

Supporting Information

Table 1(S)- Absolute values of Gibbs free energy, entropy and enthalpy for the all intermediates of the all PRs and their levels, relative Gibbs free energy for the levels, relative Gibbs free energy of activation for transition state and imaginary frequencies of them

	Species and levels	G (a.u)	H (a.u)	S (cal.mol ⁻¹ K ⁻¹)	ΔG_{rel} (kcal.mol ⁻¹)	ΔG_{rel}^\ddagger (kcal.mol ⁻¹)	ν (icm ⁻¹)
P(NMe ₂) ₃ GAS	α -keto ester	-573.362535	-573.312337	105.652			
	Phenyl carbamic acid	-476.125214	-476.082035	90.878			
	P(NMe ₂) ₃	-744.898169	-744.842753	116.633			
	Product	-974.235937	-974.165949	147.303			
	In 1A	-1318.207016	-1318.124768	173.106			
	In 1B	-1318.210908	-1318.128256	173.956			
	Level 0	-1794.385918	-1794.237125	313.163	0.00		
	Level 1	-1794.375423	-1794.235998	293.446	6.59		
	Level 2	-1794.336122	-1794.210291	264.834	31.25		
	Level 3 (re face)	-1794.344121	-1794.234431	230.862	26.23		
	Level 4 (si face)	-1794.330655	-1794.221452	229.837	34.68		
	Level 5	-1794.349903	-1794.239409	232.553	22.60		
	Level Product	-1794.403809	-1794.275917	269.173	-11.23		
	TS1	-1318.188062	-1318.103256	178.49			-363.10
	Level TS1	-1794.313276	-1794.185291	269.368		45.58	
TS2 and its Level (re face)	-1794.324546	-1794.217364	225.583		31.92	-788.03	
TS2 and its Level (si face)	-1794.330655	-1794.221452	229.837		34.68	-728.02	
TS3 and its Level	-1794.337967	-1794.228512	230.369		30.09	-271.56	
P(NMe ₂) ₃ SOLVENT	α -keto ester	-573.371884	-573.321698	105.624			
	Phenyl carbamic acid	-476.13493	-476.091242	91.949			
	P(NMe ₂) ₃	-744.901066	-744.845357	117.25			
	Product	-974.248658	-974.178754	147.124			
	In 1B	-1318.234232	-1318.151700	173.704			
	Level 0	-1794.40788	-1794.258297	314.823	0.00		
	Level 1	-1794.399724	-1794.256475	301.494	5.12		
	Level 2	-1794.369162	-1794.242942	265.653			
	Level 3 (re face)	-1794.366859	-1794.257391	230.396	25.74		
	Level 4 (si face)	-1794.358633	-1794.248429	231.945	30.90		
	Level 5	-1794.380841	-1794.268782	235.848	17.00		
	Level Product	-1794.42586	-1794.298216	268.647	-11.28		
	TS1	-1318.205322	-1318.119231	181.195			318.16
	Level TS1	-1794.340252	-1794.210473	273.144		42.44	
	TS2 and its Level (re face)	-1794.350796	-1794.243564	225.687		35.82	939.47
TS2 and its Level (si face)	-1794.353414	-1794.246315	225.409		34.18	865.14	
TS3 and its Level	-1794.359592	-1794.248615	233.57		30.30	304.25	

Phase	PR ₃	Reactants and TSs	G (a.u)	H (a.u)	S (cal.mol ⁻¹ K ⁻¹)	v (icm ⁻¹)
GAS	P(NMe ₂) ₃	Reactants	-1318.250209	-1318.153963	202.568	
		TS1	-1318.188062	-1318.103256	178.49	363.10
	P(NC ₄ H ₈) ₃	Reactants	-1550.419709	-1550.31553	219.262	
		TS1	-1550.362184	-1550.269128	195.853	340.54
	P(Et) ₃	Reactants	-1152.244515	-1152.157274	183.615	
		TS1	-1152.191161	-1152.114731	160.86	342.23
	P(Me) ₃	Reactants	-1034.38573	-1034.310401	158.544	
		TS1	-1034.325646	-1034.259925	138.322	350.17
	P(NMe ₂) ₂ Et	Reactants	-1262.907399	-1262.816751	190.784	
		TS1	-1262.851481	-1262.768549	174.544	364.44
	P(NMe ₂)Et ₂	Reactants	-1207.575831	-1207.487664	185.562	
		TS1	-1207.520253	-1207.441872	164.967	321.38
	PPh ₃	Reactants	-1609.472512	-1609.371227	213.172	
		TS1	-1609.413027	-1609.324098	187.167	317.89
P(NEt) ₃	Reactants	-1318.287307	-1318.191798	201.015		
	TS1	-1318.235862	-1318.15025	180.186	317.95	
SOLVENT	P(NMe ₂) ₃	Reactants	-1318.264794	-1318.165233	209.545	
		TS1	-1318.205322	-1318.119231	181.195	318.16
	P(NC ₄ H ₈) ₃	Reactants	-1550.432808	-1550.326294	224.177	
		TS1	-1550.381139	-1550.286156	199.91	300.99
	P(Et) ₃	Reactants	-1152.257323	-1152.169066	185.752	
		TS1	-1152.207816	-1152.130708	162.288	314.17
	P(Me) ₃	Reactants	-1034.397618	-1034.320071	163.212	
		TS1	-1034.343906	-1034.276872	141.084	326.14
	P(NMe ₂) ₂ Et	Reactants	-1262.921676	-1262.826798	199.688	
		TS1	-1262.868202	-1262.785618	173.812	364.44
	P(NMe ₂)Et ₂	Reactants	-1207.58968	-1207.499367	190.081	
		TS1	-1207.537079	-1207.458538	165.304	321.92
	PPh ₃	Reactants	-1609.487256	-1609.384865	215.501	
		TS1	-1609.429389	-1609.339925	188.294	320.43
P(NEt) ₃	Reactants	-1318.306201	-1318.208418	205.801		
	TS1	-1318.255638	-1318.170094	180.041	349.03	

Phase	PR ₃	B3LYP			MPWB95	
		G (a.u)	H (a.u)	S (cal.mol ⁻¹ K ⁻¹)	E (kcal.mol ⁻¹)	E (kcal.mol ⁻¹)
GAS	P(NMe ₂) ₃	-744.898169	-744.842753	116.633	-745.1070894	-744.8887612
	PO(NMe ₂) ₃	-820.167872	-820.109968	121.870	-820.3809752	-820.1411175
	P(NC ₄ H ₈) ₃	-977.069733	-977.003425	139.555	-977.3801344	-977.0606733
	PO(NC ₄ H ₈) ₃	-1052.34250	-1052.275322	141.397	-1052.659006	-1052.317645
	P(Et) ₃	-578.893766	-578.846146	100.226	-579.0566507	-578.918477
	PO(Et) ₃	-654.151981	-654.102777	103.559	-654.3191198	-654.153349
	P(Me) ₃	-461.034443	-460.997348	78.073	-461.1175544	-461.0518196
	PO(Me) ₃	-536.291036	-536.251832	82.513	-536.3775525	-536.2845332
	P(NMe ₂) ₂ Et	-689.556594	-689.503748	111.225	-689.7500621	-689.5582148
	PO(NMe ₂) ₂ Et	-764.827948	-764.773229	115.166	-765.0260304	-764.8106671
	P(NMe ₂)Et ₂	-634.227310	-634.176452	107.039	-634.4046777	-634.2385421
	PO(NMe ₂)Et ₂	-709.490733	-709.437481	112.080	-709.6717024	-709.4805868
	PPh ₃	-1036.12132	-1036.058616	131.978	-1036.348929	-1036.01116
	POPh ₃	-1111.37377	-1111.308976	136.384	-1111.604969	-1111.239987
P(NEt) ₃	-744.940385	-744.882388	122.066	-745.1479067	-744.9260242	
PO(NEt) ₃	-820.210370	-820.151407	124.097	-820.4234278	-820.1803554	
SOLVENT	P(NMe ₂) ₃	-744.901066	-744.845357	117.25	-745.109256	-744.8912082
	PO(NMe ₂) ₃	-820.177202	-820.119462	121.523	-820.390247	-820.1507834
	P(NC ₄ H ₈) ₃	-977.073844	-977.006243	142.279	-977.3825183	-977.0635945
	PO(NC ₄ H ₈) ₃	-1052.35410	-1052.287046	141.128	-1052.670324	-1052.329514
	P(Et) ₃	-578.896840	-578.849144	100.383	-579.0594004	-578.9210397
	PO(Et) ₃	-654.164655	-654.115565	103.317	-654.3317884	-654.1661374
	P(Me) ₃	-461.037075	-461.000101	77.818	-461.1202332	-461.0547817
	PO(Me) ₃	-536.304586	-536.265346	82.586	-536.3909291	-536.2982629
	P(NMe ₂) ₂ Et	-689.559872	-689.506658	111.998	-689.7526012	-689.5608467
	PO(NMe ₂) ₂ Et	-764.838871	-764.784095	115.286	-765.0366305	-764.8215088
	P(NMe ₂)Et ₂	-634.229760	-634.179400	105.992	-634.4073751	-634.2414499
	PO(NMe ₂)Et ₂	-709.501876	-709.449131	111.011	-709.6832867	-709.4922571
	PPh ₃	-1036.12744	-1036.064444	132.602	-1036.354645	-1036.017548
	POPh ₃	-1111.38611	-1111.321378	136.243	-1111.617381	-1111.252748
P(NEt) ₃	-744.945423	-744.887492	121.927	-745.1525984	-744.9308978	
PO(NEt) ₃	-820.224203	-820.164806	125.012	-820.4363926	-820.1936324	

Cartesian coordinate of the specious

Gas Phase

α -keto ester:

0 1
C -0.51441500 0.86827500 0.16996900
C 0.84820200 0.28691300 0.05748500
C 1.07586100 -1.09885200 0.00571100
C 1.93686800 1.17354400 -0.02843400
C 2.37583800 -1.58742200 -0.13152600
H 0.24654500 -1.79188800 0.09148500
C 3.23135900 0.68119300 -0.16332300
H 1.74266700 2.24028300 0.01057300
C 3.45261500 -0.70086100 -0.21570500
H 2.54783000 -2.65885400 -0.16714700
H 4.06886200 1.36924900 -0.22884000
H 4.46347300 -1.08437100 -0.32088200
C -1.71886300 -0.08424300 0.28574600
O -0.73430700 2.06768600 0.22145600
O -1.82729100 -0.91813400 1.16218600
O -2.63616100 0.17295700 -0.65146900
C -3.85771100 -0.59496400 -0.57217600
H -4.36854400 -0.38733400 0.37054000
H -3.63958400 -1.66314700 -0.64070700
H -4.45770500 -0.26550700 -1.41887600

Phenyl carbamic acid:

0 1
C 2.18351100 0.10888300 -0.00037900
O 3.30446600 -0.67504800 0.00046400
O 2.22711100 1.32625000 0.00026200
N 1.07514100 -0.68707800 -0.00046400
H 1.26135300 -1.68039500 -0.00039200
C -0.28359800 -0.29973600 -0.00022900
C -0.70182000 1.03906100 -0.00010200
C -1.24050400 -1.32748400 -0.00016000
C -2.06905700 1.32670600 0.00010000
H 0.03307200 1.83222400 -0.00016500
C -2.60036700 -1.02308300 0.00003600
H -0.91785100 -2.36626400 -0.00026900
C -3.02482100 0.30864100 0.00016800
H -2.38404100 2.36625800 0.00020000
H -3.32681300 -1.83038900 0.00008500
H -4.08376600 0.54738200 0.00032700
H 4.05937000 -0.06681300 0.00104300

P(NMe₂)₃:

0 1
P 0.00000300 -0.03909500 -0.74327200
N 0.00000500 1.53014600 0.07142800
N -1.42407500 -0.67334800 0.00091900
N 1.42410400 -0.67332700 0.00089900
C -1.20279400 2.33543600 -0.16367000
H -2.10088600 1.74545100 0.02272900
H -1.19935200 3.19012400 0.52343600
H -1.25761600 2.73135400 -1.19379600
C 1.20281500 2.33542600 -0.16364400
H 1.19935800 3.19011900 0.52345600
H 2.10089600 1.74543400 0.02278300
H 1.25766700 2.73133700 -1.19377100

C	-2.14655400	-1.71438200	-0.71923200
H	-1.91004200	-2.72507000	-0.34626200
H	-3.23111400	-1.56708400	-0.61674000
H	-1.89609500	-1.67546000	-1.78307500
C	-1.71024700	-0.64552500	1.43029600
H	-2.78827200	-0.50542100	1.59530900
H	-1.41570800	-1.58208000	1.93159700
H	-1.18309300	0.18642400	1.90053700
C	2.14651700	-1.71442100	-0.71923600
H	3.23108500	-1.56721900	-0.61669200
H	1.90989800	-2.72509300	-0.34629000
H	1.89610900	-1.67545900	-1.78308900
C	1.71023900	-0.64554400	1.43028600
H	2.78827200	-0.50554200	1.59532400
H	1.18315000	0.18645100	1.90052000
H	1.41560100	-1.58207500	1.93157400

Product:

0 1			
C	-1.77977500	0.63118700	-0.84908500
C	-2.52212800	-0.56387800	-0.28750700
C	-2.40733400	-0.97470300	1.04890200
C	-3.33171100	-1.30448800	-1.15987000
C	-3.08934000	-2.10826400	1.49326800
H	-1.78955100	-0.40774700	1.73372400
C	-4.01393400	-2.43916100	-0.71498000
H	-3.43161900	-0.99109100	-2.19651900
C	-3.89209400	-2.84371900	0.61586000
H	-2.99612400	-2.41530400	2.53092500
H	-4.63910300	-2.99977200	-1.40382900
H	-4.42253400	-3.72340100	0.96924800
C	-1.81752200	1.90145400	0.01566100
O	-2.61460100	2.09930600	0.90497400
O	-0.93799000	2.81399400	-0.43390100
C	-0.89948900	4.05660900	0.29642400
H	-1.87795900	4.54176500	0.27414200
H	-0.15243600	4.66596100	-0.21090800
C	0.53808400	0.20208900	-0.34043000
O	0.37202900	0.44345200	0.84243200
O	-0.43734000	0.29504100	-1.28977200
N	1.69852400	-0.19048600	-0.94640300
H	1.62583000	-0.34183100	-1.94296900
C	2.96760200	-0.40116300	-0.36509000
C	3.22564800	-0.24223100	1.00490100
C	4.00683400	-0.79097200	-1.22606100
C	4.51519000	-0.47591600	1.48912600
H	2.42792900	0.05687400	1.67049400
C	5.28725500	-1.02029200	-0.72675200
H	3.80968900	-0.91469200	-2.28852400
C	5.55124700	-0.86385100	0.63701600
H	4.70488300	-0.35107700	2.55140000
H	6.07815200	-1.32157000	-1.40738700
H	6.54827900	-1.04206500	1.02760700
H	-2.25523100	0.91574900	-1.79342400
H	-0.60785500	3.87105500	1.33268200

In 1A:

0 1			
P	1.38962500	-0.21524100	0.00001700
N	2.19485400	0.23224600	-1.43591400
N	2.19471700	0.23268500	1.43587500
N	1.93708600	-1.85130000	0.00026500
C	2.47975000	1.60867600	-1.85068600
H	2.70245200	2.24947500	-1.00246800
H	3.36369300	1.58213100	-2.49944700
H	1.64865200	2.05718600	-2.41136200
C	2.08579100	-0.64634200	-2.60816300

H	3.03912100	-0.64808000	-3.15088500
H	1.85275500	-1.66724700	-2.31356500
H	1.30113100	-0.29336000	-3.29355200
C	2.08600800	-0.64571500	2.60829600
H	3.03945500	-0.64727300	3.15081500
H	1.30146800	-0.29267100	3.29378900
H	1.85298900	-1.66669300	2.31394300
C	2.47943900	1.60923200	1.85038100
H	1.64833500	2.05766900	2.41111200
H	3.36347300	1.58295400	2.49902800
H	2.70188400	2.24994500	1.00203600
C	1.14819700	-3.07432800	0.00054500
H	1.37982300	-3.68686700	-0.88625600
H	1.37993600	-3.68654300	0.88754200
H	0.08539600	-2.85800000	0.00057200
C	3.36889700	-2.12135900	0.00027200
H	3.65834400	-2.70584700	-0.88733300
H	3.94186800	-1.19499000	0.00010500
H	3.65838900	-2.70556300	0.88804900
C	-1.23257300	0.26397700	-0.00017300
C	-2.58371200	-0.25019800	-0.00013700
C	-3.70735000	0.61301600	-0.00048800
C	-2.83025200	-1.64191700	0.00025500
C	-5.00135700	0.09906300	-0.00041300
H	-3.55523800	1.68522400	-0.00082300
C	-4.13163200	-2.14431700	0.00031400
H	-1.99399800	-2.33039600	0.00052100
C	-5.23064100	-1.28215000	-0.00001300
H	-5.84242100	0.78785200	-0.00068500
H	-4.28431100	-3.22065000	0.00061900
H	-6.24300500	-1.67505200	0.00003100
C	-0.70432400	1.51634900	-0.00037000
O	-0.18132100	-0.69549100	-0.00002200
O	0.60436000	1.61488300	-0.00027700
O	-1.45188900	2.64642300	-0.00080900
C	-0.74785600	3.89349400	0.00071000
H	-0.12436700	3.99424600	0.89389800
H	-1.52439100	4.65929100	0.00000300
H	-0.12190500	3.99505600	-0.89064700

In 1B:

0 1			
P	1.24088900	-0.58891400	-0.01326900
N	1.25518000	-0.01670900	1.53823400
N	0.98252000	-2.22250200	0.12386800
N	2.67499000	-0.33943000	-0.80005400
C	0.06621600	-0.14532000	2.40509500
H	-0.63012000	-0.88369500	2.00686500
H	0.38829800	-0.45785900	3.40636200
H	-0.46360300	0.80958500	2.47055300
C	2.16509900	1.05991100	1.94963200
H	2.50577700	0.85888200	2.97167200
H	3.03538600	1.09869200	1.29392300
H	1.66212500	2.03180200	1.91926000
C	0.72357600	-3.00708100	-1.08862800
H	1.57400000	-3.66788000	-1.30500100
H	-0.17413000	-3.61986100	-0.95320300
H	0.56306300	-2.35155500	-1.94534700
C	1.18613400	-3.02775500	1.32827400
H	0.25391700	-3.53313400	1.60861500
H	1.95216800	-3.79375100	1.14481700
H	1.51203500	-2.40319600	2.15854800
C	2.93623600	0.80054200	-1.69103100
H	3.71202300	1.44914300	-1.26292900
H	3.28973300	0.42511300	-2.65868900
H	2.02842100	1.38347000	-1.82861100
C	3.84932500	-1.16055700	-0.50394200
H	4.59614800	-0.59576500	0.07078100

H	3.57132700	-2.04780600	0.06704400
H	4.31382500	-1.48659700	-1.44208600
C	-0.95792300	0.83488400	-0.45636000
C	-2.21635000	0.14043300	-0.35772100
C	-3.36346300	0.75200900	0.22475900
C	-2.38148800	-1.18505000	-0.83786900
C	-4.56998200	0.06532400	0.32576800
H	-3.28217100	1.77216800	0.57740400
C	-3.59808100	-1.85969700	-0.72865900
H	-1.55449800	-1.67481100	-1.33468300
C	-4.70831300	-1.24904100	-0.14029500
H	-5.42128000	0.57037000	0.77664500
H	-3.67891900	-2.87108100	-1.12195100
H	-5.65525700	-1.77424200	-0.05745700
C	-0.70755700	2.19655000	-0.22530200
O	0.16544000	0.05388700	-0.98900000
O	-1.50125800	3.04798900	0.20447900
O	0.62352500	2.58000200	-0.50683600
C	0.86968600	3.98143400	-0.37466000
H	0.23587000	4.55954000	-1.05365300
H	1.92220400	4.12335600	-0.63373000
H	0.68114000	4.32878400	0.64605000

In 2:

O 1			
P	-1.93795200	-1.50238000	-0.10819800
N	-1.38908800	-1.45748000	-1.65031800
N	-1.34393000	-2.78419400	0.73890800
N	-3.59556100	-1.55738200	-0.20065500
C	-0.25297900	-2.26509800	-2.13054100
H	0.02624100	-3.01426900	-1.39160900
H	-0.55409000	-2.77151900	-3.05565300
H	0.60083500	-1.61107300	-2.31720700
C	-1.78067400	-0.38363800	-2.58458800
H	-2.12457300	-0.83537200	-3.52312700
H	-2.59202900	0.21447500	-2.16653000
H	-0.91333700	0.25600300	-2.77151300
C	-0.01305000	-2.75889100	1.37853200
H	-0.12835100	-2.86359000	2.46321300
H	0.58582500	-3.59561800	0.99965700
H	0.51971500	-1.83641500	1.14478600
C	-1.99403300	-4.09474300	0.72059000
H	-1.45181000	-4.80317200	0.07969600
H	-2.01435800	-4.49915800	1.73906000
H	-3.02231200	-4.01696600	0.36413800
C	-4.42502000	-1.22909500	0.96400700
H	-5.21159200	-0.52532400	0.66900800
H	-4.89697500	-2.13295400	1.37243200
H	-3.82146600	-0.76314900	1.74170200
C	-4.32966800	-2.17116900	-1.30865000
H	-5.08439400	-1.47047300	-1.68547900
H	-3.65187900	-2.42457800	-2.12327100
H	-4.84377400	-3.08500900	-0.97969600
C	-0.89464400	0.98290000	0.47427300
C	-1.85365600	2.09455000	0.09871300
C	-1.54518600	2.90581600	-0.99998700
C	-3.00847400	2.35810200	0.84781400
C	-2.38973800	3.96284800	-1.35081200
H	-0.63917400	2.70679100	-1.56577300
C	-3.85440200	3.41038900	0.49253900
H	-3.24192200	1.74458300	1.71338000
C	-3.54666400	4.21517700	-0.60953500
H	-2.14046900	4.58998000	-2.20199600
H	-4.74609800	3.60943200	1.08058100
H	-4.20209900	5.03720200	-0.88298500
C	-0.00371400	1.38104900	1.65213200
O	-1.61688100	-0.24616600	0.81619000
O	0.60531000	2.42813300	1.64792000

O	0.03992100	0.47944100	2.64474000
C	0.97897900	0.78196900	3.69856200
H	0.73512600	1.73997300	4.16340000
H	1.99183800	0.82018900	3.29209300
C	2.03209100	0.19008500	-1.04818600
O	1.15849000	0.68454100	-1.83011800
O	1.81220000	-0.56100500	-0.05940600
N	3.36201800	0.54567600	-1.37225300
H	3.40738400	1.17529700	-2.16072300
C	4.57331600	0.24016500	-0.75295300
C	4.69250100	-0.61196300	0.36318400
C	5.74761500	0.81338200	-1.28617700
C	5.95020300	-0.86697200	0.91331400
H	3.79447500	-1.05204100	0.77455000
C	6.99492200	0.54842900	-0.72566000
H	5.67245500	1.47426300	-2.14731800
C	7.11104000	-0.29653300	0.38301400
H	6.01924700	-1.52671800	1.77516600
H	7.88005800	1.00732400	-1.15874900
H	8.08247500	-0.50349200	0.82206100
H	-0.20384900	0.77737000	-0.35774000
H	0.87918200	-0.03273500	4.41552400

TS1:

0 1

P	1.28912600	-0.56594900	-0.10849800
N	0.89409900	-0.26431600	1.49514900
N	1.42221900	-2.25548500	-0.15293300
N	2.75516800	0.23293800	-0.35651700
C	-0.18051200	-1.00966800	2.16537300
H	-0.51611400	-1.84262100	1.54821200
H	0.18420800	-1.39992500	3.12482800
H	-1.04170300	-0.35900900	2.35197100
C	1.28606100	0.95907800	2.20073700
H	1.71819100	0.69506000	3.17537600
H	2.02347000	1.50977400	1.61919900
H	0.41647500	1.60550700	2.36676800
C	1.22783400	-2.91839400	-1.44402800
H	2.18365900	-3.24969100	-1.87541600
H	0.58184500	-3.79682500	-1.32100700
H	0.74602100	-2.23775900	-2.14935800
C	2.05220300	-3.09636900	0.86801200
H	1.43011700	-3.98112300	1.05623900
H	3.04768400	-3.43873200	0.54859600
H	2.15462200	-2.54442100	1.80305000
C	2.96044200	1.03868300	-1.56742800
H	3.58543500	1.90401500	-1.31602700
H	3.47059100	0.46292000	-2.35377000
H	2.00193800	1.39949400	-1.93610900
C	3.99051100	-0.24889800	0.26529700
H	4.65716700	0.60249100	0.45096200
H	3.77961100	-0.72464200	1.22528900
H	4.52435500	-0.96661700	-0.37514900
C	-1.05223700	0.88240000	-0.71368200
C	-2.25071100	0.08671700	-0.45742500
C	-3.36910600	0.55819900	0.27667600
C	-2.31719600	-1.23863800	-0.95410800
C	-4.47243100	-0.26268000	0.50488600
H	-3.35941000	1.57358400	0.65053200
C	-3.42399800	-2.05248500	-0.71591600
H	-1.49744800	-1.61332600	-1.55520600
C	-4.51313200	-1.57482900	0.01926300
H	-5.31394100	0.13113800	1.06961700
H	-3.44104100	-3.06210100	-1.11971700

H	-5.37891600	-2.20563200	0.19944900
C	-0.87994100	2.24687000	-0.26395600
O	-0.01695500	0.29452800	-1.32410300
O	-1.72884600	2.97700900	0.25101500
O	0.40116800	2.71978800	-0.48950600
C	0.60267200	4.09420700	-0.14490500
H	-0.05193100	4.74378600	-0.73306000
H	1.64888500	4.30445800	-0.37577300
H	0.40324700	4.27171900	0.91606200

TS2 si face:

O 1

P	1.33389000	-0.54609200	-0.11439200
N	0.91178700	-0.25541300	1.48470400
N	1.47047100	-2.22993800	-0.18009000
N	2.77745600	0.29953800	-0.33638100
C	-0.09810700	-1.06313900	2.17804400
H	-0.42339800	-1.89428500	1.55325500
H	0.32200600	-1.46425400	3.10921400
H	-0.97275600	-0.45035600	2.42382100
C	1.31831500	0.94137500	2.22623300
H	1.81669500	0.64482000	3.15837100
H	2.00431600	1.54073900	1.63076000
H	0.44258300	1.55022800	2.47986100
C	1.31292000	-2.87420900	-1.48825400
H	2.28507200	-3.13693200	-1.92785500
H	0.72295200	-3.79212700	-1.37972300
H	0.78911500	-2.20913500	-2.17808800
C	2.16280500	-3.06024200	0.81403800
H	1.58885600	-3.97903000	0.98546500
H	3.16828500	-3.33865700	0.46955800
H	2.25173400	-2.52799400	1.76142700
C	2.98641200	1.05963000	-1.57603100
H	3.60421500	1.93707800	-1.35265200
H	3.50370800	0.46027400	-2.33883500
H	2.02768500	1.39965100	-1.96456300
C	4.01796900	-0.14832700	0.30936800
H	4.66203400	0.72119100	0.48532800
H	3.80420400	-0.61094900	1.27464300
H	4.56922800	-0.86629000	-0.31372900
C	-1.10697600	0.87819700	-0.72037400
C	-2.28582900	0.05072200	-0.44198400
C	-3.40873900	0.48398800	0.30799300
C	-2.32013500	-1.27401200	-0.94470000
C	-4.49132900	-0.36604700	0.53853000
H	-3.42122600	1.49199800	0.70037900
C	-3.40386800	-2.11843200	-0.70523700
H	-1.48690500	-1.62857300	-1.53955500
C	-4.50248000	-1.67399800	0.03938300
H	-5.33590700	-0.00047100	1.11750700
H	-3.39292800	-3.12766700	-1.10941800
H	-5.34923700	-2.32933000	0.22212000
C	-0.96872800	2.25304000	-0.27191900
O	-0.08681100	0.33458500	-1.36215800
O	-1.84494000	2.95869400	0.24721900
O	0.28356300	2.75808700	-0.51056300
C	0.48914000	4.12636400	-0.13119400
H	-0.17768600	4.79002300	-0.68852000
H	1.52839700	4.34423800	-0.37949700
H	0.31987700	4.26749400	0.93961000

TS2 re face:

0 1			
P	-2.27686900	-1.18202100	-0.41238300
N	-1.05816200	-1.31935700	-1.50519100
N	-2.36288600	-2.52091300	0.56500800
N	-3.68868000	-1.01443800	-1.27385400
C	-0.05173700	-2.39141700	-1.48416900
H	-0.22130200	-3.07100000	-0.65033500
H	-0.10358100	-2.96148400	-2.42097700
H	0.94276300	-1.94965800	-1.38848500
C	-0.77967600	-0.26725700	-2.50434300
H	-0.75987500	-0.71874400	-3.50443700
H	-1.55065400	0.50221500	-2.47699800
H	0.18817100	0.19118200	-2.28453400
C	-1.57393700	-2.64859700	1.79931800
H	-2.18679800	-3.16178200	2.54887000
H	-0.65815900	-3.23188200	1.63549700
H	-1.31751300	-1.66462700	2.18719500
C	-2.92837500	-3.77748600	0.07123500
H	-2.14761700	-4.49276200	-0.22396700
H	-3.52929000	-4.23529300	0.86525800
H	-3.57889400	-3.59978400	-0.78652100
C	-4.90932100	-0.53516800	-0.61456900
H	-5.37470100	0.24696200	-1.22586200
H	-5.63093600	-1.35361000	-0.48708000
H	-4.67374600	-0.11299500	0.36199700
C	-3.89645500	-1.54367600	-2.62077400
H	-4.26525900	-0.74922000	-3.28106100
H	-2.96324900	-1.92876400	-3.03107500
H	-4.63882400	-2.35423800	-2.61295600
C	-1.13064300	0.99947100	0.85516300
C	-1.17144700	2.19552800	-0.03541900
C	-0.06619600	3.06763300	-0.07576700
C	-2.28315000	2.51058700	-0.83828900
C	-0.07730900	4.20341100	-0.88374300
H	0.80189500	2.85058000	0.53515400
C	-2.28749000	3.64386300	-1.65732600
H	-3.15959700	1.87219700	-0.81162500
C	-1.18477600	4.49929000	-1.68605000
H	0.79126300	4.85626700	-0.89420600
H	-3.16311400	3.86236300	-2.26397700
H	-1.18640400	5.38050000	-2.32118300
C	-1.11158000	1.28893300	2.29473700
O	-2.25068300	0.06550600	0.54649900
O	-0.50150000	2.21796500	2.80474700
O	-1.76806400	0.35784400	3.06291700
C	-1.65480500	0.55971000	4.48020400
H	-2.22798500	-0.24925600	4.93638300
H	-2.06937800	1.52915300	4.76792200
C	2.30780900	-0.19165000	0.21354300
O	1.34618700	-0.33624600	1.11365700
O	2.14469900	0.10333600	-0.97172700
N	3.54510600	-0.44882200	0.77964500
H	3.50871400	-0.64137600	1.77066300
C	4.81808400	-0.45471700	0.18433700
C	5.04841300	-0.12665900	-1.16274800
C	5.91019100	-0.80447400	0.99987600
C	6.35169400	-0.15495200	-1.66486300
H	4.21272600	0.15008800	-1.79036600
C	7.20429800	-0.82544100	0.48399400
H	5.73992200	-1.05789900	2.04403200
C	7.43666100	-0.50142100	-0.85609900

H	6.51515500	0.10430300	-2.70746800
H	8.03188700	-1.09598500	1.13382900
H	8.44446200	-0.51624700	-1.25973700
H	0.35772500	0.19939500	0.82794500
H	-0.60904200	0.51613000	4.79636600

TS3:

O 1			
P	-3.05894800	-0.52779300	-0.09307400
N	-2.47874200	-1.55692900	-1.27059800
N	-3.69764400	-1.56918000	1.06074400
N	-4.20258600	0.39378000	-0.92790500
C	-1.72927200	-2.77810800	-0.92274100
H	-1.86680200	-3.02592000	0.12837700
H	-2.08944700	-3.60929800	-1.54274300
H	-0.65953100	-2.63351800	-1.10689200
C	-2.17683700	-1.08515800	-2.63232200
H	-2.52164400	-1.83376800	-3.35722700
H	-2.68794900	-0.14347300	-2.83247900
H	-1.09661000	-0.94927400	-2.76169600
C	-3.63130600	-1.24750600	2.48630000
H	-4.61642700	-0.94695700	2.87340300
H	-3.29346300	-2.12828000	3.04708000
H	-2.92288900	-0.43724000	2.65069800
C	-4.62268700	-2.65113100	0.73732400
H	-4.35665100	-3.54796800	1.31197000
H	-5.66190900	-2.38687700	0.98382900
H	-4.56806300	-2.90386100	-0.32229600
C	-4.48870200	1.75962200	-0.47995700
H	-4.75684300	2.37202400	-1.34927100
H	-5.32761400	1.79102400	0.23284500
H	-3.60516900	2.18603700	-0.00698700
C	-5.31988800	-0.23825000	-1.62666300
H	-5.62102600	0.39273400	-2.47167900
H	-5.02445300	-1.21161800	-2.02185600
H	-6.19772500	-0.37242700	-0.97559400
C	0.00181200	0.50494600	0.29202300
C	0.04697500	1.94021200	0.02375300
C	0.10714600	2.32694000	-1.33051800
C	0.00513100	2.93575300	1.01590900
C	0.13170300	3.67273600	-1.68356600
H	0.16475100	1.55689100	-2.09394400
C	0.02058900	4.28297400	0.65673300
H	-0.04452000	2.65216600	2.05845800
C	0.08550200	4.65615100	-0.68905800
H	0.19139800	3.95646500	-2.73013400
H	-0.01495600	5.04445500	1.43040000
H	0.10367100	5.70762500	-0.96185000
C	0.17187300	-0.23500700	1.59355400
O	-2.11637400	0.44738900	0.60279700
O	-0.04763800	-1.42301200	1.70332700
O	0.60720900	0.53969900	2.60177600
C	0.90223000	-0.15096800	3.83141900
H	1.68356000	-0.89547900	3.66327300
H	0.00711600	-0.64475000	4.21686400
C	2.21179100	-0.62816100	-1.07777200
O	1.29931100	-0.96467600	-1.86359300
O	2.08237800	0.07576100	0.00052100
N	3.50735500	-1.04699500	-1.39823200
H	3.51805300	-1.59881500	-2.24467900
C	4.74022900	-0.87259400	-0.75460700
C	4.92440500	-0.08931800	0.39918200
C	5.85833400	-1.52052300	-1.31674600

C	6.19707300	0.02756300	0.96231300
H	4.07389800	0.41568300	0.83559600
C	7.12190000	-1.39246900	-0.74430600
H	5.72963900	-2.12955000	-2.20898100
C	7.30436200	-0.61619100	0.40426100
H	6.31908300	0.63843700	1.85310900
H	7.96576900	-1.90394900	-1.19944900
H	8.28816400	-0.51520700	0.85241200
H	-0.14532600	-0.15400400	-0.54800900
H	1.24617900	0.62049100	4.51980300

PO(NMe₂)₃:

0 1

P	0.00001400	-0.02518300	-0.48675800
N	-0.00025300	1.55403900	0.13223600
N	-1.41925600	-0.65510000	0.19025300
N	1.41947200	-0.65465100	0.19027800
C	-1.21458000	2.36037800	-0.04638700
H	-2.10362300	1.74373900	0.08606000
H	-1.22534600	3.16079800	0.70288200
H	-1.25564300	2.82050800	-1.04488900
C	1.21381200	2.36078300	-0.04633600
H	1.22427900	3.16120700	0.70293200
H	2.10305600	1.74444300	0.08614900
H	1.25476400	2.82092800	-1.04483600
C	-2.14849400	-1.69015300	-0.54281100
H	-1.89783300	-2.70153600	-0.18537300
H	-3.22775700	-1.54086000	-0.40774900
H	-1.91224000	-1.62018800	-1.60459600
C	-1.70515600	-0.62597300	1.62021200
H	-2.78554400	-0.50464900	1.77528300
H	-1.39725800	-1.55353500	2.12831100
H	-1.20022500	0.21703700	2.09469700
C	2.14908100	-1.68943500	-0.54279900
H	3.22828800	-1.53981600	-0.40764600
H	1.89870800	-2.70092000	-0.18544900
H	1.91288400	-1.61947200	-1.60459600
C	1.70528800	-0.62550500	1.62025400
H	2.78562900	-0.50385900	1.77538800
H	1.20007500	0.21733000	2.09475200
H	1.39764600	-1.55318300	2.12829700
O	0.00006000	-0.24010100	-1.96880200

P(NC₄H₈)₃:

0 1

P	-0.00045800	-0.00166700	-0.93676000
C	1.62859800	-1.24231200	1.04759000
C	2.73721700	-0.43599000	-0.95227500
C	3.10034500	-1.70779000	1.04211400
H	0.93308500	-2.09273900	1.03334400
H	1.40035700	-0.65148500	1.94643300
C	3.49266300	-1.67190000	-0.44493400
H	3.32637700	0.47646000	-0.75760500
H	2.52874500	-0.46559900	-2.02812500
H	3.72140300	-1.00133100	1.60596400
H	3.22418400	-2.69440600	1.49969300
H	4.57414200	-1.60787500	-0.60282300
H	3.12472300	-2.56868000	-0.95804400
C	-1.88193700	-0.79388600	1.05400400
C	-1.75553500	-2.14687100	-0.95415700
C	-3.02779400	-1.82809000	1.04787300

H	-2.26388100	0.23623500	1.04672500
H	-1.25349600	-0.90056500	1.94991400
C	-3.20133200	-2.17692600	-0.44033700
H	-1.26528900	-3.11767300	-0.76813100
H	-1.68084100	-1.94510700	-2.02908200
H	-2.72972800	-2.72401600	1.60572600
H	-3.93971500	-1.43859900	1.51135200
H	-3.69317000	-3.14174100	-0.60099800
H	-3.79190200	-1.40381400	-0.94671700
C	0.27045700	2.03016800	1.04626900
C	-0.99747700	2.58500000	-0.94447000
C	-0.06300400	3.53733800	1.04233800
H	1.35462600	1.85349400	1.02439700
H	-0.12021900	1.53802700	1.94862600
C	-0.30275500	3.85834800	-0.44294700
H	-2.08094100	2.63761200	-0.74227800
H	-0.87504500	2.41891600	-2.02115900
H	-0.98074700	3.72193400	1.61365800
H	0.73286300	4.13881400	1.49287000
H	-0.90149300	4.76203700	-0.59617500
H	0.65345100	3.98951900	-0.96382500
N	1.48492700	-0.44929200	-0.18360300
N	-1.13009500	-1.06418000	-0.18189500
N	-0.35301900	1.50819400	-0.18003800

TS1 when the PR is P(NC₄H₈)₃:

0 1			
P	0.84709800	-0.29136200	0.01732800
C	3.01085600	-1.66674800	-1.04371500
C	1.16167300	-1.25321700	-2.59877200
C	3.49842400	-1.84343700	-2.48886800
H	2.99318600	-2.63281100	-0.51747600
H	3.63839400	-0.98143800	-0.46484100
C	2.20470900	-2.17403000	-3.24884100
H	1.13020800	-0.27299100	-3.08509500
H	0.15372100	-1.67306400	-2.63682900
H	3.92428400	-0.90336900	-2.85865700
H	4.26439100	-2.61959000	-2.57632300
H	2.28184000	-2.00668700	-4.32693100
H	1.93511200	-3.22514000	-3.09000100
C	0.16117600	-2.84452700	0.87334400
C	-0.42547200	-1.01823500	2.35551900
C	-0.77312000	-3.35290900	1.99339600
H	1.10271600	-3.40487900	0.83795600
H	-0.31822800	-2.93224300	-0.10801100
C	-0.61151800	-2.32577000	3.12694600
H	-1.39572000	-0.64730500	1.99689000
H	0.05014700	-0.22901200	2.94382200
H	-1.80891300	-3.35066200	1.63965200
H	-0.52448200	-4.37307300	2.29978700
H	-1.47467900	-2.29140900	3.79786700
H	0.28145500	-2.54106200	3.72553600
C	2.69788200	0.36863100	2.07518300
C	2.48929900	1.89792800	0.17205100
C	3.84789800	1.39018700	2.08240300
H	3.04736300	-0.66796600	2.08569600
H	2.05369100	0.50938800	2.95217700
C	3.27814400	2.58058500	1.29402100
H	1.67320400	2.50050900	-0.22906600
H	3.16202000	1.62508600	-0.65688600
H	4.15800600	1.64886900	3.09937100
H	4.72152500	0.98025800	1.56113800
H	2.59979400	3.16654400	1.92533800

H	4.05106900	3.25322100	0.91093000
N	1.64315200	-1.12378800	-1.19630600
N	0.45084400	-1.42947500	1.22852300
N	1.95364200	0.68051400	0.82784200
C	-1.56204000	1.23680900	-0.80168600
C	-2.70505400	0.35609400	-0.58217700
C	-2.61264200	-1.00566800	-0.96787200
C	-3.91845300	0.76769700	0.03019700
C	-3.66106000	-1.90124600	-0.75483100
H	-1.71991700	-1.34334300	-1.48098600
C	-4.95852600	-0.13493900	0.23975800
H	-4.02995900	1.80353600	0.32192100
C	-4.84552300	-1.47659200	-0.14676800
H	-3.55731600	-2.93303600	-1.08321100
H	-5.87370000	0.21642000	0.70999400
H	-5.66645000	-2.17013900	0.01166300
C	-1.59238400	2.65781700	-0.52285100
O	-0.41237300	0.68437600	-1.18314300
O	-2.58611000	3.33724600	-0.25887300
O	-0.35122600	3.25814700	-0.62763500
C	-0.35973600	4.67916700	-0.45190500
H	-0.74020900	4.95407700	0.53617900
H	-0.98194400	5.16212300	-1.21068100
H	0.67992700	4.99512500	-0.56124100

PO(NC₄H₈)₃:

O 1			
P	-0.01169800	-0.14314900	0.65678200
C	1.85044600	0.31622100	-1.37743300
C	2.72783000	-0.58866700	0.71531900
C	3.34949500	0.00059400	-1.53071000
H	1.67066900	1.39911200	-1.45335700
H	1.24344200	-0.17388800	-2.14993100
C	3.87015400	0.05118200	-0.08482300
H	2.83096800	-1.68490400	0.72702300
H	2.67319200	-0.25122400	1.75221000
H	3.48018800	-1.00865500	-1.93938200
H	3.85438400	0.70130300	-2.20260700
H	4.82067700	-0.47422700	0.04873100
H	4.01174400	1.09228500	0.22998600
C	-1.42924400	1.68732800	-0.96784900
C	-0.65756700	2.45441800	1.22017100
C	-1.54036000	3.21963800	-0.87603800
H	-2.42513400	1.23179200	-1.05375400
H	-0.84787800	1.36522900	-1.83760100
C	-1.63793300	3.47886000	0.63596900
H	0.36859600	2.85465200	1.21313800
H	-0.89229600	2.15780100	2.24508200
H	-0.63330200	3.68850200	-1.27679200
H	-2.39364800	3.60659400	-1.44148300
H	-1.38629100	4.50607900	0.91637000
H	-2.65422300	3.26993500	0.99125200
C	-0.26404400	-2.53229400	-0.65096500
C	-2.33449100	-1.45353700	0.04139800
C	-1.45327800	-3.45881600	-0.93821100
H	0.34145200	-2.93848400	0.17135000
H	0.38997200	-2.40580200	-1.51971900
C	-2.50749500	-2.97921000	0.06983500
H	-2.95982700	-1.00767300	-0.74426500
H	-2.60276400	-0.98688400	0.99367600
H	-1.81265100	-3.30786900	-1.96364100
H	-1.18983300	-4.51484400	-0.82552200
H	-3.52588300	-3.28989000	-0.18360100

H	-2.27377000	-3.36354600	1.06944100
N	1.52043500	-0.17782100	-0.03062900
N	-0.78994400	1.29931500	0.30696700
N	-0.89586900	-1.24043300	-0.27707800
O	0.08882700	-0.38029400	2.13394700

P(NMe₂)₂Et:

0 1			
P	-0.01337700	-0.01569900	-0.87585900
N	1.12657900	-0.79107600	0.24703600
N	-1.46175800	-0.19243500	0.02358800
C	2.53886200	-0.57441800	-0.07524300
H	2.77617200	0.49090300	-0.10243200
H	3.15588000	-1.02951700	0.70827500
H	2.84062100	-1.02172500	-1.04056500
C	0.85760300	-2.22232300	0.41825400
H	1.47098200	-2.60538100	1.24249200
H	-0.19281500	-2.37925700	0.67313200
H	1.08693800	-2.81738500	-0.48448000
C	0.73739900	2.40155600	0.70233500
H	1.16661100	3.40615600	0.60716600
H	-0.20486300	2.49923900	1.24757000
H	1.41509800	1.80302000	1.31815100
C	-2.69938300	-0.49233700	-0.68158800
H	-3.21603100	-1.34504200	-0.21502900
H	-3.39520100	0.36218800	-0.67703900
H	-2.48249100	-0.74906400	-1.72177300
C	-1.62712700	0.08506200	1.44413200
H	-2.18887300	-0.73071700	1.92315000
H	-0.65054600	0.15104800	1.92611400
H	-2.18217200	1.01986800	1.62381000
C	0.52197400	1.77791100	-0.68407300
H	-0.25549200	2.32835800	-1.23068800
H	1.42713500	1.88466700	-1.29723000

TS1 when the PR is P(NMe₂)₂Et:

0 1			
C	-1.19042600	0.77486300	-0.64724600
C	-2.30121500	-0.11252600	-0.30073000
C	-3.46312300	0.32107500	0.38617200
C	-2.23917000	-1.48196100	-0.66062100
C	-4.48454200	-0.57352700	0.70166900
H	-3.55410800	1.36590800	0.65315900
C	-3.26370100	-2.36966900	-0.33525700
H	-1.38386100	-1.84087300	-1.22187900
C	-4.39774800	-1.92590000	0.35219400
H	-5.36189800	-0.20630300	1.22834700
H	-3.18146000	-3.41211400	-0.63379900
H	-5.20005900	-2.61506600	0.59939500
C	-1.17761100	2.19432700	-0.36219100
O	-0.08371100	0.24820600	-1.17496000
O	-2.13243900	2.90143100	-0.03888700
O	0.08853500	2.74174800	-0.49012000
C	0.13719900	4.16495000	-0.33309400
H	-0.20568200	4.46792800	0.66050600
H	-0.48912500	4.65916500	-1.08120600
H	1.18359500	4.44184800	-0.47725700
P	1.36761500	-0.43783900	0.01393500
N	2.77252600	0.43691700	0.47989100
N	1.98904100	-1.76722700	-0.79994900
C	2.64577900	1.48262400	1.50440500
H	2.06564600	1.12833400	2.35665900
H	3.64881000	1.73601200	1.86416200
H	2.16946100	2.38915200	1.10792100
C	3.65423200	0.86307900	-0.61776900

H	4.65375900	1.05281900	-0.21184800
H	3.73142700	0.07627800	-1.36991600
H	3.28949500	1.77891200	-1.10340400
C	1.40799600	-1.65600200	2.65775200
H	0.79915700	-1.84716300	3.54789400
H	1.75447800	-2.62322400	2.28368700
H	2.28456500	-1.08125500	2.96933400
C	1.46441500	-2.18745200	-2.10399000
H	2.25995500	-2.14499200	-2.86081400
H	1.09513100	-3.22021600	-2.05265800
H	0.65122800	-1.53356300	-2.41494200
C	3.12483600	-2.56267800	-0.32501700
H	3.91956200	-2.58009200	-1.08382100
H	3.53783700	-2.13610300	0.58931100
H	2.81699500	-3.59918400	-0.13096600
C	0.56088600	-0.92213300	1.60700600
H	-0.27880700	-1.54543900	1.28379200
H	0.10277300	-0.01651400	2.02178700

PO(NMe₂)₂Et:

0 1

P	-0.00350700	0.01654000	0.60795400
N	-1.17586400	-0.71144400	-0.39791100
N	1.41774300	-0.24400500	-0.26680200
C	-2.58677300	-0.39911800	-0.14143300
H	-2.73600500	0.67438900	-0.01775500
H	-3.18137000	-0.71900800	-1.00453100
H	-2.97423000	-0.91067900	0.75289300
C	-0.98771600	-2.14330500	-0.67412500
H	-1.55513000	-2.41021300	-1.57322100
H	0.06709200	-2.35774100	-0.85217300
H	-1.33372600	-2.77331000	0.15848700
C	-0.57016700	2.54949400	-0.71547600
H	-0.85020300	3.59394800	-0.54044600
H	0.36945400	2.55217400	-1.27440900
H	-1.33597900	2.10044600	-1.35535500
C	2.67208200	-0.47374800	0.44619900
H	3.19249100	-1.34078200	0.01650400
H	3.34330500	0.39589600	0.37386200
H	2.46266000	-0.67851400	1.49660000
C	1.56023100	-0.01716800	-1.69923300
H	2.07221900	-0.87132300	-2.16496700
H	0.58013800	0.08780400	-2.16626500
H	2.15472400	0.88414000	-1.91426600
C	-0.42924000	1.80852900	0.62106300
H	0.37664300	2.24835100	1.22091000
H	-1.33376700	1.91429600	1.23068800
O	0.13633000	-0.48724200	2.01564300

P(NEt)₃:

0 1

P	0.10379800	0.17323900	-0.35177400
N	-0.47714800	1.46414000	0.68714700
N	-0.85509600	-1.05320500	0.37722100
N	1.69301500	0.22488100	0.32391900
H	1.73670700	0.24868000	1.34162800
H	0.19323800	2.22888400	0.66834700
H	-0.91499800	-1.04828400	1.39346700
C	-1.85255600	1.95509400	0.52047900
H	-2.51391800	1.08293000	0.52872000
H	-2.10201500	2.54444800	1.41236000
C	-2.10719300	2.79538900	-0.73837500

H	-1.90373800	2.21893800	-1.64691900
H	-3.14992800	3.13326900	-0.77410300
H	-1.46641900	3.68544000	-0.75451600
C	-1.05646000	-2.36086800	-0.24393800
H	-0.89840700	-2.23809400	-1.32180500
H	-0.30924500	-3.09423100	0.10002600
C	-2.46131800	-2.91185700	0.01246900
H	-2.64691500	-3.03375000	1.08634600
H	-3.22221400	-2.23323100	-0.38608900
H	-2.58494400	-3.89331200	-0.46000600
C	2.79407200	-0.51877300	-0.29132500
H	2.81832600	-1.56874300	0.04412300
H	2.61272100	-0.54025000	-1.37201400
C	4.14839800	0.13445300	-0.00880600
H	4.35049500	0.17374600	1.06831400
H	4.95840300	-0.43528700	-0.47860400
H	4.17082800	1.15892500	-0.39369900

TS1 when the PR is P(NEt)₃:

0 1

P	-1.03548900	0.45125200	-0.50875000
N	-0.66908300	0.33431200	1.12660200
N	-1.96871800	1.89171400	-0.61192000
N	-2.13620400	-0.64592400	-1.10005200
C	1.47840400	-0.87014000	-0.62755600
C	2.61491200	0.00762000	-0.36461700
C	3.71611600	-0.34483900	0.45734200
C	2.61342100	1.30437800	-0.93759300
C	4.74531200	0.56291000	0.69243200
H	3.74792100	-1.33365900	0.89618100
C	3.64872500	2.20587800	-0.68833900
H	1.80496600	1.58041600	-1.60482900
C	4.72276700	1.84539600	0.12871500
H	5.57832500	0.26481600	1.32404300
H	3.62062700	3.19112000	-1.14721300
H	5.53296700	2.54431300	0.31589300
C	1.31413600	-2.19479400	-0.05564900
O	0.48988000	-0.39780900	-1.38266800
O	2.15034900	-2.84085200	0.57359600
O	0.06574000	-2.73395900	-0.32289300
C	-0.12171400	-4.07245400	0.15460400
H	0.57907300	-4.75884600	-0.32866700
H	-1.14866900	-4.33620600	-0.10485100
H	0.02473600	-4.12954500	1.23681500
H	-1.67835400	-1.49708700	-1.41312700
H	-2.33064400	2.01782100	-1.55548600
H	0.31497100	0.10375800	1.25077000
C	-1.46079000	3.15807000	-0.05217700
H	-1.09263300	2.94255700	0.95313000
H	-0.60855400	3.53823700	-0.63379900
C	-2.57053500	4.20673000	-0.00500500
H	-2.18451200	5.14339300	0.41066900
H	-2.95841700	4.42494400	-1.00721200
H	-3.40506800	3.86903800	0.61721900
C	-1.54005300	-0.27508000	2.15397400
H	-0.88566100	-0.76226500	2.88411900
H	-2.15032900	-1.06781500	1.70341900
C	-2.43413700	0.74746000	2.85598000
H	-3.05503800	0.25229200	3.61131400
H	-1.83199900	1.51341000	3.35483000
H	-3.09904500	1.24648400	2.14379000
C	-3.60378200	-0.63135500	-1.11914400
H	-3.95729800	-0.45357100	-2.14482800
H	-3.94484400	0.21276400	-0.51456300
C	-4.20367000	-1.93925800	-0.60039600
H	-5.29662800	-1.90552000	-0.66603600

H	-3.86169300	-2.79364000	-1.19538200
H	-3.92625700	-2.11887300	0.44294600

PO(NEt)₃:

O 1			
P	0.05390800	-0.18455900	0.75815700
N	1.47953400	-0.72323700	0.03329300
N	-0.88434200	-1.58290700	0.64072500
N	-0.36820600	1.03453500	-0.32440200
O	0.02660600	0.31441500	2.16782800
H	-1.47602600	-1.70901200	1.45430500
H	-0.29599400	0.80366200	-1.30920300
H	1.70187900	-1.66707900	0.33689900
C	2.67107900	0.13870000	-0.06337200
H	3.15580500	0.25278900	0.91652300
H	2.33347600	1.13212000	-0.37054800
C	3.66699600	-0.41821000	-1.07935500
H	3.21397200	-0.48883400	-2.07361300
H	4.54916500	0.22791900	-1.14312100
H	4.00985600	-1.41942600	-0.79182800
C	-1.37071400	-2.20115000	-0.59479700
H	-0.63995100	-1.98831400	-1.38194400
H	-1.36837400	-3.29100600	-0.46232800
C	-2.76790700	-1.74102600	-1.02684800
H	-3.50966100	-1.96411100	-0.25137200
H	-2.79018400	-0.66227100	-1.21194500
H	-3.07770400	-2.25534800	-1.94417000
C	-1.37057700	2.05470900	0.00320900
H	-1.31910600	2.21410000	1.08333400
H	-2.38941100	1.70417700	-0.22633200
C	-1.09769000	3.36269100	-0.73919300
H	-1.85749900	4.11029200	-0.48633000
H	-0.11435300	3.76184500	-0.47203400
H	-1.12339300	3.21854200	-1.82644200

P(NMe₂)Et₂:

O 1			
P	0.10919800	0.19032900	-0.86057200
N	-1.20437200	-0.40481000	0.09963700
C	-0.19980200	2.78794800	0.23489900
H	-1.16101500	2.50863600	0.67808700
H	0.22140900	3.60646300	0.82970500
H	-0.39838100	3.17008300	-0.77221600
C	-2.29531200	-1.06174700	-0.61312100
H	-2.16789600	-2.15705000	-0.67302300
H	-3.24873100	-0.86706500	-0.10239900
H	-2.36399200	-0.66885900	-1.63043500
C	-1.10365700	-0.83161000	1.48906400
H	-2.06063900	-0.65700100	2.00018900
H	-0.86637300	-1.90490400	1.58997800
H	-0.33729200	-0.26165900	2.01836600
C	2.25616400	-1.30013500	0.60428900
H	3.07982700	-2.01056000	0.46276700
H	2.68784200	-0.38447400	1.02125600
H	1.58520700	-1.72520300	1.35569300
C	1.53816400	-1.04005000	-0.72892600
H	2.26491100	-0.68598400	-1.47415200
H	1.14368700	-1.98058700	-1.13536300
C	0.75646400	1.58889900	0.19520600
H	1.71246600	1.88221400	-0.25919100
H	0.98947800	1.25484100	1.21338400

TS1 when the PR is P(NMe₂)Et₂:

0 1			
C	-0.88904600	0.76886700	-0.73270300
C	-2.07078300	-0.05984100	-0.52993400
C	-3.23584100	0.36610200	0.15976200
C	-2.05199400	-1.39368300	-1.01245100
C	-4.30227600	-0.50592300	0.36220400
H	-3.28520700	1.38402200	0.52397800
C	-3.12660900	-2.25902400	-0.79861000
H	-1.19943500	-1.72737200	-1.59295500
C	-4.25996200	-1.82621100	-0.10651800
H	-5.18173500	-0.14960200	0.89287900
H	-3.08201400	-3.27258100	-1.19017600
H	-5.09985500	-2.49631900	0.05327800
C	-0.74535600	2.11442700	-0.21535800
O	0.16463100	0.20465000	-1.32163800
O	-1.63070200	2.82215400	0.26609400
O	0.54528100	2.60620000	-0.34486300
C	0.69646600	3.98408700	0.01602800
H	1.75020300	4.21825200	-0.14913200
H	0.42713800	4.15380200	1.06263500
H	0.06719500	4.62189000	-0.61114200
P	1.44698700	-0.68151400	-0.12634700
N	1.08698100	-0.33359900	1.47907700
C	3.35290300	-0.01706500	-2.05267300
H	2.52643200	0.17829300	-2.74118400
H	4.18716900	0.63231100	-2.33498800
H	3.68239500	-1.05225100	-2.18798400
C	0.03485900	-1.09022500	2.16800800
H	0.45248100	-1.63245200	3.02734200
H	-0.74855500	-0.41139400	2.52337000
H	-0.44117900	-1.80335100	1.49250300
C	1.59369900	0.80349500	2.24697900
H	0.78390000	1.50495400	2.48132400
H	2.03243200	0.44580800	3.18881500
H	2.36099600	1.34486400	1.69638500
C	3.22150300	-2.86737300	0.58394900
H	3.39207800	-3.94847000	0.51947800
H	4.10988700	-2.37021900	0.18325500
H	3.13237400	-2.60444100	1.64222100
C	1.95201200	-2.48727100	-0.19275600
H	2.04764500	-2.72632200	-1.25827300
H	1.08786000	-3.05396200	0.16750200
C	2.93784200	0.27852100	-0.60034600
H	3.75987900	0.07720900	0.09577300
H	2.64605100	1.32790900	-0.51347000

PO(NMe₂)Et₂:

0 1			
P	-0.07359900	-0.27688200	0.54683000
N	-0.10971200	1.23612300	-0.22788500
C	-2.46452000	-1.08154800	-0.70468800
H	-2.60881400	-0.10524800	-1.17738600
H	-2.97917900	-1.83313400	-1.31228500
H	-2.93908500	-1.04976800	0.27979300
C	-0.09590800	2.44423600	0.59537100
H	0.90070000	2.91321600	0.62148700
H	-0.80543600	3.17600600	0.18706500
H	-0.40198900	2.19434200	1.61219100
C	0.21503600	1.46209600	-1.62894300
H	-0.49989300	2.17169600	-2.06768500
H	1.22486100	1.88206900	-1.76101900
H	0.15693300	0.53549600	-2.20326200
C	2.45343400	-1.07312700	-0.66271400
H	3.44867800	-1.47890500	-0.45231300
H	1.96491400	-1.76029600	-1.36180300
H	2.59320300	-0.11577500	-1.17331200

C	1.65740800	-0.91548300	0.64068800
H	1.58251800	-1.87510300	1.16742000
H	2.17006800	-0.23251800	1.32890000
C	-0.97373000	-1.42383800	-0.57561900
H	-0.84638500	-2.41547500	-0.12339200
H	-0.49040900	-1.46566300	-1.55818900
O	-0.66863000	-0.18932300	1.92524600

P(Et)₃:

0 1			
P	0.06129500	-0.39333000	-0.91075000
C	2.56992800	-0.76485400	0.37331100
H	2.83170100	0.29341100	0.26187300
H	3.13209800	-1.15273400	1.23051100
H	2.92026800	-1.28623500	-0.52378300
C	0.15891200	2.16122700	0.62781100
H	0.16653300	3.25228800	0.51568900
H	-0.68293000	1.90265100	1.27510400
H	1.07777000	1.88502000	1.15491500
C	1.05920100	-0.95842300	0.57302300
H	0.83993000	-2.02738700	0.69141200
H	0.73231100	-0.46590000	1.49605200
C	-1.68180600	-0.88933200	-0.41138200
H	-1.68094600	-1.98537700	-0.48277100
H	-2.32550700	-0.54901800	-1.23291000
C	0.07121500	1.48772900	-0.74984100
H	0.91279100	1.82442500	-1.36741900
H	-0.82834400	1.82602100	-1.28142400
C	-2.28659500	-0.46147200	0.93379500
H	-2.43348900	0.62116700	0.98727100
H	-3.26826300	-0.92965800	1.07654200
H	-1.65847700	-0.75796600	1.77987900

TS1 when the PR is P(Et)₃:

0 1			
P	1.57904000	-0.56142200	0.01852200
C	0.29208600	-1.59180300	2.35529900
H	0.94528100	-2.46323300	2.46302000
H	-0.08428400	-1.33570900	3.35031400
H	-0.56789700	-1.87401600	1.74124000
C	3.39614800	-2.78547300	0.40019500
H	3.59958100	-3.83045600	0.13917500
H	4.26858000	-2.19674600	0.10265900
H	3.30304800	-2.72808600	1.48899300
C	-0.82609000	0.83656100	-0.57984000
C	-1.97441000	-0.05591000	-0.48667500
C	-3.20242600	0.29727100	0.13056800
C	-1.86320400	-1.36837300	-1.01100000
C	-4.24191300	-0.62346700	0.22515200
H	-3.32181100	1.29934400	0.52193700
C	-2.91178500	-2.28421400	-0.90454000
H	-0.95913600	-1.64660600	-1.54077500
C	-4.10919400	-1.92296300	-0.28339400
H	-5.17160500	-0.32263800	0.70161300
H	-2.79543800	-3.28028700	-1.32496200
H	-4.92883100	-2.63178600	-0.20829900
C	-0.78467000	2.17296700	-0.02191000
O	0.29697300	0.34963800	-1.11881000
O	-1.74367500	2.85149500	0.34396900
O	0.50314000	2.68286400	0.04627900
C	0.58368900	4.04200700	0.49370800
H	0.03587800	4.70624900	-0.18037700
H	1.64656900	4.29151700	0.48676500
H	0.17260200	4.15197700	1.50136000
C	2.11585800	-2.30997800	-0.30966600
H	2.22886900	-2.39023900	-1.39713600

H	1.26268400	-2.94246300	-0.04533000
C	3.04415500	0.51991200	-0.22024900
H	3.84905100	0.20113400	0.45375400
H	2.70723200	1.51136800	0.09648500
C	1.03071700	-0.38370200	1.76193500
H	1.89499400	-0.09698400	2.37305800
H	0.35889200	0.48640300	1.74220000
C	3.52667400	0.56904000	-1.67867900
H	4.35670600	1.27633900	-1.77228200
H	3.88504400	-0.40588700	-2.02609700
H	2.72307200	0.89891700	-2.34206600

PO(Et)₃:

0 1			
P	0.06780900	-0.45275600	-0.45410400
C	2.50019900	-0.18824300	0.95231900
H	2.68834300	0.82310600	0.57560500
H	3.02926200	-0.28933600	1.90558500
H	2.93314400	-0.89600400	0.24028900
C	-0.13242300	2.43425100	-0.01612200
H	-0.15708900	3.40316700	-0.52620200
H	-1.04632400	2.35510500	0.57883200
H	0.71492100	2.45243400	0.67621200
C	0.99886000	-0.45760100	1.13793600
H	0.84810900	-1.45659500	1.56575200
H	0.55035500	0.26036200	1.83479600
C	-1.64780400	-0.98754200	-0.02899900
H	-1.53371400	-2.03652400	0.27140900
H	-2.18422000	-1.00847000	-0.98539100
C	0.00096700	1.30044200	-1.04437900
H	0.92535500	1.41709100	-1.62182500
H	-0.81461700	1.33834900	-1.77736900
C	-2.44671200	-0.20905100	1.02632300
H	-2.66718500	0.81227700	0.70258500
H	-3.40601600	-0.70381400	1.21173700
H	-1.91951600	-0.15315000	1.98429300
O	0.67294200	-1.36002400	-1.49840100

P(Me)₃:

0 1			
P	0.00033800	-0.00021500	-0.60368500
C	1.63521200	-0.17419700	0.28013900
H	2.11366100	-1.11305600	-0.01676500
H	2.29993900	0.64382400	-0.01568300
H	1.52693900	-0.16338400	1.37176300
C	-0.66679000	1.50287100	0.27971200
H	-0.09203200	2.38665500	-0.01534700
H	-1.70707800	1.67034800	-0.01743700
H	-0.62388800	1.40246100	1.37132400
C	-0.96884300	-1.32837200	0.27991400
H	-2.02087400	-1.27295000	-0.01786800
H	-0.59301000	-2.31344700	-0.01483900
H	-0.90619200	-1.23903800	1.37153800

TS1 when the PR is P(Me)₃:

0 1			
P	-1.59914300	-1.47621700	0.10214800
C	-1.44166000	-0.74698500	1.76159200
H	-0.59543100	-0.04406300	1.72568400
H	-2.33464800	-0.18140800	2.03747300
H	-1.23521800	-1.51824300	2.50636300
C	-3.27410900	-1.19888000	-0.55714700
H	-3.44391400	-0.12100700	-0.59248200
H	-3.32042400	-1.58973700	-1.57822700

H	-4.03942800	-1.69094700	0.05189400
C	-1.43424600	-3.31271200	0.26837900
H	-1.40341900	-3.75985200	-0.72915900
H	-0.49897600	-3.54587900	0.78239300
H	-2.27740400	-3.74411200	0.82385500
C	0.18408600	0.60085800	-0.55935000
C	1.57394600	0.23543600	-0.31780200
C	2.53359800	1.11458100	0.24664600
C	1.99783500	-1.07972400	-0.63244800
C	3.83501500	0.68450000	0.48871400
H	2.23994500	2.12952200	0.48187000
C	3.30423100	-1.50031200	-0.37718300
H	1.30040000	-1.75583800	-1.11369600
C	4.23422200	-0.62458900	0.18669900
H	4.54972600	1.38142300	0.91902500
H	3.59887500	-2.51434200	-0.63639600
H	5.25352800	-0.94842200	0.37638400
C	-0.41310700	1.86441200	-0.17848100
O	-0.62464600	-0.33488900	-1.07411600
O	0.17669300	2.89643300	0.13664400
O	-1.79903400	1.83095000	-0.22404500
C	-2.43476300	3.08467200	0.05849400
H	-2.13608300	3.84407400	-0.66918700
H	-2.17754000	3.44064000	1.06007000
H	-3.50723900	2.89395500	-0.01462800

PO(Me)₃:

O 1			
P	-0.00014500	0.00013300	0.18198800
C	-1.65656900	-0.26958200	-0.55708900
H	-2.04788500	-1.23032500	-0.21037000
H	-2.33168900	0.51917900	-0.21298800
H	-1.62372400	-0.26585400	-1.65121300
C	0.59576100	1.56891200	-0.55716400
H	-0.04178100	2.38835800	-0.21305500
H	1.61543200	1.75985300	-0.21049200
H	0.58553100	1.53750200	-1.65128200
C	1.06188400	-1.30073500	-0.55498800
H	2.08996600	-1.15736600	-0.21022400
H	0.71790100	-2.27927600	-0.20788100
H	1.04071000	-1.27719300	-1.64917900
O	-0.00109200	0.00144400	1.68778800

PPh₃:

O 1			
P	-0.00035300	-0.00073400	-1.20810700
C	0.28042700	1.64661100	-0.40227100
C	-0.32399600	2.76228200	-1.00856100
C	1.07874400	1.85227500	0.73392300
C	-0.15655800	4.04389800	-0.48060600
H	-0.92811600	2.62553500	-1.90230300
C	1.25861500	3.13743100	1.25511400
H	1.56597200	1.00884700	1.21290000
C	0.63880300	4.23535300	0.65332300
H	-0.63610900	4.89225700	-0.96091400
H	1.88273300	3.27806200	2.13346700
H	0.77967800	5.23287700	1.05969800
C	1.28673100	-1.06778400	-0.40314900
C	1.06592900	-1.86541500	0.73073800
C	2.55600400	-1.09833600	-1.00792200
C	2.09024900	-2.66244400	1.25156400
H	0.09149200	-1.86971100	1.20889400
C	3.58326400	-1.88309400	-0.48049300
H	2.73960500	-0.50460800	-1.90025900
C	3.35180400	-2.67047600	0.65157900
H	1.90018800	-3.27544000	2.12845000

H	4.55833800	-1.88880500	-0.95964100
H	4.14615800	-3.29015400	1.05784000
C	-1.56796000	-0.58063200	-0.40214600
C	-2.23837400	-1.65480900	-1.01390100
C	-2.13932500	0.00229300	0.74021400
C	-3.43230300	-2.14955800	-0.48541800
H	-1.82285100	-2.10465800	-1.91244200
C	-3.34208900	-0.48385600	1.26227400
H	-1.64866700	0.84126000	1.22370300
C	-3.98929300	-1.56272600	0.65490200
H	-3.93247200	-2.98340800	-0.97007500
H	-3.77110600	-0.01823800	2.14541000
H	-4.92358800	-1.93888000	1.06191400

TS1 when the PR is PPh₃:

0 1

C	1.45597600	-0.93362800	-1.14492800
C	2.66847100	-0.12846600	-1.05320100
C	3.95759800	-0.67307300	-0.81624100
C	2.57352700	1.27875900	-1.19116600
C	5.07352200	0.15434700	-0.71843700
H	4.06354700	-1.74534000	-0.71936400
C	3.69753600	2.09695000	-1.08279100
H	1.61081600	1.72568000	-1.40577800
C	4.95871300	1.54449600	-0.84460900
H	6.04770200	-0.29408800	-0.54039500
H	3.58524000	3.17243100	-1.19450500
H	5.83543100	2.18101100	-0.76616200
C	1.41926900	-2.37443800	-0.96571900
O	0.29221300	-0.31125700	-1.36082100
O	2.38302600	-3.13228300	-0.86905800
O	0.13104600	-2.87103800	-0.94658200
C	0.03818000	-4.29000700	-0.76914000
H	0.49435500	-4.59630000	0.17629200
H	0.53678600	-4.81787000	-1.58665800
H	-1.02979200	-4.51560100	-0.76534300
P	-0.83632300	0.34502000	0.04213900
C	-0.75206400	2.12431300	0.34092200
C	-0.99374100	2.99229200	-0.74573000
C	-0.37578600	2.67324600	1.58241200
C	-0.87204400	4.37133800	-0.58577800
H	-1.27305800	2.58758600	-1.71431500
C	-0.25214800	4.05423300	1.73043300
H	-0.18765200	2.02371300	2.43047000
C	-0.49855800	4.90857800	0.65075800
H	-1.06312900	5.02666600	-1.43051000
H	0.03250500	4.46378700	2.69526400
H	-0.40024100	5.98314400	0.77134400
C	-0.49656000	-0.57528400	1.54380500
C	-1.45519900	-1.41104400	2.14925200
C	0.82228900	-0.55661800	2.04199300
C	-1.10806800	-2.18147700	3.25592600
H	-2.46649200	-1.45064700	1.75756500
C	1.15874200	-1.33477400	3.15307300
H	1.58051500	0.06138300	1.57134100
C	0.19835200	-2.14388800	3.76134200
H	-1.85662400	-2.81149000	3.72750000
H	2.17662800	-1.31444400	3.53006300
H	0.46466900	-2.75052000	4.62186800
C	-2.47506000	-0.03454500	-0.62347300
C	-2.63236300	-1.18193500	-1.42211400
C	-3.58492500	0.79003200	-0.36097600
C	-3.89047500	-1.49767700	-1.94054600
H	-1.77189300	-1.80913200	-1.62765800
C	-4.83622100	0.46509300	-0.88431400
H	-3.47206300	1.68013300	0.24929700
C	-4.99080400	-0.67892500	-1.67457000

H	-4.00678300	-2.38238300	-2.55963800
H	-5.68899200	1.10409700	-0.67471900
H	-5.96587700	-0.92787000	-2.08344200

POPh₃:

O 1			
P	0.00096100	-0.00053400	0.91797300
C	-0.48660800	1.62248800	0.21901200
C	-0.18150900	2.76004100	0.98448400
C	-1.14225400	1.77581000	-1.01202000
C	-0.51026000	4.03200800	0.51330700
H	0.30021000	2.63739500	1.94986900
C	-1.47439500	3.05072700	-1.47838300
H	-1.40748200	0.90461000	-1.60412800
C	-1.15792800	4.17850500	-0.71773000
H	-0.27075100	4.90750000	1.10993100
H	-1.98653800	3.16096000	-2.42998700
H	-1.41885800	5.16878500	-1.08017600
C	-1.16392600	-1.23507800	0.22090200
C	-0.97252400	-1.87169600	-1.01477800
C	-2.30030200	-1.54184100	0.98728200
C	-1.91067800	-2.79538900	-1.48274700
H	-0.08538700	-1.66254200	-1.60465800
C	-3.23865800	-2.46088300	0.51386400
H	-2.43130900	-1.06975000	1.95666500
C	-3.04675200	-3.08482000	-0.72257200
H	-1.75521500	-3.28440900	-2.44010400
H	-4.11374400	-2.69608200	1.11286700
H	-3.77578000	-3.80198700	-1.08905600
C	1.65134700	-0.39285700	0.21702600
C	2.48437300	-1.22656600	0.98037200
C	2.11136500	0.10362800	-1.01186300
C	3.75063600	-1.57597200	0.50923500
H	2.14069700	-1.57931500	1.94824100
C	3.38041200	-0.24902400	-1.48126300
H	1.49024600	0.77351400	-1.60020200
C	4.19923300	-1.09024300	-0.72269300
H	4.39024400	-2.21973600	1.10632500
H	3.73175800	0.14362600	-2.43098400
H	5.18717800	-1.35996500	-1.08490500
O	0.00511000	-0.00095400	2.42526100

Solvent Phase

α -keto ester:

O 1			
C	-0.50722100	0.89419500	0.12668200
C	0.84490500	0.30016000	0.04008800
C	1.04222800	-1.09148700	-0.01253300
C	1.95477100	1.16385200	-0.02478700
C	2.33257100	-1.60931400	-0.12860200
H	0.19702900	-1.76882400	0.04240700
C	3.24007100	0.64225400	-0.13604500
H	1.79050000	2.23544000	0.01266500
C	3.43025300	-0.74532400	-0.18873600
H	2.48102300	-2.68364700	-0.16942400
H	4.09414700	1.31054300	-0.18322200
H	4.43371600	-1.15091800	-0.27667500
C	-1.71719500	-0.03991500	0.31009800
O	-0.72873300	2.09890900	0.11340200
O	-1.85289600	-0.75309700	1.28685400
O	-2.59609900	0.09636600	-0.67964100
C	-3.82390500	-0.67132700	-0.57175600
H	-4.37367200	-0.36524800	0.31982300
H	-3.59425800	-1.73712900	-0.52356500
H	-4.38553700	-0.43619900	-1.47339200

Phenyl carbamic acid:

0 1

C	-2.18585700	0.10493700	-0.00007300
O	-3.30457800	-0.67178700	-0.00004300
O	-2.22550700	1.32821300	-0.00021700
N	-1.07715700	-0.68523900	0.00006700
H	-1.25845800	-1.68069800	0.00014700
C	0.28163600	-0.29764500	0.00005000
C	0.70516500	1.04037200	-0.00003300
C	1.23708800	-1.32829500	0.00013400
C	2.07384200	1.32680900	-0.00003500
H	-0.02462100	1.83778500	-0.00009600
C	2.59797100	-1.02586100	0.00013300
H	0.91201000	-2.36550300	0.00020100
C	3.02709600	0.30567500	0.00004800
H	2.39089700	2.36573000	-0.00010000
H	3.32204800	-1.83518500	0.00019900
H	4.08670200	0.54147600	0.00004700
H	-4.06944000	-0.07428600	-0.00014000

P(NMe₂)₃:

0 1

P	0.00000300	-0.02803200	-0.73447100
N	-0.00006000	1.54051700	0.07836800
N	-1.42709500	-0.66674000	-0.00462900
N	1.42715900	-0.66662000	-0.00463200
C	-1.20374800	2.34459900	-0.16621900
H	-2.10214300	1.76505500	0.04866800
H	-1.18757700	3.21833200	0.49540000
H	-1.26869500	2.71205000	-1.20629700
C	1.20355800	2.34470300	-0.16622700
H	1.18731400	3.21843600	0.49539100
H	2.10200500	1.76523800	0.04865600
H	1.26846700	2.71215800	-1.20630600
C	-2.12067900	-1.73399700	-0.71945700
H	-1.84821300	-2.73507100	-0.34674300
H	-3.20769700	-1.62106300	-0.60700100
H	-1.88133300	-1.69001600	-1.78571800
C	-1.71124300	-0.65046900	1.42760600
H	-2.79102200	-0.53099500	1.59263500
H	-1.39810500	-1.58363500	1.92251400
H	-1.19838600	0.18789700	1.90164100
C	2.12080900	-1.73383900	-0.71945400
H	3.20781900	-1.62084200	-0.60698600
H	1.84839900	-2.73493100	-0.34674500
H	1.88147200	-1.68986900	-1.78571700
C	1.71129600	-0.65033700	1.42760600
H	2.79106600	-0.53079600	1.59264100
H	1.19838400	0.18799600	1.90164000
H	1.39821200	-1.58352300	1.92250900

Product:

0 1

C	-1.78199300	0.61792100	-0.83804600
C	-2.51392900	-0.58367400	-0.27543100
C	-2.34717100	-1.03378200	1.04392500
C	-3.37061000	-1.29088100	-1.13160600
C	-3.02416800	-2.17100300	1.48900800
H	-1.69107300	-0.49578400	1.71684300
C	-4.04823800	-2.42938600	-0.68612600
H	-3.51143300	-0.94927500	-2.15392200
C	-3.87477600	-2.87243500	0.62734100
H	-2.88902300	-2.50827000	2.51252600
H	-4.70905400	-2.96364700	-1.36225100
H	-4.40039600	-3.75528100	0.97941500

C	-1.83230300	1.89142100	0.02062000
O	-2.62483000	2.07492300	0.92312500
O	-0.98411000	2.81778900	-0.44170900
C	-0.98043300	4.08928800	0.24864800
H	-1.96875700	4.54971600	0.19468200
H	-0.24303900	4.69657400	-0.27323000
C	0.54897700	0.21473500	-0.33912800
O	0.39005300	0.48023100	0.84367700
O	-0.43620200	0.29401600	-1.27849600
N	1.70158000	-0.18971400	-0.94278100
H	1.62240000	-0.37766300	-1.93389000
C	2.97514000	-0.39152000	-0.36581100
C	3.26586000	-0.13577800	0.98344800
C	3.98755700	-0.87051300	-1.21493000
C	4.55985800	-0.36393500	1.46175100
H	2.49229400	0.23303200	1.64223100
C	5.27265300	-1.09204200	-0.72268600
H	3.76533500	-1.06940600	-2.26010700
C	5.56887900	-0.84045200	0.62133400
H	4.77398200	-0.16298200	2.50752600
H	6.04194800	-1.46288000	-1.39347100
H	6.56938500	-1.01331700	1.00533600
H	-2.26192300	0.89724100	-1.78099600
H	-0.69280900	3.94649400	1.29213300

In 1B:

O 1			
P	1.27088900	-0.56703000	-0.01039100
N	1.33582900	0.04976500	1.51686300
N	1.02106000	-2.19410100	0.16357300
N	2.64146500	-0.29814600	-0.88563300
C	0.22402100	-0.11708800	2.46926100
H	-0.48559100	-0.86363200	2.11212900
H	0.62365000	-0.44151300	3.43701900
H	-0.30924300	0.82986500	2.59929900
C	2.29547900	1.09343700	1.89973700
H	2.70475100	0.85047500	2.88604700
H	3.11729100	1.14381900	1.18594000
H	1.80726900	2.07270300	1.94393800
C	0.76550200	-3.00942100	-1.03320500
H	1.64757900	-3.61408700	-1.27835400
H	-0.08028300	-3.67997000	-0.84989200
H	0.52867500	-2.37826400	-1.89027400
C	1.36818900	-2.98158000	1.35321200
H	0.49487400	-3.55261700	1.68746400
H	2.17479800	-3.68641100	1.11559700
H	1.70006100	-2.33503600	2.16340700
C	2.84828800	0.84593800	-1.78629900
H	3.63183300	1.50495100	-1.39201400
H	3.16597700	0.47276400	-2.76635800
H	1.92842500	1.41524500	-1.88889500
C	3.84502400	-1.10882800	-0.65963100
H	4.61624900	-0.52777800	-0.13913300
H	3.61731100	-1.99388000	-0.06530300
H	4.24575100	-1.43480100	-1.62534600
C	-1.00144900	0.80522300	-0.41236800
C	-2.25516600	0.09867100	-0.31651400
C	-3.42821800	0.69720900	0.23083500
C	-2.39114200	-1.23993900	-0.77545600
C	-4.63041500	-0.00352700	0.30984700
H	-3.37139900	1.71832200	0.58419800
C	-3.60077000	-1.92935800	-0.68920600
H	-1.53859300	-1.73543500	-1.21894700
C	-4.73937000	-1.32512000	-0.14430900
H	-5.49844900	0.49437500	0.73666100

H	-3.65183800	-2.95091200	-1.05962000
H	-5.68042800	-1.86323800	-0.07844400
C	-0.78608000	2.17848800	-0.21644300
O	0.11877300	0.04505600	-0.94321600
O	-1.62185500	3.02566800	0.17386400
O	0.52098400	2.58507500	-0.49410400
C	0.78616400	3.98116800	-0.33130700
H	0.15886500	4.58515800	-0.99344700
H	1.83706700	4.11212700	-0.59602300
H	0.62003600	4.30257100	0.70132100

In 2:

0 1

P	-2.01011300	-1.52714000	-0.13145200
N	-1.33057100	-1.49583200	-1.62265800
N	-1.47844800	-2.79198800	0.77433600
N	-3.64638800	-1.53085400	-0.33489600
C	-0.20673000	-2.36222500	-2.01556000
H	-0.07771300	-3.17204800	-1.29922100
H	-0.43043400	-2.79797000	-2.99508000
H	0.71371800	-1.77598900	-2.07123400
C	-1.65748900	-0.45707200	-2.61679700
H	-1.95042500	-0.93881000	-3.55624800
H	-2.48637400	0.16238000	-2.27208200
H	-0.77939900	0.17334800	-2.78254200
C	-0.17265200	-2.77631000	1.45836700
H	-0.32326700	-2.87813800	2.53868000
H	0.43646500	-3.61664900	1.10586700
H	0.36768400	-1.85220800	1.25254400
C	-2.17332600	-4.08456200	0.79904400
H	-1.62233000	-4.84003100	0.22579100
H	-2.25728500	-4.42383300	1.83675700
H	-3.17796800	-3.99482700	0.38548600
C	-4.54851900	-1.17166000	0.77031200
H	-5.30819800	-0.47345300	0.40437600
H	-5.04863100	-2.06468100	1.16411100
H	-3.99487600	-0.69092800	1.57528500
C	-4.31794100	-2.17078500	-1.47507600
H	-5.02592100	-1.46470100	-1.92187900
H	-3.59294100	-2.46944300	-2.23106400
H	-4.87057000	-3.05903700	-1.14570300
C	-0.97050000	0.95974400	0.45522500
C	-1.92784900	2.06592700	0.04712600
C	-1.64308900	2.83571500	-1.08714800
C	-3.06790700	2.35852900	0.80968300
C	-2.49245400	3.88190100	-1.46117600
H	-0.75488100	2.61418900	-1.67124800
C	-3.91873200	3.39968400	0.43285900
H	-3.29185900	1.77393000	1.69712700
C	-3.63270100	4.16425100	-0.70422100
H	-2.26306700	4.47233300	-2.34342000
H	-4.80056100	3.61741100	1.02836000
H	-4.29417000	4.97489500	-0.99556200
C	-0.12450300	1.39200300	1.65766300
O	-1.68353000	-0.26073000	0.79975200
O	0.52664500	2.42004100	1.62863500
O	-0.17461700	0.56032600	2.69942400
C	0.64129600	0.92177500	3.83970500
H	0.32876800	1.89071600	4.23370800
H	1.69271900	0.96046900	3.54949700
C	2.22949100	0.28528200	-0.94803200
O	1.36335700	0.79739500	-1.72357400
O	2.01340900	-0.44578200	0.05483000

N	3.57137100	0.60296500	-1.29747200
H	3.63096100	1.21155500	-2.10218900
C	4.78613700	0.25485200	-0.70652600
C	4.90597100	-0.60069300	0.40819700
C	5.96701300	0.78970100	-1.26899600
C	6.16849600	-0.89799200	0.92928500
H	4.00724800	-1.01388300	0.84496100
C	7.21841200	0.48289000	-0.73813500
H	5.89360800	1.45140200	-2.12914100
C	7.33428600	-0.36588100	0.36957900
H	6.23564600	-1.55935200	1.78969500
H	8.10710200	0.91161300	-1.19386800
H	8.30882100	-0.60465000	0.78468200
H	-0.24644900	0.75809900	-0.34742800
H	0.47216100	0.13492200	4.57279900

TS1:

0 1

P	1.33389000	-0.54609200	-0.11439200
N	0.91178700	-0.25541300	1.48470400
N	1.47047100	-2.22993800	-0.18009000
N	2.77745600	0.29953800	-0.33638100
C	-0.09810700	-1.06313900	2.17804400
H	-0.42339800	-1.89428500	1.55325500
H	0.32200600	-1.46425400	3.10921400
H	-0.97275600	-0.45035600	2.42382100
C	1.31831500	0.94137500	2.22623300
H	1.81669500	0.64482000	3.15837100
H	2.00431600	1.54073900	1.63076000
H	0.44258300	1.55022800	2.47986100
C	1.31292000	-2.87420900	-1.48825400
H	2.28507200	-3.13693200	-1.92785500
H	0.72295200	-3.79212700	-1.37972300
H	0.78911500	-2.20913500	-2.17808800
C	2.16280500	-3.06024200	0.81403800
H	1.58885600	-3.97903000	0.98546500
H	3.16828500	-3.33865700	0.46955800
H	2.25173400	-2.52799400	1.76142700
C	2.98641200	1.05963000	-1.57603100
H	3.60421500	1.93707800	-1.35265200
H	3.50370800	0.46027400	-2.33883500
H	2.02768500	1.39965100	-1.96456300
C	4.01796900	-0.14832700	0.30936800
H	4.66203400	0.72119100	0.48532800
H	3.80420400	-0.61094900	1.27464300
H	4.56922800	-0.86629000	-0.31372900
C	-1.10697600	0.87819700	-0.72037400
C	-2.28582900	0.05072200	-0.44198400
C	-3.40873900	0.48398800	0.30799300
C	-2.32013500	-1.27401200	-0.94470000
C	-4.49132900	-0.36604700	0.53853000
H	-3.42122600	1.49199800	0.70037900
C	-3.40386800	-2.11843200	-0.70523700
H	-1.48690500	-1.62857300	-1.53955500
C	-4.50248000	-1.67399800	0.03938300
H	-5.33590700	-0.00047100	1.11750700
H	-3.39292800	-3.12766700	-1.10941800
H	-5.34923700	-2.32933000	0.22212000
C	-0.96872800	2.25304000	-0.27191900
O	-0.08681100	0.33458500	-1.36215800
O	-1.84494000	2.95869400	0.24721900
O	0.28356300	2.75808700	-0.51056300
C	0.48914000	4.12636400	-0.13119400

H	-0.17768600	4.79002300	-0.68852000
H	1.52839700	4.34423800	-0.37949700
H	0.31987700	4.26749400	0.93961000

TS2 si face:

0 1

P	2.43088800	-1.04459600	-0.51224800
N	3.73766300	-0.46442800	0.30755900
N	2.18320300	-2.65806900	-0.28592700
N	2.70039800	-0.72750000	-2.11303900
C	4.39517700	-1.21310900	1.38606300
H	4.01503300	-2.23244400	1.43697700
H	5.47300700	-1.24814100	1.19301800
H	4.22168600	-0.72644800	2.35130400
C	4.19456500	0.92921300	0.17741300
H	5.26736100	0.94297900	-0.04562700
H	3.66185300	1.43927200	-0.62500300
H	4.02015500	1.47461700	1.11111000
C	1.27038700	-3.24387700	0.70636500
H	0.61438100	-3.96122400	0.20136300
H	1.83632900	-3.77147100	1.48385600
H	0.67130500	-2.46677700	1.17166000
C	3.01787200	-3.64175600	-0.98928100
H	3.70930800	-4.13485800	-0.29521100
H	2.37382100	-4.40336000	-1.44135500
H	3.59982900	-3.16912300	-1.78095600
C	1.61979700	-0.97004000	-3.08109900
H	1.55248900	-0.12556900	-3.77449300
H	1.81922700	-1.88264400	-3.65624200
H	0.66133800	-1.07993800	-2.57303800
C	4.02353400	-0.56150600	-2.72714500
H	4.06042800	0.38342700	-3.28040800
H	4.80599600	-0.55997600	-1.97021800
H	4.21874500	-1.38315000	-3.42733000
C	0.80823200	0.79169700	0.71739100
C	0.87388200	2.06857900	-0.02172300
C	1.05826600	3.31783000	0.61866600
C	0.67660800	2.08958200	-1.42134000
C	1.06928900	4.50772000	-0.11241300
H	1.19159900	3.34318100	1.69174500
C	0.69079500	3.28271200	-2.14497000
H	0.49578700	1.16092300	-1.94527100
C	0.89079500	4.50703500	-1.49964000
H	1.22087900	5.44646000	0.41476700
H	0.53524200	3.25155300	-3.22039500
H	0.89961100	5.43632500	-2.06165000
C	1.12880200	0.65089800	2.11406800
O	1.02226800	-0.40166900	-0.09369300
O	1.11025700	1.55767100	2.95736900
O	1.36563300	-0.64865100	2.49345000
C	1.49438600	-0.87786400	3.90617200
H	1.67132300	-1.94865600	4.01052300
H	0.57760900	-0.59468300	4.42968600
C	-2.78038900	0.17565600	0.39617900
O	-1.96877500	0.69240700	1.31205900
O	-2.43274700	-0.27446600	-0.69719400
N	-4.08826600	0.20933000	0.84056600
H	-4.20579100	0.61305300	1.76008700
C	-5.26119200	-0.23154000	0.20255800
C	-5.28388800	-0.82471500	-1.07190300
C	-6.47298800	-0.06037800	0.89909200
C	-6.50253000	-1.23342100	-1.62253900
H	-4.35847500	-0.95836400	-1.61415800

C	-7.67941500	-0.47320600	0.33644900
H	-6.46474300	0.39808800	1.88483500
C	-7.70524700	-1.06471200	-0.93164000
H	-6.50338400	-1.68991900	-2.60861700
H	-8.60114800	-0.33072900	0.89332600
H	-8.64452800	-1.38646200	-1.37081700
H	-0.85775500	0.68087200	0.97873500
H	2.33363400	-0.31434100	4.32115500

TS2 re face:

0 1

P	-2.28735000	-1.18570300	-0.48015500
N	-0.99459000	-1.28800900	-1.49053000
N	-2.48818500	-2.56368500	0.41201400
N	-3.62692200	-0.88749100	-1.40403600
C	-0.06535000	-2.42517800	-1.50869600
H	-0.38342600	-3.19905300	-0.81262800
H	-0.03349500	-2.85356700	-2.51700200
H	0.93949100	-2.09573300	-1.22951800
C	-0.63504300	-0.20225000	-2.42192900
H	-0.57571400	-0.60527500	-3.43973100
H	-1.38740700	0.58604600	-2.40203700
H	0.33187000	0.22441400	-2.13929400
C	-1.73028100	-2.83591500	1.64235100
H	-2.40384300	-3.30072100	2.37013800
H	-0.89532500	-3.52292200	1.45359900
H	-1.35550100	-1.90815200	2.06930600
C	-3.15839100	-3.74128600	-0.15592600
H	-2.43391400	-4.50304300	-0.47112000
H	-3.81172200	-4.17795000	0.60643400
H	-3.77036400	-3.46484400	-1.01435900
C	-4.88388600	-0.45618400	-0.77370400
H	-5.31753200	0.36559500	-1.35367500
H	-5.60549800	-1.28217000	-0.74285100
H	-4.70256900	-0.10549800	0.24203100
C	-3.77266600	-1.32306500	-2.79783900
H	-4.09200000	-0.47540800	-3.41409600
H	-2.82781900	-1.70166100	-3.18519000
H	-4.52731500	-2.11561600	-2.87869400
C	-1.15185800	0.93586300	0.91024400
C	-1.24074400	2.19890900	0.12205700
C	-0.18823700	3.13769300	0.16813900
C	-2.35379600	2.51006400	-0.68279800
C	-0.25622000	4.33378100	-0.54692300
H	0.68909400	2.92138200	0.76501500
C	-2.41497800	3.70471500	-1.40795600
H	-3.18421400	1.81649400	-0.73817600
C	-1.36883500	4.62819900	-1.34435300
H	0.57232100	5.03496700	-0.48976000
H	-3.29021800	3.91272500	-2.01819900
H	-1.41528700	5.55610900	-1.90705600
C	-1.05621900	1.09608300	2.36262700
O	-2.24076500	0.00078200	0.57567300
O	-0.42538300	1.99239400	2.92588500
O	-1.65905300	0.10199000	3.07751700
C	-1.47578100	0.15302400	4.50405700
H	-2.01243400	-0.71159000	4.89519100
H	-1.89364500	1.07494300	4.91520000
C	2.36436500	-0.01066900	0.18795400
O	1.35258600	-0.37074100	0.96497900
O	2.28624300	0.72853100	-0.79642500
N	3.54088500	-0.59349200	0.62300600
H	3.44115400	-1.15855200	1.45546700

C	4.83685300	-0.50645000	0.08408200
C	5.16057000	0.24581900	-1.05876400
C	5.85518600	-1.22186900	0.74310100
C	6.48058000	0.27030500	-1.51937500
H	4.38518500	0.79982600	-1.56880000
C	7.16634300	-1.18679000	0.27162500
H	5.61404000	-1.80573300	1.62804100
C	7.49144300	-0.43941300	-0.86604100
H	6.71474500	0.85731700	-2.40328200
H	7.93482800	-1.74626600	0.79741500
H	8.51260300	-0.41092600	-1.23351600
H	0.36395500	0.20259700	0.76625400
H	-0.41546600	0.09059600	4.76142200

TS3:

0 1			
P	-3.13664600	-0.46312100	-0.09418800
N	-2.73444500	-1.33524600	-1.45894100
N	-3.79529300	-1.62676700	0.92542100
N	-4.21239700	0.69115300	-0.68223900
C	-2.12656100	-2.67165100	-1.37539900
H	-2.28060300	-3.10144200	-0.38694100
H	-2.58831400	-3.32598900	-2.12444600
H	-1.04918200	-2.61993700	-1.57286600
C	-2.49408100	-0.68451300	-2.75405700
H	-2.96071500	-1.27703600	-3.54999900
H	-2.92090600	0.31754300	-2.76544700
H	-1.41864800	-0.61667200	-2.96159800
C	-3.71104400	-1.46105400	2.38004300
H	-4.61006600	-0.97551400	2.78700500
H	-3.61355100	-2.44817600	2.84649300
H	-2.83767800	-0.86393200	2.63681800
C	-4.90988400	-2.47856000	0.50107600
H	-4.80496000	-3.46593400	0.96565300
H	-5.88120300	-2.06072000	0.80130800
H	-4.90450300	-2.61057200	-0.58139800
C	-4.34379300	1.98329300	0.00006400
H	-4.55989300	2.75909000	-0.74366100
H	-5.16346900	1.97424400	0.73352100
H	-3.41434400	2.23281800	0.50918600
C	-5.41661400	0.30612700	-1.42446700
H	-5.64739100	1.08479100	-2.16071900
H	-5.25925000	-0.63041000	-1.96077200
H	-6.28728200	0.19272300	-0.76310700
C	0.05870400	0.32906400	0.25138500
C	0.11442900	1.77923300	0.09281200
C	0.03311700	2.26677100	-1.22849300
C	0.23322200	2.70029600	1.15116500
C	0.07354700	3.63354400	-1.48836100
H	-0.04812500	1.56049000	-2.04881200
C	0.26906300	4.06920300	0.88644200
H	0.29196000	2.34604900	2.17113300
C	0.19117300	4.54052900	-0.42849500
H	0.01474600	3.99206000	-2.51140500
H	0.35849600	4.77097100	1.71014000
H	0.22169700	5.60792400	-0.62642200
C	0.22332000	-0.52789800	1.48198000
O	-2.04035100	0.27862500	0.67334100
O	0.09866800	-1.73719300	1.44830100
O	0.53326900	0.16169000	2.58484500
C	0.75146200	-0.61397700	3.78626800
H	1.57788400	-1.31117900	3.63622900
H	-0.15426400	-1.16312500	4.05002300

C	2.35223400	-0.67475100	-1.14953000
O	1.47909400	-1.02770400	-1.97359400
O	2.15060200	-0.03917900	-0.04236200
N	3.67960900	-0.99364400	-1.45932700
H	3.75220400	-1.50060700	-2.33124100
C	4.88476100	-0.78426900	-0.77221300
C	4.99672000	-0.06406000	0.43162100
C	6.05264500	-1.33063100	-1.34400200
C	6.24802300	0.09306800	1.03522900
H	4.10996700	0.36113200	0.88033900
C	7.29325800	-1.16385100	-0.73135100
H	5.98071400	-1.88975500	-2.27390400
C	7.40387000	-0.44968100	0.46730700
H	6.31258300	0.65251200	1.96475400
H	8.17585800	-1.59636100	-1.19441900
H	8.36962000	-0.31991300	0.94606300
H	-0.10737100	-0.25940800	-0.63750600
H	0.99768100	0.11539300	4.55602200

PO(NMe₂)₃:

0 1

P	0.00002900	-0.02553000	-0.48945000
N	-0.00188500	1.56032400	0.08862000
N	-1.42184200	-0.64642000	0.18137300
N	1.42339200	-0.64300800	0.18136600
C	-1.21925400	2.36907600	-0.06248100
H	-2.10797700	1.74998800	0.05672200
H	-1.22748800	3.14818500	0.70796500
H	-1.26110100	2.85907000	-1.04647300
C	1.21355200	2.37200000	-0.06240900
H	1.21986000	3.15113600	0.70802800
H	2.10376000	1.75506600	0.05686400
H	1.25428900	2.86208400	-1.04640300
C	-2.10679300	-1.74933700	-0.49717700
H	-1.79974000	-2.72993900	-0.10220500
H	-3.18879500	-1.64785000	-0.34844600
H	-1.89518200	-1.71638300	-1.56559700
C	-1.70742000	-0.57945800	1.61504300
H	-2.78994900	-0.48225200	1.76338200
H	-1.37281200	-1.48253500	2.14679300
H	-1.22497300	0.29012200	2.06273300
C	2.11099700	-1.74425900	-0.49721300
H	3.19275700	-1.64011900	-0.34856000
H	1.80640200	-2.72561900	-0.10221600
H	1.89922000	-1.71183700	-1.56561700
C	1.70881000	-0.57540700	1.61504000
H	2.79110500	-0.47562700	1.76338100
H	1.22429100	0.29300600	2.06275300
H	1.37636200	-1.47929300	2.14677400
O	0.00031600	-0.26077800	-1.97905700

P(NC₄H₈)₃:

0 1

P	0.02435900	0.06525300	-1.01050300
C	1.55089600	-1.24254600	1.01111600
C	2.73716100	-0.53858700	-0.98674500
C	3.00373000	-1.76091000	1.05424800
H	0.82841700	-2.07006500	1.00522000
H	1.32278400	-0.61858600	1.88643000
C	3.43141700	-1.78544700	-0.42314200
H	3.35647100	0.35602600	-0.80601500
H	2.55400200	-0.59622700	-2.06625300

H	3.63644700	-1.05939200	1.61083900
H	3.07942400	-2.73672900	1.54372300
H	4.51766400	-1.76477100	-0.55586400
H	3.04305700	-2.68374700	-0.91827000
C	-1.90035700	-0.67448100	0.97901600
C	-1.68870700	-2.12191200	-0.95804300
C	-2.93757500	-1.81729400	1.06331000
H	-2.37961200	0.31345300	0.97450300
H	-1.21787200	-0.69896300	1.84015300
C	-3.10521600	-2.28733000	-0.39294900
H	-1.07462800	-3.00587300	-0.71191100
H	-1.66807200	-2.00355400	-2.04812500
H	-2.53988800	-2.63792600	1.67172900
H	-3.87608100	-1.49094900	1.52173700
H	-3.47795400	-3.31342300	-0.47033000
H	-3.79807700	-1.62952500	-0.93112700
C	0.33067000	2.06200600	1.01106800
C	-0.97685600	2.65577800	-0.94673800
C	-0.09172800	3.54563700	1.09335900
H	1.42312000	1.94861400	1.00522700
H	-0.04944200	1.49425100	1.87187700
C	-0.36873300	3.94016500	-0.36806000
H	-2.05839800	2.61472200	-0.73013000
H	-0.85803100	2.57265600	-2.03383600
H	-1.01166400	3.64076800	1.68205500
H	0.67243300	4.16676700	1.57059900
H	-1.03306900	4.80518600	-0.45924500
H	0.56941900	4.17264600	-0.88619100
N	1.46683800	-0.48130200	-0.24770900
N	-1.20303600	-0.90454100	-0.29880200
N	-0.23501500	1.58971500	-0.26370700

TS1 when the PR is P(NC₄H₈)₃:

O 1			
P	0.88579400	-0.24630900	0.00613900
C	3.10533900	-1.58479300	-0.99808800
C	1.22132800	-1.34357400	-2.55216800
C	3.57111800	-1.87539200	-2.43132100
H	3.11618700	-2.49906100	-0.38861000
H	3.72556200	-0.83648000	-0.49605200
C	2.27411200	-2.29396100	-3.14028200
H	1.16912500	-0.40886600	-3.12098500
H	0.22302600	-1.78766600	-2.54197100
H	3.97490000	-0.96359300	-2.88630800
H	4.34827800	-2.64406300	-2.46282800
H	2.33206900	-2.21329800	-4.22930700
H	2.02718800	-3.33234800	-2.89005000
C	0.20836300	-2.77732400	0.92018000
C	-0.30812800	-0.93558900	2.41223900
C	-0.61963300	-3.28957400	2.12070600
H	1.15298100	-3.31992200	0.81032500
H	-0.35121000	-2.88358900	-0.01651300
C	-0.41285200	-2.23137800	3.21844300
H	-1.30862700	-0.59225700	2.11227200
H	0.18583600	-0.12440100	2.95188900
H	-1.67879000	-3.33915600	1.84806700
H	-0.30781400	-4.29109500	2.42905600
H	-1.23126900	-2.20295000	3.94330600
H	0.52185000	-2.41002600	3.76191200
C	2.74902100	0.51535300	2.01229000
C	2.43561600	2.00461300	0.08926400
C	3.92584800	1.49608000	1.90052500
H	3.06347200	-0.53085900	2.04393700

H	2.16507200	0.71858400	2.91827100
C	3.32789000	2.68542500	1.13326500
H	1.60195900	2.62240500	-0.24679800
H	3.02921600	1.71441800	-0.79074200
H	4.32346200	1.76809700	2.88257400
H	4.73905100	1.04620500	1.31907700
H	2.71936400	3.30348300	1.80386800
H	4.08452200	3.32666600	0.67276500
N	1.71776400	-1.08759100	-1.17360500
N	0.49790900	-1.35300800	1.23944100
N	1.93272300	0.79963700	0.79832900
C	-1.66924700	1.19192200	-0.82880700
C	-2.77425900	0.25937900	-0.58341700
C	-2.64889600	-1.07888000	-1.03487300
C	-3.96579900	0.59343600	0.111105400
C	-3.65044700	-2.02400400	-0.81162700
H	-1.76321100	-1.36009100	-1.59218600
C	-4.96206000	-0.35774300	0.33145600
H	-4.10096600	1.60621800	0.46679900
C	-4.81893600	-1.67366100	-0.12656000
H	-3.52013000	-3.03732200	-1.18333500
H	-5.86115400	-0.06678400	0.86909600
H	-5.60166900	-2.40725000	0.04386000
C	-1.76429700	2.61310800	-0.54273100
O	-0.52220600	0.70713300	-1.25830800
O	-2.79634100	3.24420300	-0.27238100
O	-0.56204100	3.26497800	-0.65240800
C	-0.60278900	4.68540200	-0.44955000
H	-0.96623900	4.92950700	0.55231100
H	-1.24683500	5.16648900	-1.19053900
H	0.42607800	5.02678200	-0.56961400

PO(NC₄H₈)₃:

O 1			
P	-0.04609500	-0.12316300	0.73363400
C	1.75740600	0.37897100	-1.33147000
C	2.70855500	-0.53250000	0.72865500
C	3.22746700	-0.01497900	-1.56028300
H	1.61948000	1.46368900	-1.43721100
H	1.08532900	-0.11299400	-2.04508300
C	3.83415600	0.02995500	-0.14871600
H	2.74524800	-1.63232300	0.74535700
H	2.75056200	-0.17978800	1.76134000
H	3.28439500	-1.03471200	-1.95851300
H	3.72672300	0.65107600	-2.26978000
H	4.75824800	-0.54837800	-0.05921800
H	4.05089600	1.06580100	0.13831900
C	-1.53291900	1.64489100	-0.87973900
C	-0.68698300	2.47356400	1.25824200
C	-1.43856300	3.17716800	-0.91432600
H	-2.58293200	1.32353900	-0.90000700
H	-1.02678800	1.17228400	-1.72509700
C	-1.52053200	3.56340200	0.57036700
H	0.37727700	2.75171700	1.27385000
H	-0.99966200	2.28603600	2.28892100
H	-0.47200100	3.48616000	-1.32998800
H	-2.22824800	3.62581700	-1.52414800
H	-1.13978600	4.56701000	0.77997800
H	-2.56018900	3.51645600	0.91562700
C	-0.19159700	-2.52920300	-0.56913700
C	-2.32312200	-1.51912700	0.05616600
C	-1.34295500	-3.44136900	-1.00860800
H	0.34463600	-2.97942100	0.27870900
H	0.53280700	-2.34634200	-1.36798600
C	-2.47444100	-3.04492400	-0.04884500

H	-2.91815000	-1.01431300	-0.71518400
H	-2.64281400	-1.13614300	1.03018100
H	-1.62660500	-3.21802600	-2.04408100
H	-1.07444700	-4.50006900	-0.95070200
H	-3.46719700	-3.33877600	-0.40191700
H	-2.31258600	-3.50849600	0.93131300
N	1.48387400	-0.04512200	0.05801000
N	-0.91149100	1.27343200	0.41541500
N	-0.87372300	-1.26758000	-0.18048200
O	0.07981500	-0.36449400	2.21969300

P(NMe₂)₂Et:

0 1			
P	-0.01042800	-0.02448200	-0.85809100
N	1.15328700	-0.77088400	0.25699100
N	-1.45610400	-0.25580500	0.02907000
C	2.55681600	-0.51390500	-0.08502800
H	2.76534000	0.55721000	-0.10789500
H	3.19680100	-0.96041100	0.68415700
H	2.85333700	-0.94598500	-1.05842200
C	0.92569400	-2.21206700	0.41882300
H	1.56915700	-2.58733300	1.22289300
H	-0.11398800	-2.39971800	0.69529000
H	1.15196900	-2.79014900	-0.49566300
C	0.68229200	2.42628800	0.69426800
H	1.06201000	3.44856200	0.58049600
H	-0.25186800	2.48388200	1.25840800
H	1.40260500	1.86772600	1.29905700
C	-2.69154200	-0.52828400	-0.69468800
H	-3.24118200	-1.35303200	-0.21826500
H	-3.35935300	0.34770800	-0.72038700
H	-2.46688400	-0.81475900	-1.72545500
C	-1.64758900	0.05886800	1.44029700
H	-2.22028500	-0.74399700	1.92607100
H	-0.68077800	0.13605800	1.93950400
H	-2.20249000	0.99927100	1.58529100
C	0.47047000	1.78398000	-0.68436400
H	-0.33075700	2.30574600	-1.22489900
H	1.36566500	1.91399300	-1.30709000

TS1 when the PR is P(NMe₂)₂Et:

0 1			
P	-0.01042800	-0.02448200	-0.85809100
N	1.15328700	-0.77088400	0.25699100
N	-1.45610400	-0.25580500	0.02907000
C	2.55681600	-0.51390500	-0.08502800
H	2.76534000	0.55721000	-0.10789500
H	3.19680100	-0.96041100	0.68415700
H	2.85333700	-0.94598500	-1.05842200
C	0.92569400	-2.21206700	0.41882300
H	1.56915700	-2.58733300	1.22289300
H	-0.11398800	-2.39971800	0.69529000
H	1.15196900	-2.79014900	-0.49566300
C	0.68229200	2.42628800	0.69426800
H	1.06201000	3.44856200	0.58049600
H	-0.25186800	2.48388200	1.25840800
H	1.40260500	1.86772600	1.29905700
C	-2.69154200	-0.52828400	-0.69468800
H	-3.24118200	-1.35303200	-0.21826500
H	-3.35935300	0.34770800	-0.72038700
H	-2.46688400	-0.81475900	-1.72545500
C	-1.64758900	0.05886800	1.44029700
H	-2.22028500	-0.74399700	1.92607100
H	-0.68077800	0.13605800	1.93950400
H	-2.20249000	0.99927100	1.58529100
C	0.47047000	1.78398000	-0.68436400

H	-0.33075700	2.30574600	-1.22489900
H	1.36566500	1.91399300	-1.30709000

PO(NMe₂)₂Et:

0 1

P	0.00041700	0.02180800	0.60326600
N	-1.22162900	-0.66773800	-0.35156600
N	1.39267700	-0.36036300	-0.26608100
C	-2.61135100	-0.24103300	-0.14048600
H	-2.68204800	0.84191600	-0.03695000
H	-3.20376900	-0.53082300	-1.01471900
H	-3.06108200	-0.70829900	0.74842500
C	-1.13061300	-2.11299400	-0.60967100
H	-1.69294600	-2.34824900	-1.51982900
H	-0.09068500	-2.40677500	-0.75788800
H	-1.54859200	-2.70484600	0.21788300
C	-0.41195300	2.54625200	-0.76588800
H	-0.62104000	3.60996000	-0.61236200
H	0.52399200	2.47179500	-1.32540200
H	-1.21013200	2.13517400	-1.39089400
C	2.66989900	-0.50162700	0.43362900
H	3.21883200	-1.36016000	0.02631300
H	3.29870300	0.39332100	0.31331400
H	2.49511200	-0.67370800	1.49571100
C	1.52314400	-0.18889600	-1.71228700
H	2.02428100	-1.06579600	-2.14278800
H	0.54115500	-0.09252600	-2.17608800
H	2.12201400	0.69858300	-1.96330000
C	-0.31625900	1.83270100	0.59005600
H	0.51907600	2.23788600	1.17389500
H	-1.21263500	2.01073100	1.19451600
O	0.12987200	-0.45562800	2.03407400

P (NEt)₃:

0 1

P	0.07241900	0.23025700	-0.35179300
N	-0.50579200	1.51370100	0.69715700
N	-0.87680800	-1.01298600	0.36132400
N	1.67138300	0.27299400	0.30596900
H	1.71289900	0.25920800	1.32482800
H	0.16236700	2.28113900	0.67298400
H	-0.89120700	-1.03871500	1.37973300
C	-1.88024600	2.01357400	0.52201200
H	-2.55033500	1.14850400	0.54267200
H	-2.12258900	2.61801100	1.40497600
C	-2.12791300	2.84154700	-0.74568200
H	-1.94059100	2.25166100	-1.64930500
H	-3.16588300	3.19330200	-0.77787900
H	-1.47342100	3.72083400	-0.77376100
C	-1.00975200	-2.33061600	-0.26728500
H	-0.90074700	-2.19220500	-1.34926900
H	-0.20287200	-3.01157800	0.04524000
C	-2.36266000	-2.97704600	0.03698600
H	-2.49942600	-3.11206900	1.11634100
H	-3.18438100	-2.35569900	-0.33440400
H	-2.43147200	-3.96383600	-0.43482800
C	2.73896000	-0.52490800	-0.31118900
H	2.69075000	-1.58070000	-0.00086500
H	2.58099500	-0.50865100	-1.39560100
C	4.12371300	0.03462400	0.01739000
H	4.29965400	0.03770700	1.09953200
H	4.90492200	-0.57803000	-0.44642300
H	4.22552400	1.06254700	-0.34627000

TS1 when the PR is P(NEt)₃:

0 1			
P	-1.20336600	0.29704700	-0.66880900
N	-0.88297500	0.28396500	0.95388500
N	-1.95063200	1.75798700	-0.96551000
N	-2.21505900	-0.79599000	-1.38670700
C	1.47029600	-0.85693300	-0.56063400
C	2.52184900	0.07797700	-0.16821500
C	3.57002000	-0.23916500	0.73601000
C	2.51237000	1.39127900	-0.70616800
C	4.53722400	0.70617100	1.07628400
H	3.61130200	-1.23377200	1.16092400
C	3.48189400	2.33065600	-0.35323800
H	1.73915000	1.66015800	-1.41714900
C	4.50647600	2.00072100	0.54094000
H	5.32607600	0.42698800	1.77085000
H	3.43968500	3.32667800	-0.78773400
H	5.26462500	2.73051600	0.81005100
C	1.34620700	-2.20538000	-0.08274900
O	0.53417800	-0.42402200	-1.43119500
O	2.16262300	-2.84579800	0.60043800
O	0.15556500	-2.79699300	-0.47760900
C	-0.03073900	-4.15606700	-0.05855900
H	0.73669900	-4.80671000	-0.48710100
H	-1.01461900	-4.44469100	-0.43093000
H	-0.00152100	-4.24122200	1.03115600
H	-1.73295000	-1.66915900	-1.58603400
H	-2.32626100	1.82863700	-1.90749000
H	-0.00982800	-0.20544400	1.15834700
C	-1.50557200	3.05138200	-0.40969300
H	-1.09118100	2.85963200	0.58142000
H	-0.70111800	3.46877400	-1.02803100
C	-2.67281900	4.03245500	-0.32607000
H	-2.32189900	4.98988300	0.07222300
H	-3.10619700	4.21968700	-1.31475400
H	-3.46115100	3.65111200	0.33007700
C	-1.88530300	0.22098400	2.03882300
H	-2.25761600	-0.80510700	2.15394200
H	-2.73294400	0.84831300	1.74753300
C	-1.29218600	0.71477000	3.35566500
H	-2.04430800	0.65134800	4.14865200
H	-0.43541000	0.10171700	3.65581100
H	-0.96002400	1.75403500	3.27294800
C	-3.69085200	-0.85274400	-1.39821800
H	-4.01170300	-1.02922900	-2.43102000
H	-4.06881700	0.13045800	-1.10820300
C	-4.25742900	-1.93673100	-0.48096900
H	-5.34988500	-1.95736700	-0.55923300
H	-3.88127600	-2.92616100	-0.76233300
H	-3.99117600	-1.75279400	0.56458600

PO(NEt)₃:

0 1			
P	0.08867600	-0.17271700	0.76968100
N	1.54902100	-0.58965100	0.05297800
N	-0.74341600	-1.63085000	0.65644000
N	-0.42286200	1.04052400	-0.27699800
O	0.03421500	0.30845400	2.19732400
H	-1.37193100	-1.77953100	1.43875400
H	-0.33521600	0.81744500	-1.26387700
H	1.84610100	-1.52219000	0.32610800
C	2.67296600	0.35580000	-0.08146900
H	3.18261700	0.49854200	0.88177000
H	2.25869700	1.32325600	-0.37569400
C	3.67278800	-0.12895800	-1.12961700
H	3.19708700	-0.22208300	-2.11135300
H	4.50563300	0.57730100	-1.21240600

H	4.08900700	-1.10569500	-0.85696700
C	-1.15418200	-2.29064900	-0.59209500
H	-0.42430800	-2.02825100	-1.36378300
H	-1.07480000	-3.37475700	-0.44617100
C	-2.57061500	-1.93677700	-1.05446200
H	-3.30855000	-2.20502400	-0.28998200
H	-2.66669300	-0.86581500	-1.25931600
H	-2.82026900	-2.48509300	-1.96999700
C	-1.56688900	1.91010800	0.03635500
H	-1.51829200	2.13997700	1.10379000
H	-2.52235900	1.39407200	-0.14206400
C	-1.51856200	3.19792400	-0.78405100
H	-2.37921500	3.83118700	-0.54426200
H	-0.60329500	3.76089900	-0.57439100
H	-1.55031600	2.98403700	-1.85887200

P(NMe₂)Et₂:

0 1			
P	0.16701800	0.13712600	-0.84741300
N	-1.27801900	0.17821900	0.11374800
C	1.04421100	2.62220200	0.21382700
H	0.06832600	2.81180800	0.67239100
H	1.79735400	3.17201800	0.78951500
H	1.02427500	3.04054700	-0.79864900
C	-2.53209400	-0.04122000	-0.60668100
H	-2.79536200	-1.10981200	-0.69193700
H	-3.35463600	0.46113800	-0.08075200
H	-2.46284100	0.37563000	-1.61465500
C	-1.34847900	-0.29783400	1.49358100
H	-2.18454300	0.19440000	2.00736300
H	-1.51227100	-1.38645000	1.55949400
H	-0.43446800	-0.05408800	2.03855100
C	1.51290800	-2.11587800	0.58606700
H	1.91218800	-3.12736800	0.44304500
H	2.33935500	-1.48714500	0.93199200
H	0.77218800	-2.16650500	1.38838900
C	0.90979900	-1.59414800	-0.72706300
H	1.67618100	-1.61397300	-1.51455700
H	0.11704600	-2.26957100	-1.07481600
C	1.36406800	1.12180800	0.19174400
H	2.34874200	0.95278500	-0.26383400
H	1.42684200	0.73258800	1.21457400

TS1 when the PR is P(NMe₂)Et₂:

0 1			
C	-0.94193100	0.77336700	-0.72843800
C	-2.11293500	-0.07825300	-0.50716000
C	-3.27784200	0.31681900	0.20005300
C	-2.07907900	-1.40464900	-1.00826400
C	-4.33588200	-0.57060400	0.39173400
H	-3.33749600	1.32308100	0.59290700
C	-3.14149500	-2.28747600	-0.80526900
H	-1.21431000	-1.72610600	-1.57719500
C	-4.28058600	-1.88048700	-0.10398100
H	-5.21484100	-0.23576600	0.93704600
H	-3.08014400	-3.29653900	-1.20534500
H	-5.11043200	-2.56457000	0.04856500
C	-0.81620900	2.12130100	-0.19520900
O	0.08421600	0.25750800	-1.37414200
O	-1.71696900	2.80207100	0.31290200
O	0.44472900	2.64155800	-0.35472100
C	0.61758300	3.99955300	0.07748100
H	1.66328000	4.23765500	-0.12048900
H	0.40248900	4.10331500	1.14435800
H	-0.03388800	4.67338100	-0.48548900
P	1.49604100	-0.66322200	-0.16381900

N	1.06748600	-0.28311300	1.41598600
C	3.43731900	0.02314900	-2.05716900
H	2.63226700	0.18539600	-2.77954600
H	4.26467400	0.68863100	-2.32068500
H	3.79422900	-1.00538500	-2.16478300
C	0.16592200	-1.17333400	2.15374100
H	0.71930300	-1.81871800	2.84986900
H	-0.54722100	-0.57227200	2.72758700
H	-0.40777100	-1.79938600	1.46754400
C	1.68587400	0.76327100	2.23327100
H	0.90630900	1.29870400	2.78599600
H	2.39313100	0.33201300	2.95554500
H	2.21338300	1.48759800	1.61478000
C	3.26386000	-2.81361900	0.61152400
H	3.45441400	-3.89057200	0.54164700
H	4.15575200	-2.29550300	0.24833400
H	3.12969100	-2.56421000	1.66809200
C	2.01753400	-2.45804100	-0.21359200
H	2.15919400	-2.69454600	-1.27401700
H	1.15075700	-3.03941800	0.11441900
C	2.97318300	0.32975500	-0.62260000
H	3.78010500	0.15406200	0.09685600
H	2.66639900	1.37567000	-0.54965200

PO(NMe₂)Et₂:

O 1			
P	-0.14469900	-0.24705500	0.54723500
N	0.27631200	1.22434400	-0.18666300
C	-2.74300700	-0.14161800	-0.56994700
H	-2.57173300	0.82480100	-1.05291700
H	-3.50915200	-0.67425500	-1.14201800
H	-3.13860000	0.04687500	0.43220400
C	1.02971100	2.19684800	0.61022300
H	2.11532700	2.11001100	0.44910100
H	0.72357000	3.21117800	0.32765800
H	0.81423800	2.05540900	1.67016900
C	0.46378000	1.39082200	-1.62801600
H	0.11543100	2.38783400	-1.92429800
H	1.51970000	1.30089600	-1.92304000
H	-0.11203700	0.65564200	-2.19131800
C	1.88050700	-1.78546500	-0.84045000
H	2.68736700	-2.51359600	-0.70857800
H	1.14668800	-2.23018800	-1.52006300
H	2.30906700	-0.90742400	-1.33179400
C	1.26450100	-1.43438900	0.52218800
H	0.89956700	-2.33841500	1.02524100
H	2.02053800	-0.99673000	1.18541200
C	-1.45684700	-0.97735600	-0.50697200
H	-1.65780000	-1.95399400	-0.04956700
H	-1.07003400	-1.18315100	-1.51009400
O	-0.58596200	-0.01906600	1.97998300

P(Et)₃:

O 1			
P	0.05688700	-0.38692600	-0.90387600
C	2.57225100	-0.76860900	0.36689800
H	2.83219800	0.28990000	0.25511000
H	3.13259900	-1.15550800	1.22557900
H	2.92594800	-1.29204100	-0.52811400
C	0.16134700	2.15982700	0.63244900
H	0.17228600	3.25077300	0.52067900
H	-0.68346500	1.90216300	1.27599600
H	1.07854300	1.87927000	1.15986400
C	1.06201300	-0.96526200	0.56681500
H	0.84133500	-2.03423400	0.67935200
H	0.73522600	-0.47645000	1.49137800

C	-1.68499300	-0.88839400	-0.41564100
H	-1.68290200	-1.98401700	-0.49006200
H	-2.32736100	-0.54117000	-1.23502500
C	0.07417200	1.49176600	-0.74781000
H	0.91935900	1.82632800	-1.36136900
H	-0.82441500	1.83220000	-1.27903400
C	-2.28699200	-0.46461600	0.93197100
H	-2.43296700	0.61780800	0.98856500
H	-3.26850300	-0.93385400	1.07149500
H	-1.65796200	-0.76554800	1.77562600

TS1 when the PR is P(Et)₃:

0 1			
P	1.64241800	-0.54636400	0.00641000
C	0.36803900	-1.60534900	2.33800600
H	1.02912600	-2.47189900	2.42769500
H	0.00048600	-1.36365900	3.33990400
H	-0.49368900	-1.89095700	1.72772300
C	3.49927200	-2.71650200	0.41905900
H	3.72751900	-3.75725400	0.16380400
H	4.36295600	-2.10894400	0.13561800
H	3.38107400	-2.65659900	1.50479000
C	-0.87811000	0.82815800	-0.57890400
C	-2.01297100	-0.09091700	-0.47203300
C	-3.23835700	0.22129800	0.17065300
C	-1.88140100	-1.39058000	-1.02237500
C	-4.26262800	-0.72031600	0.25558400
H	-3.37306200	1.20736100	0.59549600
C	-2.91123700	-2.32822500	-0.92680500
H	-0.96781800	-1.64802600	-1.54596200
C	-4.11164300	-2.00339100	-0.28769300
H	-5.19033400	-0.44959300	0.75346100
H	-2.77595200	-3.31504100	-1.36229700
H	-4.91596400	-2.73013600	-0.21933100
C	-0.86771700	2.17007700	-0.01625200
O	0.22841400	0.38971500	-1.15230100
O	-1.85048100	2.81538600	0.36866300
O	0.38981100	2.71790400	0.01700200
C	0.47139800	4.06671900	0.50434400
H	-0.10673200	4.74434500	-0.12934800
H	1.52954400	4.32684300	0.46478500
H	0.10365200	4.13525700	1.53160100
C	2.22365500	-2.27814900	-0.32214800
H	2.36537000	-2.35122500	-1.40607800
H	1.38275200	-2.93426800	-0.07740100
C	3.07671800	0.58233300	-0.22239300
H	3.87365600	0.28510000	0.46971500
H	2.71683700	1.56736500	0.08875400
C	1.09443900	-0.38542800	1.75438200
H	1.96504800	-0.11090200	2.36132500
H	0.42493200	0.48575300	1.76067200
C	3.59433600	0.63198100	-1.66804500
H	4.41321500	1.35420600	-1.74184400
H	3.97921000	-0.33822000	-1.99742000
H	2.80718800	0.94165300	-2.36099700

PO(Et)₃:

0 1			
P	0.05727000	-0.44642600	-0.44713100
C	2.50836100	-0.19672700	0.94781900
H	2.69090500	0.81278300	0.56493100
H	3.02544600	-0.28474200	1.90845000
H	2.96230900	-0.90802700	0.25212800
C	-0.11800600	2.43081000	-0.01393700
H	-0.12172700	3.39787500	-0.52702800
H	-1.04374700	2.36092900	0.56241200

H	0.71775400	2.43715500	0.69192400
C	1.00871900	-0.47930900	1.12664600
H	0.85927000	-1.48103300	1.54752800
H	0.55887100	0.23063200	1.82972100
C	-1.65489800	-0.97744500	-0.02342200
H	-1.54567200	-2.02500400	0.28361700
H	-2.19566400	-0.99257700	-0.97733800
C	0.01882600	1.29931100	-1.04486000
H	0.95271100	1.41349400	-1.60749300
H	-0.78956500	1.34569400	-1.78476700
C	-2.44617900	-0.19128300	1.03241600
H	-2.66590000	0.82772600	0.70289300
H	-3.40402700	-0.68741100	1.21906000
H	-1.91535200	-0.13451000	1.98772600
O	0.64429900	-1.36609100	-1.51184800

P(Me)₃:

O 1			
P	-0.00031000	-0.00009500	-0.59527500
C	0.84421400	1.41493500	0.27551700
H	1.89630100	1.45304200	-0.02432900
H	0.37571600	2.35891400	-0.02038200
H	0.79004000	1.31900700	1.36663900
C	-1.64773100	0.02333100	0.27586400
H	-2.20574700	0.91707300	-0.02093000
H	-2.23187600	-0.85272500	-0.02328100
H	-1.53755600	0.02026600	1.36694100
C	0.80392700	-1.43813600	0.27564600
H	0.30892300	-2.36838300	-0.02069300
H	1.85460000	-1.50591200	-0.02373800
H	0.75179000	-1.34063700	1.36673100

TS1 when the PR is P(Me)₃:

O 1			
P	-1.68679900	-1.48319200	0.09767100
C	-1.47293400	-0.78166900	1.76626200
H	-0.68213000	-0.01952900	1.71657400
H	-2.39023300	-0.30010500	2.11335600
H	-1.16870300	-1.55883600	2.47010300
C	-3.37700000	-1.14195500	-0.49665100
H	-3.53339800	-0.06162900	-0.49533300
H	-3.47840500	-1.51380000	-1.52012700
H	-4.12255500	-1.63098600	0.13857500
C	-1.54364100	-3.31711400	0.21698600
H	-1.59386800	-3.74635000	-0.78689700
H	-0.58314500	-3.57739000	0.66678100
H	-2.35833200	-3.72816300	0.82508600
C	0.21202900	0.62213500	-0.57289900
C	1.59413500	0.21212200	-0.31149300
C	2.57813100	1.04509500	0.27882200
C	1.97675200	-1.11076900	-0.64567600
C	3.86661300	0.57016200	0.51895800
H	2.31848800	2.06219700	0.54136000
C	3.26726000	-1.57906600	-0.39315800
H	1.25239400	-1.76145000	-1.12185800
C	4.22509000	-0.74403800	0.19021700
H	4.59963200	1.23397600	0.97034200
H	3.52643600	-2.59976600	-0.66277600
H	5.23173000	-1.10540600	0.37949100
C	-0.34127000	1.91161400	-0.18100100
O	-0.60549900	-0.25384400	-1.12570700
O	0.29680500	2.91638800	0.15344000
O	-1.70988900	1.93725600	-0.25386200
C	-2.33003400	3.19156200	0.07271800
H	-2.00344100	3.97642600	-0.61440600
H	-2.09268900	3.48984500	1.09724600

H -3.40192300 3.02197400 -0.03205200

PO(Me)₃:

0 1

P 0.00025000 -0.00003600 0.16631900
C -0.80914000 1.47503500 -0.54652800
H -1.84702500 1.51567900 -0.20406300
H -0.28898400 2.37268900 -0.20038100
H -0.79167400 1.44760000 -1.63993400
C 1.68179100 -0.03703500 -0.54808400
H 2.23824900 0.83834200 -0.20133700
H 2.19696400 -0.93935800 -0.20678900
H 1.64909000 -0.03288100 -1.64147200
C -0.87368400 -1.43737100 -0.54740900
H -0.39167400 -2.35726000 -0.20444400
H -1.91142300 -1.43396100 -0.20211800
H -0.85798000 -1.40852200 -1.64080800
O 0.00086400 -0.00069600 1.68733500

PPh₃:

0 1

P -0.00359600 0.00449300 -1.19825600
C 0.27919500 1.65460200 -0.39939900
C -0.30634200 2.77302100 -1.02024800
C 1.06092500 1.85819200 0.74944400
C -0.13575800 4.05623600 -0.49466900
H -0.89869400 2.64013500 -1.92241600
C 1.24340100 3.14422900 1.26893900
H 1.53257100 1.01412700 1.24274000
C 0.64299400 4.24555400 0.65193500
H -0.60021600 4.90646900 -0.98603900
H 1.85313500 3.28277600 2.15745300
H 0.78542800 5.24332700 1.05676100
C 1.28663400 -1.06480300 -0.40243500
C 1.07132100 -1.85267800 0.73979600
C 2.55006900 -1.10702000 -1.01983000
C 2.09495000 -2.65452800 1.25596600
H 0.10306000 -1.84410700 1.23009600
C 3.57705700 -1.89716300 -0.49760400
H 2.73175600 -0.51908200 -1.91637800
C 3.35064500 -2.67631000 0.64210000
H 1.90984000 -3.25905600 2.13953900
H 4.54719800 -1.91293400 -0.98610200
H 4.14435200 -3.29929400 1.04414200
C -1.57156800 -0.58033600 -0.39807100
C -2.23792800 -1.65469600 -1.01523300
C -2.14394300 -0.00495700 0.74774800
C -3.43044500 -2.15677000 -0.48848800
H -1.82169200 -2.10160700 -1.91495700
C -3.34546100 -0.49787300 1.26813700
H -1.65444100 0.83039400 1.23840500
C -3.98940700 -1.57669600 0.65528400
H -3.92693400 -2.99065700 -0.97652000
H -3.77489600 -0.03923900 2.15451600
H -4.92163200 -1.95853100 1.06134300

TS1 when the PR is PPh₃:

0 1

C	1.49701400	-0.94460100	-1.14645000
C	2.70503500	-0.12391500	-1.03788400
C	3.99782900	-0.64114400	-0.76544800
C	2.59292100	1.27889000	-1.20670000
C	5.10272500	0.20406100	-0.66838600
H	4.12121500	-1.70782200	-0.63623500
C	3.70312800	2.11663000	-1.10022800
H	1.62446000	1.70676100	-1.43470500
C	4.97015800	1.58887000	-0.83072000
H	6.07939600	-0.22569100	-0.46066100
H	3.57640000	3.18774100	-1.23496600
H	5.83569000	2.24027000	-0.75212400
C	1.47694600	-2.38665200	-0.95264900
O	0.34366600	-0.34573700	-1.40693300
O	2.45893200	-3.12872800	-0.83203500
O	0.20694300	-2.90096900	-0.95872800
C	0.10840000	-4.32343300	-0.78360600
H	0.54167400	-4.62954300	0.17206500
H	0.61761400	-4.85056400	-1.59450200
H	-0.95890800	-4.54550400	-0.80162800
P	-0.86601100	0.34826400	0.03476600
C	-0.77832000	2.13243600	0.32929400
C	-0.96655600	2.99658200	-0.76951000
C	-0.46197200	2.67922800	1.58722500
C	-0.85121000	4.37644500	-0.60596400
H	-1.20349800	2.59263500	-1.74951600
C	-0.34310300	4.06161300	1.73963300
H	-0.31846500	2.03227300	2.44560400
C	-0.53606900	4.91357300	0.64738300
H	-1.00278800	5.03117500	-1.45871600
H	-0.10589400	4.47230400	2.71644900
H	-0.44314200	5.98813300	0.77133000
C	-0.52169700	-0.56973800	1.54126500
C	-1.47317400	-1.42298200	2.13390100
C	0.78530800	-0.51699600	2.06697200
C	-1.12864500	-2.18272900	3.25006900
H	-2.47790600	-1.48451100	1.72925100
C	1.11941000	-1.28178000	3.18807400
H	1.53527200	0.12485000	1.61577000
C	0.16653100	-2.11339000	3.78011200
H	-1.87200500	-2.82662000	3.71028400
H	2.12602200	-1.22905100	3.59119100
H	0.42940100	-2.70833100	4.64954000
C	-2.50060100	-0.04862900	-0.63005500
C	-2.66530300	-1.25232000	-1.34103500
C	-3.59775900	0.81650000	-0.46041900
C	-3.91732300	-1.58540300	-1.86271200
H	-1.81673700	-1.91292600	-1.47991800
C	-4.84325300	0.47550900	-0.98902500
H	-3.48351100	1.74719500	0.08471200
C	-5.00525500	-0.72463800	-1.68997700
H	-4.03939500	-2.51517600	-2.41010300
H	-5.68621600	1.14571400	-0.85075400
H	-5.97582900	-0.98572600	-2.10123000

POPh₃:

0 1

P	0.00408400	-0.01508400	0.91651000
C	1.19150500	-1.21722300	0.21054900
C	1.43916800	-2.39190400	0.93997900
C	1.85540500	-1.01043000	-1.00854000
C	2.33047700	-3.34947000	0.45085600
H	0.94188000	-2.54843200	1.89229800
C	2.74674000	-1.97079700	-1.49570000
H	1.68811600	-0.10130000	-1.57775600
C	2.98398700	-3.14073400	-0.76825200

H	2.51767500	-4.25357300	1.02254800
H	3.25808100	-1.80101200	-2.43854800
H	3.67935900	-3.88420300	-1.14665500
C	0.45443800	1.62706000	0.24380000
C	-0.05576900	2.12125300	-0.96659700
C	1.35177400	2.41231200	0.98630200
C	0.33581500	3.37964100	-1.43295600
H	-0.76276600	1.53374300	-1.54428400
C	1.73984800	3.66969900	0.51873300
H	1.73563500	2.04185800	1.93195700
C	1.23387400	4.15375600	-0.69238600
H	-0.06513300	3.75516800	-2.36970600
H	2.43163100	4.27153900	1.10053500
H	1.53405000	5.13270000	-1.05441700
C	-1.64150400	-0.42793100	0.22758200
C	-2.77090400	0.05572200	0.91001000
C	-1.81614800	-1.20223300	-0.92931200
C	-4.05382000	-0.22471100	0.43618800
H	-2.64470900	0.64304500	1.81455200
C	-3.10241400	-1.48203500	-1.40128100
H	-0.95555600	-1.59425500	-1.46195200
C	-4.22106900	-0.99335600	-0.72101100
H	-4.92054400	0.15191300	0.97115500
H	-3.22758100	-2.08461300	-2.29599200
H	-5.21931900	-1.21376500	-1.08760800
O	0.00974400	-0.03143200	2.43297200