

# Electronic Supplementary Information

## Theoretical Insights into the Reductive Metabolism of CCl<sub>4</sub> by Cytochrome

### P450 Enzymes and the CCl<sub>4</sub>-dependent Suicidal Inactivation of P450

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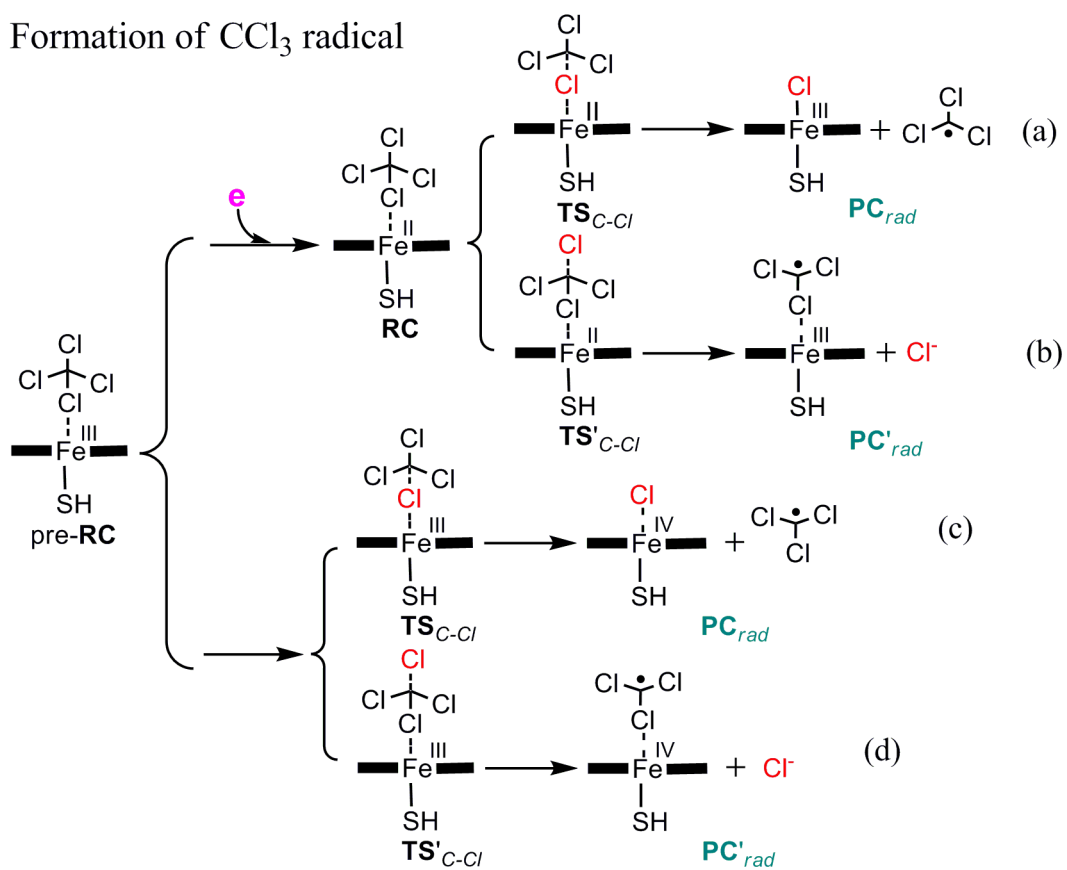
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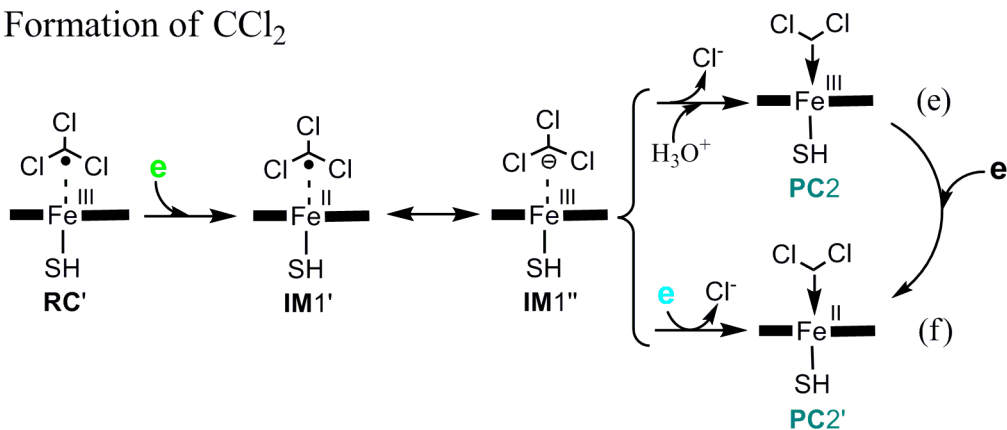
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**Scheme S1** Proposed reductive metabolism of  $\text{CCl}_4$  by P450.

**(A) Formation of  $\text{CCl}_3$  radical**



**(B) Formation of  $\text{CCl}_2$**



**Table S1** Calculated vertical electron affinity (VEA) values of various species appeared in the reductively metabolic process. All data were calculated at the UB3LYP/ B1 level, with dispersion corrections incorporated.

Species	VEA (kcal/mol)
pre-RC <sup>a</sup>	48.3
RC <sup>b</sup>	-46.8
RC <sup>c</sup>	-36.6
Ferric-Carbene complex	55.8

<sup>a</sup> The ferric-CCl<sub>4</sub> complex. <sup>b</sup> The ferrous-CCl<sub>4</sub> complex. <sup>c</sup> The ferric-CCl<sub>3</sub> complex.

**Table S2** Various energies (in kcal/mol) in reductive dechlorination of CCl<sub>4</sub> by P450 calculated at the UB3LYP/B2//B1 level, with ZPE and dispersion corrections incorporated.

	SPE		SPE+ZPE		SOLV		SOLV+ZPE	
<sup>6</sup> pre-RC	-3390.050959	0.0	-3389.758691	0.0	-3390.061055	0.0	-3389.768787	0.0
<sup>4</sup> pre-RC	-3390.046861	2.6	-3389.752977	3.0	-3390.059390	1.0	-3389.765506	2.1
<sup>2</sup> pre-RC	-3390.045557	3.4	-3389.750684	5.0	-3390.055065	3.8	-3389.760192	5.4
<sup>5</sup> RC	-3390.134191	0.0	-3389.844691	0.0	-3390.194450	0.0	-3389.904950	0.0
<sup>3</sup> RC	-3390.121819	7.8	-3389.830603	8.8	-3390.186477	5.0	-3389.895261	6.1
<sup>1</sup> RC	-3390.116704	11.0	-3389.825036	12.3	-3390.179788	9.2	-3389.888120	10.6
<sup>5</sup> TS <sub>C-Cl</sub>	-3390.102376	20.0	-3389.813355	19.7	-3390.162588	20.0	-3389.873567	19.7
<sup>3</sup> TS <sub>C-Cl</sub>	-3390.113120	13.2	-3389.822104	14.2	-3390.173801	13.0	-3389.882785	13.9
<sup>1</sup> TS <sub>C-Cl</sub>	-3390.110607	14.8	-3389.819107	16.1	-3390.168599	16.2	-3389.877099	17.5
<sup>5</sup> PC <sub>rad</sub>	-3390.118260	10.0	-3389.827715	10.7	-3390.187572	4.3	-3389.897027	5.0
<sup>3</sup> PC <sub>rad</sub>	-3390.130276	2.5	-3389.838110	4.1	-3390.193971	0.3	-3389.901805	2.0
<sup>1</sup> PC <sub>rad</sub>	-3390.130334	2.4	-3389.838109	4.1	-3390.194059	0.2	-3389.901834	2.0

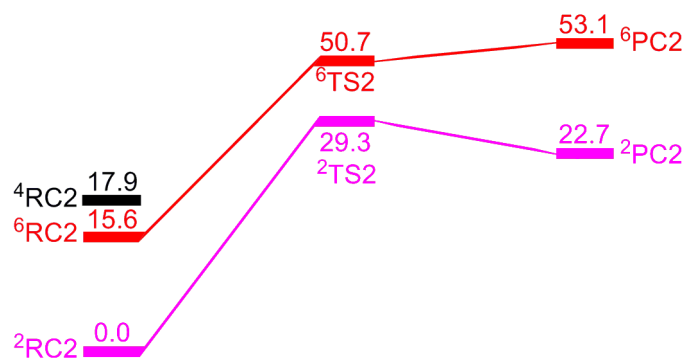
**Table S3** Various energies (in kcal/mol) during further reductive dechlorination of CCl<sub>3</sub> radical by P450 via a S<sub>E</sub>3 mechanism. All data were calculated at the UB3LYP/B2//B1 level, with ZPE and dispersion corrections incorporated.

	SPE		SPE+ZPE		SOLV		SOLV+ZPE	
<sup>2</sup> RC <sub>S<sub>E</sub>3</sub>	-3006.851718	0.0	-3006.523468	0.0	-3006.866097	0.0	-3006.537847	0.0
<sup>4</sup> RC <sub>S<sub>E</sub>3</sub>	-3006.829429	14.0	-3006.503640	12.4	-3006.842991	14.5	-3006.517202	13.0
<sup>6</sup> RC <sub>S<sub>E</sub>3</sub>	-3006.833787	11.3	-3006.509362	8.9	-3006.848908	10.8	-3006.524483	8.4
<sup>2</sup> TS <sub>S<sub>E</sub>3</sub>	-3006.848203	2.2	-3006.523511	0.0	-3006.861695	2.8	-3006.537003	0.5
<sup>4</sup> TS <sub>S<sub>E</sub>3</sub>	-3006.819395	20.3	-3006.496652	16.8	-3006.832532	21.1	-3006.509789	17.6
<sup>6</sup> TS <sub>S<sub>E</sub>3</sub>	-3006.832781	11.9	-3006.511229	7.7	-3006.847144	11.9	-3006.525592	7.7
<sup>2</sup> PC <sub>S<sub>E</sub>3</sub>	-3006.861312	-6.0	-3006.535788	-7.7	-3006.875242	-5.7	-3006.549718	-7.4
<sup>4</sup> PC <sub>S<sub>E</sub>3</sub>	-3006.847073	2.9	-3006.522742	0.5	-3006.862998	1.9	-3006.538667	-0.5
<sup>6</sup> PC <sub>S<sub>E</sub>3</sub>	-3006.849755	1.2	-3006.527011	-2.2	-3006.863679	1.5	-3006.540935	-1.9

**Table S4** Mulliken group spin densities and group charges for key moieties during further reduction of  $\text{CCl}_3$  radical by P450 via a  $\text{S}_{\text{E}3}$  mechanism. All data were computed at the UB3LYP/B1 level.

	Spin densities							Charges						
	Fe	Por	SH	$\text{CCl}_2$	$\text{H}_2\text{O}$	H	Cl	Fe	Por	SH	$\text{CCl}_2$	$\text{H}_2\text{O}$	H	Cl
$^2\text{RC}_{\text{SE}3}$	1.03	-0.07	0.07	-0.02	0.00	0.00	0.00	0.13	-0.32	0.01	-0.33	0.26	0.36	-0.10
$^4\text{RC}_{\text{SE}3}$	3.06	0.14	-0.16	-0.04	0.00	0.00	0.00	0.29	-0.51	0.02	-0.34	0.26	0.36	-0.08
$^6\text{RC}_{\text{SE}3}$	3.96	0.47	0.49	0.07	0.00	0.00	0.02	0.49	-0.53	-0.07	-0.35	0.25	0.36	-0.15
$^2\text{TS}_{\text{SE}3}$	1.02	-0.07	0.06	-0.02	0.00	0.00	0.00	0.12	-0.30	0.02	-0.06	0.20	0.32	-0.30
$^4\text{TS}_{\text{SE}3}$	3.31	0.11	-0.43	0.00	0.00	0.00	0.01	0.34	-0.49	0.01	-0.08	0.21	0.32	-0.30
$^6\text{TS}_{\text{SE}3}$	3.95	0.50	0.50	0.03	0.00	0.00	0.02	0.50	-0.52	-0.06	-0.13	0.21	0.32	-0.32
$^2\text{PC}_{\text{SE}3}$	0.96	-0.07	0.13	-0.03	0.00	0.00	0.00	0.17	-0.23	0.00	0.08	0.08	0.20	-0.30
$^4\text{PC}_{\text{SE}3}$	2.44	0.07	0.48	0.00	0.01	0.00	0.00	0.30	-0.20	-0.07	0.00	0.10	0.21	-0.33
$^6\text{PC}_{\text{SE}3}$	3.92	0.61	0.50	-0.03	0.00	0.00	0.00	0.56	-0.46	-0.06	-0.01	0.10	0.21	-0.34

**Fig. S1** Energy profiles (in kcal/mol) for the direct reduction of  $\cdot\text{CCl}_3$  without the assistance of proton calculated at the UB3LYP/B2//B1. All energy data include ZPE, solvation and dispersion corrections.



## Cartesian Coordinates of the Key Reaction Species

Formation of CCl <sub>3</sub> radical				<sup>4</sup> pre-RC			
<sup>6</sup> pre-RC				26	0.472581000	-0.641212000	0.144575000
26	0.431032000	-0.458204000	0.012475000	7	1.066190000	0.354993000	1.787657000
7	1.062169000	0.400818000	1.804726000	6	2.325773000	0.851958000	2.033583000
6	2.335363000	0.840718000	2.074583000	6	2.323073000	1.664985000	3.220068000
6	2.335348000	1.629300000	3.282355000	1	3.195197000	2.164766000	3.621187000
1	3.212757000	2.090708000	3.717104000	6	1.049523000	1.648781000	3.703795000
6	1.051240000	1.646205000	3.743726000	1	0.651728000	2.136305000	4.584385000
1	0.661696000	2.127447000	4.631680000	6	0.274046000	0.838893000	2.802563000
6	0.261608000	0.876574000	2.813413000	6	-1.083400000	0.602931000	2.943345000
6	-1.106758000	0.645070000	2.928194000	1	-1.585747000	1.040788000	3.799308000
1	-1.607925000	1.077463000	3.788557000	7	-1.381867000	-0.744601000	0.915610000
7	-1.438539000	-0.703988000	0.905332000	6	-1.849085000	-0.132421000	2.053731000
6	-1.891743000	-0.094449000	2.046889000	6	-3.267478000	-0.333443000	2.187811000
6	-3.307075000	-0.331098000	2.200757000	1	-3.864647000	0.047796000	3.006031000
1	-3.907562000	0.036974000	3.022828000	6	-3.664487000	-1.059243000	1.105224000
6	-3.699950000	-1.084859000	1.133420000	1	-4.656148000	-1.407653000	0.847416000
1	-4.687123000	-1.465216000	0.904223000	6	-2.484430000	-1.314184000	0.323521000
6	-2.523101000	-1.318829000	0.332389000	6	-2.470477000	-2.082676000	-0.827342000
6	-2.485064000	-2.111722000	-0.810833000	1	-3.415946000	-2.478503000	-1.182174000
1	-3.424926000	-2.543311000	-1.140382000	7	-0.046446000	-2.032646000	-1.205304000
7	-0.070710000	-2.032295000	-1.255993000	6	-1.324007000	-2.436829000	-1.517742000
6	-1.345416000	-2.463645000	-1.529257000	6	-1.305283000	-3.347490000	-2.629550000
6	-1.320808000	-3.399945000	-2.625024000	1	-2.186064000	-3.807083000	-3.058801000
1	-2.193394000	-3.893047000	-3.033907000	6	0.000986000	-3.503725000	-2.987080000
6	-0.015058000	-3.536134000	-3.000090000	1	0.420167000	-4.113843000	-3.776737000
1	0.398994000	-4.160014000	-3.781851000	6	0.774502000	-2.674054000	-2.103254000
6	0.758958000	-2.674577000	-2.140626000	6	2.151173000	-2.535865000	-2.175682000
6	2.142538000	-2.522929000	-2.199907000	1	2.674601000	-3.096410000	-2.942940000
1	2.666876000	-3.091389000	-2.961754000	7	2.404813000	-0.947974000	-0.323851000
7	2.432025000	-0.943216000	-0.344827000	6	2.902811000	-1.716947000	-1.349586000
6	2.916914000	-1.718581000	-1.367809000	6	4.325824000	-1.538369000	-1.467861000
6	4.350836000	-1.576831000	-1.453488000	1	4.946922000	-2.041250000	-2.197785000
1	4.978692000	-2.087296000	-2.172588000	6	4.689455000	-0.640547000	-0.510142000
6	4.721319000	-0.704440000	-0.472345000	1	5.673567000	-0.251880000	-0.282666000
1	5.715040000	-0.356283000	-0.221215000	6	3.490277000	-0.284060000	0.200347000
6	3.515862000	-0.318138000	0.220753000	6	3.458067000	0.575651000	1.285412000
6	3.468497000	0.524880000	1.328534000	1	4.391469000	1.033919000	1.594351000
1	4.411309000	0.942367000	1.667995000	16	0.135673000	1.269884000	-1.254020000
16	0.134498000	1.398852000	-1.361879000	1	0.643932000	0.630844000	-2.327712000
1	0.595336000	0.735548000	-2.443187000	6	-0.126056000	-4.389146000	2.162692000
6	-0.059300000	-4.324086000	2.122444000	17	0.310829000	-5.741954000	3.268172000
17	0.479589000	-5.614425000	3.259434000	17	1.109660000	-3.096553000	2.289356000
17	1.106943000	-2.969028000	2.159782000	17	-0.191342000	-4.995693000	0.476892000
17	-0.149165000	-4.997012000	0.461664000	17	-1.728115000	-3.732404000	2.628991000
17	-1.680008000	-3.734100000	2.619420000				

<sup>2</sup>pre-RC

26	0.483280000	-0.701374000	0.188749000	6	2.346193000	1.574351000	3.342388000
7	1.060289000	0.345120000	1.794363000	1	3.229315000	1.997817000	3.806758000
6	2.308468000	0.881733000	2.008455000	6	1.053469000	1.624767000	3.777809000
6	2.312553000	1.696780000	3.196603000	1	0.662654000	2.099372000	4.670529000
1	3.180083000	2.220853000	3.576499000	6	0.260689000	0.892984000	2.808220000
6	1.053826000	1.643857000	3.712162000	6	-1.116479000	0.670859000	2.904519000
1	0.663802000	2.119794000	4.602536000	1	-1.618185000	1.097404000	3.769809000
6	0.279524000	0.813755000	2.825836000	7	-1.469680000	-0.676017000	0.885153000
6	-1.073470000	0.560811000	2.977783000	6	-1.910841000	-0.074122000	2.025886000
1	-1.572771000	0.985271000	3.842631000	6	-3.322725000	-0.347640000	2.216349000
7	-1.373569000	-0.743585000	0.925750000	1	-3.919357000	0.008710000	3.048224000
6	-1.844221000	-0.152616000	2.074674000	6	-3.712438000	-1.129016000	1.166752000
6	-3.266919000	-0.338791000	2.194974000	1	-4.692688000	-1.544972000	0.964534000
1	-3.865062000	0.027166000	3.019464000	6	-2.535346000	-1.332590000	0.344150000
6	-3.664721000	-1.027460000	1.089528000	6	-2.489447000	-2.147661000	-0.790589000
1	-4.658953000	-1.355951000	0.815399000	1	-3.423397000	-2.616146000	-1.091062000
6	-2.479982000	-1.278825000	0.310174000	7	-0.094863000	-2.013927000	-1.297565000
6	-2.462417000	-2.033520000	-0.850434000	6	-1.352289000	-2.488104000	-1.529341000
1	-3.411437000	-2.406676000	-1.221318000	6	-1.323168000	-3.465056000	-2.600006000
7	-0.034413000	-2.045802000	-1.192114000	1	-2.186496000	-3.999469000	-2.979340000
6	-1.315965000	-2.413867000	-1.528084000	6	-0.019128000	-3.573844000	-2.992028000
6	-1.304372000	-3.329650000	-2.638838000	1	0.401370000	-4.213476000	-3.759565000
1	-2.190331000	-3.767471000	-3.080354000	6	0.739996000	-2.658601000	-2.161622000
6	0.001692000	-3.522453000	-2.974653000	6	2.128910000	-2.494438000	-2.216945000
1	0.417493000	-4.145596000	-3.755898000	1	2.655860000	-3.072351000	-2.972553000
6	0.781493000	-2.706317000	-2.081520000	7	2.443783000	-0.926857000	-0.356939000
6	2.159283000	-2.577883000	-2.145822000	6	2.915959000	-1.700267000	-1.377014000
1	2.684614000	-3.148562000	-2.904701000	6	4.362718000	-1.605351000	-1.440710000
7	2.397731000	-0.953568000	-0.327570000	1	4.989670000	-2.123069000	-2.157594000
6	2.906727000	-1.735785000	-1.339414000	6	4.742799000	-0.765547000	-0.434312000
6	4.325347000	-1.530103000	-1.475217000	1	5.744420000	-0.456678000	-0.158161000
1	4.952144000	-2.039995000	-2.195361000	6	3.527051000	-0.354076000	0.242649000
6	4.674533000	-0.596129000	-0.548157000	6	3.478068000	0.467980000	1.373183000
1	5.651367000	-0.179000000	-0.339847000	1	4.427931000	0.848466000	1.740863000
6	3.471782000	-0.248478000	0.164407000	16	0.114375000	1.622299000	-1.558015000
6	3.430416000	0.628264000	1.236549000	1	0.570718000	0.923824000	-2.620296000
1	4.357349000	1.114353000	1.523116000	6	-0.030559000	-4.232039000	2.084781000
16	0.159150000	1.064217000	-1.111580000	17	0.605986000	-5.481555000	3.255934000
1	0.778493000	0.561048000	-2.200569000	17	1.058438000	-2.839467000	2.037604000
6	-0.151296000	-4.386505000	2.135776000	17	-0.150611000	-4.980867000	0.458418000
17	0.285963000	-5.730846000	3.251996000	17	-1.663385000	-3.718265000	2.630064000
17	1.091081000	-3.095566000	2.255558000	<sup>3</sup> RC			
17	-0.217010000	-5.004225000	0.455672000	26	0.413075000	-0.669251000	0.151946000
17	-1.749762000	-3.722590000	2.598595000	7	1.008220000	0.413165000	1.737069000
<sup>5</sup> RC				6	2.293892000	0.756200000	2.071719000
26	0.398948000	-0.283588000	-0.116636000	6	2.303185000	1.604019000	3.246270000
7	1.064489000	0.422465000	1.810416000	1	3.197731000	2.010196000	3.703178000
6	2.339086000	0.807592000	2.111098000	6	1.007358000	1.744967000	3.633982000







1	-3.414556000	-2.674507000	-1.447858000	6	-1.261446000	-3.130154000	-3.188534000	
7	-0.083137000	-2.046183000	-1.488249000	1	-2.118661000	-3.597369000	-3.657387000	
6	-1.333153000	-2.488232000	-1.817877000	6	0.020483000	-3.044825000	-3.642453000	
6	-1.297832000	-3.216463000	-3.066669000	1	0.442750000	-3.430601000	-4.562090000	
1	-2.161343000	-3.669261000	-3.539140000	6	0.768961000	-2.330957000	-2.636470000	
6	-0.003976000	-3.197074000	-3.490753000	6	2.131407000	-2.078784000	-2.711321000	
1	0.425298000	-3.633952000	-4.384381000	1	2.655148000	-2.422645000	-3.597944000	
6	0.745716000	-2.465390000	-2.493140000	7	2.401197000	-0.965456000	-0.544624000	
6	2.118192000	-2.257580000	-2.544079000	6	2.884596000	-1.457584000	-1.725087000	
1	2.648134000	-2.653354000	-3.406103000	6	4.314362000	-1.272802000	-1.790816000	
7	2.388107000	-1.062842000	-0.420821000	1	4.934467000	-1.578548000	-2.624399000	
6	2.877242000	-1.617164000	-1.572735000	6	4.685067000	-0.675043000	-0.623768000	
6	4.315189000	-1.471895000	-1.628692000	1	5.674348000	-0.381235000	-0.295126000	
1	4.937960000	-1.830924000	-2.439236000	6	3.478999000	-0.487435000	0.146174000	
6	4.684970000	-0.824201000	-0.489099000	6	3.433010000	0.114551000	1.396570000	
1	5.676812000	-0.533741000	-0.163773000	1	4.372080000	0.448029000	1.827320000	
6	3.470383000	-0.569541000	0.252741000	16	0.095670000	1.252426000	-1.118402000	
6	3.415028000	0.102910000	1.468548000	1	1.205906000	1.758545000	-0.543373000	
1	4.355392000	0.436301000	1.898718000	6	-0.103612000	-3.616330000	3.768810000	
16	0.212226000	0.988180000	-1.120758000	17	0.375861000	-5.248081000	4.234453000	
1	1.305568000	1.602065000	-0.621414000	17	0.964292000	-3.291966000	1.171534000	
6	0.156827000	-3.601746000	3.085235000	17	-1.834130000	-3.416861000	3.557459000	
17	0.675747000	-5.301514000	3.472722000	17	0.656906000	-2.353542000	4.722491000	
17	0.834170000	-3.125401000	1.224623000					
17	-1.629385000	-3.486147000	3.094869000	<sup>3</sup> PC <sub>rad</sub>	26	0.557641000	-0.828592000	0.270655000
17	0.868549000	-2.457388000	4.264916000	7	1.063809000	0.482510000	1.715797000	
				6	2.297322000	1.012066000	1.970251000	
<sup>5</sup> PC <sub>rad</sub>				6	2.231059000	1.919714000	3.092367000	
26	0.473987000	-0.961983000	0.056913000	1	3.077187000	2.465871000	3.491377000	
7	1.009281000	-0.005513000	1.746950000	6	0.936204000	1.920540000	3.513871000	
6	2.276454000	0.341630000	2.129502000	1	0.488001000	2.469257000	4.333294000	
6	2.240610000	1.026633000	3.398495000	6	0.216810000	1.017649000	2.643931000	
1	3.114656000	1.398429000	3.918800000	6	-1.140856000	0.748207000	2.756023000	
6	0.931120000	1.097312000	3.768439000	1	-1.682566000	1.250926000	3.551917000	
1	0.499368000	1.532099000	4.661202000	7	-1.365224000	-0.817818000	0.883957000	
6	0.172446000	0.441540000	2.732292000	6	-1.866707000	-0.101447000	1.932636000	
6	-1.202932000	0.264784000	2.767277000	6	-3.287493000	-0.336303000	2.064560000	
1	-1.738320000	0.670272000	3.619688000	1	-3.914878000	0.113126000	2.824698000	
7	-1.434905000	-1.026039000	0.697276000	6	-3.633289000	-1.199239000	1.070362000	
6	-1.939077000	-0.432052000	1.821389000	1	-4.604773000	-1.618224000	0.838676000	
6	-3.359610000	-0.665829000	1.912700000	6	-2.420558000	-1.494220000	0.342554000	
1	-3.988831000	-0.304397000	2.716361000	6	-2.349696000	-2.357925000	-0.741068000	
6	-3.701462000	-1.419938000	0.831315000	1	-3.268484000	-2.838451000	-1.062633000	
1	-4.674493000	-1.803353000	0.550143000	7	0.054807000	-2.173583000	-1.147611000	
6	-2.491303000	-1.630261000	0.073718000	6	-1.184329000	-2.675659000	-1.423836000	
6	-2.434855000	-2.310244000	-1.134433000	6	-1.115156000	-3.605218000	-2.527797000	
1	-3.357416000	-2.741252000	-1.510724000	1	-1.964715000	-4.142033000	-2.931697000	
7	-0.052305000	-1.980787000	-1.600285000	6	0.190512000	-3.656556000	-2.908950000	
6	-1.293846000	-2.458874000	-1.911662000					

1	0.646629000	-4.241810000	-3.698149000	1	2.644563000	-2.387098000	-3.599205000
6	0.910479000	-2.750966000	-2.041353000	7	2.404054000	-0.961139000	-0.531377000
6	2.274166000	-2.508348000	-2.132976000	6	2.878681000	-1.439537000	-1.719411000
1	2.824049000	-3.047489000	-2.898885000	6	4.310614000	-1.255597000	-1.793988000
7	2.484155000	-0.870291000	-0.320441000	1	4.924119000	-1.553516000	-2.635619000
6	2.994449000	-1.629741000	-1.334412000	6	4.690207000	-0.670528000	-0.624226000
6	4.414938000	-1.396587000	-1.466264000	1	5.681771000	-0.380255000	-0.298751000
1	5.050477000	-1.882446000	-2.196660000	6	3.486824000	-0.490625000	0.155001000
6	4.750466000	-0.483094000	-0.513745000	6	3.444481000	0.101815000	1.410413000
1	5.721212000	-0.057101000	-0.291015000	1	4.384035000	0.433098000	1.842631000
6	3.534058000	-0.166652000	0.198711000	16	0.109423000	1.028136000	-1.003668000
6	3.455983000	0.723153000	1.261789000	1	1.230486000	1.621077000	-0.543870000
1	4.371792000	1.217445000	1.572193000	6	-0.111733000	-3.568105000	3.819058000
16	0.114376000	0.904602000	-1.184271000	17	0.411864000	-5.206854000	4.164932000
1	1.237190000	1.595310000	-0.897382000	17	0.892390000	-3.105431000	1.107756000
6	-0.797416000	-4.899910000	2.070736000	17	-1.833146000	-3.370030000	3.631881000
17	-0.830847000	-5.571117000	0.461806000	17	0.688779000	-2.329358000	4.748623000
17	1.045304000	-2.619628000	1.793008000				
17	-2.274116000	-4.136978000	2.596164000				
17	-0.015746000	-5.907441000	3.276192000				

<sup>1</sup>PC<sub>rad</sub>

26	0.479056000	-0.980528000	0.063497000
7	1.023333000	-0.017092000	1.746200000
6	2.285559000	0.328745000	2.140175000
6	2.242622000	1.016353000	3.410169000
1	3.113358000	1.387310000	3.936993000
6	0.930474000	1.091499000	3.766302000
1	0.490294000	1.529623000	4.653694000
6	0.179591000	0.435259000	2.720529000
6	-1.197551000	0.262881000	2.744880000
1	-1.734817000	0.672686000	3.594791000
7	-1.439840000	-1.031978000	0.678776000
6	-1.938325000	-0.433512000	1.800282000
6	-3.361061000	-0.667665000	1.901681000
1	-3.986156000	-0.301724000	2.706979000
6	-3.708011000	-1.427684000	0.826917000
1	-4.681975000	-1.813622000	0.551736000
6	-2.498261000	-1.639439000	0.065097000
6	-2.441981000	-2.324056000	-1.140933000
1	-3.363604000	-2.758777000	-1.516284000
7	-0.064845000	-1.979354000	-1.601349000
6	-1.300468000	-2.464422000	-1.919085000
6	-1.263426000	-3.128026000	-3.202628000
1	-2.116910000	-3.598498000	-3.675443000
6	0.017344000	-3.028241000	-3.653394000
1	0.445128000	-3.403370000	-4.575218000
6	0.758657000	-2.313984000	-2.637803000
6	2.120630000	-2.052926000	-2.708366000

**Formation of CCl<sub>2</sub> via a S<sub>E</sub>3 mechanism**

<sup>6</sup>RC<sub>S<sub>E</sub>3</sub>

26	0.085791000	0.006168000	-0.711004000
7	1.514165000	1.484621000	-0.503122000
6	2.866889000	1.283124000	-0.538777000
6	3.540478000	2.562625000	-0.498623000
1	4.614467000	2.697242000	-0.509992000
6	2.569270000	3.519860000	-0.436852000
1	2.689460000	4.594746000	-0.392756000
6	1.297729000	2.828377000	-0.451289000
6	0.037545000	3.440131000	-0.471031000
1	0.025796000	4.525557000	-0.447295000
7	-1.401283000	1.450069000	-0.597408000
6	-1.200511000	2.807447000	-0.567039000
6	-2.473832000	3.478525000	-0.703592000
1	-2.608807000	4.552657000	-0.708050000
6	-3.425616000	2.508938000	-0.842398000
1	-4.492516000	2.631307000	-0.979820000
6	-2.736571000	1.237561000	-0.786600000
6	-3.354134000	-0.028405000	-0.833960000
1	-4.426766000	-0.038626000	-1.003158000
7	-1.377834000	-1.468759000	-0.573065000
6	-2.716253000	-1.283247000	-0.758759000
6	-3.383994000	-2.567351000	-0.790061000
1	-4.449305000	-2.710367000	-0.919738000
6	-2.414768000	-3.517638000	-0.640996000
1	-2.530731000	-4.593916000	-0.626779000
6	-1.152562000	-2.821059000	-0.522422000
6	0.098241000	-3.428986000	-0.430809000
1	0.106874000	-4.513974000	-0.389259000

7	1.541138000	-1.447395000	-0.504839000	7	-1.322641000	1.632951000	-0.485276000
6	1.347916000	-2.794711000	-0.429499000	6	-0.939062000	2.942390000	-0.468049000
6	2.631147000	-3.462045000	-0.402851000	6	-2.115550000	3.785140000	-0.506466000
1	2.771012000	-4.533684000	-0.340124000	1	-2.098929000	4.867477000	-0.496637000
6	3.585679000	-2.487753000	-0.475422000	6	-3.196506000	2.955223000	-0.565261000
1	4.661923000	-2.603487000	-0.479100000	1	-4.245129000	3.220586000	-0.608106000
6	2.889960000	-1.221869000	-0.534617000	6	-2.689959000	1.599837000	-0.551907000
6	3.496971000	0.037001000	-0.571590000	6	-3.481552000	0.446748000	-0.577724000
1	4.582625000	0.046964000	-0.591822000	1	-4.553854000	0.606018000	-0.645043000
16	0.145634000	-0.025829000	-3.106661000	16	-0.085934000	-0.030243000	-2.797364000
1	0.302333000	-1.364772000	-3.139870000	1	-0.831138000	1.080970000	-2.964109000
6	0.285625000	0.005602000	1.794563000	6	-0.252383000	0.029820000	1.734092000
17	-0.595071000	-1.541305000	2.661933000	17	0.793259000	1.405280000	2.558035000
17	-0.575886000	1.575891000	2.627544000	17	0.363917000	-1.604323000	2.529353000
17	1.937124000	0.002072000	2.471857000	17	-1.890372000	0.261507000	2.402474000
8	-2.956958000	0.022605000	2.002525000	8	3.002985000	-0.442391000	1.942151000
1	-2.325679000	0.802632000	2.162252000	1	2.271865000	-1.121549000	2.087786000
1	-3.186347000	0.008984000	1.014054000	1	3.233995000	-0.458954000	0.934543000
1	-2.332775000	-0.758916000	2.186071000	1	2.501143000	0.414725000	2.110314000
<sup>4</sup> RC <sub>SE3</sub>				<sup>2</sup> RC <sub>SE3</sub>			
26	-0.093415000	0.018509000	-0.484890000	26	0.096288000	-0.000229000	-0.517774000
7	-1.746215000	-1.264831000	-0.423650000	7	1.484871000	1.447205000	-0.461856000
6	-3.050416000	-0.880504000	-0.518512000	6	2.838223000	1.261542000	-0.554055000
6	-3.894879000	-2.057219000	-0.565706000	6	3.519538000	2.534567000	-0.533386000
1	-4.975174000	-2.045085000	-0.636299000	1	4.593516000	2.656511000	-0.589664000
6	-3.063851000	-3.138979000	-0.515474000	6	2.557100000	3.490444000	-0.424415000
1	-3.327806000	-4.188640000	-0.539869000	1	2.669580000	4.565959000	-0.381085000
6	-1.711171000	-2.620999000	-0.447506000	6	1.290664000	2.796957000	-0.401176000
6	-0.535187000	-3.383008000	-0.497047000	6	0.050728000	3.428276000	-0.409569000
1	-0.659459000	-4.461411000	-0.531963000	1	0.040787000	4.512964000	-0.379760000
7	1.173278000	-1.599303000	-0.566305000	7	-1.338443000	1.416850000	-0.585576000
6	0.773124000	-2.914992000	-0.592389000	6	-1.164145000	2.780422000	-0.541269000
6	1.933007000	-3.758353000	-0.793657000	6	-2.427808000	3.451517000	-0.725772000
1	1.905205000	-4.839253000	-0.847568000	1	-2.557516000	4.526090000	-0.725442000
6	3.010947000	-2.934259000	-0.924042000	6	-3.362098000	2.481099000	-0.923080000
1	4.044744000	-3.201362000	-1.103134000	1	-4.422284000	2.587900000	-1.114069000
6	2.515761000	-1.577292000	-0.800917000	6	-2.663880000	1.217869000	-0.846994000
6	3.324700000	-0.419281000	-0.836137000	6	-3.290985000	-0.031705000	-0.933422000
1	4.374456000	-0.573604000	-1.067787000	1	-4.349952000	-0.043083000	-1.171637000
7	1.600875000	1.285196000	-0.496318000	7	-1.310379000	-1.441112000	-0.573550000
6	2.882488000	0.918813000	-0.753592000	6	-2.640859000	-1.268673000	-0.830631000
6	3.713595000	2.099220000	-0.888870000	6	-3.316295000	-2.544488000	-0.887500000
1	4.777793000	2.094012000	-1.088458000	1	-4.375311000	-2.672362000	-1.072011000
6	2.884672000	3.175423000	-0.751047000	6	-2.364143000	-3.496333000	-0.681815000
1	3.136357000	4.226326000	-0.818575000	1	-2.475717000	-4.572847000	-0.666339000
6	1.549905000	2.652899000	-0.535426000	6	-1.112147000	-2.801391000	-0.510796000
6	0.383576000	3.410650000	-0.475208000	6	0.115449000	-3.425024000	-0.377285000
1	0.505462000	4.489650000	-0.499075000	1	0.125565000	-4.509274000	-0.333626000

7	1.512023000	-1.417274000	-0.455915000	7	1.436722000	-1.536688000	-0.572254000
6	1.343590000	-2.770856000	-0.378617000	6	1.138810000	-2.867484000	-0.503155000
6	2.622769000	-3.439413000	-0.393865000	6	2.365456000	-3.631918000	-0.455998000
1	2.756159000	-4.512013000	-0.337773000	1	2.419382000	-4.711288000	-0.393931000
6	3.567043000	-2.465853000	-0.511474000	6	3.393879000	-2.734954000	-0.503086000
1	4.643286000	-2.567903000	-0.564034000	1	4.457814000	-2.933150000	-0.481693000
6	2.862045000	-1.206672000	-0.545895000	6	2.799685000	-1.418920000	-0.564043000
6	3.481248000	0.033791000	-0.612704000	6	3.502499000	-0.211512000	-0.540051000
1	4.564346000	0.043894000	-0.681626000	1	4.585927000	-0.282416000	-0.534558000
16	0.186222000	0.016030000	-2.791832000	16	0.171142000	0.082177000	-3.169005000
1	0.239979000	-1.322591000	-2.947152000	1	0.230531000	-1.262576000	-3.252896000
6	0.225284000	0.012133000	1.682941000	6	0.351322000	0.034549000	1.792200000
17	-0.623003000	-1.507131000	2.517764000	17	-1.122311000	-1.586525000	2.747814000
17	-0.634723000	1.532283000	2.500157000	17	-0.169005000	1.593252000	2.650333000
17	1.870216000	0.021913000	2.378076000	17	1.886586000	-0.447545000	2.492487000
8	-3.056129000	-0.000763000	1.873142000	8	-2.939193000	0.372966000	2.050121000
1	-2.436979000	0.780007000	2.039557000	1	-2.296221000	1.116646000	2.093907000
1	-3.253441000	-0.012778000	0.863712000	1	-3.179417000	0.279055000	1.092231000
1	-2.432813000	-0.773947000	2.058234000	1	-2.282616000	-0.523888000	2.344260000
${}^6\text{TS}_{\text{SE}^3}$				${}^4\text{TS}_{\text{SE}^3}$			
26	0.097196000	0.019786000	-0.796916000	26	0.096380000	0.017874000	-0.451270000
7	1.626807000	1.373690000	-0.448277000	7	1.588596000	1.435716000	-0.386752000
6	2.963899000	1.074265000	-0.466541000	6	2.931737000	1.192174000	-0.464496000
6	3.728447000	2.296304000	-0.365014000	6	3.647059000	2.452668000	-0.452423000
1	4.809521000	2.349498000	-0.352260000	1	4.724098000	2.551106000	-0.499553000
6	2.830456000	3.321894000	-0.287612000	6	2.709915000	3.439623000	-0.385718000
1	3.030008000	4.382417000	-0.202596000	1	2.862802000	4.511156000	-0.368797000
6	1.512313000	2.732099000	-0.351880000	6	1.414498000	2.789258000	-0.362916000
6	0.306733000	3.439696000	-0.368373000	6	0.182027000	3.449968000	-0.385356000
1	0.377401000	4.521344000	-0.307199000	1	0.220678000	4.535358000	-0.389063000
7	-1.271723000	1.567508000	-0.583690000	7	-1.347403000	1.529953000	-0.503510000
6	-0.974501000	2.904812000	-0.505002000	6	-1.086343000	2.875797000	-0.502758000
6	-2.190717000	3.672723000	-0.637352000	6	-2.315200000	3.599715000	-0.732284000
1	-2.245771000	4.753429000	-0.605187000	1	-2.400520000	4.678239000	-0.774056000
6	-3.209268000	2.781349000	-0.825435000	6	-3.299090000	2.668241000	-0.920099000
1	-4.261743000	2.987579000	-0.973254000	1	-4.345598000	2.835568000	-1.141673000
6	-2.620131000	1.461953000	-0.800440000	6	-2.673749000	1.371493000	-0.797829000
6	-3.327254000	0.251680000	-0.897551000	6	-3.319230000	0.128373000	-0.928329000
1	-4.398651000	0.326374000	-1.058413000	1	-4.379549000	0.154939000	-1.162390000
7	-1.465468000	-1.335123000	-0.661846000	7	-1.404299000	-1.385930000	-0.620842000
6	-2.790367000	-1.044130000	-0.822333000	6	-2.725296000	-1.142813000	-0.860480000
6	-3.557216000	-2.271552000	-0.844176000	6	-3.432274000	-2.401066000	-1.017004000
1	-4.632638000	-2.329045000	-0.954419000	1	-4.494137000	-2.494933000	-1.205971000
6	-2.665648000	-3.294154000	-0.699916000	6	-2.503242000	-3.388316000	-0.896099000
1	-2.865475000	-4.357541000	-0.669949000	1	-2.647701000	-4.458693000	-0.967821000
6	-1.351438000	-2.698286000	-0.600121000	6	-1.223625000	-2.740453000	-0.676158000
6	-0.152742000	-3.404275000	-0.510454000	6	0.001137000	-3.403465000	-0.613129000
1	-0.229106000	-4.486076000	-0.461424000	1	-0.036373000	-4.488081000	-0.650594000

7	1.522593000	-1.483979000	-0.561976000	7	1.344017000	-1.572328000	-0.494846000
6	1.276245000	-2.825654000	-0.577897000	6	1.007336000	-2.896847000	-0.438568000
6	2.531619000	-3.542382000	-0.610346000	6	2.194488000	-3.717552000	-0.446236000
1	2.630363000	-4.620361000	-0.626818000	1	2.193053000	-4.799024000	-0.404565000
6	3.524198000	-2.602517000	-0.625135000	6	3.253757000	-2.867243000	-0.532760000
1	4.594869000	-2.760865000	-0.652138000	1	4.309934000	-3.101180000	-0.568531000
6	2.877983000	-1.310217000	-0.589915000	6	2.711411000	-1.529513000	-0.553873000
6	3.524321000	-0.070099000	-0.552298000	6	3.482749000	-0.375514000	-0.553493000
1	4.609467000	-0.089627000	-0.592401000	1	4.560223000	-0.498831000	-0.593847000
16	0.082993000	0.181709000	-2.884919000	16	0.250432000	0.074247000	-2.801573000
1	1.006878000	-0.789559000	-3.023451000	1	0.039248000	-1.242611000	-3.002468000
6	0.344887000	0.052386000	1.724104000	6	0.309631000	0.077523000	1.631560000
17	-1.083874000	-1.642996000	2.674664000	17	-1.240309000	-1.511752000	2.583410000
17	-0.236799000	1.534743000	2.574851000	17	-0.217348000	1.584056000	2.484886000
17	1.865686000	-0.424240000	2.424537000	17	1.775663000	-0.476819000	2.395131000
8	-3.031819000	0.190031000	2.002064000	8	-3.083750000	0.428677000	1.914745000
1	-2.462347000	0.986985000	1.986430000	1	-2.474729000	1.194822000	1.960228000
1	-3.283416000	0.041171000	1.052855000	1	-3.291552000	0.327367000	0.947860000
1	-2.285814000	-0.658933000	2.302703000	1	-2.387924000	-0.465249000	2.211380000
<sup>2</sup> Ts <sub>SE<sup>3</sup></sub>				<sup>6</sup> PC <sub>SE<sup>3</sup></sub>			
26	0.114673000	0.004200000	-0.544115000	26	0.444896000	0.170116000	-0.911758000
7	1.672152000	1.270439000	-0.402731000	7	1.906064000	-1.179436000	-0.282919000
6	2.995788000	0.920572000	-0.462389000	6	1.852588000	-2.544695000	-0.435303000
6	3.825275000	2.098840000	-0.386202000	6	3.146158000	-3.118010000	-0.149096000
1	4.907306000	2.089055000	-0.410744000	1	3.372977000	-4.175664000	-0.187816000
6	2.984665000	3.164901000	-0.281758000	6	3.977243000	-2.084588000	0.167876000
1	3.228957000	4.216696000	-0.208699000	1	5.024039000	-2.122888000	0.440586000
6	1.642780000	2.636917000	-0.312464000	6	3.196946000	-0.873577000	0.073925000
6	0.491152000	3.412731000	-0.329401000	6	3.677928000	0.409654000	0.311540000
1	0.611569000	4.489796000	-0.275230000	1	4.722683000	0.498082000	0.592477000
7	-1.131810000	1.589685000	-0.577288000	7	1.619385000	1.679160000	-0.103512000
6	-0.793442000	2.919503000	-0.500108000	6	2.943703000	1.595511000	0.232556000
6	-1.958945000	3.744063000	-0.697083000	6	3.458434000	2.909160000	0.533255000
1	-1.955958000	4.826194000	-0.673907000	1	4.477968000	3.119552000	0.829680000
6	-3.000517000	2.899732000	-0.940430000	6	2.422251000	3.784189000	0.380647000
1	-4.033908000	3.141603000	-1.153684000	1	2.420779000	4.856620000	0.527203000
6	-2.468485000	1.559911000	-0.876169000	6	1.272638000	3.006975000	-0.013033000
6	-3.233192000	0.402113000	-1.026956000	6	-0.003289000	3.520303000	-0.220998000
1	-4.284279000	0.525230000	-1.268937000	1	-0.125548000	4.591230000	-0.091106000
7	-1.449150000	-1.243605000	-0.652154000	7	-1.198558000	1.437283000	-0.742661000
6	-2.748198000	-0.901358000	-0.912958000	6	-1.152174000	2.792990000	-0.539079000
6	-3.577385000	-2.082909000	-0.986748000	6	-2.481930000	3.344830000	-0.641097000
1	-4.643002000	-2.074924000	-1.177108000	1	-2.728453000	4.391196000	-0.514268000
6	-2.755875000	-3.146510000	-0.775665000	6	-3.324597000	2.301203000	-0.910395000
1	-3.001901000	-4.200232000	-0.758437000	1	-4.399170000	2.317469000	-1.035049000
6	-1.427584000	-2.614377000	-0.591046000	6	-2.510091000	1.114593000	-0.976654000
6	-0.290288000	-3.391600000	-0.451685000	6	-2.992650000	-0.175223000	-1.198571000
1	-0.418740000	-4.468158000	-0.411646000	1	-4.062893000	-0.278376000	-1.335092000

7	-0.886431000	-1.421231000	-0.990915000	7	-0.814656000	-1.438614000	-0.954820000
6	-2.244034000	-1.347049000	-1.195924000	6	-2.170716000	-1.395758000	-1.195871000
6	-2.782881000	-2.672120000	-1.377119000	6	-2.683911000	-2.721329000	-1.408096000
1	-3.829636000	-2.892357000	-1.539889000	1	-3.723574000	-2.948439000	-1.602729000
6	-1.736128000	-3.541966000	-1.277418000	6	-1.626938000	-3.574086000	-1.296441000
1	-1.750685000	-4.622069000	-1.345642000	1	-1.613140000	-4.652636000	-1.383342000
6	-0.557183000	-2.750108000	-1.024988000	6	-0.473419000	-2.767011000	-1.005571000
6	0.717701000	-3.268439000	-0.784571000	6	0.790539000	-3.283390000	-0.751811000
1	0.826187000	-4.346558000	-0.849923000	1	0.917456000	-4.358218000	-0.824326000
16	0.969364000	0.421418000	-3.173053000	16	0.947234000	0.389363000	-3.019861000
1	-0.184883000	-0.159490000	-3.561531000	1	-0.188675000	-0.223802000	-3.409627000
6	0.148176000	-0.466299000	1.967675000	6	0.109937000	-0.379932000	1.897396000
17	-4.724900000	-0.313548000	1.739814000	17	-4.760901000	-0.286107000	1.683728000
17	1.499922000	0.087547000	2.899649000	17	1.426414000	0.214290000	2.856207000
17	-0.192897000	-2.133133000	2.280654000	17	-0.237772000	-2.035522000	2.262912000
8	-2.212580000	1.190147000	2.120101000	8	-2.269918000	1.266977000	2.082048000
1	-1.433610000	0.699291000	1.769293000	1	-1.489828000	0.773464000	1.740585000
1	-2.302286000	1.965938000	1.549218000	1	-2.368781000	2.022437000	1.485425000
1	-3.556164000	0.341998000	1.924297000	1	-3.609553000	0.388779000	1.882928000
${}^4\text{PC}_{\text{SE}^3}$				${}^2\text{PC}_{\text{SE}^3}$			
26	0.418534000	0.113843000	-0.684346000	26	0.254243000	0.032107000	-0.558556000
7	1.909082000	-1.160396000	-0.249056000	7	2.100017000	0.744551000	-0.137711000
6	1.892225000	-2.529951000	-0.392368000	6	3.250891000	-0.000894000	-0.067971000
6	3.191628000	-3.079858000	-0.107227000	6	4.372876000	0.857458000	0.219253000
1	3.430684000	-4.134560000	-0.146445000	1	5.394612000	0.515127000	0.320867000
6	4.003653000	-2.031569000	0.199715000	6	3.886628000	2.126675000	0.320586000
1	5.052829000	-2.040869000	0.464875000	1	4.425982000	3.043801000	0.518756000
6	3.202003000	-0.840160000	0.097541000	6	2.468322000	2.050130000	0.080569000
6	3.682250000	0.440699000	0.299607000	6	1.611391000	3.137739000	0.008458000
1	4.728360000	0.550789000	0.564424000	1	2.035900000	4.121748000	0.178301000
7	1.589813000	1.643783000	-0.138284000	7	-0.439914000	1.920747000	-0.576145000
6	2.923929000	1.597794000	0.177432000	6	0.268219000	3.071934000	-0.342896000
6	3.436074000	2.922767000	0.400574000	6	-0.568295000	4.225418000	-0.556991000
1	4.461314000	3.146505000	0.665013000	1	-0.243772000	5.250290000	-0.431485000
6	2.394054000	3.781636000	0.217956000	6	-1.784509000	3.758411000	-0.956336000
1	2.381263000	4.860459000	0.302077000	1	-2.671401000	4.318426000	-1.223636000
6	1.248317000	2.978499000	-0.113168000	6	-1.690944000	2.319328000	-0.968866000
6	-0.017658000	3.490040000	-0.332886000	6	-2.739575000	1.469368000	-1.301102000
1	-0.144099000	4.565256000	-0.263261000	1	-3.676903000	1.925925000	-1.603664000
7	-1.164499000	1.360872000	-0.746884000	7	-1.589683000	-0.661039000	-0.909422000
6	-1.142259000	2.728195000	-0.616363000	6	-2.690342000	0.079885000	-1.246172000
6	-2.466664000	3.268058000	-0.779533000	6	-3.825855000	-0.782593000	-1.481190000
1	-2.712730000	4.320078000	-0.716130000	1	-4.813724000	-0.435982000	-1.756221000
6	-3.294756000	2.209333000	-1.021348000	6	-3.394234000	-2.056358000	-1.278024000
1	-4.364108000	2.205294000	-1.184359000	1	-3.950003000	-2.981668000	-1.352925000
6	-2.471470000	1.031618000	-1.009556000	6	-1.993041000	-1.970036000	-0.944664000
6	-2.948928000	-0.252798000	-1.220112000	6	-1.164802000	-3.069991000	-0.777041000
1	-4.012817000	-0.371621000	-1.385046000	1	-1.620643000	-4.053174000	-0.826169000

7	0.940281000	-1.849362000	-0.536312000	6	0.246415000	-2.721799000	0.681492000
6	0.212249000	-3.005254000	-0.624975000	6	-0.896766000	-3.405961000	0.309572000
6	1.088450000	-4.150902000	-0.589037000	1	-0.859095000	-4.490694000	0.346550000
1	0.755866000	-5.179337000	-0.643392000	7	-2.335065000	-1.486690000	-0.185792000
6	2.357431000	-3.667589000	-0.491474000	6	-2.092897000	-2.826377000	-0.103068000
1	3.289449000	-4.215536000	-0.440597000	6	-3.260786000	-3.570880000	-0.504771000
6	2.251864000	-2.228834000	-0.444773000	1	-3.322725000	-4.651875000	-0.526041000
6	3.328338000	-1.375855000	-0.233418000	6	-4.213049000	-2.652748000	-0.836026000
1	4.311915000	-1.828390000	-0.160114000	1	-5.223785000	-2.818756000	-1.187825000
16	0.693476000	0.163664000	-2.771795000	6	-3.620938000	-1.353578000	-0.632202000
1	-0.042644000	-0.904705000	-3.139614000	6	-4.278750000	-0.148834000	-0.846186000
6	0.312332000	0.000954000	1.471686000	1	-5.304457000	-0.197513000	-1.199407000
17	-2.579174000	-1.492225000	2.612358000	16	-1.845854000	-0.016069000	2.654142000
17	-0.046515000	1.392944000	2.447942000	1	-3.128969000	-0.110377000	2.249560000
17	1.135489000	-1.175103000	2.402845000	6	3.785099000	0.024615000	-0.652148000
8	-3.376496000	1.263532000	1.747084000	17	3.046107000	-1.002496000	-1.845289000
1	-2.582689000	1.796944000	1.893068000	17	-0.428270000	0.027709000	-2.221011000
1	-3.413234000	1.179503000	0.779600000	17	5.257717000	-0.698894000	0.091853000
1	-2.978554000	-0.268356000	2.251682000	17	4.084051000	1.674161000	-1.213296000

<sup>3</sup>TS<sub>C-inact</sub>

**Suicidal inactivation of P450 by CCl<sub>4</sub> via covalent binding to the *meso*-carbon of haem moiety**

<sup>5</sup>TS<sub>C-inact</sub>

26	-1.023883000	0.002152000	0.218729000	26	-1.021584000	0.000175000	0.272871000
7	-2.464465000	1.364580000	-0.202281000	7	-2.393789000	1.396056000	-0.212205000
6	-3.733625000	1.112518000	-0.643071000	6	-3.647173000	1.199393000	-0.720581000
6	-4.440762000	2.351753000	-0.858402000	6	-4.305349000	2.465521000	-0.937410000
1	-5.463148000	2.422840000	-1.208539000	1	-5.306046000	2.578268000	-1.336253000
6	-3.573839000	3.354637000	-0.540960000	6	-3.426038000	3.430183000	-0.545156000
1	-3.732135000	4.425461000	-0.574085000	1	-3.548604000	4.506347000	-0.554937000
6	-2.342206000	2.721544000	-0.135873000	6	-2.235198000	2.746006000	-0.099211000
6	-1.200685000	3.407893000	0.263088000	6	-1.091316000	3.391688000	0.362375000
1	-1.256942000	4.492174000	0.286675000	1	-1.123324000	4.476699000	0.407400000
7	0.274170000	1.482261000	0.651134000	7	0.328015000	1.428731000	0.739991000
6	0.001796000	2.829683000	0.633827000	6	0.090384000	2.780124000	0.744946000
6	1.155122000	3.571651000	1.071074000	6	1.266349000	3.489790000	1.189041000
1	1.199160000	4.651146000	1.143464000	1	1.337317000	4.566935000	1.276764000
6	2.123660000	2.654348000	1.357116000	6	2.215248000	2.545685000	1.444212000
1	3.135934000	2.818313000	1.702304000	1	3.237433000	2.676806000	1.775408000
6	1.557324000	1.359714000	1.086086000	6	1.608193000	1.269637000	1.157215000
6	2.252537000	0.152378000	1.256588000	6	2.273800000	0.039826000	1.282824000
1	3.198348000	0.202642000	1.781165000	1	3.239168000	0.053109000	1.773295000
7	0.400569000	-1.354131000	0.680436000	7	0.359892000	-1.395403000	0.750672000
6	1.659622000	-1.115301000	1.129713000	6	1.633772000	-1.205179000	1.172391000
6	2.336573000	-2.350855000	1.425577000	6	2.268679000	-2.465009000	1.471078000
1	3.357192000	-2.417793000	1.777495000	1	3.292882000	-2.570092000	1.805304000
6	1.456288000	-3.352960000	1.140933000	6	1.342626000	-3.431918000	1.218023000
1	1.594676000	-4.423379000	1.228461000	1	1.437847000	-4.506603000	1.312665000
				6	0.152527000	-2.752166000	0.764494000
				6	-1.013092000	-3.392586000	0.381452000
				1	-1.020259000	-4.477790000	0.431957000





6	-3.533245000	-1.243623000	-0.660730000	16	-1.411859000	-0.001799000	-2.424672000
6	-4.112958000	-0.008837000	-0.939547000	1	-2.752920000	0.020275000	-2.286485000
1	-5.118377000	-0.010667000	-1.348179000	6	3.492274000	0.000393000	0.564902000
16	-1.497852000	0.003714000	2.678095000	17	2.540191000	-0.002276000	2.045558000
1	-2.818326000	-0.039952000	2.406897000	17	-0.695033000	-0.004483000	2.207301000
6	3.406454000	-0.001966000	-0.632933000	17	4.611018000	1.457234000	0.553047000
17	2.318237000	-0.012839000	-2.013923000	17	4.615749000	-1.452546000	0.551020000
17	-0.798697000	0.014280000	-2.469849000				
17	4.519931000	-1.461349000	-0.681737000	<sup>1</sup> PC <sub>C-inact</sub>			
17	4.517390000	1.458294000	-0.704115000	26	-0.971840000	0.047365000	0.136257000
				7	-2.330369000	1.428381000	-0.141990000
<sup>3</sup> PC <sub>C-inact</sub>				6	-3.613596000	1.258814000	-0.616571000
26	-0.965943000	0.000238000	-0.149975000	6	-4.283395000	2.532577000	-0.734008000
7	-2.381031000	-1.400121000	0.134683000	1	-5.298168000	2.665316000	-1.088333000
6	-3.656222000	-1.232360000	0.589391000	6	-3.400847000	3.472467000	-0.293601000
6	-4.316923000	-2.508346000	0.710412000	1	-3.532154000	4.545025000	-0.218007000
1	-5.335545000	-2.643641000	1.052566000	6	-2.192781000	2.763797000	0.061530000
6	-3.418416000	-3.450977000	0.300942000	6	-1.026664000	3.371535000	0.545702000
1	-3.541188000	-4.525588000	0.241767000	1	-1.085795000	4.439021000	0.746164000
6	-2.212147000	-2.745393000	-0.046914000	7	0.479884000	1.432034000	0.500828000
6	-1.048084000	-3.349048000	-0.503642000	6	0.188906000	2.772917000	0.770445000
1	-1.092991000	-4.421681000	-0.675238000	6	1.341570000	3.436671000	1.307757000
7	0.475152000	-1.404666000	-0.506520000	1	1.376623000	4.476271000	1.608077000
6	0.169758000	-2.737862000	-0.758375000	6	2.327879000	2.493817000	1.363440000
6	1.304168000	-3.406840000	-1.304309000	1	3.345446000	2.601032000	1.711416000
1	1.329659000	-4.451558000	-1.588151000	6	1.759984000	1.279633000	0.835875000
6	2.303607000	-2.467840000	-1.388261000	6	2.552630000	0.007551000	0.719339000
1	3.316309000	-2.589675000	-1.744962000	1	3.284136000	0.009067000	1.536615000
6	1.763501000	-1.257954000	-0.861974000	7	0.472931000	-1.390588000	0.523334000
6	2.567163000	-0.000351000	-0.733073000	6	1.749641000	-1.257090000	0.852251000
1	3.304764000	-0.000007000	-1.544093000	6	2.302649000	-2.476970000	1.394808000
7	0.475311000	1.404542000	-0.504872000	1	3.317785000	-2.595401000	1.745613000
6	1.763008000	1.256846000	-0.862327000	6	1.302909000	-3.401849000	1.344782000
6	2.302790000	2.465648000	-1.391176000	1	1.322156000	-4.440038000	1.651632000
1	3.315161000	2.586259000	-1.749189000	6	0.156774000	-2.726151000	0.796600000
6	1.303942000	3.405223000	-1.307109000	6	-1.048329000	-3.328407000	0.536576000
1	1.329442000	4.449413000	-1.592855000	1	-1.101058000	-4.399002000	0.722386000
6	0.170229000	2.737636000	-0.758107000	7	-2.374910000	-1.386477000	-0.111103000
6	-1.047057000	3.349972000	-0.503560000	6	-2.222459000	-2.722748000	0.063317000
1	-1.091596000	4.422310000	-0.676965000	6	-3.424445000	-3.431887000	-0.299982000
7	-2.380149000	1.401770000	0.135368000	1	-3.551714000	-4.506141000	-0.244177000
6	-2.211232000	2.746971000	-0.046214000	6	-4.315032000	-2.484949000	-0.721264000
6	-3.416745000	3.452914000	0.303514000	1	-5.329172000	-2.617217000	-1.077806000
1	-3.539087000	4.527604000	0.244836000	6	-3.643529000	-1.216479000	-0.589477000
6	-4.314914000	2.510456000	0.714246000	6	-4.209098000	0.030135000	-0.847910000
1	-5.333034000	2.646013000	1.057816000	1	-5.232671000	0.041205000	-1.214903000
6	-3.654958000	1.234223000	0.591651000	16	-1.368868000	-0.069853000	2.499619000
6	-4.255626000	0.001028000	0.837091000	1	-2.707965000	-0.206589000	2.408783000
1	-5.281095000	0.001366000	1.194060000	6	3.464498000	-0.007389000	-0.578588000

17	2.488385000	-0.014030000	-2.040152000
17	-0.721835000	-0.127144000	-2.259950000
17	4.579667000	-1.468418000	-0.565435000
17	4.596484000	1.438662000	-0.586677000