Supporting Information for

4-Dimethylaminopyridine-catalyzed Dynamic Kinetic Resolution in Asymmetric Synthesis of P-Chirogenic 1,3,2-Oxazaphospholidine-2-oxides

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CONTENTS:

S1. General Information

Unless otherwise noted, The NMR spectra were recorded on Bruker Avance III with CD_2Cl_2 or $CDCl_3$ as solvent. The ^1H NMR were recorded at 400 MHz or 300 MHz with TMS as internal standard. The ^{13}C NMR spectra were recoded at 100 MHz with solvent as internal standard. The 31P NMR were recorded at 162 MHz with tri(o-toluyl)phosphine as internal standard. All coupling constants (*J* values) were reported in Hertz (Hz). High resolution mass spectra (HRMS) were measured using a Bruker Autoflex III MALDI-TOF mass spectrometer. The purification of products with column chromatography was performed on silica gel with 100–200 mesh.

All reagents were obtained from commercial sources and were used without further purification.

S2. General Procedure for the Synthesis of P-Stereogenic Oxazaphospholidines

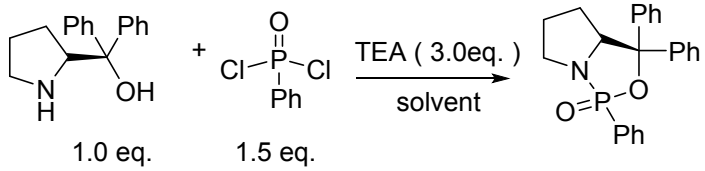
DMAP (0.06 mmol, 0.3 equiv) and the aminoethanol (0.2 mmol, 1.0 equiv) was dissolved in DCM (2.0 mL) in ice-water bath. The base (0.6 mmol, 3.0 equiv) and $PhP(O)Cl_2$ (0.3 mmol, 1.5 equiv) was added successively. The mixture was stirred at 25 ºC for 10 h. After completion of the reaction, DCM (5 mL) was added to the reaction mixture, which was washed with saturated aqueous $NaHCO_3$ for three times. The organic layer were then dried over $MgSO_4$, filtered, and tri(o-toluyl)phosphine was added as internal standard. The resulting mixture was concentrated under reduced pressure. The yield and the dr were detected by ^1H NMR.

S3. Optimization of reaction conditions

Here presented external optimization of conditions for the reaction between prolinols **2**s and phenylphosphoryl dichloride (**1**). The solvent effect was evaluated for the reaction between **2a** and **1** without using of DMAP (Table S1). The relation between DMAP loading and diastereoselectivity was checked for the reactions between **2a**

with 1.1 eq of **1** (Table S2). In comparison with the reaction using 1.5 eq of **1**, lower amount of **1** resulted in decrease of diastereoselectivity. For the reaction between **2b** with **1**, larger amount of DMAP was required to reach high diastereoselectivity, while better results could be obtained by replacement of triethylamine with imidazole as base (Table S3).

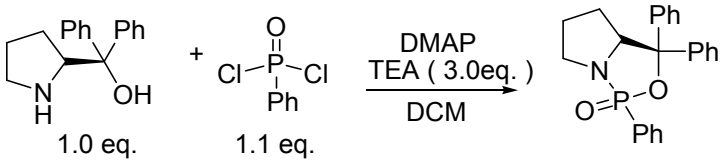
Table S1 Screening of the solvent



1.0 eq. 1.5 eq.

Entry	Solvent	Yield (%)	*dr*
1	DCM	79	83:17
3	$CHCl_3$	80	83:17
6	toluene	88	80:20
2	THF	0	-
4	DMF	0	-
5	DMF : DCM (1 : 1)	0	-

Table S2 The results of the reaction of **2a** with 1.1 eq. $PhP(O)Cl_2$

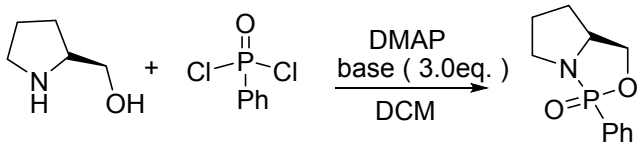


1.0 eq. 1.1 eq.

Entry	DMAP (eq.)	*dr*	Yield (%)
1	0.3	79:21	78.5
2	0.4	85:15	80.2
3	0.6	86:14	76.7
4	0.8	97:3	93.4
5	1.0	93:7	86.4

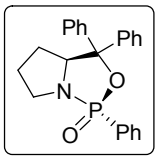
6	1.1	83:17	81.3
7	1.2	83:17	89.2

Table S3 Screening of the amount of DMAP in the reaction of **2b** with $PhP(O)Cl_2$

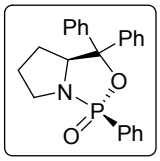


Entry	DMAP (eq.)	Base	*dr*
1	0	TEA	63:37
2	0.3	TEA	75:25
3	0.6	TEA	72:28
4	0.7	TEA	75:25
5	0.8	TEA	74:26
6	0.9	TEA	75:25
7	1.0	TEA	74:26
8	0	imidazole	75:25
9	0.5	imidazole	90:10
10	1.0	imidazole	91:9

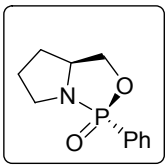
S4. Characterization of *P*-Stereogenic Oxazaphospholidines 3



(R_P)**-3a:** **^{1}H NMR** (300 MHz, $CDCl_3$): δ7.67-7.20 (m, 15H), 4.70 (dt, *J* = 12.8, 6.4 Hz, 1H), 3.84-3.64 (m, 1H), 3.10-2.87 (m, 1H), 1.91-1.44 (m, 4H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ143.61 (d, *J* = 4.4 Hz), 141.17, 132.10, 131.67, 131.57, 130.30, 128.25, 128.09, 127.97, 127.37, 128.72, 128.53, 88.67, 71.27 (d, *J* = 7.2 Hz), 44.74, 30.14, 26.26; **^{31}P NMR** (162 MHz,$CDCl_3$): δ34.97.



(S_P)-**3a:** **^{1}H NMR** (400 MHz, $CDCl_3$): δ7.27-7.85 (m, 15H), 4.75 (ddd, *J* = 16.3, 10.8, 5.1 Hz, 1H), 3.23-2.98 (m, 2H), 1.55-1.85 (m, 3H), 1.39- 1.20 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ144.76, 141.99 (d, *J* = 7.2 Hz), 133.18 (d, *J* = 10.1 Hz), 132.40, 128.76, 128.62, 128.48, 128.38, 128.17, 127.99, 127.39, 127.14, 126.32 , 125.34, 89.77, 72.61 (d, *J* = 8.5 Hz), 44.43 (d, *J*= 2.0 Hz), 30.44, 24.66; **^{31}P NMR** (162 MHz,$CDCl_3$) δ33.32.



(R_P)-**3b:** **^{1}H NMR** (400 MHz, $CDCl_3$): δ7.88-7.76 (m, 2H), 7.56-7.48 (m, 1H), 7.48-7.39 (m, 2H), 4.33 (ddd, *J* = 20.2, 8.6, 6.7 Hz, 1H), 4.11 (dd, J = 13.8, 6.7 Hz, 1H), 3.90 (td, *J* = 8.6, 2.2 Hz, 1H), 3.82-3.69 (m, 1H), 3.00-2.85 (m, 1H), 2.11-1.95 (m, 3H), 1.85-1.76 (m, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ132.00, 131.85, 131.69, 131.59, 128.41, 128.26, 69.68, 63.22 (d, *J* = 7.1 Hz), 45.36, 29.97, 27.56; **^{31}P NMR** (162 MHz,$CDCl_3$): δ38.40.

S5. MS analysis of the reaction mixture

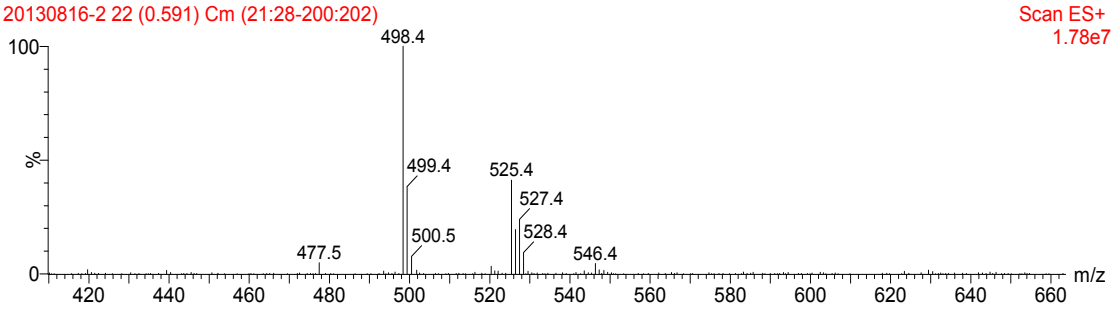


Figure S1 MS analysis of the reaction mixture of **2a** with **1**

S6. NMR Traces

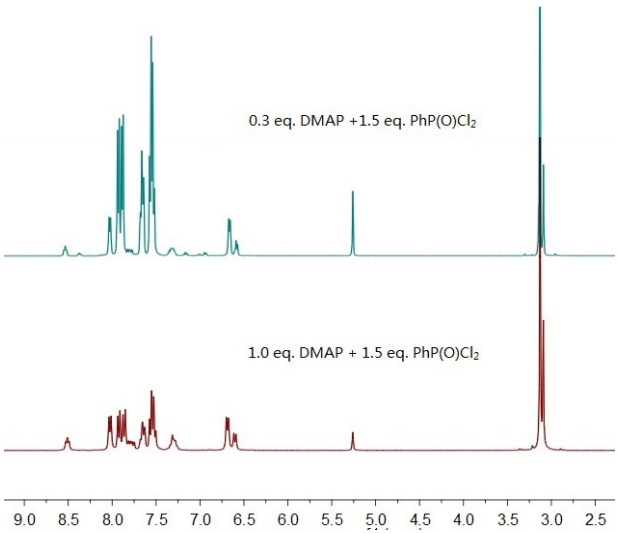


Figure S2 ^{1}H NMR spectra of mixtures of DMAP and phenylphosphoryl dichloride

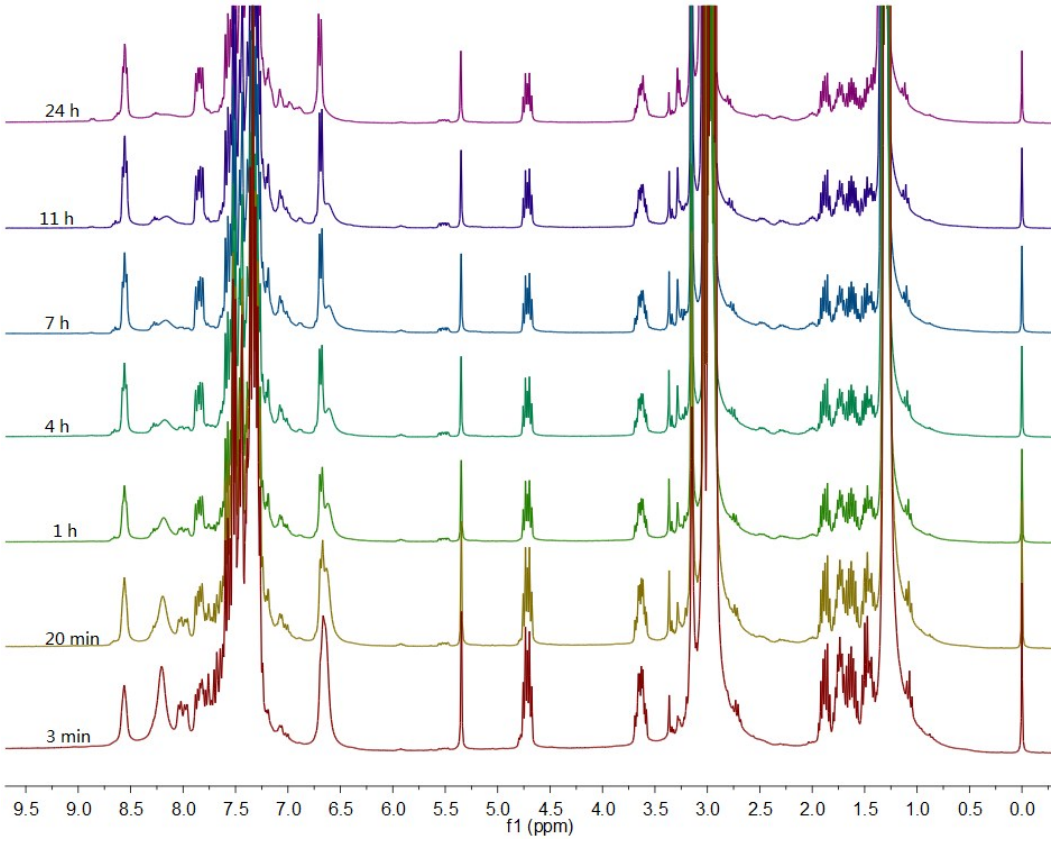


Figure S3 ^{1}H NMR traces of the reaction of **2a** with $PhP(O)Cl_2$ in presence of 1.0 equiv DMAP

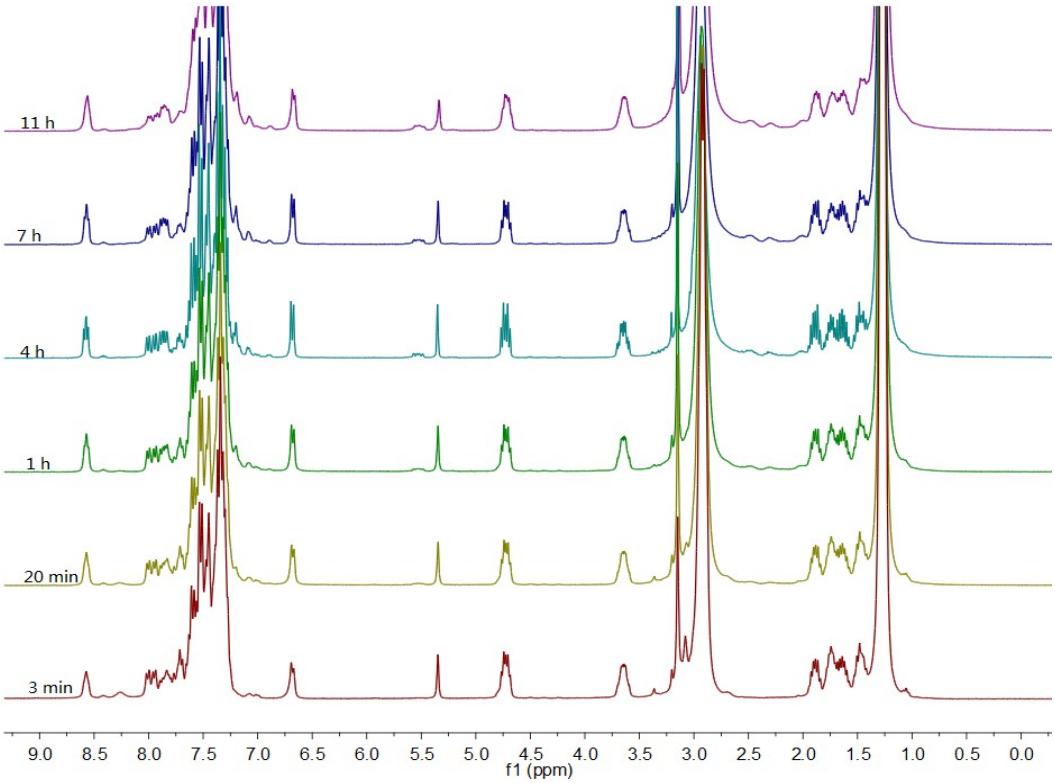


Figure S4 ^{1}H NMR traces of the reaction of **2a** with $PhP(O)Cl_2$ in presence of 0.3 equiv DMAP

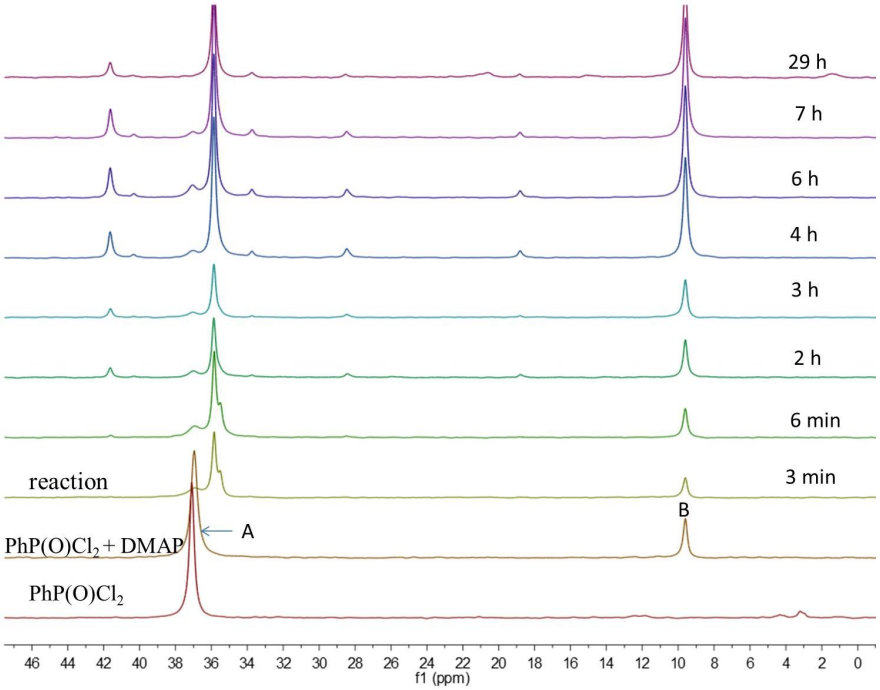


Figure S5 ^{31}P NMR traces of the reaction of **2a** with $PhP(O)Cl_2$ in presence of 1.0 equiv DMAP. The bottom spectra was the substrate $PhP(O)Cl_2$. The second from bottom was the ^{31}P NMR spectra of a mixture of $PhP(O)Cl_2$ and DMAP. The others were the ^{31}P NMR traces of the reaction of **2a** with $PhP(O)Cl_2$. A peak at 35.8 ppm was attributed to **C1** and (R_P)-**3a**. The tiny shoulder peak was probably an unspecified intermediate. No peak related to epimer of **C1** or (R_P)-**3a** was

observed.

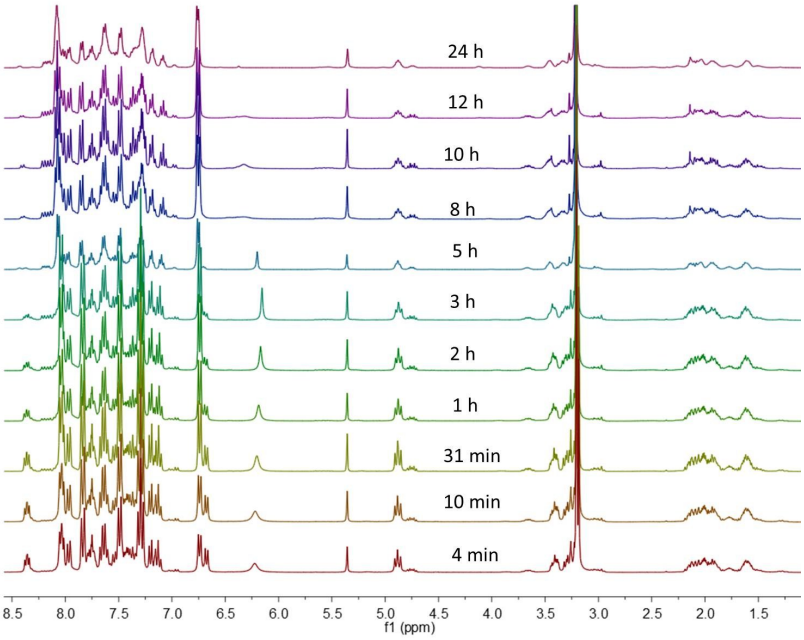


Figure S6 ^{1}H NMR traces of the reaction of **2a** with $PhP(O)Cl_2$ in presence of DMAP but without TEA

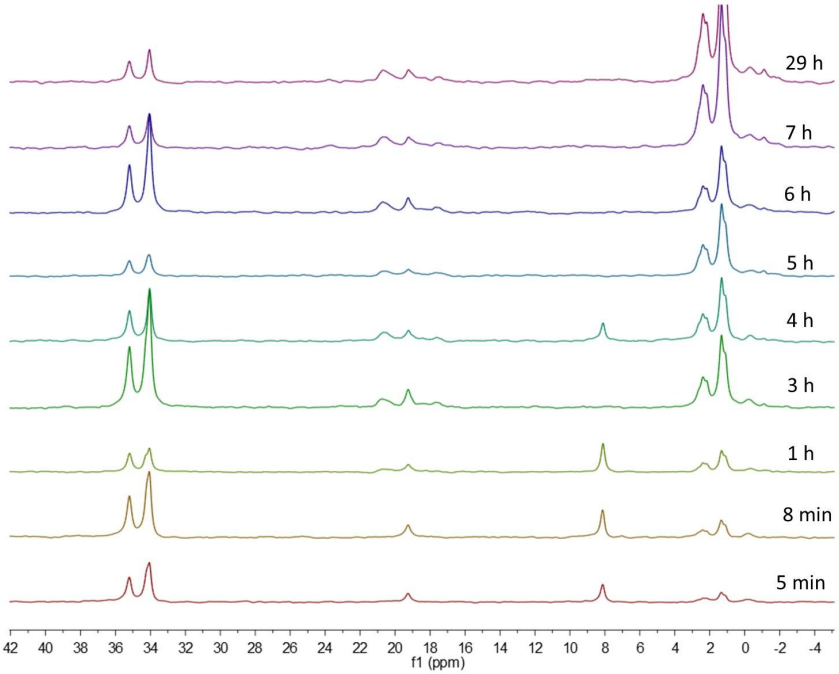


Figure S7 ^{31}P NMR traces of the reaction of **2a** with $PhP(O)Cl_2$ in presence of DMAP but without TEA

S7. NMR Spectra

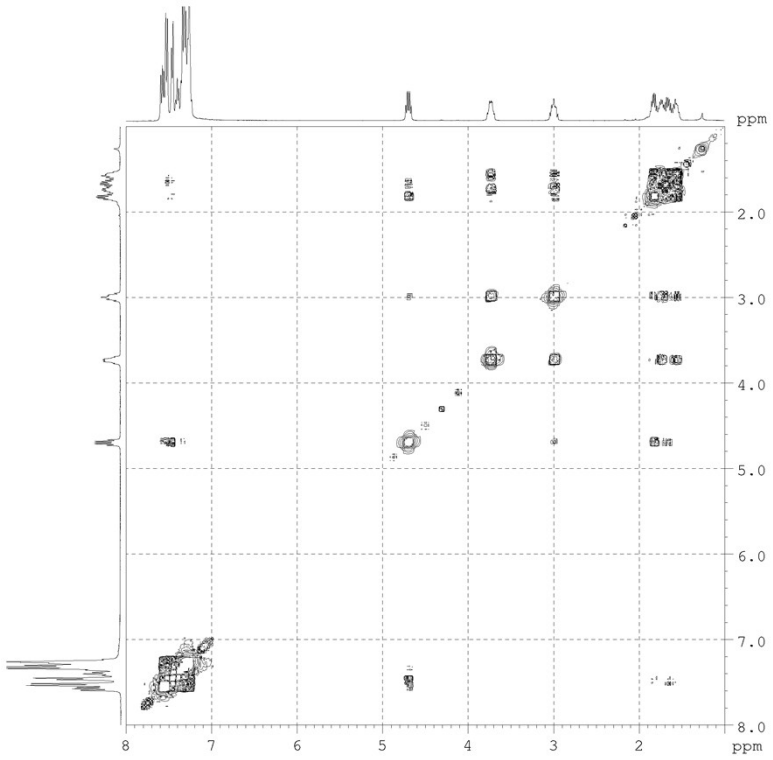


Figure S8 NOESY spectra of (R_P)-**3a**

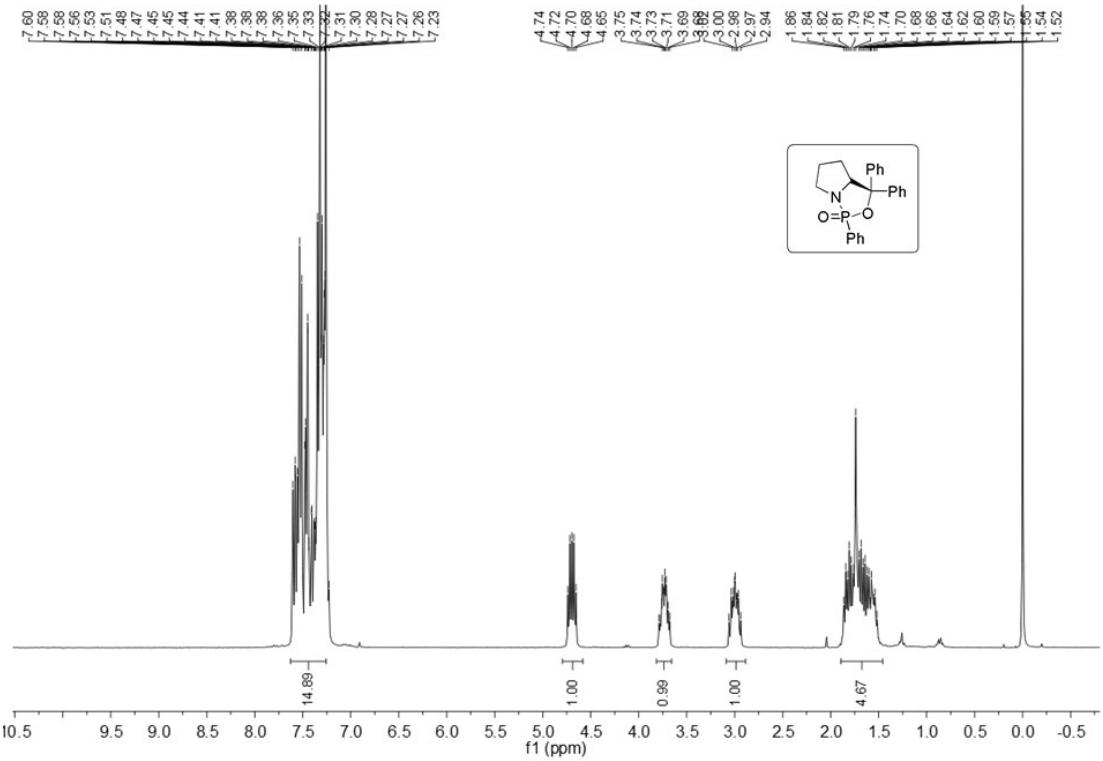


Figure S9 ^{1}H NMR of (R_P)-**3a**

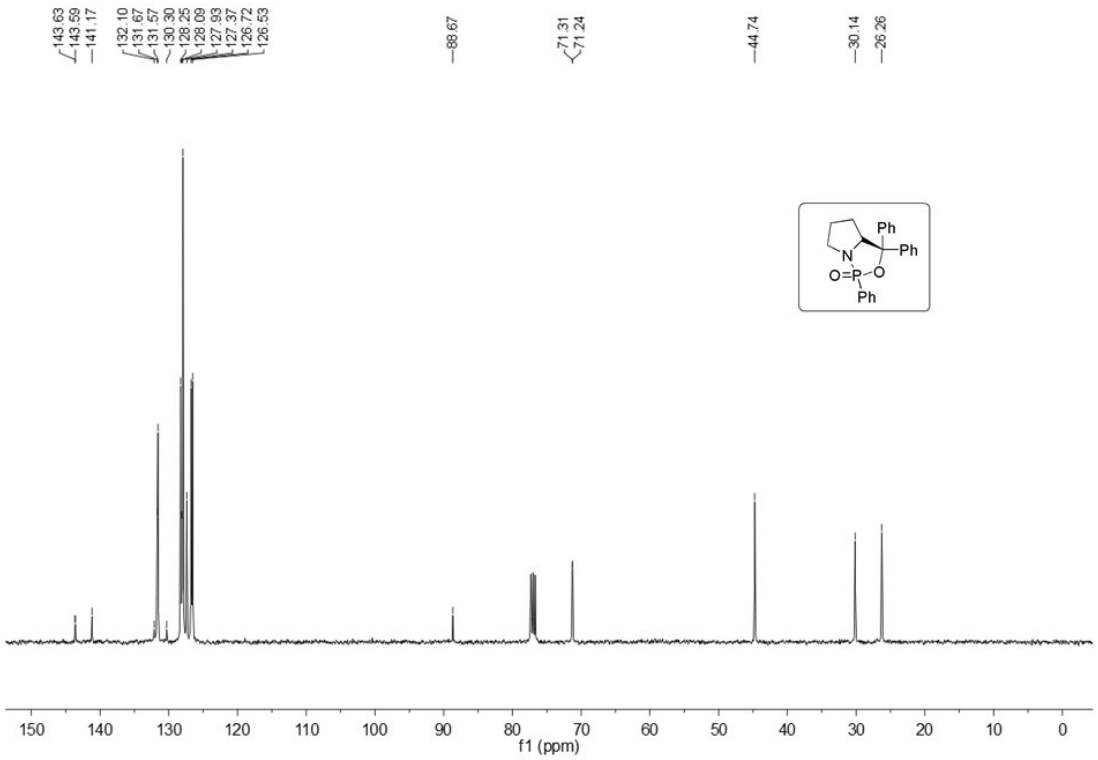


Figure S10 ^{13}C NMR of (R_P)-**3a**

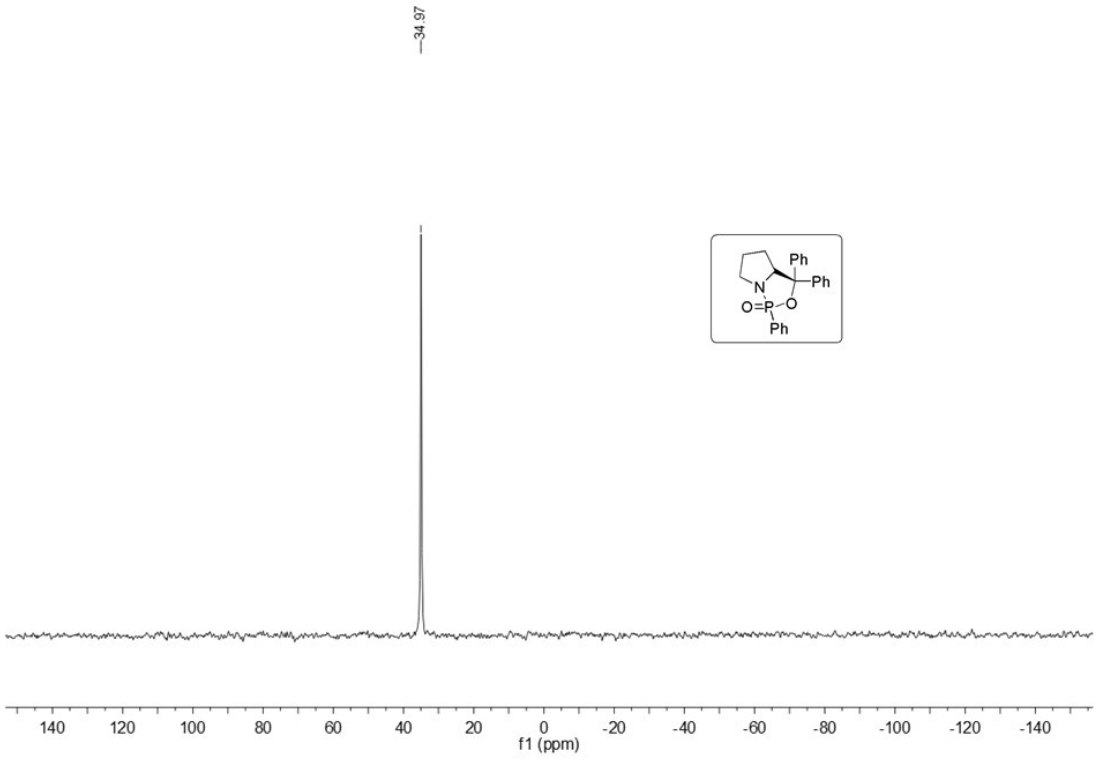


Figure S11 ^{31}P NMR of (R_P)-**3a**

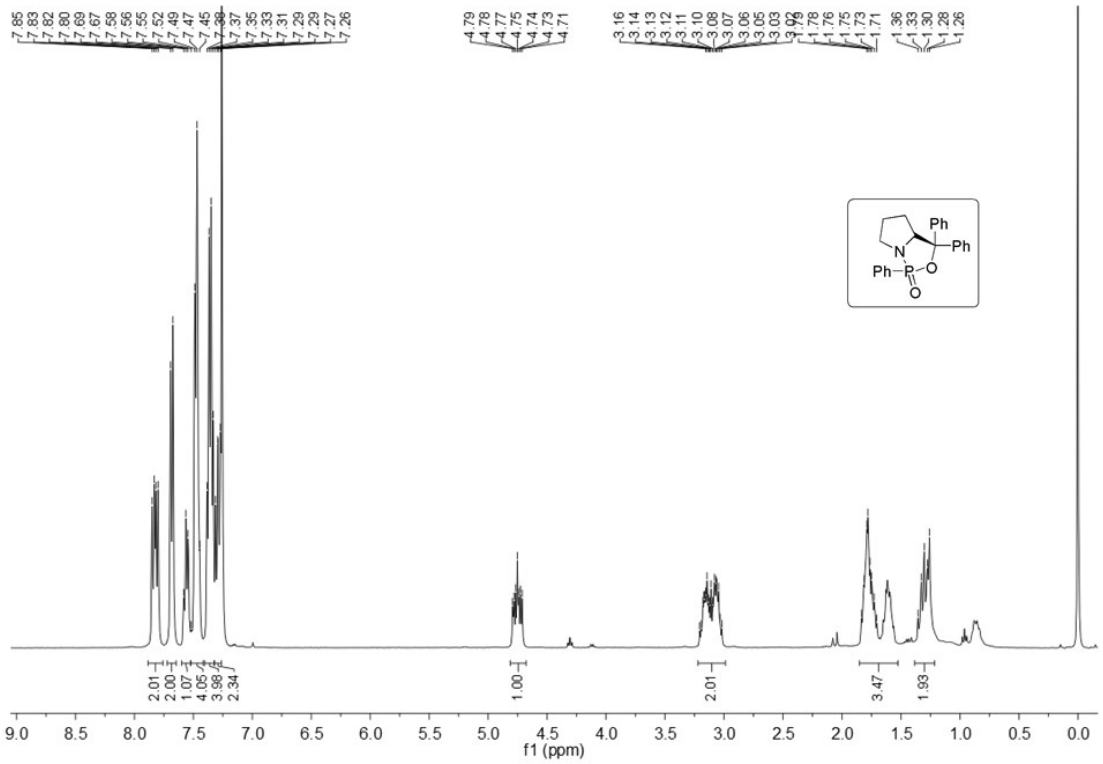


Figure S12 ^{1}H NMR of (S_P)-**3a**

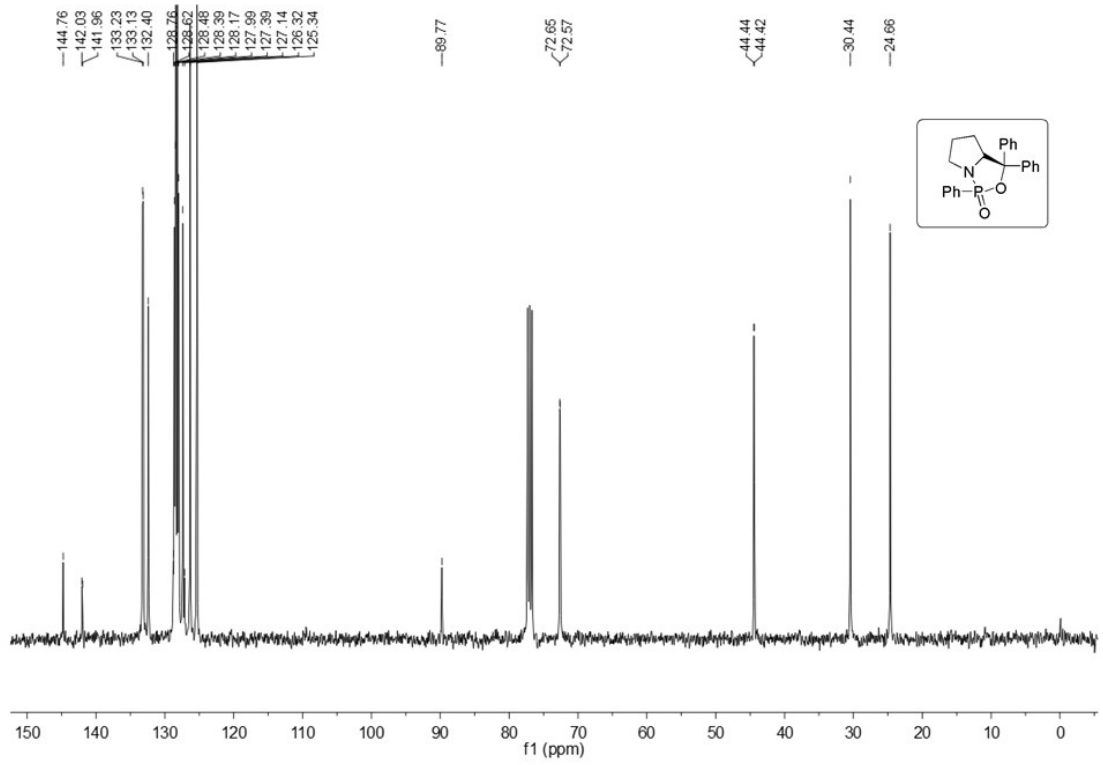


Figure S13 ^{13}C NMR of (S_P)-**3a**

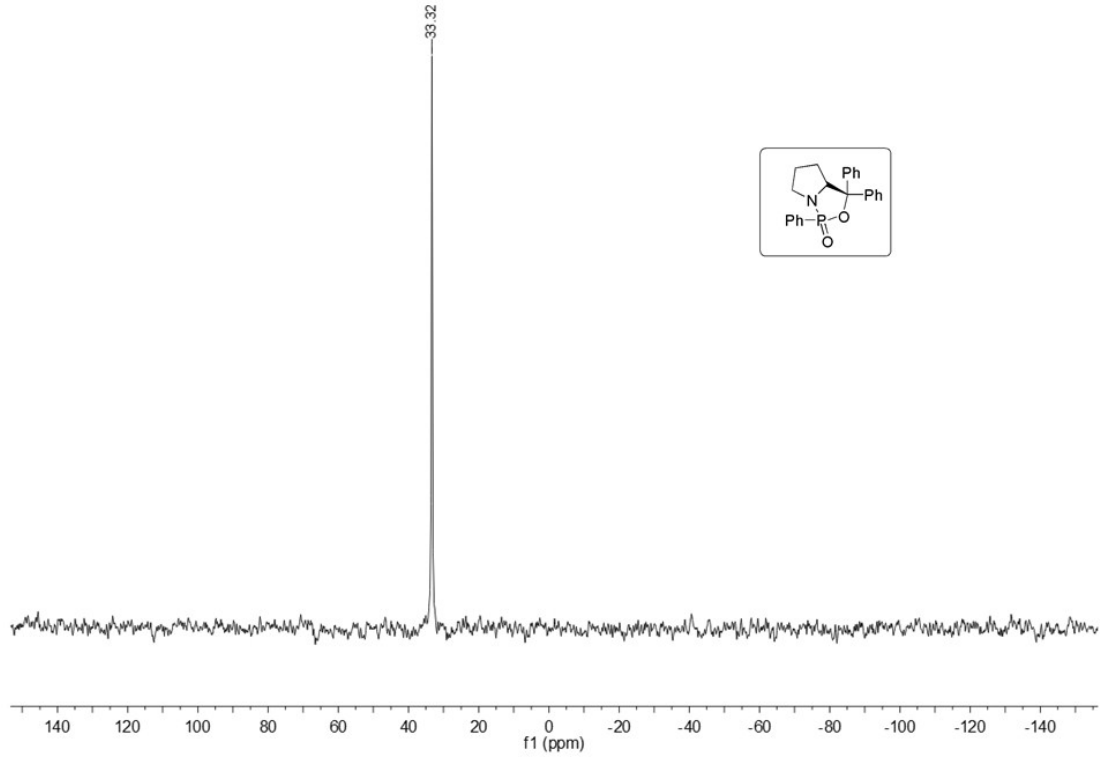


Figure S14 ^{31}P NMR of (S_P)-**3a**

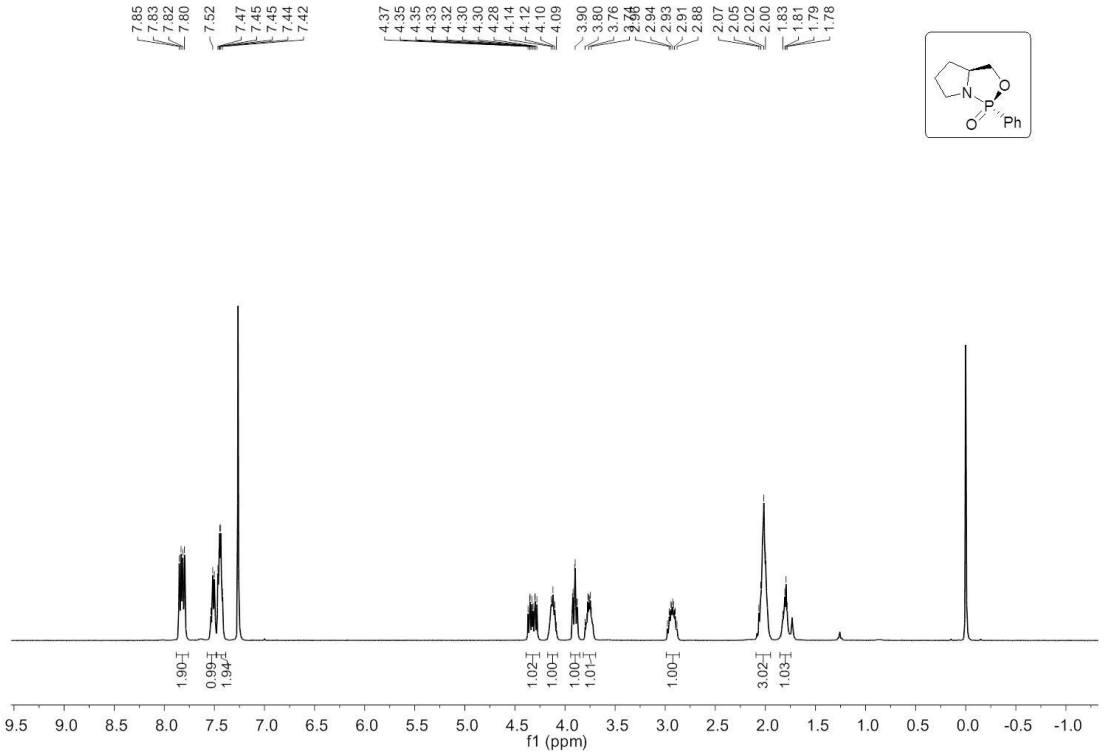


Figure S15 ^{1}H NMR of (R_P)-**3b**

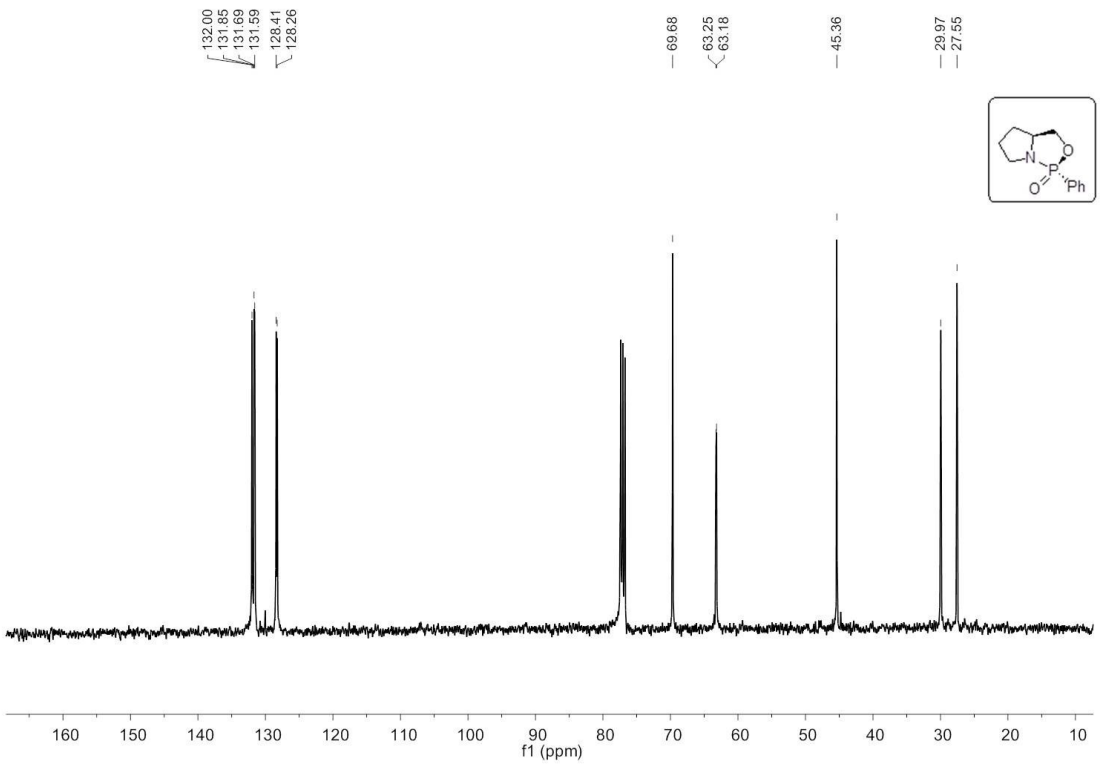


Figure S16 ^{13}C NMR of (R_P)-**3b**

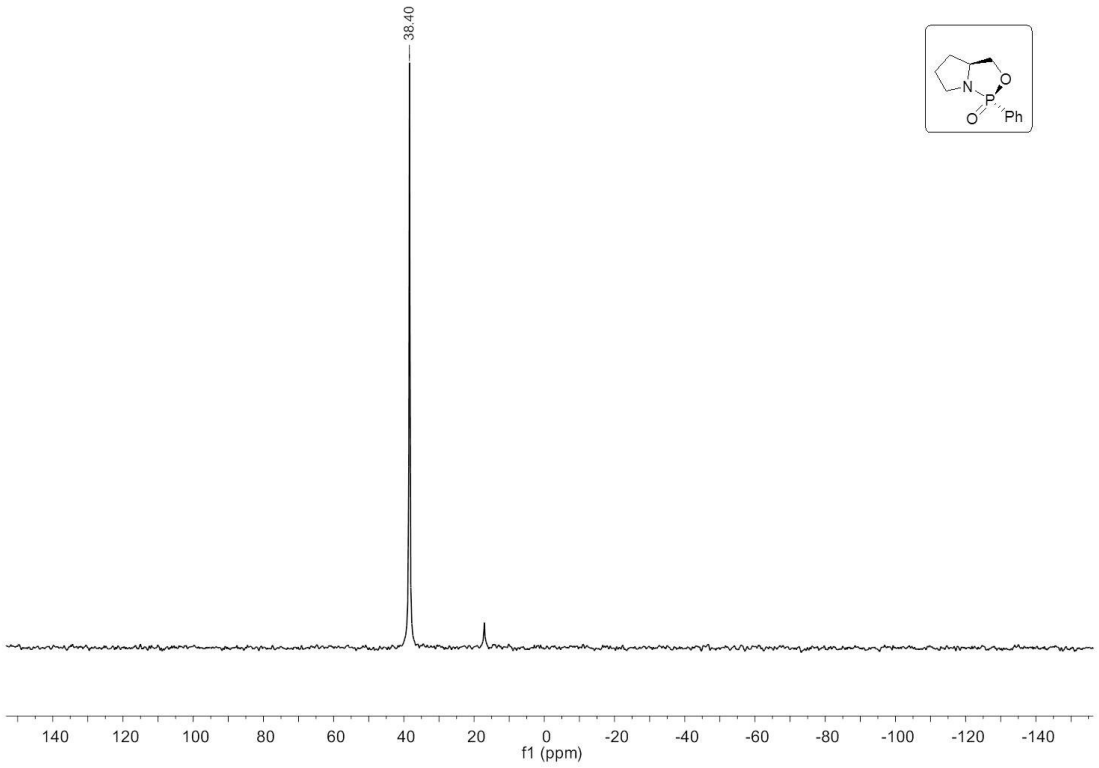


Figure S17 ^{31}P NMR of (R_P)-**3b**

S8. Computational Details

All calculations were performed using Gaussian 09 package. Geometries were optimized

using B3LYP density functional with a basis set of 6-31G (d,p) in solvent phase considering calculation cost and pratical possibility for the size of investigated system. Solvent (DCM) effects were calculated by using the PCM solvation model. All charge distributions were calculated by Natural Bond Orbital (NBO) analysis. All energies reported here are in Kcal/mol, and bond lengths are in angstroms (Å).

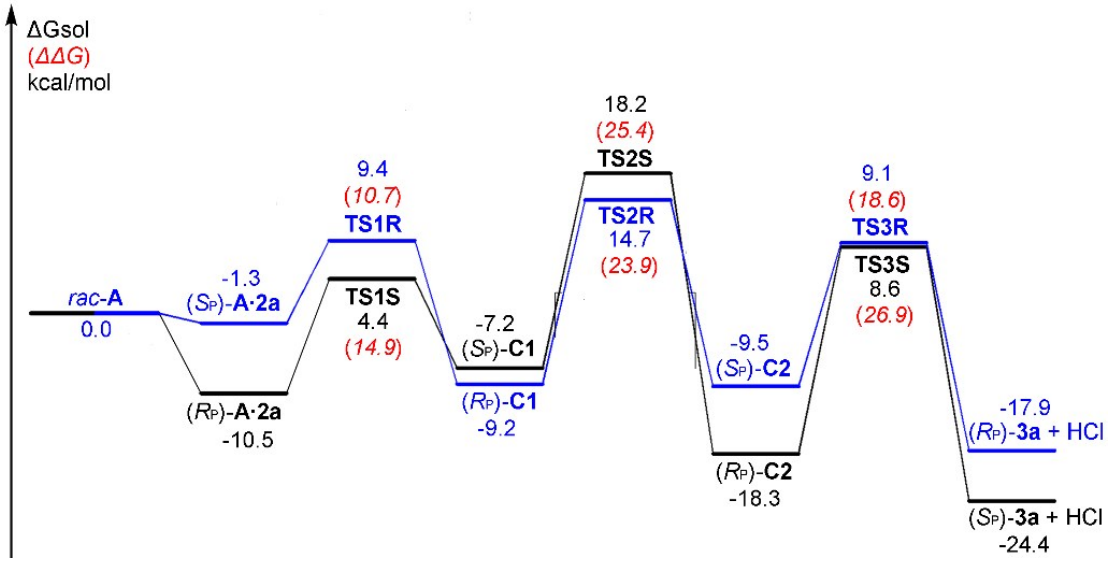
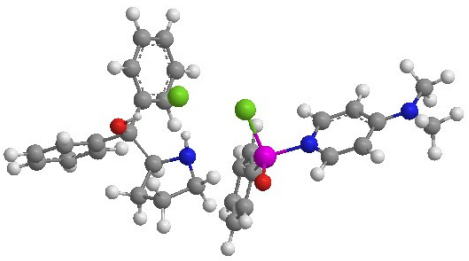
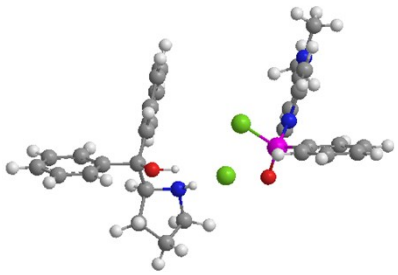
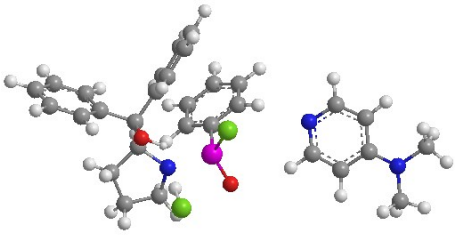
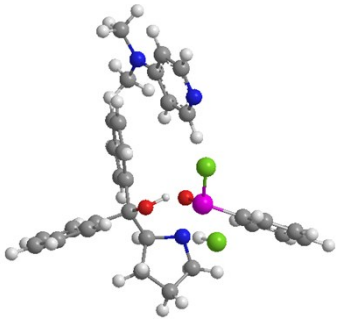
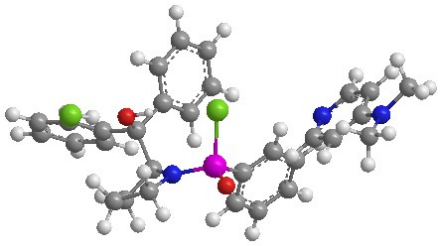


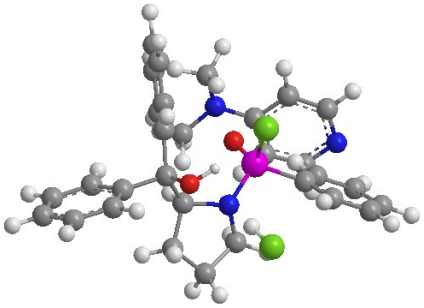
Figure S18 Reaction energy profile and geometries of stationary points and transition states

Table S4 Geometries of stationary points and transition states

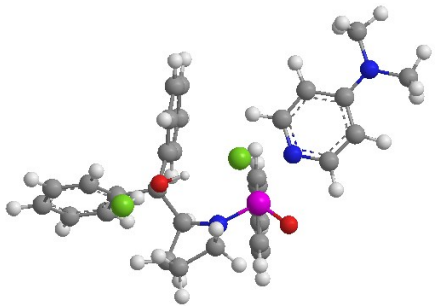
From (S_P)-**A·2a** to (R_P)-**3a**	From (R_P)-**A·2a** to (S_P)-**3a**
	
(S_P)-**A·2a**	(R_P)-**A·2a**
	
TS1R	**TS1S**



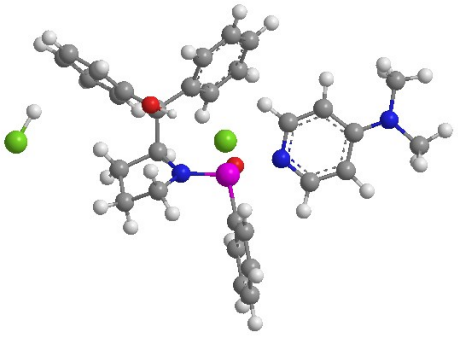
(R_P)-**C1**



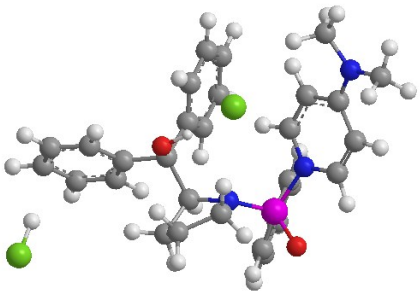
(S_P)-**C1**



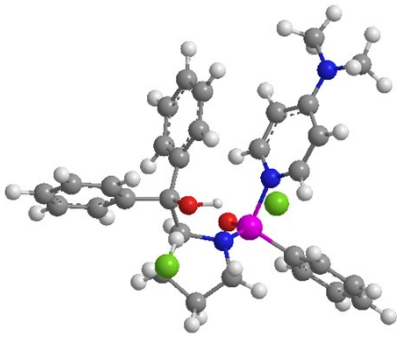
TS2R



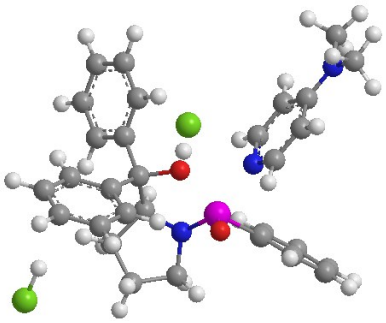
TS2S



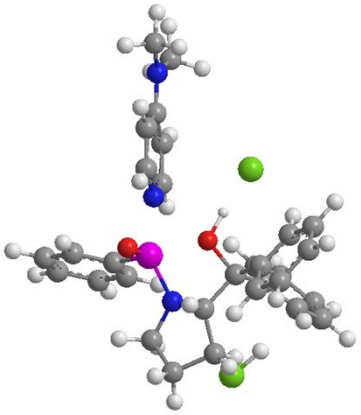
(S_P)-**C2**



(R_P)-**C2**



TS3R



TS3S

Table S5 Cartesian coordinates (in Å) and the sum of electronic and thermal Free Energies

(S_P)-**A**·**2a**	**TS1R**
Energy = -2739.704519	Energy = -2739.687400

Cl(1)	-2.624	-5.199	-0.622	Cl(1)	-1.601	4.280	-0.487
Cl(2)	0.613	-1.401	0.762	H(59)	-1.850	3.103	0.168
P(3)	1.368	-0.389	-0.814	Cl(2)	0.008	0.654	-0.940
O(4)	1.107	-0.853	-2.198	P(3)	-0.312	0.863	1.070
C(5)	1.132	1.379	-0.540	O(4)	0.644	1.793	1.724
C(6)	0.774	2.102	-1.691	C(5)	-0.355	-0.810	1.769
C(7)	1.243	2.035	0.698	C(6)	0.636	-1.726	1.387
C(8)	0.553	3.476	-1.603	C(7)	-1.263	-1.133	2.790
C(9)	1.034	3.411	0.769	C(8)	0.688	-2.972	2.013
C(10)	0.688	4.130	-0.379	C(9)	-1.203	-2.384	3.402
N(16)	6.984	-2.113	0.143	C(10)	-0.231	-3.306	3.009
N(17)	3.102	-0.760	-0.498	H(11)	1.389	-1.468	0.644
C(18)	5.727	-1.670	-0.059	H(12)	-2.013	-0.420	3.111
C(19)	7.722	-1.773	1.362	H(13)	1.459	-3.678	1.722
C(20)	7.688	-2.828	-0.923	H(14)	-1.910	-2.634	4.186
C(21)	5.018	-0.908	0.919	H(15)	-0.185	-4.280	3.487
C(22)	5.025	-1.941	-1.272	N(16)	7.259	1.094	-0.679
C(23)	3.740	-0.494	0.682	N(17)	3.497	-0.711	-0.011
C(24)	3.749	-1.489	-1.454	C(18)	6.039	0.503	-0.455
H(11)	0.655	1.578	-2.632	C(19)	8.309	0.349	-1.354
H(12)	1.472	1.487	1.608	C(20)	7.564	2.376	-0.065
H(13)	0.268	4.030	-2.492	C(21)	5.725	-0.783	-0.954
H(14)	1.123	3.921	1.723	C(22)	5.019	1.145	0.285
H(15)	0.512	5.199	-0.314	C(23)	4.469	-1.319	-0.707
H(25)	8.577	-2.440	1.452	C(24)	3.800	0.508	0.468
H(26)	7.097	-1.916	2.246	H(25)	9.188	0.985	-1.462
H(27)	8.079	-0.735	1.340	H(26)	7.996	0.040	-2.359
H(28)	7.158	-3.746	-1.195	H(27)	8.605	-0.553	-0.799
H(29)	8.682	-3.099	-0.572	H(28)	6.845	3.144	-0.373
H(30)	7.797	-2.203	-1.817	H(29)	8.554	2.700	-0.383
H(31)	5.458	-0.659	1.873	H(30)	7.556	2.325	1.034
H(32)	5.472	-2.516	-2.069	H(31)	6.442	-1.359	-1.525
H(33)	3.180	0.053	1.426	H(32)	5.165	2.128	0.714
H(34)	3.161	-1.696	-2.341	H(33)	4.231	-2.308	-1.097
O(35)	-4.724	-2.897	-0.647	H(34)	3.016	1.011	1.031
N(36)	-1.966	-1.988	-1.568	O(35)	-3.629	1.776	-1.417
C(37)	-3.192	-1.166	-1.425	N(36)	-2.111	1.735	1.100
C(38)	-4.145	-1.663	-0.284	C(37)	-3.444	1.063	0.904
C(39)	-3.906	-1.157	-2.819	C(38)	-3.832	0.659	-0.567
C(40)	-3.183	-2.248	-3.623	C(39)	-4.414	2.155	1.437
C(41)	-1.775	-2.223	-3.012	C(40)	-3.618	3.018	2.440
C(42)	-5.296	-0.643	-0.145	C(41)	-2.199	2.435	2.422

C(43)	-3.469	-1.765	1.102	C(42)	-5.353	0.373	-0.601
C(44)	-5.051	0.686	0.231	C(43)	-3.132	-0.591	-1.142
C(45)	-3.946	-2.711	2.022	C(44)	-5.910	-0.668	0.156
C(46)	-6.618	-1.028	-0.394	C(45)	-2.900	-0.646	-2.525
C(47)	-2.457	-0.898	1.521	C(46)	-6.202	1.147	-1.400
C(48)	-6.093	1.605	0.346	C(47)	-2.813	-1.716	-0.374
C(49)	-3.417	-2.793	3.308	C(48)	-7.280	-0.921	0.125
C(50)	-7.663	-0.109	-0.277	C(49)	-2.346	-1.780	-3.114
C(51)	-1.917	-0.982	2.808	C(50)	-7.574	0.887	-1.437
C(52)	-7.408	1.211	0.091	C(51)	-2.258	-2.854	-0.963
C(53)	-2.390	-1.935	3.708	C(52)	-8.121	-0.143	-0.674
H(62)	-4.049	-3.629	-0.619	C(53)	-2.018	-2.891	-2.334
H(59)	-2.097	-2.914	-1.134	H(62)	-2.688	2.004	-1.429
H(54)	-2.891	-0.136	-1.187	H(54)	-3.511	0.175	1.545
H(55)	-3.776	-0.177	-3.296	H(55)	-5.300	1.695	1.878
H(56)	-4.977	-1.343	-2.732	H(56)	-4.743	2.762	0.592
H(57)	-3.644	-3.222	-3.428	H(57)	-3.606	4.063	2.123
H(58)	-3.201	-2.065	-4.705	H(58)	-4.036	2.983	3.449
H(60)	-1.214	-3.151	-3.162	H(60)	-1.408	3.184	2.481
H(61)	-1.185	-1.402	-3.447	H(61)	-2.060	1.737	3.258
H(63)	-4.039	1.007	0.457	H(63)	-5.273	-1.301	0.766
H(64)	-4.730	-3.389	1.705	H(64)	-3.159	0.213	-3.133
H(65)	-6.806	-2.057	-0.676	H(65)	-5.782	1.951	-1.991
H(66)	-2.052	-0.176	0.822	H(66)	-2.983	-1.723	0.696
H(67)	-5.877	2.628	0.644	H(67)	-7.690	-1.732	0.721
H(68)	-3.805	-3.536	4.001	H(68)	-2.172	-1.796	-4.186
H(69)	-8.682	-0.432	-0.474	H(69)	-8.215	1.499	-2.066
H(70)	-1.109	-0.313	3.098	H(70)	-2.008	-3.708	-0.340
H(71)	-8.222	1.925	0.184	H(71)	-9.188	-0.343	-0.703
H(72)	-1.963	-2.007	4.705	H(72)	-1.584	-3.775	-2.793
(R_P)-**C1** Energy = -2739.717128				**TS2R** Energy = -2739.679009			
Cl(1)	-4.146	4.843	-0.328	Cl(1)	-5.002	-4.598	-2.099
H(59)	-3.928	3.554	-0.255	H(59)	-4.233	-3.696	-1.529
Cl(2)	-0.018	0.998	-0.357	Cl(2)	-0.119	-3.213	-1.434
P(3)	-0.379	0.689	1.706	P(3)	0.136	-0.738	-2.066
O(4)	0.547	1.551	2.492	O(4)	0.746	-0.787	-3.431
C(5)	-0.194	-1.098	1.937	C(5)	0.313	0.915	-1.240
C(6)	0.721	-1.848	1.186	C(6)	0.837	1.195	0.025
C(7)	-0.869	-1.693	3.016	C(7)	-0.073	1.987	-2.067
C(8)	0.924	-3.193	1.495	C(8)	0.959	2.515	0.464
C(9)	-0.667	-3.040	3.310	C(9)	0.062	3.304	-1.631

C(10)	0.225	-3.794	2.543	C(10)	0.575	3.572	-0.360
O(35)	-3.453	1.790	-0.265	O(35)	-3.072	-2.593	-0.726
N(36)	-1.977	1.091	1.943	N(36)	-1.549	-0.725	-2.204
C(37)	-3.223	0.329	1.694	C(37)	-2.597	-0.249	-1.278
C(38)	-3.770	0.468	0.207	C(38)	-3.020	-1.288	-0.151
C(39)	-4.140	0.910	2.794	C(39)	-3.717	0.090	-2.291
C(40)	-3.767	2.395	2.863	C(40)	-3.625	-1.005	-3.365
C(41)	-2.259	2.424	2.562	C(41)	-2.136	-1.395	-3.397
C(42)	-5.297	0.306	0.160	C(42)	-4.414	-0.980	0.430
C(43)	-3.165	-0.556	-0.783	C(43)	-2.060	-1.294	1.069
C(44)	-5.875	-0.923	0.514	C(44)	-4.809	0.334	0.728
C(45)	-3.110	-0.205	-2.142	C(45)	-1.660	-2.510	1.641
C(46)	-6.140	1.351	-0.231	C(46)	-5.290	-2.023	0.750
C(47)	-2.754	-1.844	-0.417	C(47)	-1.678	-0.109	1.713
C(48)	-7.257	-1.095	0.496	C(48)	-6.047	0.596	1.313
C(49)	-2.639	-1.102	-3.097	C(49)	-0.889	-2.539	2.804
C(50)	-7.526	1.176	-0.256	C(50)	-6.531	-1.761	1.334
C(51)	-2.282	-2.744	-1.375	C(51)	-0.910	-0.135	2.878
C(52)	-8.092	-0.043	0.111	C(52)	-6.917	-0.452	1.618
C(53)	-2.219	-2.378	-2.717	C(53)	-0.508	-1.351	3.430
H(11)	1.308	-1.390	0.394	H(11)	1.143	0.395	0.685
H(12)	-1.541	-1.102	3.630	H(12)	-0.465	1.785	-3.057
H(13)	1.640	-3.768	0.916	H(13)	1.359	2.713	1.454
H(14)	-1.197	-3.498	4.140	H(14)	-0.231	4.118	-2.286
H(15)	0.386	-4.843	2.774	H(15)	0.679	4.598	-0.018
H(62)	-2.487	1.820	-0.367	H(62)	-2.156	-2.859	-0.981
H(54)	-3.044	-0.728	1.888	H(54)	-2.242	0.658	-0.786
H(55)	-3.884	0.414	3.738	H(55)	-3.485	1.069	-2.726
H(56)	-5.199	0.739	2.605	H(56)	-4.704	0.154	-1.836
H(57)	-4.318	2.962	2.110	H(57)	-4.241	-1.863	-3.091
H(58)	-3.991	2.836	3.838	H(58)	-3.969	-0.650	-4.341
H(60)	-1.995	3.240	1.882	H(60)	-1.986	-2.477	-3.357
H(61)	-1.648	2.532	3.461	H(61)	-1.612	-1.023	-4.281
H(63)	-5.243	-1.759	0.794	H(63)	-4.156	1.169	0.498
H(64)	-3.438	0.782	-2.445	H(64)	-1.958	-3.440	1.174
H(65)	-5.723	2.305	-0.526	H(65)	-5.002	-3.046	0.546
H(66)	-2.780	-2.170	0.616	H(66)	-1.985	0.854	1.321
H(67)	-7.682	-2.055	0.775	H(67)	-6.332	1.622	1.527
H(68)	-2.601	-0.803	-4.140	H(68)	-0.596	-3.497	3.224
H(69)	-8.160	2.001	-0.565	H(69)	-7.195	-2.589	1.565
H(70)	-1.956	-3.732	-1.061	H(70)	-0.633	0.801	3.355
H(71)	-9.169	-0.177	0.091	H(71)	-7.883	-0.249	2.071
H(72)	-1.849	-3.078	-3.460	H(72)	0.083	-1.373	4.341

N(16)	7.248	1.569	0.152	N(16)	5.818	-2.295	0.357
N(17)	3.577	-0.531	0.007	N(17)	2.011	-1.295	-1.072
C(18)	6.048	0.893	0.096	C(18)	4.576	-1.971	-0.112
C(19)	8.285	1.281	-0.824	C(19)	5.961	-2.956	1.648
C(20)	7.360	2.769	0.967	C(20)	6.990	-2.096	-0.484
C(21)	5.837	-0.188	-0.791	C(21)	3.403	-2.198	0.654
C(22)	4.955	1.233	0.925	C(22)	4.382	-1.397	-1.392
C(23)	4.612	-0.843	-0.785	C(23)	2.167	-1.860	0.139
C(24)	3.776	0.504	0.841	C(24)	3.106	-1.080	-1.820
H(25)	9.169	1.877	-0.593	H(25)	7.019	-3.126	1.846
H(26)	7.975	1.514	-1.854	H(26)	5.449	-3.926	1.670
H(27)	8.578	0.226	-0.789	H(27)	5.562	-2.338	2.461
H(28)	6.687	3.572	0.632	H(28)	6.952	-2.709	-1.394
H(29)	8.385	3.140	0.917	H(29)	7.883	-2.375	0.076
H(30)	7.135	2.555	2.018	H(30)	7.094	-1.046	-0.781
H(31)	6.605	-0.515	-1.480	H(31)	3.446	-2.650	1.635
H(32)	5.009	2.057	1.625	H(32)	5.211	-1.208	-2.060
Cl(1)	-4.146	4.843	-0.328	H(33)	1.262	-2.066	0.699
H(59)	-3.928	3.554	-0.255	H(34)	2.916	-0.666	-2.804
(R_P)-**C2** Energy = -2739.717631				**TS3R** Energy = -2739.687870			
Cl(1)	-7.162	-2.362	-2.500	Cl(1)	-6.956	1.150	-1.223
H(59)	-6.536	-2.483	-1.365	H(59)	-6.161	0.246	-1.714
Cl(2)	1.550	-4.083	-1.165	Cl(2)	0.149	-2.393	-2.465
P(3)	0.849	0.533	-1.897	P(3)	0.036	1.112	-0.589
O(4)	1.282	1.078	-3.221	O(4)	-0.160	1.376	-2.054
C(5)	0.374	1.827	-0.710	C(5)	1.130	2.472	0.073
C(6)	0.937	1.999	0.568	C(6)	1.311	2.688	1.445
C(7)	-0.551	2.781	-1.195	C(7)	1.803	3.300	-0.838
C(8)	0.560	3.089	1.362	C(8)	2.160	3.699	1.901
C(9)	-0.934	3.863	-0.396	C(9)	2.639	4.320	-0.383
C(10)	-0.381	4.017	0.886	C(10)	2.825	4.517	0.987
N(16)	5.367	-2.988	-0.389	O(35)	-0.551	-0.698	-0.385
N(17)	2.345	-0.241	-1.204	N(36)	-1.221	1.402	0.516
C(18)	4.455	-2.004	-0.591	C(37)	-2.057	0.352	1.085
C(19)	5.040	-4.088	0.538	C(38)	-1.853	-0.940	0.213
C(20)	6.466	-3.183	-1.339	C(39)	-3.473	0.981	1.214
C(21)	3.323	-1.861	0.264	C(40)	-3.382	2.317	0.451
C(22)	4.538	-1.082	-1.685	C(41)	-1.903	2.705	0.589
C(23)	2.292	-1.036	-0.089	C(42)	-2.924	-1.116	-0.884
C(24)	3.481	-0.252	-1.971	C(43)	-1.754	-2.173	1.127
O(35)	-1.443	-3.172	-0.855	C(44)	-4.027	-1.959	-0.684

N(36)	-0.251	-0.711	-1.897	C(45)	-0.893	-3.236	0.826
C(37)	-1.604	-0.758	-1.266	C(46)	-2.838	-0.401	-2.090
C(38)	-1.774	-1.950	-0.232	C(47)	-2.553	-2.270	2.278
C(39)	-2.516	-0.911	-2.512	C(48)	-5.023	-2.083	-1.654
C(40)	-1.726	-1.820	-3.479	C(49)	-0.826	-4.353	1.661
C(41)	-0.232	-1.585	-3.136	C(50)	-3.835	-0.526	-3.058
C(42)	-3.271	-2.052	0.178	C(51)	-2.491	-3.391	3.106
C(43)	-0.976	-1.761	1.088	C(52)	-4.933	-1.365	-2.850
C(44)	-4.012	-0.929	0.599	C(53)	-1.622	-4.438	2.803
C(45)	-0.328	-2.872	1.662	H(11)	0.771	2.075	2.162
C(46)	-3.911	-3.304	0.168	H(12)	1.643	3.149	-1.901
C(47)	-0.945	-0.541	1.793	H(13)	2.292	3.854	2.968
C(48)	-5.347	-1.049	0.998	H(14)	3.141	4.965	-1.098
C(49)	0.341	-2.760	2.888	H(15)	3.478	5.310	1.340
C(50)	-5.247	-3.430	0.576	H(54)	-1.686	0.106	2.087
C(51)	-0.276	-0.429	3.019	H(55)	-3.689	1.161	2.272
C(52)	-5.974	-2.305	0.994	H(56)	-4.262	0.336	0.823
C(53)	0.373	-1.539	3.573	H(57)	-3.620	2.165	-0.605
H(11)	1.670	1.291	0.956	H(58)	-4.060	3.077	0.847
H(12)	-0.948	2.685	-2.203	H(60)	-1.559	3.372	-0.204
H(13)	1.001	3.212	2.351	H(61)	-1.707	3.196	1.554
H(14)	-1.649	4.593	-0.779	H(63)	-4.109	-2.540	0.227
H(15)	-0.675	4.862	1.507	H(64)	-0.281	-3.202	-0.068
H(25)	5.804	-4.862	0.445	H(65)	-1.982	0.233	-2.295
H(26)	4.052	-4.509	0.286	H(66)	-3.241	-1.471	2.536
H(27)	5.040	-3.735	1.576	H(67)	-5.860	-2.752	-1.479
H(28)	6.103	-3.544	-2.316	H(68)	-0.150	-5.165	1.406
H(29)	7.162	-3.919	-0.928	H(69)	-3.741	0.025	-3.989
H(30)	7.023	-2.249	-1.490	H(70)	-3.123	-3.441	3.989
H(31)	3.178	-2.499	1.129	H(71)	-5.693	-1.480	-3.618
H(32)	5.387	-1.077	-2.361	H(72)	-1.568	-5.310	3.448
H(33)	1.363	-1.029	0.472	N(16)	5.384	-2.035	-0.956
H(34)	3.456	0.402	-2.839	N(17)	1.760	0.010	-0.631
H(62)	-0.459	-3.330	-0.917	C(18)	4.197	-1.371	-0.852
H(54)	-1.791	0.192	-0.753	C(19)	5.936	-2.735	0.197
H(55)	-2.660	0.087	-2.955	C(20)	6.020	-2.190	-2.260
H(56)	-3.507	-1.312	-2.271	C(21)	3.495	-1.282	0.380
H(57)	-1.984	-2.869	-3.304	C(22)	3.593	-0.735	-1.964
H(58)	-1.940	-1.578	-4.529	C(23)	2.302	-0.597	0.441
H(60)	0.308	-2.513	-2.909	C(24)	2.390	-0.078	-1.817
H(61)	0.292	-1.045	-3.934	H(25)	6.902	-3.160	-0.073
H(63)	-3.554	0.060	0.618	H(26)	5.285	-3.552	0.535
H(64)	-0.328	-3.822	1.134	H(27)	6.095	-2.050	1.038

H(65)	-3.346	-4.172	-0.163	H(28)	5.386	-2.749	-2.959
H(66)	-1.444	0.341	1.395	H(29)	6.956	-2.735	-2.136
H(67)	-5.897	-0.163	1.314	H(30)	6.253	-1.217	-2.705
H(68)	0.835	-3.638	3.307	H(31)	3.865	-1.755	1.279
H(69)	-5.719	-4.413	0.573	H(32)	4.034	-0.780	-2.950
H(70)	-0.269	0.529	3.540	H(33)	1.744	-0.534	1.368
H(71)	-7.009	-2.404	1.321	H(34)	1.874	0.390	-2.647
H(72)	0.892	-1.454	4.529	H(62)	-0.261	-1.428	-1.344
(R_P)-**A**·**2a** Energy = -2739.722044				**TS1S** Energy = -2739.695172			
Cl(1)	1.618	-0.422	-0.517	Cl(1)	1.891	1.049	1.564
P(3)	3.016	0.489	0.659	P(3)	2.375	1.418	-0.393
O(4)	2.643	0.578	2.093	O(4)	1.375	1.016	-1.416
C(5)	3.553	1.964	-0.209	C(5)	2.807	3.173	-0.439
C(6)	4.897	2.366	-0.112	C(6)	2.274	3.916	-1.504
C(7)	2.606	2.773	-0.860	C(7)	3.614	3.791	0.527
C(8)	5.294	3.571	-0.689	C(8)	2.554	5.278	-1.600
C(9)	3.021	3.978	-1.426	C(9)	3.891	5.152	0.415
C(10)	4.358	4.373	-1.347	C(10)	3.363	5.894	-0.644
N(16)	7.161	-3.730	0.243	H(11)	1.641	3.425	-2.235
N(17)	4.370	-0.667	0.513	H(12)	4.033	3.220	1.349
C(18)	6.281	-2.726	0.335	H(13)	2.139	5.857	-2.419
C(19)	7.505	-4.529	1.426	H(14)	4.519	5.632	1.159
C(20)	7.769	-4.074	-1.049	H(15)	3.580	6.955	-0.721
C(21)	5.667	-2.368	1.577	Cl(2)	5.903	1.207	1.738
C(22)	5.892	-1.952	-0.807	H(59)	5.034	0.761	0.742
C(23)	4.739	-1.371	1.631	N(16)	-5.232	-0.816	-0.868
C(24)	4.956	-0.968	-0.691	N(17)	-1.971	0.860	1.258
H(11)	5.629	1.754	0.405	C(18)	-4.158	-0.288	-0.178
H(12)	1.557	2.489	-0.917	C(19)	-5.205	-0.843	-2.321
H(13)	6.332	3.880	-0.624	C(20)	-6.171	-1.684	-0.177
H(14)	2.293	4.607	-1.929	C(21)	-3.110	0.400	-0.829
H(15)	4.673	5.311	-1.796	C(22)	-4.042	-0.398	1.227
H(25)	7.982	-3.911	2.192	C(23)	-2.070	0.937	-0.077
H(26)	8.201	-5.311	1.130	C(24)	-2.956	0.189	1.868
H(27)	6.614	-5.002	1.849	H(25)	-5.081	0.166	-2.729
H(28)	7.006	-4.377	-1.772	H(26)	-6.156	-1.232	-2.689
H(29)	8.456	-4.904	-0.903	H(27)	-4.396	-1.474	-2.722
H(30)	8.333	-3.228	-1.453	H(28)	-5.704	-2.608	0.196
H(31)	5.915	-2.879	2.497	H(29)	-6.973	-1.960	-0.863
H(32)	6.315	-2.135	-1.783	H(30)	-6.629	-1.168	0.674
H(33)	4.240	-1.083	2.547	H(31)	-3.090	0.514	-1.906

H(34)	4.638	-0.383	-1.545	H(32)	-4.780	-0.925	1.818
Cl(2)	-1.171	2.558	-0.816	H(33)	-1.254	1.442	-0.591
O(35)	-3.683	0.622	-0.694	H(34)	-2.875	0.103	2.951
N(36)	-1.685	0.014	1.551	O(35)	4.236	-1.708	1.381
C(37)	-3.068	-0.475	1.410	N(36)	4.120	0.448	-0.516
C(38)	-3.523	-0.646	-0.071	C(37)	4.091	-1.003	-0.940
C(39)	-3.979	0.486	2.238	C(38)	3.614	-2.034	0.146
C(40)	-2.997	1.278	3.140	C(39)	5.572	-1.213	-1.337
C(41)	-1.634	0.584	2.904	C(40)	6.065	0.146	-1.881
C(42)	-4.919	-1.306	-0.068	C(41)	4.909	1.121	-1.598
C(43)	-2.564	-1.524	-0.906	C(42)	4.146	-3.434	-0.242
C(44)	-5.084	-2.631	0.364	C(43)	2.086	-2.162	0.322
C(45)	-2.594	-1.401	-2.303	C(44)	3.691	-4.080	-1.400
C(46)	-6.054	-0.594	-0.475	C(45)	1.593	-2.557	1.575
C(47)	-1.706	-2.480	-0.345	C(46)	5.093	-4.081	0.560
C(48)	-6.346	-3.224	0.396	C(47)	1.174	-2.009	-0.730
C(49)	-1.796	-2.207	-3.115	C(48)	4.181	-5.335	-1.756
C(50)	-7.319	-1.188	-0.446	C(49)	0.231	-2.766	1.777
C(51)	-0.908	-3.292	-1.157	C(50)	5.575	-5.344	0.207
C(52)	-7.472	-2.504	-0.009	C(51)	-0.190	-2.230	-0.531
C(53)	-0.949	-3.159	-2.546	C(52)	5.127	-5.974	-0.953
H(62)	-2.824	1.101	-0.737	C(53)	-0.669	-2.603	0.723
H(59)	-1.521	0.772	0.883	H(62)	3.841	-0.892	1.719
H(54)	-3.106	-1.465	1.884	H(54)	3.462	-1.093	-1.833
H(55)	-4.717	-0.072	2.820	H(55)	5.666	-2.022	-2.062
H(56)	-4.518	1.156	1.566	H(56)	6.134	-1.497	-0.445
H(57)	-2.942	2.323	2.817	H(57)	6.973	0.465	-1.365
H(58)	-3.292	1.276	4.195	H(58)	6.284	0.112	-2.951
H(60)	-0.775	1.255	3.001	H(60)	5.245	2.098	-1.249
H(61)	-1.499	-0.232	3.628	H(61)	4.293	1.262	-2.495
H(63)	-4.218	-3.213	0.664	H(63)	2.935	-3.611	-2.022
H(64)	-3.246	-0.656	-2.746	H(64)	2.292	-2.698	2.393
H(65)	-5.937	0.428	-0.815	H(65)	5.445	-3.593	1.459
H(66)	-1.632	-2.578	0.732	H(66)	1.503	-1.690	-1.711
H(67)	-6.448	-4.252	0.734	H(67)	3.815	-5.817	-2.658
H(68)	-1.836	-2.087	-4.195	H(68)	-0.127	-3.058	2.760
H(69)	-8.186	-0.616	-0.767	H(69)	6.308	-5.832	0.844
H(70)	-0.247	-4.022	-0.699	H(70)	-0.878	-2.090	-1.358
H(71)	-8.456	-2.965	0.014	H(71)	5.504	-6.955	-1.226
H(72)	-0.327	-3.788	-3.176	H(72)	-1.734	-2.748	0.880
(S_P)-**C1** Energy = -2739.713488				**TS2S** Energy = -2739.673128			

Cl(1)	0.152	-0.800	2.167	Cl(1)	-0.455	-0.068	2.453
P(3)	1.007	-0.428	0.301	Cl(2)	7.612	0.722	-0.391
O(4)	1.485	0.975	0.137	H(59)	7.235	-0.517	-0.291
C(5)	2.330	-1.659	0.224	P(3)	-0.376	0.447	-0.007
C(6)	3.600	-1.191	-0.139	O(4)	-0.301	-0.320	-1.302
C(7)	2.137	-3.016	0.532	C(5)	-1.139	2.111	-0.035
C(8)	4.676	-2.079	-0.206	C(6)	-1.131	2.751	-1.284
C(9)	3.214	-3.895	0.455	C(7)	-1.708	2.752	1.072
C(10)	4.480	-3.428	0.087	C(8)	-1.682	4.026	-1.419
O(35)	-2.850	-0.824	0.483	C(9)	-2.257	4.028	0.929
N(36)	-0.239	-0.930	-0.786	C(10)	-2.244	4.666	-0.313
C(37)	-1.330	0.044	-1.204	O(35)	2.675	-0.999	1.924
C(38)	-2.431	0.389	-0.131	N(36)	1.257	0.832	0.270
C(39)	-1.947	-0.692	-2.417	C(37)	2.399	0.047	-0.258
C(40)	-0.821	-1.535	-3.044	C(38)	2.682	-1.296	0.536
C(41)	0.370	-1.390	-2.089	C(39)	3.597	1.037	-0.117
C(42)	-3.662	0.952	-0.879	C(40)	2.999	2.361	0.388
C(43)	-2.057	1.436	0.939	C(41)	1.751	1.905	1.146
C(44)	-3.585	2.171	-1.567	C(42)	4.096	-1.813	0.204
C(45)	-2.779	1.422	2.143	C(43)	1.715	-2.470	0.237
C(46)	-4.877	0.258	-0.875	C(44)	4.494	-2.036	-1.123
C(47)	-1.128	2.462	0.734	C(45)	1.377	-3.346	1.280
C(48)	-4.691	2.675	-2.249	C(46)	5.010	-2.087	1.229
C(49)	-2.564	2.390	3.120	C(47)	1.253	-2.771	-1.052
C(50)	-5.987	0.769	-1.550	C(48)	5.769	-2.513	-1.418
C(51)	-0.915	3.435	1.713	C(49)	0.601	-4.481	1.045
C(52)	-5.899	1.975	-2.243	C(50)	6.288	-2.570	0.937
C(53)	-1.628	3.405	2.909	C(51)	0.480	-3.907	-1.289
H(11)	3.746	-0.138	-0.354	C(52)	6.677	-2.783	-0.388
H(12)	1.161	-3.385	0.827	C(53)	0.152	-4.771	-0.244
H(13)	5.658	-1.702	-0.475	H(11)	-0.704	2.242	-2.142
H(14)	3.066	-4.945	0.689	H(12)	-1.714	2.252	2.034
H(15)	5.316	-4.120	0.036	H(13)	-1.672	4.517	-2.388
H(62)	-2.188	-1.065	1.146	H(14)	-2.693	4.523	1.791
H(54)	-0.852	0.970	-1.543	H(15)	-2.671	5.660	-0.419
H(55)	-2.380	0.023	-3.117	H(62)	1.765	-0.747	2.170
H(56)	-2.755	-1.335	-2.063	H(54)	2.190	-0.186	-1.303
H(57)	-1.122	-2.582	-3.128	H(55)	4.135	1.151	-1.060
H(58)	-0.548	-1.190	-4.045	H(56)	4.309	0.656	0.616
H(60)	0.909	-2.324	-1.931	H(57)	3.696	2.920	1.021
H(61)	1.079	-0.641	-2.464	H(58)	2.705	3.005	-0.447
H(63)	-2.663	2.743	-1.557	H(60)	2.006	1.532	2.144
H(64)	-3.516	0.643	2.306	H(61)	1.003	2.690	1.257

H(65)	-4.947	-0.681	-0.339	H(63)	3.805	-1.842	-1.938
H(66)	-0.531	2.499	-0.169	H(64)	1.735	-3.132	2.280
H(67)	-4.611	3.621	-2.776	H(65)	4.713	-1.914	2.256
H(68)	-3.132	2.355	4.045	H(66)	1.456	-2.101	-1.878
H(69)	-6.923	0.218	-1.533	H(67)	6.056	-2.676	-2.453
H(70)	-0.179	4.214	1.537	H(68)	0.357	-5.143	1.872
H(71)	-6.763	2.371	-2.769	H(69)	6.979	-2.776	1.750
H(72)	-1.458	4.162	3.669	H(70)	0.127	-4.110	-2.297
Cl(2)	-1.455	-3.870	-0.168	H(71)	7.666	-3.170	-0.616
H(59)	-1.087	-2.606	-0.317	H(72)	-0.445	-5.660	-0.432
N(16)	3.977	3.716	-0.872	N(16)	-5.647	-2.842	-0.087
N(17)	6.923	0.673	-0.725	N(17)	-2.202	-0.470	0.257
C(18)	4.931	2.725	-0.827	C(18)	-4.523	-2.071	0.013
C(19)	3.196	4.011	0.327	C(19)	-5.566	-4.279	0.142
C(20)	3.403	4.092	-2.155	C(20)	-6.869	-2.276	-0.641
C(21)	5.402	2.190	0.396	C(21)	-3.282	-2.603	0.446
C(22)	5.513	2.179	-1.996	C(22)	-4.523	-0.694	-0.310
C(23)	6.375	1.200	0.381	C(23)	-2.179	-1.786	0.553
C(24)	6.477	1.185	-1.882	C(24)	-3.363	0.047	-0.181
H(25)	2.594	3.151	0.648	H(25)	-4.929	-4.783	-0.598
H(26)	2.531	4.849	0.113	H(26)	-6.566	-4.708	0.080
H(27)	3.851	4.319	1.149	H(27)	-5.171	-4.497	1.140
H(28)	4.184	4.401	-2.855	H(28)	-7.188	-1.396	-0.071
H(29)	2.738	4.945	-2.009	H(29)	-7.666	-3.017	-0.581
H(30)	2.824	3.278	-2.618	H(30)	-6.752	-1.980	-1.693
H(31)	5.010	2.526	1.347	H(31)	-3.167	-3.648	0.699
H(32)	5.215	2.509	-2.983	H(32)	-5.413	-0.194	-0.669
H(33)	6.728	0.793	1.328	H(33)	-1.233	-2.176	0.904
H(34)	6.912	0.766	-2.788	H(34)	-3.357	1.098	-0.440
(R_P)-**C2** Energy = -2739.731221				**TS3S** Energy = -2739.688389			
Cl(1)	-1.093	0.588	2.985	Cl(1)	-0.057	-2.507	0.649
Cl(2)	3.400	1.724	2.825	Cl(2)	4.585	3.384	1.634
H(59)	2.541	0.920	2.218	H(59)	4.494	2.150	2.031
P(3)	-1.737	1.143	-1.148	P(3)	0.654	0.825	-2.114
O(4)	-1.648	0.784	-2.598	O(4)	0.339	0.363	-3.505
C(5)	-2.905	2.475	-0.749	C(5)	-0.043	2.496	-1.733
C(6)	-3.576	3.018	-1.856	C(6)	-0.954	3.039	-2.650
C(7)	-3.194	2.948	0.546	C(7)	0.291	3.226	-0.584
C(8)	-4.526	4.024	-1.673	C(8)	-1.518	4.294	-2.420
C(9)	-4.147	3.951	0.716	C(9)	-0.284	4.476	-0.351
C(10)	-4.813	4.490	-0.390	C(10)	-1.188	5.012	-1.269

N(16)	-5.149	-3.408	0.785	O(35)	1.327	-0.874	-1.237
N(17)	-2.636	-0.308	-0.431	N(36)	2.274	1.233	-1.828
C(18)	-4.308	-2.415	0.400	C(37)	3.217	0.131	-2.060
C(19)	-5.349	-4.579	-0.065	C(38)	2.779	-1.001	-1.092
C(20)	-5.862	-3.312	2.059	C(39)	4.589	0.801	-1.963
C(21)	-3.660	-2.425	-0.871	C(40)	4.322	2.148	-2.651
C(22)	-4.020	-1.308	1.241	C(41)	2.907	2.533	-2.175
C(23)	-2.869	-1.372	-1.253	C(42)	3.225	-0.711	0.349
C(24)	-3.184	-0.308	0.816	C(43)	3.232	-2.399	-1.548
O(35)	1.402	-0.113	1.357	C(44)	4.539	-1.021	0.732
N(36)	-0.310	1.380	-0.358	C(45)	2.866	-3.519	-0.783
C(37)	0.952	0.753	-0.878	C(46)	2.391	-0.091	1.284
C(38)	1.411	-0.476	-0.017	C(47)	4.029	-2.604	-2.683
C(39)	1.994	1.913	-0.839	C(48)	5.011	-0.702	2.003
C(40)	1.218	3.179	-0.453	C(49)	3.271	-4.799	-1.156
C(41)	0.050	2.638	0.368	C(50)	2.857	0.223	2.564
C(42)	2.866	-0.870	-0.366	C(51)	4.445	-3.886	-3.047
C(43)	0.572	-1.756	-0.256	C(52)	4.174	-0.073	2.930
C(44)	3.370	-0.795	-1.673	C(53)	4.065	-4.990	-2.287
C(45)	0.083	-2.501	0.825	H(11)	-1.203	2.475	-3.544
C(46)	3.697	-1.387	0.636	H(12)	1.013	2.825	0.122
C(47)	0.428	-2.287	-1.550	H(13)	-2.212	4.713	-3.143
C(48)	4.668	-1.210	-1.967	H(14)	-0.018	5.034	0.543
C(49)	-0.503	-3.754	0.618	H(15)	-1.630	5.988	-1.091
C(50)	4.996	-1.802	0.342	H(62)	0.766	-1.500	-0.547
C(51)	-0.151	-3.539	-1.755	H(54)	3.075	-0.252	-3.079
C(52)	5.489	-1.715	-0.960	H(55)	5.379	0.220	-2.447
C(53)	-0.609	-4.285	-0.668	H(56)	4.871	0.960	-0.921
H(11)	-3.348	2.645	-2.850	H(57)	5.062	2.912	-2.397
H(12)	-2.673	2.554	1.417	H(58)	4.327	2.024	-3.740
H(13)	-5.036	4.445	-2.535	H(60)	2.946	3.165	-1.282
H(14)	-4.364	4.315	1.716	H(61)	2.353	3.070	-2.949
H(15)	-5.551	5.275	-0.248	H(63)	5.198	-1.519	0.028
H(25)	-5.706	-4.302	-1.063	H(64)	2.234	-3.390	0.090
H(26)	-6.096	-5.227	0.394	H(65)	1.359	0.106	1.033
H(27)	-4.419	-5.149	-0.175	H(66)	4.343	-1.772	-3.302
H(28)	-5.174	-3.268	2.911	H(67)	6.031	-0.955	2.277
H(29)	-6.496	-4.191	2.179	H(68)	2.961	-5.649	-0.555
H(30)	-6.503	-2.422	2.082	H(69)	2.183	0.686	3.279
H(31)	-3.773	-3.251	-1.564	H(70)	5.065	-4.015	-3.930
H(32)	-4.410	-1.238	2.250	H(71)	4.531	0.155	3.930
H(33)	-2.396	-1.317	-2.227	H(72)	4.384	-5.988	-2.574
H(34)	-2.870	0.471	1.500	N(16)	-4.513	-1.627	0.274

H(62)	0.489	0.075	1.726	N(17)	-1.001	0.072	-1.217
H(54)	0.763	0.434	-1.905	C(18)	-3.378	-1.059	-0.222
H(55)	2.508	2.013	-1.797	C(19)	-5.151	-2.723	-0.448
H(56)	2.754	1.701	-0.084	C(20)	-4.927	-1.348	1.645
H(57)	1.829	3.882	0.118	C(21)	-2.865	-1.396	-1.499
H(58)	0.838	3.695	-1.342	C(22)	-2.646	-0.089	0.509
H(60)	0.327	2.383	1.393	C(23)	-1.695	-0.828	-1.945
H(61)	-0.791	3.323	0.407	C(24)	-1.482	0.426	-0.008
H(63)	2.759	-0.400	-2.479	H(25)	-5.481	-2.402	-1.442
H(64)	0.172	-2.105	1.830	H(26)	-6.031	-3.048	0.106
H(65)	3.322	-1.456	1.651	H(27)	-4.477	-3.581	-0.564
H(66)	0.805	-1.742	-2.410	H(28)	-4.187	-1.699	2.375
H(67)	5.037	-1.130	-2.985	H(29)	-5.873	-1.854	1.839
H(68)	-0.857	-4.321	1.475	H(30)	-5.087	-0.275	1.796
H(69)	5.625	-2.191	1.139	H(31)	-3.357	-2.119	-2.135
H(70)	-0.224	-3.937	-2.764	H(32)	-2.952	0.229	1.496
H(71)	6.503	-2.035	-1.186	H(33)	-1.262	-1.061	-2.911
H(72)	-1.034	-5.275	-0.821	H(34)	-0.913	1.162	0.546