Electronic Supplementary Material (ESI) for Dalton Transactions

On the mechanism of the reaction of white phosphorus with silylenes

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Table S1a Relative energies of complexes, transition states (TS), intermediates (IM) (in reaction paths: I, II, III and IV) and products in kJ/mol at various computational methods for the reaction of SiH_2 + P_4. The energies are relative to the sum of the energies of SiH_2 and P_4 molecules.

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	B3LYP / cc-pVTZ	B3LYP-D/ cc-pVTZ	ωB97X-D/ cc-pVTZ	MP2/ cc-pVTZ	SOS-MP2/ cc-pVTZ	CCSD(T)/ cc-pVTZ*
Complex1	-49	-58	-58	-63	-50	-60
Complex2	-33	-42	-38	-58	-35	-45
TS_I	-29	-41	-26	-55	-28	-42
TS_{II}	66	56	79	63	85	63
$TS_{III}1$	48	39	34	30	46	31
$IM_{III}1$	20	10	-1	-12	12	-1
$TS_{III}2$	25	14	5	11	27	10
$IM_{III}2$	-116	-128	-139	-123	-118	-131
$TS_{III}3$	8	-4	-17	-14	2	-13
$TS_{IV}1$	16	5	31	8	1	7
$IM_{IV}1$	-40	-51	-38	-23	-22	-32
$TS_{IV}2$	-27	-43	-29	-14	-11	-23
$IM_{IV}2$	-29	-47	-29	-	-14	-26
$TS_{IV}3$	-6	-21	-8	-	-4	-16
Product	-196	-205	-232	-224	-218	-226
RMS**	15	12	10	7	13	-

* using B3LYP/cc-pVTZ geometry. ** Root mean squares (RMS) are compared to CCSD(T)/cc-pVTZ//B3LYP/cc-pVTZ results.

Table S1b Relative energies of complexes, transition states (TS), intermediates (IM) (in reaction paths: I, II, III and IV) and products in hartree at various computational methods for the reaction of $SiH_2 + P_4$. The energies are relative to the sum of the energies of SiH_2 and P_4 molecules.

	$SiH_2 + P_4$					
	B3LYP / cc-pVTZ	B3LYP-D/ cc-pVTZ	ωB97X-D/ cc-pVTZ	MP2/ cc-pVTZ	SOS-MP2/ cc-pVTZ	CCSD(T)/ cc-pVTZ*
Complex1	-1656.243745	-1656.247402	-1656.124305	-1653.797862	-1653.992306	-1654.119378
Complex2	-1656.237338	-1656.241496	-1656.116790	-1653.795968	-1653.986517	-1654.113497
TS_I	-1656.235767	-1656.240943	-1656.112022	-1653.795057	-1653.983864	-1654.112452
TS_{II}	-1656.206697	-1656.210619	-1656.089178	-1653.762734	-1653.955868	-1654.08465
$TS_{III}1$	-1656.217392	-1656.221659	-1656.102357	-1653.778801	-1653.968588	-1654.096629
$IM_{III}1$	-1656.215415	-1656.219977	-1656.100292	-1653.769820	-1653.963113	-1654.092889
$TS_{III}2$	-1656.26895	-1656.274128	-1656.155051	-1653.821074	-1654.018369	-1654.146471
$IM_{III}2$	-1656.221865	-1656.226748	-1656.108557	-1653.779341	-1653.972585	-1654.101678
$TS_{III}3$	-1656.199677	-1656.204089	-1656.07207	-1653.750145	-1653.94102	-1654.072675
$TS_{IV}1$	-1656.218721	-1656.223407	-1656.090455	-1653.771033	-1653.97742	-1654.093812
$IM_{IV}1$	-1656.240012	-1656.244777	-1656.116797	-1653.782757	-1653.981574	-1654.108875
$TS_{IV}2$	-1656.235381	-1656.241962	-1656.113186	-1653.779298	-1653.97762	-1654.10521
$IM_{IV}2$	-1656.235885	-1656.243455	-1656.113337	-	-1653.978481	-1654.106259
$TS_{IV}3$	-1656.227371	-1656.233475	-1656.105133	-	-1653.974841	-1654.102781
Product	-1656.29956	-1656.303519	-1656.190464	-1653.859318	-1654.056361	-1654.182569

Table S2 Relative energies of transition states (TS), intermediates (IM) and products of the reactions of **9b** + P_4, respectively, at various computational methods in hartree.

	9b + P_4*			
	B3LYP / cc-pVTZ	B3LYP-D/ cc-pVTZ	ωB97X-D/ cc-pVTZ	SOS-MP2/ cc-pVTZ
TS_I	-1960.030304	-1960.054797	-1959.80904	-1957.145157
TS_{II}	-1960.012437	-1960.035424	-1959.783167	-1957.114656
$TS_{III}1$	-1960.034176	-1960.056688	-1959.815168	-1957.149412
$IM_{III}1$	-1960.034368	-1960.05705	-1959.816279	-1957.151721
$TS_{III}2$	-1960.023803	-1960.047165	-1959.805336	-1957.13838
$IM_{III}2$	-1960.08036	-1960.105072	-1959.864722	-1957.196189
$TS_{III}3$	-1960.033733	-1960.058655	-1959.816316	-1957.148873
$TS_{IV}1$	-1960.04579	-1960.067345	-1959.81497	-1957.152233
$IM_{IV}1$	-1960.063258	-1960.08566	-1959.838742	-1957.170686
$TS_{IV}2$	-1960.055653	-1960.0809	-1959.831186	-1957.162822
$IM_{IV}2$	-1960.056088	-1960.081926	-1959.831532	-1957.163762
$TS_{IV}3$	-1960.052193	-1960.077787	-1959.827821	-1957.16335
TS_V1	-	-	-	-
Product	-1960.118254	-1960.141431	-1959.907181	-1957.242258

* using B3LYP/cc-pVTZ geometry.

Table S3 Relative energies of transition states (TS), intermediates (IM) and products of the reactions of **1** + P_4, respectively, at various computational methods in hartree.

	1 + P_4*			
	B3LYP / cc-pVTZ	B3LYP-D/ cc-pVTZ	ωB97X-D/ cc-pVTZ	SOS-MP2/ cc-pVTZ
TS_I	-2893.580336	-2894.1719	-2894.330522	-2893.690243
TS_{II}	-2893.567076	-2894.1554	-2894.306108	-2893.657732
$TS_{III}1$	-2893.584279	-2894.1758	-2894.33045	-2893.694523
$IM_{III}1$	-2893.584366	-2894.1759	-2894.331643	-2893.696548
$TS_{III}2$	-2893.575561	-2894.1647	-2894.323425	-2893.688498
$IM_{III}2$	-2893.630737	-2894.2171	-2894.378538	-2893.743167
$TS_{III}3$	-2893.571352	-2894.1625	-2894.323283	-2893.687353
$TS_{IV}1$	-2893.607286	-2894.1957	-2894.341255	-2893.698451
$IM_{IV}1$	-2893.625007	-2894.2129	-2894.36217	-2893.721271
$TS_{IV}2$	-2893.608757	-2894.194	-2894.346465	-2893.706545
$IM_{IV}2$	-2893.609419	-2894.1951	-2894.34862	-2893.706355
$TS_{IV}3$	-2893.59793	-2894.1854	-2894.344957	-2893.700795
TS_V1	-2893.594361	-2894.1814	-2894.338048	-2893.696463
Product	-2893.670738	-2894.2591	-2894.41949	-2893.791915

* using B3LYP/6-31G* geometry.

Table S4 Calculated geometrical parameters in the reaction of SiH_2 + P_4 at B3LYP/cc-pVTZ level in Cartesian coordinates in Angstrom.

Molecule	Atomic Symbol	Coordinates X	Y	Z	Molecule	Atomic Symbol	Coordinates X	Y	Z
SiH_2	H	0.000000	1.092804	-0.931644					
	Si	0.000000	0.000000	0.133092	**$IM_{III}2$**	Si	1.602091	-0.000023	0.857804
	H	0.000000	-1.092804	-0.931644		P	0.544489	-1.153622	-0.769677
						P	0.544458	1.153737	-0.769543
P_4	P	-1.208389	0.270098	-0.553977		P	-1.430088	1.038463	0.268148
	P	0.702153	-0.818124	-0.823197		P	-1.429990	-1.038548	0.268154
	P	-0.178209	-0.609441	1.198639		H	3.085972	-0.000018	0.807949
	P	0.684446	1.157467	0.178536		H	1.051729	-0.000117	2.226554
Complex1	P	0.530123	-0.137560	-0.154619	**$TS_{III}3$**	P	1.482747	-1.046207	-0.387551
	Si	2.905766	0.081589	0.085987		P	1.204154	1.029745	-0.216659
	P	-1.109402	1.300224	-0.237901		P	-0.015483	-0.189042	1.306596
	P	-1.101765	-0.327683	1.282262		P	-1.031304	1.261515	-0.308204
	P	-1.429492	-0.827426	-0.882046		Si	-1.466738	-0.913579	-0.347051
	H	2.992877	0.183143	-1.430597		H	-2.842157	-1.016589	0.215971
	H	2.984448	-1.438704	0.111331		H	-1.225226	-2.033472	-1.269981
Complex2	P	0.530283	-0.137028	-0.153725	**$TS_{IV}1$**	P	-2.093066	-0.156615	-0.584134
	P	-1.428785	-0.831854	-0.878615		P	-0.661602	-0.676820	1.094537
	P	-1.101383	-0.322543	1.283603		P	-0.755416	1.287396	0.120183
	P	-1.110588	1.299024	-0.243463		P	0.685753	-0.697654	-0.670273
	Si	2.905731	0.082275	0.085147		Si	2.602118	0.128801	0.029611
	H	2.994214	0.171970	-1.432000		H	2.602584	1.006407	1.235294
	H	2.982647	-1.437808	0.122930		H	3.332731	0.845787	-1.054543
TS_I	P	-0.143217	-1.241886	-0.000087	**$IM_{IV}1$**	P	-0.265312	0.000073	0.814333
	P	1.368741	-0.014910	1.105775		P	1.173290	-0.000128	-0.919889
	P	1.369098	-0.014938	-1.105548		Si	2.907071	0.000040	0.237538
	P	-0.080442	1.264129	-0.000121		P	-2.051682	1.010826	-0.102399
	Si	-2.336646	-0.107027	0.000002		P	-2.051710	-1.010822	-0.102188
	H	-2.499906	0.805999	-1.182070		H	2.985172	0.000229	1.717914
	H	-2.499737	0.806447	1.181751		H	4.247063	-0.000021	-0.391301
TS_{II}	P	1.271109	1.352132	0.093248	**$TS_{IV}2$**	P	-1.439259	1.201806	-0.367981
	P	1.005295	-0.610312	1.124526		P	-1.931254	-0.322662	0.867921
	P	1.407427	-0.403729	-1.053748		P	-0.551285	-0.816978	-0.821442
	P	-0.821214	-0.799104	-0.115315		P	1.497624	-1.080396	0.116094
	Si	-2.596106	0.474173	-0.085079		Si	2.231175	0.859437	0.186901
	H	-3.059592	0.662740	1.318058		H	1.497698	2.108984	-0.128616
	H	-3.534189	-0.385970	-0.857617		H	3.628470	1.132348	0.593125

$TS_{III}1$	P	2.182539	0.229075	-0.360832	**$IM_{IV}2$**	P	-0.660854	1.256440	-0.003373
	P	0.764351	-0.626960	1.039505		P	1.589070	1.010898	0.000311
	P	-0.622341	-0.997348	-0.822947		Si	2.005032	-1.031943	0.000510
	P	0.053071	1.103313	-0.094195		P	-1.550065	-0.533524	-1.011010
	Si	-2.152795	0.216573	0.181074		P	-1.550211	-0.527812	1.013536
	H	-2.480539	0.226655	1.626206		H	1.086434	-2.190698	-0.001175
	H	-3.044628	1.120111	-0.584219		H	3.424000	-1.452126	0.002059
$IM_{III}1$	P	-0.116059	1.053388	0.403232	**$TS_{IV}3$**	Si	-1.676275	-0.993362	-0.090172
	Si	1.876718	0.384039	-0.538866		H	-1.121855	-2.184648	-0.753068
	P	0.820798	-0.901190	1.031993		H	-3.094954	-1.289665	0.253471
	P	-0.588990	-0.832472	-0.820903		P	-1.379660	1.135710	-0.122839
	P	-2.207569	0.243954	0.021543		P	0.808172	1.295245	0.204076
	H	2.156930	-0.152476	-1.887018		P	1.474791	-0.497077	-0.964688
	H	2.946318	1.320725	-0.106826		P	0.942342	-0.775120	1.000918
$TS_{III}2$	P	-0.671763	-1.048602	-0.605524	Product	Si	1.757176	-0.000001	-0.000001
	P	-2.153174	0.313277	-0.059464		P	0.114095	-1.568426	0.000000
	P	-0.053851	1.175487	0.334398		P	-1.109985	0.000001	1.095260
	P	0.849316	-0.767414	1.105060		P	-1.109987	0.000000	-1.095259
	Si	1.822655	0.297944	-0.661265		P	0.114097	1.568426	-0.000001
	H	3.013347	1.148615	-0.405249		H	2.638119	-0.000001	-1.201241
	H	1.911575	-0.411063	-1.954081		H	2.638120	-0.000002	1.201239

Table S5 Calculated geometrical parameters in the reaction of **9b** + P_4 at B3LYP/cc-pVTZ level in Cartesian coordinates in Angstrom.

Molecule	Atomic Symbol	Coordinates X	Y	Z	Molecule	Atomic Symbol	Coordinates X	Y	Z
9b	C	2.586511	-1.095183	0.000008					
	C	1.214656	-0.488095	-0.000001	**TS_{III}3**	C	2.588909	2.854156	-0.432883
	N	1.175461	0.907882	-0.000023		C	2.195079	1.577809	-0.277124
	Si	-0.236175	1.944881	0.000000		C	3.145202	0.503159	-0.031379
	N	-1.410169	0.666003	0.000022		C	2.858595	-0.797564	0.172010
	C	-1.268814	-0.737250	0.000002		N	1.554006	-1.300977	0.169327
	C	-2.336900	-1.557093	-0.000018		Si	0.160449	-0.320666	-0.112601
	C	0.096232	-1.238403	0.000009		N	0.828557	1.227859	-0.351154
	H	-2.206947	-2.628177	-0.000028		P	-1.661179	-0.730292	1.212242
	H	-3.347970	-1.174201	-0.000020		P	-3.166400	-0.022519	-0.533165
	H	0.207057	-2.312709	0.000023		P	-1.491358	-1.356576	-1.198759
	H	-2.378847	0.953940	0.000035		P	-2.423226	1.452012	0.747384
	H	2.084303	1.344880	-0.000035		C	3.922275	-1.824368	0.422323
	H	3.151314	-0.775755	0.880600		H	3.892264	-2.607689	-0.340294
	H	2.539064	-2.181577	0.000028		H	3.772660	-2.307510	1.391950
	H	3.151312	-0.775788	-0.880597		H	4.911981	-1.375204	0.412612
						H	4.183929	0.795474	-0.011037
P_4	P	-1.208389	0.270098	-0.553977		H	3.633780	3.114397	-0.370618
	P	0.702153	-0.818124	-0.823197		H	1.882558	3.650328	-0.620762
	P	-0.178209	-0.609441	1.198639		H	0.196368	2.007313	-0.454156
	P	0.684446	1.157467	0.178536		H	1.474319	-2.294490	0.308295
TS_I	C	-3.177668	-2.336192	-0.606301	**TS_{IV}1**	C	4.219232	-1.955822	0.573153
	C	-2.477976	-1.100647	-0.120041		C	3.224598	-0.892491	0.218105
	N	-1.440484	-1.325213	0.779878		N	2.007448	-1.369927	-0.289420
	Si	-0.327680	-0.060046	1.253217		Si	0.709167	-0.369795	-0.818781
	N	-1.303976	1.342439	0.923266		N	1.317737	1.186150	-0.463776
	C	-2.292587	1.406918	-0.079500		C	2.587956	1.527379	0.057725
	C	-2.750709	2.585449	-0.543395		C	2.936827	2.810156	0.251340
	C	-2.831373	0.134068	-0.541685		C	3.480218	0.420386	0.371998
	P	2.125668	-0.409514	1.176996		P	-1.466974	-0.986255	-0.725746
	P	2.688703	1.148999	-0.303266		P	-2.409193	1.018246	-0.439032
	P	0.848431	0.132428	-1.048591		P	-4.165811	-0.263056	0.107059

	P	2.800061	-0.988036	-0.865504		P	-2.530955	-0.120606	1.422696
	H	-3.558798	2.618105	-1.257666		H	3.904070	3.058657	0.658885
	H	-2.345061	3.527388	-0.200923		H	2.267440	3.625315	0.015568
	H	-3.619511	0.202770	-1.276515		H	4.444457	0.698466	0.769858
	H	-1.047340	2.237553	1.307267		H	0.727020	1.984479	-0.647193
	H	-1.325420	-2.276016	1.086710		H	1.936998	-2.372524	-0.359210
	H	-3.602916	-2.892034	0.234452		H	4.471897	-2.558218	-0.303847
	H	-3.984397	-2.089333	-1.292054		H	5.135373	-1.521956	0.965472
	H	-2.478881	-3.004116	-1.117320		H	3.809138	-2.633217	1.327198
TS_{II}	C	-4.143221	-2.017623	0.190172	**$IM_{IV}1$**	C	4.712513	-1.684109	0.001227
	C	-3.131921	-0.918660	0.056216		C	3.554807	-0.732716	0.000567
	N	-1.823097	-1.346938	-0.189186		N	2.293654	-1.346844	0.000187
	Si	-0.486941	-0.289563	-0.521017		Si	0.813008	-0.484913	-0.000565
	N	-1.187095	1.222943	-0.124459		N	1.327354	1.136174	-0.000691
	C	-2.555307	1.520207	0.054519		C	2.660143	1.610082	-0.000266
	C	-2.982529	2.790962	0.156754		C	2.926313	2.926848	-0.000431
	C	-3.460959	0.383898	0.159892		C	3.713400	0.604219	0.000356
	P	1.531766	-1.332990	0.160738		P	-1.096738	-1.363227	-0.001043
	P	3.133578	-0.219804	-1.044468		P	-2.163374	0.618442	-0.001736
	P	2.285772	1.468522	0.028795		P	-4.067661	0.047526	-1.014804
	P	3.171528	-0.291786	1.168763		P	-4.065067	0.049730	1.017554
	H	-4.025099	3.004776	0.332730		H	3.946078	3.278020	-0.000101
	H	-2.303855	3.628233	0.077499		H	2.139825	3.668202	-0.000893
	H	-4.495035	0.626656	0.352516		H	4.722503	0.987380	0.000679
	H	-0.571487	2.021874	-0.080167		H	0.627716	1.864310	-0.001117
	H	-1.713428	-2.344809	-0.276647		H	2.301612	-2.353883	0.000410
	H	-3.875745	-2.690903	1.009166		H	4.681891	-2.331468	-0.879579
	H	-5.135374	-1.618735	0.385341		H	5.659575	-1.150989	0.001504
	H	-4.187504	-2.617097	-0.723441		H	4.681179	-2.331112	0.882269
$TS_{III}1$	C	-2.992565	2.732738	-0.294969	**$TS_{IV}2$**	C	-2.154769	2.989421	-0.260191
	C	-2.502191	1.498218	-0.097818		C	-2.138830	1.496132	-0.133863
	C	-3.291618	0.298621	-0.337067		N	-0.865900	0.916012	-0.258967
	C	-2.890946	-0.976994	-0.186177		Si	-0.571475	-0.765019	-0.141125
	N	-1.599100	-1.318254	0.247314		N	-2.131409	-1.391817	0.134454
	Si	-0.361992	-0.171411	0.542842		C	-3.344929	-0.672784	0.214710
	N	-1.178976	1.307024	0.370303		C	-4.514703	-1.302423	0.416324

	P	1.589090	-0.609297	1.472508		C	-3.254759	0.773594	0.074551
	P	1.687863	-0.759943	-0.822416		P	1.095800	-2.032093	-0.321409
	P	3.864432	-0.133868	-0.778558		P	2.944661	-0.775907	-0.514691
	P	2.333086	1.142309	0.032268		P	2.560952	1.428722	-0.426818
	C	-3.787238	-2.145894	-0.459869		P	3.026530	0.502226	1.320099
	H	-0.658934	2.163499	0.492006		H	-5.433553	-0.741373	0.480186
	H	-2.399425	3.618162	-0.115146		H	-4.574150	-2.376711	0.520157
	H	-4.004500	2.869614	-0.642000		H	-4.189419	1.308348	0.149256
	H	-4.303383	0.467973	-0.672853		H	-2.236937	-2.388132	0.255462
	H	-4.773735	-1.818290	-0.777379		H	-0.104396	1.562013	-0.402168
	H	-3.366565	-2.781388	-1.243960		H	-1.757852	3.299457	-1.230567
	H	-3.901047	-2.763558	0.435215		H	-3.164216	3.379888	-0.160935
	H	-1.407709	-2.305778	0.299387		H	-1.528856	3.449540	0.509050
$IM_{III}1$	C	-3.031668	2.721559	-0.259329	**$IM_{IV}2$**	C	4.601802	-1.188486	-0.000083
	C	-2.510800	1.493782	-0.096231		C	3.294044	-0.456974	-0.000010
	C	-3.295464	0.284790	-0.298247		C	3.213784	0.886865	-0.000073
	C	-2.867785	-0.984968	-0.171382		C	1.997608	1.686269	-0.000033
	N	-1.553067	-1.307943	0.195294		C	2.022331	3.029657	-0.000030
	Si	-0.305465	-0.145746	0.410123		N	2.160911	-1.280981	0.000088
	P	1.586343	-0.615763	1.507471		Si	0.547000	-0.701741	0.000031
	P	2.275698	1.123711	0.102944		P	-1.042147	-2.079641	-0.000109
	P	3.825342	-0.058858	-0.823746		P	-2.990686	-0.973170	0.000082
	P	1.703831	-0.817377	-0.772740		P	-2.792426	1.005706	-1.018255
	N	-1.160443	1.322748	0.291783		P	-2.791788	1.005639	1.018322
	C	-3.761623	-2.165418	-0.401989		N	0.767399	0.985297	0.000001
	H	-0.647091	2.187354	0.374564		H	2.962525	3.558211	-0.000053
	H	-2.443834	3.615918	-0.108295		H	1.115623	3.617661	-0.000011
	H	-4.063758	2.843270	-0.547733		H	4.137891	1.444578	-0.000167
	H	-4.325429	0.440309	-0.581076		H	-0.047673	1.580830	0.000044
	H	-4.767125	-1.850469	-0.668793		H	2.342687	-2.271663	0.000192
	H	-3.372812	-2.794785	-1.207256		H	4.685797	-1.830818	-0.881037
	H	-3.822507	-2.785736	0.496543		H	5.439382	-0.495792	-0.000115
	H	-1.350535	-2.293211	0.244923		H	4.685884	-1.830837	0.880849
$TS_{III}2$	C	-2.825241	2.826999	-0.147079	**$TS_{IV}3$**	C	4.042713	-1.717088	0.698932
	C	-2.360542	1.566386	-0.082153		C	2.964711	-0.761475	0.287428
	C	-3.243911	0.415785	-0.196186		C	3.191301	0.548357	0.079296
	C	-2.887197	-0.881715	-0.144563		C	2.209033	1.546783	-0.316901

	N	-1.565023	-1.300395	0.037801		C	2.522028	2.846186	-0.455528
	Si	-0.221094	-0.220947	0.165498		N	1.692809	-1.332814	0.141206
	P	1.530966	-0.807066	1.502439		Si	0.281173	-0.484289	-0.334178
	P	2.305565	1.063269	0.460080		P	-1.367456	-1.669445	-1.026121
	P	3.590906	0.217963	-0.948659		P	-3.124457	-0.647180	-0.132752
	P	1.687890	-1.067436	-0.801637		P	-2.493987	1.497956	-0.076697
	N	-0.983094	1.311144	0.098044		P	-2.079070	0.316931	1.556268
	C	-3.883708	-1.994427	-0.273334		N	0.895778	1.084862	-0.573353
	H	-0.415553	2.143319	0.133765		H	3.528576	3.187856	-0.272542
	H	-2.170072	3.682642	-0.062096		H	1.788596	3.581249	-0.754871
	H	-3.878094	3.013899	-0.287544		H	4.197699	0.912984	0.218602
	H	-4.289408	0.643579	-0.336977		H	0.249323	1.808438	-0.852971
	H	-4.890533	-1.607138	-0.406448		H	1.624692	-2.310216	0.376655
	H	-3.643439	-2.631961	-1.128734		H	4.154467	-2.515925	-0.039233
	H	-3.874006	-2.627988	0.618148		H	4.998617	-1.210348	0.803525
	H	-1.433061	-2.297464	0.078537		H	3.797346	-2.188810	1.654537
$IM_{III}2$	C	-4.014437	-1.735924	0.000407	Product	C	-3.342948	-2.428075	0.000022
	C	-2.899847	-0.733947	0.000018		C	-2.581431	-1.136202	-0.000060
	N	-1.613940	-1.290901	-0.000484		N	-1.190623	-1.277401	-0.000357
	Si	-0.168278	-0.359043	-0.000591		Si	-0.065383	0.041708	-0.000165
	N	-0.756080	1.240397	-0.001615		P	1.569656	-0.004718	-1.578369
	C	-2.110392	1.643662	-0.000182		P	2.751597	-1.129212	-0.000005
	C	-2.441805	2.946464	0.000578		P	2.814491	1.048505	0.000275
	C	-3.118877	0.593989	0.000206		P	1.569341	-0.005111	1.578391
	P	1.615510	-1.160782	1.165949		C	-3.198515	0.060998	0.000114
	P	1.616181	-1.161394	-1.165171		C	-2.555084	1.365811	0.000037
	P	2.729111	0.744004	-1.046687		N	-1.145541	1.383047	-0.000270
	P	2.729235	0.744083	1.046919		C	-3.267325	2.507921	0.000209
	H	-3.477841	3.246112	0.001427		H	-4.345506	2.480692	0.000393
	H	-1.693492	3.726439	0.000300		H	-2.790019	3.478159	0.000156
	H	-4.143528	0.932795	0.000738		H	-4.277774	0.070810	0.000315
	H	-0.099711	2.005455	-0.001897		H	-0.761194	2.315531	-0.000396
	H	-1.583349	-2.297228	-0.000423		H	-0.862112	-2.228974	-0.000219
	H	-3.954754	-2.381244	0.881348		H	-3.091618	-3.025734	0.880886
	H	-4.984214	-1.245191	0.000833		H	-4.415756	-2.252951	0.000241
	H	-3.955468	-2.381119	-0.880673		H	-3.091955	-3.025637	-0.881003

Table S5 Calculated geometrical parameters in the reaction of **1** + P_4 at B3LYP/6-31G* level in Cartesian coordinates in Angstrom.

Molecule	Atomic Symbol	Coordinates X	Y	Z	Molecule	Atomic Symbol	Coordinates X	Y	Z
1	C	-2.492849	0.000012	2.709537					
	C	-1.223494	0.000027	1.894438	**TS_{IV}1**	C	-3.138362	-1.235511	-0.980213
	N	-1.343574	0.000067	0.486800		C	-2.493371	-0.954930	0.245661
	Si	0.010911	0.000069	-0.659024		C	-3.150793	-0.263451	1.289566
	N	1.347293	0.000104	0.483835		C	-4.462973	0.168954	1.064107
	C	1.306929	0.000099	1.906984		C	-5.106847	-0.075197	-0.144989
	C	2.421030	0.000146	2.677313		C	-4.449096	-0.773040	-1.152440
	C	-0.018719	0.000056	2.513307		N	-1.120991	-1.388310	0.445459
	H	2.323587	0.000170	3.757245		Si	0.115432	-0.325407	-0.129718
	H	3.421073	0.000205	2.264992		P	0.191375	1.993738	-0.790322
	H	-0.021912	0.000055	3.598029		P	-1.876052	2.679054	-1.185619
	H	-3.112190	-0.878662	2.496049		P	-0.600819	4.308768	-2.038376
	H	-2.253550	-0.000143	3.775711		P	-0.868019	4.215833	0.047700
	H	-3.112036	0.878847	2.496275		C	-2.501358	-0.001257	2.646490
	C	2.658574	0.000010	-0.135761		C	-2.440812	1.501411	2.981513
	C	3.283019	1.231815	-0.437458		C	-2.474043	-2.026980	-2.104196
	C	4.527714	1.203470	-1.078448		C	-3.250196	-3.321195	-2.417943
	C	5.146122	-0.000244	-1.401592		C	-0.907875	-2.669576	1.042887
	C	4.527603	-1.203819	-1.078262		C	-1.927580	-3.487268	1.387427
	C	3.282866	-1.231868	-0.437258		C	0.478653	-3.067683	1.256713
	H	5.019039	2.139976	-1.328751		C	1.612467	-2.388614	0.963872
	H	6.111482	-0.000312	-1.901289		C	2.959958	-3.002613	1.241878
	H	5.018774	-2.140440	-1.328415		N	1.592486	-1.100898	0.368370
	C	2.654974	2.577323	-0.084263		C	2.841340	-0.398885	0.115627
	C	3.544957	3.384221	0.880767		C	3.394177	0.412740	1.135231
	C	2.322653	3.394691	-1.347722		C	4.582405	1.098926	0.857581
	H	1.715086	2.380930	0.438655		C	5.205677	0.994606	-0.381566
	H	3.045539	4.317884	1.166540		C	4.648491	0.192005	-1.370859
	H	3.747882	2.813985	1.792911		C	3.463984	-0.520984	-1.148666
	H	4.505340	3.649265	0.422627		C	2.750067	0.575278	2.511216
	H	1.830762	4.336903	-1.077020		C	3.687762	0.118156	3.647135
	H	3.227899	3.643251	-1.914352		C	2.899586	-1.381943	-2.277137
	H	1.654528	2.839727	-2.015779		C	2.450795	-0.518386	-3.473520
	C	2.654708	-2.577298	-0.083770		C	3.898892	-2.463211	-2.735100

H	1.714530	-2.380762	0.438586
C	2.323140	-3.395200	-1.346962
C	3.544321	-3.383493	0.882111
H	3.045466	-4.317649	1.167304
H	4.505477	-3.647648	0.425089
H	3.745693	-2.813126	1.794522
H	1.830978	-4.337253	-1.076155
H	1.655457	-2.840507	-2.015699
H	3.228628	-3.644203	-1.913021
C	-2.663696	0.000000	-0.114499
C	-3.287288	-1.231476	-0.424168
C	-4.536783	-1.203331	-1.055862
C	-5.159533	-0.000049	-1.371047
C	-4.537037	1.203279	-1.055490
C	-3.287561	1.231432	-0.423807
H	-5.027132	-2.139203	-1.309224
H	-6.128330	-0.000079	-1.863839
H	-5.027553	2.139118	-1.308641
C	-2.635862	-2.578128	-0.116872
H	-1.750671	-2.390729	0.498208
C	-3.559797	-3.509599	0.690816
H	-3.023887	-4.425500	0.965979
H	-3.908002	-3.032103	1.613602
H	-4.444399	-3.807851	0.116239
C	-2.161472	-3.269784	-1.410780
H	-1.660792	-4.217762	-1.179853
H	-3.006152	-3.488224	-2.075159
H	-1.458499	-2.637587	-1.964297
C	-2.636142	2.578115	-0.116229
H	-1.751260	2.390618	0.499258
C	-2.161061	3.269560	-1.409946
C	-3.560306	3.509688	0.690974
H	-1.659833	4.217221	-1.178872
H	-1.458363	2.636981	-1.963376
H	-3.005442	3.488605	-2.074521
H	-3.024663	4.425872	0.965739
H	-4.444999	3.807496	0.116309
H	-3.908391	3.032538	1.613985
C	2.290151	2.027444	2.752594
C	-3.217671	-0.782673	3.766617
C	-2.288318	-1.170495	-3.371939
H	-1.710621	-4.448370	1.839464
H	-2.966522	-3.227852	1.235603
H	0.599249	-4.049638	1.700559
H	3.544199	-3.122064	0.322553
H	3.560155	-2.383860	1.916400
H	2.833061	-3.986856	1.698464
H	-4.961640	-0.965443	-2.090796
H	-6.123470	0.275799	-0.300676
H	-4.986915	0.707529	1.848618
H	-1.480007	-2.330638	-1.763137
H	-2.726868	-3.899204	-3.188813
H	-3.342564	-3.948858	-1.525635
H	-4.258833	-3.108236	-2.790731
H	-1.774871	-1.747288	-4.150519
H	-3.251615	-0.844015	-3.780318
H	-1.695467	-0.272282	-3.166022
H	-1.472720	-0.370933	2.605244
H	-2.713567	-0.617560	4.726369
H	-4.259029	-0.457667	3.877146
H	-3.214633	-1.857584	3.560667
H	-1.915905	1.655345	3.931785
H	-1.914573	2.068163	2.206475
H	-3.443016	1.932998	3.085650
H	5.021326	1.732036	1.623520
H	6.124207	1.541465	-0.576972
H	5.138463	0.119020	-2.337639
H	1.861285	-0.062346	2.547560
H	3.172568	0.189005	4.612086
H	4.016958	-0.918609	3.517333
H	4.584334	0.746025	3.704915
H	1.777164	2.106023	3.718602
H	3.143414	2.715626	2.773210
H	1.605043	2.369009	1.970766
H	2.015347	-1.903342	-1.897609
H	1.999547	-1.148020	-4.249769
H	1.716667	0.235951	-3.171506

P_4	P	0.000372	-0.000313	0.000726		H	3.300292	0.008506	-3.923523
	P	0.000395	-0.000178	2.219316		H	3.441203	-3.099747	-3.501187
	P	1.921761	-0.000313	1.110041		H	4.802115	-2.020113	-3.169933
	P	0.640768	-1.811720	1.110158		H	4.211794	-3.106479	-1.904967
TS_I	C	3.707036	-0.395686	0.118947	**$IM_{IV}1$**	C	2.963898	-1.120846	-1.196616
	C	2.464305	-0.975259	-0.259519		C	2.310777	-1.190015	0.054928
	C	2.414475	-1.924158	-1.311108		C	3.005587	-0.984748	1.268554
	C	3.594870	-2.227921	-2.003404		C	4.370232	-0.679930	1.198367
	C	4.810006	-1.657403	-1.650619		C	5.027504	-0.588326	-0.024244
	C	4.858347	-0.762577	-0.587379		C	4.329091	-0.811165	-1.206622
	N	1.251791	-0.599116	0.436729		N	0.895488	-1.506304	0.094777
	Si	-0.021722	0.330464	-0.387156		Si	-0.232883	-0.208469	0.036293
	P	0.697231	2.418589	-1.641515		P	-0.114690	1.907025	-0.068180
	P	1.842295	3.762525	-0.288728		P	2.101750	2.348748	-0.125262
	P	-0.328465	4.066119	-0.564814		P	2.026230	4.392890	0.805786
	P	0.387281	2.560944	0.943156		P	1.988925	4.302854	-1.229548
	C	1.147814	-2.677487	-1.706399		C	2.336066	-1.109938	2.634652
	C	0.706906	-2.355405	-3.146965		C	2.911870	-2.296734	3.433329
	C	3.863068	0.599802	1.267616		C	2.248249	-1.387802	-2.518713
	C	4.578210	-0.028851	2.481784		C	2.266985	-0.153603	-3.441416
	C	1.033726	-1.097716	1.747705		C	0.528790	-2.887184	0.170270
	C	1.769862	-2.089501	2.300298		C	1.450659	-3.875417	0.205471
	C	-0.072162	-0.498618	2.518398		C	-0.895376	-3.196346	0.204328
	C	-1.243891	-0.042372	2.018560		C	-1.951853	-2.350802	0.161899
	C	-2.343829	0.480353	2.907671		C	-3.357218	-2.892383	0.203201
	N	-1.456216	0.009570	0.614733		N	-1.801982	-0.943831	0.079427
	C	-2.744486	-0.424121	0.104735		C	-2.975926	-0.089452	0.009669
	C	-3.112951	-1.792076	0.225704		C	-3.541739	0.410973	1.205767
	C	-4.386179	-2.185487	-0.204482		C	-4.668168	1.236504	1.106433
	C	-5.277180	-1.282342	-0.772019		C	-5.219273	1.561861	-0.128187
	C	-4.898325	0.045883	-0.910828		C	-4.647822	1.063371	-1.294258
	C	-3.648584	0.501781	-0.470735		C	-3.521351	0.233204	-1.255585
	C	-2.192315	-2.865672	0.804941		C	-2.976081	0.098294	2.589910
	C	-2.640317	-3.304091	2.214057		C	-2.463014	1.372769	3.290242
	C	-3.341475	1.984849	-0.626060		C	-2.930180	-0.273486	-2.570041
	C	-3.315948	2.405842	-2.108377		C	-3.945884	-1.101277	-3.382703
	C	-4.321914	2.864543	0.174345		C	-2.377897	0.886251	-3.423618
	C	-2.089663	-4.094285	-0.119907		C	-4.002322	-0.627232	3.483486

C	1.331159	-4.196672	-1.512612	C	2.431101	0.195315	3.448245
C	4.625183	1.867729	0.831380	C	2.833443	-2.620747	-3.235672
H	1.557394	-2.417946	3.311436	H	1.121324	-4.906555	0.261596
H	2.577612	-2.580656	1.772249	H	2.515724	-3.690092	0.180594
H	0.051900	-0.503771	3.596743	H	-1.120507	-4.254741	0.268166
H	-2.519024	1.546727	2.715645	H	-3.912534	-2.513774	1.067655
H	-3.291135	-0.038259	2.724979	H	-3.929026	-2.606810	-0.685873
H	-2.081372	0.357823	3.962118	H	-3.332480	-3.982846	0.260833
H	5.812782	-0.329260	-0.302658	H	4.925303	-0.512809	2.117199
H	5.716228	-1.914402	-2.192972	H	6.086696	-0.346822	-0.055536
H	3.558686	-2.941725	-2.821744	H	4.852002	-0.743848	-2.156508
H	2.862722	0.901871	1.591384	H	1.274746	-1.319777	2.471378
H	4.664059	0.706250	3.291424	H	2.390058	-2.397370	4.392508
H	4.030607	-0.893826	2.863524	H	2.795543	-3.234919	2.881934
H	5.592372	-0.351080	2.215321	H	3.977927	-2.155378	3.647506
H	4.568224	2.632879	1.614253	H	1.891569	0.089604	4.397021
H	5.687346	1.659841	0.657299	H	3.471089	0.446900	3.686507
H	4.219732	2.293136	-0.092018	H	1.999902	1.041174	2.902879
H	0.342129	-2.363422	-1.036866	H	1.201974	-1.616401	-2.295551
H	0.405443	-4.729086	-1.756633	H	2.273285	-2.826130	-4.155758
H	2.121938	-4.593199	-2.159717	H	3.882403	-2.464466	-3.513862
H	1.596740	-4.430599	-0.475994	H	2.778061	-3.508831	-2.598181
H	-0.230301	-2.872517	-3.386095	H	1.707676	-0.359496	-4.361885
H	0.543775	-1.280513	-3.280348	H	1.814239	0.716843	-2.955079
H	1.458461	-2.675267	-3.878555	H	3.289338	0.118395	-3.728474
H	-4.680283	-3.225993	-0.102203	H	-5.080886	1.327543	-2.254907
H	-6.257288	-1.613001	-1.105731	H	-6.092637	2.206456	-0.182142
H	-5.591488	0.754276	-1.356034	H	-5.116611	1.633334	2.012930
H	-1.188500	-2.446754	0.897387	H	-2.092137	-0.935745	-2.331115
H	-1.952146	-4.058114	2.614109	H	-3.471386	-1.497007	-4.288226
H	-2.658114	-2.462674	2.913004	H	-4.335318	-1.949566	-2.809142
H	-3.644874	-3.744001	2.189414	H	-4.801455	-0.492725	-3.697673
H	-1.319287	-4.779208	0.251512	H	-1.906459	0.495912	-4.333659
H	-3.030356	-4.655023	-0.165447	H	-3.178986	1.568816	-3.730912
H	-1.825399	-3.805036	-1.142382	H	-1.633585	1.467758	-2.871166
H	-2.346765	2.159366	-0.212120	H	-2.121858	-0.573926	2.462737
H	-3.045124	3.464011	-2.204268	H	-2.006409	1.117513	4.254128
H	-2.590787	1.814504	-2.678189	H	-1.715679	1.887435	2.678976
H	-4.296834	2.271700	-2.579433	H	-3.281444	2.075594	3.486578

	H	-4.029985	3.919378	0.106236		H	-3.547649	-0.888004	4.446309
	H	-5.345894	2.778819	-0.207607		H	-4.872534	0.006595	3.689368
	H	-4.337742	2.583939	1.233069		H	-4.367593	-1.551745	3.022910
TS_{II}	C	-3.260339	1.390517	-0.022236	**$TS_{IV}2$**	C	-2.965120	1.456306	-0.577402
	C	-2.585021	0.332317	-0.669800		C	-2.246463	0.320746	-1.018997
	C	-3.208179	-0.918998	-0.890597		C	-2.889693	-0.913963	-1.269495
	C	-4.505142	-1.100840	-0.397031		C	-4.268455	-0.995166	-1.036424
	C	-5.169737	-0.084621	0.283115		C	-4.990494	0.106499	-0.588843
	C	-4.552970	1.149136	0.459656		C	-4.342724	1.317747	-0.363223
	N	-1.227107	0.535033	-1.140810		N	-0.823930	0.440843	-1.275713
	Si	0.062387	0.397197	0.026324		C	-0.402015	0.825349	-2.582638
	P	0.363915	-1.519169	1.348787		C	-1.479752	1.144933	-3.587597
	P	0.302011	-1.066257	3.633963		C	-2.144539	-2.135175	-1.808117
	P	-1.771310	-0.577920	3.235500		C	-2.792677	-2.689193	-3.092948
	P	-0.963092	-2.630829	2.709076		C	-2.296426	2.813043	-0.356942
	C	-2.542947	-2.045988	-1.678929		C	-2.147757	3.142158	1.141873
	C	-2.540144	-3.383682	-0.915597		C	0.898359	0.907187	-2.940274
	C	-2.651040	2.780180	0.149395		C	2.085047	0.638549	-2.139728
	C	-3.506977	3.859737	-0.542146		C	3.316889	0.765785	-2.683532
	C	-1.058256	1.033601	-2.467989		N	1.875811	0.248573	-0.785701
	C	-2.107341	1.296218	-3.280915		Si	0.329615	0.068517	-0.031290
	C	0.305818	1.298231	-2.910791		P	0.433858	-0.553366	1.994426
	C	1.470663	1.099184	-2.246477		P	-1.297744	-0.578457	3.427059
	C	2.770369	1.564945	-2.855402		P	-2.904924	-2.066923	2.886048
	N	1.521432	0.536550	-0.951962		P	-3.369279	-0.095375	2.719746
	C	2.802770	0.223793	-0.349484		C	3.059605	-0.010151	0.014308
	C	3.415500	-1.020996	-0.648184		C	3.660069	1.055903	0.722379
	C	4.652665	-1.305179	-0.059489		C	4.811015	0.781528	1.469832
	C	5.262993	-0.410308	0.814221		C	5.355441	-0.497930	1.515607
	C	4.645446	0.800357	1.104228		C	4.755158	-1.531838	0.804739
	C	3.417563	1.150038	0.526565		C	3.602820	-1.314800	0.040097
	C	2.787432	-2.055252	-1.583444		C	3.117691	2.482209	0.689641
	C	3.565785	-2.187285	-2.909490		C	4.088561	3.435319	-0.036352
	C	2.815568	2.514591	0.859607		C	3.000504	-2.479494	-0.741709
	C	2.392518	2.602268	2.339290		C	2.615007	-3.652859	0.179288
	C	3.772470	3.670435	0.504355		C	3.944473	-2.948062	-1.867507
	C	2.670453	-3.441718	-0.918502		C	2.785756	3.005080	2.100472
	C	-3.209665	-2.224694	-3.059089		C	-2.021474	-3.247124	-0.747654

C	-2.418099	3.124390	1.632967	C	-3.034841	3.954454	-1.083724
H	-1.924393	1.666416	-4.283194	H	3.410518	1.069101	-3.719945
H	-3.135845	1.152319	-2.979707	H	4.227541	0.579095	-2.131492
H	0.376018	1.753714	-3.892116	H	1.104465	1.212487	-3.959793
H	3.197088	2.393846	-2.278018	H	-2.137850	0.288528	-3.768991
H	3.529957	0.779557	-2.882244	H	-2.119886	1.969200	-3.255692
H	2.598159	1.915101	-3.875738	H	-1.021031	1.429859	-4.537041
H	-5.084418	1.942537	0.977816	H	5.187841	-2.527686	0.842056
H	-6.173138	-0.251809	0.665857	H	6.249334	-0.688542	2.103877
H	-5.003047	-2.054450	-0.548340	H	5.287607	1.584555	2.025128
H	-1.676523	2.786921	-0.347569	H	2.083106	-2.125269	-1.220800
H	-3.022754	4.839765	-0.455035	H	3.478511	-3.758382	-2.441249
H	-3.635232	3.636611	-1.606380	H	4.171971	-2.128895	-2.556919
H	-4.501806	3.940765	-0.088860	H	4.890684	-3.327708	-1.463847
H	-1.934017	4.104118	1.726612	H	2.126174	-4.444161	-0.402126
H	-3.363174	3.164946	2.187208	H	3.495650	-4.094883	0.659977
H	-1.784627	2.375455	2.121041	H	1.927423	-3.327034	0.966207
H	-1.500560	-1.762411	-1.854097	H	2.185670	2.474910	0.116245
H	-2.700039	-3.011888	-3.627946	H	3.662291	4.444532	-0.089667
H	-4.261755	-2.516357	-2.953606	H	5.046785	3.506721	0.492274
H	-3.166530	-1.300545	-3.642444	H	4.286390	3.093767	-1.057304
H	-1.977548	-4.137471	-1.478933	H	2.328669	4.000081	2.036389
H	-2.080665	-3.284984	0.072524	H	2.088848	2.337111	2.615986
H	-3.554708	-3.773145	-0.772838	H	3.686066	3.097488	2.719458
H	5.141878	-2.249191	-0.282165	H	-4.917218	2.172152	-0.017611
H	6.219368	-0.657379	1.267457	H	-6.060083	0.022332	-0.416188
H	5.127392	1.494976	1.786398	H	-4.784654	-1.934008	-1.215359
H	1.775251	-1.717431	-1.825157	H	-1.288874	2.760388	-0.780481
H	3.088384	-2.934499	-3.554265	H	-2.463531	4.885338	-0.993737
H	3.602826	-1.245376	-3.464689	H	-3.168097	3.741803	-2.150322
H	4.597829	-2.511552	-2.730782	H	-4.026446	4.137390	-0.654569
H	2.111851	-4.124201	-1.569662	H	-1.651461	4.111270	1.271127
H	3.654824	-3.890456	-0.741204	H	-3.126109	3.196457	1.633552
H	2.148663	-3.382323	0.041298	H	-1.552332	2.385597	1.662878
H	1.914462	2.645558	0.252495	H	-1.130431	-1.820372	-2.071817
H	1.936990	3.577094	2.549948	H	-1.473984	-4.104260	-1.157450
H	1.663942	1.824776	2.592819	H	-1.484538	-2.897157	0.139785
H	3.253677	2.483232	3.007246	H	-3.007985	-3.600740	-0.425765
H	3.280779	4.634306	0.680080	H	-2.180955	-3.502523	-3.499580

	H	4.681182	3.647691	1.116662		H	-3.792835	-3.094456	-2.902092
	H	4.080774	3.634276	-0.546338		H	-2.887458	-1.919665	-3.867116
$TS_{III}1$	C	3.346789	1.362503	-0.092635	**$IM_{IV}2$**	C	-3.644404	-1.238442	0.413488
	C	2.664946	0.204741	-0.532890		C	-3.078766	-0.001573	0.024195
	C	3.277473	-1.071116	-0.511141		C	-3.648097	1.228856	0.428280
	C	4.576609	-1.164152	0.000663		C	-4.795484	1.192085	1.229342
	C	5.251485	-0.042403	0.471386		C	-5.364826	-0.014534	1.622124
	C	4.641963	1.206523	0.417203		C	-4.791837	-1.214650	1.214973
	N	1.315745	0.333154	-1.057665		N	-1.885755	0.005049	-0.807279
	Si	-0.016817	0.267801	0.040695		C	-2.020721	0.014149	-2.215772
	P	-0.525979	-1.231780	2.026020		C	-3.419115	0.016362	-2.778223
	P	0.153733	-1.563599	4.154657		C	-3.063895	2.585286	0.037638
	P	1.507379	-0.693113	2.671952		C	-2.572745	3.365865	1.273671
	P	-0.062761	0.940925	2.232802		C	-3.056438	-2.588289	0.006141
	C	2.602683	-2.332237	-1.048699		C	-4.054548	-3.432947	-0.811301
	C	3.316080	-2.850496	-2.314891		C	-0.957297	0.020644	-3.053176
	C	2.755989	2.767111	-0.196541		C	0.460749	0.019293	-2.725603
	C	2.770566	3.517730	1.148721		C	1.393667	0.026564	-3.704921
	C	1.185051	0.498397	-2.472782		N	0.813665	0.010114	-1.337437
	C	2.253929	0.544747	-3.299233		Si	-0.322261	0.001172	-0.038543
	C	-0.161040	0.669345	-3.000380		P	-0.399699	-0.010898	2.080109
	C	-1.344208	0.637931	-2.347092		P	1.372254	-0.024089	3.463176
	C	-2.616891	0.937300	-3.099576		P	3.256835	0.996242	2.797235
	N	-1.450174	0.402291	-0.947165		P	3.254393	-1.039202	2.783098
	C	-2.758956	0.073735	-0.398283		C	2.228411	0.008810	-1.027995
	C	-3.221914	-1.265941	-0.493828		C	2.907799	-1.226412	-0.924263
	C	-4.500135	-1.557489	-0.004248		C	4.281628	-1.196904	-0.645171
	C	-5.297372	-0.574591	0.573187		C	4.963326	0.007390	-0.498474
	C	-4.824849	0.728150	0.668139		C	4.279600	1.212450	-0.628201
	C	-3.558574	1.085969	0.185542		C	2.905679	1.243486	-0.906598
	C	-2.405853	-2.395120	-1.129007		C	2.217618	-2.567382	-1.168916
	C	-2.371281	-3.664605	-0.255580		C	2.219497	-3.470824	0.078685
	C	-3.131509	2.549539	0.300028		C	2.212834	2.586347	-1.131883
	C	-4.032949	3.479617	-0.539435		C	2.830545	3.335842	-2.330106
	C	-3.124322	3.036215	1.763615		C	2.217479	3.474031	0.126992
	C	-2.922347	-2.753848	-2.538928		C	2.840599	-3.300818	-2.374263
	C	2.514740	-3.447226	0.010863		C	-4.064343	3.437600	-0.768953
	C	3.479971	3.589201	-1.283484		C	-2.563168	-3.383186	1.232167

H	2.095927	0.689301	-4.361910	H	1.072847	0.033508	-4.740257
H	3.273745	0.450283	-2.953257	H	2.457231	0.026122	-3.511564
H	-0.198535	0.881475	-4.062802	H	-1.170739	0.027532	-4.115761
H	-3.394385	0.187721	-2.933714	H	-3.986801	-0.863541	-2.459133
H	-3.034020	1.900912	-2.788701	H	-3.988259	0.891488	-2.448823
H	-2.408568	0.989678	-4.170730	H	-3.378449	0.022822	-3.869743
H	5.065367	-2.133604	0.034459	H	4.825122	-2.133167	-0.556015
H	6.257410	-0.140186	0.871045	H	6.029015	0.006779	-0.285744
H	5.183125	2.080179	0.768980	H	4.821436	2.148329	-0.525932
H	1.579897	-2.072673	-1.337335	H	1.174219	-2.364132	-1.424971
H	2.794660	-3.731313	-2.708471	H	2.291274	-4.227989	-2.576018
H	3.335880	-2.088607	-3.099714	H	2.802366	-2.680491	-3.275070
H	4.349259	-3.146136	-2.096506	H	3.886837	-3.569907	-2.187071
H	1.968942	-4.307830	-0.393788	H	1.708079	-4.415831	-0.139807
H	3.508211	-3.800226	0.310620	H	3.238786	-3.711325	0.402478
H	1.996056	-3.103998	0.910315	H	1.704714	-2.995124	0.919877
H	1.711923	2.674246	-0.510688	H	1.168871	2.384576	-1.386942
H	3.020052	4.580077	-1.380352	H	2.279098	4.264591	-2.518341
H	4.537350	3.734695	-1.031873	H	3.877008	3.604137	-2.143054
H	3.425799	3.090591	-2.256146	H	2.790196	2.726766	-3.238464
H	2.271377	4.488196	1.043976	H	1.702364	4.420152	-0.077480
H	2.255563	2.954046	1.933681	H	1.707762	2.986203	0.964306
H	3.792529	3.711630	1.494131	H	3.237414	3.713557	0.449480
H	-5.452262	1.489776	1.121801	H	-5.246545	2.125637	1.554008
H	-6.285266	-0.825710	0.949937	H	-6.254275	-0.019621	2.246700
H	-4.876001	-2.573704	-0.074066	H	-5.240130	-2.153308	1.528557
H	-2.111168	2.636203	-0.087416	H	-2.196419	2.407448	-0.605706
H	-3.668509	4.511747	-0.479832	H	-3.596033	4.380110	-1.075991
H	-4.062421	3.193185	-1.595140	H	-4.407326	2.922955	-1.673115
H	-5.064141	3.470862	-0.167802	H	-4.950180	3.687391	-0.173592
H	-2.732327	4.058692	1.817681	H	-2.095875	4.303826	0.964058
H	-4.136549	3.049680	2.184425	H	-3.406026	3.621664	1.939031
H	-2.503068	2.401612	2.401328	H	-1.848695	2.781448	1.848941
H	-1.373687	-2.049152	-1.238508	H	-2.189464	-2.399986	-0.634924
H	-1.670454	-4.390215	-0.684150	H	-2.086000	-4.316974	0.910642
H	-2.050572	-3.445011	0.766612	H	-1.838716	-2.805247	1.813464
H	-3.351707	-4.151889	-0.205727	H	-3.395386	-3.647747	1.895432
H	-2.329904	-3.574971	-2.959219	H	-3.583451	-4.369840	-1.131029
H	-3.968416	-3.080796	-2.501563	H	-4.939340	-3.693348	-0.218932

	H	-2.856697	-1.909751	-3.231113		H	-4.399485	-2.907382	-1.708404
$IM_{III}1$	C	-3.580628	1.069511	0.186264	**$TS_{IV}3$**	C	-3.014673	1.441206	-0.605009
	C	-2.766374	0.057471	-0.377996		C	-2.546939	0.520684	0.363415
	C	-3.213842	-1.289066	-0.451959		C	-3.422178	-0.413211	0.977790
	C	-4.489391	-1.588378	0.039899		C	-4.759397	-0.426072	0.568990
	C	-5.300161	-0.605657	0.598293		C	-5.229496	0.448266	-0.406610
	C	-4.843846	0.704254	0.671431		C	-4.363982	1.371344	-0.979392
	N	-1.461042	0.391656	-0.930653		N	-1.165516	0.580094	0.809657
	C	-1.356205	0.599451	-2.334318		Si	0.150003	-0.057297	-0.138096
	C	-2.630018	0.880910	-3.091909		P	0.590012	-0.155284	-2.271136
	C	-2.383984	-2.418473	-1.068645		P	-0.369360	-2.032224	-2.952923
	C	-2.897284	-2.806605	-2.471828		P	-0.814191	-2.958285	-0.987966
	C	-3.173669	2.540551	0.276220		P	-2.368640	-1.992460	-1.948094
	C	-3.182701	3.054526	1.730479		C	-2.987519	-1.374042	2.085653
	C	-0.174136	0.619358	-2.989882		C	-3.572238	-0.954771	3.452149
	C	1.172441	0.458444	-2.461116		C	-2.148978	2.546341	-1.208504
	C	2.238333	0.489931	-3.292504		C	-2.224220	2.589988	-2.745685
	N	1.309177	0.317033	-1.043969		C	-0.957886	1.270269	2.053871
	Si	-0.023356	0.282742	0.056882		C	-1.911528	2.039367	2.624458
	P	-0.074362	1.048917	2.202777		C	0.323726	1.092981	2.723764
	P	1.526877	-0.583134	2.641052		C	1.471414	0.607453	2.206262
	P	0.229420	-1.576662	4.085007		C	2.702573	0.486330	3.066980
	P	-0.501479	-1.146255	1.989328		N	1.559668	0.182630	0.854155
	C	2.661525	0.195694	-0.527173		C	2.888681	0.126393	0.254982
	C	3.352239	1.360219	-0.119925		C	3.596900	-1.095418	0.193375
	C	4.651469	1.210428	0.381595		C	4.888375	-1.079733	-0.348598
	C	5.256792	-0.039362	0.458224		C	5.468204	0.095752	-0.811316
	C	4.573265	-1.168736	0.018921		C	4.755185	1.288005	-0.745710
	C	3.269960	-1.081657	-0.482772		C	3.459202	1.332314	-0.220098
	C	2.766044	2.764700	-0.249406		C	3.021874	-2.427900	0.666396
	C	3.486197	3.561942	-1.357214		C	2.902376	-3.428631	-0.500981
	C	2.584237	-2.351181	-0.985275		C	2.731116	2.675850	-0.178293
	C	2.505521	-3.445227	0.096895		C	3.423328	3.670493	0.775570
	C	3.280151	-2.898280	-2.249153		C	2.582180	3.287961	-1.585311
	C	2.791685	3.543544	1.079631		C	3.852242	-3.053931	1.805632
	C	-2.332870	-3.672552	-0.173901		C	-3.375425	-2.837422	1.796025
	C	-4.082429	3.443233	-0.585088		C	-2.515347	3.920528	-0.608714
	H	2.075444	0.615008	-4.356896		H	-1.701159	2.521500	3.572630

H	3.259805	0.402057	-2.949781	H	-2.889994	2.194009	2.192292
H	-0.213011	0.811423	-4.055995	H	0.342203	1.412652	3.759588
H	-3.405738	0.133031	-2.910207	H	3.017579	-0.558354	3.160768
H	-3.048894	1.849821	-2.800564	H	3.553177	1.038956	2.656931
H	-2.422568	0.911806	-4.164067	H	2.491584	0.869127	4.068375
H	5.058754	-2.139112	0.069690	H	-5.445567	-1.134554	1.023706
H	6.266100	-0.132132	0.850536	H	-6.272545	0.416625	-0.710362
H	5.199446	2.089533	0.708410	H	-4.742754	2.064804	-1.724133
H	1.559209	-2.092783	-1.267032	H	-1.896832	-1.331509	2.162175
H	2.750776	-3.785210	-2.617539	H	-3.219168	-1.633733	4.237787
H	3.292934	-2.152876	-3.049716	H	-3.276356	0.062657	3.719582
H	4.314944	-3.193099	-2.037252	H	-4.667993	-1.001844	3.438986
H	1.952107	-4.311375	-0.285016	H	-2.959270	-3.492367	2.570360
H	3.501507	-3.796487	0.390274	H	-4.462511	-2.977674	1.801251
H	1.999819	-3.086216	0.997812	H	-2.999694	-3.178396	0.827493
H	1.719819	2.669199	-0.555105	H	-1.106713	2.348117	-0.944721
H	3.028415	4.551914	-1.471979	H	-1.870893	4.701029	-1.030886
H	4.545436	3.709765	-1.114868	H	-3.554990	4.186820	-0.835119
H	3.424728	3.043652	-2.319018	H	-2.390793	3.926894	0.478410
H	2.298068	4.514680	0.956348	H	-1.523641	3.339674	-3.131000
H	2.276452	3.000242	1.878702	H	-1.957710	1.624402	-3.184804
H	3.816467	3.738277	1.416233	H	-3.224603	2.865909	-3.098809
H	-5.482308	1.465866	1.109398	H	5.210221	2.203180	-1.113780
H	-6.286040	-0.862220	0.976693	H	6.473133	0.082700	-1.224905
H	-4.852768	-2.610125	-0.014107	H	5.447600	-2.008983	-0.408640
H	-2.152128	2.633530	-0.106355	H	1.723198	2.509930	0.213034
H	-3.731982	4.481035	-0.541976	H	2.861695	4.611144	0.816069
H	-4.102170	3.137769	-1.635582	H	3.489929	3.275318	1.794891
H	-5.115554	3.427445	-0.219042	H	4.440510	3.903785	0.439586
H	-2.801814	4.081928	1.768001	H	1.988685	4.208685	-1.534520
H	-4.198162	3.065238	2.143587	H	3.555912	3.547179	-2.017212
H	-2.559059	2.438964	2.384171	H	2.085138	2.593418	-2.269881
H	-1.356591	-2.061123	-1.185501	H	2.014655	-2.243747	1.053116
H	-1.622995	-4.396518	-0.590174	H	2.399150	-4.343659	-0.167640
H	-2.015206	-3.432628	0.844869	H	2.333188	-3.007046	-1.333842
H	-3.307070	-4.171277	-0.115278	H	3.890652	-3.712881	-0.881330
H	-2.295199	-3.627063	-2.879504	H	3.379707	-3.980926	2.150660
H	-3.939322	-3.145339	-2.428182	H	4.865058	-3.304539	1.469516
H	-2.842360	-1.972720	-3.177173	H	3.948366	-2.383800	2.666293

$TS_{III}2$					**$TS_{V}1$**				
	C	3.095278	1.517513	-0.078561		C	-3.500693	-0.647332	0.542702
	C	2.779931	0.157885	-0.337381		C	-2.684992	0.481560	0.283553
	C	3.697209	-0.873112	-0.016784		C	-3.148870	1.573261	-0.489685
	C	4.918897	-0.513618	0.569065		C	-4.442371	1.499248	-1.020281
	C	5.239909	0.813213	0.826876		C	-5.257169	0.398478	-0.785087
	C	4.332671	1.816360	0.501299		C	-4.788275	-0.656514	-0.009859
	N	1.504651	-0.152313	-0.966233		N	-1.353126	0.565820	0.874789
	C	1.391657	0.036421	-2.367646		Si	0.011741	0.122185	-0.068487
	C	2.651390	-0.089062	-3.187118		P	0.091576	-0.270201	-2.201676
	C	3.437152	-2.353625	-0.289799		P	0.902982	-2.762639	-2.412751
	C	3.495295	-3.196891	1.000349		P	-0.325776	-3.409073	-0.837346
	C	2.151771	2.669883	-0.422122		P	-1.187812	-2.134230	-2.495212
	C	2.713593	3.535507	-1.568925		C	-2.333716	2.842094	-0.736507
	C	0.215235	0.294374	-2.981531		C	-2.147747	3.131868	-2.238262
	C	-1.106512	0.457946	-2.389992		C	-3.058655	-1.827743	1.408480
	C	-2.135002	0.888003	-3.157779		C	-3.551520	-1.686063	2.865498
	N	-1.269333	0.119239	-1.012009		C	-1.256644	1.202602	2.158049
	Si	0.056558	-0.364107	0.012856		C	-2.340472	1.643320	2.833152
	P	0.012230	-2.171431	1.437873		C	0.080369	1.414336	2.697301
	P	-1.658963	-0.956858	2.416754		C	1.282207	1.157501	2.134990
	P	-0.615705	-0.182582	4.063100		C	2.547411	1.581891	2.837467
	P	0.747179	-0.122015	2.219915		N	1.407488	0.543724	0.852998
	C	-2.625903	0.126303	-0.504309		C	2.745399	0.330968	0.313525
	C	-3.130460	1.295303	0.114901		C	3.362931	1.372054	-0.418387
	C	-4.443401	1.269023	0.600071		C	4.674273	1.169876	-0.867869
	C	-5.238131	0.134682	0.473182		C	5.354145	-0.011571	-0.600944
	C	-4.735980	-0.995012	-0.166039		C	4.721915	-1.031073	0.104365
	C	-3.433181	-1.023772	-0.676374		C	3.407621	-0.896228	0.567648
	C	-2.317834	2.581991	0.242363		C	2.674460	2.695891	-0.754057
	C	-2.272843	3.111883	1.688232		C	3.447828	3.914332	-0.209579
	C	-2.955809	-2.271528	-1.417138		C	2.748417	-2.066106	1.303116
	C	-3.718309	-2.454033	-2.745892		C	3.161971	-3.434515	0.730104
	C	-3.067218	-3.545744	-0.558276		C	3.014341	-2.047032	2.823536
	C	-2.848753	3.669993	-0.714339		C	2.461947	2.847516	-2.274541
	C	4.433500	-2.930985	-1.317513		C	-2.962255	4.054733	-0.018991
	C	1.832617	3.545022	0.805604		C	-3.520764	-3.186412	0.847519
	H	-1.954798	1.118958	-4.201426		H	-2.205459	2.128150	3.793304
	H	-3.142059	1.013935	-2.784992		H	-3.350730	1.536428	2.464410

H	0.238423	0.402905	-4.059912	H	0.093781	1.891702	3.670622
H	3.440864	0.585202	-2.840647	H	3.280984	0.775936	2.909587
H	3.053126	-1.106671	-3.133718	H	3.036455	2.405623	2.307300
H	2.439578	0.138834	-4.234413	H	2.307588	1.924521	3.846748
H	-4.849231	2.152696	1.083967	H	-5.433449	-1.510373	0.168245
H	-6.253360	0.134635	0.861405	H	-6.259348	0.362243	-1.203985
H	-5.369999	-1.870206	-0.278042	H	-4.816312	2.322821	-1.621671
H	-1.290256	2.359694	-0.059763	H	-1.964367	-1.840412	1.425287
H	-2.238273	4.577653	-0.633245	H	-3.222097	-2.549203	3.456419
H	-2.820083	3.331250	-1.754232	H	-3.167972	-0.780162	3.340927
H	-3.882999	3.941015	-0.469678	H	-4.647768	-1.654867	2.902189
H	-1.598433	3.974133	1.750575	H	-3.020054	-3.996306	1.388998
H	-3.259948	3.446359	2.028271	H	-4.600030	-3.332849	0.974830
H	-1.919223	2.350784	2.390897	H	-3.283633	-3.294870	-0.214132
H	-1.900025	-2.132491	-1.666158	H	-1.337652	2.699979	-0.306260
H	-3.330228	-3.323698	-3.289768	H	-2.342201	4.946749	-0.168731
H	-4.788167	-2.620452	-2.571032	H	-3.962103	4.274571	-0.411480
H	-3.607917	-1.573815	-3.385874	H	-3.049586	3.875750	1.057044
H	-2.660940	-4.405355	-1.104105	H	-1.514007	4.016527	-2.374015
H	-2.513403	-3.451883	0.381835	H	-1.672319	2.289252	-2.750455
H	-4.108929	-3.777878	-0.308179	H	-3.105213	3.335851	-2.731082
H	5.632532	-1.292343	0.822869	H	5.167833	1.953467	-1.435575
H	6.195127	1.066338	1.279269	H	6.373801	-0.145449	-0.952231
H	4.589175	2.852694	0.702474	H	5.257720	-1.956430	0.287683
H	2.429996	-2.445000	-0.709076	H	1.687230	2.700372	-0.280771
H	4.179599	-3.972777	-1.545769	H	2.893901	4.835943	-0.422047
H	4.436017	-2.369116	-2.256335	H	3.602651	3.858163	0.873050
H	5.457078	-2.918437	-0.924937	H	4.433389	4.006396	-0.679792
H	3.218452	-4.235362	0.784950	H	1.930098	3.781738	-2.490591
H	4.506185	-3.205339	1.424437	H	3.420179	2.879189	-2.805964
H	2.812271	-2.820421	1.766585	H	1.876137	2.019599	-2.684918
H	1.207572	2.247429	-0.775826	H	1.666032	-1.982859	1.160631
H	1.093563	4.310219	0.540307	H	2.508358	-4.213599	1.136635
H	1.425320	2.948758	1.628579	H	3.079660	-3.460327	-0.360417
H	2.723253	4.064084	1.177857	H	4.190893	-3.699570	1.001597
H	2.007821	4.335167	-1.822380	H	2.598881	-2.950191	3.285342
H	3.663465	4.004174	-1.285200	H	4.090566	-2.027099	3.034966
H	2.888074	2.943096	-2.473041	H	2.552173	-1.187296	3.315661

$IM_{III}2$					Product				
	C	2.984634	1.390032	-0.358144		C	0.000000	0.000000	0.000000
	C	2.530983	0.326733	0.459570		C	0.000000	0.000000	1.418017
	C	3.386931	-0.739461	0.831996		C	1.217450	0.000000	2.145867
	C	4.688836	-0.744857	0.315112		C	2.419226	0.042143	1.427386
	C	5.139722	0.270140	-0.521850		C	2.433158	0.069049	0.037420
	C	4.298128	1.330640	-0.841112		C	1.232934	0.041998	-0.663524
	N	1.165151	0.339827	0.952385		N	-1.263438	-0.067724	2.132416
	Si	-0.104466	-0.354727	0.001279		Si	-2.082279	1.414869	2.586106
	P	-0.520621	-0.399124	-2.246399		P	-2.249467	3.042348	0.987306
	P	1.487877	-0.568227	-3.178315		P	-0.219528	3.712921	1.740980
	P	1.945146	-2.331812	-2.144117		P	-2.026895	4.518920	2.678867
	P	-0.005913	-2.370505	-1.089872		P	-0.843404	2.931127	3.774379
	C	2.980704	-1.834051	1.820622		C	1.282608	-0.101588	3.669826
	C	3.212876	-3.258734	1.283087		C	1.716896	-1.514078	4.116625
	C	2.130859	2.619154	-0.672933		C	-1.275221	-0.102070	-0.836927
	C	2.519304	3.805172	0.236827		C	-1.350761	0.969119	-1.942268
	C	0.948454	0.848728	2.270114		C	-1.743167	-1.374173	2.438596
	C	1.927564	1.444829	2.986636		C	-1.100883	-2.503550	2.055809
	C	-0.374769	0.667542	2.856842		C	-2.970914	-1.476993	3.213704
	C	-1.520442	0.273530	2.257263		C	-3.814343	-0.495166	3.604004
	C	-2.791216	0.161880	3.060100		C	-5.014882	-0.850301	4.446100
	N	-1.589355	-0.067723	0.878273		N	-3.600356	0.875173	3.304168
	C	-2.853132	0.165264	0.188476		C	-4.731731	1.787697	3.370545
	C	-3.758046	-0.897283	-0.045806		C	-4.968417	2.562018	4.534879
	C	-4.975751	-0.600767	-0.674621		C	-6.059910	3.441895	4.535933
	C	-5.302898	0.693867	-1.056679		C	-6.910289	3.549057	3.442642
	C	-4.403206	1.727946	-0.820020		C	-6.686484	2.761105	2.318931
	C	-3.170425	1.491764	-0.202877		C	-5.606474	1.872726	2.254298
	C	-3.491107	-2.348047	0.351338		C	-4.135640	2.456298	5.813626
	C	-4.497218	-2.853627	1.406780		C	-3.523984	3.806132	6.240917
	C	-2.234115	2.676572	0.032109		C	-5.455424	0.998343	1.007226
	C	-1.918116	3.430923	-1.274100		C	-6.497779	-0.140292	0.996400
	C	-2.801017	3.642021	1.092681		C	-5.547192	1.799999	-0.305712
	C	-3.523257	-3.285609	-0.873099		C	-4.973270	1.904682	6.988749
	C	3.722641	-1.660566	3.163743		C	2.214003	0.952793	4.299204
	C	2.198890	3.052615	-2.148988		C	-1.423537	-1.508599	-1.455435
	H	1.713392	1.796294	3.989452		H	-1.518044	-3.467048	2.325770
	H	2.931603	1.586398	2.611053		H	-0.179798	-2.500156	1.489733
	H	-0.427462	0.890366	3.916628		H	-3.224574	-2.486542	3.516524

	H	-3.600615	0.767114	2.639651	H	-5.936645	-0.386618	4.084421
	H	-3.145597	-0.874040	3.087013	H	-5.154190	-1.933915	4.455487
	H	-2.614747	0.490004	4.087171	H	-4.875522	-0.521261	5.481457
	H	4.668855	2.131792	-1.473137	H	3.360805	0.045199	1.968508
	H	6.153046	0.242672	-0.913747	H	3.378116	0.100897	-0.498752
	H	5.361706	-1.555220	0.580304	H	1.251241	0.043999	-1.749398
	H	1.088633	2.369050	-0.453189	H	0.274641	0.066165	4.061937
	H	1.892192	4.676716	0.012024	H	1.730813	-1.576562	5.211596
	H	2.392637	3.558377	1.294366	H	1.032627	-2.277857	3.738013
	H	3.564745	4.094311	0.073496	H	2.726636	-1.745335	3.755541
	H	1.467943	3.847764	-2.335669	H	2.131560	0.919038	5.391701
	H	3.184960	3.453087	-2.411720	H	3.264407	0.766465	4.047143
	H	1.985017	2.222588	-2.829031	H	1.964893	1.967551	3.974963
	H	1.911040	-1.729046	2.023428	H	-2.128637	0.046450	-0.168188
	H	3.389404	-2.421436	3.879806	H	-2.356070	-1.573765	-2.029340
	H	4.805400	-1.776547	3.033522	H	-0.594239	-1.725938	-2.139700
	H	3.532122	-0.676095	3.599420	H	-1.443164	-2.281276	-0.682128
	H	2.844726	-3.994579	2.007522	H	-2.325507	0.923200	-2.442054
	H	2.697281	-3.427910	0.333374	H	-1.226280	1.979910	-1.541822
	H	4.277192	-3.464173	1.120345	H	-0.584708	0.813527	-2.710658
	H	-5.680928	-1.404953	-0.863402	H	-7.365016	2.834705	1.474229
	H	-6.255346	0.897503	-1.538865	H	-7.751204	4.237057	3.469276
	H	-4.661529	2.739190	-1.121529	H	-6.250381	4.046244	5.418191
	H	-2.489481	-2.400383	0.789276	H	-4.468288	0.527566	1.037420
	H	-4.237493	-3.872493	1.717102	H	-6.369906	-0.761940	0.102480
	H	-4.517205	-2.222374	2.300474	H	-6.403022	-0.789549	1.871582
	H	-5.515691	-2.881137	1.001864	H	-7.517670	0.262614	0.982954
	H	-3.230244	-4.300184	-0.580266	H	-5.327233	1.144596	-1.156676
	H	-4.529961	-3.341092	-1.303983	H	-6.551386	2.209599	-0.464764
	H	-2.839231	-2.952350	-1.657996	H	-4.835855	2.631299	-0.326434
	H	-1.287673	2.295282	0.423969	H	-3.315820	1.755513	5.625260
	H	-1.183855	4.222673	-1.083342	H	-2.883304	3.666733	7.119402
	H	-1.508296	2.758176	-2.034677	H	-2.917791	4.254805	5.450998
	H	-2.810822	3.907007	-1.695469	H	-4.303776	4.526950	6.513494
	H	-2.099288	4.464892	1.272248	H	-4.335151	1.747399	7.866268
	H	-3.752512	4.077473	0.765274	H	-5.760121	2.612360	7.274885
	H	-2.974169	3.133657	2.046865	H	-5.459907	0.955683	6.747772
$TS_{III}3$	C	-3.100015	1.588987	-0.124131				

C	-2.803409	0.260683	0.279956
C	-3.767600	-0.767763	0.147020
C	-5.013529	-0.439360	-0.405314
C	-5.314734	0.855036	-0.808707
C	-4.361693	1.857696	-0.664484
N	-1.501369	-0.000129	0.885790
C	-1.353340	0.367753	2.250347
C	-2.547294	0.200729	3.154432
C	-3.535048	-2.217013	0.569264
C	-4.495381	-2.654819	1.695717
C	-2.113851	2.747378	0.026878
C	-1.868987	3.482442	-1.305297
C	-0.191700	0.843527	2.743315
C	1.052079	1.080947	2.019778
C	1.989569	1.892051	2.557685
N	1.255314	0.390248	0.775761
Si	-0.079916	-0.295008	-0.108743
P	-0.774465	-0.341523	-2.236312
P	0.583317	-1.890472	-3.129010
P	2.083695	-2.290070	-1.715738
P	-0.217757	-2.464974	-1.076359
C	2.637715	0.348996	0.327308
C	3.085507	1.254789	-0.657828
C	4.430244	1.192872	-1.047777
C	5.309890	0.286722	-0.468314
C	4.858411	-0.568476	0.533637
C	3.526208	-0.557239	0.955714
C	2.186522	2.314144	-1.291171
C	2.563304	3.729083	-0.806116
C	3.102877	-1.503279	2.079604
C	3.377414	-2.982827	1.745799
C	3.788023	-1.130149	3.411054
C	2.193943	2.248050	-2.829769
C	-3.681274	-3.185367	-0.622938
C	-2.577877	3.736361	1.115524
H	1.792763	2.359586	3.516083
H	2.944247	2.091096	2.091538
H	-0.165519	1.107613	3.794666
H	-3.430642	0.724833	2.776407

H	-2.318165	0.587718	4.150296
H	-2.816126	-0.856565	3.252971
H	5.554996	-1.263512	0.994228
H	6.349146	0.255492	-0.785070
H	4.793973	1.874265	-1.811760
H	2.023977	-1.396240	2.224765
H	3.429933	-1.781760	4.217412
H	3.578367	-0.093520	3.689860
H	4.875815	-1.252736	3.344119
H	3.017326	-3.623458	2.559858
H	4.449155	-3.178028	1.623913
H	2.878171	-3.291925	0.822761
H	1.160022	2.127622	-0.962631
H	1.894152	4.476488	-1.250240
H	3.589575	3.987122	-1.093792
H	2.485815	3.807119	0.282792
H	1.467254	2.957642	-3.243239
H	1.936395	1.245456	-3.185832
H	3.175363	2.507800	-3.243033
H	-4.602137	2.870644	-0.974866
H	-6.289506	1.083393	-1.231555
H	-5.762312	-1.218024	-0.517399
H	-1.152859	2.344894	0.357193
H	-1.845841	4.543611	1.235440
H	-2.691770	3.238624	2.084071
H	-3.540924	4.191004	0.854350
H	-1.087733	4.241072	-1.178568
H	-2.770100	3.995303	-1.660192
H	-1.549659	2.791184	-2.092959
H	-2.511903	-2.296176	0.951051
H	-3.395301	-4.200333	-0.324308
H	-3.051556	-2.892352	-1.467232
H	-4.718841	-3.222976	-0.975147
H	-4.256627	-3.674868	2.019082
H	-5.535847	-2.653882	1.350464
H	-4.439559	-2.000086	2.570237