482066	-2.282070	-3.854397
6	3.517514	-1.238358	-3.961155	6	3.549948	-1.177256	-3.920434

7	1.413299	-1.950175	-4.914410	7	1.466085	-1.900119	-4.912142
1	1.907026	-2.299549	-2.916408	1	1.934015	-2.262774	-2.910114
6	2.831515	-0.027407	-4.653935	6	2.867264	0.029764	-4.622901
1	4.380711	-1.578833	-4.540075	1	4.428948	-1.506726	-4.481569
1	3.873104	-0.986000	-2.959721	1	3.880839	-0.925127	-2.910482
6	1.348708	-0.409349	-4.829199	6	1.389437	-0.360561	-4.818715
6	0.094498	-2.643157	-4.759431	6	0.150243	-2.603447	-4.779921
1	2.899525	0.884277	-4.056104	1	2.922330	0.942086	-4.024782
1	3.294366	0.185023	-5.622010	1	3.342046	0.244260	-5.584840
1	0.806783	-0.239775	-3.894443	1	0.834475	-0.200038	-3.890072
6	0.608440	0.190602	-5.996153	6	0.661272	0.241674	-5.992176
1	0.257543	-3.720240	-4.832045	1	0.322109	-3.678848	-4.857007
1	-0.304805	-2.375420	-3.779591	1	-0.264473	-2.344779	-3.804002
1	-0.569858	-2.309739	-5.557782	1	-0.505209	-2.269641	-5.585457
6	-0.593326	0.883727	-5.802055	6	-0.541642	0.935843	-5.809647
6	1.088918	0.087834	-7.310623	6	1.155899	0.141160	-7.301554
6	-1.242999	1.431895	-6.905762	6	-1.178635	1.486802	-6.919394
1	-1.004502	0.998700	-4.801964	1	-0.963345	1.050375	-4.813925
7	0.469378	0.592760	-8.378200	7	0.548592	0.648674	-8.374876
1	2.029740	-0.424972	-7.521778	1	2.098612	-0.372026	-7.503422
6	-0.675864	1.255625	-8.170077	6	-0.598212	1.312278	-8.177879
1	-2.171617	1.982140	-6.792650	1	-2.107761	2.037961	-6.815202
1	-1.158141	1.664313	-9.055302	1	-1.070528	1.723074	-9.067487
1	1.788157	-2.184704	-5.839836	1	1.855241	-2.126394	-5.833693

$^{4}TS_{H}$

26	-0.084821	-0.293974	-0.345108
7	0.294858	-2.261763	-0.117456
7	1.913463	0.084227	-0.111278
7	-0.446454	1.677522	-0.355728
7	-2.040088	-0.669326	-0.509784
6	-0.625798	-3.278420	-0.174013
6	1.516653	-2.866126	0.079025
6	2.919280	-0.834801	0.093901
6	2.522374	1.317187	-0.106484
6	0.480799	2.692859	-0.341227
6	-1.670470	2.285897	-0.474461
6	-3.053547	0.248477	-0.610350
6	-2.644291	-1.899912	-0.531460
6	0.026117	-4.551815	-0.001483
6	1.355014	-4.295788	0.156074
6	4.189699	-0.163122	0.212343
6	3.944314	1.170968	0.085074
6	-0.180037	3.971165	-0.436876
6	-1.515691	3.718545	-0.513766
6	-4.329175	-0.420673	-0.725963

$^{2}TS_{H}$

26	0.007656	-0.237047	-0.334619
7	0.520887	-2.172705	-0.193746
7	1.943914	0.264789	-0.066046
7	-0.518886	1.721575	-0.304431
7	-1.944336	-0.725458	-0.468065
6	-0.331233	-3.243822	-0.293112
6	1.763755	-2.703641	0.042187
6	3.011541	-0.575355	0.166398
6	2.461786	1.537111	-0.061258
6	0.341636	2.795534	-0.285082
6	-1.783651	2.254616	-0.419534
6	-3.016281	0.118314	-0.570096
6	-2.456768	-1.994831	-0.547764
6	0.396570	-4.479795	-0.144519
6	1.700157	-4.143152	0.070545
6	4.226652	0.186626	0.310280
6	3.887539	1.496750	0.157667
6	-0.401968	4.031353	-0.364001
6	-1.717560	3.696769	-0.440102
6	-4.240439	-0.633991	-0.715944

6	-4.074883	-1.754776	-0.680293	6	-3.892092	-1.949418	-0.703948
6	-1.992333	-3.115241	-0.377101	6	-1.710677	-3.164396	-0.469985
6	2.737809	-2.208949	0.171472	6	2.928002	-1.959871	0.228020
6	1.858236	2.531621	-0.236461	6	1.723188	2.710013	-0.197878
6	-2.889111	1.625914	-0.582115	6	-2.947025	1.510677	-0.537826
1	-2.601575	-4.013523	-0.395882	1	-2.254471	-4.102636	-0.527581
1	3.619443	-2.820404	0.337736	1	3.843320	-2.507781	0.430905
1	2.462392	3.433606	-0.220625	1	2.276226	3.644355	-0.185483
1	-3.781691	2.238243	-0.662942	1	-3.881322	2.056727	-0.625360
1	-0.480787	-5.508108	0.004344	1	-0.047027	-5.466674	-0.176258
1	2.161270	-4.999359	0.319058	1	2.544245	-4.797041	0.248385
1	5.135642	-0.658966	0.388718	1	5.202285	-0.237101	0.510763
1	4.647954	1.991966	0.135682	1	4.528080	2.367639	0.210980
1	0.325813	4.928073	-0.437270	1	0.041375	5.018639	-0.354442
1	-2.331743	4.424840	-0.594077	1	-2.576013	4.352207	-0.509419
1	-5.283010	0.082466	-0.816986	1	-5.226824	-0.198229	-0.807933
1	-4.776622	-2.577614	-0.723449	1	-4.533831	-2.817539	-0.781530
8	0.069626	-0.350038	-2.098074	8	0.095283	-0.166960	-2.110786
16	-0.090962	-0.313359	2.028300	16	-0.133866	0.094661	2.043744
1	0.143072	1.001435	2.238935	1	-1.448942	0.393710	2.136835
1	3.098782	-0.858755	-2.813611	1	2.751809	-1.630560	-2.721508
6	2.304718	-0.360862	-3.365445	6	2.203683	-0.905168	-3.318454
6	2.462042	1.048859	-3.890131	6	2.848284	0.363760	-3.830838
7	1.774170	-1.195196	-4.488208	7	1.474773	-1.528762	-4.464006
1	1.093299	-0.317813	-2.443272	1	1.080396	-0.455451	-2.465873
6	1.684249	1.075791	-5.232897	6	2.173166	0.638927	-5.201365
1	3.516707	1.317179	-4.034068	1	3.935453	0.255097	-3.934962
1	2.054974	1.765866	-3.167610	1	2.682156	1.181053	-3.120713
6	0.855173	-0.220925	-5.261050	6	0.964041	-0.312734	-5.271731
6	1.121841	-2.479414	-4.067521	6	0.416642	-2.519312	-4.073685
1	1.024069	1.941177	-5.324251	1	1.838028	1.672870	-5.309107
1	2.373221	1.106352	-6.082900	1	2.865006	0.437993	-6.025244
1	-0.011434	-0.121162	-4.601621	1	0.150611	0.072804	-4.650544
6	0.449776	-0.766615	-6.604799	6	0.460473	-0.705961	-6.635318
1	1.865372	-3.089759	-3.551881	1	0.895373	-3.339412	-3.535576
1	0.307604	-2.227436	-3.388385	1	-0.286384	-2.003219	-3.419912
1	0.762565	-2.993066	-4.960224	1	-0.061995	-2.887390	-4.982072
6	-0.888403	-1.076419	-6.879107	6	-0.889451	-0.549886	-6.974555
6	1.384484	-0.983749	-7.628938	6	1.314490	-1.234701	-7.615550
6	-1.225548	-1.573177	-8.135768	6	-1.314616	-0.915562	-8.249428
1	-1.653080	-0.921888	-6.121412	1	-1.592283	-0.139644	-6.253134
7	1.079349	-1.474791	-8.830664	7	0.918791	-1.605146	-8.833819
1	2.439738	-0.746255	-7.480796	1	2.380076	-1.364883	-7.416122
6	-0.206957	-1.758372	-9.073784	6	-0.374941	-1.440925	-9.139743
1	-2.253549	-1.815586	-8.385061	1	-2.351294	-0.799984	-8.548756
1	-0.430495	-2.149667	-10.06373	1	-0.670247	-1.742608	-10.14215

			5				2
1	2.542294	-1.441097	-5.128343	1	2.145796	-2.021497	-5.069500
^{4}IM				^{2}IM			
26	0.122095	-0.222965	-0.314472	26	0.100332	-0.258698	-0.303285
7	0.469980	-1.963762	0.645521	7	0.448945	-1.979841	0.662821
7	1.783571	0.537823	0.539323	7	1.779308	0.511293	0.530975
7	-0.290625	1.560296	-1.151508	7	-0.308734	1.533023	-1.165608
7	-1.601891	-0.948431	-1.087791	7	-1.620882	-0.976934	-1.062331
6	-0.280783	-3.105165	0.536025	6	-0.308430	-3.119621	0.575850
6	1.473125	-2.258305	1.523783	6	1.465544	-2.271542	1.532851
6	2.620679	-0.068546	1.451879	6	2.626779	-0.091148	1.430869
6	2.303444	1.790987	0.334825	6	2.298791	1.762665	0.307609
6	0.517260	2.674222	-1.135552	6	0.507386	2.639909	-1.164016
6	-1.398334	1.909988	-1.899816	6	-1.408099	1.874591	-1.922623
6	-2.538249	-0.284653	-1.829729	6	-2.553952	-0.315533	-1.816586
6	-2.067615	-2.229287	-0.950741	6	-2.096799	-2.252687	-0.908435
6	0.277546	-4.153916	1.356441	6	0.254744	-4.161532	1.401428
6	1.367629	-3.623510	1.977996	6	1.355619	-3.631402	2.002097
6	3.690926	0.826096	1.823547	6	3.706137	0.801035	1.780933
6	3.501204	1.975317	1.121718	6	3.508581	1.947458	1.075598
6	-0.094586	3.746594	-1.884234	6	-0.095936	3.704707	-1.931131
6	-1.285260	3.276967	-2.348412	6	-1.287601	3.233957	-2.393246
6	-3.626543	-1.166880	-2.179351	6	-3.647159	-1.196945	-2.153055
6	-3.327934	-2.382596	-1.637277	6	-3.357915	-2.405997	-1.593109
6	-1.447667	-3.234414	-0.211019	6	-1.480831	-3.253219	-0.160677
6	2.472548	-1.365568	1.919622	6	2.475373	-1.386397	1.908876
6	1.735529	2.770696	-0.473797	6	1.728116	2.736747	-0.505345
6	-2.447499	1.057654	-2.207457	6	-2.460495	1.018312	-2.215968
1	-1.942436	-4.200910	-0.183994	1	-1.979862	-4.216904	-0.120446
1	3.204112	-1.723823	2.637422	1	3.213267	-1.746132	2.619360
1	2.262141	3.717664	-0.545372	1	2.259737	3.679855	-0.590260
1	-3.262338	1.464937	-2.798881	1	-3.275289	1.416800	-2.813391
1	-0.129674	-5.152592	1.447424	1	-0.157320	-5.156578	1.508733
1	2.041118	-4.097580	2.680000	1	2.035368	-4.102070	2.700367
1	4.475278	0.590171	2.530916	1	4.501072	0.566512	2.476865
1	4.094915	2.880086	1.139232	1	4.105943	2.850018	1.078381
1	0.333998	4.732453	-2.011178	1	0.338222	4.686318	-2.071633
1	-2.030576	3.798119	-2.935601	1	-2.028145	3.749820	-2.991085
1	-4.504018	-0.877673	-2.743863	1	-4.522043	-0.910197	-2.722841
1	-3.909133	-3.295232	-1.669933	1	-3.944961	-3.315214	-1.613506
8	1.059603	-0.810131	-1.800109	8	1.054715	-0.792205	-1.796902
16	-1.000935	0.706387	1.584081	16	-0.972400	0.761073	1.571074
1	-2.189246	1.000663	1.010252	1	-2.161271	1.064291	1.002918
1	3.560882	-1.298437	-4.234966	1	3.566844	-1.256381	-4.202597
6	2.719511	-0.694688	-4.548976	6	2.726202	-0.655343	-4.523388

6	2.428853	0.737675	-4.286803	6	2.434672	0.780029	-4.278127
7	1.522621	-1.401619	-5.027103	7	1.537263	-1.364388	-5.017250
1	1.922915	-1.073938	-1.438303	1	1.924430	-1.037772	-1.437592
6	1.115267	0.985757	-5.056136	6	1.123643	1.020488	-5.054638
1	3.246857	1.393857	-4.605373	1	3.253663	1.432426	-4.602282
1	2.271062	0.885932	-3.207702	1	2.275383	0.942242	-3.201533
6	0.364001	-0.352144	-4.970072	6	0.375319	-0.318866	-4.965993
6	1.202637	-2.676011	-4.286654	6	1.215740	-2.644642	-4.288212
1	0.512775	1.780704	-4.610069	1	0.517221	1.816123	-4.615294
1	1.317098	1.260598	-6.096280	1	1.329577	1.290615	-6.095244
1	-0.031967	-0.475240	-3.959940	1	-0.022655	-0.440429	-3.956448
6	-0.672127	-0.662843	-6.019213	6	-0.657851	-0.634976	-6.016373
1	2.047722	-3.359283	-4.391978	1	2.064004	-3.324288	-4.391449
1	1.029918	-2.398232	-3.242871	1	1.034382	-2.375065	-3.243865
1	0.310543	-3.112924	-4.739534	1	0.328743	-3.081565	-4.750884
6	-1.932454	-1.161592	-5.663866	6	-1.917956	-1.134803	-5.661712
6	-0.409737	-0.488425	-7.387750	6	-0.393408	-0.464241	-7.384933
6	-2.852409	-1.452333	-6.668655	6	-2.835581	-1.430472	-6.667145
1	-2.191018	-1.311192	-4.618397	1	-2.177797	-1.281259	-4.616153
7	-1.276824	-0.775400	-8.360164	7	-1.258196	-0.755952	-8.357993
1	0.548981	-0.091140	-7.725061	1	0.565062	-0.066065	-7.721897
6	-2.477281	-1.246042	-7.998362	6	-2.458370	-1.227766	-7.996838
1	-3.839663	-1.834884	-6.429755	1	-3.822554	-1.814093	-6.428828
1	-3.167757	-1.466672	-8.809456	1	-3.146961	-1.452247	-8.808468
1	1.647542	-1.649010	-6.018289	1	1.672632	-1.605243	-6.008796

$^{4}TS_{reb}$

26	-0.099081	-0.007611	-0.399002
7	-0.312429	-1.834919	-1.241229
7	1.814686	-0.418150	0.022133
7	0.153458	1.878344	0.293218
7	-2.043154	0.378206	-0.737642
6	-1.476900	-2.385598	-1.724247
6	0.625031	-2.840114	-1.261083
6	2.472403	-1.608743	-0.200203
6	2.733731	0.424288	0.607213
6	1.293709	2.401377	0.861779
6	-0.825181	2.835479	0.450060
6	-2.710327	1.552491	-0.474950
6	-2.959998	-0.460054	-1.330655
6	-1.253287	-3.757966	-2.104041
6	0.048051	-4.041747	-1.811208
6	3.832143	-1.511639	0.261999
6	3.994270	-0.253421	0.759367
6	1.037563	3.736009	1.341417
6	-0.272764	4.004017	1.087841

$^{2}TS_{reb}$

26	0.106491	-0.145886	-0.426385
7	0.218598	-2.085264	-0.978141
7	1.910412	-0.266492	0.479301
7	-0.021222	1.768164	0.185612
7	-1.708251	-0.043059	-1.289300
6	-0.749840	-2.847950	-1.585718
6	1.275958	-2.932616	-0.750773
6	2.738755	-1.364249	0.491467
6	2.567267	0.704765	1.203773
6	0.874101	2.484546	0.938598
6	-1.051059	2.632558	-0.090526
6	-2.507695	1.066171	-1.351329
6	-2.428158	-1.055576	-1.870572
6	-0.290446	-4.206647	-1.749953
6	0.972693	-4.255512	-1.242143
6	3.942039	-1.075664	1.236315
6	3.832853	0.204456	1.683321
6	0.399228	3.831496	1.145080
6	-0.796221	3.925010	0.500934

6	-4.085165	1.440947	-0.889136	6	-3.753699	0.756080	-2.013613
6	-4.239553	0.195584	-1.420341	6	-3.707260	-0.568255	-2.329889
6	-2.706416	-1.744715	-1.791905	6	-1.989431	-2.370394	-1.998731
6	1.928078	-2.737967	-0.794208	6	2.456593	-2.589818	-0.099497
6	2.502798	1.736889	0.994701	6	2.082441	1.987237	1.423599
6	-2.154306	2.696066	0.083614	6	-2.194534	2.314602	-0.815502
1	-3.541199	-2.301624	-2.205423	1	-2.669978	-3.080370	-2.459450
1	2.562536	-3.614475	-0.876863	1	3.206762	-3.368471	0.001332
1	3.323106	2.273708	1.459453	1	2.697936	2.660094	2.012810
1	-2.813375	3.540822	0.254643	1	-2.931398	3.102482	-0.941126
1	-2.011602	-4.416386	-2.508176	1	-0.875253	-5.010814	-2.178375
1	0.572171	-4.983291	-1.917917	1	1.637706	-5.106852	-1.173920
1	4.558203	-2.312623	0.208691	1	4.749829	-1.777545	1.398515
1	4.879975	0.188601	1.197032	1	4.533380	0.770624	2.283335
1	1.772850	4.366625	1.824109	1	0.921129	4.591674	1.711680
1	-0.833796	4.900213	1.319120	1	-1.459515	4.777610	0.432986
1	-4.824406	2.224445	-0.783739	1	-4.557859	1.460798	-2.182159
1	-5.132224	-0.252230	-1.837829	1	-4.464755	-1.172644	-2.812243
8	0.351704	0.703334	-2.148250	8	0.999809	0.427976	-2.022731
16	-0.571613	-0.828687	1.705571	16	-0.772952	-0.998557	1.582918
1	-1.911351	-0.653975	1.686840	1	-0.203644	-0.125343	2.443821
1	0.790750	2.262866	-4.228514	1	2.060558	1.991876	-3.988779
6	0.332120	1.283643	-4.295206	6	1.188204	1.371517	-4.150864
6	-1.089577	1.004381	-4.664157	6	-0.213095	1.829903	-4.362211
7	1.206999	0.223068	-4.829368	7	1.422670	0.105164	-4.859844
1	0.561103	1.619743	-1.892295	1	1.672959	1.039010	-1.679236
6	-1.055041	-0.380873	-5.356687	6	-0.910871	0.646742	-5.083337
1	-1.506113	1.777261	-5.322885	1	-0.262285	2.751642	-4.958519
1	-1.702667	0.986458	-3.756496	1	-0.677038	2.049836	-3.393553
6	0.284622	-1.017047	-4.946556	6	0.023052	-0.565335	-4.907228
6	2.484334	-0.011461	-4.071497	6	2.513735	-0.757626	-4.291661
1	-1.880290	-1.025478	-5.046943	1	-1.891673	0.420128	-4.659860
1	-1.111043	-0.278037	-6.444967	1	-1.057672	0.870108	-6.144184
1	0.224670	-1.389429	-3.921747	1	-0.089214	-0.978785	-3.903677
6	0.872655	-2.050601	-5.873089	6	-0.021523	-1.649402	-5.953607
1	3.088299	0.896235	-4.130978	1	3.459918	-0.221105	-4.388380
1	2.214584	-0.219665	-3.038132	1	2.268075	-0.921295	-3.243024
1	3.009848	-0.842980	-4.542987	1	2.549232	-1.685202	-4.864519
6	1.231590	-3.320707	-5.405035	6	-0.091702	-3.000359	-5.588132
6	1.079028	-1.783565	-7.235719	6	0.023391	-1.355566	-7.325803
6	1.766013	-4.244988	-6.299889	6	-0.118808	-3.971950	-6.585858
1	1.078466	-3.580801	-4.360653	1	-0.128298	-3.283174	-4.538739
7	1.606064	-2.651953	-8.099447	7	0.013382	-2.276120	-8.291110
1	0.800466	-0.818460	-7.664790	1	0.065630	-0.322303	-7.674475
6	1.938539	-3.862514	-7.632183	6	-0.060726	-3.560647	-7.919568
1	2.047279	-5.241361	-5.974161	1	-0.179138	-5.027063	-6.338711

1	2.359152	-4.555173	-8.357719	1	-0.074390	-4.290821	-8.725711
1	1.478935	0.463532	-5.794120	1	1.676548	0.300043	-5.840428

^{4}PC

26	-0.364570	-0.271932	0.082270	26	-0.462577	-0.367299	0.073990
7	-0.377395	-2.275663	-0.127726	7	-0.740180	-2.338479	0.019361
7	1.657609	-0.312159	0.016607	7	1.530085	-0.638716	-0.008149
7	-0.275493	1.722921	-0.325938	7	-0.150693	1.593961	-0.343334
7	-2.311876	-0.240657	-0.418508	7	-2.418062	-0.110598	-0.253737
6	-1.485675	-3.090816	-0.225354	6	-1.936764	-3.024964	-0.031714
6	0.691662	-3.129710	0.059364	6	0.222479	-3.304191	0.238513
6	2.459298	-1.425861	0.180024	6	2.192795	-1.830168	0.198792
6	2.513824	0.770381	0.093613	6	2.521902	0.320281	-0.083029
6	0.830563	2.546147	-0.155505	6	1.057261	2.284077	-0.304921
6	-1.362525	2.585931	-0.391442	6	-1.127834	2.580803	-0.331588
6	-3.117431	0.874147	-0.543741	6	-3.088532	1.093495	-0.326901
6	-3.166871	-1.321429	-0.497337	6	-3.403606	-1.074963	-0.290232
6	-1.104271	-4.474092	-0.109813	6	-1.718642	-4.438306	0.138629
6	0.245610	-4.498090	0.068487	6	-0.380222	-4.610794	0.313364
6	3.834392	-1.036303	0.333162	6	3.618049	-1.619572	0.227059
6	3.868589	0.325612	0.279603	6	3.823077	-0.285215	0.045894
6	0.432716	3.924362	-0.164137	6	0.826651	3.700142	-0.322597
6	-0.923636	3.948697	-0.309622	6	-0.525684	3.883137	-0.332694
6	-4.492345	0.484163	-0.708842	6	-4.511354	0.877195	-0.419013
6	-4.522915	-0.877083	-0.682401	6	-4.706231	-0.468358	-0.404077
6	-2.788905	-2.652065	-0.403808	6	-3.182709	-2.439697	-0.194946
6	2.014424	-2.739651	0.199295	6	1.585050	-3.070405	0.330221
6	2.132971	2.103804	0.015161	6	2.305683	1.684555	-0.224973
6	-2.684057	2.191105	-0.517424	6	-2.493714	2.345403	-0.338718
1	-3.569698	-3.402999	-0.466734	1	-4.048033	-3.094330	-0.221264
1	2.755551	-3.518812	0.345366	1	2.229080	-3.927432	0.500960
1	2.908588	2.854941	0.124895	1	3.175246	2.334926	-0.216131
1	-3.436531	2.969413	-0.589590	1	-3.149222	3.210133	-0.364055
1	-1.792844	-5.308058	-0.153470	1	-2.499847	-5.187353	0.131256
1	0.892617	-5.355631	0.200529	1	0.164594	-5.531648	0.477126
1	4.657142	-1.724641	0.477548	1	4.353812	-2.399255	0.377318
1	4.725085	0.981065	0.372004	1	4.760836	0.255311	0.023246
1	1.110658	4.761054	-0.054772	1	1.605026	4.452274	-0.303720
1	-1.579199	4.808977	-0.347014	1	-1.075931	4.815276	-0.329263
1	-5.317397	1.174492	-0.827204	1	-5.250283	1.664780	-0.490480
1	-5.378751	-1.533395	-0.773262	1	-5.638203	-1.016027	-0.457735
8	0.011772	1.319218	-3.224824	8	-0.263636	0.929761	-3.185436
16	-0.556306	-0.136712	2.450051	16	-0.523697	-0.131558	2.269584
1	-1.718673	-0.823574	2.524888	1	-1.676835	-0.800269	2.501777
1	1.891899	0.706544	-2.621398	1	1.696663	1.576379	-3.075063
6	1.282618	0.881444	-3.512621	6	0.940420	1.219523	-3.781105

6	1.947036	1.719032	-4.600510	6	0.769716	2.068893	-5.037467
7	1.156882	-0.489244	-4.249018	7	1.489808	-0.100174	-4.408176
1	-0.136686	1.338034	-2.250250	1	-0.219160	1.072793	-2.208756
6	1.269361	1.285998	-5.921344	6	0.222184	1.099740	-6.111874
1	3.023202	1.510384	-4.622681	1	1.737142	2.487446	-5.339132
1	1.817228	2.780169	-4.380220	1	0.096389	2.902368	-4.829364
6	0.676479	-0.130795	-5.671923	6	0.603203	-0.336061	-5.650015
6	0.319345	-1.508439	-3.551734	6	1.582292	-1.264833	-3.479181
1	0.457094	1.966129	-6.186203	1	-0.865097	1.168882	-6.185348
1	1.975363	1.279600	-6.753683	1	0.631718	1.320084	-7.099326
1	-0.409002	-0.067807	-5.573969	1	-0.275864	-0.844736	-5.249593
6	1.043990	-1.217844	-6.651277	6	1.304621	-1.222806	-6.648657
1	0.772316	-1.745796	-2.588498	1	2.302950	-1.037862	-2.692602
1	-0.672357	-1.085309	-3.397142	1	0.599483	-1.433670	-3.041731
1	0.265620	-2.400710	-4.177565	1	1.906078	-2.136179	-4.050540
6	0.064377	-2.011750	-7.259853	6	0.842342	-2.515216	-6.925160
6	2.382650	-1.475005	-6.986341	6	2.449354	-0.786539	-7.333819
6	0.456809	-3.003960	-8.155735	6	1.528973	-3.296085	-7.852411
1	-0.989183	-1.847769	-7.045164	1	-0.046903	-2.899283	-6.430484
7	2.774112	-2.431498	-7.828056	7	3.126304	-1.528076	-8.210394
1	3.188111	-0.872128	-6.560766	1	2.841694	0.220624	-7.175571
6	1.820808	-3.177953	-8.401782	6	2.666038	-2.760847	-8.462331
1	-0.276176	-3.631020	-8.652862	1	1.193645	-4.298580	-8.097667
1	2.165637	-3.946006	-9.090269	1	3.231641	-3.342725	-9.186441
1	2.105891	-0.867799	-4.339017	1	2.434363	0.104624	-4.751654

Table S9. Cartesian coordinates for *N*-methylhydroxylation by Cpd I. The geometries were optimized at the B3LYP/B1 level.

^{4}RC				^{2}RC			
26	0.996103	-1.199557	-2.702327	26	0.991898	-1.185692	-2.688315
7	2.739162	-0.191424	-2.773370	7	2.734038	-0.182044	-2.760776
7	1.653044	-2.412166	-4.171298	7	1.651219	-2.406504	-4.160803
7	-0.833283	-2.045852	-2.851942	7	-0.839915	-2.031680	-2.844620
7	0.228452	0.221343	-1.491098	7	0.225568	0.231635	-1.482531
6	3.083605	0.909895	-2.026772	6	3.080194	0.919469	-2.015756
6	3.863376	-0.533376	-3.475929	6	3.858469	-0.526695	-3.463557
6	2.922462	-2.444601	-4.716655	6	2.922787	-2.446235	-4.696952
6	0.978702	-3.480834	-4.731424	6	0.979566	-3.480688	-4.711306
6	-1.167773	-3.168883	-3.565043	6	-1.171375	-3.158516	-3.553815
6	-1.971291	-1.680799	-2.168760	6	-1.978064	-1.666919	-2.163374
6	-1.049971	0.290370	-1.003117	6	-1.055859	0.305109	-1.000167
6	0.902710	1.275492	-0.933069	6	0.898915	1.287729	-0.925249
6	4.460520	1.267448	-2.267882	6	4.456898	1.275984	-2.258180
6	4.945908	0.369453	-3.167391	6	4.941052	0.376620	-3.157004
6	3.031005	-3.530038	-5.658589	6	3.036360	-3.541145	-5.627828
6	1.832002	-4.171939	-5.664757	6	1.836936	-4.182370	-5.633566
6	-3.044120	-2.599799	-2.459448	6	-3.049959	-2.587682	-2.452163
6	-2.543156	-3.528089	-3.320915	6	-2.546908	-3.518106	-3.310128
6	-1.186754	1.413499	-0.109370	6	-1.194119	1.432172	-0.111939
6	0.030095	2.026044	-0.064197	6	0.023480	2.042680	-0.063466
6	2.233947	1.598792	-1.175317	6	2.230854	1.609056	-1.164187
6	3.953428	-1.582399	-4.386901	6	3.951410	-1.579482	-4.369340
6	-0.320106	-3.851299	-4.431755	6	-0.321803	-3.845934	-4.414469
6	-2.079993	-0.591185	-1.317779	6	-2.086483	-0.575187	-1.314456
1	2.637081	2.466761	-0.662911	1	2.634016	2.477065	-0.651907
1	4.906970	-1.731330	-4.883612	1	4.907004	-1.730139	-4.861620
1	-0.721139	-4.722128	-4.940722	1	-0.722235	-4.719899	-4.918593
1	-3.047813	-0.409714	-0.860484	1	-3.054570	-0.391215	-0.858752
1	4.969853	2.104575	-1.808411	1	4.967045	2.113346	-1.800063
1	5.936370	0.315244	-3.600202	1	5.931272	0.321327	-3.590245
1	3.920062	-3.758808	-6.231810	1	3.928116	-3.775962	-6.194383
1	1.533508	-5.034519	-6.246351	1	1.540669	-5.050356	-6.208242
1	-3.052073	-4.366641	-3.778535	1	-3.054368	-4.358851	-3.765367
1	-4.048259	-2.521081	-2.062877	1	-4.054490	-2.509037	-2.056588
1	-2.102240	1.692708	0.396109	1	-2.111416	1.715216	0.388076
1	0.318753	2.914014	0.483433	1	0.310988	2.932453	0.481822
8	1.479226	-2.157670	-1.463552	8	1.472598	-2.175099	-1.474253
16	0.224274	0.009415	-4.782757	16	0.221926	0.007309	-4.788402
1	1.435118	0.368123	-5.265753	1	1.434768	0.357285	-5.272885
1	1.871918	-5.848077	-0.039316	1	1.874147	-5.866681	-0.044099
6	1.225796	-4.967661	-0.055384	6	1.228282	-4.986154	-0.063789
6	-0.279828	-5.260678	0.044567	6	-0.277586	-5.278454	0.037781

7	1.529883	-4.115483	1.159535	7	1.533323	-4.128791	1.147311
1	1.462590	-4.337775	-0.915453	1	1.464896	-4.359931	-0.926529
6	-0.867385	-4.150319	0.961013	6	-0.863796	-4.168233	0.955196
1	-0.463610	-6.251736	0.469328	1	-0.461719	-6.269663	0.461966
1	-0.725270	-5.243807	-0.952538	1	-0.723878	-5.260465	-0.958912
6	0.296769	-3.194658	1.291270	6	0.299322	-3.208875	1.277062
6	2.842837	-3.397739	1.094477	6	2.845371	-3.409940	1.076958
1	-1.664889	-3.588158	0.469840	1	-1.665801	-3.609541	0.467361
1	-1.289435	-4.579159	1.874336	1	-1.279569	-4.596665	1.871630
1	0.436070	-2.480499	0.474942	1	0.435475	-2.499574	0.455894
6	0.265667	-2.489471	2.622780	6	0.270634	-2.495480	2.604173
1	3.640199	-4.138379	1.007375	1	3.643335	-4.150100	0.991184
1	2.818747	-2.746410	0.218905	1	2.818814	-2.761950	0.198923
1	2.967177	-2.818073	2.010157	1	2.970929	-2.826645	1.990167
6	0.381781	-1.095591	2.698944	6	0.387966	-1.101198	2.671058
6	0.119329	-3.191784	3.828941	6	0.125641	-3.189817	3.815076
6	0.346151	-0.482493	3.949506	6	0.354569	-0.479890	3.917591
1	0.487231	-0.501996	1.794232	1	0.493145	-0.513882	1.762244
7	0.100673	-2.619839	5.033530	7	0.109108	-2.609949	5.015932
1	0.005155	-4.277980	3.831216	1	0.010897	-4.275879	3.824629
6	0.210134	-1.285665	5.084096	6	0.219522	-1.275554	5.057590
1	0.425322	0.595636	4.045958	1	0.434668	0.598791	4.006827
1	0.185560	-0.842338	6.077136	1	0.196642	-0.825703	6.047738
1	1.540204	-4.721691	1.986850	1	1.545723	-4.731580	1.977095

$^{4}TS_{H}$ $^{2}TS_{H}$

26	0.716046	-1.201520	-2.776479	26	0.744871	-1.145665	-2.705426
7	2.637167	-0.642251	-2.338460	7	2.629640	-0.558667	-2.317377
7	1.407577	-2.476711	-4.152223	7	1.429720	-2.398512	-4.139335
7	-1.161532	-1.715651	-3.221417	7	-1.153841	-1.684400	-3.179175
7	0.052188	0.245880	-1.534660	7	0.054531	0.256272	-1.450819
6	3.045089	0.354525	-1.477095	6	3.033569	0.428871	-1.445150
6	3.787580	-1.168458	-2.875934	6	3.783060	-1.048645	-2.880906
6	2.726032	-2.756211	-4.441696	6	2.747912	-2.642088	-4.465711
6	0.660671	-3.294616	-4.965690	6	0.685125	-3.271639	-4.906763
6	-1.570728	-2.643832	-4.140354	6	-1.550118	-2.654175	-4.057271
6	-2.309969	-1.189312	-2.683102	6	-2.307026	-1.170868	-2.642232
6	-1.258492	0.512096	-1.232153	6	-1.259606	0.517318	-1.163016
6	0.801186	1.111960	-0.773810	6	0.788196	1.140845	-0.700643
6	4.484498	0.438251	-1.459408	6	4.470137	0.540784	-1.442396
6	4.945051	-0.508506	-2.323671	6	4.936564	-0.379342	-2.332939
6	2.803531	-3.763874	-5.469468	6	2.828533	-3.659196	-5.485263
6	1.524517	-4.093466	-5.798145	6	1.553721	-4.049880	-5.755148
6	-3.472461	-1.829704	-3.256212	6	-3.462755	-1.843691	-3.192209
6	-3.013483	-2.731354	-4.163049	6	-2.991551	-2.769977	-4.068462
6	-1.342433	1.580990	-0.269931	6	-1.359279	1.588984	-0.204081

6	-0.061318	1.955267	0.013407	6	-0.083520	1.978027	0.082870
6	2.192224	1.167747	-0.744729	6	2.177313	1.223996	-0.693983
6	3.829836	-2.168537	-3.840693	6	3.839082	-2.024383	-3.875288
6	-0.725610	-3.375911	-4.965102	6	-0.693003	-3.405186	-4.857715
6	-2.360782	-0.155425	-1.761748	6	-2.358876	-0.143064	-1.712646
1	2.645651	1.916793	-0.102795	1	2.628195	1.979328	-0.057471
1	4.809119	-2.492085	-4.179653	1	4.823986	-2.312138	-4.230651
1	-1.184434	-4.068839	-5.663258	1	-1.143975	-4.141877	-5.515301
1	-3.342531	0.171760	-1.433549	1	-3.341888	0.181724	-1.385169
1	5.054377	1.145337	-0.870375	1	5.034356	1.247030	-0.847001
1	5.969610	-0.734542	-2.589773	1	5.961262	-0.580991	-2.617571
1	3.725879	-4.153207	-5.880691	1	3.749809	-4.019229	-5.924748
1	1.181029	-4.811018	-6.531885	1	1.214747	-4.795497	-6.462615
1	-3.581035	-3.391965	-4.805452	1	-3.550954	-3.461942	-4.684499
1	-4.496574	-1.593097	-2.998309	1	-4.489863	-1.617568	-2.936737
1	-2.265933	1.989725	0.119680	1	-2.288671	1.992519	0.176877
1	0.280861	2.733596	0.683441	1	0.247831	2.766178	0.746758
8	0.732863	-2.412186	-1.477371	8	0.751593	-2.444711	-1.482828
16	0.905351	0.364859	-4.539712	16	0.561980	0.271325	-4.649316
1	0.922854	1.502352	-3.809124	1	1.874194	0.555899	-4.812201
1	2.806560	-5.491197	-0.067429	1	2.733201	-5.548987	-0.083911
6	1.821927	-5.034371	0.052235	6	1.757739	-5.071721	0.031154
6	0.771741	-5.920795	0.741108	6	0.685827	-5.936821	0.714376
7	1.952684	-3.821001	0.953160	7	1.910329	-3.861511	0.934127
1	1.476118	-4.640422	-0.905427	1	1.424180	-4.668298	-0.926942
6	-0.029302	-4.977119	1.682621	6	-0.090181	-4.981884	1.665152
1	1.245033	-6.725508	1.310660	1	1.138282	-6.758923	1.275873
1	0.134162	-6.389958	-0.011479	1	0.035507	-6.382055	-0.041855
6	0.497693	-3.552959	1.425161	6	0.460296	-3.567086	1.407983
6	2.621199	-2.669050	0.323054	6	2.598826	-2.720909	0.304976
1	-1.103821	-5.005647	1.487170	1	-1.166663	-4.990510	1.478848
1	0.110118	-5.261547	2.729275	1	0.053118	-5.271883	2.709832
1	0.033624	-3.125041	0.532417	1	0.004822	-3.130434	0.514962
6	0.453908	-2.568671	2.563887	6	0.436138	-2.583271	2.547633
1	3.567129	-2.930935	-0.141577	1	3.539507	-2.999645	-0.160888
1	1.606562	-2.334654	-0.917151	1	1.621945	-2.376429	-0.902391
1	2.592304	-1.776732	0.939837	1	2.588977	-1.829919	0.924431
6	-0.096748	-1.293346	2.382058	6	-0.094885	-1.299251	2.368632
6	0.958215	-2.879640	3.836150	6	0.939504	-2.903383	3.818054
6	-0.124477	-0.410239	3.458838	6	-0.105473	-0.416911	3.446364
1	-0.500310	-1.001987	1.415772	1	-0.496989	-1.000566	1.404093
7	0.953011	-2.038240	4.870827	7	0.950841	-2.062996	4.853470
1	1.388758	-3.861801	4.041234	1	1.355008	-3.892475	4.021037
6	0.413660	-0.827069	4.678468	6	0.429861	-0.843307	4.663902
1	-0.550403	0.582356	3.353862	1	-0.516075	0.582247	3.342963
1	0.412890	-0.163379	5.540398	1	0.442232	-0.180561	5.526467

1	2.479373	-4.102337	1.792430	1	2.434197	-4.150701	1.772127

^{4}IM ^{2}IM

26	0.924686	-1.373322	-2.853572	26	0.922880	-1.329670	-2.843407
7	2.385911	-0.025381	-2.469793	7	2.375275	0.015920	-2.482564
7	2.235485	-2.410617	-3.977118	7	2.240524	-2.390617	-3.958189
7	-0.543809	-2.658095	-3.331418	7	-0.548250	-2.642928	-3.300771
7	-0.417963	-0.262324	-1.831772	7	-0.417053	-0.217302	-1.846025
6	2.268237	1.079528	-1.663636	6	2.257918	1.135954	-1.696572
6	3.675170	-0.019283	-2.926791	6	3.668919	0.012966	-2.937831
6	3.553663	-2.100323	-4.256689	6	3.558159	-2.090348	-4.232297
6	1.999187	-3.618635	-4.590061	6	2.003570	-3.613094	-4.545815
6	-0.405385	-3.825185	-4.039144	6	-0.400770	-3.821782	-3.984985
6	-1.891108	-2.541671	-3.059698	6	-1.890239	-2.534050	-3.021351
6	-1.764940	-0.457803	-1.730651	6	-1.765691	-0.423719	-1.734898
6	-0.144644	0.870661	-1.112443	6	-0.151146	0.929180	-1.144442
6	3.521026	1.793447	-1.605974	6	3.510955	1.850485	-1.650352
6	4.396359	1.111876	-2.397695	6	4.387267	1.154781	-2.426976
6	4.144418	-3.128820	-5.078456	6	4.153496	-3.135466	-5.029245
6	3.186553	-4.073553	-5.275416	6	3.194708	-4.082578	-5.214062
6	-2.610826	-3.667556	-3.606136	6	-2.604912	-3.676977	-3.539064
6	-1.687465	-4.471368	-4.200077	6	-1.677619	-4.483738	-4.124371
6	-2.365989	0.565410	-0.909123	6	-2.369005	0.609310	-0.927832
6	-1.352298	1.388840	-0.514440	6	-1.360776	1.446772	-0.551099
6	1.102388	1.485660	-1.021535	6	1.092517	1.551173	-1.061334
6	4.221952	-0.986541	-3.775385	6	4.221945	-0.964929	-3.765687
6	0.785003	-4.293625	-4.587089	6	0.791987	-4.291282	-4.529058
6	-2.463415	-1.510146	-2.329528	6	-2.462733	-1.488730	-2.307100
1	1.161086	2.391339	-0.424877	1	1.148374	2.465488	-0.477995
1	5.261017	-0.863899	-4.065394	1	5.262387	-0.844305	-4.051461
1	0.745215	-5.239147	-5.119414	1	0.756896	-5.247787	-5.041834
1	-3.541586	-1.530512	-2.198605	1	-3.539821	-1.510155	-2.167740
1	3.690592	2.702243	-1.043024	1	3.679158	2.769380	-1.103655
1	5.431260	1.343642	-2.613451	1	5.422594	1.382632	-2.644958
1	5.163101	-3.116583	-5.443789	1	5.174886	-3.132808	-5.387136
1	3.256591	-4.993509	-5.841197	1	3.267645	-5.014115	-5.760250
1	-1.846539	-5.403540	-4.726675	1	-1.831635	-5.427581	-4.631397
1	-3.682359	-3.806965	-3.541745	1	-3.674606	-3.825117	-3.464182
1	-3.422512	0.643957	-0.686526	1	-3.425022	0.682769	-0.701105
1	-1.409107	2.280539	0.096635	1	-1.421864	2.347131	0.046665
8	1.375877	-2.305651	-1.314485	8	1.375812	-2.298792	-1.330140
16	0.355465	-0.341536	-4.930878	16	0.357989	-0.409241	-4.971096
1	1.561988	0.182154	-5.243553	1	1.561984	0.110719	-5.300419
1	-1.496534	-5.048154	0.288006	1	-1.503141	-5.051951	0.254541
6	-1.125153	-4.029208	0.411253	6	-1.129047	-4.035181	0.387085
6	-2.046038	-3.081753	1.183295	6	-2.044232	-3.093988	1.172617

7	0.142898	-4.067609	1.247427	7	0.141625	-4.084733	1.218156
1	-0.821527	-3.624190	-0.555772	1	-0.828674	-3.620595	-0.576794
6	-1.104738	-2.086615	1.918316	6	-1.097436	-2.100337	1.902269
1	-2.660811	-3.636507	1.899378	1	-2.649761	-3.653945	1.892655
1	-2.723974	-2.576431	0.492694	1	-2.730923	-2.587348	0.491751
6	0.341870	-2.551467	1.648813	6	0.347485	-2.573031	1.633784
6	1.269738	-4.680689	0.578283	6	1.264668	-4.694854	0.539882
1	-1.218927	-1.067378	1.540025	1	-1.206740	-1.082478	1.518772
1	-1.321694	-2.061378	2.988993	1	-1.313335	-2.068426	2.972903
1	0.718813	-2.125958	0.711962	1	0.730019	-2.141392	0.702256
6	1.354572	-2.418140	2.751459	6	1.356627	-2.456588	2.741581
1	1.504826	-4.247954	-0.388224	1	1.493946	-4.259795	-0.426874
1	2.343792	-2.223427	-1.266716	1	2.343362	-2.212769	-1.280288
1	1.935951	-5.283367	1.179909	1	1.937655	-5.294390	1.137186
6	2.619033	-1.873565	2.492220	6	2.625305	-1.916544	2.493968
6	1.091582	-2.841513	4.063191	6	1.085461	-2.893174	4.047362
6	3.540774	-1.775204	3.531341	6	3.543065	-1.835402	3.538116
1	2.865804	-1.525940	1.492081	1	2.878755	-1.559000	1.499001
7	1.969631	-2.769151	5.064790	7	1.959552	-2.837542	5.053412
1	0.118866	-3.259607	4.329025	1	0.108997	-3.308231	4.304236
6	3.170567	-2.240540	4.795729	6	3.164743	-2.313020	4.795499
1	4.526446	-1.350827	3.369179	1	4.531855	-1.414956	3.385001
1	3.865729	-2.186276	5.630665	1	3.856659	-2.272491	5.633891
1	-0.051737	-4.579250	2.114567	1	-0.051151	-4.603780	2.081334

$^{4}TS_{reb}$

26	1.089012	-1.261155	-2.725819
7	2.603336	0.024741	-2.455608
7	2.259641	-2.367842	-3.942570
7	-0.439031	-2.520399	-3.037266
7	-0.027239	-0.248922	-1.378396
6	2.633272	1.086806	-1.580441
6	3.830964	0.005849	-3.076876
6	3.520272	-2.043440	-4.397267
6	1.891659	-3.508061	-4.622540
6	-0.431604	-3.650220	-3.825247
6	-1.717092	-2.411135	-2.532413
6	-1.365106	-0.429400	-1.116498
6	0.350423	0.876140	-0.685457
6	3.904257	1.759029	-1.666305
6	4.642912	1.094396	-2.598082
6	3.967608	-3.025113	-5.352138
6	2.963973	-3.935183	-5.485370
6	-2.530046	-3.494588	-3.018597
6	-1.731685	-4.267083	-3.811006
6	-1.831185	0.583156	-0.202608

$^{2}TS_{reb}$

26	0.794924	-1.198873	-2.778773
7	2.502094	-0.358611	-2.145022
7	1.825910	-2.352748	-4.094977
7	-0.922813	-1.983015	-3.502695
7	-0.232300	-0.025431	-1.501985
6	2.653893	0.643963	-1.208399
6	3.777816	-0.678556	-2.560006
6	3.188131	-2.395592	-4.247099
6	1.317611	-3.196679	-5.056415
6	-1.078157	-2.888465	-4.515585
6	-2.186442	-1.694870	-3.060245
6	-1.594293	0.001234	-1.345803
6	0.260760	0.924995	-0.649564
6	4.049796	0.964925	-1.041679
6	4.745557	0.142114	-1.873239
6	3.550331	-3.301412	-5.312260
6	2.387572	-3.793052	-5.820029
6	-3.165785	-2.450565	-3.805509
6	-2.475233	-3.191497	-4.715412
6	-1.968787	0.984561	-0.355652

6	-0.766638	1.388934	0.069793	6	-0.812582	1.563007	0.075799
6	1.596936	1.483281	-0.748021	6	1.612603	1.239853	-0.510346
6	4.258716	-0.941065	-3.997689	6	4.096748	-1.639039	-3.511604
6	0.653712	-4.127234	-4.548820	6	-0.034585	-3.445389	-5.255184
6	-2.159845	-1.434653	-1.650086	6	-2.499722	-0.778741	-2.060246
1	1.758030	2.364168	-0.135067	1	1.872070	2.021231	0.197888
1	5.248269	-0.815967	-4.424490	1	5.149959	-1.775505	-3.738588
1	0.505068	-5.023619	-5.141913	1	-0.302184	-4.136982	-6.048302
1	-3.206004	-1.456136	-1.361560	1	-3.552840	-0.642508	-1.832167
1	4.179984	2.629025	-1.084452	1	4.432846	1.726160	-0.374319
1	5.649908	1.303989	-2.934687	1	5.815539	0.093668	-2.029452
1	4.926248	-3.001174	-5.853865	1	4.563932	-3.506692	-5.631510
1	2.927584	-4.808343	-6.123891	1	2.250394	-4.488316	-6.638030
1	-1.993052	-5.163749	-4.358265	1	-2.860415	-3.877136	-5.458882
1	-3.577896	-3.631402	-2.783367	1	-4.235688	-2.400680	-3.649971
1	-2.847681	0.664646	0.160371	1	-2.985426	1.206946	-0.057690
1	-0.733395	2.271149	0.696365	1	-0.685296	2.359040	0.798322
8	1.808405	-2.359498	-1.239161	8	0.828483	-2.564428	-1.496172
16	0.249505	0.021546	-4.462839	16	0.839302	0.437290	-4.457914
1	1.015280	1.116876	-4.266540	1	0.869181	1.540975	-3.677037
1	1.340723	-5.851905	-0.251281	1	3.087555	-5.499686	0.530182
6	0.667694	-4.994785	-0.172142	6	2.040627	-5.194828	0.464080
6	-0.757677	-5.326149	0.268441	6	1.060528	-6.017663	1.291583
7	1.173904	-4.074485	0.923122	7	1.893944	-3.802864	1.033378
1	0.710658	-4.394571	-1.081461	1	1.747004	-5.125599	-0.585218
6	-1.259278	-4.062791	1.019828	6	-0.159483	-5.084063	1.460007
1	-0.766488	-6.199832	0.928880	1	1.502930	-6.269865	2.262712
1	-1.376187	-5.565736	-0.599483	1	0.808982	-6.958511	0.796199
6	-0.028965	-3.148017	1.249035	6	0.365331	-3.624627	1.339943
6	2.409666	-3.362916	0.612451	6	2.468066	-2.740873	0.211280
1	-1.990662	-3.509687	0.427047	1	-0.889440	-5.260658	0.664860
1	-1.738500	-4.328519	1.964421	1	-0.668946	-5.248512	2.411500
1	0.032414	-2.386448	0.470323	1	-0.003464	-3.143503	0.432279
6	0.138061	-2.532296	2.615191	6	0.187670	-2.729468	2.538647
1	3.226098	-4.002236	0.299430	1	3.380161	-2.993929	-0.310513
1	2.570296	-2.746251	-1.707296	1	0.979773	-3.364806	-2.029840
1	2.606417	-2.501635	1.234259	1	2.269180	-1.735909	0.549621
6	0.391685	-1.163363	2.767835	6	-0.371445	-1.452283	2.410400
6	0.061216	-3.309306	3.781906	6	0.574804	-3.140326	3.824179
6	0.551808	-0.646486	4.051960	6	-0.514351	-0.662739	3.549571
1	0.450114	-0.515250	1.897353	1	-0.697098	-1.086962	1.440354
7	0.228554	-2.830855	5.015028	7	0.459743	-2.388736	4.919489
1	-0.153503	-4.378739	3.724872	1	0.994132	-4.136226	3.985700
6	0.466908	-1.518341	5.139649	6	-0.080024	-1.170772	4.775888
1	0.741152	0.410474	4.209929	1	-0.952078	0.328484	3.488279
1	0.592952	-1.150759	6.155603	1	-0.170637	-0.579375	5.684364

1	1.323054	-4.648224	1.766582	1	2.353528	-3.806570	1.956368

^{4}PC

26	0.710402	-0.804966	-2.840956	26	0.721672	-0.842804	-2.758767
7	2.444007	-0.169127	-2.027680	7	2.454958	-0.160557	-2.008233
7	1.762845	-2.280215	-3.783649	7	1.748170	-2.270471	-3.764864
7	-0.978717	-1.815569	-3.252388	7	-0.967691	-1.832397	-3.174421
7	-0.288674	0.239012	-1.435807	7	-0.257804	0.292104	-1.438942
6	2.601728	0.858420	-1.115893	6	2.635084	0.853181	-1.084898
6	3.724485	-0.499976	-2.432379	6	3.724462	-0.460982	-2.465918
6	3.133349	-2.288064	-4.011940	6	3.107892	-2.242550	-4.050048
6	1.240904	-3.205394	-4.678254	6	1.224043	-3.241001	-4.609775
6	-1.133609	-2.841509	-4.161407	6	-1.138951	-2.903133	-4.029111
6	-2.257330	-1.477856	-2.858642	6	-2.243663	-1.446975	-2.819366
6	-1.659287	0.321150	-1.297326	6	-1.628664	0.417357	-1.335737
6	0.223967	1.227716	-0.622568	6	0.261115	1.269727	-0.612614
6	3.995366	1.162170	-0.939488	6	4.032956	1.163540	-0.938655
6	4.691247	0.320347	-1.755538	6	4.708063	0.352779	-1.799342
6	3.466052	-3.255440	-5.017681	6	3.430994	-3.221544	-5.049163
6	2.295795	-3.822901	-5.429220	6	2.266285	-3.843290	-5.390981
6	-3.224397	-2.311030	-3.522161	6	-3.224071	-2.304661	-3.437393
6	-2.527389	-3.156707	-4.330680	6	-2.538406	-3.211367	-4.183686
6	-2.008644	1.366611	-0.371074	6	-1.971298	1.482685	-0.428314
6	-0.840012	1.930676	0.045749	6	-0.798269	2.009437	0.022896
6	1.570454	1.517415	-0.463896	6	1.612344	1.519482	-0.427552
6	4.050138	-1.478480	-3.362183	6	4.027906	-1.413476	-3.429150
6	-0.106031	-3.485075	-4.836434	6	-0.120473	-3.563255	-4.699767
6	-2.581428	-0.480911	-1.951938	6	-2.555409	-0.391520	-1.977280
1	1.836843	2.322926	0.212730	1	1.888578	2.316359	0.255847
1	5.098381	-1.602401	-3.614256	1	5.068763	-1.515259	-3.720179
1	-0.379411	-4.251262	-5.554454	1	-0.401240	-4.362167	-5.378703
1	-3.633205	-0.309684	-1.747046	1	-3.606442	-0.188713	-1.796928
1	4.379746	1.929444	-0.279815	1	4.430523	1.918548	-0.272668
1	5.761948	0.257221	-1.901431	1	5.773756	0.304660	-1.983117
1	4.469735	-3.457692	-5.368680	1	4.425468	-3.399567	-5.437685
1	2.148318	-4.583517	-6.184964	1	2.114230	-4.631728	-6.116716
1	-2.909013	-3.924522	-4.991079	1	-2.928507	-4.011752	-4.798963
1	-4.295453	-2.242133	-3.382728	1	-4.294612	-2.207629	-3.310547
1	-3.021534	1.634856	-0.099375	1	-2.982509	1.782653	-0.184623
1	-0.696886	2.758097	0.729038	1	-0.648992	2.832541	0.710072
8	1.694188	-3.888872	-1.369495	8	1.837640	-3.922523	-1.377385
16	0.505771	0.729644	-4.650088	16	0.564527	0.559889	-4.457441
1	1.309653	1.679365	-4.120292	1	0.910033	1.694387	-3.805707
1	2.844908	-5.893935	1.648831	1	2.823626	-5.921605	1.704830
6	2.256380	-5.610931	0.773018	6	2.282450	-5.638024	0.799136
6	0.888146	-6.294904	0.752140	6	0.913485	-6.314605	0.709641

7	1.945777	-4.114167	0.911619	7	1.973637	-4.138928	0.917592
1	2.845074	-5.760647	-0.130954	1	2.916655	-5.794069	-0.072515
6	0.027310	-5.402890	1.655639	6	0.012880	-5.416310	1.566838
1	0.954522	-7.326175	1.107998	1	0.956180	-7.345472	1.070284
1	0.494760	-6.307124	-0.268577	1	0.572361	-6.327036	-0.329717
6	0.426595	-3.975472	1.256369	6	0.441095	-3.991232	1.188692
6	2.347753	-3.305869	-0.302466	6	2.440551	-3.340088	-0.281541
1	-1.045837	-5.550755	1.509146	1	-1.052161	-5.557395	1.364991
1	0.243020	-5.588559	2.713699	1	0.172104	-5.602748	2.634732
1	-0.033342	-3.725679	0.298296	1	0.028617	-3.738287	0.209993
6	0.207595	-2.868924	2.255184	6	0.180238	-2.885260	2.178060
1	3.442865	-3.372389	-0.365434	1	3.536620	-3.418597	-0.288339
1	1.699213	-3.287943	-2.155725	1	1.801918	-3.294282	-2.141050
1	2.052055	-2.267624	-0.108504	1	2.146568	-2.297720	-0.108959
6	-0.474551	-1.699451	1.896767	6	-0.486446	-1.715477	1.792886
6	0.678034	-2.966104	3.574851	6	0.593761	-2.985017	3.516411
6	-0.658476	-0.705344	2.855220	6	-0.711248	-0.723107	2.744577
1	-0.859311	-1.570041	0.888187	1	-0.827550	-1.583606	0.769075
7	0.523743	-2.015072	4.496408	7	0.400068	-2.035949	4.432443
1	1.203856	-3.860355	3.915000	1	1.104807	-3.880003	3.876737
6	-0.139299	-0.908067	4.135875	6	-0.247236	-0.928350	4.045806
1	-1.186183	0.209591	2.608414	1	-1.227732	0.192389	2.476899
1	-0.259327	-0.151915	4.908576	1	-0.400368	-0.173695	4.814118
1	2.470772	-3.732936	1.703817	1	2.463015	-3.757451	1.732230

Table S10. Cartesian coordinates for *N*-(hydroxymethyl)nornicotine decomposition.

RC(protonated, without water)

8	2.004196	-1.546953	-0.736046
1	0.184229	-4.181180	-2.007813
6	0.060880	-3.903829	-0.959330
6	-0.669539	-4.984693	-0.154602
7	1.458203	-3.826736	-0.341010
1	-0.401934	-2.916326	-0.916721
6	0.453446	-5.939552	0.270522
1	-1.441317	-5.470139	-0.756634
1	-1.159794	-4.548088	0.722453
6	1.600005	-5.001767	0.673773
6	1.816232	-2.470539	0.268297
1	0.176426	-6.586859	1.106270
1	0.757366	-6.586216	-0.559796
1	1.370075	-4.551818	1.645806
6	3.005632	-5.544334	0.681476
1	1.214894	-0.998551	-0.866849
1	1.019608	-2.227984	0.979251
1	2.761672	-2.627826	0.792283
6	3.813265	-5.446438	1.821709
6	3.553479	-6.170063	-0.449477
6	5.103680	-5.967129	1.782376
1	3.435070	-4.981619	2.729745
7	4.791736	-6.658634	-0.504929
1	2.965494	-6.291574	-1.361564
6	5.547596	-6.557823	0.596385
1	5.754567	-5.915610	2.648966
1	6.551277	-6.970060	0.525401
1	2.154854	-3.965847	-1.080606

RC(protonated, with water)

8	1.783128	-1.972624	-1.140287
1	-0.240815	-3.839625	-1.676901
6	-0.108779	-4.237792	-0.670387
6	-0.423056	-5.721477	-0.503429
7	1.351339	-4.154867	-0.296946
1	-0.657376	-3.609694	0.037652
6	0.366087	-6.132008	0.758388
1	-0.081385	-6.280714	-1.382029
1	-1.497175	-5.895477	-0.404876
6	1.581102	-5.160331	0.856970
6	1.865890	-2.732630	-0.009882
1	-0.252751	-6.023571	1.653458
1	0.697531	-7.171012	0.717556
1	1.509223	-4.558964	1.767733
6	2.961696	-5.763659	0.763515
1	0.941432	-1.450824	-1.128409
1	1.265646	-2.372828	0.834400
1	2.909111	-2.864017	0.289727
6	3.940784	-5.494810	1.727105
6	3.310780	-6.619932	-0.292696
6	5.198114	-6.078783	1.594949
1	3.720472	-4.848988	2.574362
7	4.513651	-7.174393	-0.438830
1	2.580265	-6.881929	-1.061094
6	5.436473	-6.905135	0.494286
1	5.978529	-5.898537	2.326991
1	6.407238	-7.374804	0.354641
1	1.899664	-4.476457	-1.103390
1	-1.093545	-0.513140	-1.667372
8	-0.596308	-0.704545	-0.855560
1	-0.553182	0.145903	-0.388595

TS(protonated, without water)

8	3.134991	-2.033867	-1.131071
1	-0.833517	-3.545201	-1.376249
6	-0.491147	-3.947870	-0.419789
6	-0.968550	-5.407404	-0.147192
7	0.998148	-3.979113	-0.389239
1	-0.833539	-3.270972	0.369548
6	0.307790	-6.167157	0.303128
1	-1.402327	-5.860864	-1.042264
1	-1.740691	-5.420430	0.626749
6	1.308117	-5.029622	0.617339

TS(protonated, with water)

8	2.724060	-1.921414	-1.299135
1	-1.026311	-4.094960	-1.468072
6	-0.676264	-4.427678	-0.485720
6	-1.030602	-5.913114	-0.178196
7	0.807189	-4.304157	-0.406259
1	-1.116171	-3.772041	0.276975
6	0.284806	-6.523065	0.369570
1	-1.365045	-6.435809	-1.078162
1	-1.843517	-5.972564	0.550463
6	1.184666	-5.294652	0.647927

6	3.306539	-2.602744	-0.002655
1	0.139120	-6.818441	1.164823
1	0.704916	-6.791493	-0.505607
1	1.037865	-4.600706	1.592556
6	2.779270	-5.366608	0.649687
1	2.226035	-1.669780	-1.216509
1	2.588712	-2.495353	0.800933
1	4.284917	-3.050419	0.140308
6	3.468037	-5.489889	1.869221
6	3.532319	-5.558606	-0.526186
6	4.828957	-5.771311	1.861108
1	2.935909	-5.366732	2.809736
7	4.846543	-5.808208	-0.549723
1	3.056189	-5.519995	-1.506175
6	5.476889	-5.913900	0.625083
1	5.385898	-5.876386	2.786779
1	6.543058	-6.124249	0.579992
1	1.304478	-4.332153	-1.299414

6	3.072814	-2.601772	-0.308255
1	0.134520	-7.128167	1.267639
1	0.761413	-7.166467	-0.378278
1	0.877144	-4.849076	1.603441
6	2.674987	-5.537699	0.695792
1	1.791447	-1.443641	-1.108125
1	2.540101	-2.534243	0.638254
1	3.973980	-3.205216	-0.405614
6	3.400110	-5.390769	1.886374
6	3.403152	-5.898657	-0.450776
6	4.778633	-5.589524	1.878851
1	2.886989	-5.128053	2.808947
7	4.729037	-6.066419	-0.481714
1	2.895454	-6.064542	-1.402208
6	5.398818	-5.916049	0.668699
1	5.364500	-5.490644	2.787266
1	6.475007	-6.065739	0.619061
1	1.178350	-4.656045	-1.291836
1	-0.044992	-1.891754	-0.558497
8	0.497180	-1.083251	-0.602196
1	-0.017675	-0.400448	-1.065165

PC(protonated, without water)

8	0.879766	2.374659	-1.924095
1	2.682295	0.447050	1.747484
6	2.605818	0.544718	0.662648
6	3.025363	-0.739869	-0.059183
7	1.126850	0.700941	0.321546
1	3.136176	1.443963	0.346238
6	1.763527	-1.610944	0.001571
1	3.889393	-1.201721	0.424695
1	3.299001	-0.523095	-1.097545
6	0.617888	-0.633918	-0.306366
6	0.714278	3.500340	-2.355844
1	1.771077	-2.430119	-0.721685
1	1.638693	-2.051139	0.996847
1	0.591632	-0.424303	-1.378922
6	-0.764504	-0.976417	0.184663
1	0.982528	1.469381	-0.362802
1	0.581346	4.371960	-1.691213
1	0.691179	3.693069	-3.440879
6	-1.854026	-1.005277	-0.694116
6	-1.011039	-1.278655	1.532875
6	-3.112809	-1.334221	-0.199360
1	-1.716668	-0.782407	-1.749730
7	-2.214098	-1.577758	2.023223

PC(protonated, with water)

8	2.776956	-2.383436	-1.021119
1	-0.367646	-4.703499	-2.023387
6	-0.667371	-4.522869	-0.988826
6	-1.158517	-5.804393	-0.306014
7	0.578300	-4.131418	-0.210748
1	-1.375539	-3.693128	-0.966019
6	0.138852	-6.473510	0.168099
1	-1.735888	-6.426956	-0.993755
1	-1.803680	-5.562511	0.545932
6	0.978856	-5.305214	0.711645
6	3.918087	-2.311590	-1.442053
1	-0.021981	-7.228476	0.941645
1	0.655571	-6.961193	-0.666347
1	0.612055	-5.021673	1.702015
6	2.476740	-5.479607	0.758395
1	1.586007	-1.422743	0.446115
1	4.510727	-1.387456	-1.336502
1	4.406060	-3.166571	-1.938104
6	3.181197	-5.386185	1.962633
6	3.217394	-5.727591	-0.406227
6	4.565375	-5.545619	1.951103
1	2.656044	-5.193605	2.895059
7	4.545671	-5.846763	-0.439465

1	-0.197851	-1.285972	2.261252
6	-3.241821	-1.607448	1.164803
1	-3.978154	-1.375494	-0.852780
1	-4.210192	-1.862491	1.588865
1	0.572433	0.921981	1.152999

1	2.717062	-5.829879	-1.371159
6	5.201272	-5.763268	0.727654
1	5.142197	-5.490705	2.868626
1	6.281903	-5.875279	0.677017
1	1.362775	-3.882091	-0.829315
1	0.447777	-3.253509	0.346597
8	0.863532	-1.718027	1.029516
1	0.310162	-0.940076	1.197767

RC(deprotonated, without water)

8	-0.932635	2.156746	-1.935013
1	-1.223574	4.662546	-2.971048
6	-1.139461	4.280780	-3.991312
6	-0.422642	5.231244	-4.959298
7	-0.306291	3.074659	-4.018562
1	-2.164432	4.061094	-4.350422
6	0.259761	4.285364	-5.983097
1	0.329815	5.819976	-4.425638
1	-1.117104	5.933745	-5.429490
6	0.021795	2.845386	-5.435010
6	-0.881394	1.936869	-3.328251
1	-0.156174	4.382097	-6.990599
1	1.331491	4.490410	-6.055331
1	-0.848313	2.413024	-5.968403
6	1.199326	1.912087	-5.630576
1	-0.023442	2.362320	-1.660849
1	-1.927327	1.748235	-3.627710
1	-0.283567	1.049701	-3.582077
6	1.192569	0.917968	-6.611521
6	2.363649	2.037639	-4.857298
6	2.321321	0.117537	-6.784436
1	0.310789	0.772196	-7.232416
7	3.453894	1.278246	-5.004938
1	2.401189	2.789879	-4.071621
6	3.423300	0.337657	-5.959193
1	2.345117	-0.663954	-7.538413
1	4.322202	-0.267925	-6.063559

RC(deprotonated, with water)

8	0.189216	1.801862	-1.742791
1	0.348425	4.472224	-2.052897
6	-0.385079	4.435055	-2.860359
6	-0.209365	5.524370	-3.925581
7	-0.240279	3.183895	-3.624305
1	-1.390557	4.492781	-2.403605
6	-0.754940	4.876825	-5.225980
1	0.850168	5.774145	-4.039489
1	-0.736352	6.444584	-3.657323
6	-1.034050	3.389904	-4.856711
6	-0.626048	1.986034	-2.861442
1	-1.672408	5.354712	-5.582192
1	-0.024452	4.941594	-6.037246
1	-2.109794	3.287438	-4.618896
6	-0.705093	2.392741	-5.949483
1	1.108620	1.710067	-2.079237
1	-1.659124	2.079805	-2.485624
1	-0.589596	1.134263	-3.558466
6	-1.690885	1.598805	-6.540607
6	0.605819	2.234539	-6.425395
6	-1.339078	0.704715	-7.551459
1	-2.724124	1.678960	-6.209330
7	0.965798	1.377066	-7.384947
1	1.410617	2.834835	-6.003225
6	-0.000864	0.628276	-7.934095
1	-2.084841	0.075337	-8.028084
1	0.313785	-0.062337	-8.714549
1	2.556988	1.490902	-4.053236
8	2.423159	2.176574	-3.380726
1	1.649079	2.694902	-3.706878

TS(deprotonated, without water)

8	0.165789	2.320451	-2.013782
1	-1.377401	4.753594	-3.116704
6	-1.305680	4.269964	-4.093849
6	-0.683233	5.144596	-5.203255

TS(deprotonated, with water)

8	0.274949	1.765778	-1.756156
1	0.534867	4.430096	-2.142188
6	-0.255154	4.445739	-2.892389
6	-0.064937	5.453693	-4.025447

7	-0.394285	3.102700	-3.978965
1	-2.302641	3.914251	-4.378776
6	0.304239	4.201406	-5.942625
1	-0.156477	6.004903	-4.781226
1	-1.458530	5.534146	-5.869139
6	0.014220	2.788946	-5.376424
6	-0.776379	2.002901	-2.927948
1	0.190355	4.227176	-7.029806
1	1.341109	4.467440	-5.714621
1	-0.873261	2.381657	-5.884181
6	1.157292	1.807855	-5.539184
1	0.404602	3.200606	-3.080202
1	-1.835288	2.166328	-2.644345
1	-0.695834	1.022962	-3.439482
6	1.442334	1.335691	-6.827226
6	1.980303	1.365017	-4.491981
6	2.524831	0.485377	-7.023075
1	0.819955	1.632850	-7.669297
7	3.026794	0.544442	-4.671463
1	1.771260	1.650583	-3.461139
6	3.291460	0.127306	-5.912231
1	2.769425	0.105372	-8.010651
1	4.151660	-0.531205	-6.024393

7	-0.263100	3.139827	-3.605790
1	-1.222270	4.571488	-2.388786
6	-0.876263	4.854205	-5.200038
1	0.997186	5.516042	-4.285042
1	-0.399071	6.457475	-3.748282
6	-1.060728	3.338989	-4.858315
6	-0.667223	1.932591	-2.688053
1	-1.857595	5.329305	-5.294369
1	-0.363269	4.981686	-6.156491
1	-2.108711	3.155474	-4.588248
6	-0.677091	2.374442	-5.960315
1	1.312919	1.874614	-2.389736
1	-1.661766	2.193552	-2.283298
1	-0.792471	1.107766	-3.421091
6	-1.636561	1.565859	-6.575314
6	0.641778	2.277376	-6.433644
6	-1.254334	0.717419	-7.612845
1	-2.672266	1.600037	-6.244266
7	1.025727	1.465253	-7.422512
1	1.432932	2.874245	-5.981720
6	0.085597	0.703940	-7.997890
1	-1.977533	0.077562	-8.109414
1	0.423644	0.053710	-8.802756
1	2.367306	1.511241	-3.781668
8	2.075252	2.280576	-3.268212
1	0.814615	2.853038	-3.765993

PC(deprotonated, without water)

8	0.116699	1.683053	-1.296698
1	-1.199595	4.900912	-3.290784
6	-1.199095	4.357349	-4.239758
6	-0.681267	5.199749	-5.441536
7	-0.340853	3.163511	-4.135422
1	-2.227233	4.023709	-4.427647
6	0.238887	4.226965	-6.222537
1	-0.121860	6.076449	-5.099697
1	-1.510029	5.567853	-6.055129
6	0.015255	2.848036	-5.531119
6	-0.911411	1.567633	-1.925199
1	0.011022	4.198851	-7.292981
1	1.291251	4.515597	-6.121115
1	-0.883152	2.392053	-5.976340
6	1.163725	1.871201	-5.677531
1	0.511067	3.415200	-3.631002
1	-1.789220	2.223578	-1.750916
1	-1.061932	0.778883	-2.686456

PC(deprotonated, with water)

8	0.462464	1.239041	-1.578674
1	0.158010	4.653225	-2.141896
6	-0.542596	4.629069	-2.980828
6	-0.283527	5.732108	-4.043272
7	-0.446118	3.336908	-3.678245
1	-1.556373	4.728842	-2.571066
6	-0.562355	5.034039	-5.401579
1	0.753675	6.079053	-3.995080
1	-0.924137	6.605644	-3.883618
6	-1.026113	3.595165	-5.014619
6	-0.566613	1.202386	-2.230895
1	-1.321333	5.548898	-5.999946
1	0.346524	4.986443	-6.009867
1	-2.117454	3.615094	-4.883888
6	-0.696524	2.507743	-6.014179
1	1.916644	1.652178	-2.735734
1	-1.535252	1.522911	-1.807762
1	-0.615868	0.763576	-3.241847

6	1.711739	1.618542	-6.942593
6	1.721214	1.175362	-4.594637
6	2.764139	0.718070	-7.070782
1	1.315754	2.123172	-7.820681
7	2.739173	0.308654	-4.702229
1	1.336223	1.312641	-3.587121
6	3.244329	0.091230	-5.919489
1	3.205996	0.506229	-8.040233
1	4.069201	-0.617497	-5.978353

6	-1.694532	1.724384	-6.600009
6	0.628059	2.227089	-6.386975
6	-1.343233	0.722350	-7.504041
1	-2.738536	1.898604	-6.348421
7	0.986994	1.261553	-7.239774
1	1.446779	2.806579	-5.964188
6	0.007865	0.527225	-7.785748
1	-2.099594	0.101637	-7.975586
1	0.322676	-0.250965	-8.479119
1	2.496266	1.383581	-4.137666
8	2.347389	2.095240	-3.496761
1	0.543024	3.081123	-3.775443