

B3LYP/6-31G* optimised coordinates of compounds **2**, **4**, **9** and Mes*₂P(=O)*t*Bu (in Å, xyz format).

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Compound **2**

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P 2.467712408 4.3262770653 3.3222460887
O 1.3229023233 3.8326448025 4.1685132387
C 4.0312862187 3.3436289769 3.5575823227
C 4.9421123302 3.5288247579 4.640338202
C 6.2522553849 3.030972395 4.4881078679
C 6.6839108829 2.322469807 3.3771897397
C 5.6980792136 1.961171102 2.4531332396
C 4.3697602972 2.3848636329 2.5254331581
C 4.6776641562 4.0880958159 6.0807939548
C 3.2601670503 4.5903181852 6.397117242
C 5.6577657173 5.2361833516 6.4247895534
C 4.9224013186 2.8984710797 7.0550543857
C 8.1390513461 1.86477548 3.1768249264
C 9.0760923454 2.3904568208 4.2808414815
C 8.2044186933 0.3186595214 3.1832571296
C 8.6536107884 2.3940582942 1.8169295191
C 3.3785328185 1.6682841164 1.5279025184
C 3.9554886782 0.2869755203 1.1004511964
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C 2.0275195294 1.3166340541 2.2015978368
C 2.7027558136 6.1811525345 3.4769282759
C 3.9418046886 6.8687915384 3.297796678
C 4.2100851213 7.973230655 4.1248983156
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C 1.9816517093 7.9913020499 4.9204991889
C 1.6328665876 6.8970602837 4.1228830097
C 4.9549604683 6.6712403268 2.127852525
C 4.5119119786 5.6430114567 1.0754578648
C 6.3743351017 6.3152535391 2.6186067667

C 5.0217541432 8.0296984811 1.3694754625
C 3.605766188 9.6242800755 6.0151449418
C 5.0920648232 10.0278712997 5.980422626
C 2.7592669658 10.8750785492 5.6774814393
C 3.2681044179 9.1499896207 7.4487522652
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C -0.2396592343 5.8761100223 2.6272767222
H 2.2675155442 4.1232588691 1.9493989976
H 6.9564308347 3.2149296091 5.2871633393
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H 5.4841635148 6.1004767639 5.7767715098
H 6.7097358276 4.9482839346 6.3343742601
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H 4.2273123664 2.0780433516 6.844388848
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H 5.9393106627 2.4999372755 6.9998384029
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Compound 4

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O 5.0922764362 2.0084937689 5.6232294063
C 5.9958117951 3.8936755023 3.7496706045
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C 7.458471965 5.4860592516 4.8734548779
C 7.0018745154 6.547777138 4.0999978316
C 6.2265636257 6.1986080079 2.9965363217
C 5.73472536 4.9059603841 2.7601080083
C 7.9546153738 3.1316917363 5.4925635456
C 7.9617068975 1.6897218839 4.9401257699
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C 8.19444385 8.1851516721 5.6614891343
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C 4.6311089109 3.3705618453 0.9006814569
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(Mes*)₂P(=O)tBu

P 0.0599186144 1.8071578942 -0.4580429489
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C -3.3145118427 2.5750873882 0.184234985
C -2.8649521973 3.686073191 -0.7834688117
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