Spin Transfer and Magnetic Interaction via Phosphorus in

Nitronyl Nitroxide Radical Substituted Triphenylphosphine Derivatives

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Supporting Information

Table S1. Experimental details of the solid-state NMR measurements.

		Compound				
		1d	**2d**	**3d**	**1e**	Mo(**1e**)$(CO)_5$
ν_{rot}[a]		15	15	15	15	14[d]/12[e]
T[b]		309.1	309.1	309.4	308.0	309.0[d]/300.0[e]
CH_3	δ^{exp}_T	–11.4	–13.5	–14.1	[c]	–10.0/–15.6[f]
	δ^{dia}	1.1	1.1	1.1		1.1
	δ^{para}_T	–12.5	–14.6	–15.3		–11.1/–16.7[f]
	δ^{pcon}_{298}	–13.0	–15.1	–15.8		–11.5/–17.3[f]
H_o	δ^{exp}_T	41.7	39.5	47.0	[c]	40.1
	δ^{dia}	7.5	7.5	7.5		7.5
	δ^{para}_T	34.2	32.0	39.5		32.6
	δ^{pcon}_{298}	35.5	33.2	41.0		33.8
H_m	δ^{exp}_T	–4.5	–3.5	–4.5	[c]	0.4
	δ^{dia}	7.5	7.5	7.5		7.5
	δ^{para}_T	–12.0	–11.0	–12.0		–7.1
	δ^{pcon}_{298}	–12.4	–11.4	–12.5		–7.4
C_6H_5	δ^{exp}_T	7.9	7.7		[c]	7.8
	δ^{dia}	7.5	7.5			7.5
	δ^{para}_T	0.4	0.2			0.3
	δ^{pcon}_{298}	0.4	0.2			0.3
P	δ^{exp}_T	128.4	233.2	341.4/374.9	–101.0	59.3
	δ^{dia}	28.5	28.5	28.5	–9.2	37.5
	δ^{para}_T	99.9	204.7	312.9/346.4	–91.8	21.8
	δ^{pcon}_{298}	103.6	212.3	324.9/359.7	–94.9	21.9

[a] Rotor spinning frequency in kHz. [b] Absolute temperature in K. [c] No data.

[d] ^{1}H NMR. [e] ^{31}P NMR. [f] Axial and equatorial methyl groups resolved.

Table S2a: Spin density computed for mono-radical **1d** (labeling as shown in Figure 1).

pPONit1	spin density $\rho_{\alpha-\beta}$ in *a.u.* (x-ray structure)	spin density $\rho_{\alpha-\beta}$ in *a.u.* (optimized)
P1	0.0007	0.0017
O2	–0.0004	–0.0006
C11 (P-C)	–0.0017	–0.0020
C12 - C16 (phenyl)	< ± 0.0002	< ± 0.0005
C21 (P-C)	0.0005	0.0004
C22 - C26 (phenyl)	< ± 0.0001	< ± 0.0001
C31 (P-C)	–0.0387	–0.0534
C32 (meta)	0.0220	0.0317
C33 (ortho)	–0.0421	–0.0587
C34 (C-NIT)	0.0514	0.0635
C35 (ortho)	–0.0419	–0.0584
C36 (meta)	0.0214	0.0316
C41 (NIT C2)	–0.2410	–0.2421
N42	0.2580	0.2672
O52	0.3747	0.3701
N45	0.2560	0.2656
O55	0.3710	0.3786
C43 (methylene)	–0.0143	–0.0145
C44 (methylene)	–0.0146	–0.0145
C53 (methyl)	0.0037	0.0030
C63 (methyl)	0.0201	0.0172
C54 (methyl)	0.0172	0.0172
C64 (methyl)	0.0023	0.0030

Table S2b: Optimized geometry of mono-radical **1d** (labeling as shown in Figure 1).

pPONit1	bond distances (in Å) and angles (in °)		bond distances (in Å) and angles (in °)
P1-O2	1.614	C43-C44	1.572
P1-C11	1.871	O2-P1-C11	112.0
P1-C21	1.871	O2-P1-C21	112.0
P1-C31	1.870	O2-P1-C31	111.8
C31-C32	1.408	C11-P1-C21	107.1
C32-C33	1.402	C11-P1-C31	106.7
C33-C34	1.423	C33-C34-C41	120.6
C34-C35	1.424	C41-N42-O52	127.6
C35-C36	1.402	C41-N45-O55	127.6
C36-C31	1.408	N42-C41-N45	107.7
C34-C41	1.465	C41-N42-C43	112.1
C41-N42	1.379	C41-N45-C44	112.1
N42-O52	1.324	C33-C34-C41-N42	0.5
N42-C43	1.528	C32-C31-P1-O2	156.2
C41-N45	1.379	C31-P1-C11-C13	–82.4
N45-O55	1.323	C31-P1-C21-C22	–145.8
N45-C44	1.528		

Table S3a: Spin density computed for mono-radical **1e**.

pPNit1	spin density $\rho_{\alpha-\beta}$ in e/a_0^3
P12	0.0008
C13 (phenyl)	–0.0032
C14-C18 (phenyl)	< ± 0.0002
C25-C30 (phenyl)	< –0.0001
C9 (P-C)	–0.0540
C8 (meta)	0.0320
C7 (ortho)	–0.0590
C6 (C-NIT)	0.0626
C10 (meta)	0.0321
C11 (ortho)	–0.0564
C2 (NIT C2)	–0.2387
N1	0.2674
O24	0.3729
N3	0.2670
O19	0.3717
C4 (methylene)	–0.0146
C5 (methylene)	–0.0146
C20 (methyl)	0.0029
C21 (methyl)	0.0173
C22 (methyl)	0.0173
C23 (methyl)	0.0029

Table S3b: Optimized geometry of mono-radical **1e**.

pPNit1	bond distances (in Å) and angles (in °)
P12-C9 (P-C)	1.894
P12-C13 (P-C)	1.895
P12-C25 (P-C)	1.895
C9-C10	1.414
C10-C11	1.401
C11-C6	1.424
C6-C7	1.423
C7-C8	1.404
C8-C9	1.410
C6-C2	1.464
C2-N1	1.379
N1-O24	1.324
N1-C5	1.527
C2-N3	1.379
N3-O19	1.325
N3-C4	1.527
C4-C5	1.571
C2-N1-O24	127.6
C2-N3-O19	127.6
C2-N2-C5	112.1
C2-N3-C4	112.1
C6-C2-N1	126.2
C11-C6-C2-N1	0.3
C9-P12-C13	101.2
C9-P12-C25	101.6
C9-P12-C13-C14	–161.4
C9-P12-C25-C26	–94.0

Table S4a: Spin density computed for di-radical **2d**.

pPONit2	spin density $\rho_{\alpha-\beta}$ in *a.u.* (S = 0)	spin density $\rho_{\alpha-\beta}$ in *a.u.* (S = 1)
P12	0.0000	0.0033
O25	0.0000	–0.0012
C26 - C31 (phenyl)	< ± 0.0016	< ± 0.0025
C9 (P-C)	–0.0529	–0.0538
C10 (meta)	0.0316	0.0317
C11 (ortho)	–0.0585	–0.0585
C6 (C-NIT)	0.0636	0.0635
C7 (ortho)	–0.0586	–0.0587
C8 (meta)	0.0317	0.0318
C2 (NIT C2)	–0.2423	–0.2423
N1	0.2656	0.2656
O24	0.3781	0.3781
N3	0.2670	0.2670
O19	0.3710	0.3709
C4 (methylene)	–0.0145	–0.0145
C5 (methylene)	–0.0145	–0.0145
C20 (methyl)	0.0029	0.0029
C21 (methyl)	0.0172	0.0172
C22 (methyl)	0.0172	0.0172
C23 (methyl)	0.0030	0.0030
C13 (P-C)	0.0512	–0.0556
C14 (meta)	–0.0315	0.0318
C15 (ortho)	0.0583	–0.0585
C16 (C-NIT)	–0.0635	0.0635
C17 (ortho)	0.0588	–0.0588
C18 (meta)	–0.0313	0.0323
C39 (NIT C2)	0.2424	–0.2424
N58	–0.2670	0.2670
O63	–0.3710	0.3710
N59	–0.2655	0.2655
O62	–0.3782	0.3782
C60 (methylene)	0.0145	–0.0145
C61 (methylene)	0.0145	–0.0145
C64 (methyl)	–0.0172	0.0172
C65 (methyl)	–0.0029	0.0029
C66 (methyl)	–0.0029	0.0029
C67 (methyl)	–0.0173	0.0173

Table S4b: Optimized geometry for di-radical **2d**.

pPONit2	bond distances (in Å) and angles (in °)		bond distances (in Å) and angles (in °)
P12-O25	1.614	C39-N59	1.379
P12-C26	1.871	N58-C60	1.528
P12-C9	1.870	N59-C61	1.528
C9-C8	1.408	C60-C62	1.571
C8-C7	1.402	C16-C39-N58	126.2
C7-C6	1.423	C16-C39-N59	126.1
C6-C11	1.424	C39-N58-O63	127.6
C11-C10	1.402	C39-N59-O62	127.6
C10-C9	1.408	N58-C39-N59	107.7
C6-C2	1.465	C15-C16-C39-N58	178.7
C2-N3	1.378	C6-C2-N1	126.1
C2-N1	1.379	C6-C2-N3	126.1
N3-O19	1.324	C2-N1-O24	127.6
N1-O24	1.323	C2-N3-O19	127.6
N3-C4	1.528	N1-C2-N3	107.7
N1-C2	1.527	C7-C6-C2-N1	–178.6
C2-C4	1.572	O25-P12-C9	111.9
P12-C13	1.871	O25-P12-C9-C8	156.7
C13-C14	1.408	O25-P12-C13	112.0
C14-C15	1.402	O25-P12-C13-C14	–23.7
C15-C16	1.424	O25-P12-C26	112.0
C16-C17	1.423	O25-P12-C26-C27	155.9
C17-C18	1.402	C26-P12-C9	106.9
C18-C13	1.408	C26-P12-C9-C8	33.7
C16-C39	1.465	C26-P12-C13	106.9
C39-N58	1.378	C26-P12-C13-C14	99.3

Table S5a: Spin density computed for tri-radical **3d**.

pPONit3	spin density $\rho_{\alpha-\beta}$ in e/a_0^3
P12	0.0049
O25	–0.0019
C9 (P-C)	–0.0560
C10 (meta)	0.0319
C11 (ortho)	–0.0586
C6 (C-NIT)	0.0635
C7 (ortho)	–0.0589
C8 (meta)	0.0324
C2 (NIT C2)	–0.2424
N1	0.2654
O24	0.3777
N3	0.2670
O19	0.3717
C4 (methylene)	–0.0145
C5 (methylene)	–0.0145
C20 (methyl)	0.0029
C21 (methyl)	0.0172
C22 (methyl)	0.0172
C23 (methyl)	0.0029
C13 (P-C)	–0.0560
C14 (meta)	0.0319
C15 (ortho)	–0.0586
C16 (C-NIT)	0.0635
C17 (ortho)	–0.0589
C18 (meta)	0.0324
C39 (NIT C2)	–0.2425
N60	0.2667
O67	0.3715
N61	0.2658
O66	0.3780
C62 (methylene)	–0.0145
C63 (methylene)	–0.0145
C70 (methyl)	0.0172
C71 (methyl)	0.0029
C74 (methyl)	0.0029
C75 (methyl)	0.0172
C26 (P-C)	–0.0561
C27 (meta)	0.0324
C28 (ortho)	–0.0589
C29 (C-NIT)	0.0635
C30 (ortho)	–0.0586
C31 (meta)	0.0319
C34 (NIT C2)	–0.2428
N58	0.2668
O69	0.3714
N59	0.2657
O68	0.3784
C64 (methylene)	–0.0145
C65 (methylene)	–0.0145
C72 (methyl)	–0.0173
C73 (methyl)	–0.0028
C76 (methyl)	–0.0028
C77 (methyl)	–0.0173

Table S5b: Optimized geometry of tri-radical **3d**.

pPONit3	bond distances (in Å) and angles (in °)		bond distances (in Å) and angles (in °)
P12-O25	1.614	C32-C26	1.408
P12-C9	1.870	C29-C34	1.465
C9-C10	1.408	C34-N58	1.378
C10-C11	1.402	C34-N59	1.379
C11-C6	1.424	N58-O69	1.324
C6-C7	1.424	N59-O68	1.323
C7-C8	1.402	N58-C64	1.528
C8-C9	1.408	N59-C65	1.528
C6-C2	1.465	C64-C65	1.571
C2-N1	1.379	O25-P12-C9	112.0
C2-N3	1.379	O25-P12-C13	112.0
N1-O24	1.323	O25-P12-C26	112.0
N3-O19	1.324	O25-P12-C9-C8	156.0
N1-C5	1.528	O25-P12-C13-C14	–23.3
N3-C4	1.528	O25-P12-C26-C27	156.0
C4-C5	1.571	C9-P12-C13	106.8
P12-C13	1.870	C9-P12-C26	106.8
C13-C14	1.408	C9-P12-C13-C14	–81.0
C14-C15	1.402	C9-P12-C26-C27	–146.3
C15-C16	1.424	C6-C2-N1	126.1
C16-C17	1.423	C6-C2-N3	126.2
C17-C18	1.402	C2-N1-O24	127.6
C18-C13	1.408	C2-N3-O19	127.6
C16-C39	1.465	N1-C2-N3	107.7
C39-N60	1.378	C7-C6-C2-N1	179.3
C39-N61	1.379	C16-C39-N60	126.2
N60-O67	1.324	C16-C39-N61	126.1
N61-O66	1.323	C39-N60-O67	127.6
N60-C62	1.528	C39-N61-O66	127.6
N61-C63	1.528	N60-C39-N61	107.7
C62-C63	1.571	C17-C16-C39-N61	179.8
P12-C26	1.870	C29-C34-N58	126.1
C26-C27	1.408	C29-C34-N59	126.2
C27-C28	1.402	C34-N58-O69	127.7
C28-C29	1.423	C34-N59-O68	127.6
C29-C30	1.424	N58-C34-N59	107.7
C30-C31	1.402	C28-C29-C34-N59	178.2

Table S6a: Spin density computed for the hypothetical di-radical phosphine derivative.

pPNit2	spin density $\rho_{\alpha-\beta}$ in *a.u.* (S = 0)	spin density $\rho_{\alpha-\beta}$ in *a.u.* (S = 1)
P7	–0.0003	0.0017
C2 (P-C)	–0.0539	–0.0540
C1 (meta)	0.0320	0.0321
C6 (ortho)	–0.0566	–0.0566
C5 (C-NIT)	0.0628	0.0627
C4 (ortho)	–0.0591	–0.0590
C3 (meta)	0.0322	0.0319
C8 (P-C)	0.0032	–0.0033
C9-C13 (phenyl)	< ± 0.0002	< ± 0.0001
C14 (P-C)	0.0509	–0.0573
C15 (meta)	–0.0319	0.0321
C16 (ortho)	0.0588	–0.0588
C17 (C-NIT)	–0.0628	0.0627
C18 (ortho)	0.0567	–0.0567
C19 (meta)	–0.0322	0.0320
C20 (NIT C2)	0.2391	–0.2391
N21	–0.2672	0.2672
O25	–0.3728	0.3728
N24	–0.2669	0.2669
O26	–0.3723	0.3723
C22 (methylene)	0.0146	–0.0146
C23 (methylene)	0.0146	–0.0146
C28 (methyl)	–0.0173	0.0173
C29 (methyl)	–0.0173	0.0173
C30 (methyl)	–0.0029	0.0029
C33 (NIT C2)	–0.2392	–0.2392
N57	0.2669	0.2668
O62	0.3721	0.3721
N58	0.2674	0.2674
O61	0.3731	0.3730
C59 (methylene)	–0.0146	–0.0146
C60 (methylene)	–0.0146	–0.0146
C63 (methyl)	0.0173	0.0173
C64 (methyl)	0.0029	0.0029
C65 (methyl)	0.0174	0.0174
C66 (methyl)	0.0029	0.0029

Table S6b: Optimized geometry of the hypothetical di-radical phosphine derivative.

pPNit2	bond distances (in Å) and angles (in °)		bond distances (in Å) and angles (in °)
P7-C8	1.894	C17-C20	1.464
P7-C2	1.893	C20-N21	1.379
P7-C14	1.893	C20-N24	1.379
C8-C9	1.414	N21-O25	1.324
C9-C10	1.408	N21-C22	1.527
C10-C11	1.409	N24-O26	1.325
C11-C12	1.408	N24-C23	1.527
C12-C13	1.409	C22-C23	1.571
C13-C8	1.412	C17-C20-N21	126.2
C2-C3	1.410	C17-C20-N24	126.2
C3-C4	1.404	C21-N21-O25	127.6
C4-C5	1.423	C21-N24-O26	127.6
C5-C6	1.424	N21-C21-N24	107.7
C6-C1	1.401	C16-C17-C21-N21	–179.0
C1-C2	1.414	C5-C33-N57	126.2
C5-C33	1.464	C5-C33-N58	126.2
C33-N57	1.379	C33-N57-O62	127.6
C33-N58	1.379	C33-N58-O61	127.6
N57-O62	1.324	N57-C33-N58	107.6
N57-C60	1.527	C4-C5-C33-N57	1.2
N58-O61	1.324	P7-C14-C15	124.5
N58-C59	1.527	P7-C2-C1	117.5
C59-C60	1.571	P7-C8-C9	117.0
C14-C15	1.410	C8-P7-C14	101.5
C15-C16	1.404	C8-P7-C2	101.9
C16-C17	1.423	C2-P7-C14	101.6
C17-C18	1.424	C15-C14-P7-C2	10.2
C18-C19	1.401	C15-C14-P7-C8	–94.6
C19-C14	1.414	C1-C2-P7-C8	–171.1

Table S6c: Spin density computed for the hypothetical tri-radical phosphine derivative.

pPNit3	spin density $\rho_{\alpha-\beta}$ in e/a_0^3
P12	0.0033
C9 (P-C)	–0.0575
C10 (meta)	0.0321
C11 (ortho)	–0.0568
C6 (C-NIT)	0.0626
C7 (ortho)	–0.0589
C8 (meta)	0.0321
C3 (NIT C2)	–0.2393
N4	0.2668
O13	0.3725
N2	0.2672
O14	0.3730
C1 (methylene)	–0.0146
C5 (methylene)	–0.0146
C15 (methyl)	0.0173
C16 (methyl)	0.0029
C17 (methyl)	0.0029
C18 (methyl)	0.0174
C19 (P-C)	–0.0574
C20 (meta)	0.0321
C21 (ortho)	–0.0586
C22 (C-NIT)	0.0626
C23 (ortho)	–0.0571
C24 (meta)	0.0320
C25 (NIT C2)	–0.2394
N29	0.2667
O31	0.3725
N26	0.2672
O30	0.3730
C27 (methylene)	–0.0146
C28 (methylene)	–0.0146
C32 (methyl)	0.0030
C33 (methyl)	0.0173
C34 (methyl)	0.0173
C35 (methyl)	0.0030
C36 (P-C)	–0.0574
C37 (meta)	0.0321
C38 (ortho)	–0.0570
C39 (C-NIT)	0.0627
C40 (ortho)	–0.0588
C41 (meta)	0.0322
C42 (NIT C2)	–0.2394
N43	0.2666
O47	0.3725
N46	0.3730
O48	0.3730
C44 (methylene)	–0.0146
C45 (methylene)	–0.0146
C49 (methyl)	0.0029
C50 (methyl)	0.0173
C51 (methyl)	0.0174
C52 (methyl)	0.0029

Table S6d: Optimized geometry of the hypothetical tri-radical phosphine derivative.

pPNit3	bond distances (in Å) and angles (in °)		bond distances (in Å) and angles (in °)
P12-C9	1.893	C41-C36	1.410
P12-C19	1.893	C39-C42	1.464
P12-C36	1.893	C42-N43	1.379
C9-C10	1.414	N43-O47	1.324
C10-C11	1.401	C42-N46	1.379
C11-C6	1.424	N46-O48	1.324
C6-C7	1.423	N43-C44	1.527
C7-C8	1.403	N46-C45	1.527
C8-C9	1.410	C44-C45	1.571
C6-C3	1.464	C6-C3-N2	126.2
C3-N2	1.379	C6-C3-N4	126.2
N2-O14	1.324	C3-N2-O14	127.6
C3-N4	1.379	C3-N4-O13	127.6
N4-O13	1.324	N2-C3-N4	107.7
N2-C1	1.527	C7-C6-C3-N2	178.6
N4-C5	1.527	C22-C25-N26	126.2
C1-C5	1.571	C22-C25-N29	126.2
C19-C20	1.410	C25-N26-O30	127.6
C20-C21	1.403	C25-N29-O31	127.6
C21-C22	1.423	N26-C25-N29	107.7
C22-C23	1.424	C21-C22-C25-N26	–179.4
C23-C24	1.401	C39-C42-N43	126.2
C24-C19	1.413	C39-C42-N46	126.2
C22-C25	1.464	C42-N43-O47	127.6
C25-N26	1.379	C42-N46-O48	127.6
N26-O30	1.324	N43-C42-N46	107.7
C25-N29	1.379	C38-C39-C42-N43	179.9
N29-O31	1.324	C9-P12-C19	101.6
N26-C27	1.527	C9-P12-C36	101.7
N29-C28	1.527	C19-P12-C36	101.7
C27-C28	1.572	C10-C9-P12	117.3
C36-C37	1.414	C24-C19-P12	117.3
C37-C38	1.401	C37-C36-P12	117.4
C38-C39	1.424	C10-C9-P12-C19	85.9
C39-C40	1.423	C10-C9-P12-C36	–169.3
C40-C41	1.403	C20-C19-P12-C36	–90.9
C40-C41	1.403	C20-C19-P12-C36	–90.9

Table S7a: Spin density computed for di-radical **5**.

oPONit2	spin density $\rho_{\alpha-\beta}$ in *a.u.* (S = 0) optimized	spin density $\rho_{\alpha-\beta}$ in *a.u.* (S = 1) optimized	spin density $\rho_{\alpha-\beta}$ in *a.u.* (S = 0) x-ray structure	spin density $\rho_{\alpha-\beta}$ in *a.u.* (S = 1) x-ray structure
C1 - C6 (phenyl)	< ± 0.0015	< ± 0.0015	< ±0.0005	< ±0.0005
P7	–0.0003	0.0036	–0.0009	0.0044
O8 (P=O)	–0.0000	–0.0034	0.0007	–0.0051
C9 (C-P)	–0.0177	–0.0233	0.0123	–0.0142
C10	0.0053	0.0105	–0.0021	0.0041
C11	–0.0128	–0.0156	0.0053	–0.0065
C12	0.0053	0.0100	–0.0019	0.0033
C13	–0.0177	–0.0205	0.0103	–0.0113
C14 (C-NIT)	0.0354	0.0404	–0.0303	0.0317
C15 (C2 of NIT)	–0.2587	–0.2593	0.2555	–0.2555
N16	0.2632	0.2533	–0.2582	0.2582
O20	0.3705	0.3707	–0.3589	0.3589
N19	0.2576	0.2579	–0.2545	0.2546
O21	0.3610	0.3611	–0.3672	0.3672
C17 (methylene)	–0.0151	–0.0151	0.0150	–0.0150
C18 (methylene)	–0.0138	–0.0138	0.0139	–0.0139
C22 (methyl)	0.0165	0.0165	–0.0186	0.0186
C23 (methyl)	0.0041	0.0041	–0.0035	0.0035
C24 (methyl)	0.0029	0.0029	–0.0030	0.0030
C25 (methyl)	0.0168	0.0168	–0.0185	0.0185
C26 (C-P)	0.0292	–0.0289	–0.0175	–0.0174
C27	–0.0126	0.0127	0.0059	0.0060
C28	0.0236	–0.0235	–0.0109	–0.0109
C29	–0.0122	0.0123	0.0048	0.0048
C30	0.0276	–0.0276	–0.0139	–0.0139
C31 (C-NIT)	–0.0436	0.0438	0.0322	0.0324
C32 (C2 of NIT)	0.2537	–0.2538	–0.2457	–0.2458
N33	–0.2576	0.2576	0.2623	0.2623
O37	–0.3512	0.3510	0.3619	0.3618
N36	–0.2704	0.2704	0.2529	0.2529
O42	–0.3778	0.3777	0.3601	0.3601
C34 (methylene)	0.0135	–0.0130	–0.0147	–0.0144
C35 (methylene)	0.0155	–0.0154	–0.0149	–0.0148
C38 (methyl)	–0.0164	0.0164	0.0178	0.0180
C39 (methyl)	–0.0030	0.0049	0.0039	0.0065
C40 (methyl)	–0.0026	0.0026	0.0045	0.0045
C41 (methyl)	–0.0175	0.0175	0.0175	0.0174

Table S7b: Optimized geometry for di-radical **5**.

oPONit2	bond distances (in Å) and angles (in °)		bond distances (in Å) and angles (in °)
P7-O8	1.620	N36-C35	1.531
P7-C5	1.871	C34-C35	1.581
P7-C9	1.882	C31-C32-N33	124.8
P7-C26	1.895	C31-C32-N36	125.3
C9-C10	1.406	C32-N33-O37	125.6
C10-C11	1.405	C32-N36-O42	126.7
C11-C12	1.405	N33-C32-N36	109.7
C12-C13	1.403	C26-C31-C32-N33	52.1
C13-C14	1.411	C31-C32-N33-O37	–2.5
C14-C9	1.419	C14-C15-N16	125.8
C14-C15	1.476	C14-C15-N19	124.3
C15-N16	1.366	C15-N19-O21	126.0
C15-N19	1.362	C15-N16-O20	126.8
N16-O20	1.323	N16-C15-N19	109.7
N19-O21	1.322	C9-C14-C15-N19	62.8
N16-C17	1.532	C14-C15-N19-O21	–1.6
N19-C18	1.524	O8-P7-C5	111.7
C17-C18	1.581	O8-P7-C5-C6	35.7
C26-C27	1.411	O8-P7-C9	114.1
C27-C28	1.405	O8-P7-C9-C14	28.0
C28-C29	1.406	P7-C9-C14-C15	9.0
C29-C30	1.402	O8-P7-C26	112.0
C30-C31	1.415	O8-P7-C26-C31	23.6
C31-C26	1.421	P7-C26-C31-C32	11.0
C31-C32	1.470	C9-P7-C26	108.2
C32-N33	1.359	C9-P7-C26-C31	–102.9
C32-N36	1.369	C9-P7-C5	108.1
N33-O37	1.320	C9-P7-C5-C6	162.0
N36-O42	1.323	C26-P7-C5	102.0
N33-C34	1.526	C26-P7-C5-C6	–84.1