Predictive Elucidation of Conformational Characteristics and Configurational Properties of Poly(1-methylphosphirane) and Poly(1-phenylphosphirane) as a Molecular Design

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Supplementary Information

(Tables S1 – S4)

Table S1 Geometrical parameters for *ll* form of poly(1-methylphosphirane), used in the refined RIS calculations [a]

Conformation					
Bond					
$j-1$	j	$j+1$	l_j [b]	$\angle j \wedge (j+1)$ [c]	ϕ_j [d]
$j-1=c$, $j=a$, and $j+1=b$					
t	t	t	1.880	113.1	2.9
	g^+		1.885	119.3	125.1
	g^-		1.881	113.2	−101.2
g^+	t		1.881	112.9	3.3
	g^+		1.885	119.2	130.5
	g^-		1.883	114.5	−99.4
g^-	t		1.881	112.2	−1.0
	g^+		1.891	120.2	101.0
	g^-		1.880	113.0	−109.4
t	t	g^+	1.880	115.7	−1.8
	g^+		1.883	120.5	121.5
	g^-		1.886	116.3	−80.7
g^+	t		1.880	115.6	2.7
	g^+		1.884	120.2	120.9
	g^-		–	–	–
g^-	t		1.880	114.9	−3.4
	g^+		1.892	121.6	97.8
	g^-		1.894	116.2	−87.1
t	t	g^-	1.885	115.4	−15.0
	g^+		1.884	121.0	133.6
	g^-		1.884	116.2	−114.6
g^+	t		1.886	115.2	−16.6
	g^+		1.886	121.7	125.7
	g^-		1.885	117.3	−107.2
g^-	t		1.886	114.6	−19.6
	g^+		–	–	–
	g^-		1.883	115.8	−117.1
$j-1=a$, $j=b$, and $j+1=c$					
t	t	t	1.537	113.1	0.0
	g^+		1.541	115.4	108.9
	g^-		1.541	115.8	−108.9
g^+	t		1.536	113.0	−5.8
	g^+		1.547	114.0	83.1
	g^-		1.549	117.3	−104.8
g^-	t		1.536	113.2	−4.6
	g^+		1.541	116.3	111.4
	g^-		1.539	116.1	−129.8
t	t	g^+	1.536	113.2	4.6
	g^+		1.539	116.1	129.8
	g^-		1.541	116.3	−111.4
g^+	t		1.536	112.9	3.6
	g^+		1.547	114.0	83.1
	g^-		–	–	–
g^-	t	g^+	1.537	113.0	−1.5
	g^+		1.541	116.0	109.7
	g^-		1.541	115.5	−109.7
t	t	g^-	1.536	119.3	5.8
	g^+		1.549	123.0	104.8
	g^-		1.547	120.5	−83.1
g^+	t		1.535	119.2	0.0
	g^+		–	–	–
	g^-		–	–	–
g^-	t		1.536	119.4	−3.6
	g^+		–	–	–
	g^-		1.547	120.5	−83.1
$j-1=b$, $j=c$, and $j+1=a$					
t	t	t	1.880	98.6	−2.9
	g^+		1.881	99.8	101.2
	g^-		1.885	101.1	−125.1
g^+	t		1.885	97.8	15.0
	g^+		1.884	99.8	114.6
	g^-		1.888	103.3	−133.6
g^-	t		1.880	98.1	1.8
	g^+		1.886	100.4	80.7
	g^-		1.883	100.6	−121.5
t	t	g^+	1.881	101.2	1.0
	g^+		1.880	102.4	109.4
	g^-		1.891	103.9	−101.0
g^+	t		1.886	100.2	19.6
	g^+		1.883	102.2	117.1
	g^-		–	–	–
g^-	t		1.880	101.0	3.4
	g^+		1.884	104.0	87.1
	g^-		1.892	102.2	−97.8
t	t	g^-	1.881	99.7	−3.3
	g^+		1.883	102.2	99.4
	g^-		1.885	102.4	−130.5
g^+	t		1.886	99.0	16.6
	g^+		1.885	101.8	107.2
	g^-		1.886	104.7	−125.7
g^-	t		1.880	99.3	−2.7
	g^+		–	–	–
	g^-		1.884	101.5	−120.9

[a] Obtained from the geometrical optimization for 1,2-bis(ethylmethylphosphino)ethane at the B3LYP/6-31G(d) level. j denotes the current bond. Geometrical parameters of the *dd* form can be derived from the above ones. [b] Length of bond j. [c] Angle formed between bonds j and $j+1$. [d] Dihedral angle of bond j. For the bond designations, see Figure 2.

Table S2 Geometrical parameters for *ld* form of poly(1-methylphosphirane), used in the refined RIS calculations [a]

Conformation					
Bond					
$j-1$	j	$j+1$	l_j [b]	$\angle j \wedge (j+1)$ [c]	ϕ_j [d]
$j-1=c$, $j=a$, and $j+1=b$					
t	t	t	1.880	113.1	2.1
	g^+		1.884	119.4	130.1
	g^-		1.881	113.2	−102.6
g^+	t		1.880	113.0	2.6
	g^+		1.885	119.2	130.5
	g^-		1.884	114.4	−95.3
g^-	t		1.880	112.4	−0.2
	g^+		1.891	120.5	101.4
	g^-		1.880	112.8	−107.9
t	t	g^+	1.883	115.9	14.0
	g^+		1.887	122.8	144.1
	g^-		1.886	115.4	−84.3
g^+	t		1.884	115.7	14.0
	g^+		1.886	122.8	140.5
	g^-		1.884	116.4	−93.5
g^-	t		1.882	115.3	12.1
	g^+		1.892	121.5	99.4
	g^-		1.886	114.9	−86.8
t	t	g^-	1.886	116.2	−19.6
	g^+		1.883	120.6	134.1
	g^-		1.880	115.8	−102.3
g^+	t		1.887	116.3	−19.5
	g^+		1.885	122.8	115.5
	g^-		1.885	116.7	−88.9
g^-	t		1.886	115.6	−20.5
	g^+		1.884	122.9	127.6
	g^-		1.880	115.8	−108.6
$j-1=a$, $j=b$, and $j+1=c$					
t	t	t	1.537	113.1	5.3
	g^+		1.539	115.9	128.8
	g^-		1.541	116.2	−111.9
g^+	t		1.536	112.8	5.6
	g^+		1.544	117.1	104.2
	g^-		1.547	114.0	−83.5
g^-	t		1.536	113.1	0.2
	g^+		1.541	115.7	109.6
	g^-		1.541	115.4	−108.4
t	t	g^+	1.536	119.4	5.6
	g^+		1.544	122.8	104.2
	g^-		1.547	120.6	−83.5
g^+	t		1.535	119.1	3.1
	g^+		–	–	–
	g^-		–	–	–
g^-	t	g^+	1.536	119.4	−2.7
	g^+		–	–	–
	g^-		1.543	122.8	−105.2
t	t	g^-	1.536	113.2	0.2
	g^+		1.541	115.4	109.6
	g^-		1.541	115.8	−108.4
g^+	t		1.536	112.9	−2.7
	g^+		–	–	–
	g^-		1.543	117.4	−105.2
g^-	t		1.536	113.2	−6.4
	g^+		–	–	–
	g^-		1.539	116.1	−129.1
$j-1=b$, $j=c$, and $j+1=a$					
t	t	t	1.880	98.6	2.1
	g^+		1.884	101.5	130.1
	g^-		1.881	99.7	−102.6
g^+	t		1.883	97.6	14.0
	g^+		1.887	101.6	144.1
	g^-		1.886	101.3	−84.3
g^-	t		1.886	98.2	−19.6
	g^+		1.883	102.9	134.1
	g^-		1.880	99.5	−102.3
t	t	g^+	1.880	99.8	2.6
	g^+		1.885	102.4	130.5
	g^-		1.884	102.2	−95.3
g^+	t		1.884	98.8	14.0
	g^+		1.886	102.7	140.5
	g^-		1.884	104.3	−93.5
g^-	t		1.887	99.3	−19.5
	g^+		1.885	104.7	115.5
	g^-		1.885	101.6	−88.9
t	t	g^-	1.880	101.2	−0.2
	g^+		1.891	104.1	101.4
	g^-		1.880	102.3	−107.9
g^+	t		1.882	100.5	12.1
	g^+		1.892	102.4	99.4
	g^-		1.886	104.4	−86.8
g^-	t		1.886	100.4	−20.5
	g^+		1.884	106.0	127.6
	g^-		1.880	102.2	−108.6

[a] Obtained from the geometrical optimization for 1,2-bis(ethylmethylphosphino)ethane at the B3LYP/6-31G(d) level. j denotes the current bond. Geometrical parameters of the *dl* form can be derived from the above ones. [b] Length of bond j. [c] Angle formed between bonds j and $j+1$. [d] Dihedral angle of bond j. For the bond designations, see Figure 2.

Table S3 Geometrical parameters for *ll* form of poly(1-phenylphosphirane), used in the refined RIS calculations [a]

Conformation					
Bond					
$j-1$	j	$j+1$	l_j [b]	$\angle j \wedge (j+1)$ [c]	ϕ_j [d]
$j-1=c$, $j=a$, and $j+1=b$					
t	t	t	1.880	112.6	4.2
	g^+		1.887	118.7	128.6
	g^-		1.883	112.4	−100.9
g^+	t		1.879	112.4	5.9
	g^+		1.887	118.1	129.5
	g^-		1.885	113.6	−105.5
g^-	t		1.875	112.3	1.1
	g^+		1.888	121.1	111.0
	g^-		1.876	111.6	−105.7
t	t	g^+	1.881	115.2	4.4
	g^+		1.887	122.9	144.8
	g^-		1.889	115.6	−82.8
g^+	t		1.881	115.0	3.1
	g^+		1.886	122.7	141.8
	g^-		–	–	–
g^-	t		1.876	114.6	2.5
	g^+		–	–	–
	g^-		1.882	115.3	−87.0
t	t	g^-	1.888	114.7	−20.4
	g^+		1.891	122.6	108.8
	g^-		1.886	115.7	−115.0
g^+	t		1.887	114.6	−19.5
	g^+		1.890	121.3	118.7
	g^-		1.888	116.4	−111.5
g^-	t		1.883	113.9	−23.3
	g^+		1.909	120.6	70.6
	g^-		1.878	114.6	−116.4
$j-1=a$, $j=b$, and $j+1=c$					
t	t	t	1.535	112.6	0.2
	g^+		1.539	114.7	113.6
	g^-		1.539	115.2	−113.6
g^+	t		1.533	112.5	0.3
	g^+		1.543	115.9	99.1
	g^-		1.540	116.8	−105.4
g^-	t		1.536	112.4	−4.5
	g^+		1.542	116.4	101.9
	g^-		1.538	115.4	−127.1
t	t	g^+	1.536	112.4	4.5
	g^+		1.538	115.7	127.1
	g^-		1.542	115.6	−101.9
g^+	t		1.534	112.5	7.1
	g^+		–	–	–
	g^-		–	–	–
g^-	t	g^+	1.537	112.4	0.1
	g^+		1.542	115.4	108.3
	g^-		1.542	114.8	−108.3
t	t	g^-	1.533	118.7	−0.3
	g^+		1.540	122.6	105.4
	g^-		1.543	122.5	−99.1
g^+	t		1.531	119.0	1.1
	g^+		–	–	–
	g^-		–	–	–
g^-	t		1.534	118.8	−7.1
	g^+		–	–	–
	g^-		–	–	–
$j-1=b$, $j=c$, and $j+1=a$					
t	t	t	1.880	98.9	−4.2
	g^+		1.883	99.9	100.9
	g^-		1.887	101.5	−128.6
g^+	t		1.888	97.9	20.4
	g^+		1.886	100.2	115.0
	g^-		1.891	103.4	−108.8
g^-	t		1.881	98.2	−4.4
	g^+		1.889	100.9	82.8
	g^-		1.887	102.0	−144.8
t	t	g^+	1.875	101.3	−1.1
	g^+		1.879	102.2	105.7
	g^-		1.888	105.3	−111.0
g^+	t		1.883	100.2	23.3
	g^+		1.878	101.8	116.4
	g^-		1.909	104.5	−70.6
g^-	t		1.876	100.7	−2.5
	g^+		1.882	104.5	87.0
	g^-		–	–	–
t	t	g^-	1.879	100.0	−5.9
	g^+		1.885	101.6	105.5
	g^-		1.887	102.2	−129.5
g^+	t		1.887	99.1	19.5
	g^+		1.888	101.2	111.5
	g^-		1.890	104.5	−118.7
g^-	t		1.881	99.2	−3.1
	g^+		–	–	–
	g^-		1.886	102.6	−141.8

[a] Obtained from the geometrical optimization for 1,2-bis(ethylphenylphosphino)ethane at the B3LYP/6-31G(d) level. j denotes the current bond. Geometrical parameters of the *dd* form can be derived from the above ones. [b] Length of bond j. [c] Angle formed between bonds j and $j+1$. [d] Dihedral angle of bond j. For the bond designations, see Figure 2.

Table S4 Geometrical parameters for *ld* form of poly(1-phenylphosphirane), used in the refined RIS calculations [a]

Conformation					
Bond					
$j-1$	j	$j+1$	l_j [b]	$\angle j \wedge (j+1)$ [c]	ϕ_j [d]
$j-1=c$, $j=a$, and $j+1=b$					
t	t	t	1.880	112.5	4.2
	g^+		1.887	119.1	126.2
	g^-		1.883	112.1	−100.3
g^+	t		1.881	112.5	6.9
	g^+		1.887	118.3	128.3
	g^-		1.885	113.7	−103.0
g^-	t		1.874	112.4	−1.7
	g^+		1.893	120.1	102.3
	g^-		1.875	111.5	−105.5
t	t	g^+	1.884	115.3	11.5
	g^+		1.894	122.4	154.2
	g^-		–	–	–
g^+	t		1.885	115.2	13.8
	g^+		1.888	122.5	142.6
	g^-		1.890	116.2	−90.5
g^-	t		1.878	114.9	5.2
	g^+		–	–	–
	g^-		1.884	113.8	−86.4
t	t	g^-	1.884	116.3	−16.9
	g^+		1.887	121.5	125.8
	g^-		1.884	115.7	−108.0
g^+	t		1.883	116.2	−15.9
	g^+		–	–	–
	g^-		1.887	116.1	−91.9
g^-	t		1.879	115.7	−17.0
	g^+		–	–	–
	g^-		1.876	114.3	−109.6
$j-1=a$, $j=b$, and $j+1=c$					
t	t	t	1.535	112.5	3.9
	g^+		1.537	115.3	123.5
	g^-		1.540	116.3	−100.2
g^+	t		1.532	112.2	3.7
	g^+		1.542	115.9	97.5
	g^-		1.543	114.6	−92.7
g^-	t		1.536	112.8	3.2
	g^+		1.540	115.2	108.1
	g^-		1.539	114.9	−118.4
t	t	g^+	1.532	119.1	3.7
	g^+		1.542	122.4	97.5
	g^-		1.543	121.5	−92.7
g^+	t		1.531	118.7	3.7
	g^+		–	–	–
	g^-		–	–	–
g^-	t	g^+	1.534	118.9	−1.9
	g^+		–	–	–
	g^-		1.542	122.9	−102.6
t	t	g^-	1.536	112.1	3.2
	g^+		1.540	114.3	108.1
	g^-		1.539	115.7	−118.4
g^+	t		1.534	112.2	−1.9
	g^+		–	–	–
	g^-		1.542	116.6	−102.6
g^-	t		1.537	112.6	−10.2
	g^+		–	–	–
	g^-		1.540	115.8	−129.5
$j-1=b$, $j=c$, and $j+1=a$					
t	t	t	1.880	98.9	4.2
	g^+		1.887	101.5	126.2
	g^-		1.883	99.7	−100.3
g^+	t		1.884	98.0	11.5
	g^+		1.894	102.7	154.2
	g^-		–	–	–
g^-	t		1.884	97.5	−16.9
	g^+		1.887	103.6	125.8
	g^-		1.884	100.1	−108.0
t	t	g^+	1.881	99.9	6.9
	g^+		1.887	102.1	128.3
	g^-		1.885	101.9	−103.0
g^+	t		1.885	99.1	13.8
	g^+		1.888	102.7	142.6
	g^-		1.890	104.2	−90.5
g^-	t		1.883	98.6	−15.9
	g^+		–	–	–
	g^-		1.887	101.9	−91.9
t	t	g^-	1.874	101.1	−1.7
	g^+		1.893	103.8	102.3
	g^-		1.875	102.2	−105.5
g^+	t		1.878	100.6	5.2
	g^+		–	–	–
	g^-		1.884	104.6	−86.4
g^-	t		1.879	99.8	−17.0
	g^+		–	–	–
	g^-		1.876	102.1	−109.6

[a] Obtained from the geometrical optimization for 1,2-bis(ethylphenylphosphino)ethane at the B3LYP/6-31G(d) level. j denotes the current bond. Geometrical parameters of the *dl* form can be derived from the above ones. [b] Length of bond j. [c] Angle formed between bonds j and $j+1$. [d] Dihedral angle of bond j. For the bond designations, see Figure 2.