Spectral data of representative compounds

Table S1: Bond lengths (Å), bond angles and torsion angles in comparison with calculated values.

Bond length (Å)	X-ray analysis	B3LYP/6-311++G(2d,2p)
P(1)-O(1)	1.448(3)	1.475
P(1)-O(2)	1.558(3)	1.609
P(1)-(O3)	1.552(3)	1.597
P(1)-C(3)	1.804(4)	1.855
O(3)-C(1)	1.458(6)	1.441
O(2)-C(2)	1.442(6)	1.443
C(3)-C(4)	1.532(6)	1.517
C(9)-O(4)	1.373(6)	1.361
O(4)-C(10)	1.428(7)	1.421
C(3)-N(1)	1.453(5)	1.453
N(1)-C(11)	1.371(5)	1.379
C(16)-N(2)	1.438(6)	1.404
N(2)-N(3)	1.221(4)	1.256
N(3)-C(17)	1.453(5)	1.417
N(1)-H(1)	0.96(5)	1.004
C(3)-H(3)	0.980	1.090
bond angles (◦)		
C(1)-O(3)-P(1)	119.3(3)	119.7
C(2)-O(2)-P(1)	121.7(4)	121.1
O(3)-P(1)-O(1)	115.2(2)	116.5
O(2)-P(1)-O(1)	113.47(19)	114.0
O(1)-P(1)-C(3)	115.0(2)	114.9
O(3)-P(1)-O(2)	104.7(2)	103.1
O(3)-P(1)-C(3)	102.8(2)	100.4
O(2)-P(1)-C(3)	104.33(19)	106.2
P(1)-C(3)-N(1)	109.7(3)	113.2
P(1)-C(3)-C(4)	108.3(3)	109.7
P(1)-C(3)-H(3)	108.2	104.0
N(1)-C(3)-C(4)	114.1(4)	112.5
C(3)-N(1)-H(1)	117(3)	114.9
C(3)-N(1)-C(11)	122.8(4)	125.4
C(11)-N(1)-H(1)	115(3)	115.1
C(3)-C(4)-C(5)	120.7(4)	120.8
N(1)-C(11)-C(13)	119.1(4)	118.4
C(14)-C(16)-N(2)	125.3(4)	125.1
C(15)-C(16)-N(2)	116.2(5)	116.3
C(16)-N(2)-N(3)	113.6(4)	115.9
N(2)-N(3)-C(17)	112.8(4)	115.1
N(3)-C(17)-C(18)	115.8(4)	115.6
N(3)-C(17)-C(19)	124.9(4)	124.8
Torsion angles		
C(1)-O(3)-P(1)-O(1)	-49.8(4)	51.7
C(1)-O(3)-P(1)-O(2)	75.5(4)	-74.1
C(1)-O(3)-P(1)-C(3)	-175.7(4)	176.4
O(3)-P(1)-O(2)-C(2)	-146.5(4)	137.9
O(3)-P(1)-C(3)-N(1)	64.5(4)	46.8
O(3)-P(1)-C(3)-C(4)	-170.5(3)	173.4
P(1)-C(3)-N(1)-C(11)	-173.7(3)	-100.5
P(1)-C(3)-C(4)-C(5)	-67.6(5)	-79.8
P(1)-C(3)-C(4)-C(6)	-126.2(4)	99.9
C(3)-N(1)-C(11)-C(13)	-170.3(4)	-163.8
C(3)-N(1)-C(11)-C(12)	10.0(7)	16.9
C(14)-C(16)-N(2)-N(3)	-6.6(7)	-0.04
C(15)-C(16)-N(2)-N(3)	177.3(4)	179.8
C(16)-N(2)-N(3)-C(17)	176.4(4)	179.9
N(2)-N(3)-C(17)-C(18)	169.9(4)	179.9
N(2)-N(3)-C(17)-C(19)	-13.8(7)	-0.06

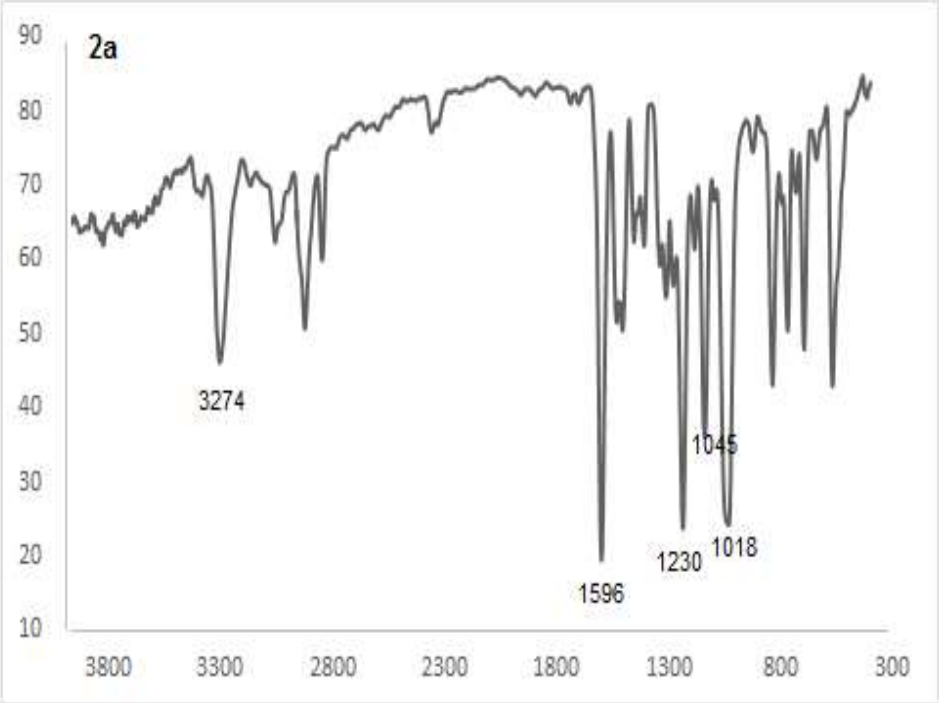

Fig. S1: FT-IR spectrum of 2a.

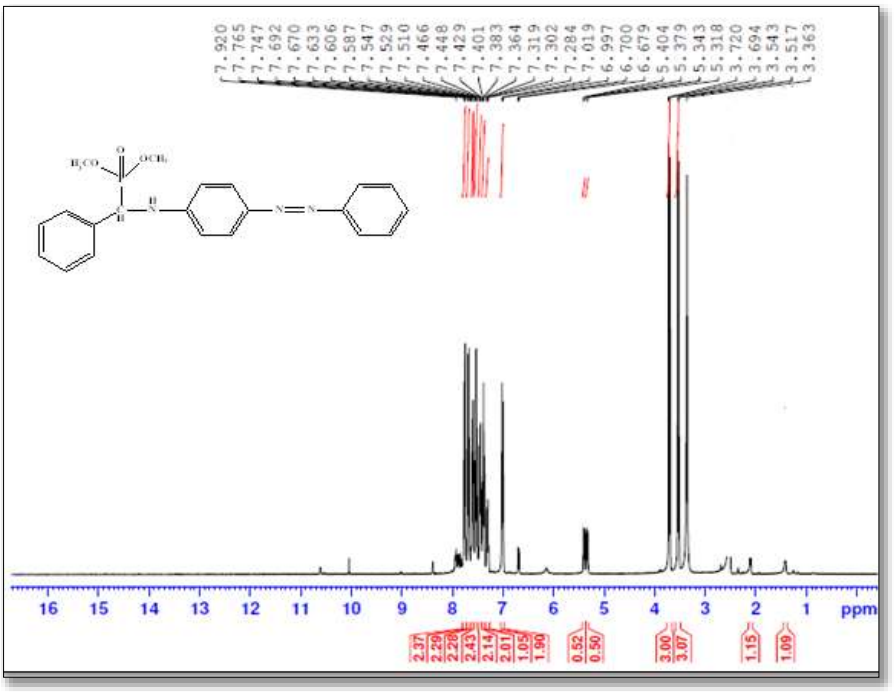

Fig. S2: ^{1}H NMR spectrum of 2a.

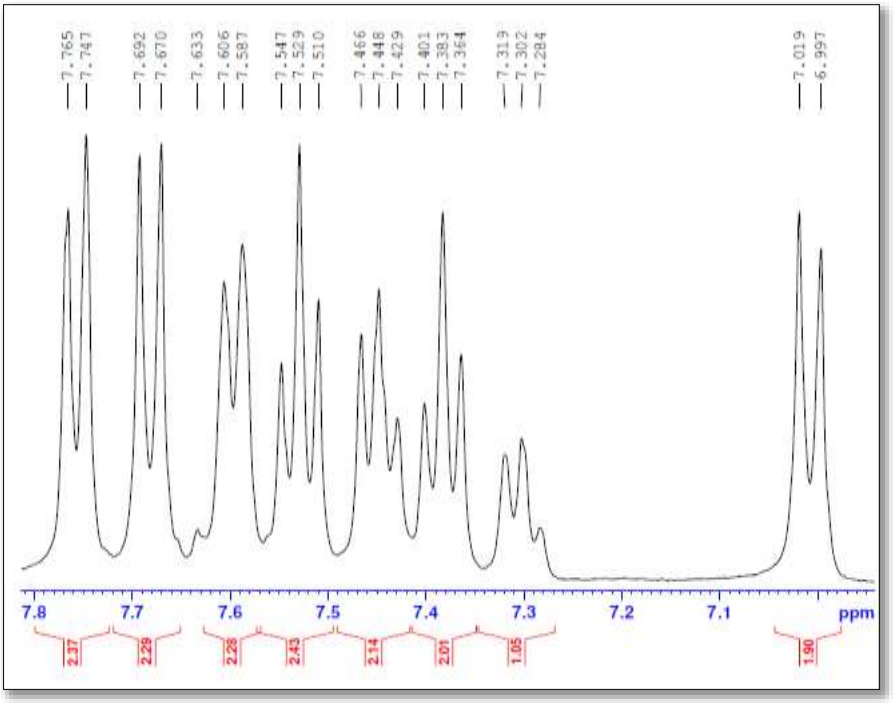

Fig. S2: [1]H NMR spectrum of 2a (Exp. 6.8-7.9 ppm)

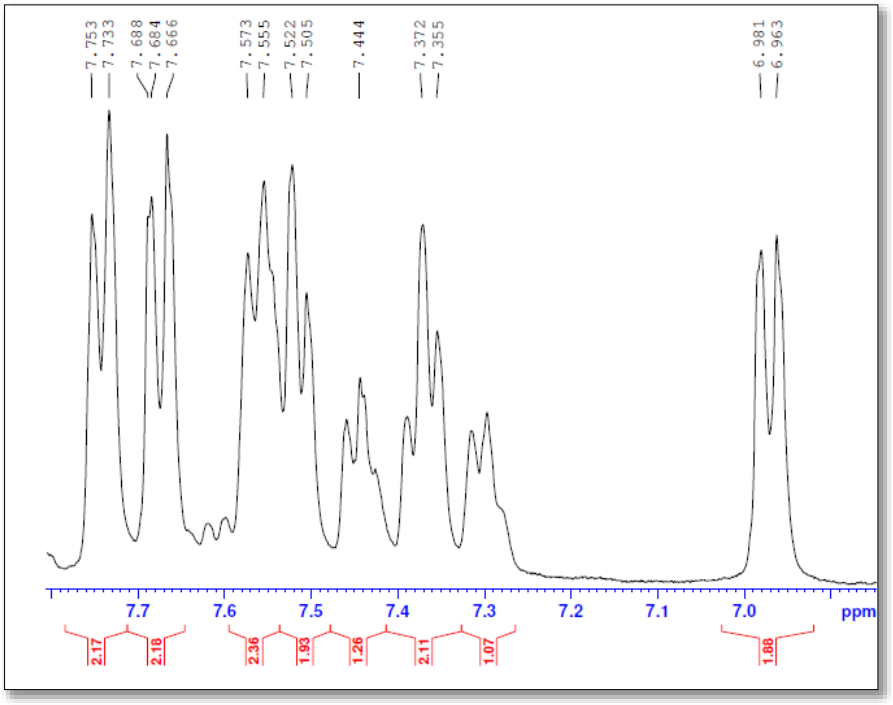

Figure S2: [1]H NMR spectrum of 2a (Exp. D2O exchangeable).

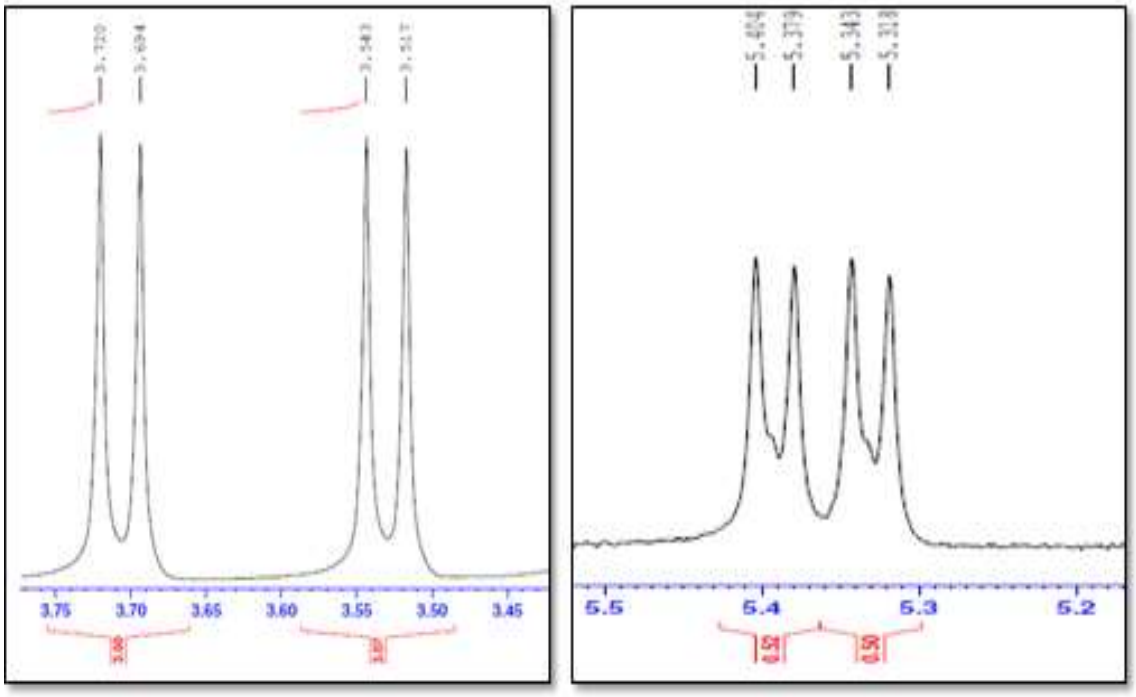

Fig. S2: ^{1}H NMR spectrum of 2a (Exp. 3.45 -5.5 ppm).

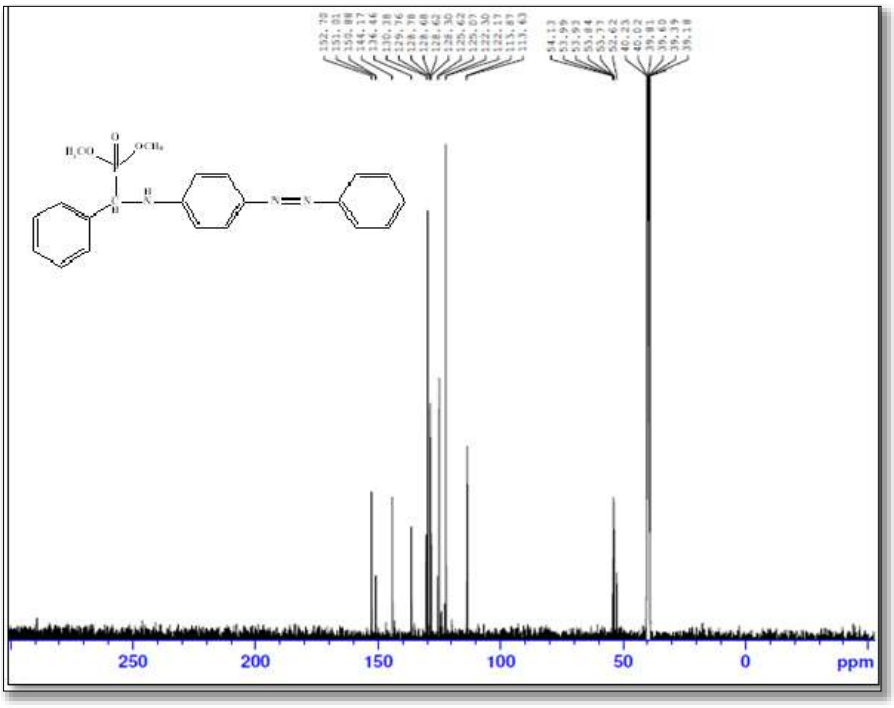

Figure S3: ^{13}C NMR spectrum of 2a.

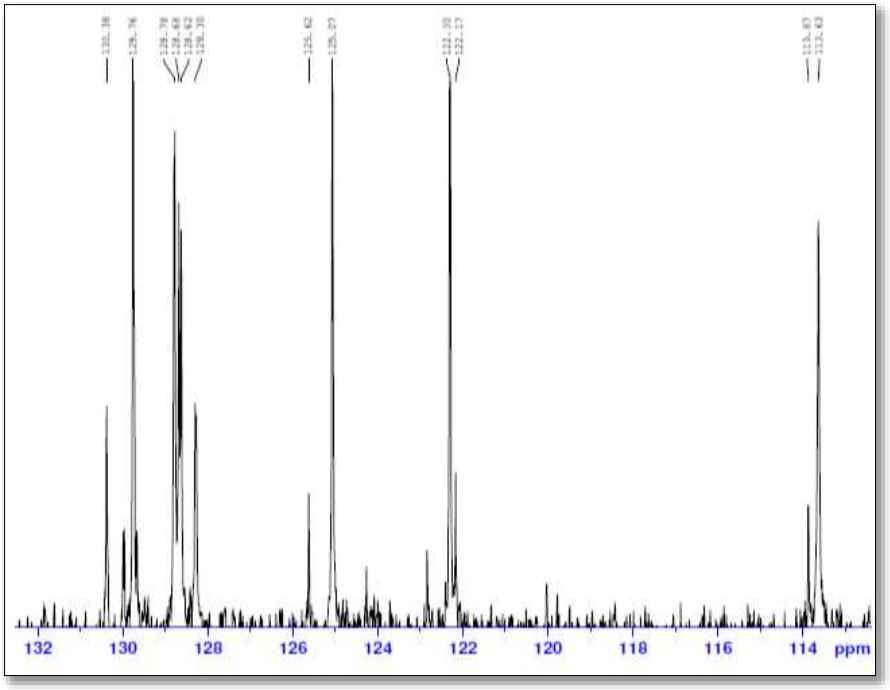

Fig. S3: ^{13}C NMR spectrum of 2a(Exp.).

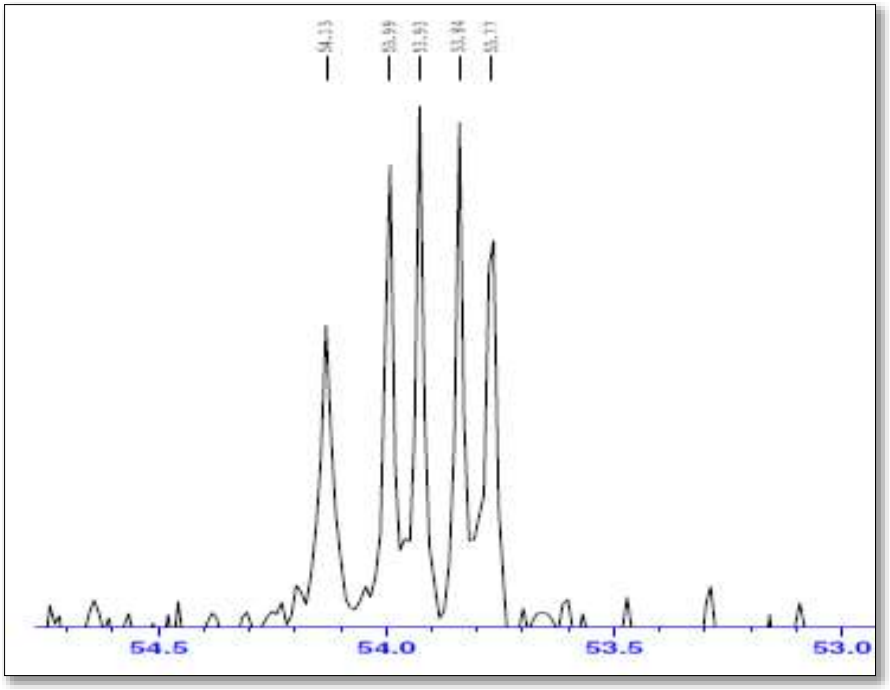

Fig. S3: ^{13}C NMR spectrum of 2a (Exp.).

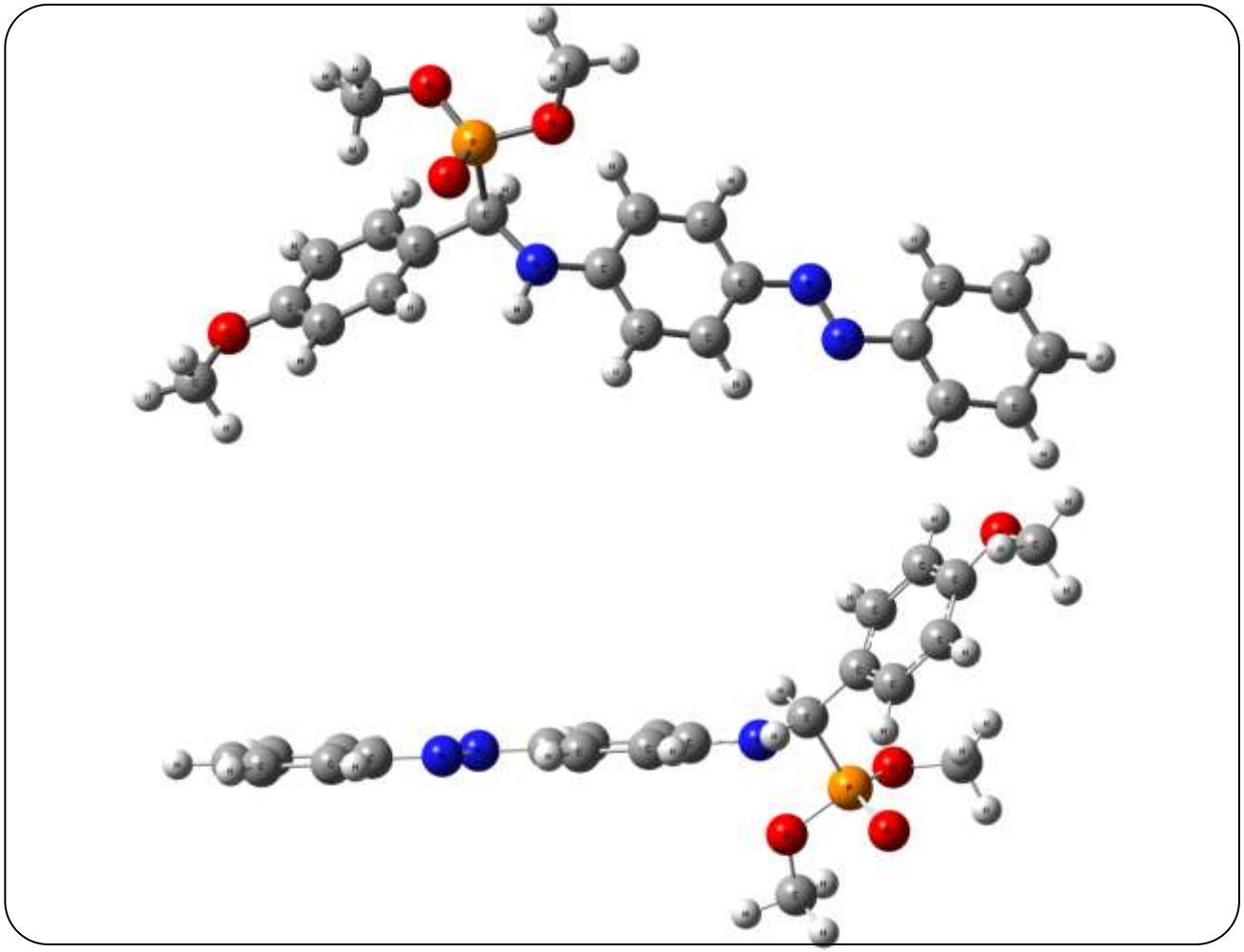

Fig. S4: The geometry of dimethyl[(4-methoxyphenyl((4-phenyldiazenyl)phenyl)amino) methyl]phosphonate (2b)