Supplementary Material (ESI) for PCCP

Theoretical Studies of ^{31}P NMR Spectral Properties of Phosphanes and Related Compounds in Solution

Boris Maryasin, Hendrik Zipse*[a]

Supporting information

Theoretical methods and computational details

The geometries of all systems have been optimized at the MPW1K/6-31G(d) level of theory. The conformational space of the systems has first been searched using the MM3 force field and the systematic search routine in the TINKER program, and, in some cases, also with MM3* and OPLS force fields and the systematic routine implemented in MACROMODEL 9.7.[1,2] All stationary points located at force field level have then been reoptimized at MPW1K/6-31G(d) level.

The thermal corrections to Gibbs free energy to 298.15 K have been calculated for all minima from unscaled vibrational frequencies obtained at the same level.

These MPW1K/6-31G(d) geometries have been directly used for gas-phase NMR chemical shift calculations.

For conformationally flexible systems thermal corrections to Gibbs free energy have been combined with single point energies calculated at the MP2(FC)/6-31+G(2d,p)//MPW1K/6-31G(d) level to yield Gibbs free energies G_{298} at 298.15 K. For these conformationally flexible systems chemical shifts have been calculated as Boltzmann-averaged values over all available conformers, relying on the Gibbs free energies in the gas phase calculated as written before.

For the consideration of solvent effect we have compared two approaches:
a)Solution model 1: use of the Polarized Continuum Model (PCM) in combination with the NMR shift calculations. In this case for Boltzmann averaging of chemical shifts Gibbs free energies in solution $G_{298,\mathrm{solvent}}$ have been used, yielded from Gibbs free energies G_{298} in the gas phase (calculated as described before), combined with PCM determined solvation free energies.
b)Solution model 2: inclusion of one explicit solvent molecule in the geometry optimization of the substrate and subsequent NMR shift calculations on this solvent/solute complex in combination with PCM approach. The conformational flexibility of the complexes has been treated analogously to the *vide supra* situation.

All quantum mechanical calculations have been performed with Gaussian 03.[3]

Table 1 Experimental chemical shifts of Ph_3P (**1**) measured in different solvents

Chemical shift, ppm	Solvent
-4.73 [b]	Chloroform-d_1[11]
-4.45	Chloroform-d_1[5]
-5.64	Chloroform-d_1[7]
-4.98	Chloroform-d_1[12]
-8.0	Chloroform-d_1[14]
-5.4	Chloroform-d_1[15]
-5.9	Benzene-d_6[29]
-4.7 [b]	Benzene-d_6[34]
-5.0	Benzene-d_6[16]
-5.0	Benzene-d_6[32]
-4.93	Benzene-d_6[33]
-4.6	Dimethylformamide[6]
-5.37	Pyridine[7]
-5.3	Tetrahydrofuran[8]
-6.0	Tetrahydrofuran-d_8[1]
-5.9	Tetrahydrofuran[9]
-6.3	Dichlormethane + 10%benzene[13]

[a] The value has been used for present study

Table 2 Experimental chemical shifts of Ph_3PO (**2**) measured in different solvents

Chemical shift, ppm	Solvent
+29.65 [b]	Chloroform-d_1[11]
+29.4	Chloroform-d_1[15]
+28.51	Chloroform-d_1[7]
+29.4	Chloroform-d_1[26]
+26.4	Chloroform-d_1[14]
+24.7 [b]	Benzene-d_6[27]
+26.4	Benzene-d_6[28]
+28.4	Benzene-d_6[16]
+30.1	Benzene-d_6[29]
+25.4	Toluene-d_8[31,35-39]
+28.1	Toluene-d_8[30]
+34.7	Acetonitril-d_3[29]
+26.0	Dichlormethane[9]
+30.0	Dichlormethane[25]
+25.0	Dimethylformamide[25]
+27.2	Tetrahydrofuran[9]

[b] The value has been used for present study

Table 3 Experimental chemical shifts of Me_3P (**6**) measured in different solvents

Chemical shift, ppm	Solvent
-61.58	Chloroform-d1[22]
-60.5	Chloroform-d_1[21]
-61.0 [b]	Benzene-d_6[17]
-61.1	Dichlormethane[18]
-61.5	Tetrahydrofuran[19]
-61.0	Neat (no solvent)[20]
-63.0	Gas-phase[23]

[b] The value has been used for present study

Table 4 Experimental chemical shifts[40] of PH_3 (**3**) measured in different solvents

Temperature, °C			Solvent
29	50	71	
-238.4	-239.7	-241.0	Tetrachlormethane
-242.4 [b]	-243.5	-244.5	Benzene
-243.3	-244.0	-244.8	Toluene
-246.3	-247.0	-247.6	Cyclohexane

[b] -242 ppm - The value has been used for present study

Table 5 Experimental chemicals shifts of PH_3 (**3**) measured in gas-phase

-254.2	Gas-phase[40]
-266.1	Gas-phase[23]

Table 6 Chemical shifts and energetic characteristics for solvent-solute complexes of **22** with $CHCl_3$ as employed for solvent model 2

		Free energies, kJ/mol					
Complex	Chem. shift ppm[a]	MPW1K/ 6-311++G(2d,2p)		MP2(FC)/ 6-31+G(2d,p)		MP2(FC)/ G3MP2large	
		ΔG_{298} [b]	$\Delta G_{298,CHCl3}$ [c]	ΔG_{298} [d]	$\Delta G_{298,CHCl3}$ [e]	ΔG_{298} [f]	$\Delta G_{298,CHCl3}$ [g]
22_1*$CHCl_3$_1	+62.4	0.0	0.0	0.0	0.0	0.0	0.0
22_1*$CHCl_3$_2	+65.9	5.8	4.5	4.9	3.5	5.7	4.4
22_2*$CHCl_3$_1	+52.1	2.9	5.7	4.0	6.7	4.0	6.7
22_2*$CHCl_3$_2	+50.8	3.9	1.8	11.8	9.7	12.0	10.0
22_3*$CHCl_3$_1	+82.7	13.6	14.9	9.8	11.1	11.7	13.0
22_3*$CHCl_3$_2	+85.1	17.0	13.4	17.7	14.1	19.8	16.2
<δ> [g]		+59.2	+59.1	+61.5	+62.6	+61.2	+62.3

[a] relative to PPh_3, GIAO-MPW1K/6-311++G(2d,2p) + PCM/UAHF/MPW1K/6-311++G(2d,2p); [b] MPW1K/6-311++G(2d,2p), free en. corr.: MPW1K/6-31G(d); [c] MPW1K/6-311++G(2d,2p) + PCM/UAHF/MPW1K/6-311++G(2d,2p), free en. corr.: MPW1K/6-31G(d); [d] MP2(FC)/6-31+G(2d,p)//MPW1K/6-31G(d), free en. corr.: MPW1K/6-31G(d); [e] MP2(FC)/6-31+G(2d,p)//MPW1K/6-31G(d) + PCM/UAHF/MPW1K/6-311++G(2d,2p), free en. corr.: MPW1K/6-31G(d); [e] MP2(FC)/G3MP2large//MPW1K/6-31G(d), free en. corr.: MPW1K/6-31G(d); [f] MP2(FC)/G3MP2large//MPW1K/6-31G(d) + PCM/UAHF/MPW1K/6-311++G(2d,2p), free en. corr.: MPW1K/6-31G(d); [g] Boltzmann-averaged chemical shift

References

[a] M. Sci. Boris Maryasin, Prof. Dr. Hendrik Zipse, Department of Chemistry, LMU München, Butenandtstrasse 5-13, D-81377 München, Germany. Fax: +49 89 2180 77738;
E-mail: zipse@cup.uni-muenchen.de

1. J. W. Ponder, TINKER; 4.2 ed., 2004.
2. Schrödinger, LLC., MacroModel 9.7, 2009
3. Gaussian 03, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.
4. V. Farina and B. Krishnan, *J. Am. Chem. Soc*., 1991, 113, 9585

5. V. F. Slagt, P. W. N. M. van Leeuwen and J. N. H. Reek, *Dalton Trans*., 2007, 22, 2302.
6. J. M. Berg' and R. H. Holm, J*. Am. Chem. Soc*, 1985, 107, 925.
7. T. Wilczewski, J*. Organomet. Chem*., 1990, 382, 431.
8. D. Crich, H. Dyker and R. J. Harris, *J. Org. Chem*., 1989, 54, 257.
9. W. Levason, R. Patel, G. Reid, *J. Organomet. Chem*., 2003, 688, 280.
10. I. Mathieu-Pelta and S. A. Evans, Jr., *J. Org. Chem*., 1994, 59, 2234
11. W.-N. Chou, M. Pomerantz, *J. Org. Chem*., 1991, 56, 2762.
12. A. J. Bellamy, R. O. Gould and M. D. Walkinshaw, *J. Chem. Soc Perk. T 2*, 1981, 1099.
13. T. Allman and R. G. Goel, *Can. J. Chem*., 1982, 60, 716.
14. R. Appel und L. Willms, *Chem. Ber*., 1981, 114. 858.
15. G. F. de la Fuente and J. E. Huheey, *Phosphorus Sulfur*, 1993, 78, 23.
16. H. J. Lawson and J. D. Atwood, *J. Am. Chem. Soc*., 1989, 111, 6223.
17. C. A. Jaska, T. J. Clark, S. B. Clendenning, D. Grozea, A. Turak, Z.-H. Lu and I. Manners, *J. Am. Chem. Soc*., 2005, 127, 5116.
18. F. Palacios, J. Vicario and D. Aparicio, *J. Org. Chem*., 2006, 71.
19. K. Abdur-Rashid, T. P. Fong, B. Greaves, D. G. Gusev, J. G. Hinman, S. E. Landau, A. J. Lough and R. H. Morris, *J. Am. Chem. Soc*., 2000, 122, 38, 9157.
20. H. Karsch, *Chem. Ber*., 1982, 115, 823.
21. L. K. Krannich, R. K. Kanjolia, C. L. Watkins, *Magn. Reson. Chem*., 1987, 25, 320.
22. M. Alajarin, P. Molina, A. Vidal, F. Tovar, *Tetrahedron*, 1997, 53, 13449.
23. C. J. Jameson, A. de Dios, *Chem. Phys. Lett.,* 1990, 167, 575.
24. N. Burford, B. W. Royan, R. E. v. H. Spence and R. D. Rogers, *J. Chem. Soc., Dalton Trans*., 1990, 7, 2111.
25. F. El Khatib, J. Bellan, M. Koenig, *Phosphorus Sulfur*, 1998, 134, 391.
26. M. Varasi, K. A. M. Walker and M. L. Maddox, *J. Org. Chem*., 1987, 52, 4235
27. K. L. McKillop, G. R. Gillette, D. R. Powell and R. West, *J. Am. Chem. Soc*., 1992, 114, 5203.
28. I. Mathieu-Pelta, S. A. Evans, *J. Org. Chem*., 1994, 59, 2234.
29. C. D. Hall, P. D. Beer, R. L. Powell and M. P. Naan, *Phosphorus Sulfur,* 1995, 105, 145.
30. N. Lowther, C. D. Hall, *J. Chem. Soc., Chem. Commun*., 1985, 19, 1303.
31. I. D. Grice, P. J. Harvey, I. D. Jenkins, M. J. Gallagher, M. G. Ranasinghe, *Tetrahedron Lett.,* 1996, 37, 1087.
32. R. U. Kirss, *Journal Organomet. Chem*., 1995, 498, 171.
33. M. C. Potyen and I. P Rothwell, *J. Chem. Soc., Chem. Commun*., 1995, 8, 849.
34. J. Schraml, M. Čapka and V. Blechta, *Magn. Reson. Chem*., 1992, 30, 544.
35. P. Harvey, I. D. Jenkins*, Tetrahedron Lett*., 1994, 35, 9775.
36. D. Camp, I. D. Jenkins, *Aust. J. Chem*., 1992, 45, 47.
37. D. Camp, I. D. Jenkins, *J. Org. Chem*., 1989, 54, 3045.
38. M. Von Itzstein, I. D. Jenkins, *J.Chem. Soc Perkin Trans. 1*, 1987, 2057; 1986, 437.
39. M. Von Itzstein, I. D. Jenkins, *Aust. J. Chem*., 1984, 37, 2447; 1983, 36, 557.
40. N. Zumbulyadis and B. P. Dailey, *Mol. Phys*., 1974, 27, 633.

Archive Entries and calculated shielding values

1 C_3

1\1\GINC-NODE8\FOpt\RmPWPW91\6-31G(d)\C18H15P1\ZIP04\22-May-2009\0\\#m
pwpw91/6-31g(d) opt=(maxcycle=50) scf=tight int=finegrid IOp(3/76=0572

004280)\\molnmr_001\\0,1\P,-0.0000000005,0.0000000009,-1.2625464489\C,
1.6467724861,-0.0166469133,-0.4561888184\C,2.6359006163,-0.8028094913,
-1.0455859646\C,1.9655033457,0.7121086664,0.6863380921\C,3.9040720353,
-0.8770497646,-0.4951204537\H,2.4088755994,-1.3591385681,-1.9447377934
\C,3.2388120641,0.6474707111,1.2305990265\H,1.2159650756,1.334970259,1
.1517185947\C,4.2087560127,-0.149436005,0.6448032035\H,4.6572040897,-1
.4951555232,-0.9619431118\H,3.4719470094,1.2207970145,2.1163155827\H,5
.2002554821,-0.1989856586,1.0708906449\C,-0.8089695932,1.4344702656,-0
.4561888184\C,-1.5994558682,1.3461214972,0.6863380921\C,-0.6226968943,
2.6841616429,-1.0455859646\C,-2.180132116,2.4811581718,1.2305990265\H,
-1.7641006954,0.3855715178,1.1517185947\C,-1.1924886412,3.8195504448,-
0.4951204537\H,-0.0273892725,2.7657167494,-1.9447377934\C,-1.974962629
8,3.7196076296,0.6448032035\H,-2.7932147322,2.3963958052,2.1163155827\
H,-1.0337593792,4.7808348156,-0.9619431118\H,-2.4278011057,4.603046184
7,1.0708906449\C,-0.8378028944,-1.4178233497,-0.4561888184\C,-2.013203
7235,-1.881352149,-1.0455859646\C,-0.366047479,-2.058230161,0.68633809
21\C,-2.7115833957,-2.9425006776,-0.4951204537\H,-2.3814863285,-1.4065
781787,-1.9447377934\C,-1.0586799496,-3.1286288803,1.2305990265\H,0.54
81356183,-1.7205417742,1.1517185947\C,-2.2337933844,-3.570171622,0.644
8032035\H,-3.623444712,-3.2856792898,-0.9619431118\H,-0.6787322788,-3.
6171928172,2.1163155827\H,-2.7724543779,-4.4040605235,1.0708906449\\Ve
rsion=AM64L-G03RevD.01\State=1-A\HF=-1036.1138845\RMSD=6.789e-09\RMSF=
1.760e-05\Thermal=0.\Dipole=0.,0.,0.6303467\PG=C03 [C3(P1),X(C18H15)]\
\@

Level of theory	Shielding, ppm
MPW1K/6-311+G(d,p)	346.9819
B98/6-311+G(d,p)	323.3616
B3LYP/6-311+G(d,p)	305.7122
HF/6-311+G(d,p)	379.9194
MP2/6-311+G(d,p)	362.4713
MPW1K/6-311++G(2d,2p)	337.0432
MPW1K/IGLOIII	342.6872
MPW1K/3-21G	504.5147
MPW1K/6-31G(d)	403.1655
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	337.3980
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAKS)	337.4117
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAHF)	337.3727
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAKS)	337.3857
MPW1K/IGLOIII + PCM($CHCl_3$,UAHF)	343.0746
MPW1K/IGLOIII + PCM($CHCl_3$,UAKS)	343.0750
MPW1K/IGLOIII + PCM(C_6H_6,UAHF)	343.0124
MPW1K/IGLOIII + PCM(C_6H_6,UAKS)	343.0147

1*$CHCl_3$_1

1\1\GINC-GOLEM\SP\RmPWPW91\6-311++G(2d,2p)\C19H16Cl3P1\BORIS\03-Jun-20
08\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0
572004280) scrf=(PCM,Read,solvent=chloroform)\\bm_mbh_pph3chcl3_002_PC
M_UAHF_001\\0,1\P\C,1,1.83216898\C,2,1.3945326,1,116.93928043\C,2,1.39
200014,1,124.27380644,3,178.6546928,0\C,3,1.38424428,2,120.73059313,1,
179.83120967,0\H,3,1.0814748,2,119.62092072,1,-0.02212224,0\C,4,1.3863
8162,2,120.45984265,1,-179.03830225,0\H,4,1.08004035,2,119.82616144,1,
0.67306442,0\C,7,1.38533038,4,120.25971912,2,-0.33971247,0\H,5,1.08022
838,3,119.802023,2,179.61958693,0\H,7,1.0805,4,119.67637146,2,179.7468
5327,0\H,9,1.08029664,7,120.1218069,4,-179.9701115,0\C,1,1.83229784,2,
102.6527508,4,11.01897739,0\C,13,1.39238045,1,124.42983521,2,-89.14399
691,0\C,13,1.39398965,1,116.86133475,2,91.80801992,0\C,14,1.3860554,13
,120.5085353,1,-179.38942644,0\H,14,1.08018368,13,119.83026526,1,0.329
65593,0\C,15,1.38453388,13,120.79494295,1,-179.94454614,0\H,15,1.08135
652,13,119.4859785,1,0.35615921,0\C,16,1.38567587,14,120.24380513,13,-
0.28581501,0\H,16,1.08049542,14,119.69612031,13,179.77786943,0\H,18,1.
08029077,15,119.84977301,13,179.80489648,0\H,20,1.08028945,16,120.1096
0228,14,179.94788715,0\C,1,1.83543062,2,102.1853141,4,-94.38716534,0\C

- ,24,1.39575565,1,116.98442523,2,-167.59450114,0\C,24,1.39290677,1,124.
41551535,2,11.05546294,0\C,25,1.38505702,24,120.87302454,1,179.8220189
9,0\H,25,1.08131763,24,119.46621726,1,0.0806484,0\C,26,1.38803436,24,1
20.56181579,1,-179.13347666,0\H,26,1.08002294,24,119.75898809,1,0.5948
4431,0\C,29,1.38625014,26,120.2846266,24,-0.22486989,0\H,27,1.08011583
,25,119.86590378,24,179.91692132,0\H,29,1.08029735,26,119.64605155,24,
179.67523776,0\H,31,1.08000865,29,120.1743269,26,179.79699267,0\H,29,2
.76768842,26,76.74649532,24,64.2573078,0\C,31,3.72123591,29,79.4863941
6,26,73.48299321,0\Cl,36,1.75933871,31,129.31338881,29,-94.1926956,0\C
l,36,1.75940497,31,104.25882377,29,39.38301065,0\Cl,36,1.75950761,31,8
7.33488034,29,150.49006328,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-2
455.7221962\RMSD=3.930e-09\Thermal=0.\Dipole=-1.2593168,-0.2805186,0.1
856684\PG=C01 [X(C19H16Cl3P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	336.8437
MPW1K/IGLOIII	342.6131
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	336.7176
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAKS)	336.6920
MPW1K/IGLOIII + PCM($CHCl_3$,UAHF)	342.6838
MPW1K/IGLOIII + PCM($CHCl_3$,UAKS)	342.6780

1*$CHCl_3$_2

1\1\GINC-CIPCLU05\SP\RMP2-FC\6-31+G(2d,p)\C19H16Cl3P1\BRYCH\19-Nov-200
9\0\\#p mp2(fc)/6-31+g(2d,p) scf=tight int=finegrid\\pph3_chcl3_p_spmp
\\0,1\P,0,-0.40934,0.001162,0.001975\C,0,-1.199791,-0.673606,1.507701\
C,0,-0.602517,-1.78678,2.097211\C,0,-2.33872,-0.131563,2.096384\C,0,-1
.143274,-2.358258,3.236074\H,0,0.29473,-2.206385,1.662885\C,0,-2.87308
8,-0.6978,3.243251\H,0,-2.80698,0.738326,1.659864\C,0,-2.279874,-1.812
793,3.812547\H,0,-0.670682,-3.222361,3.679692\H,0,-3.75575,-0.26555,3.
691993\H,0,-2.69762,-2.2517,4.70685\C,0,-1.189563,1.646606,-0.172599\C
,0,-2.331228,1.88817,-0.93147\C,0,-0.581626,2.713783,0.486691\C,0,-2.8
57485,3.167428,-1.019736\H,0,-2.807394,1.075088,-1.459401\C,0,-1.11414
6,3.989061,0.406947\H,0,0.31782,2.545055,1.063119\C,0,-2.253321,4.2183
28,-0.34881\H,0,-3.742266,3.342078,-1.614691\H,0,-0.633105,4.805414,0.
925566\H,0,-2.664785,5.214601,-0.420022\C,0,-1.1865,-0.969176,-1.34047
3\C,0,-0.574188,-0.931381,-2.592252\C,0,-2.330103,-1.745395,-1.17516\C
,0,-1.10417,-1.636185,-3.659308\H,0,0.32664,-0.349043,-2.730624\C,0,-2
.853864,-2.45948,-2.241487\H,0,-2.809921,-1.796005,-0.208853\C,0,-2.24
5226,-2.403695,-3.484775\H,0,-0.619716,-1.595068,-4.623893\H,0,-3.7401
71,-3.060707,-2.099034\H,0,-2.654622,-2.961992,-4.314011\H,0,2.275223,
-0.000999,0.00748\C,0,3.360693,-0.001958,0.008689\Cl,0,3.898421,0.3839
36,-1.622274\Cl,0,3.89629,1.217343,1.159385\Cl,0,3.894503,-1.608339,0.
490354\\Version=AM64L-G03RevD.01\State=1-A\HF=-2448.0412175\MP2=-2451.
2952851\RMSD=8.116e-09\Thermal=0.\PG=C01 [X(C19H16Cl3P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	334.7652
MPW1K/IGLOIII	
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	334.6193
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAKS)	334.6221
MPW1K/IGLOIII + PCM($CHCl_3$,UAHF)	
MPW1K/IGLOIII + PCM(CHCl,UAKS)	

	MPW1K/6-311++G(2d,2p) + PCM/UAHF/MPW1K/6-311++G(2d,2p)	MP2(FC)/6-31+G(2d,p)/MPW1K/6-31G(d) + PCM/UAHF/MPW1K/6-311++G(2d,2p)		
	Shielding, ppm	E_{tot}	„G“$_{298,\ gas}$	„G“$_{298,CHCl3}$
1*$CHCl_3$_1	336.7176	-2451.298781	-2451.055107	-2451.043044
1*$CHCl_3$_2	334.6193	-2451.295285	-2451.052558	-2451.040463

<σ> = 336.5897 ppm

1*C_6H_6_1

1\1\GINC-NODE6\SP\RmPWPW91\6-311++G(2d,2p)\C24H21P1\ZIP04\06-Jun-2008\
0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0572
004280) scrf=(PCM,Read,solvent=benzene)\\bm_mbh_pph3benz_001_PCM_UAHF_
001\\0,1\P\C,1,1.83259186\C,2,1.39503414,1,116.89010278\C,2,1.39155357
,1,124.34200973,3,178.60048926,0\C,3,1.38394349,2,120.70542349,1,179.8
0383427,0\H,3,1.08134483,2,119.79434981,1,-0.52329957,0\C,4,1.3868962,
2,120.48350192,1,-178.94223432,0\H,4,1.07999589,2,119.84459242,1,0.944
78607,0\C,7,1.38497162,4,120.28124426,2,-0.39750437,0\H,5,1.08035996,3
,119.64146575,2,179.51424539,0\H,7,1.08057669,4,119.64272448,2,179.792
27953,0\H,9,1.08037823,7,120.14457001,4,-179.92413622,0\C,1,1.83271301
,2,102.60422957,4,6.5464726,0\C,13,1.3921868,1,124.41161889,2,-90.4723
6048,0\C,13,1.39419206,1,116.92225911,2,90.62487765,0\C,14,1.3861177,1
3,120.53172618,1,-179.28372198,0\H,14,1.08008829,13,119.81860787,1,0.4
0680298,0\C,15,1.38454057,13,120.82221447,1,-179.99138552,0\H,15,1.081
44519,13,119.48341415,1,0.28209041,0\C,16,1.38553903,14,120.2653839,13
,-0.31406669,0\H,16,1.08053502,14,119.68184773,13,179.76103928,0\H,18,
1.08035047,15,119.84590891,13,179.73631168,0\H,20,1.08032212,16,120.13
203869,14,179.99530051,0\C,1,1.83387693,2,101.89462555,4,-99.26648206,
0\C,24,1.39405315,1,117.12386338,2,-162.86410846,0\C,24,1.39283791,1,1
24.20010682,2,15.67608751,0\C,25,1.38511564,24,120.82493537,1,179.3904
388,0\H,25,1.08137373,24,119.441485,1,-0.21049915,0\C,26,1.38658396,24
,120.54214237,1,-178.74312826,0\H,26,1.08019597,24,119.67681396,1,0.88
63007,0\C,29,1.38604271,26,120.24069228,24,-0.25865504,0\H,27,1.080362
2,25,119.87211671,24,179.83628291,0\H,29,1.08054864,26,119.73362181,24
,179.81739028,0\H,31,1.08024236,29,120.12290081,26,179.85160932,0\C,26
,3.97582597,24,80.2628895,1,-100.12598035,0\C,35,1.38647324,26,145.397
05455,24,-17.63183547,0\C,36,1.38633015,35,120.11498584,26,153.1658011
4,0\C,37,1.38624794,36,120.00009797,35,-0.01010736,0\C,38,1.38642817,3
7,119.96095899,36,-0.03827346,0\C,39,1.38657054,38,120.00463001,37,0.0
4305314,0\H,35,1.08021323,26,31.60318523,24,-65.8334194,0\H,36,1.08044
711,35,119.88846788,26,-26.77027178,0\H,37,1.08052706,36,120.0221163,3
5,-179.9819964,0\H,38,1.08053757,37,120.01430801,36,179.96300546,0\H,3
9,1.08069743,38,119.97677442,37,179.90496157,0\H,40,1.0803079,39,120.1
6248826,38,-179.79744849,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-126
8.5727758\RMSD=5.532e-09\Thermal=0.\Dipole=-0.494992,-0.4178277,0.1856
017\PG=C01 [X(C24H21P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	335.7529
MPW1K/IGLOIII	341.6665
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAHF)	335.7325
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAKS)	335.7386
MPW1K/IGLOIII + PCM(C_6H_6,UAHF)	341.7266
MPW1K/IGLOIII + PCM(C_6H_6,UAKS)	341.7323

1*C_6H_6_2

1\1\GINC-CIPCLU04\SP\RmPWPW91\6-311++G(2d,2p)\C24H21P1\BRYCH\23-Nov-20
09\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0
572004280) geom=check guess=read\\pph3_c6h6_p4_nmr\\0,1\P,0,-0.5881325
141,-0.4376005705,1.0912247405\C,0,-0.2561243108,1.2255915344,0.393910
368\C,0,0.1479566529,2.2173515255,1.2876327347\C,0,-0.3480322788,1.542
8250172,-0.9581297891\C,0,0.4362391785,3.4970847006,0.8450545886\H,0,0
.2399132268,1.9819615525,2.3392922302\C,0,-0.0480252201,2.821514021,-1
.4035379001\H,0,-0.6486394502,0.7855141524,-1.6668494677\C,0,0.3417489
699,3.8013723908,-0.504829518\H,0,0.7441485576,4.2540151945,1.55175576
08\H,0,-0.1212203309,3.0514045747,-2.4567988891\H,0,0.5748229436,4.796
7719942,-0.8540410741\C,0,-0.7347786824,-1.4734295643,-0.413012938\C,0
,-1.9449375269,-1.8522624887,-0.9862432819\C,0,0.4521070376,-1.9335838
829,-0.9840037571\C,0,-1.9675036264,-2.6684092492,-2.1071144184\H,0,-2
.8743047312,-1.5117235298,-0.5544166319\C,0,0.4282494895,-2.735535904,
-2.1117587894\H,0,1.4018036636,-1.6584731045,-0.5458988468\C,0,-0.7830

804382,-3.1086048796,-2.6740514273\H,0,-2.9150318594,-2.9578278855,-2.
5384691726\H,0,1.3571269685,-3.0763864094,-2.5453715308\H,0,-0.8029247
343,-3.7434985114,-3.5479828938\C,0,-2.3283101638,-0.2801019699,1.6439
920804\C,0,-2.7830824336,-1.2022515001,2.5847850658\C,0,-3.2050948469,
0.7040104655,1.1942596119\C,0,-4.0863567563,-1.1555121425,3.0509120869
\H,0,-2.107003978,-1.9595704631,2.9572538117\C,0,-4.5059378954,0.75809
5521,1.6688178019\H,0,-2.8674558711,1.433963863,0.4731609138\C,0,-4.95
01510532,-0.1725634734,2.5946486001\H,0,-4.4238166385,-1.8798400663,3.
7779648329\H,0,-5.174167719,1.5291664502,1.313219315\H,0,-5.964430486,
-0.1281600899,2.9639803431\H,0,2.9644134424,-0.0140072066,1.4328298212
\C,0,3.6284335327,-0.0164490884,0.5802846409\C,0,4.5833198105,-1.01336
07781,0.4448661853\C,0,3.5200949767,0.9770013645,-0.3818167918\C,0,5.4
322364951,-1.0162797735,-0.6513699307\H,0,4.6663128076,-1.78673451,1.1
94934147\C,0,4.3700046805,0.9728209474,-1.4770586993\H,0,2.771954749,1
.7490314967,-0.2771742676\C,0,5.3255765858,-0.0225096051,-1.6120531202
\H,0,6.1770734397,-1.7920209922,-0.7563651587\H,0,4.2860024077,1.74596
84366,-2.2271926348\H,0,5.9873959293,-0.0241625635,-2.4662737516\\Vers
ion=AM64L-G03RevD.01\State=1-A\HF=-1268.5710585\RMSD=2.941e-09\Thermal
=0.\Dipole=-0.4741169,0.222277,-0.3733812\PG=C01 [X(C24H21P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	333.6551
MPW1K/IGLOIII	
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAHF)	333.7080
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAKS)	
MPW1K/IGLOIII + PCM(C_6H_6,UAHF)	
MPW1K/IGLOIII + PCM(C_6H_6,UAKS)	

	MPW1K/6-311++G(2d,2p) + PCM/UAHF/MPW1K/6-311++G(2d,2p)	MP2(FC)/6-31+G(2d,p)/MPW1K/6-31G(d) + PCM/UAHF/MPW1K/6-311++G(2d,2p)		
	Shielding, ppm	E_{tot}	„G“$_{298,\ gas}$	„G“$_{298,CHCl3}$
1*C_6H_6_1	335.7325	-1265.382840	-1265.055205	-1265.046041
1*C_6H_6_2	333.7080	-1265.383835	-1265.056668	-1265.045672

<σ> = 334.9158 ppm

2_1 C_1

1\1\GINC-NODE-27\SP\RmPWPW91\6-31G(d)\C18H15O1P1\ZIP04\23-Jan-2008\0\\
#mpwpw91/6-31g(d) nmr scf=tight int=finegrid IOp(3/76=0572004280) geom
=check guess=read\\bm_mbh_nmr_0006\\0,1\P,0,0.0771897347,-0.0233721421
,0.087035764\O,0,0.1013452401,-0.0517421853,1.5744800712\C,0,1.7017033
874,-0.0177401193,-0.7151183797\C,0,2.449612173,-1.1940375228,-0.72268
82917\C,0,2.2635949777,1.1474463547,-1.2267409394\C,0,3.7308766651,-1.
2057266664,-1.2439827567\H,0,2.0264681315,-2.1026875272,-0.3189532822\
C,0,3.5470700981,1.1338788847,-1.7493482468\H,0,1.6987968203,2.0678073
871,-1.2173364489\C,0,4.2797317143,-0.0412399994,-1.759970406\H,0,4.30
22883409,-2.1222301229,-1.2466164357\H,0,3.9745903143,2.0429120756,-2.
1462188721\H,0,5.2800531988,-0.0504605189,-2.1678033838\C,0,-0.7934749
274,1.4428689352,-0.5272471801\C,0,-1.0722724419,1.6695807187,-1.87222
26908\C,0,-1.2116949589,2.363139586,0.4266401529\C,0,-1.7561414579,2.8
089250626,-2.2571394494\H,0,-0.7595220938,0.9567810091,-2.621788238\C,
0,-1.8971619403,3.503927227,0.038350185\H,0,-0.9948174397,2.1664526862
,1.4664107396\C,0,-2.1682179834,3.7268168679,-1.3011703308\H,0,-1.9713
148922,2.9812011771,-3.301537492\H,0,-2.2207671461,4.2164095376,0.7828
848126\H,0,-2.7040652373,4.6147948607,-1.6037482456\C,0,-0.7861282962,
-1.4592826736,-0.6025632843\C,0,-1.6644659828,-2.1250766534,0.24620441
52\C,0,-0.6336042138,-1.8982921277,-1.9145895442\C,0,-2.3914419681,-3.
2094010994,-0.2163491373\H,0,-1.7550853053,-1.7905244349,1.2692581721\
C,0,-1.3624217314,-2.9820495447,-2.3748378399\H,0,0.0695941786,-1.4091
138753,-2.5739607567\C,0,-2.2434376589,-3.6355557703,-1.5267114695\H,0
,-3.0699038181,-3.7248311181,0.447493444\H,0,-1.2372706662,-3.32153458

33,-3.3926411154\H,0,-2.8092554613,-4.4826946155,-1.8863798865\\Versio
n=IA32L-G03RevD.01\State=1-A\HF=-1111.3389231\RMSD=1.773e-09\Thermal=0
.\Dipole=-0.0542574,0.0212194,-1.7243145\PG=C01 [X(C18H15O1P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311+G(d,p)	319.7633
B98/6-311+G(d,p)	307.4676
B3LYP/6-311+G(d,p)	292.8302
HF/6-311+G(d,p)	351.0237
MP2(FC)/6-311+G(d,p)	336.2062
MPW1K/6-311+G(2d,p)	308.0225
MPW1K/6-311+G(2df,2pd)	307.1925
MPW1K/3-21G	481.4436
MPW1K/6-31G(d)	371.5699
MPW1K/6-311++G(2d,2p)	308.0144
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	306.4356
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAKS)	306.2551
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAHF)	307.0724
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAKS)	306.9890
MPW1K/IGLOIII	312.4864
MPW1K/IGLOIII + PCM($CHCl_3$,UAHF)	308.9998
MPW1K/IGLOIII + PCM($CHCl_3$,UAKS)	310.7379
MPW1K/IGLOIII + PCM(C_6H_6,UAHF)	311.5517
MPW1K/IGLOIII + PCM(C_6H_6,UAKS)	311.4672

2_2 C_3

1\1\GINC-NODE8\FOpt\RmPWPW91\6-31G(d)\C18H15O1P1\ZIP04\22-May-2009\0\\
#mpwpw91/6-31g(d) opt=(maxcycle=50) scf=tight int=finegrid IOp(3/76=05
72004280)\\molnmr_002\\0,1\P,-0.0000000005,0.0000000008,-1.0561830201\
C,1.6728278569,-0.0369653746,-0.3626184568\C,2.661514111,-0.6147847731
,-1.1536496978\C,2.0054128371,0.4765728702,0.8869141165\C,3.9634978359
,-0.6960707427,-0.6898595354\H,2.4010124946,-0.9797285845,-2.136344623
6\C,3.3085311177,0.3907922372,1.3493446331\H,1.2534930529,0.9626775166
,1.4923252484\C,4.2862098404,-0.1982821947,0.5629822512\H,4.7279043135
,-1.1425425669,-1.3087125787\H,3.562777307,0.7937946808,2.318764897\H,
5.3028080832,-0.2598596911,0.9232944549\C,-0.804400975,1.4671941092,-0
.3626184568\C,-1.415430631,1.4984520286,0.8869141165\C,-0.7983378241,2
.6123312209,-1.1536496978\C,-1.9927015639,2.6698758802,1.3493446331\H,
-1.4604497115,0.6042180706,1.4923252484\C,-1.3789339719,3.7805251867,-
0.6898595354\H,-0.3520364043,2.569202109,-2.1363446236\C,-1.9713875025
,3.8111077068,0.5629822512\H,-2.4688350124,2.6885583171,2.318764897\H,
-1.3744812689,4.6657565273,-1.3087125787\H,-2.4263589477,4.7222963587,
0.9232944549\C,-0.8684268834,-1.4302287321,-0.3626184568\C,-1.86317628
83,-1.9975464453,-1.1536496978\C,-0.5899822076,-1.9750248963,0.8869141
165\C,-2.5845638654,-3.0844544415,-0.6898595354\H,-2.0489760917,-1.589
4735221,-2.1363446236\C,-1.3158295553,-3.0606681149,1.3493446331\H,0.2
069566572,-1.5668955847,1.4923252484\C,-2.3148223394,-3.6128255096,0.5
629822512\H,-3.353423046,-3.5232139579,-1.3087125787\H,-1.093942296,-3
.4823529954,2.318764897\H,-2.876449137,-4.4624366651,0.9232944549\O,-0
.0000000005,0.0000000008,-2.5433745508\\Version=AM64L-G03RevD.01\State
=1-A\HF=-1111.3394967\RMSD=7.081e-09\RMSF=3.363e-06\Thermal=0.\Dipole=
0.,0.,1.640972\PG=C03 [C3(P1O1),X(C18H15)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311+G(d,p)	320.9482
B98/6-311+G(d,p)	308.9801
B3LYP/6-311+G(d,p)	294.3596
HF/6-311+G(d,p)	352.6781
MP2(FC)/6-311+G(d,p)	337.2729
MPW1K/6-311++G(2d,2p)	308.4744
MPW1K/IGLOIII	312.9412
MPW1K/3-21G	484.0238

MPW1K/6-31G(d)	372.7677
MPW1K/6-311++G(2d,2p)	308.4744
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	305.3405
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAKS)	306.9241
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAHF)	307.6548
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAKS)	307.5553
MPW1K/IGLOIII	312.9412
MPW1K/IGLOIII + PCM(CHCl3,UAHF)	311.5801
MPW1K/IGLOIII + PCM(CHCl3,UAKS)	311.4219
MPW1K/IGLOIII + PCM(C_6H_6,UAHF)	312.1449
MPW1K/IGLOIII + PCM(C_6H_6,UAKS)	312.0409

	MPW1K/6-311++G(2d,2p)//MPW1K/6-31G(d)	MP2(FC)/6-31+G(2d,p)/MPW1K/6-31G(d)	
	Chemical shift, ppm (relative to PPh_3)	E_{tot}	„G“$_{298,\ gas}$
2_1	24.3	-1108.914974	-1108.673297
2_2	23.9	-1108.915735	-1108.673065

<δ> = 24.1 ppm

	MPW1K/6-311++G(2d,2p) + PCM/UAHF/MPW1K/6-311++G(2d,2p)	MP2(FC)/6-31+G(2d,p)/MPW1K/6-31G(d) + PCM/UAHF/MPW1K/6-311++G(2d,2p)		
	Chemical shift, ppm (relative to PPh_3)	E_{tot}	„G“$_{298,\ gas}$	„G“$_{298,CHCl3}$
2_1	26.3	-1108.914974	-1108.673297	-1108.672978
2_2	27.4	-1108.915735	-1108.673065	-1108.672204

<δ> = 26.6 ppm

	MPW1K/6-311++G(2d,2p) + PCM/UAHF/MPW1K/6-311++G(2d,2p)	MP2(FC)/6-31+G(2d,p)/MPW1K/6-31G(d) + PCM/UAHF/MPW1K/6-311++G(2d,2p)		
	Chemical shift, ppm (relative to PPh_3)	E_{tot}	„G“$_{298,\ gas}$	„G“$_{298,C6H6}$
2_1	26.2	-1108.914974	-1108.673297	-1108.671161
2_2	27.3	-1108.915735	-1108.673065	-1108.670563

<δ> = 26.6 ppm

2*$CHCl_3$

1\1\GINC-GRETEL\SP\RmPWPW91\6-311++G(2d,2p)\C19H16Cl3O1P1\BORIS\04-Jun
-2008\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/7
6=0572004280) scrf=(PCM,Read,solvent=chloroform)\\bm_mbh_ph3pochcl3_PC
M_UA0_001\\0,1\P\O,1,1.49197838\C,1,1.80804692,2,112.40284548\C,3,1.39
266952,1,116.96935507,2,34.37685889,0\C,3,1.39099589,1,123.35738423,2,
-146.19173296,0\C,4,1.38387471,3,120.08999033,1,178.73509668,0\H,4,1.0
8008991,3,119.51957474,1,-2.36443037,0\C,5,1.38568169,3,120.05322526,1
,-178.46880105,0\H,5,1.08043672,3,120.12832421,1,2.25004421,0\C,8,1.38
562591,5,120.03039338,3,-0.50427747,0\H,6,1.07989812,4,119.82214718,3,
179.72964478,0\H,8,1.08007351,5,119.83717242,3,-179.8721385,0\H,10,1.0
8024682,8,119.91113851,5,-179.6528136,0\C,1,1.80729847,2,111.78898555,
3,-120.31546344,0\C,14,1.39149917,1,123.35148326,2,-153.88191431,0\C,1
4,1.39159674,1,116.92811886,2,25.86239497,0\C,15,1.38504615,14,120.036
016,1,-179.10904943,0\H,15,1.08077097,14,120.22539963,1,2.03503065,0\C
,16,1.38456897,14,120.05741478,1,179.273517,0\H,16,1.08000117,14,119.2
4953491,1,-1.81025254,0\C,19,1.38619809,16,120.02621936,14,0.1660839,0
\H,17,1.08009293,15,119.85306778,14,-179.79505785,0\H,19,1.07993914,16
,119.82986405,14,179.76816273,0\H,21,1.08023327,19,119.98059752,16,179
.84524431,0\C,1,1.80766514,2,112.31272579,14,-119.85462719,0\C,25,1.39
184211,1,117.17172622,2,28.92416542,0\C,25,1.39142709,1,123.12169298,2
,-151.46015232,0\C,26,1.38437667,25,120.05277299,1,178.7949282,0\H,26,
1.0798942,25,119.42395145,1,-2.09743878,0\C,27,1.38534184,25,120.05460

72,1,-178.49796882,0\H,27,1.08084524,25,120.16060122,1,2.53917733,0\C,
30,1.38595273,27,120.00745724,25,-0.57142427,0\H,28,1.07990414,26,119.
81430807,25,179.69009858,0\H,30,1.08008304,27,119.84986606,25,-179.878
89126,0\H,32,1.08023087,30,119.90826218,27,-179.59146913,0\H,2,1.92315
256,1,162.96628282,14,161.61898483,0\C,2,3.00807809,1,162.68566114,14,
160.66127257,0\Cl,37,1.76313696,2,108.33591818,1,79.42857303,0\Cl,37,1
.7607142,2,108.62288389,1,-159.99570684,0\Cl,37,1.7635419,2,107.190583
8,1,-40.13167091,0\\Version=IA32L-G03RevD.01\State=1-A\HF=-2530.996541
2\RMSD=2.040e-09\Thermal=0.\Dipole=-0.0593821,0.2790084,-3.1921681\PG=
C01 [X(C19H16Cl3O1P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	302.9821
MPW1K/IGLOIII	306.9763
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	302.2425
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAKS)	302.2417
MPW1K/IGLOIII + PCM($CHCl_3$,UAHF)	306.2497
MPW1K/IGLOIII + PCM($CHCl_3$,UAKS)	306.2487

2*C_6H_6

1\1\GINC-CIPCLU08\SP\RmPWPW91\6-311++G(2d,2p)\C24H21O1P1\BRYCH\21-Nov-
2009\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76
=0572004280) geom=check guess=read\\nmrfreq_004_2_nmr\\0,1\P,0,-0.7568
638211,0.1050430913,-0.2811151164\O,0,0.4428556317,0.4398679793,-1.099
0833104\C,0,-1.7924268006,-1.2191597428,-0.9539801579\C,0,-1.294561059
3,-2.5215726458,-0.9405221273\C,0,-3.0159389575,-0.9657742051,-1.56431
29445\C,0,-2.0133667452,-3.5512042828,-1.5192602871\H,0,-0.3404298929,
-2.7284580156,-0.4771521347\C,0,-3.7361276822,-1.9996932506,-2.1422680
856\H,0,-3.4086317053,0.0397680584,-1.5907796097\C,0,-3.2368489308,-3.
2907993008,-2.1193718688\H,0,-1.6201398412,-4.5569678069,-1.5045140748
\H,0,-4.6863616844,-1.7936260981,-2.6125304925\H,0,-3.7983528608,-4.09
56315232,-2.5709410838\C,0,-1.8325759658,1.5484721044,-0.0833092615\C,
0,-2.9262398732,1.5862330985,0.7778878878\C,0,-1.5096455009,2.67198421
2,-0.8350951838\C,0,-3.6921575172,2.7338161794,0.8762203944\H,0,-3.177
7029062,0.7241560492,1.3788655579\C,0,-2.278847654,3.8210596756,-0.733
8424049\H,0,-0.6491651047,2.6311668963,-1.4865709557\C,0,-3.3690401367
,3.8513677913,0.1189432939\H,0,-4.5384887157,2.760832196,1.546805344\H
,0,-2.0230371992,4.6920293949,-1.3190929248\H,0,-3.9676522605,4.746977
0973,0.2002943793\C,0,-0.3068012202,-0.4440385689,1.3837921114\C,0,0.9
428593363,-0.0569081099,1.8576721228\C,0,-1.1461674093,-1.2010618705,2
.1965422471\C,0,1.3427361722,-0.4141170845,3.1349043719\H,0,1.59974945
12,0.5098095151,1.2142754125\C,0,-0.7448303945,-1.5532959365,3.4741847
414\H,0,-2.1048796039,-1.5357921872,1.8258323274\C,0,0.4983932246,-1.1
575839097,3.9439647871\H,0,2.3161759766,-0.1152019612,3.494742644\H,0,
-1.3978183777,-2.1440123818,4.0998134146\H,0,0.8115590862,-1.436808645
,4.9394901145\C,0,3.7611079572,0.3053063398,-1.0878623347\C,0,4.610964
3399,1.2686050689,-1.6120556924\C,0,5.9742581523,1.2071152463,-1.36847
40168\C,0,6.4957067426,0.1798410045,-0.596742242\C,0,5.6511503884,-0.7
851876789,-0.0705238548\C,0,4.2880363603,-0.7209281881,-0.3166675534\H
,0,2.6957234466,0.3524217845,-1.2703178961\H,0,4.2060606565,2.06993609
82,-2.2134905009\H,0,6.6321024582,1.9596288523,-1.7797324377\H,0,7.558
- 5463955,0.1314765761,-0.4070110527\H,0,6.0560947699,-1.5875516685,0.52
99518992\H,0,3.6289392176,-1.4735981093,0.0925116461\\Version=AM64L-G0
3RevD.01\State=1-A\HF=-1343.8304369\RMSD=1.216e-09\Thermal=0.\Dipole=-
1.7291503,-0.3570922,0.9376229\PG=C01 [X(C24H21O1P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	305.4242
MPW1K/IGLOIII	309.7354
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAHF)	304.8235
MPW1K/IGLOIII + PCM(C_6H_6,UAHF)	309.1385

3

1\1\GINC-NODE8\SP\RmPWPW91\Gen\H3P1\ZIP04\12-Jun-2010\0\\#p mpwpw91/ge
n nmr scf=tight int=finegrid IOp(3/76=0572004280) geom=check guess=rea
d\\title\\0,1\P,0,0.,-0.0000000556,0.1210924934\H,0,0.,1.1902459939,-0
.6371094978\H,0,-1.0307833156,-0.5951230803,-0.6371094978\H,0,1.030783
3156,-0.5951230803,-0.6371094978\\Version=AM64L-G03RevD.01\State=1-A1\
HF=-343.1686902\RMSD=9.759e-09\Thermal=0.\Dipole=0.,0.,-0.2586942\PG=C
03V [C3(P1),3SGV(H1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311+G(d,p)	588.6318
MPW1K/6-311++G(2d,2p)	586.2645
MPW1K/IGLO-III	592.0708
HF/6-311++G(2d,2p)	595.2526
B98/6-311++G(2d,2p)	577.3875
B3LYP/6-311++G(2d,2p)	568.2426
MP2/6-311++G(2d,2p)	611.7305

4

1\1\GINC-NODE3\SP\RmPWPW91\Gen\F3P1\ZIP04\14-Jun-2010\0\\#p mpwpw91/ge
n nmr scf=tight int=finegrid IOp(3/76=0572004280) geom=check guess=rea
d\\title\\0,1\P,0,0.,-0.0000001886,0.0577911145\F,0,-1.1830837135,-0.6
830538738,-0.7266667595\F,0,0.0000000132,1.3661072048,-0.7266667595\F,
0,1.1830837003,-0.6830538967,-0.7266667595\\Version=AM64L-G03RevD.01\S
tate=1-A1\HF=-641.0412291\RMSD=2.913e-09\Thermal=0.\Dipole=0.,0.,0.447
9424\PG=C03V [C3(P1),3SGV(F1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	194.0557
MPW1K/IGLO-III	207.9761

5

1\1\GINC-NODE8\SP\RmPWPW91\Gen\Cl3P1\ZIP04\12-Jun-2010\0\\#p mpwpw91/g
en nmr scf=tight int=finegrid IOp(3/76=0572004280) geom=check guess=re
ad\\title\\0,1\P,0,0.,-0.0000002833,0.0034634307\Cl,0,-1.5790774493,-0
.9116809577,-0.9293794308\Cl,0,0.0000001005,1.8233612395,-0.9293794308
\Cl,0,1.5790773488,-0.9116811318,-0.9293794308\\Version=AM64L-G03RevD.
01\State=1-A1\HF=-1722.1249811\RMSD=4.923e-09\Thermal=0.\Dipole=0.,0.,
0.1748308\PG=C03V [C3(P1),3SGV(Cl1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	73.7237
MPW1K/IGLO-III	80.7244

6

1\1\GINC-NODE8\SP\RmPWPW91\Gen\C3H9P1\ZIP04\11-Jun-2010\0\\#p mpwpw91/
gen nmr scf=tight int=finegrid IOp(3/76=0572004280) geom=check guess=r
ead\\title\\0,1\P,0,0.,-0.0000001667,0.59705\C,0,0.,1.624301,-0.276069
\H,0,-0.877929,2.198107,0.016281\H,0,0.877929,2.198107,0.016281\H,0,0.
,1.516673,-1.361399\C,0,-1.4066860737,-0.81215075,-0.276069\H,0,-1.464
6521466,-1.8593625667,0.016281\H,0,-2.3425811466,-0.3387449333,0.01628
1\H,0,-1.3134774916,-0.75833675,-1.361399\C,0,1.4066860737,-0.81215075
,-0.276069\H,0,2.3425811466,-0.3387449333,0.016281\H,0,1.4646521466,-1
.8593625667,0.016281\H,0,1.3134774916,-0.75833675,-1.361399\\Version=A
M64L-G03RevD.01\State=1-A1\HF=-461.1516115\RMSD=4.076e-09\Thermal=0.\D
ipole=0.,0.,-0.4733679\PG=C03V [C3(P1),3SGV(C1H1),X(H6)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	397.9419
MPW1K/6-311+G(d,p)	409.5647
MPW1K/IGLO-III	401.9422
HF/6-311++G(2d,2p)	435.2273
B98/6-311++G(2d,2p)	384.0079
B3LYP/6-311++G(2d,2p)	366.9421

MP2/6-311++G(2d,2p)	427.8159

7_1

1\1\GINC-NODE23\SP\RmPWPW91\6-311++G(2d,2p)\C9H21P1\ZIP04\07-Aug-2010\
0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0572
004280) geom=check guess=read\\vw_005_0810_1\\0,1\P,0,0.2169073574,1.0
963470206,0.0467654619\C,0,1.3536120378,-0.1696579976,0.8108029886\H,0
,0.7733007031,-0.962111228,1.2867461814\C,0,-1.1187326663,1.3612529495
,1.3429959633\H,0,-2.0381407112,1.431628894,0.7559112407\C,0,-0.677789
4052,0.1159725529,-1.2692748105\H,0,0.1254635397,-0.1844616016,-1.9459
481498\C,0,2.2152970043,0.5089705783,1.8697853326\H,0,1.6236631617,0.9
621303162,2.6633309846\H,0,2.8883208724,-0.213431462,2.3340066773\H,0,
2.8239916515,1.2958428232,1.4246341088\C,0,2.2457381349,-0.7968117263,
-0.2527786388\H,0,2.7705731825,-0.0327185241,-0.8275629308\H,0,2.99936
21615,-1.4313408592,0.215505492\H,0,1.686678596,-1.4174282744,-0.95051
27963\C,0,-0.9138901271,2.7119078289,2.0218320761\H,0,-1.7367975065,2.
9288004292,2.7049781313\H,0,0.0078933614,2.7293346108,2.6033068216\H,0
,-0.8537273774,3.5184723674,1.2938534964\C,0,-1.3161248261,0.265289367
2,2.3816779371\H,0,-0.4511120913,0.1722537788,3.0369273453\H,0,-2.1723
523332,0.5031613326,3.0152121803\H,0,-1.4983818099,-0.7085803612,1.934
0734347\C,0,-1.5936829194,1.0453888581,-2.0575456981\H,0,-1.0559043479
,1.9165172272,-2.427726833\H,0,-2.4260362363,1.4018132886,-1.449637760
3\H,0,-2.0231616031,0.5224689286,-2.9130469454\C,0,-1.4235009635,-1.13
46556256,-0.8301696912\H,0,-1.8013228455,-1.6764189943,-1.6992335349\H
,0,-0.7910373546,-1.8196052024,-0.267122817\H,0,-2.2841066394,-0.88473
12957,-0.2103852479\\Version=AM64L-G03RevD.01\State=1-A\HF=-697.027359
6\RMSD=2.119e-09\Thermal=0.\Dipole=-0.2458879,-0.4772464,0.1238028\PG=
C01 [X(C9H21P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	317.6473

7_2

1\1\GINC-NODE23\SP\RmPWPW91\6-311++G(2d,2p)\C9H21P1\ZIP04\07-Aug-2010\
0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0572
004280) geom=check guess=read\\vw_005_0810_5\\0,1\P,0,-0.5412643301,-0
.0528705959,0.509269838\C,0,1.2739737325,-0.5154410439,0.5019975134\H,
0,1.3801045152,-1.0497095191,-0.4434285976\C,0,-0.7792819759,0.7187808
443,-1.1901924087\H,0,-0.5008377686,1.7746173148,-1.1333865855\C,0,-0.
5906658957,1.4777109773,1.5851563364\H,0,0.1827267437,2.1705048845,1.2
447410237\C,0,1.5895904224,-1.5318927643,1.5950725182\H,0,0.9057620394
,-2.3778311268,1.5562370566\H,0,2.6051977009,-1.9118384819,1.473525641
6\H,0,1.5231361846,-1.1017631182,2.5925724836\C,0,2.2697605482,0.63446
53198,0.5045832902\H,0,2.2665951792,1.1649227011,1.4561547834\H,0,3.28
35019271,0.2615321735,0.3487480314\H,0,2.0615093138,1.3615654278,-0.27
96474951\C,0,-2.2540411028,0.6141995348,-1.5712616263\H,0,-2.445270398
6,1.1389958788,-2.5087420666\H,0,-2.53452955,-0.4299640252,-1.70778975
47\H,0,-2.9174516853,1.0280652214,-0.8159250794\C,0,0.0547364778,0.067
4718267,-2.2852429901\H,0,-0.1090777211,-1.0105528499,-2.3230510591\H,
0,-0.2344075814,0.4703834066,-3.2568308662\H,0,1.1214798234,0.24337737
28,-2.1656539883\C,0,-0.3227812185,1.1215210832,3.0415422776\H,0,0.679
7639481,0.7301640054,3.1962605742\H,0,-1.0314598866,0.3739504048,3.398
2302846\H,0,-0.4275543579,2.0059196759,3.6717578909\C,0,-1.9356617934,
2.184724242,1.4742847212\H,0,-1.9751118112,3.0188244053,2.176339495\H,
0,-2.1108733591,2.5913641942,0.4806529667\H,0,-2.7587681202,1.51160263
03,1.716325791\\Version=AM64L-G03RevD.01\State=1-A\HF=-697.0262134\RMS
D=4.501e-09\Thermal=0.\Dipole=0.3683908,0.4079788,-0.1641438\PG=C01 [X
(C9H21P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	316.7730

7_3

1\1\GINC-NODE19\SP\RmPWPW91\6-311++G(2d,2p)\C9H21P1\ZIP04\07-Aug-2010\
0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0572
004280) geom=check guess=read\\vw_005_0810_12\\0,1\P,0,-0.2815549551,-
0.2579987135,0.5217203811\C,0,-0.8464840014,0.1141125961,-1.2274344003
\H,0,-0.1956579907,-0.5376084296,-1.8177571407\C,0,1.5867454601,-0.128
8227067,0.3315094292\H,0,1.7572781068,-0.4821024418,-0.689098556\C,0,-
0.7345706399,1.2463770027,1.5290405056\H,0,-0.248648049,2.1338378857,1
.1189461558\C,0,-0.670347849,1.5341585806,-1.7453647265\H,0,-1.0211415
871,1.6064942196,-2.7764704975\H,0,-1.240267087,2.2545809299,-1.159862
4759\H,0,0.3709539829,1.847039576,-1.7356539511\C,0,-2.27117741,-0.384
0036091,-1.4506787595\H,0,-2.526072173,-0.3356899116,-2.51045864\H,0,-
2.3857655274,-1.4148948366,-1.1210723962\H,0,-3.0036468233,0.216258402
1,-0.914274226\C,0,2.2692646654,-1.1219996372,1.2676543869\H,0,2.12531
33456,-0.8508946263,2.3133050496\H,0,1.875792554,-2.1278794624,1.13560
70673\H,0,3.3442775963,-1.1483261126,1.0817801926\C,0,2.2287830636,1.2
466282699,0.4570956559\H,0,1.803157198,1.9756988935,-0.2278532117\H,0,
2.1324316639,1.6471261259,1.4650774337\H,0,3.2964444503,1.1784019045,0
.2416876781\C,0,-0.2585163767,1.0407438149,2.9632265607\H,0,-0.5172253
544,1.9060920457,3.5753395992\H,0,-0.735283613,0.1655071187,3.40446051
53\H,0,0.8176973534,0.8993841838,3.0352793011\C,0,-2.2408324581,1.4739
229789,1.5319844683\H,0,-2.49716714,2.2693561504,2.2334855685\H,0,-2.6
209832425,1.7674646432,0.5566568598\H,0,-2.7739971627,0.575335165,1.84
35221724\\Version=AM64L-G03RevD.01\State=1-A\HF=-697.0245237\RMSD=2.43
5e-09\Thermal=0.\Dipole=0.1954779,0.4582776,-0.2372366\PG=C01 [X(C9H21
P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	315.6641

7_4

1\1\GINC-NODE23\SP\RmPWPW91\6-311++G(2d,2p)\C9H21P1\ZIP04\07-Aug-2010\
0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0572
004280) geom=check guess=read\\vw_005_0810_3\\0,1\P,0,-0.0183324957,-0
.2633970682,0.7285881746\C,0,-0.8368723858,1.0212005249,1.8150707372\H
,0,-0.0979132144,1.1284892995,2.6130289653\C,0,1.6569686682,0.49650088
7,0.4108668661\H,0,1.5434180638,1.4915699136,-0.0250160492\C,0,-0.8025
801594,-0.186695439,-0.9721347098\H,0,-0.3097425398,-1.0247738467,-1.4
727001911\C,0,-2.0915094266,0.4549482369,2.4732907529\H,0,-2.448303513
2,1.1324830086,3.2504690172\H,0,-2.9025146005,0.3267080604,1.758532506
\H,0,-1.8973024443,-0.5129213316,2.9318198943\C,0,-1.1004386172,2.4061
59758,1.2433368446\H,0,-1.3924722061,3.092730829,2.0401777879\H,0,-0.2
258088235,2.8274139232,0.750818764\H,0,-1.9166081941,2.3878253713,0.52
27410059\C,0,2.4287134697,-0.380470745,-0.5685817301\H,0,3.4283677352,
0.0236361501,-0.7333508478\H,0,2.5400966259,-1.3916855241,-0.176424804
2\H,0,1.9420492635,-0.4530819539,-1.5395403399\C,0,2.4456553636,0.6290
582119,1.7078783984\H,0,2.5240254094,-0.3308219024,2.2189564001\H,0,3.
4580194764,0.9763073117,1.4972805818\H,0,1.9985800105,1.3415144156,2.3
984195659\C,0,-0.5818138588,1.0483125428,-1.835729762\H,0,-0.971745336
7,0.8697874852,-2.8397048056\H,0,0.4714062924,1.301821976,-1.938817264
7\H,0,-1.0954884773,1.9204743658,-1.4396497663\C,0,-2.2840706285,-0.53
72722562,-0.9000819958\H,0,-2.4631186917,-1.419661268,-0.2869941784\H,
0,-2.8670826268,0.2844843977,-0.4861999257\H,0,-2.6744821385,-0.738145
3343,-1.8984498918\\Version=AM64L-G03RevD.01\State=1-A\HF=-697.0254699
\RMSD=2.401e-09\Thermal=0.\Dipole=0.020315,0.4804936,-0.2164483\PG=C01
 [X(C9H21P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	318.1632

7_5

1\1\GINC-NODE23\SP\RmPWPW91\6-311++G(2d,2p)\C9H21P1\ZIP04\07-Aug-2010\
0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0572
004280) geom=check guess=read\\vw_005_0810_11\\0,1\P,0,0.1732950004,1.

0445876147,0.1415878509\C,0,-0.7565583105,0.1030015716,-1.1898669013\H
,0,-0.7989645015,-0.9493737278,-0.9008185478\C,0,1.4282258523,-0.28912
08378,0.5557800717\H,0,1.7807767626,-0.575480183,-0.4384260997\C,0,-1.
0033757285,1.0844107879,1.5976863721\H,0,-1.5689229252,0.150422899,1.6
494982391\C,0,0.0315074361,0.2152684586,-2.4914224894\H,0,0.0572808194
,1.2485476234,-2.8363621416\H,0,1.0621763445,-0.1219419934,-2.39208367
11\H,0,-0.4348159654,-0.3883592915,-3.2713991979\C,0,-2.1841559771,0.5
7199596,-1.4238652\H,0,-2.6126104075,0.0358498415,-2.2719491298\H,0,-2
.8264942555,0.3866423262,-0.5657996852\H,0,-2.2228755761,1.6357282956,
-1.6596866024\C,0,0.9069365801,-1.5540825575,1.2251724058\H,0,0.579208
6386,-1.3723315239,2.2465421783\H,0,0.0706114532,-1.9953708786,0.68590
64135\H,0,1.6958688524,-2.3067522359,1.2701616604\C,0,2.6376325693,0.2
784157269,1.2904335515\H,0,3.4262742223,-0.4725250917,1.3595557046\H,0
,3.0417692571,1.1453345325,0.7708605409\H,0,2.394584009,0.5871164835,2
.3052084294\C,0,-1.9694247798,2.2569351141,1.442223359\H,0,-2.66256337
89,2.283883275,2.2845848077\H,0,-2.5590531129,2.2161956706,0.532046999
9\H,0,-1.4198203012,3.1980905848,1.4341093723\C,0,-0.251163453,1.27972
65548,2.9100608872\H,0,-0.9613965472,1.434896296,3.7234273384\H,0,0.36
98936565,0.4306422097,3.1788557378\H,0,0.3883537664,2.1620464948,2.864
1777457\\Version=AM64L-G03RevD.01\State=1-A\HF=-697.0248252\RMSD=2.259
e-09\Thermal=0.\Dipole=-0.2111284,-0.520464,0.1110261\PG=C01 [X(C9H21P
1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	315.8336

7_6

1\1\GINC-NODE19\SP\RmPWPW91\6-311++G(2d,2p)\C9H21P1\ZIP04\08-Aug-2010\
0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0572
004280) geom=check guess=read\\vw_005_0810_20\\0,1\P,0,0.0463614985,1.
0286588624,0.2527271454\C,0,-1.1218957261,0.8755917519,1.7194204787\H,
0,-1.6593581754,-0.0721358948,1.6287089849\C,0,-0.8525213461,0.0176979
339,-1.0541461633\H,0,-0.7061649746,-1.0412968538,-0.8250092855\C,0,1.
4329615957,-0.141431666,0.7521121777\H,0,1.0091032049,-0.9127391735,1.
4006565776\C,0,-2.1212335117,2.0277072515,1.6868379401\H,0,-2.84960345
68,1.9224440725,2.4926969396\H,0,-1.6034480305,2.9765285316,1.82570203
66\H,0,-2.6693969719,2.0915088904,0.7512458132\C,0,-0.4300596121,0.883
7440253,3.0755331458\H,0,0.2421032833,0.0409103223,3.2169694754\H,0,0.
1356955072,1.8030250101,3.2265009697\H,0,-1.1815706325,0.8353186906,3.
8648188101\C,0,-0.2567082592,0.3263470384,-2.4242394196\H,0,-0.4435244
97,1.3670807643,-2.6879839489\H,0,0.8169344264,0.168302242,-2.46894583
04\H,0,-0.717455731,-0.3008594648,-3.1892279687\C,0,-2.3523477866,0.27
23281222,-1.1195980817\H,0,-2.8704416261,0.0078039625,-0.201012077\H,0
,-2.5672653459,1.3167253279,-1.3455759369\H,0,-2.7861270585,-0.3260813
233,-1.921980325\C,0,2.4939074312,0.6385105124,1.5226072529\H,0,3.2748
085197,-0.0344421576,1.8808499565\H,0,2.0957014505,1.1699590505,2.3823
475971\H,0,2.9617927599,1.3772849115,0.8723838888\C,0,2.1125548515,-0.
8440369822,-0.4154137581\H,0,2.5547992803,-0.126486841,-1.1063629107\H
,0,2.9234495658,-1.4691468551,-0.0387833407\H,0,1.4398493673,-1.488820
062,-0.9760401436\\Version=AM64L-G03RevD.01\State=1-A\HF=-697.0229917\
RMSD=6.458e-09\Thermal=0.\Dipole=-0.1635046,-0.5608965,0.1572924\PG=C0
1 [X(C9H21P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	322.2977

7_7

1\1\GINC-NODE19\SP\RmPWPW91\6-311++G(2d,2p)\C9H21P1\ZIP04\07-Aug-2010\
0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0572
004280) geom=check guess=read\\vw_005_0810_14\\0,1\P,0,-0.2815045079,-
0.2794192867,0.6445098696\C,0,1.5246176101,-0.0196192664,0.2258375998\
H,0,1.6079980971,-0.3946803372,-0.7985863431\C,0,-1.2274155892,0.24789
29822,-0.88291511\H,0,-2.2054186253,0.5437917296,-0.4919970625\C,0,-0.
6840087005,1.0030056219,1.9480630382\H,0,0.1837080381,0.9759792517,2.6

139380779\C,0,2.3505528639,-0.9416506726,1.1190007109\H,0,2.0235432566
,-1.9760485536,1.0393369605\H,0,3.4070920916,-0.8923835116,0.851164129
1\H,0,2.2677117113,-0.6506586689,2.1673346788\C,0,2.1002142235,1.38883
1062,0.2687889339\H,0,2.0540395742,1.8026124142,1.2758768258\H,0,3.152
917732,1.3690006888,-0.0194532936\H,0,1.5905217701,2.0748642502,-0.401
5215382\C,0,-1.4373801283,-0.988374969,-1.7533098653\H,0,-2.0616263797
,-0.751131021,-2.616129953\H,0,-0.4873711036,-1.3665479374,-2.13429379
61\H,0,-1.9111916139,-1.7943330182,-1.1972108556\C,0,-0.6849009695,1.3
895350896,-1.7309746216\H,0,0.2867364949,1.1377828728,-2.1554269203\H,
0,-1.3580993636,1.5833626263,-2.5681201946\H,0,-0.579723897,2.31610995
09,-1.1739999726\C,0,-1.8864328763,0.4998566977,2.7422896529\H,0,-1.71
44680991,-0.4977066582,3.1404944774\H,0,-2.7791279095,0.4543257722,2.1
164620035\H,0,-2.1072632979,1.1701726126,3.5743644641\C,0,-0.915124756
7,2.4448772822,1.5191340868\H,0,-1.1193350532,3.0653861755,2.393738782
6\H,0,-0.0596215786,2.874147003,1.0056104393\H,0,-1.7806390132,2.52661
98177,0.8619947954\\Version=AM64L-G03RevD.01\State=1-A\HF=-697.022092\
RMSD=6.310e-10\Thermal=0.\Dipole=0.1072981,0.4837841,-0.1492082\PG=C01
[X(C9H21P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	311.6041

	MPW1K/6-311++G(2d,2p)//MPW1K/6-31G(d)		MP2(FC)/6-31+G(2d,p)//MPW1K/6-31G(d)	
	Chemical shift, ppm (relative to PH_3)	Chemical shift, ppm (relative to PPh_3)	E_{tot}	„G“$_{298,\ gas}$
7_1	2.5172	14.7	-695.337277	-695.082770
7_3	3.3915	15.6	-695.336113	-695.080627
7_5	4.5004	16.7	-695.334107	-695.080404
7_2	2.0013	14.2	-695.335158	-695.080115
7_4	4.3309	16.5	-695.334409	-695.080070
7_7	-2.1332	10.0	-695.332921	-695.076711
7_6	8.5604	20.7	-695.331065	-695.076146

<δ> = 14.9 ppm (relative to PPh3)
<δ> = 2.8 ppm (relative to PH3)

8_1

1\1\GINC-NODE3\SP\RmPWPW91\Gen\C3H9O3P1\ZIP04\14-Jun-2010\0\\#p mpwpw9
1/gen nmr scf=tight int=finegrid IOp(3/76=0572004280) geom=check guess
=read\\title\\0,1\P,0,0.2379289522,-0.6249421117,0.0098765968\O,0,0.73
42069932,0.3671805957,1.2091190597\O,0,0.761721303,0.3886418256,-1.159
2928459\O,0,-1.3696026002,-0.3696637032,-0.0063493668\C,0,0.7688362267
,-0.1152055566,-2.4749009091\H,0,1.3630958993,0.5660592188,-3.07570263
71\H,0,1.2147869143,-1.1096713038,-2.5228935479\H,0,-0.2394404432,-0.1
63244709,-2.8863076297\C,0,-1.9051764789,0.9410083903,-0.0007398433\H,
0,-2.985882044,0.8420223198,-0.0144326404\H,0,-1.5987096882,1.48077437
71,0.8921967039\H,0,-1.5777658583,1.4968858161,-0.8761824296\C,0,0.708
4796718,-0.159862438,2.5153745819\H,0,1.2873291191,0.5105644375,3.1428
188257\H,0,-0.3097689697,-0.215008867,2.9005004834\H,0,1.1533640028,-1
.1550992917,2.5569155983\\Version=AM64L-G03RevD.01\State=1-A\HF=-686.8
505417\RMSD=4.407e-09\Thermal=0.\Dipole=-0.1531146,0.1080622,-0.000953
2\PG=C01 [X(C3H9O3P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	164.2884

8_2

1\1\GINC-NODE8\SP\RmPWPW91\Gen\C3H9O3P1\ZIP04\11-Jun-2010\0\\#p mpwpw9
1/gen nmr scf=tight int=finegrid IOp(3/76=0572004280) geom=check guess

=read\\title\\0,1\P,0,-0.0754547367,0.0646112531,0.5390006865\O,0,1.00
39637097,-1.128627544,0.6533199902\O,0,-1.246663889,-0.7646833945,-0.2
392254849\O,0,0.4416147615,0.9101832945,-0.7755826978\C,0,1.3077039735
,-1.967621328,-0.4479213951\H,0,1.4709261597,-1.3809883159,-1.34883211
54\H,0,2.2151937368,-2.5052904082,-0.1923159127\H,0,0.4987043081,-2.67
21841546,-0.6184162416\C,0,-2.3989459968,-0.0514622457,-0.6205270755\H
,0,-3.1496104356,-0.7807141233,-0.908672236\H,0,-2.7904366437,0.547599
6479,0.204160415\H,0,-2.1876814795,0.6020988709,-1.4649074428\C,0,1.30
0166705,2.0018914063,-0.5416111903\H,0,1.2377684873,2.6597892449,-1.40
34360182\H,0,1.0095154067,2.5596340522,0.350324719\H,0,2.331175933,1.6
696107445,-0.4245270004\\Version=AM64L-G03RevD.01\State=1-A\HF=-686.85
1786\RMSD=3.633e-09\Thermal=0.\Dipole=-0.0234238,0.3680916,-0.4974643\
PG=C01 [X(C3H9O3P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	167.6754

8_3

1\1\GINC-NODE19\SP\RmPWPW91\6-311++G(2d,2p)\C3H9O3P1\ZIP04\17-Aug-2010
\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=057
2004280) geom=check guess=read\\vw_006_mae_manynmr_1\\0,1\P,-0.127502,
-0.107105,-0.904343\O,-0.895365,-0.755945,0.401529\O,1.35363,-0.661424
,-0.548144\O,-0.083019,1.467625,-0.49247\C,0.422803,1.934624,0.738636\
H,0.106957,2.967815,0.848441\H,0.035084,1.351089,1.572059\H,1.510854,1
.896415,0.740989\C,1.793863,-1.158376,0.698301\H,1.109691,-1.909415,1.
081832\H,2.768184,-1.604932,0.525136\H,1.894686,-0.362905,1.434146\C,-
2.299876,-0.649685,0.422622\H,-2.662982,-1.299337,1.213134\H,-2.738267
,-0.966537,-0.524701\H,-2.614393,0.372953,0.629433\\Version=AM64L-G03R
evD.01\State=1-A\HF=-686.8079354\RMSD=4.091e-09\Thermal=0.\Dipole=-0.2
056353,-0.0261829,1.0672457\PG=C01 [X(C3H9O3P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	191.2445

8_4

1\1\GINC-NODE8\SP\RmPWPW91\Gen\C3H9O3P1\ZIP04\11-Jun-2010\0\\#p mpwpw9
1/gen nmr scf=tight int=finegrid IOp(3/76=0572004280) geom=check guess
=read\\title\\0,1\P,0,0.,-0.0000001061,0.2900962448\O,0,-0.5107803866,
1.3249735993,-0.5062018696\O,0,1.4028510815,-0.2201381682,-0.506201869
6\O,0,-0.8920706949,-1.1048357493,-0.5062018696\C,0,0.0016019852,2.568
8426917,-0.0883734358\H,0,-0.6599310038,3.3389579285,-0.472752265\H,0,
0.0379677943,2.6461920033,1.0001959012\H,0,1.0022572113,2.7252523725,-
0.4875170773\C,0,2.2238821286,-1.2858088649,-0.0883734358\H,0,3.221587
982,-1.0979621093,-0.472752265\H,0,2.2726856928,-1.3559772351,1.000195
9012\H,0,1.8590092725,-2.2306065515,-0.4875170773\C,0,-2.2254841138,-1
.283034145,-0.0883734358\H,0,-2.5616569782,-2.2409961373,-0.472752265\
H,0,-2.3106534871,-1.2902150864,1.0001959012\H,0,-2.8612664839,-0.4946
461392,-0.4875170773\\Version=AM64L-G03RevD.01\State=1-A\HF=-686.84868
38\RMSD=1.533e-09\Thermal=0.\Dipole=0.,0.,0.5107526\PG=C03 [C3(P1),X(C
3H9O3)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	145.5871

8_5

1\1\GINC-NODE24\SP\RmPWPW91\6-311++G(2d,2p)\C3H9O3P1\ZIP04\19-Aug-2010
\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=057
2004280) geom=check guess=read\\vw_006_mae_manynmr_12c3\\0,1\P,0,-0.00
00000009,0.0000000012,-1.0812894249\O,0,0.8741847902,-1.1806678812,-0.
3599223586\O,0,0.5853959831,1.3474001792,-0.3599223586\O,0,-1.45958077
61,-0.1667322943,-0.3599223586\C,0,-1.7111808539,-0.8922125333,0.82004
50228\H,0,-1.1959357621,-1.8500060438,0.8065551563\H,0,-1.407614711,-0
.333125926,1.7059947956\H,0,-2.782382369,-1.0638747077,0.8677005189\C,

0,0.0829117051,1.9280323576,0.8200450228\H,0,0.4153118385,1.3855930625
,1.7059947956\H,0,0.4698486587,2.9415511695,0.8677005189\H,0,-1.004184
3525,1.9607137742,0.8065551563\C,0,1.628269146,-1.0358198207,0.8200450
228\H,0,2.3125337075,-1.8776764581,0.8677005189\H,0,0.9923028698,-1.05
24671329,1.7059947956\H,0,2.2001201118,-0.1107077267,0.8065551563\\Ver
sion=AM64L-G03RevD.01\State=1-A\HF=-686.8012421\RMSD=6.675e-09\Thermal
=0.\Dipole=0.,0.,1.4269379\PG=C03 [C3(P1),X(C3H9O3)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	199.1895

	MPW1K/6-311++G(2d,2p)//MPW1K/6-31G(d)	MP2(FC)/6-31+G(2d,p)/MPW1K/6-31G(d)	
	Chemical shift, ppm (relative to PPh_3)	E_{tot}	„G“$_{298,\ gas}$
8_1	168.1	-685.411875	-685.316081
8_2	164.7	-685.413133	-685.315107
8_3	141.1	-685.410670	-685.312847
8_4	186.8	-685.408176	-685.310219
8_5	133.2	-685.404419	-685.303744

<δ> = 166.6 ppm (relative to PPh_3)

8_1*$CHCl_3$_1

1\1\GINC-PHOENIX\SP\RmPWPW91\6-311++G(2d,2p)\C4H10Cl3O3P1\BORIS\27-Oct
-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/7
6=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read
\\vw_8_solmod2_1_006c_2_2\\0,1\P,0,2.3280984269,-0.022129925,-0.685715
8622\O,0,1.2032820993,1.1643029724,-0.5812675793\O,0,1.1937851652,-1.1
729642253,-0.4161583196\O,0,3.0755939979,0.0763177378,0.7500287677\C,0
,1.569461519,-2.5196979112,-0.6141464214\H,0,0.6559071012,-3.104170446
8,-0.6339542888\H,0,2.0969526481,-2.6500584587,-1.5591914021\H,0,2.203
5228392,-2.8728627629,0.1980624435\C,0,2.3527911592,0.1647729845,1.966
3313871\H,0,3.085448272,0.2208120342,2.7644169529\H,0,1.727253415,1.05
38068279,1.981351442\H,0,1.7244758821,-0.7110647075,2.1079158319\C,0,1
.5895334264,2.4667853021,-0.9664165634\H,0,0.6806800409,3.0500614126,-
1.0682070977\H,0,2.2273481019,2.9253819701,-0.2118871581\H,0,2.1169821
365,2.4587897277,-1.9203976238\H,0,-0.7077408671,0.0270019748,-0.17399
5449\C,0,-1.7634635501,0.0475903573,0.0569970716\Cl,0,-2.4675321219,1.
4489761775,-0.7427173495\Cl,0,-1.9290047958,0.1713880425,1.8068823949\
Cl,0,-2.4794008958,-1.4461930841,-0.5389851767\\Version=AM64L-G03RevD.
01\State=1-A\HF=-2106.2129614\RMSD=1.917e-09\Thermal=0.\Dipole=0.83727
75,0.0033481,0.0965061\PG=C01 [X(C4H10Cl3O3P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	165.5506

8_2*$CHCl_3$_1

1\1\GINC-PHOENIX\SP\RmPWPW91\6-311++G(2d,2p)\C4H10Cl3O3P1\BORIS\26-Oct
-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/7
6=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read
\\vw_8_solmod2_1_006b\\0,1\P,0,-0.0678940367,-0.1270485805,-0.68737264
\O,0,0.7962581859,1.2254697376,-0.5615945403\O,0,-1.3887071884,0.34441
89801,0.1462655465\O,0,0.5458053594,-1.0650475757,0.5290402442\C,0,0.9
285432101,1.9399320881,0.6559411454\H,0,1.3415772379,1.3031300712,1.43
50786399\H,0,1.610701002,2.7609345967,0.4628466588\H,0,-0.0337298547,2
.3291212056,0.9755635132\C,0,-2.525678459,-0.4909943713,0.0950511463\H
,0,-3.3568209204,0.0748704782,0.5019591624\H,0,-2.7591578809,-0.780618
9837,-0.9300748112\H,0,-2.3790451189,-1.3884279436,0.6943981557\C,0,1.
6402097218,-1.9025983252,0.2188619092\H,0,1.6964728022,-2.6642621513,0
.9899610101\H,0,1.5058611644,-2.3859402074,-0.7492761524\H,0,2.5709261
324,-1.3376727038,0.206619528\H,0,-0.3078818931,-0.6881949516,2.427968

2616\C,0,-0.5318064622,-0.7741628636,3.4835435841\Cl,0,-1.2483594852,-2.3622009963,3.7467328241\Cl,0,0.987448792,-0.6149373188,4.3609901624\Cl,0,-1.6536195088,0.5069927955,3.9219052918\\Version=AM64L-G03RevD.01\State=1-A\HF=-2106.2124829\RMSD=2.885e-09\Thermal=0.\Dipole=0.1365864,-0.3145265,-0.3984648\PG=C01 [X(C4H10Cl3O3P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	166.3742

8_4*$CHCl_3$_1

1\1\GINC-PHOBOS\SP\RmPWPW91\6-311++G(2d,2p)\C4H10Cl3O3P1\BORIS\26-Oct-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read\\vw_8_solmod2_1_006a\\0,1\P,0,-0.1417244509,0.0770655172,0.5513602053\O,0,-0.8923755773,1.4705457808,0.1568706536\O,0,0.8389726038,0.0146129622,-0.7477773147\O,0,-1.2856650073,-0.9353094941,-0.0108208502\C,0,-0.2758821844,2.6862627523,0.5282055796\H,0,-1.0368032336,3.4585649492,0.4878188582\H,0,0.1270797146,2.6359646858,1.5407097174\H,0,0.5253170882,2.9348423366,-0.1645073358\C,0,1.7385256329,-1.0690828084,-0.8532377504\H,0,2.4755430607,-0.8020289622,-1.6031171183\H,0,2.24634632,-1.2590555555,0.0934441708\H,0,1.2164675705,-1.9699492744,-1.1683561535\C,0,-2.3818478585,-1.2277886064,0.8297418244\H,0,-2.8805964575,-2.0974630011,0.4153372903\H,0,-2.0564490011,-1.4546271379,1.8461039663\H,0,-3.0790246461,-0.3928901248,0.8537725088\H,0,-1.175410668,0.6167439323,-2.071344756\C,0,-1.5879110865,0.6867119799,-3.0664471951\Cl,0,-0.7913594326,-0.5163818737,-4.0729399315\Cl,0,-1.2744690168,2.3152379834,-3.6616251646\Cl,0,-3.3171643,0.3776771288,-2.9600106146\\Version=AM64L-G03RevD.01\State=1-A\HF=-2106.2102372\RMSD=1.910e-09\Thermal=0.\Dipole=0.5228216,-0.1838685,1.326293\PG=C01 [X(C4H10Cl3O3P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	146.8236

8_1*$CHCl_3$_2

1\1\GINC-PHOENIX\SP\RmPWPW91\6-311++G(2d,2p)\C4H10Cl3O3P1\BORIS\25-Oct-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read\\vw_8_solmod2_2_006c_2\\0,1\P,0,0.0002906863,-0.3171463521,-0.3879508108\O,0,-1.1853941672,-0.5668267137,0.6977148697\O,0,1.1857423953,-0.565619745,0.6982396244\O,0,-0.0005014949,1.2947758637,-0.5656543512\C,0,2.5030481978,-0.6613286299,0.2010373224\H,0,3.1188709716,-1.0471006303,1.0066365259\H,0,2.5636178324,-1.3429940083,-0.6480855969\H,0,2.8821549394,0.3140337391,-0.1022093665\C,0,-0.0011255429,2.1638450307,0.5544914614\H,0,-0.0015850769,3.1769491893,0.166436799\H,0,-0.8859200754,2.0045774173,1.1659228303\H,0,0.8836390896,2.0054837031,1.1661999415\C,0,-2.5024262588,-0.6633618799,0.1999507305\H,0,-3.1182496352,-1.0500740986,1.005099722\H,0,-2.8822112094,0.3118500061,-0.1029272856\H,0,-2.5621100507,-1.3446247179,-0.6495605621\H,0,0.0014339358,-1.6300743577,-2.758424964\C,0,0.0018152674,-2.2095907879,-3.6738873032\Cl,0,-1.4521116292,-1.7923128338,-4.5722967892\Cl,0,0.0055365463,-3.9113167685,-3.2245748426\Cl,0,1.4526365988,-1.7865986457,-4.574681615\\Version=AM64L-G03RevD.01\State=1-A\HF=-2106.2105854\RMSD=2.175e-09\Thermal=0.\Dipole=-0.0005028,0.7130473,0.7767277\PG=C01 [X(C4H10Cl3O3P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	169.6337

8_3*$CHCl_3$_1

1\1\GINC-PHOENIX\SP\RmPWPW91\6-311++G(2d,2p)\C4H10Cl3O3P1\BORIS\26-Oct-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read\\vw_8_solmod2_1_006_mae_manynmr_1\\0,1\P,0,-0.3255797029,-0.1251950627,-0.9092285184\O,0,-0.9638547773,-0.7409999687,0.4737176933\O,0,1.177

5261242,-0.7307881339,-0.7013846657\O,0,-0.1760270467,1.4457460442,-0.
529224695\C,0,0.4636852974,1.9155433388,0.6389501594\H,0,0.1835750574,
2.9568719335,0.7636740296\H,0,0.1488879848,1.3514370259,1.5150137316\H
,0,1.5446607959,1.8512567676,0.5290135787\C,0,1.7293081492,-1.22736212
,0.5064153729\H,0,1.0300366814,-1.8909700503,1.0039761394\H,0,2.625995
7815,-1.7756315074,0.2348967911\H,0,1.9982296747,-0.4158476638,1.17852
68814\C,0,-2.3607772097,-0.6272955884,0.6340728071\H,0,-2.6417401187,-
1.2580142884,1.4714943178\H,0,-2.8921786014,-0.9632095434,-0.256907673
3\H,0,-2.6483748301,0.4010486162,0.8496201037\H,0,2.6240320701,-0.5995
872484,-2.2302881223\C,0,3.5523978887,-0.5594515977,-2.7860576585\Cl,0
,3.1952868324,-0.032016239,-4.4236246088\Cl,0,4.2507865187,-2.17702788
96,-2.7762544038\Cl,0,4.6089939404,0.5874081356,-1.9644546601\\Version
=AM64L-G03RevD.01\State=1-A\HF=-2106.2086533\RMSD=2.191e-09\Thermal=0.
\Dipole=-0.8421016,0.0059563,1.6639601\PG=C01 [X(C4H10Cl3O3P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	190.3348

8_3*CHCl$_3$_2

1\1\GINC-PHOENIX\SP\RmPWPW91\6-311++G(2d,2p)\C4H10Cl3O3P1\BORIS\26-Oct
-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/7
6=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read
\\vw_8_solmod2_2_006_mae_manynmr_1\\0,1\P,0,-0.0376314621,-0.061557810
3,-0.7427287987\O,0,-0.8975426804,-0.6640456498,0.5172581524\O,0,1.393
5147622,-0.690249122,-0.3345001511\O,0,0.0713100158,1.5098950585,-0.35
53283188\C,0,0.566240412,1.9723745459,0.8842861259\H,0,0.3130641808,3.
0252201596,0.9591714473\H,0,0.1133388703,1.433655971,1.7147421371\H,0,
1.6484513114,1.8638173134,0.9231068212\C,0,1.7543562086,-1.2222701481,
0.9250469346\H,0,1.0236175381,-1.9511340966,1.2619142926\H,0,2.7176822
24,-1.7032190109,0.7894462007\H,0,1.8489686843,-0.440337514,1.67559541
33\C,0,-2.2971110977,-0.4821611893,0.4853617933\H,0,-2.7217789279,-1.1
18487931,1.2550865508\H,0,-2.713718006,-0.7677279385,-0.4810357718\H,0
,-2.5615304439,0.5541842141,0.6912242116\H,0,-0.8359829483,-0.54873048
62,-3.305143623\C,0,-1.3319949782,-0.8223447775,-4.2283517536\Cl,0,-0.
903376813,-2.4882960173,-4.5958393778\Cl,0,-0.7835092532,0.2714201848,
-5.4896298946\Cl,0,-3.0658627168,-0.6602158861,-3.9553653714\\Version=
AM64L-G03RevD.01\State=1-A\HF=-2106.2086654\RMSD=3.806e-09\Thermal=0.\
Dipole=0.0757744,0.1878844,1.9168565\PG=C01 [X(C4H10Cl3O3P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	193.5683

8_4*CHCl$_3$_2

1\1\GINC-PHOENIX\SP\RmPWPW91\6-311++G(2d,2p)\C4H10Cl3O3P1\BORIS\26-Oct
-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/7
6=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read
\\vw_8_solmod2_2_006a\\0,1\P,0,-0.005706533,0.0004353782,0.2723094518\
O,0,-0.4279810025,1.3601878683,-0.5037119709\O,0,1.3843196243,-0.30822
64681,-0.5037801006\O,0,-0.9657039685,-1.0447705778,-0.5103840104\C,0,
0.1811519746,2.5662070046,-0.0941310726\H,0,-0.4200410944,3.3796420467
,-0.4865437482\H,0,0.2205181697,2.6474302297,0.993586249\H,0,1.1902280
511,2.6376505215,-0.4945015\C,0,2.1303885873,-1.4354066347,-0.09597777
94\H,0,3.1339552544,-1.3164403785,-0.4908004445\H,0,2.1848398624,-1.51
04799617,0.9915559642\H,0,1.6916307297,-2.3473272365,-0.4954679968\C,0
,-2.3147029186,-1.1384362686,-0.1065084651\H,0,-2.7079667868,-2.064282
2298,-0.513020133\H,0,-2.4086344992,-1.1609632391,0.980614449\H,0,-2.8
889773793,-0.3011044319,-0.4974746007\H,0,-0.0011253769,0.0031066934,2
.9363008855\C,0,0.0034927203,0.0067181303,4.0207297992\Cl,0,-1.5684749
645,-0.5658597013,4.5643114881\Cl,0,1.2918461475,-1.0684263482,4.55151
74479\Cl,0,0.2969465267,1.6603429404,4.5470253475\\Version=AM64L-G03Re
vD.01\State=1-A\HF=-2106.2086136\RMSD=6.244e-09\Thermal=0.\Dipole=-0.0
050013,-0.0116709,-0.2345563\PG=C01 [X(C4H10Cl3O3P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	152.2356

8_5*CHCl$_3$_2

1\1\GINC-PHOENIX\SP\RmPWPW91\6-311++G(2d,2p)\C4H10Cl3O3P1\BORIS\26-Oct
-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/7
6=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read
\\vw_8_solmod2_2_006_mae_manynmr_12c3\\0,1\P,0,0.001691966,0.002918861
3,0.9023345248\O,0,0.0062948234,1.4708900537,0.1947406298\O,0,1.270975
1818,-0.7361490231,0.196425271\O,0,-1.2725210594,-0.7285669372,0.19741
45071\C,0,-1.9218633608,-0.2930584687,-0.9760463479\H,0,-2.0813519385,
0.7822982148,-0.9557824514\H,0,-1.3510378751,-0.5574659416,-1.86646527
98\H,0,-2.8819452183,-0.7979331405,-1.0131747957\C,0,1.215629518,-1.51
77145462,-0.9760415604\H,0,1.1576295518,-0.8924258161,-1.8672259017\H,
0,2.1325809965,-2.0971690088,-1.0143029323\H,0,0.3638223058,-2.1930478
931,-0.9530576053\C,0,0.7065357817,1.812193835,-0.9808123835\H,0,0.747
9639122,2.8960115712,-1.0216073974\H,0,0.1919592546,1.4464407066,-1.86
96440657\H,0,1.7181400983,1.4141546259,-0.9599449754\H,0,0.0006043561,
-0.0005118709,3.6081388949\C,0,-0.0006678393,-0.0021118156,4.691292086
4\Cl,0,-0.138565179,-1.6731235971,5.2254724803\Cl,0,-1.3793709369,0.95
08795634,5.2276492031\Cl,0,1.513495636,0.7134935877,5.2312773691\\Vers
ion=AM64L-G03RevD.01\State=1-A\HF=-2106.2025789\RMSD=2.507e-09\Thermal
=0.\Dipole=-0.0012087,-0.0009413,-2.4913331\PG=C01 [X(C4H10Cl3O3P1)]\\
@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	201.0740

	MPW1K/6-311++G(2d,2p) + PCM/UAHF/MPW1K/6-311++G(2d,2p)	MP2(FC)/6-31+G(2d,p)//MPW1K/6-31G(d) + PCM/UAHF/MPW1K/6-311++G(2d,2p)		
	Chemical shift, ppm (relative to PPh_3)	E_{tot}	„G“$_{298,\ gas}$	„G“$_{298,CHCl3}$
8_1*CHCl$_3$_1	166.3391	-2102.905420	-2102.802752	-2102.795629
8_2*CHCl$_3$_1	165.5155	-2102.905303	-2102.800769	-2102.793199
8_4*CHCl$_3$_1	185.0661	-2102.902432	-2102.800623	-2102.793149
8_1*CHCl$_3$_2	162.256	-2102.898157	-2102.797380	-2102.791404
8_3*CHCl$_3$_1	141.5549	-2102.899183	-2102.796847	-2102.790839
8_3*CHCl$_3$_2	138.3214	-2102.896857	-2102.793321	-2102.787855
8_4*CHCl$_3$_2	179.6541	-2102.894943	-2102.791641	-2102.785203
8_5*CHCl$_3$_2	130.8157	-2102.890032	-2102.785269	-2102.781364

<δ> = 167.3 ppm

9

1\1\GINC-NODE14\FOpt\RmPWPW91\6-31G(d)\C3H9O1P1\ZIP04\25-Jun-2009\0\\#
mpwpw91/6-31g(d) scf=tight int=finegrid IOp(3/76=0572004280) opt=(maxc
ycle=50)\\gas_001\\0,1\P,0.,0.,-0.1934828527\C,-1.4325334132,-0.827073
551,0.5476994774\H,-2.3434505963,-0.3366854614,0.2109940158\H,-1.46330
34622,-1.8611450171,0.2109940158\H,-1.3999862499,-0.8082824376,1.63563
43667\C,1.4325334126,-0.8270735521,0.5476994774\H,1.4633034608,-1.8611
450182,0.2109940158\H,2.343450596,-0.3366854631,0.2109940158\H,1.39998
62493,-0.8082824386,1.6356343667\C,0.0000000006,1.6541471031,0.5476994
774\H,0.8801471355,2.1978304796,0.2109940158\H,-0.8801471338,2.1978304
802,0.2109940158\H,0.0000000006,1.6165648762,1.6356343667\O,0.,0.,-1.6
790775924\\Version=AM64L-G03RevD.01\State=1-A1\HF=-536.3011092\RMSD=3.
474e-09\RMSF=9.705e-06\Thermal=0.\Dipole=0.,0.,1.7496116\PG=C03V [C3(P
1O1),3SGV(C1H1),X(H6)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	307.0808
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	302.8686
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAKS)	302.4897

MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAHF)	304.5230
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAKS)	304.3111
MPW1K/IGLOIII	309.7277
MPW1K/IGLOIII + PCM($CHCl_3$,UAHF)	305.6400
MPW1K/IGLOIII + PCM($CHCl_3$,UAKS)	305.3037
MPW1K/IGLOIII + PCM(C_6H_6,UAHF)	307.2554
MPW1K/IGLOIII + PCM(C_6H_6,UAKS)	307.0572

9*C_6H_6

1\1\GINC-NODE4\SP\RmPWPW91\6-311++G(2d,2p)\C9H15O1P1\ZIP04\16-Jun-2008
\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=057
2004280) scrf=(PCM,Read,solvent=benzene) geom=check guess=read\\bm_mbh
_pme3o_benz_001_nmr001_pcm_uahf\\0,1\P,0,2.6749045065,0.0116197793,-0.
0311627465\C,0,2.7103649917,-0.1371196498,1.7732748854\H,0,2.229404376
8,0.7331244348,2.2147205059\H,0,2.1478368423,-1.0191209082,2.071999202
7\H,0,3.7256856335,-0.2159640323,2.1576533123\C,0,3.6046727007,-1.4231
466436,-0.629066103\H,0,3.0619955126,-2.3323072539,-0.3791004133\H,0,3
.6911559424,-1.3692503225,-1.7121862262\H,0,4.6014828531,-1.4734933558
,-0.1946780188\C,0,3.736394444,1.4325361192,-0.3979352344\H,0,3.818756
1929,1.5492038146,-1.4764350537\H,0,3.2804939035,2.3344172383,0.004985
7834\H,0,4.7331213044,1.3189295253,0.0244851707\O,0,1.3054263054,0.121
9362197,-0.6016890954\C,0,-2.6122862035,-1.1379736531,-0.1724356181\C,
0,-3.9746008584,-1.2477228275,0.060221081\C,0,-4.7498625886,-0.1054603
016,0.1879092873\C,0,-4.1596503371,1.144415223,0.0818513713\C,0,-2.796
8539916,1.2499560149,-0.1508501168\C,0,-2.0164015432,0.110242971,-0.27
87472589\H,0,-2.0080725575,-2.0282803619,-0.2735351658\H,0,-4.43356326
64,-2.2229761604,0.1414809166\H,0,-5.8120891884,-0.1892480112,0.368703
9318\H,0,-4.762798009,2.0359923352,0.1799325523\H,0,-2.3383239239,2.22
50711487,-0.2345945265\H,0,-0.9527233396,0.1897519482,-0.4578117733\\V
ersion=AM64L-G03RevD.01\State=1-A\HF=-768.6586504\RMSD=4.316e-09\Therm
al=0.\Dipole=2.1772998,-0.1312115,0.7047314\PG=C01 [X(C9H15O1P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	304.6040
MPW1K/IGLOIII	307.3231
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAHF)	302.9428
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAKS)	302.8898
MPW1K/IGLOIII + PCM(C_6H_6,UAHF)	305.7132
MPW1K/IGLOIII + PCM(C_6H_6,UAKS)	305.6632

9*$CHCl_3$

1\1\GINC-CIPCLU08\SP\RmPWPW91\6-311++G(2d,2p)\C4H10Cl3O1P1\BRYCH\20-No
v-2009\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/
76=0572004280) geom=check guess=read\\nmrfreq_006_3_nmr\\0,1\P,0,2.369
4931142,0.0060538742,-0.187813593\C,0,2.3013054352,0.972678659,1.33904
03203\H,0,2.0814006254,2.0107295974,1.0990685274\H,0,1.496951035,0.593
6937715,1.9662227002\H,0,3.2371430443,0.9255772614,1.8927315637\C,0,2.
8480432377,-1.6594019911,0.3304936106\H,0,2.0559558721,-2.0841866915,0
.9436655819\H,0,2.9709497115,-2.2894590205,-0.5477918981\H,0,3.7759183
574,-1.6571436724,0.8994064054\C,0,3.7934077021,0.6498772099,-1.097454
2587\H,0,3.9350669056,0.0651770556,-2.0037672124\H,0,3.5976647499,1.68
00568677,-1.3868751178\H,0,4.7052669585,0.6140548106,-0.5043079079\O,0
,1.1038110944,0.0451235502,-0.9786331025\H,0,-0.7739273294,-0.00718500
39,-0.588193932\C,0,-1.7585021065,-0.0034053605,-0.1273267251\Cl,0,-2.
8922236159,-0.8327588793,-1.1847521736\Cl,0,-1.6078558104,-0.850910650
7,1.418606096\Cl,0,-2.2384090088,1.6712653717,0.1287166473\\Version=AM
64L-G03RevD.01\State=1-A\HF=-1955.8091152\RMSD=6.543e-09\Thermal=0.\Di
pole=2.4557558,-0.0334147,0.6414452\PG=C01 [X(C4H10Cl3O1P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	298.4922
MPW1K/IGLOIII	301.2428
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	295.6368

MPW1K/IGLOIII + PCM($CHCl_3$,UAHF)	298.4888

10_1 C_3

1\1\GINC-NODE15\FOpt\RmPWPW91\6-31G(d)\C3H9O4P1\ZIP04\25-Jun-2009\0\\#
mpwpw91/6-31g(d) scf=tight int=finegrid IOp(3/76=0572004280) opt=(maxc
ycle=50)\\gas_002\\0,1\P,0.0000000001,-0.0000000011,0.114995915\O,1.22
64074677,0.7235841803,-0.5789130635\O,0.0134385492,-1.4238921141,-0.57
89130635\O,-1.2398460165,0.7003079305,-0.5789130635\O,0.0000000001,-0.
0000000011,1.5799617789\C,2.5314831454,0.4846430467,-0.0748674993\H,3.
1836591907,1.2110741709,-0.5462941044\H,2.5527039207,0.6098598236,1.00
43489414\H,2.8557974073,-0.5196113012,-0.3377410255\C,-0.8460283814,-2
.434650238,-0.0748674993\H,-0.5430085964,-3.3626668231,-0.5462941044\H
,-0.7481978592,-2.515636357,1.0043489414\H,-1.8778952894,-2.2133874537
,-0.3377410255\C,-1.6854547637,1.9500071881,-0.0748674993\H,-2.6406505
939,2.151592649,-0.5462941044\H,-1.8045060611,1.9057765301,1.004348941
4\H,-0.9779021175,2.7329987516,-0.3377410255\\Version=AM64L-G03RevD.01
\State=1-A\HF=-761.9104737\RMSD=8.721e-09\RMSF=1.452e-05\Thermal=0.\Di
pole=0.,0.,-0.3046985\PG=C03 [C3(P1O1),X(C3H9O3)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	313.1888
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	312.8775
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAKS)	312.8453
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAHF)	312.9986
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAKS)	312.9823
MPW1K/IGLOIII	322.5535
MPW1K/IGLOIII + PCM($CHCl_3$,UAHF)	322.2479
MPW1K/IGLOIII + PCM($CHCl_3$,UAKS)	322.2172
MPW1K/IGLOIII + PCM(C_6H_6,UAHF)	322.3696
MPW1K/IGLOIII + PCM(C_6H_6,UAKS)	322.3541

10_2 C_1

1\1\GINC-NODE16\FOpt\RmPWPW91\6-31G(d)\C3H9O4P1\ZIP04\25-Jun-2009\0\\#
mpwpw91/6-31g(d) scf=tight int=finegrid IOp(3/76=0572004280) opt=(maxc
ycle=50)\\gas_003\\0,1\P,1.9640155132,-0.0110737743,-0.2455446356\O,2.
6902183797,-1.3607943824,-0.6295555612\O,3.1626350839,1.0254915881,-0.
3038504427\O,1.703191652,-0.0811694953,1.3293271738\O,0.7762951451,0.2
684997672,-1.0456932443\C,3.8906333714,-1.7579734549,0.0111008398\H,3.
762809261,-1.7774611823,1.0909728462\H,4.1152719671,-2.7558137092,-0.3
483606792\H,4.698600491,-1.080607795,-0.2504642589\C,2.8869189625,2.39
72632061,-0.0689741542\H,3.8034324173,2.9381303949,-0.2752910549\H,2.0
974172367,2.7433527051,-0.7307961174\H,2.596494181,2.5499475095,0.9678
494926\C,0.4695842112,-0.6129049612,1.7886122175\H,0.4133577858,-0.395
0111339,2.849463335\H,-0.3624063452,-0.1510147065,1.2652967063\H,0.439
8636862,-1.690119576,1.6380645371\\Version=AM64L-G03RevD.01\State=1-A\
HF=-761.9090844\RMSD=4.577e-09\RMSF=2.995e-05\Thermal=0.\Dipole=0.7582
613,0.0522977,1.2634754\PG=C01 [X(C3H9O4P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	319.4004
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	318.3833
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAKS)	318.3086
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAHF)	318.7836
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAKS)	318.7424
MPW1K/IGLOIII	328.7141
MPW1K/IGLOIII + PCM($CHCl_3$,UAHF)	327.7280
MPW1K/IGLOIII + PCM($CHCl_3$,UAKS)	327.6565
MPW1K/IGLOIII + PCM(C_6H_6,UAHF)	328.1158
MPW1K/IGLOIII + PCM(C_6H_6,UAKS)	328.0757

10_3 C_S

1\1\GINC-NODE11\FOpt\RmPWPW91\6-31G(d)\C3H9O4P1\ZIP04\25-Jun-2009\0\\#

mpwpw91/6-31g(d) scf=tight int=finegrid IOp(3/76=0572004280) opt=(maxc
ycle=50)\\gas_004\\0,1\P,0.2657329954,0.2140217421,0.\O,0.303814964,-0
.8222949562,-1.2020174703\O,0.303814964,-0.8222949562,1.2020174703\O,-
1.2121344654,0.8069474286,0.\O,1.2732605973,1.269465217,0.\C,0.6664193
717,-0.338344653,2.4871633137\H,0.7834953135,-1.2098997001,3.121003171
7\H,1.5992754125,0.2152396071,2.4353725749\H,-0.1150643676,0.302588012
9,2.8905211026\C,-2.3336905061,-0.0578109254,0.\H,-3.2136500984,0.5757
007544,0.\H,-2.3351534258,-0.6872968291,-0.8867739089\H,-2.3351534258,
-0.6872968291,0.8867739089\C,0.6664193717,-0.338344653,-2.4871633137\H
,0.7834953135,-1.2098997001,-3.1210031717\H,-0.1150643676,0.3025880129
,-2.8905211026\H,1.5992754125,0.2152396071,-2.4353725749\\Version=AM64
L-G03RevD.01\State=1-A'\HF=-761.9073501\RMSD=6.192e-09\RMSF=3.841e-05\
Thermal=0.\Dipole=-0.8968342,-0.7556395,0.\PG=CS [SG(C1H1O2P1),X(C2H8O
2)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	316.8600
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	315.3937
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAKS)	315.9187
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAHF)	316.3318
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAKS)	316.2902
MPW1K/IGLOIII	326.5091
MPW1K/IGLOIII + PCM($CHCl_3$,UAHF)	325.6488
MPW1K/IGLOIII + PCM($CHCl_3$,UAKS)	325.5763
MPW1K/IGLOIII + PCM(C_6H_6,UAHF)	325.9871
MPW1K/IGLOIII + PCM(C_6H_6,UAKS)	325.9485

	MPW1K/6-311++G(2d,2p)//MPW1K/6-31G(d)		MP2(FC)/6-31+G(2d,p)/MPW1K/6-31G(d)	
	Chemical shift, ppm (relative to PH_3)	Chemical shift, ppm (relative to PPh_3)	E_{tot}	„G“$_{298,\ gas}$
10_1	6.9757	19.1544	-760.547654	-760.444018
10_2	0.7641	12.9428	-760.546429	-760.443496
10_3	3.3045	15.4832	-760.544752	-760.442762

<δ> = 16.7 ppm (relative to PPh_3)
<δ> = 4.5 ppm (relative to PH_3)

10_3*C_6H_6

1\1\GINC-SOLARIS\SP\RmPWPW91\6-311++G(2d,2p)\C9H15O4P1\BORIS\19-Jun-20
08\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0
572004280) geom=check guess=read\\bm_mbh_tmpbenz_003_nmr001\\0,1\P,0,0
.0913455565,0.1348505194,0.0917133545\O,0,0.0451078076,0.1057518367,1.
6763099649\O,0,1.65709265,-0.022452496,-0.1032972637\O,0,-0.2434050066
,1.6348766615,-0.3193360585\O,0,-0.7616866904,-0.818960627,-0.61250972
86\C,0,2.1362437661,-0.4258254,-1.379071241\H,0,3.1950743725,-0.623998
2555,-1.2592548026\H,0,1.6225056299,-1.3229283762,-1.7113850806\H,0,1.
9943681245,0.3675992758,-2.1099446391\C,0,0.4752716044,2.7144957174,0.
2520026554\H,0,0.0684633231,3.6207157921,-0.1822623926\H,0,0.346141738
8,2.7340504221,1.3314811138\H,0,1.5343528057,2.6379459602,0.0176919798
\C,0,-1.2011432134,-0.1601128823,2.305548628\H,0,-0.9915512577,-0.2736
286951,3.3628484981\H,0,-1.8900557748,0.6689391832,2.1575586229\H,0,-1
.6390932876,-1.0716863437,1.9101230388\C,0,-4.3879540513,-4.2107746499
,-3.2489136403\C,0,-3.3806582789,-3.6242005553,-2.4982750829\C,0,-3.20
67076395,-2.2481658188,-2.5133022804\C,0,-4.0482467794,-1.4619377272,-
3.2863229239\C,0,-5.0558383178,-2.0456151762,-4.0388242298\C,0,-5.2266
85224,-3.4213007716,-4.0202687182\H,0,-4.5197468735,-5.2834074464,-3.2
335432485\H,0,-2.7278344648,-4.240379498,-1.8965223027\H,0,-2.42289872
01,-1.7924783465,-1.9251736385\H,0,-3.9161812577,-0.3894382777,-3.2998
170961\H,0,-5.709408273,-1.4286383611,-4.639111419\H,0,-6.011997336,-3

.8773518477,-4.6060874961\\Version=AM64L-G03RevD.01\State=1-A\HF=-994.
3417616\RMSD=3.946e-09\Thermal=0.\Dipole=0.9090215,1.0471177,0.7249262
\PG=C01 [X(C9H15O4P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	317.3162
MPW1K/IGLOIII	326.7555
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAHF)	316.9913
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAKS)	316.9829
MPW1K/IGLOIII + PCM(C_6H_6,UAHF)	326.4295
MPW1K/IGLOIII + PCM(C_6H_6,UAKS)	326.4222

10_1*C_6H_6

1\1\GINC-NODE8\SP\RmPWPW91\6-311++G(2d,2p)\C9H15O4P1\ZIP04\17-Jun-2008
\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=057
2004280) scrf=(PCM,Read,solvent=benzene)\\bm_mbh_tmpbenz_001_nmr001_pc
m_uahf\\0,1\P\O,1,1.58312892\O,1,1.58294554,2,102.46935528\O,1,1.58072
8,3,102.40881351,2,105.92963775,0\O,1,1.46694977,4,116.18600956,3,-126
.95549398,0\C,2,1.41934917,1,118.88575951,5,44.07224897,0\H,6,1.084052
02,2,106.59887553,1,-168.38292654,0\H,6,1.08668831,2,110.58011031,1,-4
8.77864536,0\H,6,1.08745723,2,110.07915241,1,72.88174614,0\C,3,1.41947
73,1,118.88003089,5,44.21534186,0\H,10,1.08404634,3,106.60904479,1,-16
7.60416231,0\H,10,1.08665262,3,110.55643885,1,-48.02958303,0\H,10,1.08
743498,3,110.0676731,1,73.65363573,0\C,4,1.42163662,1,119.21206307,5,4
6.85064694,0\H,14,1.08386826,4,106.45291788,1,-170.66480107,0\H,14,1.0
8654364,4,110.84333375,1,-51.1019297,0\H,14,1.08732755,4,109.99936903,
1,70.73817106,0\C,5,3.37021442,1,133.63605918,4,-26.11692277,0\C,18,1.
38762177,5,113.62328636,1,-74.54053477,0\C,19,1.38632559,18,120.313658
82,5,164.8284717,0\C,20,1.38642476,19,119.96077276,18,-0.0648531,0\C,2
1,1.38634941,20,119.92268825,19,0.0103054,0\C,22,1.38642527,21,120.003
68065,20,0.00486342,0\H,18,1.08111893,5,14.64906057,1,166.52465229,0\H
,19,1.08068823,18,119.66307214,5,-15.34902944,0\H,20,1.08070369,19,120
.07389684,18,179.86175912,0\H,21,1.08060854,20,120.04383996,19,179.948
04113,0\H,22,1.08068941,21,119.95092789,20,179.94245939,0\H,23,1.08068
293,22,119.94619932,21,179.88633354,0\\Version=AM64L-G03RevD.01\State=
1-A\HF=-994.3470868\RMSD=5.375e-09\Thermal=0.\Dipole=0.4364668,0.31766
83,0.2716308\PG=C01 [X(C9H15O4P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	313.2352
MPW1K/IGLOIII	322.4000
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAHF)	313.1300
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAKS)	313.1220
MPW1K/IGLOIII + PCM(C_6H_6,UAKS)	322.2874

10_2*C_6H_6

1\1\GINC-NODE2\SP\RmPWPW91\6-311++G(2d,2p)\C9H15O4P1\ZIP04\18-Jun-2008
\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=057
2004280) scrf=(PCM,Read,solvent=benzene) geom=check guess=read\\bm_mbh
_tmpbenz_002_nmr001_pcm_uahf\\0,1\P,0,-2.0422788518,0.0927464093,0.101
020105\O,0,-2.7360881135,1.4928330382,0.3311604104\O,0,-3.2796602287,-
0.8254843586,-0.2690165514\O,0,-1.6704530539,-0.4656839595,1.547378140
2\O,0,-0.9272760477,0.1435374778,-0.8412689626\C,0,-3.8685218374,1.620
8209591,1.1748116129\H,0,-3.6645339197,1.2052707797,2.1588568126\H,0,-
4.0692601607,2.6826962257,1.260461117\H,0,-4.7240297661,1.117234523,0.
7338610402\C,0,-3.0477428733,-2.1852231867,-0.6016289935\H,0,-3.993916
3644,-2.5859593945,-0.9467922429\H,0,-2.3058966696,-2.2603753305,-1.39
23399459\H,0,-2.7145161355,-2.7348526396,0.2754847897\C,0,-0.402503511
4,-0.1433891909,2.1045156901\H,0,-0.3060012049,-0.732192506,3.00977515
93\H,0,0.3968017833,-0.3882217729,1.4115849047\H,0,-0.3549494602,0.914
511831,2.3538432805\C,0,2.4287622743,0.0417914962,-0.7060433849\C,0,3.
0940429038,1.2082222079,-0.3562331179\C,0,4.4072390973,1.1582997377,0.
0850105666\C,0,5.0609119382,-0.060828427,0.1798901972\C,0,4.3999867119

,-1.2286968697,-0.1678275231\C,0,3.0867149235,-1.1760744046,-0.6096837
923\H,0,1.402110187,0.0834570223,-1.0417077393\H,0,2.5843021685,2.1580
128084,-0.4319726241\H,0,4.9228026194,2.0691931312,0.3541534103\H,0,6.
0848845021,-0.1003454681,0.5229778916\H,0,4.9093375224,-2.1791650831,-
0.0960805656\H,0,2.5727807471,-2.0864319856,-0.8839100844\\Version=AM6
4L-G03RevD.01\State=1-A\HF=-994.3459608\RMSD=4.165e-09\Thermal=0.\Dipo
le=-0.985981,-0.5027117,1.2613599\PG=C01 [X(C9H15O4P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	319.3150
MPW1K/IGLOIII	328.4058
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAHF)	318.8362
MPW1K/6-311++G(2d,2p) + PCM(C_6H_6,UAKS)	318.8070
MPW1K/IGLOIII + PCM(C_6H_6,UAHF)	327.9443
MPW1K/IGLOIII + PCM(C_6H_6,UAKS)	327.9139

	MPW1K/6-311++G(2d,2p) + PCM/UAHF/MPW1K/6-311++G(2d,2p)	MP2(FC)/6-31+G(2d,p)//MPW1K/6-31G(d) + PCM/UAHF/MPW1K/6-311++G(2d,2p)		
	Chemical shift, ppm (relative to PPh3)	E_{tot}	„G“$_{298,\ gas}$	„G“$_{298,C6H6}$
10_3*C_6H_6	13.2	-992.116994	-991.928039	-991.925569
10_1*C_6H_6	17.1	-992.1211642	-991.929749	-991.925478
10_2*C_6H_6	11.4	-992.1200939	-991.927889	-991.924367

<δ> = 14.6 ppm (relative to PPh_3)

10_1*$CHCl_3$

1\1\GINC-NODE7\SP\RmPWPW91\6-311++G(2d,2p)\C4H10Cl3O4P1\ZIP04\17-Jun-2
008\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=
0572004280) scrf=(PCM,Read,solvent=chloroform)\\bm_mbh_tmpchcl3_001_nm
r001_pcm_uahf\\0,1\P\O,1,1.57862557\O,1,1.57919597,2,102.89360768\O,1,
1.57854638,2,102.86378954,3,-106.57769223,0\O,1,1.46972653,4,115.57436
888,3,-126.42332415,0\C,2,1.42148284,1,119.38584102,5,44.65830265,0\H,
6,1.08362742,2,106.43328336,1,-171.30334908,0\H,6,1.08643379,2,110.564
7337,1,-51.86710415,0\H,6,1.08713305,2,110.0751647,1,69.97940493,0\C,3
,1.42107277,1,119.1166204,5,45.56635467,0\H,10,1.08370522,3,106.490377
92,1,-170.45732874,0\H,10,1.08648227,3,110.50268927,1,-50.94538976,0\H
,10,1.08712974,3,110.05068906,1,70.79018165,0\C,4,1.42170289,1,119.366
66006,5,46.12302087,0\H,14,1.08368598,4,106.47936248,1,-168.78789639,0
\H,14,1.08647331,4,110.6317029,1,-49.29769072,0\H,14,1.08702684,4,109.
97912071,1,72.48004565,0\H,5,1.96548253,1,157.95724815,4,-76.56548682,
0\C,5,3.04049354,1,154.86392565,4,-75.01310197,0\Cl,19,1.75919428,5,11
4.20065532,1,178.24499382,0\Cl,19,1.76282506,5,105.84175418,1,-59.3367
7529,0\Cl,19,1.76357942,5,103.71910081,1,57.35263586,0\\Version=AM64L-
G03RevD.01\State=1-A\HF=-2181.4992667\RMSD=3.962e-09\Thermal=0.\Dipole
=1.0293539,0.887277,0.3189906\PG=C01 [X(C4H10Cl3O4P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	315.0754
MPW1K/IGLOIII	324.3176
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	314.8869
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAKS)	314.8881
MPW1K/IGLOIII + PCM($CHCl_3$,UAHF)	324.1264
MPW1K/IGLOIII + PCM($CHCl_3$,UAKS)	324.1285

10_2*$CHCl_3$

1\1\GINC-NODE3\SP\RmPWPW91\6-311++G(2d,2p)\C4H10Cl3O4P1\ZIP04\18-Jun-2
008\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=
0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read\\
bm_mbh_tmpchcl3_002_nmr001_pcm_uahf\\0,1\P,0,2.0566399291,0.0054673042

,-0.1286509327\O,0,2.3916589524,1.0567428744,-1.2535563804\O,0,3.17115
1201,0.3032327119,0.9518885695\O,0,2.5190648522,-1.4162479567,-0.67526
58508\O,0,0.6614795086,0.0570903891,0.3096785768\C,0,3.7075011357,1.19
74075538,-1.767088583\H,0,4.0861553063,0.2414658683,-2.1207235978\H,0,
3.6392418014,1.8934858664,-2.5949340745\H,0,4.3673240779,1.5952997573,
-1.0016977312\C,0,3.1693025713,-0.4309029078,2.1682831801\H,0,3.940764
1085,0.0045469219,2.7923992719\H,0,2.2042498143,-0.34408185,2.66003403
64\H,0,3.3980309738,-1.476029278,1.9754786458\C,0,1.5931234411,-2.2081
103384,-1.409232752\H,0,2.0586234739,-3.1774343189,-1.5460454743\H,0,0
.6622749599,-2.3130249954,-0.8602839793\H,0,1.3957071514,-1.759255257,
-2.3800761795\H,0,-1.3156819273,0.1173411032,0.2249113769\C,0,-2.38257
19369,-0.0077758091,0.0851481289\Cl,0,-3.1901136935,0.3683839169,1.603
2377962\Cl,0,-2.9007917579,1.0833379288,-1.1946483103\Cl,0,-2.66148595
32,-1.6900349149,-0.3735836267\\Version=AM64L-G03RevD.01\State=1-A\HF=
-2181.4983135\RMSD=4.277e-09\Thermal=0.\Dipole=2.4027402,-0.6712497,-0
.3014513\PG=C01 [X(C4H10Cl3O4P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	320.3781
MPW1K/IGLOIII	329.6535
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	319.7309
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAKS)	319.7176
MPW1K/IGLOIII + PCM($CHCl_3$,UAHF)	329.0210
MPW1K/IGLOIII + PCM($CHCl_3$,UAKS)	329.0062

10_3*$CHCl_3$

1\1\GINC-EDDY\SP\RmPWPW91\6-311++G(2d,2p)\C4H10Cl3O4P1\BORIS\19-Jun-20
08\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0
572004280) geom=check guess=read\\bm_mbh_tmpchcl3_003_nmr001\\0,1\P,0,
-0.0560997144,0.0033112606,0.0805908817\O,0,0.0769312662,-0.0141011231
,1.6576347732\O,0,1.4790043244,-0.0374604575,-0.2975797901\O,0,-0.5659
196753,1.4576907814,-0.2995562998\O,0,-0.9093554782,-1.0272245964,-0.5
147870616\C,0,1.8501418372,-0.4849577547,-1.5966784379\H,0,2.933003537
2,-0.522971394,-1.6056580437\H,0,1.4397271534,-1.4714198667,-1.7887661
725\H,0,1.5015107993,0.2097111315,-2.3572607545\C,0,0.1247370467,2.610
4072821,0.1539262311\H,0,-0.4188378614,3.4657761196,-0.2302256612\H,0,
0.1435362849,2.6439689654,1.2405751085\H,0,1.1432586088,2.6206205159,-
0.2258576289\C,0,-1.0768357008,-0.3224391147,2.4296290397\H,0,-0.74309
86033,-0.4021658256,3.4574923923\H,0,-1.816684092,0.4707773802,2.34624
59746\H,0,-1.5105213068,-1.2627758069,2.102921211\H,0,-1.9541292183,-1
.5080915589,-2.1208173169\C,0,-2.3862797113,-1.7173204715,-3.092693343
3\Cl,0,-1.5626111635,-0.6897916314,-4.2679918691\Cl,0,-2.120990855,-3.
4198298252,-3.4566989491\Cl,0,-4.104839868,-1.3447828201,-3.029368494\
\Version=AM64L-G03RevD.01\State=1-A\HF=-2181.493124\RMSD=4.537e-09\The
rmal=0.\Dipole=1.0463204,1.2079511,1.2458854\PG=C01 [X(C4H10Cl3O4P1)]\
\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	316.8740
MPW1K/IGLOIII	326.4599
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	316.3608
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAKS)	316.3450
MPW1K/IGLOIII + PCM($CHCl_3$,UAHF)	325.9458
MPW1K/IGLOIII + PCM($CHCl_3$,UAKS)	325.9300

	MPW1K/6-311++G(2d,2p) + PCM/UAHF/MPW1K/6-311++G(2d,2p)	MP2(FC)/6-31+G(2d,p)//MPW1K/6-31G(d) + PCM/UAHF/MPW1K/6-311++G(2d,2p)		
	Chemical shift, ppm (relative to PPh3)	E_{tot}	„G“$_{298,\ gas}$	„G“$_{298,C6H6}$

10_1*$CHCl_3$	17.0	-2178.038722	-2177.932073	-2177.925826
10_2*$CHCl_3$	12.2	-2178.037242	-2177.929764	-2177.924680
10_3*$CHCl_3$	15.5	-2178.035824	-2177.928884	-2177.923609

<δ> = 15.9 ppm (relative to PPh_3)

11

1\1\GINC-NODE20\SP\RmPWPW91\6-311++G(2d,2p)\H8P4Si1\ZIP04\16-Aug-2010\
0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0572
004280) geom=check guess=read\\vw_009_s4\\0,1\Si,0,0.,0.,0.\P,0,-0.009
8584221,-0.0043858159,2.257870871\H,0,1.3939177628,-0.0288492564,2.419
1767131\H,0,-0.1144924245,1.3979683421,2.3906215629\P,0,1.4586772518,1
.5210953291,-0.810325224\H,0,2.6162800717,0.8218142476,-0.4027348836\H
,0,1.4847701316,1.0222270672,-2.132314343\P,0,0.5709880392,-2.09461724
8,-0.6202004009\H,0,-0.6655380221,-2.6957820243,-0.2933826792\H,0,0.25
34308434,-1.9176916966,-1.9851263995\P,0,-2.0198068689,0.5779077348,-0
.827345246\H,0,-2.7552184906,-0.3020908931,-0.0027602797\H,0,-2.213149
8723,1.7024042136,0.0065203092\\Version=AM64L-G03RevD.01\State=1-A\HF=
-1659.8729972\RMSD=2.333e-09\Thermal=0.\Dipole=0.,0.,0.\PG=S04 [O(Si1)
,X(H8P4)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	556.6147

12

1\1\GINC-IBLIS\SP\RmPWPW91\6-311++G(2d,2p)\C5H3Cr1O5P1\BORIS\12-Aug-20
10\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0
572004280) geom=check guess=read\\vw_010_0810_1\\0,1\Cr,0,-0.011603398
3,-0.1015747783,-0.018155916\C,0,-0.03125894,-0.1609642462,1.860386635
9\C,0,1.8650026264,0.0044446008,0.0153534132\C,0,0.0927799766,-1.94596
48646,-0.1031054106\C,0,0.0170915755,0.0094643929,-1.8938488141\C,0,-1
.8876393769,-0.2109816105,-0.0406051134\O,0,-0.037579983,-0.1953529087
,2.9996682032\O,0,0.154678854,-3.0842710755,-0.1606962738\O,0,3.003848
2968,0.0469146573,0.0381361658\O,0,0.0389577373,0.0937715244,-3.030166
8747\O,0,-3.0254606575,-0.2731007744,-0.0480197225\P,0,-0.1492670635,2
.2361599793,0.0832307121\H,0,-1.3904446862,2.8571017649,0.2952260277\H
,0,0.571915321,2.9410901836,1.0597817907\H,0,0.2443375082,3.0073542828
,-1.0219762854\\Version=AM64L-G03RevD.01\State=1-A\HF=-1954.3119813\RM
SD=2.575e-09\Thermal=0.\Dipole=-0.1001202,1.5371304,0.0627649\PG=C01 [
X(C5H3Cr1O5P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	447.6852

13

1\1\GINC-NODE8\SP\RmPWPW91\Gen\H4P1(1+)\ZIP04\12-Jun-2010\0\\#p mpwpw9
1/gen nmr scf=tight int=finegrid IOp(3/76=0572004280) geom=check guess
=read\\title\\1,1\P,0,0.,-0.0000000005,0.\H,0,-0.0000000008,-0.0000000
076,1.3894725882\H,0,0.,-1.3100073173,-0.4631575361\H,0,-1.1344996172,
0.6550036617,-0.4631575267\H,0,1.1344996179,0.6550036612,-0.4631575254
\\Version=AM64L-G03RevD.01\State=1-A1\HF=-343.4816132\RMSD=7.532e-09\T
hermal=0.\Dipole=0.,0.,0.\PG=TD [O(P1),4C3(H1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	448.1596

14

1\1\GINC-CIP-D-16\FOpt\RmPWPW91\6-31G(d)\C4H12P1(1+)\BRYCH\31-Mar-2010
\0\\#mpwpw91/6-31G(d) scf=tight int=finegrid IOp(3/76=0572004280) opt=
(maxcycle=50)\\title\\1,1\P,0.,0.,-0.0000000006\C,-0.0000000022,0.0000
000022,-1.7969703846\H,-0.0000000015,-1.0216561894,-2.1717890807\H,-0.
8847802195,0.5108280975,-2.1717890777\H,0.8847802128,0.5108280997,-2.1
717890799\C,-0.0000000013,1.6941999248,0.5989901295\H,-0.8847802186,2.

2178584106,0.2423163486\H,0.,1.7070303139,1.6871563896\H,0.8847802138,
2.2178584127,0.2423163463\C,-1.4672201728,-0.8470999653,0.5989901282\H
,-1.478331616,-1.8751713521,0.2423163444\H,-1.4783316155,-0.8535151618
,1.6871563884\H,-2.3631118341,-0.3426870652,0.2423163473\C,1.467220176
4,-0.8470999617,0.5989901246\H,2.3631118356,-0.3426870594,0.2423163414
\H,1.4783316218,-0.8535151582,1.6871563847\H,1.4783316213,-1.875171348
4,0.2423163407\\Version=IA32L-G03RevE.01\State=1-A1\HF=-500.7788442\RM
SD=3.332e-09\RMSF=2.058e-04\Thermal=0.\Dipole=0.,0.,0.\PG=TD [O(P1),4C
3(C1),6SGD(H2)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	306.9167
MPW1K/IGLOIII	307.9990

15

1\1\GINC-NODE11\SP\RmPWPW91\6-311++G(2d,2p)\F6P1(1-)\ZIP04\19-Aug-2010
\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=057
2004280) geom=check guess=read\\vw_013_oh\\-1,1\P,0,0.,0.,0.\F,0,0.,0.
,1.61580428\F,0,0.,1.61580428,0.\F,0,1.61580428,0.,0.\F,0,0.,-1.615804
28,0.\F,0,0.,0.,-1.61580428\F,0,-1.61580428,0.,0.\\Version=AM64L-G03Re
vD.01\State=1-A1G\HF=-940.7233914\RMSD=1.631e-09\Thermal=0.\Dipole=0.,
0.,0.\PG=OH [O(P1),3C4(F1.F1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	458.8171

16

1\1\GINC-NODE8\SP\RmPWPW91\Gen\P4\ZIP04\12-Jun-2010\0\\#p mpwpw91/gen
nmr scf=tight int=finegrid IOp(3/76=0572004280) geom=check guess=read\
\title\\0,1\P,0,-0.0000000019,-0.0000000003,1.3326851436\P,0,0.0000000
046,-1.2564676038,-0.4442283758\P,0,-1.0881328625,0.6282337936,-0.4442
283805\P,0,1.0881328598,0.6282338005,-0.4442283773\\Version=AM64L-G03R
evD.01\State=1-A1\HF=-1365.5477528\RMSD=3.133e-09\Thermal=0.\Dipole=0.
,0.,0.\PG=TD [4C3(P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	904.4006

17

1\1\GINC-NODE8\SP\RmPWPW91\6-311++G(2d,2p)\N1P1\ZIP04\12-Jun-2010\0\\#
p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=05720042
80) geom=check guess=read\\title\\0,1\P,0,0.,0.,-0.4194477901\N,0,0.,0
.,1.0558114301\\Version=AM64L-G03RevD.01\State=1-SG\HF=-396.0668181\RM
SD=2.546e-09\Thermal=0.\Dipole=0.,0.,-1.1865693\PG=C*V [C*(N1P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	-46.2557

18_cation

1\1\GINC-CIPCLU10\SP\RmPWPW91\6-311++G(2d,2p)\C19H18P1(1+)\BRYCH\23-Ma
r-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/
76=0572004280) geom=check guess=read\\pph3me_nmr_001\\1,1\P,0,0.514575
3339,-0.4956597584,-0.2104389302\C,0,0.4721578844,-0.4424445039,1.5795
762025\C,0,1.6687098525,-0.33210017,2.2903927515\C,0,-0.7429932567,-0.
4951394497,2.2577116603\C,0,1.6428742596,-0.2800249851,3.6710242626\H,
0,2.6177819974,-0.2795153901,1.776436864\C,0,-0.7575212993,-0.44199657
08,3.6416315092\H,0,-1.6708194557,-0.5809685246,1.7124624063\C,0,0.430
8660274,-0.3368571964,4.3452151004\H,0,2.5671955776,-0.1972130389,4.22
18316628\H,0,-1.6984791119,-0.4852455938,4.1682363498\H,0,0.4152188003
,-0.2988773896,5.4239524094\C,0,-1.0740023364,-1.0134325966,-0.8562853
144\C,0,-1.9023652785,-0.1012184952,-1.505066496\C,0,-1.4824741133,-2.
3380965431,-0.6901862866\C,0,-3.1319420125,-0.5166209402,-1.9886481763
\H,0,-1.5906646201,0.9240286691,-1.6363516297\C,0,-2.7111598285,-2.742

069375,-1.1766634563\H,0,-0.8542174112,-3.0536498635,-0.1793725127\C,0
,-3.5335747479,-1.8322239107,-1.8266958188\H,0,-3.7735938128,0.1888840
998,-2.4937524693\H,0,-3.0271056099,-3.7662954547,-1.0511417037\H,0,-4
.4914059031,-2.1525484442,-2.2078954445\C,0,0.9632062804,1.1077987819,
-0.8710721582\C,0,1.3200538353,1.2192777174,-2.216213385\C,0,0.9422795
975,2.2368324059,-0.0561599532\C,0,1.6572609902,2.4547694298,-2.735226
1359\H,0,1.330168822,0.3531562011,-2.8622667541\C,0,1.2818635192,3.470
3630155,-0.5865884338\H,0,0.6675040665,2.1555662342,0.9847142235\C,0,1
.6397602419,3.5782522051,-1.9202369837\H,0,1.9356744567,2.5419925561,-
3.7742134204\H,0,1.2683645339,4.3455433064,0.0446500131\H,0,1.90674321
2,4.5411218657,-2.3288487723\C,0,1.7619025021,-1.6971356972,-0.7205414
9\H,0,1.5544060628,-2.6635095705,-0.2684725941\H,0,1.7541864602,-1.805
0159699,-1.8020228035\H,0,2.7481758298,-1.3655985208,-0.4064594216\\Ve
rsion=AM64L-G03RevD.01\State=1-A\HF=-1076.0471025\RMSD=1.378e-09\Therm
al=0.\Dipole=0.317088,-0.305432,-0.1296752\PG=C03 [C3(P1C1),X(C18H18)]
\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	304.9854
MPW1K/IGLOIII	308.2132
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	304.5109
MPW1K/IGLOIII + PCM($CHCl_3$,UAHF)	307.8174

18_cation*$CHCl_3$

1\1\GINC-CIPCLU09\SP\RmPWPW91\6-311++G(2d,2p)\C20H19Cl3P1(1+)\BRYCH\29
-Mar-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp
(3/76=0572004280) scrf=(PCM,Read,solvent=chloroform)\\title\\1,1\P,0,-
1.372281,-0.047934,0.555788\C,0,-1.253148,1.643571,-0.019615\C,0,-0.10
8503,2.385845,0.27686\C,0,-2.278394,2.204905,-0.777276\C,0,0.000347,3.
684846,-0.182285\H,0,0.699951,1.959125,0.853058\C,0,-2.157544,3.507081
,-1.232751\H,0,-3.165338,1.63384,-1.007138\C,0,-1.023099,4.244161,-0.9
34627\H,0,0.883669,4.260687,0.047213\H,0,-2.951569,3.944829,-1.817988\
H,0,-0.933983,5.259826,-1.289485\C,0,-3.049968,-0.651265,0.379358\C,0,
-3.351848,-1.642805,-0.550108\C,0,-4.055815,-0.111429,1.18329\C,0,-4.6
55931,-2.09352,-0.670904\H,0,-2.577005,-2.063338,-1.173139\C,0,-5.3535
77,-0.568284,1.054552\H,0,-3.83577,0.666531,1.900404\C,0,-5.652076,-1.
559201,0.129378\H,0,-4.891225,-2.863414,-1.389548\H,0,-6.132264,-0.153
294,1.675884\H,0,-6.666841,-1.914783,0.033642\C,0,-0.240946,-1.089529,
-0.369939\C,0,0.147465,-2.327836,0.143498\C,0,0.221456,-0.673078,-1.61
6427\C,0,0.994148,-3.139789,-0.589617\H,0,-0.205991,-2.665869,1.106496
\C,0,1.066034,-1.494819,-2.345555\H,0,-0.068988,0.287615,-2.014472\C,0
,1.451623,-2.724098,-1.83337\H,0,1.296544,-4.096456,-0.191922\H,0,1.42
402,-1.171883,-3.311056\H,0,2.110965,-3.361659,-2.402979\C,0,-0.921958
,-0.104944,2.301726\H,0,-1.53133,0.602566,2.858264\H,0,-1.093203,-1.10
2105,2.698926\H,0,0.126516,0.153207,2.42576\H,0,2.948747,-0.884918,-0.
177255\C,0,3.667165,-0.210113,0.265385\Cl,0,3.105704,0.147144,1.904526
\Cl,0,5.221848,-1.009458,0.292825\Cl,0,3.700372,1.247626,-0.716816\\Ve
rsion=AM64L-G03RevD.01\State=1-A\HF=-2495.4836096\RMSD=5.872e-09\Therm
al=0.\Dipole=-3.101455,-0.4220751,-0.0601577\PG=C01 [X(C20H19Cl3P1)]\\
@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	304.7771
MPW1K/IGLOIII	308.0217
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	304.5229
MPW1K/IGLOIII + PCM($CHCl_3$,UAHF)	307.7840

18_ionic_associate_1

1\1\GINC-PHOBOS\SP\RMP2-FC\Gen\C19H18I1P1\BORIS\26-Oct-2010\0\\#p MP2(
FC)/gen scf=tight int=finegrid geom=check guess=read\\pph3me_i_salt1_0
1\\0,1\P,0,0.4660849724,0.2016512727,0.\C,0,0.4616100842,2.0030673045,
0.\C,0,1.6655635066,2.7006532857,0.\C,0,-0.7420466212,2.712151771,0.\C
,0,1.6672780674,4.0865188402,0.\H,0,2.6055073583,2.1711154924,0.\C,0,-

0.7338846812,4.0953730602,0.\H,0,-1.6860488153,2.1860528626,0.\C,0,0.4
710061395,4.7830693277,0.\H,0,2.6062053293,4.6189224997,0.\H,0,-1.6683
191413,4.635918821,0.\H,0,0.4749443903,5.8627766462,0.\C,0,-0.34147492
46,-0.3908925277,1.4976483501\C,0,-0.2838459722,-1.7568302472,1.773318
2244\C,0,-0.9795786811,0.4753930862,2.3841128331\C,0,-0.8823505163,-2.
2464926204,2.9213392127\H,0,0.252628618,-2.4537550806,1.1355732333\C,0
,-1.5764084332,-0.0282410408,3.5265065038\H,0,-0.9993216086,1.53814824
04,2.2028313043\C,0,-1.5333334023,-1.388247666,3.792429916\H,0,-0.8210
363568,-3.3039712961,3.1285727341\H,0,-2.0676069278,0.645341123,4.2126
504127\H,0,-1.9973575993,-1.7764643373,4.6871477535\C,0,-0.3414749246,
-0.3908925277,-1.4976483501\C,0,-0.2838459722,-1.7568302472,-1.7733182
244\C,0,-0.9795786811,0.4753930862,-2.3841128331\C,0,-0.8823505163,-2.
2464926204,-2.9213392127\H,0,0.252628618,-2.4537550806,-1.1355732333\C
,0,-1.5764084332,-0.0282410408,-3.5265065038\H,0,-0.9993216086,1.53814
82404,-2.2028313043\C,0,-1.5333334023,-1.388247666,-3.792429916\H,0,-0
.8210363568,-3.3039712961,-3.1285727341\H,0,-2.0676069278,0.645341123,
-4.2126504127\H,0,-1.9973575993,-1.7764643373,-4.6871477535\C,0,2.1534
23584,-0.4032062236,0.\H,0,2.672072178,-0.0684918528,0.8953511409\H,0,
2.1473250113,-1.5043070214,0.\H,0,2.672072178,-0.0684918528,-0.8953511
409\I,0,2.0135140748,-4.2435823801,0.\\Version=AM64L-G03RevD.01\State=
1-A'\HF=-7987.5885349\MP2=-7990.5753193\RMSD=5.139e-09\Thermal=0.\PG=C
S [SG(C7H6I1P1),X(C12H12)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p); for I atom: MPW1K/6-311G(d,p)	313.0141
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF); for I atom: MPW1K/6-311G(d,p)	313.0282

18_ionic_associate_2

1\1\GINC-PHOBOS\SP\RMP2-FC\Gen\C19H18I1P1\BORIS\28-Oct-2010\0\\#p MP2(
FC)/gen scf=tight int=finegrid geom=check guess=read\\pph3me_i_salt2_0
1_qadhoc\\0,1\P,0,-1.882277719,0.0121560876,0.0056467384\C,0,-1.317446
2983,1.6510650421,-0.4539363071\C,0,-2.1466816035,2.758049417,-0.26529
97485\C,0,-0.0299697209,1.8149812726,-0.9576547965\C,0,-1.6862996522,4
.0202984674,-0.5891226103\H,0,-3.144151972,2.6467103742,0.1331079565\C
,0,0.4264736275,3.0872703956,-1.2604737306\H,0,0.64972157,0.9811573096
,-1.0820467846\C,0,-0.3998232508,4.1839254032,-1.085223043\H,0,-2.3284
419495,4.8767253734,-0.4484819933\H,0,1.4373379502,3.2028257901,-1.619
9508124\H,0,-0.0409415207,5.1731122998,-1.3282073493\C,0,-1.3412273441
,-1.2105784507,-1.189392869\C,0,-0.0556547615,-1.7365824976,-1.0949798
049\C,0,-2.1873710837,-1.5992406828,-2.229207288\C,0,0.3821033101,-2.6
408540353,-2.0486583742\H,0,0.636218407,-1.430575083,-0.3199582388\C,0
,-1.7453680281,-2.5164331128,-3.1638634468\H,0,-3.1837114922,-1.192674
4692,-2.3194290141\C,0,-0.460665279,-3.0352316602,-3.0736494131\H,0,1.
3912267319,-3.0170049364,-1.9809439174\H,0,-2.4004189589,-2.8212879004
,-3.9660970098\H,0,-0.1162381323,-3.7447230538,-3.8114247441\C,0,-1.32
28597103,-0.4173556558,1.6546063395\C,0,-2.1581033253,-1.1322979796,2.
5147662268\C,0,-0.0337934882,-0.0729369116,2.0516586697\C,0,-1.7024805
758,-1.4896960875,3.7696043954\H,0,-3.156941593,-1.4140069703,2.216289
2236\C,0,0.4178601335,-0.4536451443,3.3046914702\H,0,0.6498582901,0.44
9735734,1.3944467828\C,0,-0.4145197516,-1.1512342565,4.1629162018\H,0,
-2.3493803308,-2.0376861838,4.438049184\H,0,1.42960767,-0.2070846915,3
.5875372066\H,0,-0.0593843347,-1.4407939608,5.1408459939\C,0,-3.689271
7456,0.0258542465,0.0135857932\H,0,-4.0606799566,0.4772029677,-0.90260
5679\H,0,-4.0678234792,-0.9902525276,0.0857284015\H,0,-4.0515069358,0.
5990567171,0.8628256723\I,0,3.165847303,-0.0149356464,-0.0100912812\\V
ersion=AM64L-G03RevD.01\State=1-A\HF=-7987.5883991\MP2=-7990.5741048\R
MSD=2.738e-09\Thermal=0.\PG=C01 [X(C19H18I1P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p); for I atom: MPW1K/6-311G(d,p)	319.9455
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF); for I atom: MPW1K/6-311G(d,p)	319.8243

	MPW1K/6-311++G(2d,2p) [+ PCM/UAHF/MPW1K/6-311++G(2d,2p)][a]		MP2(FC)/6-31+G(2d,p)/MPW1K/6-31G(d) + PCM/UAHF/MPW1K/6-311++G(2d,2p)		
	Chemical shift, ppm (relative to PPh_3)		E_{tot}	„G“$_{298,\ gas}$	„G“$_{298,CHCl3}$
	Gas-phase	Solution model 1			
18_ionic_associate_1	19.3	19.7	-7990.575319	-7990.302402	-7990.311295
18_ionic_associate_2	12.4	12.9	-7990.574105	-7990.302606	-7990.310829
[a]the theory shown in square brackets relates to solution model 1 and not to gas-phase calculations					

<δ> =15.5 ppm (gas-phase)
<δ> = 17.1 ppm (solution modell 1)

18_ionic_associate_1*$CHCl_3$_1

1\1\GINC-PHOENIX\SP\RmPWPW91\Gen\C20H19Cl3I1P1\BORIS\27-Oct-2010\0\\#p
mpwpw91/gen nmr scf=tight int=finegrid IOp(3/76=0572004280) scrf=(PCM
,Read,solvent=chloroform) geom=check guess=read\\pph3me_i_salt1_01_chc
l01\\0,1\P,0,0.5006377174,-0.1023004595,-0.2476330001\C,0,0.5614348784
,1.6629488031,0.102790019\C,0,1.7358780633,2.2354816052,0.5841292357\C
,0,-0.5785022274,2.4509558178,-0.0533926762\C,0,1.7692956419,3.5823061
443,0.9042914392\H,0,2.6259002913,1.6375966814,0.7095642639\C,0,-0.539
1624954,3.795809686,0.2714987374\H,0,-1.4898151076,2.0168030367,-0.438
2800266\C,0,0.633630851,4.3609175564,0.7494069538\H,0,2.683459195,4.02
19806627,1.2731895649\H,0,-1.4230645968,4.4028643491,0.1467775799\H,0,
0.6626501372,5.411125815,0.9986699645\C,0,-0.1487411884,-0.9543865081,
1.1925763768\C,0,0.10908216,-2.315463726,1.347854434\C,0,-0.8947253736
,-0.2634097217,2.147021217\C,0,-0.3897705313,-2.978864466,2.4569113298
\H,0,0.6682095109,-2.872365638,0.6024391186\C,0,-1.3857211998,-0.93823
62932,3.2496285014\H,0,-1.081643132,0.7943280339,2.0399810888\C,0,-1.1
325613808,-2.2937217303,3.4043013255\H,0,-0.1865465373,-4.0325232172,2
.5717638601\H,0,-1.9604018771,-0.4042660127,3.9913915665\H,0,-1.514070
6296,-2.8155490376,4.2695282557\C,0,-0.5314608744,-0.3524622699,-1.693
9939237\C,0,-1.2801571259,-1.5187064379,-1.8169694237\C,0,-0.487177977
1,0.5685794282,-2.7418021488\C,0,-1.9938633981,-1.7521235887,-2.980663
3455\H,0,-1.2927114672,-2.2542090544,-1.0285520795\C,0,-1.2072248092,0
.3276662388,-3.8964609384\H,0,0.103374958,1.4693836516,-2.6579227422\C
,0,-1.9609414638,-0.8320312233,-4.0137552858\H,0,-2.5578364096,-2.6661
924178,-3.0801955318\H,0,-1.1745809328,1.039912635,-4.7070247982\H,0,-
2.515588366,-1.0219032226,-4.9205806125\C,0,2.156174364,-0.7034461895,
-0.5915856353\H,0,2.7685842024,-0.692703261,0.3064808178\H,0,2.0754208
2,-1.7367216224,-0.9558292989\H,0,2.6081691096,-0.094737413,-1.3715645
488\I,0,1.390554938,-4.3017581268,-1.6750736129\H,0,3.0016085854,-5.03
10181208,0.3736293576\C,0,3.5869600248,-5.1843247229,1.2804319717\Cl,0
,2.5731102534,-6.0286559665,2.4488513617\Cl,0,5.0115572503,-6.12843773
71,0.8823717477\Cl,0,4.042172499,-3.5896398904,1.8961721\\Version=AM64
L-G03RevD.01\State=1-A\HF=-9415.6226106\RMSD=1.840e-09\Thermal=0.\Dipo
le=-2.4549,7.0311752,1.4731524\PG=C01 [X(C20H19Cl3I1P1)]\\@

MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF); for I atom: MPW1K/6-311G(d,p)	305.4268

18_ionic_associate_2*$CHCl_3$_1

1\1\GINC-IBLIS\SP\RmPWPW91\Gen\C20H19Cl3I1P1\BORIS\27-Oct-2010\0\\#p m
pwpw91/gen nmr scf=tight int=finegrid IOp(3/76=0572004280) scrf=(PCM,R
ead,solvent=chloroform) geom=check guess=read\\pph3me_i_salt2_01_chcl0
1\\0,1\P,0,0.006937472,0.0401465964,-1.0150895602\C,0,-1.7581953142,-0
.0110300265,-0.7122337387\C,0,-2.6117981937,-0.6388060287,-1.620809278
3\C,0,-2.261384582,0.5394079653,0.4631497485\C,0,-3.965506932,-0.70517

57278,-1.3513429234\H,0,-2.2308195756,-1.0772936855,-2.5314196169\C,0,
-3.6176797958,0.449460984,0.7310909431\H,0,-1.6124000276,1.0003963675,
1.1957171622\C,0,-4.4664188205,-0.1626367477,-0.1751104049\H,0,-4.6290
911692,-1.1858255283,-2.0542892647\H,0,-3.9929093766,0.8502656745,1.65
99118924\H,0,-5.5236267477,-0.2261183723,0.0358959291\C,0,0.710027383,
1.5719042522,-0.4073098829\C,0,1.2118612658,1.6294990819,0.8893943832\
C,0,0.7140798825,2.7087873708,-1.2181346535\C,0,1.7138115584,2.8275325
6,1.3727137516\H,0,1.1885983587,0.7688685794,1.542019719\C,0,1.2297182
358,3.8935016219,-0.7297962433\H,0,0.3168545539,2.6777417166,-2.222226
5909\C,0,1.7288545898,3.9511341745,0.5653334552\H,0,2.0803706173,2.868
758195,2.386399605\H,0,1.2383224046,4.7730599971,-1.3557163855\H,0,2.1
245615524,4.8811361962,0.9456882533\C,0,0.8246445869,-1.3668064655,-0.
2674950305\C,0,1.9705115803,-1.9026478438,-0.8583185275\C,0,0.34721854
26,-1.8791773559,0.9356632561\C,0,2.6273866438,-2.9523888486,-0.245972
4933\H,0,2.3566606022,-1.5055268941,-1.7855813604\C,0,1.0251130273,-2.
9205507892,1.5486436785\H,0,-0.5167527183,-1.4555239354,1.4283500485\C
,0,2.1557553369,-3.4580109356,0.9583924562\H,0,3.5128054738,-3.3695506
969,-0.7013168776\H,0,0.6692595998,-3.2889060728,2.4980859655\H,0,2.68
13220539,-4.267431917,1.4425075484\C,0,0.274375642,-0.0322207787,-2.80
16229169\H,0,-0.3769188183,0.6783588829,-3.3035397536\H,0,1.3076648934
,0.2142990358,-3.0306341457\H,0,0.0589463918,-1.0318535895,-3.16963822
91\I,0,-0.7205955031,0.243810196,3.9295020733\H,0,1.7586664189,-0.3659
949458,4.8053697186\C,0,2.8070242932,-0.6017008123,4.9898475781\Cl,0,3
.3269906178,0.2375636145,6.4423823274\Cl,0,2.9539585987,-2.347336708,5
.1821966108\Cl,0,3.728093577,-0.0531181617,3.5845037437\\Version=AM64L
-G03RevD.01\State=1-A\HF=-9415.6187997\RMSD=2.738e-09\Thermal=0.\Dipol
e=0.1233792,-0.0775463,-7.4010759\PG=C01 [X(C20H19Cl3I1P1)]\\@

MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	315.5837

18_ionic_associate_1*$CHCl_3$_2

1\1\GINC-PHOBOS\SP\RmPWPW91\Gen\C20H19Cl3I1P1\BORIS\27-Oct-2010\0\\#p
mpwpw91/gen nmr scf=tight int=finegrid IOp(3/76=0572004280) scrf=(PCM,
Read,solvent=chloroform) geom=check guess=read\\pph3me_i_salt1_01_chcl
02\\0,1\P,0,0.5332141748,0.1070641668,-0.0393159141\C,0,0.3335199848,1
.8956926014,-0.0513035838\C,0,1.4321932728,2.7182756455,-0.2836588366\
C,0,-0.9281539003,2.4624445787,0.1322852575\C,0,1.2703424137,4.0930799
729,-0.3325904342\H,0,2.4145648842,2.2939083537,-0.4240687733\C,0,-1.0
831146252,3.8363775147,0.0792667439\H,0,-1.7866400117,1.8352696757,0.3
240773387\C,0,0.0152170604,4.6510991432,-0.1528348605\H,0,2.1264451445
,4.7262391895,-0.509533305\H,0,-2.0614852727,4.2690245213,0.2235464094
\H,0,-0.1080109567,5.7231639074,-0.190445181\C,0,-0.3893648393,-0.5556
874853,1.3560016649\C,0,-0.7933499509,-1.8884705377,1.335911496\C,0,-0
.580699948,0.2185469365,2.5010984339\C,0,-1.3920612746,-2.4382997196,2
.4587718976\H,0,-0.6166528103,-2.5132699453,0.4749839437\C,0,-1.188620
8253,-0.336727315,3.6129223721\H,0,-0.2597348638,1.2490774337,2.528233
0736\C,0,-1.5922567174,-1.6655288999,3.59165056\H,0,-1.674134196,-3.47
9428247,2.4467684413\H,0,-1.3394262596,0.2641713171,4.4968226262\H,0,-
2.0538025119,-2.1010789953,4.4655213317\C,0,-0.0377686054,-0.560090843
5,-1.6066914138\C,0,0.3852853459,-1.8318836468,-1.99009595\C,0,-0.8807
789343,0.1826248587,-2.4331860229\C,0,-0.0537267599,-2.3580919912,-3.1
940295142\H,0,1.0330679056,-2.4332945671,-1.3562642018\C,0,-1.30704589
72,-0.3543057999,-3.6342352541\H,0,-1.1939486774,1.1762896729,-2.15210
72452\C,0,-0.8953743547,-1.6241112476,-4.0132345773\H,0,0.2712045145,-
3.3467324446,-3.4805170016\H,0,-1.9565205865,0.2212655569,-4.276561166
9\H,0,-1.2305683005,-2.0389414566,-4.9524699226\C,0,2.2640515923,-0.31
27985642,0.1718593578\H,0,2.6525664673,0.173830474,1.063718563\H,0,2.3
386570407,-1.4029532625,0.3092873011\H,0,2.8397296881,-0.0264767661,-0
.70479272\I,0,2.1221144324,-4.1070738172,0.5063462085\H,0,-3.473699708
2,-0.7295399587,1.8945914158\C,0,-4.3418913394,-0.2729318232,1.4393199
981\Cl,0,-4.0833169541,-0.2554979115,-0.3012127837\Cl,0,-5.7453039912,
-1.2335617969,1.8671820403\Cl,0,-4.4746668496,1.3667810122,2.074150307
6\\Version=AM64L-G03RevD.01\State=1-A\HF=-9415.6164078\RMSD=2.628e-09\
Thermal=0.\Dipole=-2.3833868,6.450258,-0.6604828\PG=C01 [X(C20H19Cl3I1

P1)]\\@

MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF); for I atom: MPW1K/6-311G(d,p)	307.6611

18_ionic_associate_1*$CHCl_3$_3

1\1\GINC-PHOENIX\SP\RmPWPW91\Gen\C20H19Cl3I1P1\BORIS\27-Oct-2010\0\\#p
mpwpw91/gen nmr scf=tight int=finegrid IOp(3/76=0572004280) scrf=(PCM
,Read,solvent=chloroform) geom=check guess=read\\pph3me_i_salt1_01_chc
l03\\0,1\P,0,0.4742800848,0.1706957577,-0.0111830525\C,0,0.4782421853,
1.9703742018,0.0290291764\C,0,1.6841353253,2.6607168115,0.1041961379\C
,0,-0.7221436446,2.6841601495,0.0004021197\C,0,1.6902301346,4.04577859
02,0.1495941921\H,0,2.6208644554,2.1263449517,0.1305295414\C,0,-0.7091
938499,4.0664831905,0.0466579872\H,0,-1.6668031201,2.1626083777,-0.060
5358999\C,0,0.4972265187,4.7475488729,0.1214046124\H,0,2.6300220836,4.
5733914218,0.2077686559\H,0,-1.6406985886,4.6115608764,0.0239919653\H,
0,0.5049507557,5.8266118435,0.1576140431\C,0,-0.3204376637,-0.44619136
61,1.4877466372\C,0,-0.2124204616,-1.8060984762,1.7771262091\C,0,-1.00
52415787,0.4011563315,2.358319633\C,0,-0.8056608319,-2.3108924252,2.92
30697128\H,0,0.3507529459,-2.4908494712,1.1475342667\C,0,-1.5949294417
,-0.1154960825,3.4997509464\H,0,-1.0634334765,1.4607119137,2.167552851
\C,0,-1.5007004864,-1.4717598002,3.7800385283\H,0,-0.7075066429,-3.364
344943,3.1371091912\H,0,-2.1212637136,0.5441057154,4.1732572053\H,0,-1
.9607020752,-1.8701219367,4.6724075602\C,0,-0.3643687154,-0.3892585361
,-1.5037922124\C,0,-0.3942664176,-1.7603092143,-1.7577252182\C,0,-0.92
47382512,0.5038978662,-2.4158826914\C,0,-1.004037309,-2.2276935558,-2.
9087628608\H,0,0.0913954153,-2.4782778599,-1.104428184\C,0,-1.53580899
91,0.0224364391,-3.56044455\H,0,-0.872799272,1.5684494729,-2.252058886
3\C,0,-1.5816528364,-1.3416637432,-3.8036824974\H,0,-1.0077231762,-3.2
896856479,-3.1010988953\H,0,-1.967740662,0.716055632,-4.2661730453\H,0
,-2.0557546322,-1.7123371304,-4.7005193204\C,0,2.1545730497,-0.4508321
251,-0.0461759677\H,0,2.689709726,-0.1441048791,0.8494764693\H,0,2.136
4272162,-1.5516465255,-0.0745349612\H,0,2.6612112159,-0.0961843734,-0.
9407748247\I,0,1.9535874724,-4.2930128938,-0.0959712184\H,0,1.12106951
38,-0.5165917299,4.1547935407\C,0,2.1159883626,-0.2201952673,4.4565889
284\Cl,0,2.4097289473,1.384251818,3.7717222414\Cl,0,3.2494362479,-1.39
46187619,3.8270664319\Cl,0,2.1442107502,-0.1608088793,6.2133558418\\Ve
rsion=AM64L-G03RevD.01\State=1-A\HF=-9415.6152663\RMSD=2.572e-09\Therm
al=0.\Dipole=-3.1193926,6.9351744,-0.1345415\PG=C01 [X(C20H19Cl3I1P1)]
\\@

MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF); for I atom: MPW1K/6-311G(d,p)	312.1285

18_ionic_associate_2*$CHCl_3$_3

1\1\GINC-IBLIS\SP\RmPWPW91\Gen\C20H19Cl3I1P1\BORIS\27-Oct-2010\0\\#p m
pwpw91/gen nmr scf=tight int=finegrid IOp(3/76=0572004280) scrf=(PCM,R
ead,solvent=chloroform) geom=check guess=read\\pph3me_i_salt2_01_chcl0
3\\0,1\P,0,-0.031338426,-0.0863706587,-1.1594134155\C,0,-1.7281350692,
-0.0831071081,-0.582600423\C,0,-2.7485983613,-0.6165093886,-1.37045488
64\C,0,-2.0044898264,0.4265697439,0.6836877155\C,0,-4.0443799348,-0.63
20262998,-0.8891280052\H,0,-2.5430477303,-1.0185329799,-2.3516295814\C
,0,-3.3048793299,0.3907831552,1.1597567193\H,0,-1.2223739007,0.8172203
3,1.3265357409\C,0,-4.3205716142,-0.1297822233,0.3754773768\H,0,-4.837
4475892,-1.0393955709,-1.4979563675\H,0,-3.5062107251,0.7669249361,2.1
510290933\H,0,-5.3334173135,-0.1503054342,0.7498611679\C,0,0.768285492
,1.441487009,-0.663037494\C,0,1.6727745628,1.4630996608,0.3925915394\C
,0,0.417286454,2.6270119217,-1.315691402\C,0,2.2345374641,2.6702061977
,0.7859866081\H,0,1.9217655147,0.5654244808,0.9348930427\C,0,0.9914421
134,3.8205741226,-0.9251296064\H,0,-0.3042311198,2.6255695598,-2.11966
73032\C,0,1.9023804462,3.8400978726,0.1266940736\H,0,2.904455484,2.683
549658,1.6309715265\H,0,0.7240630753,4.735834181,-1.430971511\H,0,2.33
86195454,4.7767222422,0.4404470641\C,0,0.8583237883,-1.5208077014,-0.5
581017921\C,0,1.6405327058,-2.2846004529,-1.4253654737\C,0,0.765849084

4,-1.8593761219,0.7903581153\C,0,2.3231907359,-3.3848260828,-0.9401797
133\H,0,1.7254457172,-2.029672247,-2.4706975517\C,0,1.4685718015,-2.95
34287217,1.2666202724\H,0,0.1979472712,-1.2620611324,1.4950964069\C,0,
2.2376207746,-3.7173850033,0.4045967703\H,0,2.9259645514,-3.9788444182
,-1.6105102769\H,0,1.4123227052,-3.1882371539,2.3184141334\H,0,2.77872
12575,-4.5732488788,0.7802229129\C,0,-0.042845441,-0.140505697,-2.9648
922687\H,0,-0.7050320537,0.6307523851,-3.3489178163\H,0,0.9603305246,0
.0417460609,-3.341797826\H,0,-0.3897991767,-1.108841112,-3.3158987593\
I,0,0.3507093535,0.5284480908,3.7067557153\H,0,3.251452832,2.482280074
7,-1.8507327603\C,0,3.8623412839,2.1895016935,-2.6937257937\Cl,0,4.136
4041161,0.453791826,-2.5759234992\Cl,0,2.9716266868,2.5854286307,-4.16
27579285\Cl,0,5.3699252297,3.079642604,-2.6068528894\\Version=AM64L-G0
3RevD.01\State=1-A\HF=-9415.6122259\RMSD=2.189e-09\Thermal=0.\Dipole=-
0.921331,-0.7775629,-6.3882323\PG=C01 [X(C20H19Cl3I1P1)]\\@

MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF); for I atom: MPW1K/6-311G(d,p)	316.3598

18_ionic_associate_1*$CHCl_3$_4

1\1\GINC-PHOBOS\SP\RmPWPW91\Gen\C20H19Cl3I1P1\BORIS\28-Oct-2010\0\\#p
mpwpw91/gen nmr scf=tight int=finegrid IOp(3/76=0572004280) scrf=(PCM,
Read,solvent=chloroform) geom=check guess=read\\pph3me_i_salt1_01_chcl
04\\0,1\P,0,0.5730385268,0.0600270392,-0.0984616671\C,0,0.5967950436,1
.8610548297,0.0090461041\C,0,1.7757272536,2.5232611591,0.3417041735\C,
0,-0.5698861946,2.5953625392,-0.2031590658\C,0,1.7881034907,3.90442592
56,0.4571302786\H,0,2.6872916214,1.9689316162,0.5051949477\C,0,-0.5536
756982,3.9745744461,-0.0818563176\H,0,-1.4861361803,2.0914710867,-0.47
46722643\C,0,0.6251128968,4.6297538613,0.2451243123\H,0,2.7071959595,4
.4128687113,0.7065520321\H,0,-1.4595279371,4.5375749798,-0.2474759542\
C,0,-0.0659998902,-0.5993578875,1.4451884988\C,0,0.2358814918,-1.91470
20606,1.7951591961\C,0,-0.8518112109,0.1916544539,2.2833147548\C,0,-0.
2598738671,-2.4297072531,2.9821549344\H,0,0.8215475894,-2.5569718576,1
.142005048\C,0,-1.3343539869,-0.3339808598,3.467507137\H,0,-1.08418448
13,1.2130710472,2.0227829968\C,0,-1.0376295967,-1.6439588234,3.8163790
721\H,0,-0.0310376321,-3.4516990758,3.2433231646\H,0,-1.9368187918,0.2
815430357,4.1182751273\H,0,-1.4153016467,-2.0508994206,4.7428544615\C,
0,-0.4466890621,-0.3994964082,-1.500532957\C,0,-1.1026875779,-1.627158
1504,-1.4965944023\C,0,-0.4793394953,0.4129231081,-2.6352191296\C,0,-1
.8023500998,-2.0291369627,-2.6222871334\H,0,-1.0486923966,-2.283814001
,-0.6429366707\C,0,-1.1864985331,0.0040545169,-3.7497771328\H,0,0.0426
700593,1.3584481453,-2.6511236931\C,0,-1.8486117461,-1.2160148551,-3.7
409578028\H,0,-2.2903026223,-2.9910663847,-2.6233547373\H,0,-1.2144045
041,0.6322910317,-4.6272443256\H,0,-2.3927545564,-1.5372366408,-4.6166
637119\C,0,2.2420504721,-0.544494783,-0.3500473363\H,0,2.8505113641,-0
.3872831569,0.5370616626\H,0,2.183356604,-1.6247231035,-0.5596424094\H
,0,2.6827790475,-0.049341314,-1.2124815717\I,0,1.5988634453,-4.2337947
171,-0.8852276959\H,0,0.6373785418,5.7057889741,0.3332406914\H,0,0.275
7047901,3.7682872128,2.9214638835\C,0,-0.1832268506,4.146580556,3.8239
936324\Cl,0,0.4682204254,3.2450573966,5.1811577803\Cl,0,-1.921941477,3
.9078549633,3.6727775386\Cl,0,0.2124181222,5.8558626398,3.9382078306\\
Version=AM64L-G03RevD.01\State=1-A\HF=-9415.6150563\RMSD=2.180e-09\The
rmal=0.\Dipole=-1.8727517,6.6381029,0.7273746\PG=C01 [X(C20H19Cl3I1P1)
]\\@

MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF); for I atom: MPW1K/6-311G(d,p)	305.9459

18_ionic_associate_2*$CHCl_3$_2

1\1\GINC-IBLIS\SP\RmPWPW91\Gen\C20H19Cl3I1P1\BORIS\27-Oct-2010\0\\#p m
pwpw91/gen nmr scf=tight int=finegrid IOp(3/76=0572004280) scrf=(PCM,R
ead,solvent=chloroform) geom=check guess=read\\pph3me_i_salt2_01_chcl0
2\\0,1\P,0,-0.0250713996,-0.2058422155,-1.3229410956\C,0,-1.7513401745
,-0.3429547909,-0.8590537443\C,0,-2.6633508063,-0.965181866,-1.7130753

567\C,0,-2.1626330278,0.1376308767,0.3809381387\C,0,-3.9834116423,-1.0
942962844,-1.325264874\H,0,-2.3538213943,-1.3507709807,-2.6732709455\C
,0,-3.4847480977,-0.014315209,0.7660363894\H,0,-1.4683658617,0.5925584
4,1.0751895786\C,0,-4.3923391351,-0.6197354907,-0.0858377626\H,0,-4.69
19127334,-1.5704907553,-1.9862044066\H,0,-3.7852226992,0.3349928791,1.
7416871056\H,0,-5.4230836924,-0.7309802055,0.2166089521\C,0,0.66295209
33,1.3448761722,-0.7469964265\C,0,1.1892755129,1.4264038494,0.53925029
44\C,0,0.6175408982,2.4757541512,-1.5644918033\C,0,1.6602422314,2.6427
46006,1.0063632894\H,0,1.2017021848,0.5737896993,1.2047567585\C,0,1.10
52534253,3.6793092598,-1.0925603851\H,0,0.202377638,2.427086494,-2.560
4076255\C,0,1.6234730225,3.7622668196,0.193184301\H,0,2.0350831728,2.7
046727518,2.0158412863\H,0,1.0731902304,4.5547656349,-1.723522266\H,0,
0.3959143415,5.2539341833,5.8942830667\C,0,0.9151531974,-1.5952364043,
-0.690919489\C,0,1.9517135748,-2.1446274769,-1.4472958181\C,0,0.631304
374,-2.0910761741,0.5785785457\C,0,2.6916050642,-3.1926644411,-0.93350
977\H,0,2.1884606191,-1.7624140555,-2.4292488506\C,0,1.3923826841,-3.1
295519181,1.0900562044\H,0,-0.1418413685,-1.6598755314,1.2015764261\C,
0,2.4118585799,-3.683386757,0.3349846658\H,0,3.4904081282,-3.622126902
3,-1.519209138\H,0,1.1830608691,-3.4839718716,2.0874674965\H,0,2.99871
81194,-4.4963116486,0.7362738115\C,0,0.0766080083,-0.2326966024,-3.127
2362266\H,0,-0.6538948743,0.4521605229,-3.5494473089\H,0,1.0703760356,
0.070341968,-3.4460253354\H,0,-0.1239992831,-1.2350068971,-3.496161408
4\I,0,-0.3046570393,-0.1351428457,3.7107632576\H,0,1.9892632143,4.7076
255659,0.5652894594\C,0,0.3295150875,5.1450312799,4.8214073164\Cl,0,0.
0615140989,3.4605167185,4.4456491755\Cl,0,1.8632195988,5.7285889883,4.
1551441486\Cl,0,-1.0048741347,6.1655977435,4.2786456685\\Version=AM64L
-G03RevD.01\State=1-A\HF=-9415.6125105\RMSD=2.061e-09\Thermal=0.\Dipol
e=0.3293235,-0.4470769,-6.7581035\PG=C01 [X(C20H19Cl3I1P1)]\\@

MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF); for I atom: MPW1K/6-311G(d,p)	318.0986

	MPW1K/6-311++G(2d,2p) + PCM/UAHF/MPW1K/6-311++G(2d,2p)	MP2(FC)/6-31+G(2d,p)/MPW1K/6-31G(d) + PCM/UAHF/MPW1K/6-311++G(2d,2p)		
	Chemical shift, ppm (relative to PPh3)	E_{tot}	$„G“_{298,\ gas}$	$„G“_{298,CHCl3}$
18_ionic_associate_1*$CHCl_3$_1	26.5	-9408.065275	-9407.786178	-9407.783676
18_ionic_associate_2*$CHCl_3$_1	16.3	-9408.063140	-9407.786532	-9407.782994
18_ionic_associate_1*$CHCl_3$_2	24.2	-9408.062679	-9407.782659	-9407.780252
18_ionic_associate_1*$CHCl_3$_3	19.8	-9408.061179	-9407.780773	-9407.778876
18_ionic_associate_2*$CHCl_3$_3	15.5	-9408.059436	-9407.780425	-9407.777876
18_ionic_associate_1*$CHCl_3$_4	25.9	-9408.057140	-9407.778408	-9407.777404
18_ionic_associate_2*$CHCl_3$_2	13.8	-9408.051094	-9407.774153	-9407.774424

<δ> = 23.1 ppm

19

1\1\GINC-NODE13\SP\RmPWPW91\6-311++G(2d,2p)\C6H5Br2P1\ZIP04\03-Aug-201
0\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=05
72004280) geom=check guess=read\\nmr_0710_03_1cs\\0,1\P,0,-0.980112079
1,0.5303986087,0.0000000007\Br,0,0.1598865723,1.3794408559,1.709184094
8\Br,0,0.1598865723,1.3794408601,-1.7091840913\C,0,-0.3240830621,-1.16
26651041,-0.0000000014\C,0,-1.2776976631,-2.174023889,-0.0000000027\C,
0,1.0305354713,-1.4865752941,-0.0000000018\C,0,-0.8822165046,-3.504013
7578,-0.0000000044\H,0,-2.3302454149,-1.9258697962,-0.0000000024\C,0,1

.4198637753,-2.810838842,-0.0000000035\H,0,1.7706217518,-0.6996294832,
-0.0000000009\C,0,0.4640011685,-3.8200230414,-0.0000000047\H,0,-1.6258
165121,-4.2868933179,-0.0000000053\H,0,2.470166765,-3.062003165,-0.000
0000038\H,0,0.7751350195,-4.8543459897,-0.000000006\\Version=AM64L-G03
RevD.01\State=1-A'\HF=-5721.6386444\RMSD=3.357e-09\Thermal=0.\Dipole=0
.0495713,-1.186119,0.\PG=CS [SG(C6H5P1),X(Br2)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	156.9698

19*$CHCl_3$_1

1\1\GINC-NODE17\SP\RmPWPW91\6-311++G(2d,2p)\C7H6Br2Cl3P1\ZIP04\05-Aug-
2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76
=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read\
\nmr_0710_03c_3\\0,1\P,0,-0.7700597641,0.5225186116,0.0260532567\Br,0,
1.0074312852,0.8533197538,1.3227837728\Br,0,0.1619848577,0.8206540003,
-1.9739245719\C,0,-0.8491091699,-1.2884221275,0.056426828\C,0,-2.10890
02872,-1.8259677112,0.2941801778\C,0,0.2401345008,-2.1332651276,-0.149
4597711\C,0,-2.2838873357,-3.2020151785,0.32497266\H,0,-2.9556565688,-
1.1727960028,0.4551250391\C,0,0.0608042805,-3.5011815539,-0.1172338923
\H,0,1.2228753932,-1.7185934066,-0.3231948967\C,0,-1.2006820616,-4.035
9217878,0.1183972364\H,0,-3.2636122152,-3.6161752187,0.5101407876\H,0,
0.9039442403,-4.156782257,-0.2762054197\H,0,-1.3332774351,-5.107571345
,0.1415886263\H,0,2.735008934,1.2636107145,-0.9140058127\C,0,3.7779282
989,1.0974802534,-1.1415095007\Cl,0,4.6434896284,0.9630435592,0.382323
6376\Cl,0,3.8721373062,-0.3987261424,-2.0635345094\Cl,0,4.3494857626,2
.4638333361,-2.0858469979\\Version=AM64L-G03RevD.01\State=1-A\HF=-7141
.0359867\RMSD=3.686e-09\Thermal=0.\Dipole=-1.2023589,-1.3008616,0.3063
521\PG=C01 [X(C7H6Br2Cl3P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	158.1013

19*$CHCl_3$_2

1\1\GINC-NODE19\SP\RmPWPW91\6-311++G(2d,2p)\C7H6Br2Cl3P1\ZIP04\07-Aug-
2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76
=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read\
\nmr_0710_03c_2\\0,1\P,0,-1.4841280951,0.0333133385,-1.431936285\Br,0,
-0.1932021179,1.7000052376,-0.7169330887\Br,0,-0.1986360294,-1.7006086
402,-0.8873281057\C,0,-2.6797223599,-0.0329472054,-0.071195856\C,0,-4.
0179024917,-0.0118775104,-0.4476845736\C,0,-2.337953599,-0.1011241033,
1.27752887\C,0,-5.0125526035,-0.0586774199,0.5183980947\H,0,-4.2863993
155,0.0410153804,-1.4939432094\C,0,-3.3306876005,-0.1475005363,2.23504
13581\H,0,-1.2978479386,-0.1174529293,1.569032232\C,0,-4.6679465501,-0
.1263006545,1.8559672666\H,0,-6.0509421488,-0.0421723598,0.2231561176\
H,0,-3.0662135355,-0.2003548948,3.280617445\H,0,-5.4401669528,-0.16284
4822,2.6101603639\H,0,1.9385506925,-0.0392801384,-0.0918835637\C,0,2.8
700333069,-0.0681543278,0.4560409934\Cl,0,2.8960923713,1.3317064208,1.
5204542375\Cl,0,2.8931883398,-1.5690472016,1.3725851305\Cl,0,4.1855816
755,-0.0101534464,-0.7075013757\\Version=AM64L-G03RevD.01\State=1-A\HF
=-7141.0360789\RMSD=3.422e-09\Thermal=0.\Dipole=-1.911354,-0.016474,0.
3811601\PG=C01 [X(C7H6Br2Cl3P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	159.4190

19*$CHCl_3$_3

1\1\GINC-NODE23\SP\RmPWPW91\6-311++G(2d,2p)\C7H6Br2Cl3P1\ZIP04\07-Aug-
2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76
=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read\
\nmr_0710_03c_1\\0,1\P,0,-2.2226044954,-0.0541836924,-0.7991388257\Br,
0,-0.5695849417,-1.4457602023,-1.3727286589\Br,0,-2.7266578636,-0.8301
784041,1.2114817136\C,0,-1.252512256,1.4220337215,-0.3728022549\C,0,-1

.2986659381,2.4389725609,-1.3224154653\C,0,-0.4908990643,1.5883232686,
0.7809299679\C,0,-0.5777320981,3.606640085,-1.1284009579\H,0,-1.898521
2644,2.3206105652,-2.2146618814\C,0,0.2270005016,2.7543134323,0.969628
9854\H,0,-0.4737709055,0.8132819888,1.5332333423\C,0,0.1860280235,3.76
20687667,0.0151111069\H,0,-0.616813803,4.3919815077,-1.8682669626\H,0,
0.8203736001,2.8780187167,1.8631019357\H,0,0.748316141,4.6711441743,0.
1688697415\H,0,1.6294322785,-0.411305716,-0.0701916791\C,0,2.647125024
2,-0.5384268162,0.2719957901\Cl,0,3.6309533245,0.7165327913,-0.4674194
426\Cl,0,3.1642029307,-2.1398286447,-0.235006625\Cl,0,2.6475253028,-0.
3951862274,2.0272666666\\Version=AM64L-G03RevD.01\State=1-A\HF=-7141.0
361649\RMSD=1.544e-09\Thermal=0.\Dipole=-0.2439172,1.4525279,-0.152040
4\PG=C01 [X(C7H6Br2Cl3P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	154.7541

19*$CHCl_3$_4

1\1\GINC-NODE22\SP\RmPWPW91\6-311++G(2d,2p)\C7H6Br2Cl3P1\ZIP04\12-Aug-
2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76
=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read\
\nmr_0710_03c_4\\0,1\P,0,-0.5867280124,-0.487551853,-0.0063662765\Br,0
,-1.5212831779,-1.5523438046,1.7019700494\Br,0,-1.5214535202,-1.545747
656,-1.7186854164\C,0,-1.5549199504,1.044188801,-0.0033845963\C,0,-0.8
199585433,2.224153939,-0.000461235\C,0,-2.9471655624,1.0901663572,-0.0
038478457\C,0,-1.4737200938,3.4478871438,0.0020037821\H,0,0.2606843147
,2.1923706554,-0.0001002405\C,0,-3.5924155867,2.3101351558,-0.00139577
98\H,0,-3.5153410848,0.1713440124,-0.006133078\C,0,-2.8559534388,3.489
1208622,0.0015334611\H,0,-0.9008742291,4.3630236187,0.0042751204\H,0,-
4.6716344422,2.3472669618,-0.0017627442\H,0,-3.3667072534,4.4408123635
,0.0034437264\H,0,2.3983210105,-0.6278191284,-0.004202842\C,0,3.230097
4042,0.0621819313,-0.0015853806\Cl,0,3.0924141543,1.0518988557,-1.4505
010893\Cl,0,4.7177246374,-0.8700327217,-0.0021589802\Cl,0,3.0891065495
,1.0448709495,1.4517812725\\Version=AM64L-G03RevD.01\State=1-A\HF=-714
1.0363285\RMSD=3.392e-09\Thermal=0.\Dipole=-0.8233095,1.0207779,0.0013
266\PG=C01 [X(C7H6Br2Cl3P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	159.5320

	MPW1K/6-311++G(2d,2p) + PCM/UAHF/MPW1K/6-311++G(2d,2p)	MP2(FC)/6-31+G(2d,p)/MPW1K/6-31G(d) + PCM/UAHF/MPW1K/6-311++G(2d,2p)		
	Chemical shift, ppm (relative to PPh3)	E_{tot}	„G“$_{298,\ gas}$	„G“$_{298,CHCl3}$
19*$CHCl_3$_1	173.8	-7129.755150	-7129.689742	-7129.682571
19*$CHCl_3$_2	172.5	-7129.754516	-7129.688209	-7129.681245
19*$CHCl_3$_3	177.1	-7129.754901	-7129.689460	-7129.680807
19*$CHCl_3$_4	172.4	-7129.752551	-7129.688714	-7129.680395

<δ> = 173.8 ppm

20_1

1\1\GINC-GOLEM\SP\RmPWPW91\6-311++G(2d,2p)\C4H8N1O2P1\BORIS\30-Jul-201
0\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=05
72004280) geom=check guess=read\\nmr_0710_04_01\\0,1\P,0,0.0288493018,
0.1578898011,-0.1222154558\O,0,1.650054685,0.3489667522,0.1126896271\O
,0,-0.6644169873,1.6539399268,-0.0872997495\N,0,-0.2819187266,-0.13337
98152,1.5736967257\C,0,0.9961908854,-0.3068854805,2.24969475\H,0,0.922
6848896,0.0001502223,3.2904765004\H,0,1.2658031231,-1.36295736,2.23415
29831\C,0,2.0260694813,0.4948291852,1.4701943464\H,0,3.0372104961,0.11

21672792,1.581029833\H,0,2.0206716925,1.5506260068,1.7470332012\C,0,-1
.1682959816,0.9134724551,2.0626517288\H,0,-1.0053881161,1.0871885336,3
.1238699562\H,0,-2.2020272844,0.5922476608,1.934457388\C,0,-0.90876206
42,2.1495382779,1.2166010538\H,0,-1.7634901552,2.8188813616,1.16619371
37\H,0,-0.0438356648,2.7146254331,1.5686733612\\Version=AM64L-G03RevD.
01\State=1-A\HF=-703.8403963\RMSD=5.978e-09\Thermal=0.\Dipole=0.079047
,0.372692,1.5168498\PG=C01 [X(C4H8N1O2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	171.9077
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	169.3983

20_2

1\1\GINC-YANG\SP\RmPWPW91\6-311++G(2d,2p)\C4H8N1O2P1\BORIS\30-Jul-2010
\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=057
2004280) geom=check guess=read\\nmr_0710_04_02\\0,1\P,0,0.0690018167,0
.2338186004,-0.0966421956\O,0,1.6965243862,0.381001188,0.1563452261\O,
0,-0.5724239658,1.7526544097,-0.0791738953\N,0,-0.2870222559,-0.037344
9842,1.5931458372\C,0,0.9572197788,-0.5076349646,2.1836686591\H,0,0.93
28442872,-0.3987209511,3.2656307935\H,0,1.085344676,-1.5659350271,1.95
72508893\C,0,2.0667784561,0.3006921046,1.5214393389\H,0,2.1497340417,1
.3031617511,1.9441990745\H,0,3.0387621565,-0.1817021924,1.5785884489\C
,0,-0.7805954334,1.1978413697,2.1926908491\H,0,-1.518541678,0.98330458
24,2.9645674481\H,0,0.0320887023,1.7702385713,2.6509802172\C,0,-1.3795
956394,1.9977059096,1.0550865007\H,0,-2.4014074267,1.6797377642,0.8443
976345\H,0,-1.3828119025,3.0657818684,1.254725174\\Version=AM64L-G03Re
vD.01\State=1-A\HF=-703.8365432\RMSD=9.341e-09\Thermal=0.\Dipole=-0.02
9371,0.1857199,1.4275297\PG=C01 [X(C4H8N1O2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	152.5953
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	150.5037

	MPW1K/6-311++G(2d,2p) [+ PCM/UAHF/MPW1K/6-311++G(2d,2p)][a]		MP2(FC)/6-31+G(2d,p)/MPW1K/6-31G(d) + PCM/UAHF/MPW1K/6-311++G(2d,2p)		
	Chemical shift, ppm (relative to PPh_3)		E_{tot}	„G“$_{298,\ gas}$	„G“$_{298,CHCl3}$
	Gas-phase	Solution model 1			
20_1	160.4	163.3	-702.374270	-702.271149	-702.279882
20_2	179.7	182.2	-702.369998	-702.267031	-702.275763
[a]the theory shown in square brackets relates to solution model 1 and not to gas-phase calculations					

<δ> = 160.7 ppm (gas-phase)
<δ> = 163.5 ppm (solution model 1)

20_1*$CHCl_3$

1\1\GINC-NODE12\SP\RmPWPW91\6-311++G(2d,2p)\C5H9Cl3N1O2P1\ZIP04\31-Jul
-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/7
6=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read
\\nmr_0710_04c_03_2\\0,1\P,0,2.049379599,-0.0636211933,-1.16598967\O,0
,2.8035751106,-1.405640552,-0.5916917489\O,0,2.9829583075,1.233299604,
-0.7777166687\N,0,1.0459774226,0.1069122256,0.2768383948\C,0,1.2227720
54,-1.0961972175,1.0884075273\H,0,1.0709654882,-0.8708713996,2.1411195
861\H,0,0.473535545,-1.8313164177,0.7955767971\C,0,2.6092685317,-1.642
1225892,0.7916456917\H,0,2.6881676188,-2.7120032355,0.9627975699\H,0,3
.385754785,-1.1374958869,1.3680892986\C,0,1.3831809132,1.3827092023,0.
9057490584\H,0,1.2068714725,1.3364437157,1.9775257014\H,0,0.7359503774
,2.1579181865,0.4963139432\C,0,2.8279690434,1.6918322915,0.5532861602\
H,0,3.0486851072,2.7555250629,0.569368687\H,0,3.5331174633,1.179191015

,1.2090891717\H,0,-1.0338284919,0.1459882563,-0.1143331071\C,0,-2.1198
447926,0.0914269419,-0.0755878593\Cl,0,-2.7745611823,1.4689677386,-0.9
521424181\Cl,0,-2.6147506454,-1.4277162786,-0.8145677245\Cl,0,-2.58195
3727,0.1460785299,1.6263026091\\Version=AM64L-G03RevD.01\State=1-A\HF=
-2123.2450176\RMSD=1.775e-09\Thermal=0.\Dipole=0.7253044,0.1702286,1.8
041332\PG=C01 [X(C5H9Cl3N1O2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	170.1380

21_cation

1\1\GINC-NODE16\SP\RmPWPW91\6-311++G(2d,2p)\C15H21P2(1+)\ZIP04\02-Aug-
2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76
=0572004280) geom=check guess=read\\nmr_0710_05_01_2\\1,1\C,0,2.577005
3108,-0.7498690457,0.5259570279\C,0,1.2519673952,-0.5785772079,0.19852
37567\C,0,0.7366515313,0.7368700503,0.0052313631\C,0,1.6715254381,1.81
44655072,0.0332505806\C,0,3.0193551618,1.5816064385,0.3741547525\C,0,3
.4650694914,0.3244576974,0.650071104\H,0,2.9634737582,-1.748588205,0.6
667704553\C,0,-0.6411505196,1.0860632683,-0.2295416738\C,0,1.274363155
3,3.1268898218,-0.2989074417\H,0,3.6942389022,2.4244091381,0.405008597
6\H,0,4.4951880839,0.1478191153,0.9182919235\C,0,-0.013450822,3.406043
9086,-0.6341129597\C,0,-0.968170796,2.3852952675,-0.558736178\H,0,2.02
08301593,3.9077220725,-0.2888841126\H,0,-0.3168596547,4.4036148379,-0.
9096801799\H,0,-1.9928071267,2.6596141061,-0.745397689\P,0,0.213137676
,-2.0301563274,-0.1872512874\P,0,-2.0797813407,0.0258608918,0.06654956
47\C,0,-1.9884436137,-0.7930311166,1.6845193513\H,0,-2.5971811586,-0.2
334839845,2.3924306525\H,0,-2.3624041476,-1.8103339538,1.6138155959\H,
0,-0.9666440443,-0.8146184638,2.0487469585\C,0,-3.5114310982,1.1229280
324,0.299700339\H,0,-3.8093703624,1.6213540721,-0.6185467606\H,0,-4.34
25368302,0.4928206318,0.6156322852\H,0,-3.3263124572,1.8634690031,1.07
32509384\C,0,-2.6406683449,-1.0182017079,-1.3134939631\H,0,-3.56419668
95,-0.6038443598,-1.7135373407\H,0,-1.8902386364,-1.045900109,-2.09565
27527\H,0,-2.8144507144,-2.0327756979,-0.9690556252\C,0,0.7071853898,-
3.2901382433,1.0506716714\H,0,0.1595673864,-4.2082263993,0.8451469087\
H,0,1.7698148168,-3.5237425119,1.0247481212\H,0,0.4487954068,-2.964393
6527,2.0558230443\C,0,1.0222778086,-2.6665722721,-1.706435202\H,0,2.08
51204314,-2.8478675774,-1.5555164346\H,0,0.5470179395,-3.5988584979,-2
.0068816763\H,0,0.9075561142,-1.9508765269,-2.5176337151\\Version=AM64
L-G03RevD.01\State=1-A\HF=-1266.8363071\RMSD=6.901e-09\Thermal=0.\Dipo
le=-1.5147021,-0.0881009,0.1152469\PG=C01 [X(C15H21P2)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	391.4385
	329.7804

21_ionic_associate

1\1\GINC-NODE11\SP\RmPWPW91\Gen\C15H21I1P2\ZIP04\05-Aug-2010\0\\#p mpw
pw91/gen nmr scf=tight int=finegrid IOp(3/76=0572004280) geom=check gu
ess=read\\nmr_0710_05salz_01\\0,1\C,0,3.6465605128,1.5920831917,-0.688
3780302\C,0,2.5277196795,0.9625823887,-0.194941618\C,0,2.5171106177,-0
.4628136063,-0.0746280438\C,0,3.7516177448,-1.1404849517,-0.3169750726
\C,0,4.8693957902,-0.4406994448,-0.8155266437\C,0,4.8117511709,0.90082
09713,-1.0401468382\H,0,3.6488299641,2.6688297456,-0.7761624024\C,0,1.
3888354952,-1.2879335332,0.279411113\C,0,3.8905726773,-2.5183116956,-0
.0442826282\H,0,5.776165503,-0.9953292725,-1.0096249784\H,0,5.66299852
28,1.4356544728,-1.4332309743\C,0,2.8443414279,-3.2428733831,0.4305757
456\C,0,1.5920579673,-2.6241838495,0.5448604783\H,0,4.8518254324,-2.98
13405779,-0.2151030488\H,0,2.9477220769,-4.2912227967,0.6636303995\H,0
,0.7579890529,-3.2496055125,0.8177808706\P,0,1.1823138029,1.9870038655
,0.5271141302\P,0,-0.3830834858,-0.8434075819,0.2110925313\C,0,-0.7060
468426,0.212235277,-1.2242941786\H,0,-1.2884951151,-0.3659141663,-1.93
75688206\H,0,-1.3197137705,1.0574493316,-0.9295187327\H,0,0.2274995489
,0.5299375223,-1.6803674039\C,0,-1.3033234137,-2.3567005849,-0.1463742
323\H,0,-1.3220555833,-3.0418257008,0.6965566792\H,0,-2.3299208255,-2.

0182769198,-0.3304538218\H,0,-0.9128254725,-2.8571661292,-1.0289522262
\C,0,-1.0726253231,-0.3128801432,1.7874735983\H,0,-0.9600078237,-1.134
8539549,2.4924514439\H,0,-0.5920054422,0.5801073752,2.1624585243\H,0,-
2.1364056069,-0.1270279716,1.6007594949\C,0,0.9768202447,3.3539579511,
-0.682823723\H,0,0.2488387011,4.0543020698,-0.2763259216\H,0,1.8950551
325,3.9014138403,-0.8903142138\H,0,0.5762675721,2.9736926807,-1.619598
796\C,0,2.1133911568,2.8496824098,1.8592518404\H,0,2.9891964839,3.3816
476004,1.4894947595\H,0,1.4501328356,3.5632684416,2.3463509244\H,0,2.4
353157839,2.1276676438,2.6068341449\I,0,-4.2582232369,0.0909155149,-0.
2219957742\\Version=AM64L-G03RevD.01\State=1-A\HF=-8186.996332\RMSD=2.
720e-09\Thermal=0.\Dipole=6.7218369,-0.6512978,0.4144748\PG=C01 [X(C15
H21I1P2)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p);	388.6395
for I atom: MPW1K/6-311G(d,p)	304.9301

21_ionic_associate*CHCl$_3$_1

1\1\GINC-NODE18\SP\RmPWPW91\Gen\C16H22Cl3I1P2\ZIP04\17-Aug-2010\0\\#p
mpwpw91/gen nmr scf=tight int=finegrid IOp(3/76=0572004280) scrf=(PCM,
Read,solvent=chloroform) geom=check guess=read\\nmr_0710_05salz_c_01_1
\\0,1\C,0,-5.7127511324,-1.0818661218,-0.3382150474\C,0,-4.4130329004,
-0.75673382,-0.0275731551\C,0,-4.0436396072,0.6188609664,0.0996296452\
C,0,-5.1022556739,1.5778351917,0.0756238753\C,0,-6.4186541387,1.184896
7016,-0.2417371696\C,0,-6.7183079134,-0.1197623679,-0.4900966999\H,0,-
5.9870744302,-2.1223350898,-0.4328422515\C,0,-2.7094434374,1.137898218
4,0.2637513115\C,0,-4.8615103295,2.9325117276,0.3897620584\H,0,-7.1859
316951,1.9448466171,-0.2771689861\H,0,-7.723043013,-0.4200559317,-0.74
59970222\C,0,-3.6102678116,3.3649990656,0.6955578923\C,0,-2.5399514016
,2.4673582486,0.5827716082\H,0,-5.6979604285,3.616554641,0.3892365483\
H,0,-3.4213769119,4.3934495197,0.9611742885\H,0,-1.5472928953,2.865608
2424,0.7166525862\P,0,-3.2581334764,-2.0981120311,0.4721156712\P,0,-1.
1361415515,0.3047386562,-0.1438645204\C,0,-1.3359536462,-0.7470910524,
-1.6051344078\H,0,-0.7659145208,-0.3026173868,-2.4173968601\H,0,-0.910
8339026,-1.7271614075,-1.4154293205\H,0,-2.3830667683,-0.8190511845,-1
.8855655504\C,0,0.0169826649,1.5860605946,-0.6813814139\H,0,0.36877546
67,2.2031121545,0.1404610533\H,0,0.8780671946,1.0423804906,-1.08297277
24\H,0,-0.4213389322,2.2075716421,-1.458172168\C,0,-0.3014792102,-0.44
8869951,1.2620739666\H,0,-0.0735387922,0.3375186671,1.9788889177\H,0,-
0.9019064104,-1.2227359398,1.7203584691\H,0,0.6326606651,-0.8671748548
,0.8751111819\C,0,-3.6009451036,-3.4394826149,-0.735562963\H,0,-3.0037
886741,-4.3053782018,-0.454038354\H,0,-4.6453532091,-3.7458578371,-0.7
694830769\H,0,-3.2915475505,-3.139128813,-1.7340313575\C,0,-4.14090727
56,-2.7402817179,1.9534029588\H,0,-5.1721812737,-3.0204463535,1.741678
95\H,0,-3.6098755299,-3.6134573041,2.3301241123\H,0,-4.1398187801,-1.9
843257851,2.7359226334\I,0,2.3542879789,-1.4030437655,-1.363737723\H,0
,3.7409444703,0.5161797857,-0.0198096303\C,0,4.099460446,1.3747389006,
0.5482486697\Cl,0,3.8207702121,2.8204774405,-0.4218954174\Cl,0,5.80558
64146,1.1615095692,0.8909964508\Cl,0,3.1626049067,1.4510582964,2.04805
12423\\Version=AM64L-G03RevD.01\State=1-A\HF=-9606.4165937\RMSD=8.695e
-10\Thermal=0.\Dipole=-7.5358852,1.6705407,1.4612135\PG=C01 [X(C16H22C
l3I1P2)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) +	385.9969
PCM(CHCl$_3$,UAHF); for I atom: MPW1K/6-311G(d,p)	307.2375

21_ionic_associate*CHCl$_3$_2

1\1\GINC-NODE27\SP\RmPWPW91\Gen\C16H22Cl3I1P2\ZIP04\13-Aug-2010\0\\#p
mpwpw91/gen nmr scf=tight int=finegrid IOp(3/76=0572004280) scrf=(PCM,
Read,solvent=chloroform) geom=check guess=read\\nmr_0710_05salz_c_02_1
\\0,1\C,0,3.7337653287,1.5621894153,-0.5737837288\C,0,2.5929358619,0.9
404482831,-0.1210634208\C,0,2.5765361588,-0.4823707999,0.0274451088\C,

0,3.8212348592,-1.1639979696,-0.1438331973\C,0,4.9614731936,-0.4739455
454,-0.6041037452\C,0,4.9158385646,0.8649058439,-0.8560315288\H,0,3.74
04508798,2.6369183974,-0.682485562\C,0,1.4325136551,-1.3007919226,0.34
65089946\C,0,3.9486231957,-2.5363565204,0.1614190741\H,0,5.8768527874,
-1.0310451417,-0.74299293\H,0,3.7958703463,0.2572111411,-3.229474615\C
,0,2.8820162291,-3.2506595895,0.6035839499\C,0,1.6256374427,-2.6304293
739,0.6483335971\H,0,4.916162209,-3.0021103402,0.0418491647\H,0,2.9738
384595,-4.2941777257,0.8616082674\H,0,0.7806921728,-3.2521282719,0.894
2870892\P,0,1.2142591944,1.9817707758,0.5151805595\P,0,-0.3369986211,-
0.8630740865,0.1813713712\C,0,-0.5908430927,0.1570732268,-1.2919546084
\H,0,-1.1385539833,-0.439366506,-2.017516126\H,0,-1.2194250634,1.00760
06345,-1.0482158611\H,0,0.3607477884,0.4657225284,-1.7153319021\C,0,-1
.2317037386,-2.3899051587,-0.1782380749\H,0,-1.2835180322,-3.053947555
1,0.6798887349\H,0,-2.2511573814,-2.0608821487,-0.4140187296\H,0,-0.80
13222329,-2.9078213579,-1.0316520922\C,0,-1.1028481867,-0.2938921704,1
.7086533569\H,0,-1.0206599419,-1.0944855442,2.4418996384\H,0,-0.646133
5481,0.612520397,2.0809206339\H,0,-2.1575792143,-0.1199411686,1.467233
4029\C,0,1.0757906556,3.3254287459,-0.728413511\H,0,0.3292472245,4.033
786204,-0.3724758239\H,0,2.003960229,3.8687977949,-0.8990389671\H,0,0.
7232678873,2.9275882723,-1.6770529768\C,0,2.0887656994,2.8607898528,1.
8748764881\H,0,2.9855172809,3.3786504107,1.5367394807\H,0,1.4096662677
,3.5885817437,2.3169602128\H,0,2.3686693125,2.1503267956,2.6499622179\
I,0,-4.1877705978,0.0058793819,-0.4908860548\H,0,5.7867294652,1.393266
4665,-1.2143219889\C,0,3.3811851337,0.0647037869,-4.2088993183\Cl,0,2.
1221693054,1.2581033005,-4.4989286055\Cl,0,2.7232181331,-1.5659093062,
-4.1975591034\Cl,0,4.6861150931,0.2185276041,-5.376233351\\Version=AM6
4L-G03RevD.01\State=1-A\HF=-9606.4100005\RMSD=3.356e-09\Thermal=0.\Dip
ole=7.6731613,-0.687633,1.488896\PG=C01 [X(C16H22Cl3I1P2)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF); for I atom: MPW1K/6-311G(d,p)	387.0484
	305.5388

	MPW1K/6-311++G(2d,2p) + PCM/UAHF/MPW1K/6-311++G(2d,2p)	MP2(FC)/6-31+G(2d,p)/MPW1K/6-31G(d) + PCM/UAHF/MPW1K/6-311++G(2d,2p)		
	Chemical shift, ppm (relative to PPh_3)	E_{tot}	„G“$_{298,\ gas}$	„G“$_{298,CHCl3}$
21_ia*$CHCl_3$_1	-54.1	-9598.694016	-9598.407812	-9598.407541
	24.7			
21_ia*$CHCl_3$_2	-55.2	-9598.687798	-9598.403959	-9598.404373
	26.4			

$<\delta_1>$ = -54.1 ppm
$<\delta_2>$ = 24.7 ppm

22_1

1\1\GINC-YANG\SP\RmPWPW91\6-311++G(2d,2p)\C14H31N2P1\BORIS\31-Jul-2010
\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=057
2004280) geom=check guess=read\\nmr_0710_06_3\\0,1\P,0,0.2851832047,-0
.3491969647,0.2665829119\C,0,1.4501968033,-0.3810713298,-1.1256174138\
H,0,1.7086370438,-1.3781968929,-1.4662437882\C,0,2.1086001723,0.655489
7287,-1.6280631458\H,0,2.876578135,0.531808815,-2.3792972479\H,0,1.909
9091757,1.6619140554,-1.2917143308\N,0,-0.292664825,1.2551158888,0.257
111616\N,0,-0.8911387556,-1.4300451343,-0.3364113568\C,0,-0.1057733056
,2.0606898811,1.4679102371\H,0,-0.6078506028,3.0080461662,1.2737094395
\C,0,-1.1653445095,1.8019062018,-0.7756525891\H,0,-1.1658176276,1.0729
305463,-1.5833652224\C,0,-1.4507349567,-2.423898961,0.5849731395\H,0,-
2.1298809057,-3.0330500964,-0.0107637421\C,0,-1.2134454888,-1.60844187
82,-1.7513843938\H,0,-0.6530171664,-0.842926175,-2.28683528\C,0,-0.663

9382364,3.1143359019,-1.3679248442\H,0,-1.3424950028,3.4515792357,-2.1
513976004\H,0,-0.6151884634,3.9069678411,-0.6220546723\H,0,0.323616653
9,2.9984920824,-1.8059415625\C,0,-2.6023458794,1.9559797186,-0.2889996
083\H,0,-3.256925043,2.263934364,-1.1046165376\H,0,-2.9724075816,1.017
4187113,0.1170262278\H,0,-2.6777234016,2.7139753544,0.4908867891\C,0,-
0.3951225667,-3.3595093249,1.1592999595\H,0,-0.8578473879,-4.129398489
,1.7770984583\H,0,0.1631187144,-3.8506172637,0.3642873523\H,0,0.311502
4235,-2.8087293795,1.7780245356\C,0,-2.2819299425,-1.7947898305,1.6904
140827\H,0,-2.75538611,-2.5650676753,2.2994061882\H,0,-1.66088336,-1.1
882885296,2.3460362069\H,0,-3.0613446913,-1.158522798,1.2749598344\C,0
,-2.691600853,-1.3928520521,-2.0520882041\H,0,-2.8772057684,-1.4773755
73,-3.1228429515\H,0,-3.3146162395,-2.1369589037,-1.556071322\H,0,-3.0
20457769,-0.4097075107,-1.7252526609\C,0,-0.7520343404,-2.9545217629,-
2.3021773641\H,0,-0.9266596888,-3.0003193141,-3.3768325685\H,0,0.31015
00033,-3.1102385688,-2.125244653\H,0,-1.2929036129,-3.7857690342,-1.85
05532524\C,0,1.3632928323,2.3735027204,1.7119371765\H,0,1.8004961193,2
.8781985908,0.8523328685\H,0,1.4851309026,3.0157783848,2.5845202057\H,
0,1.9253488467,1.4566526104,1.8885148175\C,0,-0.7454658987,1.471441947
9,2.7169176343\H,0,-0.6704675158,2.174338314,3.5469248158\H,0,-1.79797
78238,1.2502702188,2.5520400754\H,0,-0.2428657103,0.5523261623,3.01353
174\\Version=AM64L-G03RevD.01\State=1-A\HF=-1003.0646086\RMSD=3.629e-0
9\Thermal=0.\Dipole=-0.4399094,0.0801857,-0.3924497\PG=C01 [X(C14H31N2
P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	265.7888
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	266.4206

22_2

1\1\GINC-NAUTILUS\SP\RmPWPW91\6-311++G(2d,2p)\C14H31N2P1\BORIS\02-Aug-
2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76
=0572004280) geom=check guess=read\\nmr_0710_06_2\\0,1\P,0,0.030417991
6,0.4577548513,0.763059004\C,0,-0.0211210893,-0.8118666988,2.072916460
5\H,0,0.203244241,-1.8494447438,1.8466122699\C,0,-0.2578996325,-0.4757
182383,3.3353249505\H,0,-0.2573327926,-1.2053057017,4.1342911693\H,0,-
0.4612344832,0.5488162545,3.6178476785\N,0,1.3967417054,-0.0294192195,
-0.1335441608\N,0,-1.3764803061,0.0737239751,-0.1218046341\C,0,2.55096
81128,0.8701326007,-0.1733010039\H,0,3.3022461444,0.3634372241,-0.7791
392024\C,0,1.5628851723,-1.3479123188,-0.7256659406\H,0,0.6248204385,-
1.8750893139,-0.5603890896\C,0,-2.184176172,1.1858699304,-0.6308401847
\H,0,-3.0569125899,0.7298877687,-1.0973516682\C,0,-1.976398039,-1.2534
925179,-0.2160828484\H,0,-1.2654920672,-1.9466156391,0.2282720986\C,0,
2.6643169651,-2.1729098122,-0.0677447859\H,0,2.693604023,-3.1772689419
,-0.4904514348\H,0,3.6463899961,-1.7269120512,-0.2230472\H,0,2.5008128
79,-2.2560894615,1.0049495675\C,0,1.7611477799,-1.2751935089,-2.235266
6407\H,0,1.7757553724,-2.2743751824,-2.6707573249\H,0,0.9564633898,-0.
7063826128,-2.6962141071\H,0,2.7044119856,-0.794734211,-2.4946521624\C
,0,-2.6971533218,2.1071058811,0.4683148122\H,0,-3.3605306502,2.8659736
971,0.052720296\H,0,-3.2479961676,1.5450773788,1.2202987772\H,0,-1.871
1392902,2.614990019,0.9630175382\C,0,-1.4667428298,1.9741108997,-1.715
1620541\H,0,-2.1340505283,2.7144873526,-2.1570686993\H,0,-0.6074105047
,2.5033889244,-1.3078392542\H,0,-1.1136522358,1.3118020341,-2.50338688
58\C,0,-2.1882451406,-1.7019545948,-1.657079618\H,0,-2.5510950129,-2.7
293807686,-1.6848765184\H,0,-2.9255178777,-1.085127559,-2.1699758139\H
,0,-1.2583259093,-1.650395758,-2.21929361\C,0,-3.2596208643,-1.3781040
103,0.5972018744\H,0,-3.6374845212,-2.3999071757,0.5584054936\H,0,-3.0
744506216,-1.1194035821,1.6376446513\H,0,-4.045417589,-0.7264044919,0.
2161344355\C,0,3.1638328664,1.1029692197,1.202149104\H,0,3.4164036614,
0.1591200202,1.6816797416\H,0,4.0706767235,1.7036957217,1.1261481036\H
,0,2.4642222416,1.6320846632,1.8484435248\C,0,2.2462437631,2.190676533
4,-0.862929253\H,0,3.1520445573,2.7899646042,-0.9572235258\H,0,1.83905
80421,2.0213130194,-1.8577340476\H,0,1.5228272321,2.7679306312,-0.2892
560499\\Version=AM64L-G03RevD.01\State=1-A\HF=-1003.0633391\RMSD=5.333
e-09\Thermal=0.\Dipole=-0.0489268,-0.5243259,-0.2248928\PG=C01 [X(C14H

31N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	281.5945
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	281.4732

22_3

1\1\GINC-YIN\SP\RmPWPW91\6-311++G(2d,2p)\C14H31N2P1\BORIS\31-Jul-2010\
0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0572
004280) geom=check guess=read\\nmr_0710_06_1\\0,1\P,0,0.1087497347,0.5
264104878,-0.2012812175\C,0,1.3925637193,-0.5269339807,-0.9628826189\H
,0,1.1954966278,-1.5812721755,-1.1230699573\C,0,2.5327798277,0.0015869
775,-1.3904305975\H,0,3.2848170349,-0.5845652272,-1.9018495402\H,0,2.7
562625338,1.0505425073,-1.2437349682\N,0,-1.2113745668,0.2914271809,-1
.2487001671\N,0,-0.3591545616,-0.5047297467,1.1364792215\C,0,-1.718082
6179,1.4507919181,-1.9849784983\H,0,-2.4903425311,1.0647325194,-2.6502
446844\C,0,-1.6237293492,-1.035583603,-1.6955366134\H,0,-1.133538972,-
1.7312158088,-1.0151308499\C,0,0.6666138218,-0.9112188521,2.1072893463
\H,0,0.1328908475,-1.0466415761,3.0472925603\C,0,-1.6349239909,-0.1128
972454,1.7432896282\H,0,-2.2474949534,0.2388380518,0.9152322576\C,0,-1
.1800366584,-1.3548475482,-3.1184887273\H,0,-1.4231806574,-2.386999566
,-3.3714906701\H,0,-1.6834727929,-0.7157725701,-3.8443755989\H,0,-0.10
73953282,-1.216437943,-3.2358643744\C,0,-3.1236214907,-1.2563132224,-1
.5409747186\H,0,-3.3795984297,-2.2849873051,-1.7941828725\H,0,-3.44429
1298,-1.0692162811,-0.518840591\H,0,-3.7008983346,-0.6095195287,-2.201
2596456\C,0,1.2749041452,-2.2670605731,1.7734942301\H,0,1.8560157461,-
2.6363752515,2.6192655185\H,0,0.4916187881,-2.9894071692,1.5525534086\
H,0,1.9435442859,-2.2108023831,0.9179474981\C,0,1.7559969375,0.1222035
227,2.3826820811\H,0,2.383040482,-0.2140740516,3.2085700422\H,0,2.4037
771097,0.2642660752,1.5197870524\H,0,1.3316099356,1.087337221,2.650781
1173\C,0,-1.5439693184,1.0291505979,2.7510630125\H,0,-2.541038273,1.32
9272972,3.0732362448\H,0,-0.9871318146,0.743756844,3.6437398956\H,0,-1
.0574939767,1.898505503,2.3109948074\C,0,-2.35038124,-1.3183861694,2.3
360525407\H,0,-3.3500068706,-1.0382655688,2.6682581132\H,0,-2.44064738
85,-2.1103915598,1.595404478\H,0,-1.8268144636,-1.72547764,3.201122454
4\C,0,-0.6654391066,2.1207042185,-2.8600770278\H,0,-0.1859430247,1.398
5997886,-3.5179994865\H,0,-1.1163161233,2.8994000206,-3.4758771853\H,0
,0.106430866,2.5840037147,-2.2467134829\C,0,-2.3826640373,2.4605757418
,-1.0621410173\H,0,-2.7913590261,3.29442973,-1.6329124945\H,0,-3.19463
76193,1.9986356922,-0.5030716331\H,0,-1.6627336279,2.8633212618,-0.350
4262703\\Version=AM64L-G03RevD.01\State=1-A\HF=-1003.0594558\RMSD=3.67
0e-09\Thermal=0.\Dipole=-0.1567893,-0.2717431,-0.1455554\PG=C01 [X(C14
H31N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	245.3870
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	245.5205

22_4

1\1\GINC-SOLARIS\SP\RmPWPW91\6-311++G(2d,2p)\C14H31N2P1\BORIS\01-Aug-2
010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=
0572004280) geom=check guess=read\\nmr_0710_06_10\\0,1\P,0,-0.19775767
49,0.8066476714,-0.4039054515\C,0,1.3850494209,0.2346088091,-1.1097540
102\H,0,1.534087762,-0.8133470769,-1.350277881\C,0,2.339644715,1.10085
61103,-1.4288482165\H,0,3.266656631,0.7894162747,-1.8916489591\H,0,2.2
278157915,2.1600698544,-1.2382143005\N,0,-1.3284645122,-0.1919893164,-
1.2126572011\N,0,-0.0563560071,0.2713705373,1.2086336876\C,0,-2.220243
984,0.5380528224,-2.1147250306\H,0,-2.2694171028,1.5405836072,-1.68588
84873\C,0,-1.235161625,-1.6455573912,-1.1747831636\H,0,-0.3488518803,-
1.8521126141,-0.5747251384\C,0,0.8182959627,-0.7965443342,1.6806801994
\H,0,1.2086200264,-1.289475576,0.7924091672\C,0,-0.6878657231,1.108205
8721,2.2329624725\H,0,-0.4911145826,0.6171017144,3.1856713553\C,0,-1.0
003850196,-2.3127942653,-2.525269989\H,0,-0.7810838089,-3.3708856621,-

2.3804302314\H,0,-1.8780881427,-2.251490616,-3.1664755476\H,0,-0.16283
20054,-1.8584212067,-3.0506758888\C,0,-2.388120824,-2.3229898896,-0.43
62867766\H,0,-2.1243452811,-3.3558479426,-0.2056069179\H,0,-2.59656912
62,-1.8049462778,0.4967130467\H,0,-3.3020738563,-2.345903258,-1.023996
0684\C,0,2.0247507768,-0.2673702381,2.4467631771\H,0,2.6897380479,-1.0
851194559,2.7246669106\H,0,2.5835232836,0.436603438,1.8335452892\H,0,1
.7277529253,0.2377631122,3.3656782263\C,0,0.0784677167,-1.858254457,2.
4857468481\H,0,0.7528781514,-2.6758767097,2.7400500936\H,0,-0.31284152
06,-1.4611949317,3.421977614\H,0,-0.7552505144,-2.2656912439,1.9188774
405\C,0,-2.1991792005,1.1693108827,2.0684761856\H,0,-2.6519788413,1.73
50991532,2.8828940935\H,0,-2.4683819278,1.6595120111,1.1330749547\H,0,
-2.6284120178,0.1694020221,2.0611229372\C,0,-0.0916107697,2.5080950767
,2.3160557461\H,0,-0.5298062038,3.0620710671,3.1466149302\H,0,0.985448
4848,2.4633738434,2.4647010338\H,0,-0.2834700261,3.0644966012,1.400292
6714\C,0,-3.6492549459,0.0184495053,-2.1512691314\H,0,-4.0601251354,-0
.0787457104,-1.1489635932\H,0,-4.2706823878,0.7204412552,-2.7066096028
\H,0,-3.7272970672,-0.9441463411,-2.6539885005\C,0,-1.6710851444,0.713
2951613,-3.5292022792\H,0,-2.2854727568,1.4228357476,-4.0847007942\H,0
,-0.6540927385,1.1005598388,-3.4980738089\H,0,-1.6609573419,-0.2201174
746,-4.0876311112\\Version=AM64L-G03RevD.01\State=1-A\HF=-1003.0586236
\RMSD=2.107e-09\Thermal=0.\Dipole=0.1077047,-0.4891426,0.1272784\PG=C0
1 [X(C14H31N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	246.6964
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	246.3052

22_5

1\1\GINC-YIN\SP\RmPWPW91\6-311++G(2d,2p)\C14H31N2P1\BORIS\01-Aug-2010\
0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0572
004280) geom=check guess=read\\nmr_0710_06_15\\0,1\P,0,-0.0575078604,0
.8264464644,-0.2778406869\C,0,1.5361475087,0.2199449462,-0.9225203272\
H,0,1.6441021102,-0.7965850505,-1.2866910716\C,0,2.570508608,1.0448432
376,-1.0352015548\H,0,3.514438197,0.7270383664,-1.4578305916\H,0,2.510
1237887,2.0742636496,-0.7080006179\N,0,-1.1448074176,0.1717389342,-1.4
202592793\N,0,-0.1849422091,-0.0349072988,1.1954933773\C,0,-2.01574942
45,1.099536154,-2.1440603416\H,0,-2.6016356705,0.4873127378,-2.8297094
634\C,0,-1.1729106874,-1.2255827927,-1.8269339059\H,0,-0.4580379584,-1
.7429705682,-1.1880516311\C,0,0.4743502525,-1.3152116888,1.4463734487\
H,0,0.7601512285,-1.6923149116,0.466673335\C,0,-1.0117282862,0.6369154
463,2.1993961318\H,0,-1.1225060752,1.651341882,1.8111142843\C,0,-0.722
7359192,-1.4360246036,-3.268751661\H,0,-0.6784731713,-2.4991015493,-3.
5059827849\H,0,-1.4123434459,-0.9741430476,-3.9750391336\H,0,0.2628759
356,-1.0046263436,-3.4329846019\C,0,-2.5271208323,-1.8767189408,-1.572
282499\H,0,-2.4882368771,-2.9425228909,-1.7970476947\H,0,-2.8184044706
,-1.7539157012,-0.5314691301\H,0,-3.3082702561,-1.4422960146,-2.195784
3558\C,0,1.7804727515,-1.1904369458,2.2282997202\H,0,2.3222618997,-2.1
366960148,2.1974164895\H,0,2.4122489532,-0.4228749883,1.787509255\H,0,
1.6164234388,-0.9424800407,3.2736306716\C,0,-0.4180915244,-2.390020033
2,2.0525092646\H,0,0.1147347082,-3.3408909054,2.0562720222\H,0,-0.6865
855458,-2.1699354594,3.0838411184\H,0,-1.3334316267,-2.5161896124,1.47
82855749\C,0,-0.363348478,0.7823415647,3.5690779731\H,0,-0.9762218127,
1.4366877788,4.1887550843\H,0,-0.2800410882,-0.1681702856,4.0932006653
\H,0,0.6282797432,1.2222067889,3.489412318\C,0,-2.4287957316,0.0815772
49,2.3262946207\H,0,-3.0504162524,0.7779001518,2.8901933072\H,0,-2.874
0957243,-0.0479467013,1.342662765\H,0,-2.4594866872,-0.8743560254,2.84
37309439\C,0,-1.2373741639,2.0989563737,-2.9906439411\H,0,-0.546727624
4,1.5861916133,-3.6574761878\H,0,-1.9140436582,2.7041283786,-3.5946901
037\H,0,-0.6590634695,2.7712643025,-2.3581797257\C,0,-3.0017377493,1.8
094366925,-1.2285612158\H,0,-3.6693281674,2.4503674787,-1.8048367151\H
,0,-3.6070416237,1.0904410775,-0.6797405031\H,0,-2.4762776342,2.435037
1459,-0.5082726464\\Version=AM64L-G03RevD.01\State=1-A\HF=-1003.058400
9\RMSD=2.147e-09\Thermal=0.\Dipole=-0.0294429,-0.5226057,-0.0812585\PG
=C01 [X(C14H31N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	252.3767
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	251.9034

22_6

1\1\GINC-YANG\SP\RmPWPW91\6-311++G(2d,2p)\C14H31N2P1\BORIS\01-Aug-2010
\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=057
2004280) geom=check guess=read\\nmr_0710_06_9\\0,1\P,0,0.2352946753,-0
.6257022747,-0.3804869252\C,0,1.1930915017,0.3422087212,-1.5682144267\
H,0,1.1296213013,-0.0218921522,-2.5851853194\C,0,2.093068214,1.2754885
056,-1.2823157354\H,0,2.7337291744,1.6954838283,-2.0454578931\H,0,2.23
12957477,1.6370377176,-0.2751772327\N,0,0.2283516397,0.3499787172,1.01
89404816\N,0,-1.2935480638,-0.7386858581,-1.1545590743\C,0,0.529926195
5,-0.3268542715,2.2875197677\H,0,0.3655981097,0.4176128379,3.065064418
3\C,0,-0.2815858554,1.7137064623,1.1168561925\H,0,-0.3471270767,2.0785
873083,0.0958864546\C,0,-1.9157728198,0.0740715706,-2.2035108061\H,0,-
2.9621653682,-0.233260011,-2.2112073422\C,0,-2.0460845175,-1.940398313
2,-0.7764438856\H,0,-1.412966299,-2.4617983859,-0.0591534598\C,0,0.653
7053529,2.6627147418,1.8610706835\H,0,0.2859161542,3.6844780807,1.7698
660631\H,0,0.7103378582,2.437942987,2.9255817671\H,0,1.6636265182,2.63
21122619,1.4597400175\C,0,-1.6741034787,1.771775892,1.7341206465\H,0,-
2.0624113447,2.7905410166,1.7217980684\H,0,-2.3659365653,1.1337549746,
1.1899264293\H,0,-1.657948064,1.4419546382,2.7734027915\C,0,-1.9198828
889,1.5686416746,-1.9368053301\H,0,-2.4850343389,2.0752576363,-2.71927
70989\H,0,-2.3828815589,1.8027289903,-0.9820121925\H,0,-0.9101243891,1
.9739576437,-1.9505312713\C,0,-1.3873904306,-0.1908973048,-3.614994590
1\H,0,-2.1042587665,0.1746083835,-4.35113658\H,0,-0.4498343018,0.32829
54106,-3.8006385427\H,0,-1.2316636781,-1.2509976706,-3.7940038739\C,0,
-2.2792287311,-2.9056432126,-1.9312109865\H,0,-2.7496626727,-3.8177696
192,-1.5645356642\H,0,-2.9376771173,-2.4846055158,-2.6907459446\H,0,-1
.3371124765,-3.1772118549,-2.4040011341\C,0,-3.3540746367,-1.621665991
7,-0.0632133584\H,0,-3.8258482797,-2.5391469331,0.2881541777\H,0,-3.17
78839784,-0.9794684797,0.7964447102\H,0,-4.0700539937,-1.12298755,-0.7
166777218\C,0,1.990606868,-0.7451455725,2.3629842359\H,0,2.6452742196,
0.1093465685,2.2020206813\H,0,2.2224132843,-1.1782558202,3.3364992455\
H,0,2.212158665,-1.4898653446,1.5995083212\C,0,-0.3875003262,-1.498488
1664,2.6092384938\H,0,-0.2041224691,-1.8534204506,3.6237519468\H,0,-1.
4342688906,-1.209663099,2.5348723613\H,0,-0.2104621016,-2.331462717,1.
9310484343\\Version=AM64L-G03RevD.01\State=1-A\HF=-1003.0570924\RMSD=3
.909e-09\Thermal=0.\Dipole=-0.4625851,0.3449148,0.038572\PG=C01 [X(C14
H31N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	247.6572
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	248.4291

22_7

1\1\GINC-GOLEM\SP\RmPWPW91\6-311++G(2d,2p)\C14H31N2P1\BORIS\31-Jul-201
0\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=05
72004280) geom=check guess=read\\nmr_0710_06_6\\0,1\P,0,0.40567308,-0.
4072199293,-0.4343656173\C,0,1.6419676596,0.9116615014,-0.2374531614\H
,0,2.2832391147,0.8115196728,0.6316252954\C,0,1.9363376232,1.834051909
,-1.1449107497\H,0,2.7760753213,2.5047012829,-1.0248292661\H,0,1.35263
25994,1.9387351164,-2.0481909856\N,0,-0.0955816578,-0.5671250924,1.187
595611\N,0,-0.8029120611,0.3285211528,-1.4013637325\C,0,-0.2871514423,
-1.9238868171,1.7098027081\H,0,-0.6315942513,-1.8020592581,2.736344532
9\C,0,-0.1490308791,0.5156370645,2.1679542913\H,0,0.0973186011,1.42710
13553,1.6236884764\C,0,-1.6397034538,1.4139908382,-0.893511609\H,0,-1.
2779445265,1.5873342131,0.1164487777\C,0,-1.0883712438,-0.3908196293,-
2.6478155394\H,0,-0.1965860678,-0.99732906,-2.808173161\C,0,0.89027179
84,0.3716909053,3.2750578696\H,0,0.8707441327,1.2466951406,3.924261860
8\H,0,0.698545418,-0.5000849814,3.8999031252\H,0,1.8936211689,0.276417

9245,2.8649758577\C,0,-1.5384671748,0.6981561813,2.7684346077\H,0,-1.5
591934042,1.572473553,3.4189782349\H,0,-2.2884008232,0.8297749367,1.99
21270202\H,0,-1.8307369571,-0.1608328651,3.3723337699\C,0,-1.497295113
1,2.7550183057,-1.6110753494\H,0,-2.0390934991,3.5178013418,-1.0506006
413\H,0,-0.457274929,3.0611478379,-1.6681240931\H,0,-1.909972404,2.739
9443841,-2.6159716525\C,0,-3.1160876622,1.0575538808,-0.7604517955\H,0
,-3.6261339249,1.8200307586,-0.171311946\H,0,-3.6123328703,1.017996717
9,-1.728742992\H,0,-3.2484705632,0.0973504031,-0.2668370959\C,0,-1.213
4684799,0.5100411472,-3.868194483\H,0,-1.1868152486,-0.0995456486,-4.7
711618579\H,0,-2.1546142666,1.057170354,-3.8806140498\H,0,-0.396538394
8,1.2269721607,-3.9182741218\C,0,-2.2560915751,-1.3740087226,-2.599183
2552\H,0,-2.2175955974,-2.0258463875,-3.4725505692\H,0,-2.2017465948,-
1.9996129416,-1.712376972\H,0,-3.2239751536,-0.8790507781,-2.607485057
9\C,0,1.0057522272,-2.7280903781,1.7525403199\H,0,1.772887634,-2.20858
94264,2.3234117842\H,0,0.8395156726,-3.7023328177,2.2130028796\H,0,1.3
850207789,-2.8910761249,0.7447289315\C,0,-1.3713839736,-2.6911252349,0
.9716235631\H,0,-1.5760483071,-3.6381984301,1.4709363627\H,0,-2.294835
7748,-2.1165036217,0.929651265\H,0,-1.0573545553,-2.9163518943,-0.0464
573905\\Version=AM64L-G03RevD.01\State=1-A\HF=-1003.0576962\RMSD=4.152
e-09\Thermal=0.\Dipole=-0.3135244,0.2724444,0.3693203\PG=C01 [X(C14H31
N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	231.8476
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	232.4019

22_8

1\1\GINC-SOLARIS\SP\RmPWPW91\6-311++G(2d,2p)\C14H31N2P1\BORIS\02-Aug-2
010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=
0572004280) geom=check guess=read\\nmr_0710_06_5\\0,1\P,0,0.179268975,
0.5803774661,-0.8097703128\C,0,0.2131568156,2.2790223495,-0.1410607539
\H,0,0.1107771981,2.4479049924,0.9266961885\C,0,0.4499011238,3.3091042
991,-0.9445726082\H,0,0.5469127132,4.3204087621,-0.5725058055\H,0,0.55
81316152,3.1748205164,-2.0128258508\N,0,1.3862405379,-0.2041316798,0.0
993645349\N,0,-1.2656816367,-0.0139960349,-0.035283656\C,0,2.570038218
1,-0.7024579672,-0.6015055823\H,0,3.2318220552,-1.0919691642,0.1720098
458\C,0,1.4213442408,-0.1564145641,1.5551165467\H,0,0.4528741175,0.245
2754566,1.8514164713\C,0,-2.3662043456,0.9023726808,0.2525546762\H,0,-
1.9668367741,1.89940901,0.0736803991\C,0,-1.487317379,-1.4290958973,-0
.3354528358\H,0,-0.4885088497,-1.8660711515,-0.2839482288\C,0,2.510657
204,0.7600537237,2.0995976353\H,0,2.4361783358,0.8405738042,3.18426016
23\H,0,3.5056126902,0.3775344139,1.8704688288\H,0,2.4296858688,1.75883
23727,1.6752238922\C,0,1.5194796638,-1.5460871352,2.1714714415\H,0,1.4
583180839,-1.4841995559,3.2579145708\H,0,0.7095136665,-2.1812531285,1.
8195339657\H,0,2.4633108559,-2.0336807788,1.9281121791\C,0,-3.58580607
32,0.7937029065,-0.6564199612\H,0,-4.2681525638,1.6165795155,-0.443646
416\H,0,-3.3037687933,0.8532958663,-1.70552601\H,0,-4.1390440516,-0.13
05853711,-0.5010814565\C,0,-2.7817911011,0.8834110723,1.721362466\H,0,
-3.4659288113,1.7076500796,1.9270963888\H,0,-3.2862372068,-0.038530809
2,1.9995531147\H,0,-1.9113836492,0.9966285948,2.3651919198\C,0,-2.0107
399984,-1.7375114224,-1.7392736659\H,0,-1.8798987815,-2.798313213,-1.9
556489259\H,0,-3.0675347072,-1.5088701247,-1.8518353099\H,0,-1.4573314
514,-1.1740704259,-2.4887648677\C,0,-2.3081401776,-2.1531808371,0.7202
221742\H,0,-2.2798983703,-3.2253308552,0.5271078105\H,0,-1.9102916915,
-1.9751331511,1.717095945\H,0,-3.3546671841,-1.8534806046,0.7092884728
\C,0,3.3347552382,0.3903612107,-1.338145275\H,0,3.5705635167,1.2173599
632,-0.6713754268\H,0,4.267508416,0.0004821185,-1.7466838884\H,0,2.744
0188701,0.781751662,-2.165431818\C,0,2.2370119965,-1.8596454159,-1.531
0881026\H,0,3.1391898007,-2.2450382962,-2.006320658\H,0,1.7665898368,-
2.6730101917,-0.9810128836\H,0,1.5550466729,-1.5386376307,-2.317505437
8\\Version=AM64L-G03RevD.01\State=1-A\HF=-1003.0568077\RMSD=1.428e-09\
Thermal=0.\Dipole=0.0443698,0.0869899,0.4128707\PG=C01 [X(C14H31N2P1)]
\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	229.9567
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	230.1054

22_9

1\1\GINC-AZAZEL\SP\RmPWPW91\6-311++G(2d,2p)\C14H31N2P1\BORIS\03-Aug-20
10\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0
572004280) geom=check guess=read\\nmr_0710_06_11\\0,1\P,0,0.165406452,
-0.0203732808,-0.9685991382\C,0,0.1473782993,-1.7883994316,-1.40979032
58\H,0,0.5010723209,-2.5331546246,-0.7042168775\C,0,-0.2049509677,-2.1
834320529,-2.6272885471\H,0,-0.177789268,-3.2235755864,-2.9233472623\H
,0,-0.5318450192,-1.4769638159,-3.378809488\N,0,-1.2546032133,0.129636
2907,-0.0135454506\N,0,1.5289996861,0.0355068652,0.0485357862\C,0,-1.9
063385103,1.4315814171,-0.1997431283\H,0,-1.0861725936,2.123257457,-0.
3985879463\C,0,-1.9136340734,-0.9971527193,0.6403683147\H,0,-1.2746607
249,-1.8531331334,0.4312677798\C,0,1.7000222417,-0.7923456454,1.232374
4232\H,0,0.8109784058,-1.4200256142,1.2930317591\C,0,2.5553056649,1.04
10758777,-0.2276116364\H,0,3.3206289342,0.9051077212,0.5364054534\C,0,
-3.2743312544,-1.3580312391,0.0561964436\H,0,-3.6238324965,-2.29488758
9,0.490538793\H,0,-4.0268937835,-0.6021753638,0.2736244933\H,0,-3.2117
641601,-1.4853054115,-1.0223536342\C,0,-1.9954584509,-0.9053921201,2.1
635134449\H,0,-2.250670506,-1.8835561895,2.5730399098\H,0,-1.042941690
9,-0.5998346742,2.5892946292\H,0,-2.7559251904,-0.2068710979,2.5018215
653\C,0,2.9048576023,-1.7202702711,1.1253448357\H,0,2.9623301183,-2.37
94436882,1.9916926585\H,0,2.8418531965,-2.33292921,0.2280598373\H,0,3.
8379160612,-1.1586817038,1.0811871701\C,0,1.7486961875,0.0241352008,2.
5188184813\H,0,1.7600027246,-0.6319142535,3.3891466215\H,0,2.643771554
3,0.6436385814,2.5685065133\H,0,0.8821049376,0.6779429334,2.5890907151
\C,0,2.0388035127,2.4672735623,-0.0966403698\H,0,2.851470748,3.1851301
829,-0.2103524892\H,0,1.2977975496,2.6782738594,-0.8670362647\H,0,1.57
52416574,2.6241723877,0.8756849\C,0,3.2267724772,0.8222464487,-1.57599
87259\H,0,4.0449023962,1.528500737,-1.7201481819\H,0,3.6260199135,-0.1
878732319,-1.6469340399\H,0,2.5138677164,0.9620324827,-2.3873885226\C,
0,-2.6050697543,1.9745273394,1.0366115348\H,0,-1.948368294,1.952308883
1,1.903402202\H,0,-2.894214109,3.0094676382,0.8562562494\H,0,-3.514397
1973,1.4261467743,1.276238931\C,0,-2.8204721614,1.502845579,-1.4198147
347\H,0,-3.1143305049,2.5361008212,-1.6080732318\H,0,-2.2987001449,1.1
36811129,-2.3024438963\H,0,-3.7288095195,0.9190590461,-1.292583683\\Ve
rsion=AM64L-G03RevD.01\State=1-A\HF=-1003.0580623\RMSD=5.989e-09\Therm
al=0.\Dipole=-0.0009994,-0.2493951,0.4462732\PG=C01 [X(C14H31N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	251.9917
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	251.8790

22_10

1\1\GINC-YIN\SP\RmPWPW91\6-311++G(2d,2p)\C14H31N2P1\BORIS\01-Aug-2010\
0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0572
004280) geom=check guess=read\\nmr_0710_06_8\\0,1\P,0,0.0971479269,0.4
431651993,-0.2251229792\C,0,1.3136546819,-0.6968170283,-0.9693652844\H
,0,1.1190728272,-1.7622463534,-1.0075676466\C,0,2.4401713215,-0.216396
143,-1.4824080796\H,0,3.1747608081,-0.8537931756,-1.9565377421\H,0,2.6
692120605,0.8409246853,-1.4471295277\N,0,-1.2519623978,0.3193643358,-1
.2903554323\N,0,-0.4030644977,-0.5202301324,1.1562490535\C,0,-1.626744
0475,1.6080990675,-1.8964662701\H,0,-2.5615954946,1.4289443574,-2.4204
289171\C,0,-1.430272738,-0.8812830128,-2.1279288659\H,0,-0.5063020205,
-1.0719786931,-2.6858406936\C,0,0.6110711714,-0.7552245898,2.194538223
5\H,0,0.0586965348,-0.8362313221,3.1298057262\C,0,-1.7386329211,-0.208
8573474,1.6711091087\H,0,-2.3397653078,0.0007155268,0.7881671632\C,0,-
2.5439303253,-0.7564281032,-3.158715469\H,0,-2.646119548,-1.7149564721
,-3.6656685734\H,0,-3.4999516136,-0.5319787416,-2.685563641\H,0,-2.347
5465571,-0.0080377606,-3.9231286457\C,0,-1.7250739263,-2.100735191,-1.
2673631277\H,0,-1.6987972208,-3.0030880842,-1.8783148721\H,0,-1.020037

6533,-2.2070220273,-0.4489027687\H,0,-2.7204789682,-2.015065931,-0.831
3566691\C,0,1.321175185,-2.0893003746,2.0043067799\H,0,1.9283367684,-2
.3230790741,2.8796577364\H,0,0.5966223384,-2.8891588811,1.8649574985\H
,0,1.9827587679,-2.0708691096,1.1410553323\C,0,1.6234532566,0.36998494
99,2.3947825969\H,0,2.2417656157,0.1529081242,3.2658371498\H,0,2.29086
83699,0.4730584515,1.5405004333\H,0,1.1320709317,1.327222438,2.5556148
898\C,0,-1.7997241756,1.0194665549,2.5753165173\H,0,-2.833181019,1.249
076514,2.8356305614\H,0,-1.2579107478,0.8640044389,3.5084436367\H,0,-1
.3759312911,1.8922667808,2.0812165192\C,0,-2.3606494774,-1.4184099211,
2.354527357\H,0,-3.3951208792,-1.2052086139,2.6240136759\H,0,-2.348125
2448,-2.2823951566,1.6941622418\H,0,-1.8389247811,-1.6874672088,3.2731
054835\C,0,-0.6113917373,2.1210294288,-2.9101600643\H,0,-0.3806443575,
1.3652359234,-3.6601549877\H,0,-0.9886629884,3.004008982,-3.4266050027
\H,0,0.3189023079,2.3940394925,-2.4123262422\C,0,-1.9405001249,2.66857
17921,-0.8541216098\H,0,-2.3412306523,3.5540534373,-1.3474692924\H,0,-
2.6863478588,2.3068362557,-0.1486749476\H,0,-1.0546203008,2.9679817127
,-0.2982203327\\Version=AM64L-G03RevD.01\State=1-A\HF=-1003.0508889\RM
SD=3.663e-09\Thermal=0.\Dipole=-0.0973084,-0.1489271,-0.2611156\PG=C01
[X(C14H31N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p)	245.0854
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	245.2238

	MPW1K/6-311++G(2d,2p) [+ PCM/UAHF/MPW1K/6-311++G(2d,2p)][a]		MP2(FC)/6-31+G(2d,p)/MPW1K/6-31G(d) + PCM/UAHF/MPW1K/6-311++G(2d,2p)		
	Chemical shift, ppm (relative to PPh_3)		E_{tot}	„G“$_{298,\ gas}$	„G“$_{298,CHCl3}$
	Gas-phase	Solution model 1			
22_1	66.6	66.3	-1000.520008	-1000.118416	-1000.110927
22_2	50.7	51.2	-1000.517667	-1000.117992	-1000.109468
22_3	87.0	87.2	-1000.516425	-1000.115793	-1000.108145
22_4	85.6	86.4	-1000.513206	-1000.113047	-1000.105224
22_5	80.0	80.8	-1000.512755	-1000.112136	-1000.104503
22_6	84.7	84.3	-1000.512573	-1000.110910	-1000.104106
22_7	100.5	100.3	-1000.512714	-1000.110846	-1000.103851
22_8	102.4	102.6	-1000.512417	-1000.111790	-1000.103823
22_9	80.4	80.8	-1000.511937	-1000.111630	-1000.102404
22_10	87.3	87.5	-1000.508684	-1000.106245	-1000.099648
[a]the theory shown in square brackets relates to solution model 1 and not to gas-phase calculations					

<δ> = 61.5 ppm (gas-phase)
<δ> = 64.7 ppm (solution model 1)

22_1*$CHCl_3$_1

1\1\GINC-NODE10\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\ZIP04\13-Aug
-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/7
6=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read
\\nmr_0710_06c_3_1_2\\0,1\P,0,0.5331786776,-0.0199379493,0.0190175599\
C,0,-0.040879606,0.0847893424,-1.7013128187\H,0,-0.3692286578,1.071593
8711,-2.0091222292\C,0,-0.2530052695,-0.940073913,-2.5180905489\H,0,-0
.7189850803,-0.8080073267,-3.4846171081\H,0,0.0228158056,-1.9467056774
,-2.2414703718\N,0,1.48589425,-1.4294460609,0.0227210094\N,0,1.4797922
282,1.3951310016,0.0795969136\C,0,1.1672651759,-2.4925750227,0.9824463
924\H,0,1.922543162,-3.2619146367,0.8256856389\C,0,2.7517500397,-1.545
8831097,-0.6958911292\H,0,2.8097030428,-0.6724692974,-1.3425083119\C,0
,1.4175868784,2.2374983229,1.2792852832\H,0,2.0240520224,3.1135619362,
1.0529317912\C,0,2.2012370111,1.9576259741,-1.0625280269\H,0,2.0944680
143,1.2367061857,-1.8722849739\C,0,2.8247702982,-2.7689488819,-1.60290

76272\H,0,3.7765545057,-2.78158575,-2.1336913574\H,0,2.7581309536,-3.6
998268138,-1.0407619991\H,0,2.027881046,-2.7592186053,-2.3412254539\C,
0,3.9519975116,-1.510077158,0.2434737646\H,0,4.8833914096,-1.479954035
2,-0.3219637143\H,0,3.9106992901,-0.6362834099,0.8895268286\H,0,3.9862
962159,-2.396248614,0.8772859488\C,0,0.0123268177,2.736680811,1.584731
6377\H,0,0.0307470286,3.4449823124,2.4130236363\H,0,-0.4209119071,3.23
55127186,0.7196515546\H,0,-0.6429620033,1.9136054624,1.8646301552\C,0,
2.0404988766,1.5769747871,2.497417428\H,0,2.0716777214,2.2730819977,3.
3356866925\H,0,1.4622846679,0.710038969,2.809119632\H,0,3.0570102697,1
.250957377,2.2849112785\C,0,3.6912843165,2.1287396173,-0.7956612401\H,
0,4.1965273183,2.4915220698,-1.6906148722\H,0,3.8773396907,2.853100820
4,-0.002945351\H,0,4.1491479455,1.1872408059,-0.5034627562\C,0,1.59485
46241,3.2671797172,-1.5576646914\H,0,2.1006792047,3.5952729113,-2.4652
297132\H,0,0.5363370966,3.1531887726,-1.7822315871\H,0,1.6962008754,4.
06600098,-0.8237672266\C,0,-0.1838726764,-3.1328038704,0.7014513176\H,
0,-0.2588373946,-3.454424678,-0.3351162009\H,0,-0.3357262642,-4.002108
6354,1.3414446371\H,0,-0.9940236996,-2.4330054738,0.9051143791\C,0,1.2
60428634,-2.0666116878,2.4399295066\H,0,1.1162826424,-2.9258237306,3.0
951652246\H,0,2.2301275826,-1.6267602228,2.6623644315\H,0,0.4878802777
,-1.3366180232,2.6770852998\H,0,-2.2328866282,-0.1138522468,0.03529436
71\C,0,-3.307440369,0.0096215,-0.0133328436\Cl,0,-3.9760016667,-1.3701
826158,-0.8745813161\Cl,0,-3.6339562459,1.5121195287,-0.8714698538\Cl,
0,-3.9118610228,0.0808645696,1.6372510011\\Version=AM64L-G03RevD.01\St
ate=1-A\HF=-2422.4642953\RMSD=2.428e-09\Thermal=0.\Dipole=1.5297782,0.
0208251,-0.2516951\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	269.5152

22_1*$CHCl_3$_2

1\1\GINC-NODE26\SP\RMP2-FC\6-31+G(2d,p)\C15H32Cl3N2P1\ZIP04\14-Aug-201
0\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid geom=check guess=r
ead\\nmr_0710_06c_3_1_1\\0,1\P,0,-1.7075087568,-0.0058877633,-0.965756
9466\C,0,-0.0972741569,0.0208114754,-1.8069646186\H,0,0.1642399392,0.9
796321514,-2.2422729278\C,0,0.6545337323,-1.0366764207,-2.0994994995\H
,0,1.5158235668,-0.9602060035,-2.7504843851\H,0,0.4073712921,-2.020195
7153,-1.7281383759\N,0,-1.6126992833,-1.3952611154,0.0141938938\N,0,-1
.5740737758,1.4241375875,-0.0481826249\C,0,-2.625376788,-2.440645579,-
0.1729978342\H,0,-2.421633358,-3.1882280492,0.5927792879\C,0,-0.746716
0521,-1.517002564,1.1822126878\H,0,-0.0706719261,-0.6648462123,1.14738
20649\C,0,-2.7360286896,2.3179042606,0.0112065453\H,0,-2.4187199592,3.
1757887947,0.6027570127\C,0,-0.3274929605,1.9536229518,0.5022565935\H,
0,0.4316788067,1.1970723505,0.3076475162\C,0,0.1217638519,-2.770066323
8,1.1671223974\H,0,0.7816339922,-2.776375041,2.0343177026\H,0,-0.47473
57693,-3.6808814549,1.2091162305\H,0,0.7401996677,-2.8132297071,0.2742
583776\C,0,-1.527717613,-1.4286418534,2.4885693184\H,0,-0.8505383711,-
1.4051018772,3.3422678574\H,0,-2.1418618751,-0.5312826294,2.5080464932
\H,0,-2.1839628283,-2.289380585,2.6181675396\C,0,-3.1508504508,2.84186
49573,-1.3569330445\H,0,-3.9587999134,3.5674847713,-1.2619392483\H,0,-
2.3152905289,3.3267446292,-1.8584795115\H,0,-3.5009677417,2.028540313,
-1.9906449216\C,0,-3.9175279666,1.6979512314,0.7376787238\H,0,-4.71941
2325,2.4269881361,0.8547706477\H,0,-4.3166008715,0.8537215794,0.179868
5654\H,0,-3.6258257141,1.3476601093,1.7260565272\C,0,-0.3853820402,2.1
609296798,2.010281086\H,0,0.5879870819,2.4753037013,2.3857685775\H,0,-
1.1040847327,2.9339212664,2.282229149\H,0,-0.668599076,1.2446601909,2.
5215177155\C,0,0.1372877816,3.2295497779,-0.1927077154\H,0,1.116653325
8,3.5252211171,0.1818341389\H,0,0.2164416832,3.0880625143,-1.268669424
2\H,0,-0.5440871062,4.0605092038,-0.0125837514\C,0,-2.4793316567,-3.12
96856387,-1.52151882\H,0,-1.4823519604,-3.5511366824,-1.6360206515\H,0
,-3.20464989,-3.936881527,-1.6258223567\H,0,-2.6450729368,-2.422828108
7,-2.3343203155\C,0,-4.0562688799,-1.9693062334,0.0402371755\H,0,-4.74
13364722,-2.8166396914,0.0084743615\H,0,-4.1671912401,-1.4770381021,1.
0040916182\H,0,-4.3554831962,-1.2712544861,-0.7399192075\H,0,2.4676697
907,-0.298930456,-0.4813169928\C,0,3.4633409705,-0.0901390818,-0.11071

04296\Cl,0,3.3590185361,0.1170216539,1.6341417525\Cl,0,4.019880708,1.3
839471592,-0.8930557518\Cl,0,4.4847873136,-1.4586533367,-0.5292375628\
\Version=AM64L-G03RevD.01\State=1-A\HF=-2414.7360189\MP2=-2418.0114554
\RMSD=7.860e-09\Thermal=0.\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	265.9469

22_2*$CHCl_3$_1

1\1\GINC-NODE26\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\ZIP04\14-Aug
-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/7
6=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read
\\nmr_0710_06c_2_5\\0,1\P,0,0.0030735408,0.0152458984,0.0102649314\C,0
,-0.0306937349,0.019792447,1.8347789876\C,0,1.071312444,-0.1217024745,
2.561128356\H,0,1.0412549297,-0.169116294,3.641278979\H,0,2.051713992,
-0.1936931989,2.1087054745\N,0,-1.486612805,-0.7258327159,-0.353594291
\N,0,-0.1018853145,1.6823655029,-0.3180834464\C,0,-1.4906682784,-2.023
8538469,-1.0314549972\H,0,-2.5408620539,-2.2863351011,-1.1589210909\C,
0,-2.7699074507,-0.2128340944,0.1067294099\H,0,-2.5543501218,0.7181609
933,0.6295048449\C,0,0.5621029135,2.2109619231,-1.5129388457\H,0,0.475
7589496,3.2944158623,-1.4414102105\C,0,-0.6780584684,2.6721742657,0.58
9201521\H,0,-1.1394057768,2.1130302204,1.4006213482\C,0,-3.4714579725,
-1.1350809503,1.0984903098\H,0,-4.3782221724,-0.6644675514,1.478164683
6\H,0,-3.7653028961,-2.0757544256,0.6338272769\H,0,-2.82669918,-1.3679
617493,1.9436547466\C,0,-3.6923819501,0.1398194136,-1.0538727286\H,0,-
4.6076566977,0.6069627202,-0.6903183609\H,0,-3.1996053926,0.8272325686
,-1.7376989458\H,0,-3.9825004928,-0.745629873,-1.6191968835\C,0,2.0498
88112,1.8957716829,-1.5674850386\H,0,2.51999188,2.4348451854,-2.389770
8871\H,0,2.5437883401,2.1832120388,-0.6413198745\H,0,2.2239767946,0.83
40632355,-1.7305245752\C,0,-0.1322195015,1.7914738323,-2.7992565683\H,
0,0.3252687087,2.277991059,-3.6609757076\H,0,-0.0570308648,0.715782064
2,-2.9457300906\H,0,-1.1875628018,2.0563551126,-2.7747725411\C,0,-1.77
55158815,3.5071443619,-0.0591131516\H,0,-2.2326568365,4.1655719255,0.6
79316652\H,0,-1.387970618,4.138579421,-0.8578504267\H,0,-2.5531511632,
2.8731011811,-0.4799393084\C,0,0.3870456196,3.5548331016,1.2280013014\
H,0,-0.0651428475,4.2446680714,1.9404460638\H,0,1.1149792108,2.9429415
386,1.7561679349\H,0,0.916295029,4.1529491378,0.4866954673\C,0,-0.8533
215125,-3.1265422418,-0.1962746995\H,0,-1.3147497086,-3.1868018745,0.7
875144107\H,0,-0.9601445482,-4.0947205333,-0.6858510588\H,0,0.21101245
48,-2.943777571,-0.0547035154\C,0,-0.8846544389,-1.9694067491,-2.42502
22598\H,0,-0.9727924748,-2.9386833509,-2.9154410034\H,0,-1.3940396638,
-1.228133329,-3.0375259544\H,0,0.1733748652,-1.7145020741,-2.385672486
2\H,0,-0.9867284689,0.060868881,2.3456616206\H,0,2.3911690628,-1.31222
85048,-0.3489662885\C,0,3.3563131808,-1.8076143962,-0.4015843087\Cl,0,
4.5715574903,-0.6872475555,0.2066071482\Cl,0,3.6577553938,-2.215528486
2,-2.0863297877\Cl,0,3.279706828,-3.2538753167,0.597953821\\Version=AM
64L-G03RevD.01\State=1-A\HF=-2422.4634091\RMSD=1.911e-09\Thermal=0.\Di
pole=-1.341016,0.7667123,0.2559346\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	279.7620

22_2*$CHCl_3$_2

1\1\GINC-NODE19\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\ZIP04\09-Aug
-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/7
6=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read
\\nmr_0710_06c_2_1\\0,1\P,0,-1.1348469009,-0.2023127467,0.5401109721\C
,0,-0.0262131087,-1.1090933725,-0.5970609028\H,0,2.8130175689,-0.58370
62547,0.1167893086\C,0,0.6870354819,-2.1544907727,-0.1886925928\H,0,1.
3556863686,-2.6886282941,-0.8511769833\H,0,0.6159459672,-2.525968939,0
.8256983377\N,0,-1.0018951582,1.38501299,-0.0628551342\N,0,-2.64178525
87,-0.8562436138,0.0860871287\C,0,-0.4365470989,2.4148455486,0.8117717
598\H,0,-0.4584147195,3.3390667598,0.2346502819\C,0,-1.3135020611,1.77
29929562,-1.4311837229\H,0,-1.6809800746,0.874519939,-1.9248096939\C,0

,-3.6218345745,-1.1146098639,1.1453951459\H,0,-4.4708335232,-1.5883142
426,0.6537661188\C,0,-2.9626178379,-1.3954370632,-1.2328883706\H,0,-2.
1209283727,-1.1523265442,-1.8787464051\C,0,-0.0955656398,2.2506459985,
-2.2151055285\H,0,-0.3634995641,2.4468322269,-3.2532376069\H,0,0.30994
16531,3.175239494,-1.8052237745\H,0,0.6977113881,1.5057171225,-2.20121
64909\C,0,-2.4396788584,2.7980373414,-1.4925093574\H,0,-2.7258095647,2
.9948727161,-2.5256651205\H,0,-3.3120998458,2.4362043545,-0.9528607546
\H,0,-2.1417542777,3.749062136,-1.0515276502\C,0,-3.1172137458,-2.0885
002239,2.2018784996\H,0,-3.9063595353,-2.3198495291,2.9175424507\H,0,-
2.7861493521,-3.0193058778,1.7448046691\H,0,-2.2787075336,-1.663106453
8,2.7505291834\C,0,-4.1385058344,0.1657836107,1.7816806866\H,0,-4.9461
304773,-0.0513312457,2.4809524553\H,0,-3.3488500485,0.6717506879,2.333
6866541\H,0,-4.5127354665,0.8500766525,1.022443893\C,0,-4.1982267419,-
0.7486813576,-1.8468309015\H,0,-4.3560435316,-1.1184663255,-2.85986933
37\H,0,-5.0988581748,-0.9740720104,-1.2764660248\H,0,-4.0911416126,0.3
330287447,-1.8892188209\C,0,-3.076917718,-2.9152381632,-1.2342419203\H
,0,-3.2446782162,-3.2821929541,-2.2467359224\H,0,-2.1623084233,-3.3647
954675,-0.8537426125\H,0,-3.9094901085,-3.2603392306,-0.6218169916\C,0
,1.0190224298,2.1420310702,1.166857967\H,0,1.6220482982,2.026664255,0.
2675559113\H,0,1.4384229203,2.9595148172,1.7534793876\H,0,1.105577002,
1.2305681603,1.7585726789\C,0,-1.2657390427,2.6587279801,2.0628222188\
H,0,-0.8578238693,3.494444163,2.6313560922\H,0,-2.2971412394,2.8898213
742,1.8040971997\H,0,-1.2604998074,1.7824669038,2.7092083919\H,0,0.096
1665557,-0.7655752637,-1.61942783\C,0,3.8876804847,-0.4831457048,0.038
421339\Cl,0,4.4990463014,0.0568608393,1.5945830558\Cl,0,4.2209770849,0
.6977676836,-1.2242905828\Cl,0,4.5386900986,-2.0623799471,-0.386737500
1\\Version=AM64L-G03RevD.01\State=1-A\HF=-2422.4611895\RMSD=5.047e-09\
Thermal=0.\Dipole=-1.0027611,0.0857842,-0.6057336\PG=C01 [X(C15H32Cl3N
2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	281.0781

22_3*$CHCl_3$_1

1\1\GINC-SOLARIS\SP\RMP2-FC\6-31+G(2d,p)\C15H32Cl3N2P1\BORIS\07-Oct-20
10\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid geom=check guess=
read\\nmr_1010_sys22_3c_001\\0,1\P,0,0.0155935564,0.5736488421,-0.6823
012795\C,0,-0.0723484604,2.1585227645,0.216536053\H,0,-0.1394888341,2.
1476133122,1.298570642\C,0,0.0239708117,3.3162668609,-0.4253976073\H,0
,0.038843099,4.2631961496,0.0974768195\H,0,0.0900332547,3.3643054258,-
1.5047084832\N,0,1.3630410819,-0.1777091147,0.0249552243\N,0,-1.287398
7701,-0.2902444918,0.0911989393\C,0,2.535959551,-0.4459088868,-0.80977
37262\H,0,3.2878193082,-0.8519192847,-0.1339047089\C,0,1.5290515245,-0
.250189703,1.4754910011\H,0,0.546547256,-0.0225145136,1.8880653438\C,0
,-2.6384381608,0.290100524,0.0747946575\H,0,-3.3135273745,-0.562677634
1,0.1297833377\C,0,-1.2501810582,-1.7396233132,-0.1322609486\H,0,-0.19
30970643,-1.9938899492,-0.1809622476\C,0,2.529683357,0.7640548911,2.01
67727096\H,0,2.5519195459,0.7319144283,3.1060984503\H,0,3.5396002147,0
.5520607684,1.6652484734\H,0,2.272141364,1.7752353347,1.7095127533\C,0
,1.8867987098,-1.6547474206,1.9462602359\H,0,1.8999147897,-1.690786011
,3.0352970172\H,0,1.1635750173,-2.3854110275,1.5923023857\H,0,2.874692
0398,-1.9620200255,1.6035392529\C,0,-2.9258987425,1.1308712007,1.31172
93529\H,0,-3.992687621,1.3470625588,1.3765883312\H,0,-2.6285132549,0.5
962720497,2.21169983\H,0,-2.4014201467,2.0828795276,1.286093171\C,0,-3
.0079535768,1.0445870547,-1.1987412108\H,0,-4.0601018134,1.3273419903,
-1.1688563889\H,0,-2.4311549915,1.9613538227,-1.3084645679\H,0,-2.8511
175706,0.4330194357,-2.0850897712\C,0,-1.886441901,-2.2043374434,-1.43
79702567\H,0,-1.7288597118,-3.2742255464,-1.5731568304\H,0,-2.96251800
86,-2.0311672355,-1.4537727324\H,0,-1.4493087185,-1.6923460437,-2.2938
159718\C,0,-1.8281546611,-2.486609214,1.0610260657\H,0,-1.6813391626,-
3.5599009591,0.9413898763\H,0,-1.3418946712,-2.170885845,1.9817415854\
H,0,-2.8993664359,-2.3190530808,1.1718546032\C,0,3.1323527472,0.805933
477,-1.4411959618\H,0,3.3253222929,1.5687896902,-0.6899416843\H,0,4.07
14474514,0.5721223592,-1.9428515005\H,0,2.4582515429,1.2280884387,-2.1

852415759\C,0,2.2565321741,-1.5120903483,-1.8574272577\H,0,3.1553767246,-1.7296493624,-2.4336626451\H,0,1.9178077619,-2.4351426129,-1.3902583282\H,0,1.4883807615,-1.1827713936,-2.556098411\H,0,-0.1330213943,1.0268493559,-3.378842228\C,0,-0.2925220953,1.2576888233,-4.4286845495\Cl,0,1.2809497011,1.3476944744,-5.2118607525\Cl,0,-1.1294585804,2.8049113986,-4.5148267079\Cl,0,-1.2707661285,-0.0307007582,-5.1215280085\\Version=AM64L-G03RevD.01\State=1-A\HF=-2414.7342512\MP2=-2418.0103806\RMSD=5.642e-09\Thermal=0.\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	249.2158

22_7*$CHCl_3$_2

1\1\GINC-CALYPSO\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\BORIS\28-Dec-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read\\nmr_22_7_c_02\\0,1\P,0,-0.1178350967,0.0040738311,-1.0478036396\C,0,-0.1893506728,-1.7223360254,-1.6061847491\H,0,-1.1704514031,-2.050728131,-1.9321210265\C,0,0.8548705019,-2.5142618827,-1.8341977434\H,0,0.7465598695,-3.4709179251,-2.3285792634\H,0,1.8575615117,-2.2128072184,-1.5680943992\N,0,-1.4867356483,0.0366044539,-0.0335022299\N,0,1.3380347293,0.0869803624,-0.1643368155\C,0,-2.2894847551,1.2648090584,-0.0533236485\H,0,-3.1080747971,1.0996098469,0.6467042864\C,0,-2.0605930088,-1.1111771408,0.6655474499\H,0,-1.3451457469,-1.9239824314,0.5441839386\C,0,1.5779253138,-0.717124844,1.030877097\H,0,0.827270723,-1.5068839689,0.9880313719\C,0,2.2777620225,1.1041254019,-0.6475642464\H,0,1.679701296,1.7274594244,-1.3138399403\C,0,-3.3783539811,-1.5734069892,0.0519370758\H,0,-3.7245936631,-2.4844912318,0.5389319113\H,0,-4.1589869015,-0.8225607149,0.1726315884\H,0,-3.272351522,-1.7767130268,-1.0119843207\C,0,-2.2300442955,-0.8861168589,2.1626710069\H,0,-2.5908923553,-1.7978810397,2.6377307712\H,0,-1.2889884144,-0.6104322626,2.6284494748\H,0,-2.9566428597,-0.1019636355,2.3745849925\C,0,2.9303957084,-1.4180587469,1.0774505214\H,0,2.9570562789,-2.088999337,1.935832268\H,0,3.1168613972,-2.0095547079,0.1845335096\H,0,3.7502998041,-0.7120440032,1.1954127679\C,0,1.3467245798,0.029618773,2.3445326973\H,0,1.2241344447,-0.6846661413,3.1592669961\H,0,2.1829076372,0.6742358199,2.6032636285\H,0,0.4516474417,0.6423583931,2.2864383062\C,0,3.3987704413,0.5311965186,-1.5091322463\H,0,3.9700239304,1.3394662484,-1.9668573724\H,0,4.0936454896,-0.0784340494,-0.936036615\H,0,2.9858688034,-0.0808820504,-2.3091990974\C,0,2.8318552959,2.0363369511,0.4206033605\H,0,3.3736848665,2.8488680305,-0.0625713855\H,0,2.0343400299,2.4713946068,1.0185395043\H,0,3.5323577798,1.5379264162,1.0883238587\C,0,-2.9086315714,1.550872811,-1.415393245\H,0,-3.5021825618,0.7061862913,-1.7599710857\H,0,-3.5577005936,2.4253348834,-1.3654690241\H,0,-2.1352614516,1.7458988951,-2.1565190745\C,0,-1.5083748401,2.4675676512,0.4526990025\H,0,-2.1464914916,3.3501799324,0.4947763099\H,0,-1.1124172866,2.281704461,1.4490344502\H,0,-0.6724640867,2.6945787423,-0.2090870043\H,0,0.2657059601,-4.036346041,0.1092528536\C,0,0.1547277644,-4.9487726824,0.6814445104\Cl,0,1.5434030613,-5.9684444607,0.3305062148\Cl,0,0.0980008027,-4.5139037852,2.3860076781\Cl,0,-1.34462451,-5.7141362818,0.1708688995\\Version=AM64L-G03RevD.01\State=1-A\HF=-2422.4585656\RMSD=1.959e-09\Thermal=0.\Dipole=-0.07929,0.4601325,0.3079777\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	233.1692

22_3*$CHCl_3$_2

1\1\GINC-EDDY\SP\RMP2-FC\6-31+G(2d,p)\C15H32Cl3N2P1\BORIS\07-Oct-2010\0\\#p MP2(FC)/6-31+g(2d,p) scf=tight int=finegrid geom=check guess=read\\nmr_1010_sys22_3c_002\\0,1\P,0,0.0231355168,0.6260680158,-0.6412534528\C,0,-0.0025845322,2.1774289865,0.329517673\H,0,-0.0035469911,2.1322336169,1.4132234177\C,0,0.0245558602,3.3594848455,-0.2776704113\H,0,0.0384531795,4.2912333654,0.2734727726\H,0,0.0146877703,3.4378632099,-1

.3575688526\N,0,1.3701280945,-0.1797837911,0.0110231407\N,0,-1.2833657
5,-0.2288971013,0.1532608352\C,0,2.4887716546,-0.4898053285,-0.8812997
47\H,0,3.2527244095,-0.9446501818,-0.2513390284\C,0,1.5718850615,-0.33
98275955,1.4481903266\H,0,0.6116130465,-0.0938650301,1.9007931152\C,0,
-2.6168044081,0.389102197,0.1926743397\H,0,-3.3162930015,-0.4451824151
,0.224557893\C,0,-1.2989378103,-1.6624100912,-0.1567715666\H,0,-0.2518
616495,-1.9480190688,-0.2359904535\C,0,2.6304407159,0.6014589215,2.009
5987054\H,0,2.7044757733,0.4944981539,3.0917287408\H,0,3.6149294911,0.
3871732364,1.5932027923\H,0,2.3903199311,1.6396673097,1.7895715412\C,0
,1.8822777487,-1.7807715859,1.8368443673\H,0,1.9205598361,-1.874257928
2,2.9218153479\H,0,1.1201330636,-2.4617994126,1.4659061697\H,0,2.84751
77921,-2.1097480406,1.4524451343\C,0,-2.8515807643,1.1777809297,1.4741
502562\H,0,-3.9073671142,1.4338640009,1.5686393095\H,0,-2.5622609319,0
.5867476406,2.34077141\H,0,-2.2880670339,2.1074774467,1.4876784297\C,0
,-2.9956317738,1.2127175382,-1.0354752441\H,0,-4.0446568713,1.50276128
45,-0.9755094615\H,0,-2.410064438,2.1272523852,-1.1058339948\H,0,-2.85
27390897,0.6471949273,-1.9536297853\C,0,-1.9647660694,-2.0279006479,-1
.4798580097\H,0,-1.8402197893,-3.0913237687,-1.6837936753\H,0,-3.03545
78026,-1.8235908028,-1.4691440747\H,0,-1.5214823548,-1.4738853572,-2.3
061331334\C,0,-1.8843096768,-2.4634497666,0.9972434743\H,0,-1.76893417
45,-3.5312920625,0.8118601745\H,0,-1.378376014,-2.2165900188,1.9283330
115\H,0,-2.9490636,-2.2742918875,1.132679638\C,0,3.1115833222,0.745844
6546,-1.5182677067\H,0,3.4239166115,1.4595783777,-0.7579370875\H,0,3.9
890086933,0.4763805881,-2.1061916062\H,0,2.4017552458,1.2375825454,-2.
1824636474\C,0,2.1076709396,-1.5150566433,-1.9382985138\H,0,2.96529157
06,-1.7603066589,-2.5645220666\H,0,1.7498088649,-2.4335192173,-1.47619
3355\H,0,1.3208265212,-1.1281327166,-2.5849007195\H,0,2.6521944589,3.8
230167637,0.1225978234\C,0,3.2726611577,4.6723812755,0.3743866321\Cl,0
,2.8073321233,5.2043164184,1.9861301265\Cl,0,4.9513250519,4.1525305786
,0.3363051264\Cl,0,2.9652717751,5.9251183754,-0.8212897308\\Version=AM
64L-G03RevD.01\State=1-A\HF=-2414.73179\MP2=-2418.0044731\RMSD=5.386e-
09\Thermal=0.\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM($CHCl_3$,UAHF)	246.7699

22_4*$CHCl_3$_1

1\1\GINC-YANG\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\BORIS\24-Dec-2
010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=
0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read\\
nmr_22_4_c_01\\0,1\P,0,-0.1546866067,0.4953004652,-0.063848474\C,0,-0.
4637632694,2.0785964416,0.7854013723\H,0,-0.1633940646,2.2042231325,1.
8204877431\C,0,-0.9606597241,3.1245580987,0.1357310958\H,0,-1.10032550
87,4.082926807,0.617347506\H,0,-1.2501249492,3.0653480804,-0.905409078
4\N,0,1.2908411863,-0.0368511961,0.670730855\N,0,-1.450098437,-0.45244
51551,0.4986855173\C,0,2.4381842223,-0.11192924,-0.23558798\H,0,1.9926
227396,-0.2635890334,-1.2207163532\C,0,1.3951704566,-0.1934923365,2.11
71252938\H,0,0.4245856457,0.1208385188,2.5016383027\C,0,-2.2159629282,
-0.1957515899,1.7153315923\H,0,-1.691866513,0.5976841995,2.2445426301\
C,0,-1.9747559286,-1.4783866501,-0.4081588488\H,0,-2.7802378278,-1.971
4038976,0.135115647\C,0,2.430278933,0.7033746176,2.7855266301\H,0,2.32
63374098,0.6410196391,3.8688662941\H,0,3.447018478,0.4003365284,2.5422
716611\H,0,2.305028614,1.7428450164,2.4892388141\C,0,1.563469473,-1.64
02240421,2.576007865\H,0,1.3600925436,-1.714964679,3.6447963744\H,0,0.
869686455,-2.2896330828,2.0481730761\H,0,2.5704929807,-2.0136763312,2.
4111779035\C,0,-3.6155228308,0.3297469965,1.4223515287\H,0,-4.13419223
01,0.5696496022,2.3503906157\H,0,-3.5640943862,1.2310172723,0.81512828
8\H,0,-4.2190383576,-0.4071975708,0.8931474395\C,0,-2.2655073563,-1.39
77608482,2.6505799652\H,0,-2.7658583203,-1.1288767644,3.5807044691\H,0
,-2.8193061057,-2.2297238903,2.2168246369\H,0,-1.2644696169,-1.7485316
855,2.8892519537\C,0,-0.9384782878,-2.5444223744,-0.7302193559\H,0,-1.
3758170686,-3.3292152264,-1.3472391787\H,0,-0.0996274591,-2.1198614589
,-1.2814791189\H,0,-0.5503188928,-2.9965751091,0.180145446\C,0,-2.5799
998457,-0.9039918878,-1.6822724848\H,0,-3.0609945461,-1.6900760537,-2.

2643012373\H,0,-3.3230841333,-0.1426457388,-1.4547255709\H,0,-1.814558
3543,-0.4512324424,-2.309392057\C,0,3.3549833039,-1.3032518334,-0.0040
332803\H,0,2.7928269886,-2.2333771535,0.0373988144\H,0,4.0636436261,-1
.3715370374,-0.8286964913\H,0,3.9379265846,-1.2076067992,0.9105314465\
C,0,3.243244853,1.1819837608,-0.3317317732\H,0,3.9450813258,1.12446988
95,-1.163945259\H,0,2.5851698678,2.0312746486,-0.5074187068\H,0,3.8176
700042,1.3800960845,0.5704869759\H,0,0.2112155819,1.1987100509,-2.6601
716565\C,0,0.3131265132,1.4893063197,-3.7019349805\Cl,0,0.6181794409,0
.0279431602,-4.6342757569\Cl,0,-1.1950708964,2.2535308322,-4.194858947
9\Cl,0,1.6605106174,2.6139117054,-3.8265501131\\Version=AM64L-G03RevD.
01\State=1-A\HF=-2422.4597274\RMSD=1.252e-09\Thermal=0.\Dipole=-0.2040
997,-0.3668124,1.4827074\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	248.4409

22_9*CHCl$_3$_1

1\1\GINC-AZAZEL\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\BORIS\29-Dec
-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/7
6=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read
\\nmr_22_9_c_01\\0,1\P,0,0.1990192028,0.0632206978,-0.9411844907\C,0,0
.1905233253,-1.6809491011,-1.4633151554\H,0,0.5543194857,-2.4494252713
,-0.7897113872\C,0,-0.1669947128,-2.0288234785,-2.6934570991\H,0,-0.13
25265131,-3.0564214588,-3.0292548102\H,0,-0.508915273,-1.2997385878,-3
.4163746347\N,0,-1.2467487706,0.184410721,-0.03250242\N,0,1.536445006,
0.0865566592,0.1057653712\C,0,-1.8922826112,1.4968141621,-0.1627191007
\H,0,-1.0742969482,2.1840968418,-0.3843306776\C,0,-1.9083314756,-0.963
3081278,0.5853703518\H,0,-1.2798410063,-1.8159866519,0.3346668124\C,0,
1.6918347901,-0.8167212385,1.2374724773\H,0,0.7983323562,-1.4407926258
,1.252094348\C,0,2.5868164933,1.0836120038,-0.1062445333\H,0,3.2983993
641,0.9396535155,0.7061228507\C,0,-3.2780459259,-1.2900655444,0.003085
3635\H,0,-3.6169595928,-2.2519801762,0.3878112235\H,0,-4.0284762923,-0
.551622562,0.2797598516\H,0,-3.2350971859,-1.3532142981,-1.0818296188\
C,0,-1.9761423484,-0.9292891504,2.111162665\H,0,-2.2409836735,-1.91938
70672,2.4839557597\H,0,-1.0176550999,-0.6524389251,2.5423000038\H,0,-2
.7255732124,-0.2351479385,2.4812227781\C,0,2.8920705251,-1.743907934,1
.0842884525\H,0,2.9380945125,-2.4535429695,1.9103546674\H,0,2.83485964
07,-2.302280584,0.1518650483\H,0,3.8282023502,-1.1858337579,1.08186556
22\C,0,1.7344279127,-0.0821801208,2.572584493\H,0,1.7088890427,-0.7921
236202,3.399045637\H,0,2.6445513953,0.5068810516,2.6817399735\H,0,0.88
49211967,0.5905576252,2.667254718\C,0,2.0773864004,2.5133569412,0.0023
787339\H,0,2.9037308404,3.2213264651,-0.0591815592\H,0,1.3845245876,2.
745016746,-0.8056470707\H,0,1.5610323021,2.6685334789,0.948082518\C,0,
3.3468313555,0.8590487968,-1.4056387326\H,0,4.1793072485,1.5573453565,
-1.4935739083\H,0,3.7409388249,-0.1544883565,-1.4508889493\H,0,2.69920
56178,1.0051190555,-2.2685529377\C,0,-2.5297342909,2.0177797395,1.1156
918046\H,0,-1.8402005219,1.9604625784,1.955053665\H,0,-2.8087726677,3.
0616293857,0.9756705133\H,0,-3.4380458493,1.4764510676,1.3744183255\C,
0,-2.8634774448,1.6036296904,-1.3345966329\H,0,-3.1203941172,2.6479597
821,-1.5121412475\H,0,-2.4125765373,1.2116837843,-2.2446162032\H,0,-3.
7888429409,1.0615761444,-1.1573894577\H,0,0.2196336072,1.6491389832,-3
.2134811795\C,0,0.0991773731,2.244202974,-4.1143735033\Cl,0,1.64623716
56,2.2988000344,-4.9500349449\Cl,0,-0.4140321689,3.8555131239,-3.62677
80725\Cl,0,-1.126123492,1.4632315302,-5.1106534918\\Version=AM64L-G03R
evD.01\State=1-A\HF=-2422.4589294\RMSD=5.504e-09\Thermal=0.\Dipole=0.0
65346,-0.7770129,1.2858202\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	255.3035

22_6*CHCl$_3$_1

1\1\GINC-NAUTILUS\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\BORIS\27-D

ec-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3
/76=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=re
ad\\nmr_22_6_c_01\\0,1\P,0,-0.0778456463,-0.3749511294,-0.4328078126\C
,0,-0.0157265,-2.0765365969,-1.0344562525\H,0,0.9190674622,-2.34769789
18,-1.5066271195\C,0,-1.0463723744,-2.906766705,-1.1362847991\H,0,-0.9
585845065,-3.8548204388,-1.6483932093\H,0,-2.0139321133,-2.6589524072,
-0.7281644939\N,0,-1.4612087188,-0.3382941208,0.5558834519\N,0,1.39662
63529,-0.223791391,0.4229332617\C,0,-2.3895732925,0.7868710443,0.37275
35314\H,0,-3.0910235882,0.7258791647,1.2033940949\C,0,-1.6906157196,-1
.1837097092,1.7248297014\H,0,-0.9906627701,-2.0095944654,1.6349318081\
C,0,2.2896780157,-1.2353523477,0.9982494816\H,0,2.9729709839,-0.670887
2174,1.6329686657\C,0,1.9032871401,1.1539917778,0.4802238942\H,0,1.167
4849663,1.7569106366,-0.0514848232\C,0,-3.0877538285,-1.7947988368,1.7
674694855\H,0,-3.146799577,-2.5135818906,2.5842938341\H,0,-3.860653193
5,-1.0475615396,1.9430658196\H,0,-3.3301837183,-2.3154949853,0.8443849
823\C,0,-1.401276681,-0.4541484916,3.0312916967\H,0,-1.4993546434,-1.1
286974938,3.8820411397\H,0,-0.3938553248,-0.0457532034,3.03030441\H,0,
-2.0989054463,0.369321275,3.186784279\C,0,1.6117651872,-2.2458035756,1
.9060528546\H,0,2.3668927629,-2.8881169371,2.359038839\H,0,1.061134535
7,-1.7585886826,2.7063719112\H,0,0.9333700288,-2.8877045325,1.34730460
48\C,0,3.1652752801,-1.9662845845,-0.0207593957\H,0,4.0177650269,-2.41
98521004,0.4858342671\H,0,2.6265317057,-2.7713780984,-0.5151239186\H,0
,3.545689537,-1.292084372,-0.7827545629\C,0,3.2283235457,1.3470990365,
-0.2448861801\H,0,3.4966551607,2.4030288586,-0.2511329189\H,0,4.042623
5431,0.8082072365,0.2389856648\H,0,3.1596417997,1.0124762113,-1.278343
9247\C,0,1.9759177317,1.7000279516,1.9004918767\H,0,2.2601795533,2.751
764243,1.8842869635\H,0,1.0123383477,1.6168305914,2.3978916739\H,0,2.7
159348759,1.1771053819,2.5061521393\C,0,-3.1946994844,0.6440318739,-0.
9096674317\H,0,-3.7169925423,-0.3104846889,-0.9340867974\H,0,-3.932501
9986,1.4417125133,-0.9984621807\H,0,-2.5437590484,0.6923886072,-1.7819
723415\C,0,-1.7397341423,2.1600829361,0.4621148841\H,0,-2.5049743779,2
.9362671966,0.4728292273\H,0,-1.1475416758,2.254514487,1.3705432922\H,
0,-1.0934378701,2.3499755631,-0.3928861211\H,0,0.0797172605,0.93742446
25,-2.7498607985\C,0,0.3319712741,1.4311555644,-3.6843018987\Cl,0,-1.0
649121416,1.3389907236,-4.7489653434\Cl,0,1.7143856431,0.5884465286,-4
.3768379326\Cl,0,0.734304563,3.1045806984,-3.3093264497\\Version=AM64L
-G03RevD.01\State=1-A\HF=-2422.4587231\RMSD=1.945e-09\Thermal=0.\Dipol
e=-0.0503691,-0.5385649,1.4701549\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	253.6456

22_7*CHCl$_3$_1

1\1\GINC-NAUTILUS\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\BORIS\28-D
ec-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3
/76=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=re
ad\\nmr_22_7_c_01\\0,1\P,0,-0.1774304155,0.176079629,-1.0098062002\C,0
,-0.3196352803,-1.4858098611,-1.7313315278\H,0,-1.3316470789,-1.806134
2109,-1.9528326153\C,0,0.6955229569,-2.2180073428,-2.1715043719\H,0,0.
5389638512,-3.1394867722,-2.7149550691\H,0,1.7197708679,-1.9117260398,
-2.0143649467\N,0,-1.5152383442,0.1523358972,0.0394381234\N,0,1.308601
4054,0.1271959666,-0.1678422124\C,0,-2.3613705931,1.3482699282,0.11889
19453\H,0,-3.1155011733,1.1254260353,0.8729136949\C,0,-2.0096494242,-1
.0352175231,0.7359877392\H,0,-1.3055984164,-1.8342204229,0.5046465131\
C,0,1.4846806351,-0.7066343711,1.022150511\H,0,0.5228527436,-1.1926344
717,1.1619208635\C,0,2.2757770639,1.1547124995,-0.5742701612\H,0,1.949
7996688,1.4444690837,-1.5732277631\C,0,-3.375271853,-1.4948536339,0.23
659979\H,0,-3.6586525173,-2.4262176258,0.7259669538\H,0,-4.1534221761,
-0.7641973984,0.4547158414\H,0,-3.3675678122,-1.6661126144,-0.83797665
76\C,0,-2.0305375411,-0.861702801,2.2504638506\H,0,-2.3035801139,-1.79
87937758,2.7352736186\H,0,-1.058055672,-0.551628681,2.6254869785\H,0,-
2.7609358152,-0.1141204932,2.5588317704\C,0,2.4973953921,-1.8422280197
,0.890707822\H,0,2.4323701047,-2.4805154226,1.7726481801\H,0,2.2869052

938,-2.4566541055,0.0208551451\H,0,3.5217891643,-1.4870498422,0.824446
2245\C,0,1.7517634447,0.0791090998,2.300289195\H,0,1.6479413021,-0.579
2476529,3.1628216337\H,0,2.763186291,0.4809148146,2.3251204087\H,0,1.0
512634396,0.9035519223,2.4120817465\C,0,3.6970770885,0.6364518219,-0.7
354597879\H,0,4.2963561548,1.3876130379,-1.2488488089\H,0,4.1759082799
,0.4456188798,0.2234524982\H,0,3.722824048,-0.2778188973,-1.3244827804
\C,0,2.2733405262,2.4372295951,0.2540866991\H,0,2.81964098,3.213796335
8,-0.2814515859\H,0,1.2604428726,2.7942909664,0.4182803002\H,0,2.75154
55829,2.3126205222,1.2222557763\C,0,-3.0946242937,1.6426525093,-1.1825
873592\H,0,-3.6581038873,0.7760162299,-1.5216377533\H,0,-3.7889308817,
2.4729914105,-1.0540579714\H,0,-2.3929228113,1.917199205,-1.9685658693
\C,0,-1.608316433,2.5756627072,0.6032068792\H,0,-2.2987058944,3.401701
2153,0.7726632423\H,0,-1.083087465,2.3689659977,1.5337994597\H,0,-0.88
23073577,2.9042002117,-0.1390373554\H,0,-0.0535169377,1.7707484336,-3.
1857789244\C,0,0.1182264448,2.4065008582,-4.049435172\Cl,0,0.258659609
1,4.0629547922,-3.4684557602\Cl,0,1.611627651,1.8769363532,-4.81649287
4\Cl,0,-1.2516791747,2.2301206404,-5.1390988365\\Version=AM64L-G03RevD
.01\State=1-A\HF=-2422.4589239\RMSD=5.131e-09\Thermal=0.\Dipole=-0.263
0897,-0.803348,1.3295827\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	237.4259

22_5*CHCl3_1

1\1\GINC-NAUTILUS\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\BORIS\25-D
ec-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3
/76=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=re
ad\\nmr_22_5_c_01\\0,1\P,0,0.1830375216,0.5704382636,-0.2186313647\C,0
,0.22127107,2.3575158171,0.126637258\H,0,0.4043090802,2.7166459319,1.1
336869858\C,0,0.1205385694,3.2454183685,-0.8550799466\H,0,0.1923763634
,4.3091510879,-0.6724038022\H,0,-0.0401630579,2.9455139078,-1.88209562
22\N,0,1.4256600414,0.0038908994,0.7984313047\N,0,-1.3380198175,0.1185
58183,0.409534546\C,0,2.5469604743,-0.7236414868,0.2004320461\H,0,3.21
16302836,-0.9739572973,1.0270909303\C,0,1.5056246127,0.3055270498,2.22
19125551\H,0,0.593987674,0.8487037639,2.4690786265\C,0,-2.0330393891,0
.8749292811,1.451903868\H,0,-1.2805184174,1.5319992743,1.8835563443\C,
0,-1.8945445101,-1.0961973284,-0.1909739109\H,0,-1.2886005436,-1.25189
16032,-1.086021242\C,0,2.6818171899,1.2102344609,2.5724076512\H,0,2.65
88392233,1.4757755302,3.6292719167\H,0,3.6352552633,0.718222965,2.3818
715361\H,0,2.6560736281,2.1268698455,1.9863207583\C,0,1.5041004373,-0.
9514705285,3.0831639573\H,0,1.474894412,-0.6890634391,4.1405031318\H,0
,0.6372274747,-1.5682411358,2.8575406715\H,0,2.3986957827,-1.552823861
,2.9234032445\C,0,-3.1203392827,1.8029029773,0.9151214395\H,0,-3.44183
98554,2.4867881019,1.7015216476\H,0,-2.7373255471,2.394219733,0.086938
8118\H,0,-3.9986816761,1.2614364052,0.5743705458\C,0,-2.5582658091,0.0
361975985,2.6088581779\H,0,-2.9139775116,0.6965536791,3.3995417768\H,0
,-3.3970678397,-0.5918554887,2.3155312101\H,0,-1.7800429569,-0.6009431
445,3.0234937418\C,0,-3.330171883,-0.9661875024,-0.6783102622\H,0,-3.5
917554302,-1.8504752099,-1.2585841524\H,0,-4.0426925071,-0.8985097199,
0.1418466619\H,0,-3.4510826101,-0.0948429813,-1.3177871592\C,0,-1.7174
635275,-2.3567118459,0.6516798829\H,0,-1.9299800936,-3.2379523549,0.04
59067224\H,0,-0.6936803255,-2.4333500417,1.0100628198\H,0,-2.383422145
2,-2.3832732339,1.5107408596\C,0,3.3512886846,0.1280747605,-0.77303179
54\H,0,3.6690177465,1.0570219715,-0.3034153746\H,0,4.2384147984,-0.407
2580536,-1.1118462949\H,0,2.7617050025,0.3815707435,-1.6531986993\C,0,
2.1214060998,-2.0380145299,-0.4357169743\H,0,2.9876497513,-2.576192907
8,-0.8202277639\H,0,1.6182277866,-2.6738834084,0.290099532\H,0,1.44028
81628,-1.8689174087,-1.2687042183\H,0,0.2323365437,0.1456274846,-2.864
4344598\C,0,0.0664540777,0.0303143932,-3.9321694352\Cl,0,1.5064786234,
0.5911595186,-4.7732868659\Cl,0,-0.2301234896,-1.6758497434,-4.2484180
028\Cl,0,-1.3363232834,1.0063669784,-4.3572871252\\Version=AM64L-G03Re
vD.01\State=1-A\HF=-2422.4598649\RMSD=5.772e-10\Thermal=0.\Dipole=0.05
57015,0.1570993,1.5507473\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	253.7436

22_5*$CHCl_3$_2

1\1\GINC-YIN\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\BORIS\26-Dec-20
10\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=0
572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read\\n
mr_22_5_c_02\\0,1\P,0,0.2029112039,0.6068212476,-0.1874319231\C,0,0.27
63582238,2.3856893347,0.2230071813\H,0,0.5638610811,2.7079907361,1.218
6745261\C,0,0.0513336104,3.3127840731,-0.7035576291\H,0,0.1160866605,4
.3709008004,-0.4861395032\H,0,-0.2234697474,3.0444898379,-1.7157856683
\N,0,1.434952169,-0.0007252085,0.8229442786\N,0,-1.3367367339,0.190792
2114,0.4297334465\C,0,2.5112646517,-0.7782564286,0.2034676838\H,0,3.17
77030348,-1.0669289986,1.0160612568\C,0,1.5162640593,0.2248050628,2.25
94261286\H,0,0.6352236753,0.8070914926,2.5262735966\C,0,-1.9871609626,
0.9020825921,1.5302399897\H,0,-1.2061967724,1.5133567176,1.9790182109\
C,0,-1.9514967601,-0.9560251851,-0.2427453921\H,0,-1.3648153092,-1.069
5674241,-1.1563495019\C,0,2.7380153182,1.0432557532,2.6617790005\H,0,2
.720023513,1.2585688392,3.730110517\H,0,3.6646890097,0.5088474592,2.45
39788092\H,0,2.7708982797,1.9874346347,2.1214677768\C,0,1.4372291852,-
1.0701499403,3.0591044842\H,0,1.409875628,-0.8585103414,4.1278645677\H
,0,0.5422695231,-1.6292862046,2.7954879398\H,0,2.3010065566,-1.7090079
068,2.8771798224\C,0,-3.0630202404,1.8885789977,1.0801162107\H,0,-3.33
72339686,2.5373596158,1.91281037\H,0,-2.6919156052,2.5133913819,0.2715
58339\H,0,-3.9685296653,1.3914361376,0.7430764033\C,0,-2.5116798417,0.
0113041694,2.6483918441\H,0,-2.8280009247,0.6319782611,3.4866519405\H,
0,-3.3770148636,-0.5706682051,2.3371013732\H,0,-1.746076614,-0.6747086
356,3.0036616713\C,0,-3.389597785,-0.7380684635,-0.6911023445\H,0,-3.6
950719697,-1.567013189,-1.329088322\H,0,-4.0846127864,-0.706034423,0.1
46220735\H,0,-3.4897230067,0.1830657541,-1.2607697801\C,0,-1.816181421
9,-2.2781366986,0.5091947356\H,0,-2.0689424237,-3.107334731,-0.1523582
251\H,0,-0.7934403135,-2.4194622697,0.8502408235\H,0,-2.4749244271,-2.
3386634097,1.3722043545\C,0,3.3342249041,0.0475256038,-0.7756995465\H,
0,3.7279488542,0.9398204196,-0.2916416713\H,0,4.1760258547,-0.52904239
55,-1.1594164923\H,0,2.726615136,0.3557452107,-1.6258833244\C,0,2.0170
455021,-2.0631100768,-0.4444369438\H,0,2.8528175901,-2.6362761127,-0.8
458784338\H,0,1.4928603805,-2.6857793266,0.2779900891\H,0,1.3362643645
,-1.8441537629,-1.2659002035\H,0,2.6277584865,3.4738065633,-1.26266548
68\C,0,3.4626681657,4.1043894007,-1.5388328762\Cl,0,4.51985183,4.23003
0592,-0.1371054909\Cl,0,4.289358581,3.3538833409,-2.8956472215\Cl,0,2.
8120544402,5.6785793166,-1.9832155656\\Version=AM64L-G03RevD.01\State=
1-A\HF=-2422.4563185\RMSD=1.797e-09\Thermal=0.\Dipole=-0.5758357,-0.46
70734,0.894581\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	252.9543

22_8*$CHCl_3$_1

1\1\GINC-GOLEM\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\BORIS\31-Dec-
2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76
=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read\
\nmr_22_8_c_01\\0,1\P,-0.552298,-0.164412,0.445772\C,-0.862782,-0.2064
61,2.241554\H,-1.876242,-0.09563,2.614308\C,0.124488,-0.450082,3.09493
7\H,-0.048057,-0.546875,4.158415\H,1.147636,-0.566957,2.762673\N,-1.52
6078,-1.421144,-0.147195\N,-1.485977,1.236765,0.012511\C,-0.891137,-2.
567282,-0.799724\H,-1.699229,-3.265871,-1.015086\C,-2.93382,-1.53845,0
.219826\H,-3.191158,-0.585726,0.681685\C,-1.554154,2.359421,0.948656\H
,-1.105633,1.995168,1.872085\C,-1.567405,1.423254,-1.4372\H,-1.692196,
0.410612,-1.822514\C,-3.194917,-2.649233,1.229381\H,-4.238626,-2.64201
9,1.543697\H,-2.991314,-3.631606,0.802886\H,-2.569921,-2.529797,2.1120
87\C,-3.835897,-1.684587,-0.998915\H,-4.882305,-1.681594,-0.694611\H,-

3.682034,-0.863688,-1.69566\H,-3.657789,-2.619143,-1.530798\C,-0.74783
,3.596776,0.571744\H,-0.757018,4.298374,1.405636\H,0.288444,3.345891,0
.356318\H,-1.163742,4.116258,-0.289441\C,-2.989205,2.734685,1.307374\H
,-2.99469,3.434169,2.143969\H,-3.512984,3.207944,0.480628\H,-3.553049,
1.850719,1.599837\C,-0.314152,1.980721,-2.113399\H,-0.37285,1.812112,-
3.188925\H,-0.19099,3.048998,-1.956507\H,0.582421,1.480548,-1.751038\C
,-2.804948,2.188638,-1.878981\H,-2.89677,2.130752,-2.963278\H,-3.70576
9,1.767748,-1.437307\H,-2.754516,3.244232,-1.618146\C,0.101452,-3.2989
33,0.095198\H,-0.355421,-3.569284,1.045181\H,0.453962,-4.210205,-0.388
065\H,0.971875,-2.678693,0.305662\C,-0.261535,-2.189161,-2.13107\H,0.1
63653,-3.065992,-2.618959\H,-1.00248,-1.752661,-2.79853\H,0.541076,-1.
465731,-1.993173\H,2.099801,-0.080822,0.01339\C,3.178421,0.039688,-0.0
46782\Cl,3.905024,-1.093097,1.090294\Cl,3.556731,1.702262,0.38933\Cl,3
.675616,-0.313186,-1.697024\\Version=AM64L-G03RevD.01\State=1-A\HF=-24
22.4582254\RMSD=1.490e-09\Thermal=0.\Dipole=-1.3890671,-0.1694895,0.21
32453\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	236.5452

22_4*CHCl$_3$_2

1\1\GINC-CALYPSO\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\BORIS\26-De
c-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/
76=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=rea
d\\nmr_22_4_c_02\\0,1\P,0,-0.0342252618,0.5716940687,0.0458417014\C,0,
-0.0684259943,2.0654114673,1.1011966272\H,0,0.4031855379,2.0447039709,
2.078829598\C,0,-0.5973179317,3.2084858872,0.6736322135\H,0,-0.6066750
544,4.10212929,1.2843403488\H,0,-1.0594974618,3.2876256123,-0.30204096
59\N,0,1.3643818809,-0.2244318643,0.6156689728\N,0,-1.42233188,-0.2389
299657,0.6115711398\C,0,2.4036163031,-0.4062355505,-0.4005086815\H,0,1
.8626571025,-0.3636277226,-1.3473943773\C,0,1.5405735016,-0.575116707,
2.0199869308\H,0,0.6783776069,-0.1398185392,2.5264008934\C,0,-2.056929
6418,-0.0375618295,1.9105644406\H,0,-1.3796592808,0.5909883156,2.48661
16127\C,0,-2.1648366777,-1.0352680565,-0.3699964493\H,0,-3.0116223738,
-1.4609966325,0.1676441626\C,0,2.773687041,0.0310651861,2.678917136\H,
0,2.7442447211,-0.1517536687,3.7531705928\H,0,3.6930073485,-0.41369774
76,2.302257239\H,0,2.8248346357,1.1058878442,2.516697517\C,0,1.4657251
315,-2.0740534859,2.3058501862\H,0,1.3067432857,-2.239763345,3.3719376
152\H,0,0.6399061576,-2.5250214523,1.7611933961\H,0,2.3791434322,-2.59
46805537,2.0310888452\C,0,-3.3725342649,0.7239325931,1.804343127\H,0,-
3.783879716,0.9145082806,2.7955005248\H,0,-3.2213497623,1.6792483781,1
.306272059\H,0,-4.1189954251,0.1601935547,1.2451031921\C,0,-2.23845475
67,-1.3319922797,2.6935696021\H,0,-2.6367319447,-1.1183184567,3.685370
0416\H,0,-2.9390536837,-2.0084146489,2.2047388471\H,0,-1.2924388651,-1
.8542497574,2.8103528069\C,0,-1.3431780953,-2.2010471338,-0.8998758855
\H,0,-1.9406466763,-2.8205228714,-1.5688754126\H,0,-0.4793445653,-1.84
4807421,-1.4609817675\H,0,-0.9824433057,-2.8239576633,-0.0837427268\C,
0,-2.7295111721,-0.2025106231,-1.5142748339\H,0,-3.3466704462,-0.81915
77043,-2.1679635173\H,0,-3.3424648007,0.6138052848,-1.1366888654\H,0,-
1.9270373026,0.2251185681,-2.1127934742\C,0,3.0995948703,-1.758559088,
-0.3697111875\H,0,2.3794628763,-2.5734577291,-0.3601201352\H,0,3.71646
00182,-1.8621903986,-1.2619103855\H,0,3.7601094578,-1.8678866574,0.488
8534987\C,0,3.4225968179,0.7287648033,-0.4500142104\H,0,4.0649216673,0
.6210565569,-1.3244603708\H,0,2.915793688,1.6892096919,-0.5269088312\H
,0,4.0625535616,0.753482431,0.4288433645\H,0,1.8604963415,4.1451876935
,0.3714145739\C,0,2.5805416859,4.935408708,0.538433122\Cl,0,3.49208283
56,4.52312801,1.9864436363\Cl,0,3.6271793681,5.0276996027,-0.869870598
6\Cl,0,1.6803107059,6.4314605344,0.7618085712\\Version=AM64L-G03RevD.0
1\State=1-A\HF=-2422.4561532\RMSD=1.761e-09\Thermal=0.\Dipole=-0.52886
37,-0.7969002,0.5367357\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) +	247.8256

PCM(CHCl3,UAHF)	

22_6*$CHCl_3$_2

1\1\GINC-CALYPSO\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\BORIS\29-De
c-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/
76=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=rea
d\\nmr_22_6_c_02_2\\0,1\P,0,1.7349188518,0.1106200632,-1.0399286347\C,
0,0.1676400468,-0.3710201797,-1.8015473827\H,0,0.1568307295,-1.3714253
865,-2.2135414598\C,0,-0.8325645267,0.4504693451,-2.1099438893\H,0,-1.
6513637942,0.1305731012,-2.7408163679\H,0,-0.8401628207,1.479655086,-1
.7828251273\N,0,1.3169050984,1.4777688275,-0.1127098752\N,0,2.14072230
71,-1.2711950442,-0.1095659408\C,0,2.1938159805,2.6505417032,-0.240294
4058\H,0,1.841381703,3.3644317349,0.5026234308\C,0,0.3232017713,1.5246
681603,0.9550540792\H,0,-0.2788088478,0.6279377685,0.837401299\C,0,1.3
260787274,-2.3679817964,0.4209066109\H,0,1.973215689,-2.8756882701,1.1
36637255\C,0,3.5872860832,-1.4262566118,0.0885963457\H,0,4.0410469945,
-0.5804748202,-0.4271466045\C,0,-0.6289312175,2.7118259627,0.850449381
5\H,0,-1.4209350885,2.6121801175,1.5921359916\H,0,-0.1292114824,3.6606
02455,1.041583913\H,0,-1.0934089907,2.7719351582,-0.1306509919\C,0,0.9
571695809,1.4856274408,2.3404867023\H,0,0.1918451671,1.4436024611,3.11
55890095\H,0,1.6024559275,0.6168248756,2.4459823006\H,0,1.5582709613,2
.3766671896,2.5235725891\C,0,0.0992782339,-1.9349911212,1.2017491598\H
,0,-0.3803389073,-2.8086474905,1.6423071542\H,0,0.354025326,-1.2480207
601,2.0040019413\H,0,-0.6330377892,-1.4623452107,0.5500744532\C,0,0.92
78900473,-3.4243246023,-0.6118805105\H,0,0.6500678529,-4.3489400853,-0
.1049274753\H,0,0.0647541963,-3.1151934807,-1.1975103373\H,0,1.7419829
043,-3.6467112717,-1.2957650581\C,0,4.1606585744,-2.6830374509,-0.5522
374183\H,0,5.2461221411,-2.6866523475,-0.4560612871\H,0,3.7908324832,-
3.5914128824,-0.0772596085\H,0,3.9147823474,-2.7232418184,-1.611801698
5\C,0,3.9987452568,-1.3242331991,1.5517013795\H,0,5.0846358329,-1.3434
477627,1.6404447324\H,0,3.6386793102,-0.3960195501,1.9891026968\H,0,3.
613520554,-2.1514704492,2.1481087178\C,0,2.0504735562,3.3087487813,-1.
6041783251\H,0,1.0125763705,3.5741076204,-1.7970976406\H,0,2.653284485
8,4.2152537137,-1.6646996771\H,0,2.3791665537,2.6308071358,-2.39098136
18\C,0,3.6557334447,2.3763951732,0.082948416\H,0,4.2186798676,3.309770
0966,0.1018150086\H,0,3.7588279575,1.8981816343,1.0552345668\H,0,4.109
0643138,1.7320993014,-0.6684560481\H,0,-2.5903085857,-0.1054005853,-0.
3545276343\C,0,-3.6159475712,-0.2131361037,-0.025545438\Cl,0,-3.632783
6384,-0.1625263179,1.7328624827\Cl,0,-4.5323604262,1.1232448655,-0.709
4538665\Cl,0,-4.2025945431,-1.759812174,-0.6231305523\\Version=AM64L-G
03RevD.01\State=1-A\HF=-2422.4547282\RMSD=7.533e-10\Thermal=0.\Dipole=
0.6074305,-0.0959464,0.5319707\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	247.5471

22_9*$CHCl_3$_2

1\1\GINC-SOLARIS\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\BORIS\31-De
c-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/
76=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=rea
d\\nmr_22_9_c_02_2\\0,1\P,-0.982105,-0.131703,-0.536875\C,0.080771,-0.
994274,0.671804\H,0.261684,-0.54788,1.644229\C,0.708866,-2.1258,0.3651
39\H,1.364548,-2.626154,1.065417\H,0.582306,-2.602004,-0.598832\N,-2.5
33773,-0.746639,-0.13937\N,-0.836384,1.469294,0.013672\C,-3.379684,-0.
917616,-1.327817\H,-3.06485,-0.122765,-2.005511\C,-2.860044,-1.341891,
1.15462\H,-1.95355,-1.230872,1.747564\C,-1.163687,1.904563,1.364618\H,
-1.442581,1.00518,1.913918\C,-0.514519,2.507417,-0.968298\H,-0.493871,
3.445438,-0.414166\C,-3.129751,-2.840755,1.109586\H,-3.207582,-3.22930
8,2.125046\H,-4.064454,-3.074785,0.603234\H,-2.321541,-3.365875,0.6052
65\C,-3.958527,-0.625544,1.937881\H,-3.950591,-0.971564,2.972104\H,-3.
799529,0.449722,1.941072\H,-4.951681,-0.818941,1.54168\C,0.033096,2.52
0988,2.079779\H,-0.218918,2.764433,3.111918\H,0.87879,1.835986,2.08360
5\H,0.354225,3.443783,1.597283\C,-2.367399,2.838776,1.408537\H,-2.6513

19,3.04784,2.439786\H,-2.151245,3.79462,0.932406\H,-3.21907,2.393472,0
.899058\C,-1.56869,2.652084,-2.057414\H,-1.34445,3.505149,-2.698065\H,
-1.596482,1.763087,-2.686779\H,-2.557695,2.797756,-1.626606\C,0.870446
,2.314962,-1.568087\H,1.120313,3.136733,-2.23936\H,1.626105,2.271848,-
0.785636\H,0.916622,1.389558,-2.140821\C,-4.862919,-0.684428,-1.088283
\H,-5.03777,0.262468,-0.582523\H,-5.377341,-0.656132,-2.048299\H,-5.32
1222,-1.480044,-0.503745\C,-3.145661,-2.225647,-2.078048\H,-3.660923,-
2.202894,-3.038861\H,-2.083213,-2.364134,-2.272041\H,-3.508932,-3.0907
8,-1.529006\H,2.810694,-0.5903,-0.228871\C,3.878001,-0.535352,-0.06099
1\Cl,4.122273,0.166672,1.535006\Cl,4.582447,0.473774,-1.315318\Cl,4.51
0832,-2.175774,-0.13437\\Version=AM64L-G03RevD.01\State=1-A\HF=-2422.4
56228\RMSD=1.543e-09\Thermal=0.\Dipole=-1.0150487,0.1961244,0.4758125\
PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	253.1536

22_8*CHCl$_3$_2

1\1\GINC-SOLARIS\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\BORIS\29-De
c-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/
76=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=rea
d\\nmr_22_8_c_02\\0,1\P,0,0.0864558318,0.5944741336,-0.7275671474\C,0,
0.0946999233,2.2612080849,0.0296635055\H,0,-0.0668035901,2.3791040347,
1.0970106941\C,0,0.4154183466,3.3244190915,-0.7019543957\H,0,0.5318060
924,4.3097637516,-0.2691441269\H,0,0.5974003766,3.2395211569,-1.765902
1117\N,0,1.3497489398,-0.1860017346,0.0992055197\N,0,-1.307780929,-0.0
819537108,0.0722918483\C,0,2.5164002246,-0.6240279218,-0.6687444531\H,
0,3.218640167,-1.0242814682,0.0622292074\C,0,1.444115481,-0.1937973693
,1.5543180272\H,0,0.4741099405,0.1567379495,1.90576722\C,0,-2.44880881
54,0.7826188083,0.3657700884\H,0,-2.0896112514,1.7986432032,0.20393402
39\C,0,-1.4726477927,-1.5023637768,-0.2433418108\H,0,-0.4561476166,-1.
8960877959,-0.2043505779\C,0,2.5202319275,0.7440181314,2.0880209646\H,
0,2.4949678137,0.7750679717,3.1773914277\H,0,3.5170801828,0.4132289116
,1.7956758206\H,0,2.3794739581,1.7558037413,1.7130420508\C,0,1.6229322
135,-1.6002852299,2.111445214\H,0,1.5978263886,-1.5801621078,3.2007664
873\H,0,0.8285041046,-2.25719464,1.7644324101\H,0,2.577541175,-2.03730
48931,1.8187942165\C,0,-3.6592985186,0.6345808324,-0.5490205033\H,0,-4
.3756947665,1.4266164468,-0.3322358597\H,0,-3.3767971617,0.7135661586,
-1.596771152\H,0,-4.1729801024,-0.3135344304,-0.4028178436\C,0,-2.8667
274458,0.7311023465,1.8327434168\H,0,-3.5710505614,1.5352942744,2.0477
65187\H,0,-3.3499932379,-0.2068561753,2.0944800718\H,0,-2.0006157326,0
.8545412248,2.480367617\C,0,-1.9953613478,-1.8211134349,-1.645516134\H
,0,-1.8048107758,-2.8693103916,-1.8777587801\H,0,-3.065420526,-1.65534
97165,-1.7412115849\H,0,-1.4883151367,-1.2168358387,-2.3961875373\C,0,
-2.2542511596,-2.2689056116,0.811739426\H,0,-2.176141347,-3.3375338064
,0.6130858314\H,0,-1.8618569767,-2.0769941999,1.8081505944\H,0,-3.3137
654988,-2.0190771832,0.8044644697\C,0,3.2219505393,0.5161928551,-1.391
9331639\H,0,3.4620986082,1.3249525724,-0.7044061339\H,0,4.1480949522,0
.1674910595,-1.8494613062\H,0,2.5899993017,0.9198794317,-2.1822139736\
C,0,2.1743853354,-1.7530485733,-1.6288446221\H,0,3.0653651888,-2.09403
95314,-2.156057393\H,0,1.7493042819,-2.6001131846,-1.0931463417\H,0,1.
4516144302,-1.42127035,-2.3735472969\H,0,-2.0179021461,4.0980317413,-1
.1536491371\C,0,-2.7643956798,4.8531359012,-1.3614185478\Cl,0,-1.92315
99904,6.3865917344,-1.5541330249\Cl,0,-3.6004704016,4.3954978882,-2.83
77619186\Cl,0,-3.8674724668,4.9026327487,0.0090373679\\Version=AM64L-G
03RevD.01\State=1-A\HF=-2422.4539449\RMSD=6.731e-10\Thermal=0.\Dipole=
0.545283,-0.5333623,0.6694687\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	230.8414

22_10*CHCl$_3$_1

1\1\GINC-EDDY\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\BORIS\30-Dec-2
010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/76=
0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=read\\
nmr_22_10_c_01\\0,1\P,0,0.0651484268,0.5531832835,-0.6117736713\C,0,0.
0179115018,2.1214366306,0.3162864795\H,0,-0.1754022688,2.1176118592,1.
3821870725\C,0,0.2408815575,3.2733599212,-0.3047367576\H,0,0.248869071
3,4.2171674315,0.2238411338\H,0,0.4232398778,3.3199304048,-1.370576799
6\N,0,1.4123949979,-0.268776717,0.0681123891\N,0,-1.3024633545,-0.2725
94959,0.1001646444\C,0,2.4620914632,-0.6067474976,-0.9078120992\H,0,3.
1631479595,-1.2441227082,-0.3766675113\C,0,1.8626958169,0.0581201011,1
.4360422258\H,0,2.0202284223,1.1397216636,1.5130088052\C,0,-2.63295392
37,0.3199407378,-0.1031373998\H,0,-3.3268433931,-0.519188004,-0.102794
9142\C,0,-1.2625776595,-1.7343075352,-0.0000097126\H,0,-0.2137029661,-
1.9976783853,0.1240563698\C,0,3.1783325708,-0.6002776585,1.8277506041\
H,0,3.3813482184,-0.3552759732,2.869231022\H,0,3.1186926945,-1.6860110
34,1.7525224557\H,0,4.0289130137,-0.2544215817,1.2450442133\C,0,0.8168
816169,-0.3458521171,2.4645522106\H,0,1.0969962298,0.0329534075,3.4474
390066\H,0,-0.1735956196,0.020297664,2.2143552306\H,0,0.7567543892,-1.
4325158949,2.5244666051\C,0,-3.0447615177,1.2117283047,1.0612292781\H,
0,-4.0982876739,1.4801663021,0.9762050983\H,0,-2.8981469967,0.69455234
23,2.0074474238\H,0,-2.4719664176,2.1363867398,1.0820348066\C,0,-2.837
098104,1.0383544814,-1.4332793853\H,0,-3.8825564805,1.328274406,-1.535
7206661\H,0,-2.244622896,1.9496757116,-1.5001431277\H,0,-2.5824828604,
0.399748799,-2.2768539595\C,0,-1.7274482644,-2.2886860267,-1.343547555
1\H,0,-1.5742568323,-3.3672046794,-1.3826278931\H,0,-2.7889782926,-2.1
066963866,-1.5120517407\H,0,-1.1757043473,-1.8420305217,-2.1691661019\
C,0,-2.0202508059,-2.3863643035,1.1480695264\H,0,-1.8724204507,-3.4659
373069,1.1264049109\H,0,-1.6688210804,-2.0103299506,2.1059946503\H,0,-
3.0940248612,-2.209048039,1.0881982322\C,0,3.2293964096,0.6065628235,-
1.4173905805\H,0,3.6033209118,1.2139275276,-0.5938675948\H,0,4.0810229
642,0.3011582044,-2.0253372304\H,0,2.5904641274,1.2376104808,-2.034279
9637\C,0,1.9403860339,-1.4545389089,-2.0555469663\H,0,2.776728567,-1.7
844349964,-2.6709915037\H,0,1.4250494382,-2.3373483246,-1.6819605748\H
,0,1.2576948393,-0.9053598638,-2.6994320351\H,0,-0.0580166171,1.187510
243,-3.2912630107\C,0,-0.161127973,1.4518959012,-4.3405947967\Cl,0,1.4
53573343,1.5878090805,-5.0289149122\Cl,0,-1.0779533174,0.1736857696,-5
.1293408317\Cl,0,-1.0120250981,2.9911422413,-4.4273418991\\Version=AM6
4L-G03RevD.01\State=1-A\HF=-2422.45151\RMSD=1.152e-09\Thermal=0.\Dipol
e=0.2951815,-0.2283885,1.1492483\PG=C01 [X(C15H32Cl3N2P1)]\\@

Level of theory	Shielding, ppm
MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	248.8534

22_10*CHCl$_3$_2

1\1\GINC-CALYPSO\SP\RmPWPW91\6-311++G(2d,2p)\C15H32Cl3N2P1\BORIS\31-De
c-2010\0\\#p mpwpw91/6-311++g(2d,2p) nmr scf=tight int=finegrid IOp(3/
76=0572004280) scrf=(PCM,Read,solvent=chloroform) geom=check guess=rea
d\\nmr_22_10_c_02_2\\0,1\P,1.374456,-0.078136,-0.792612\C,0.079398,-1.
284216,-0.327942\H,-0.063569,-1.57335,0.707002\C,-0.679083,-1.83332,-1
.272106\H,-1.447955,-2.560797,-1.04399\H,-0.5441,-1.584942,-2.317196\N
,0.876838,1.36348,0.004595\N,2.684748,-0.662406,0.218665\C,0.644495,2.
484397,-0.923356\H,0.498565,3.36154,-0.299191\C,0.019302,1.307067,1.20
1969\H,-0.875445,0.712764,0.979262\C,3.231652,-1.986331,-0.115507\H,4.
282263,-1.947812,0.168825\C,3.696505,0.342407,0.557975\H,3.14003,1.265
562,0.70946\C,-0.472911,2.667853,1.674388\H,-1.026293,2.525377,2.60123
6\H,0.360379,3.337335,1.887536\H,-1.144978,3.155118,0.972076\C,0.74332
8,0.642606,2.362929\H,0.046076,0.466777,3.181707\H,1.201116,-0.299592,
2.079487\H,1.537098,1.294811,2.726908\C,2.604338,-3.088435,0.72798\H,3
.145408,-4.025209,0.589783\H,2.638312,-2.825034,1.783309\H,1.567047,-3
.264801,0.451688\C,3.20856,-2.356735,-1.596488\H,3.757623,-3.286207,-1
.746914\H,2.19579,-2.516552,-1.963525\H,3.67058,-1.585254,-2.208825\C,
4.728362,0.596801,-0.537748\H,5.378661,1.426985,-0.261694\H,5.366036,-
0.271573,-0.704482\H,4.246937,0.84638,-1.481928\C,4.377353,0.011807,1.

878484\H,5.040548,0.825665,2.171404\H,3.642099,-0.133585,2.666416\H,4.985802,-0.890307,1.813787\C,-0.599254,2.307973,-1.784986\H,-1.484791,2.124423,-1.176587\H,-0.788298,3.199102,-2.383719\H,-0.473349,1.466315,-2.466183\C,1.861165,2.791987,-1.780402\H,1.687365,3.713286,-2.336047\H,2.744623,2.932808,-1.160441\H,2.064514,2.001597,-2.499435\H,-2.727686,-0.344519,-0.368031\C,-3.74311,-0.430375,-0.005605\Cl,-4.685014,-1.238229,-1.251763\Cl,-4.35,1.190909,0.302697\Cl,-3.692572,-1.383427,1.472426\\Version=AM64L-G03RevD.01\State=1-A\HF=-2422.4479518\RMSD=5.453e-10\Thermal=0.\Dipole=0.4743896,0.2104569,0.0991932\PG=C01 [X(C15H32Cl3N2P1)]\\@

MPW1K/6-311++G(2d,2p) + PCM(CHCl3,UAHF)	245.5574

	MPW1K/6-311++G(2d,2p) + PCM/UAHF/MPW1K/6-311++G(2d,2p)	MP2(FC)/6-31+G(2d,p)//MPW1K/6-31G(d) + PCM/UAHF/MPW1K/6-311++G(2d,2p)		
	Chemical shift, ppm (relative to PPh_3)	E_{tot}	„G“$_{298,\ gas}$	„G“$_{298,CHCl3}$
22_1*CHCl3_1	+62.4	-2418.012453	-2417.605115	-2417.588063
22_1*CHCl3_2	+65.9	-2418.011455	-2417.603255	-2417.586714
22_2*CHCl3_1	+52.1	-2418.011107	-2417.603583	-2417.585496
22_2*CHCl3_2	+50.8	-2418.006454	-2417.600627	-2417.584356
22_3*CHCl3_1	+82.7	-2418.010381	-2417.601381	-2417.583835
22_7*CHCl3_2	+98.7	-2418.007090	-2417.599424	-2417.583280
22_3*CHCl3_2	+85.1	-2418.004473	-2417.598363	-2417.582682
22_4*CHCl3_1	+83.4	-2418.006987	-2417.598943	-2417.581206
22_9*CHCl3_1	+76.6	-2418.005694	-2417.598336	-2417.580631
22_6*CHCl3_1	+78.2	-2418.006641	-2417.597699	-2417.580599
22_7*CHCl3_1	+94.5	-2418.006008	-2417.597546	-2417.580399
22_5*CHCl3_1	+78.1	-2418.006719	-2417.598061	-2417.580133
22_5*CHCl3_2	+78.9	-2418.001595	-2417.595216	-2417.579918
22_8*CHCl3_1	+95.3	-2418.006382	-2417.597685	-2417.579869
22_4*CHCl3_2	+84.1	-2418.001342	-2417.595296	-2417.579790
22_6*CHCl3_2	+84.3	-2418.002483	-2417.594869	-2417.579092
22_9*CHCl3_2	+78.7	-2418.000962	-2417.594742	-2417.578966
22_8*CHCl3_2	+101.0	-2418.000476	-2417.593966	-2417.578030
22_10*CHCl3_1	+83.0	-2418.002900	-2417.592096	-2417.575697
22_10*CHCl3_2	+86.3	-2417.998250	-2417.589613	-2417.573932

<δ> = 62.8 ppm