

Supplementary Information (SI)

Reactions of diphosphine-stabilized Os₃ clusters with triphenylantimony: Syntheses and structures of new antimony-containing Os₃ clusters via Sb-Ph bond cleavage

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Fig. S7. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\text{HOs}_3(\text{CO})_7(\text{SbPh}_3)\{\mu_3\text{-Ph}_2\text{PCH}_2(\text{Ph})\text{C}_6\text{H}_4\}]$ (**2**) in CD_2Cl_2 .

Fig. S8. Hydride region of the ^1H NMR spectrum of $[\text{HOs}_3(\text{CO})_7(\text{SbPh}_3)(\mu,\eta^2\text{-C}_6\text{H}_4)(\mu\text{-SbPh}_2)(\mu\text{-dppm})]$ (**3**) in CDCl_3 .

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Fig. S11. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\text{HOs}_3(\text{CO})_7(\text{SbPh}_3)(\mu,\eta^2\text{-C}_6\text{H}_4)(\mu\text{-SbPh}_2)(\mu\text{-dppm})]$ (**3**) in CDCl_3 .

Fig. S12. Aliphatic region of the ^1H NMR spectrum of $[\text{Os}_3(\text{CO})_8(\eta^1\text{-Ph})(\text{SbPh}_3)(\mu\text{-SbPh}_2)(\mu\text{-dppm})]$ (**4**) in CD_2Cl_2 .

Fig. S13. Aromatic region of the ^1H NMR spectrum of $[\text{Os}_3(\text{CO})_8(\eta^1\text{-Ph})(\text{SbPh}_3)(\mu\text{-SbPh}_2)(\mu\text{-dppm})]$ (**4**) in CD_2Cl_2 .

Fig. S14. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\text{Os}_3(\text{CO})_8(\eta^1\text{-Ph})(\text{SbPh}_3)(\mu\text{-SbPh}_2)(\mu\text{-dppm})]$ (**4**) in CD_2Cl_2 .

Table S1. Selected bond distances (\AA) and angles ($^\circ$) for clusters **1-4**.

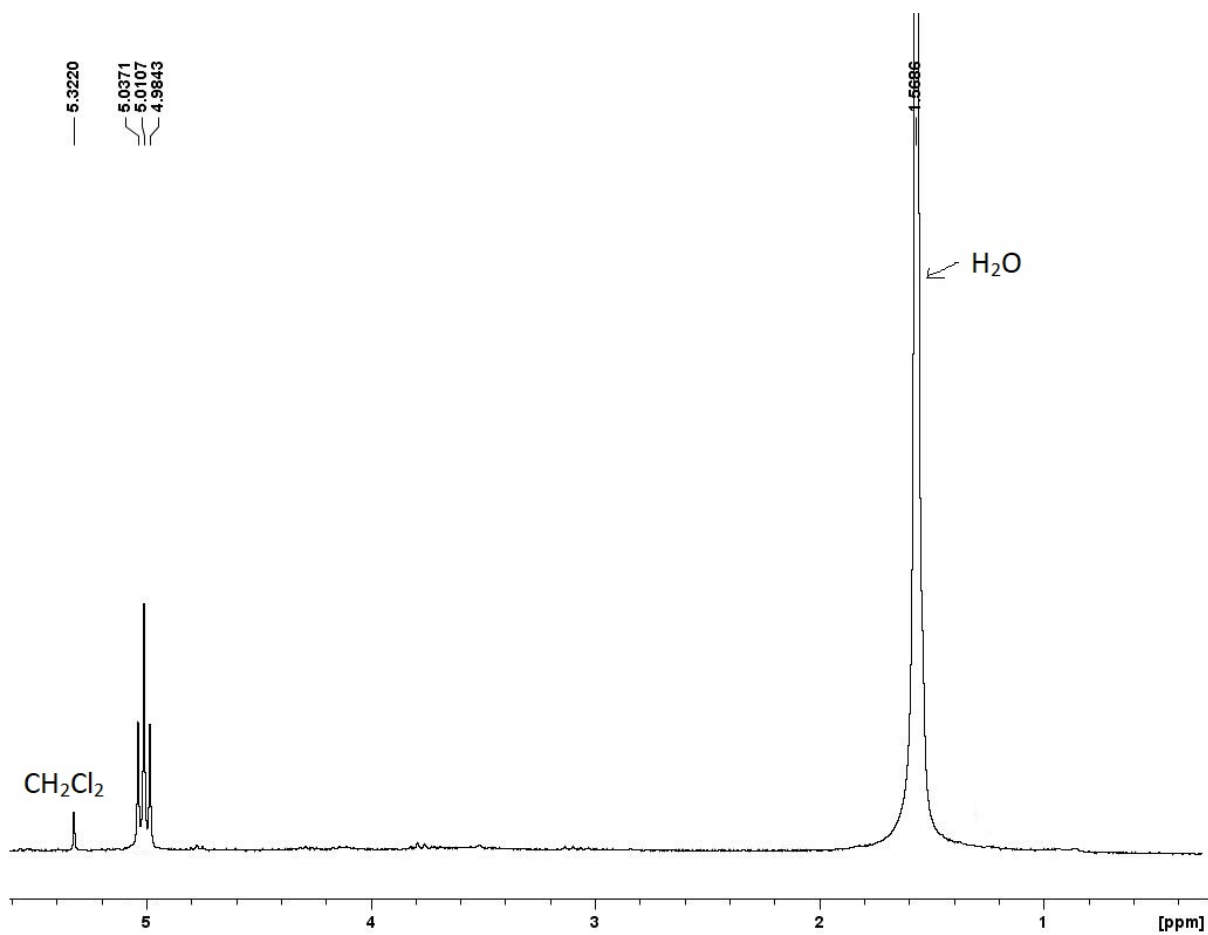


Fig. S1. Aliphatic region of the ^1H NMR spectrum of $[\text{Os}_3(\text{CO})_9(\text{SbPh}_3)(\mu\text{-dppm})]$ (1) in CDCl_3 .

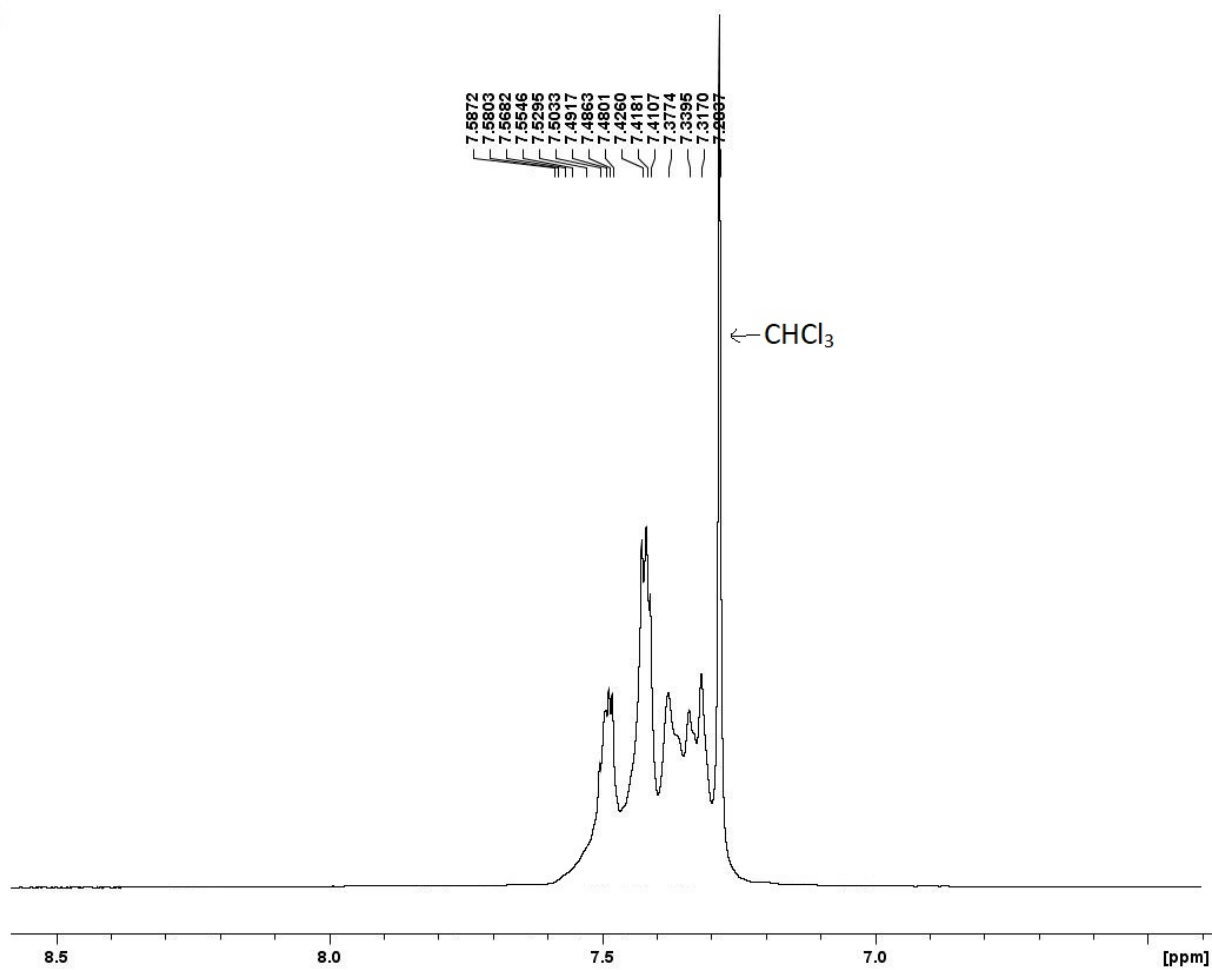


Fig. S2. Aromatic region of the ¹H NMR spectrum of [Os₃(CO)₉(SbPh₃)(μ-dppm)] (**1**) in CDCl₃.

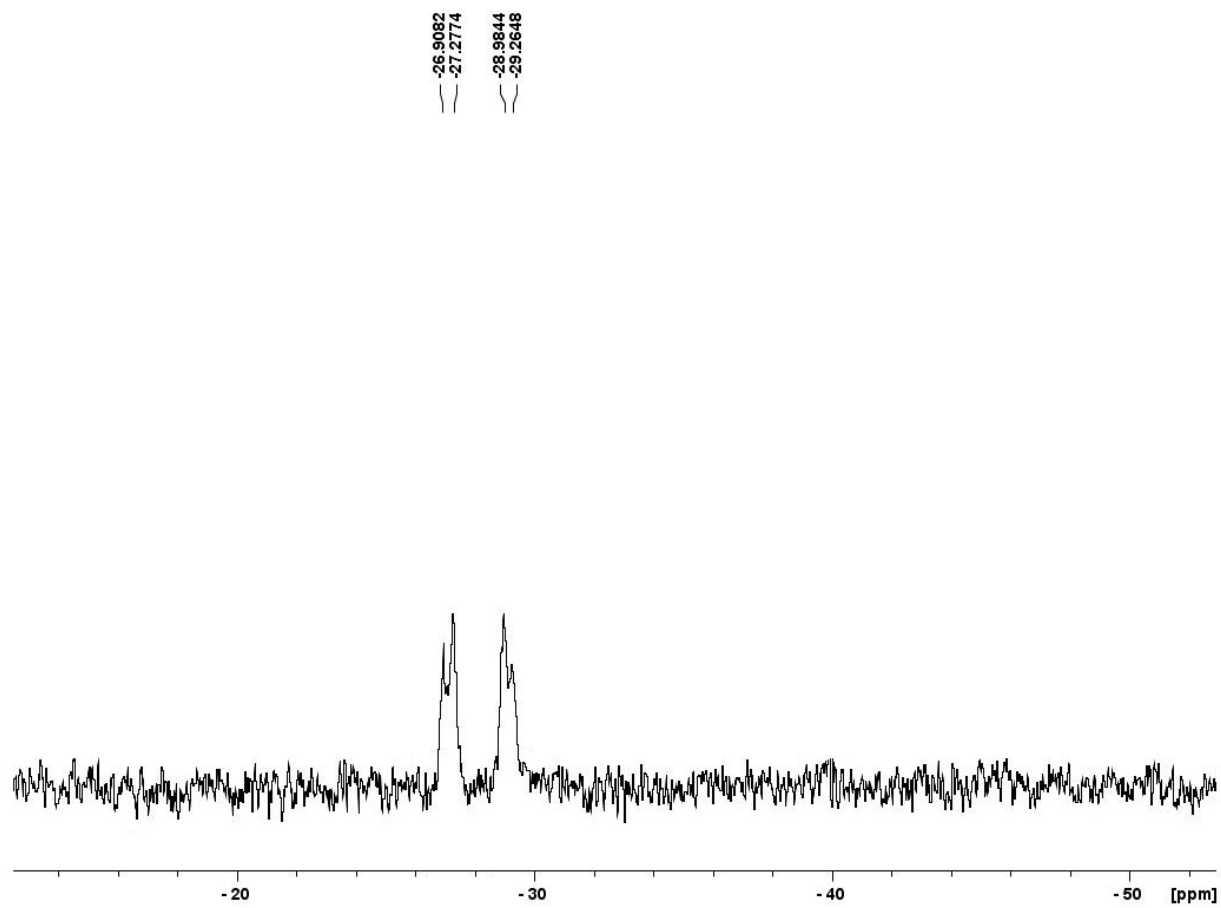


Fig. S3. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\text{Os}_3(\text{CO})_9(\text{SbPh}_3)(\mu\text{-dppm})]$ (**1**) in CDCl_3 .

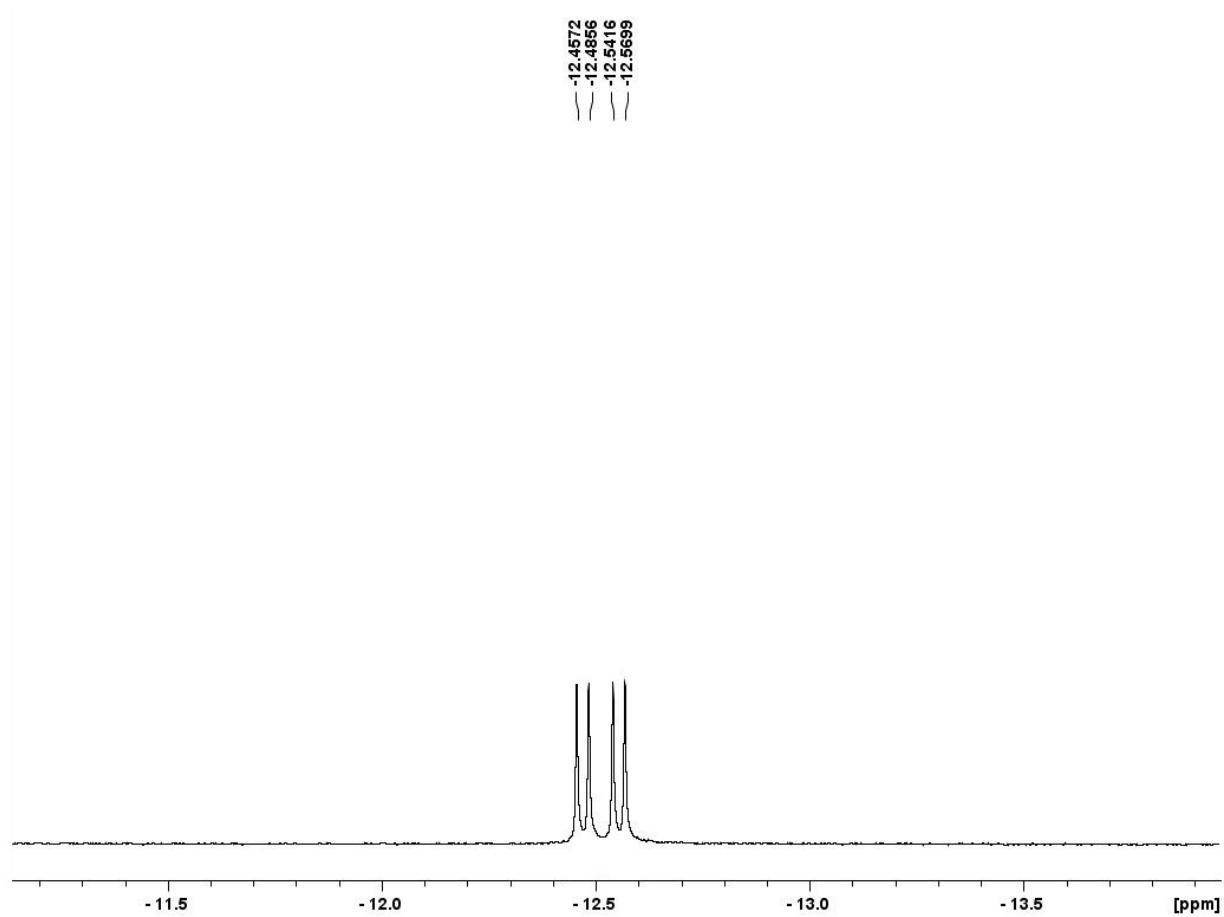


Fig. S4. Hydride region of the ^1H NMR spectrum of $[\text{HOs}_3(\text{CO})_7(\text{SbPh}_3)\{\mu_3\text{-Ph}_2\text{PCH}_2(\text{Ph})\text{C}_6\text{H}_4\}]$ (**2**) in CD_2Cl_2 .

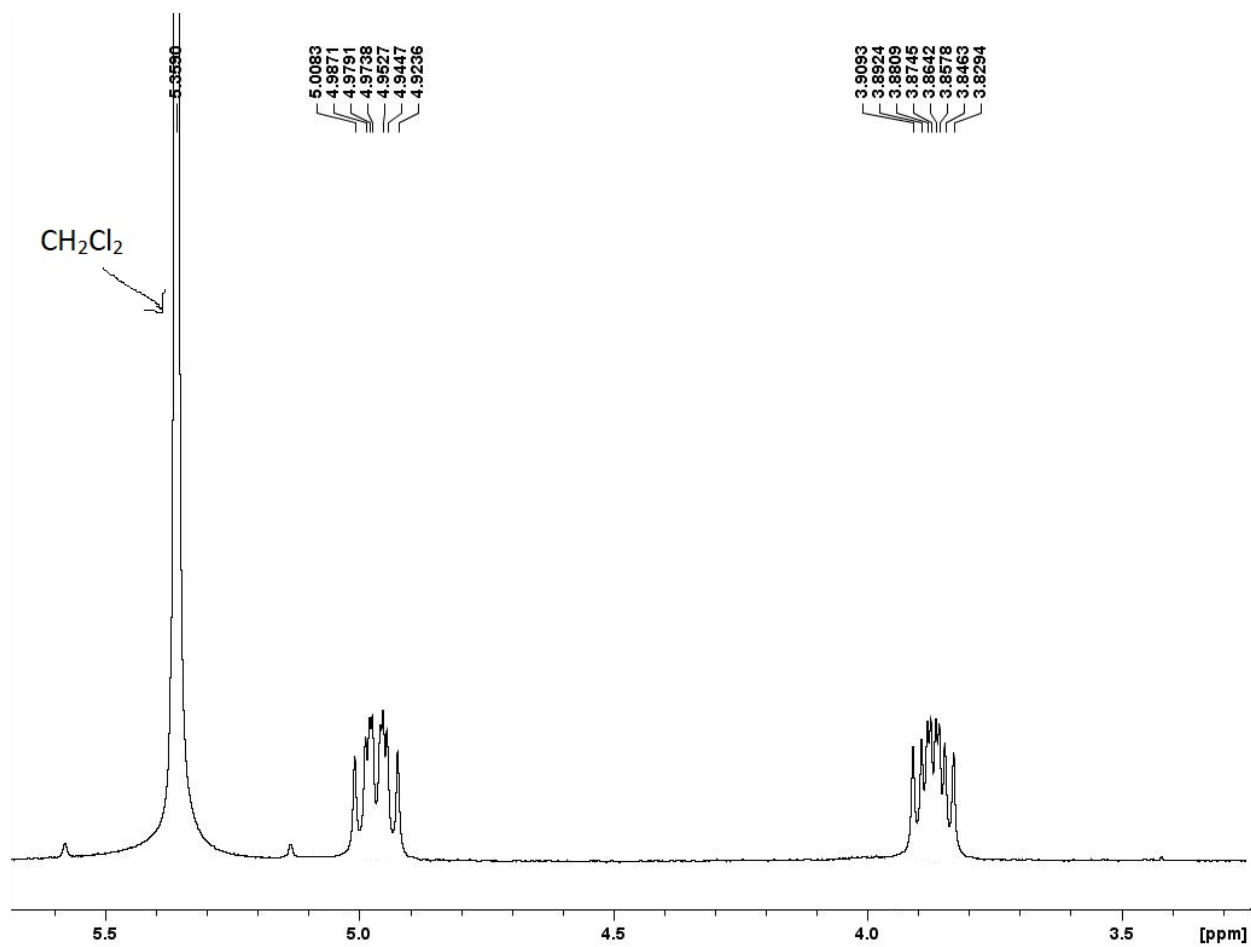


Fig. S5. Aliphatic region of the ^1H NMR spectrum of $[\text{HO}_3(\text{CO})_7(\text{SbPh}_3)\{\mu_3\text{-Ph}_2\text{PCH}_2(\text{Ph})\text{C}_6\text{H}_4\}]$ (2) in CD_2Cl_2 .

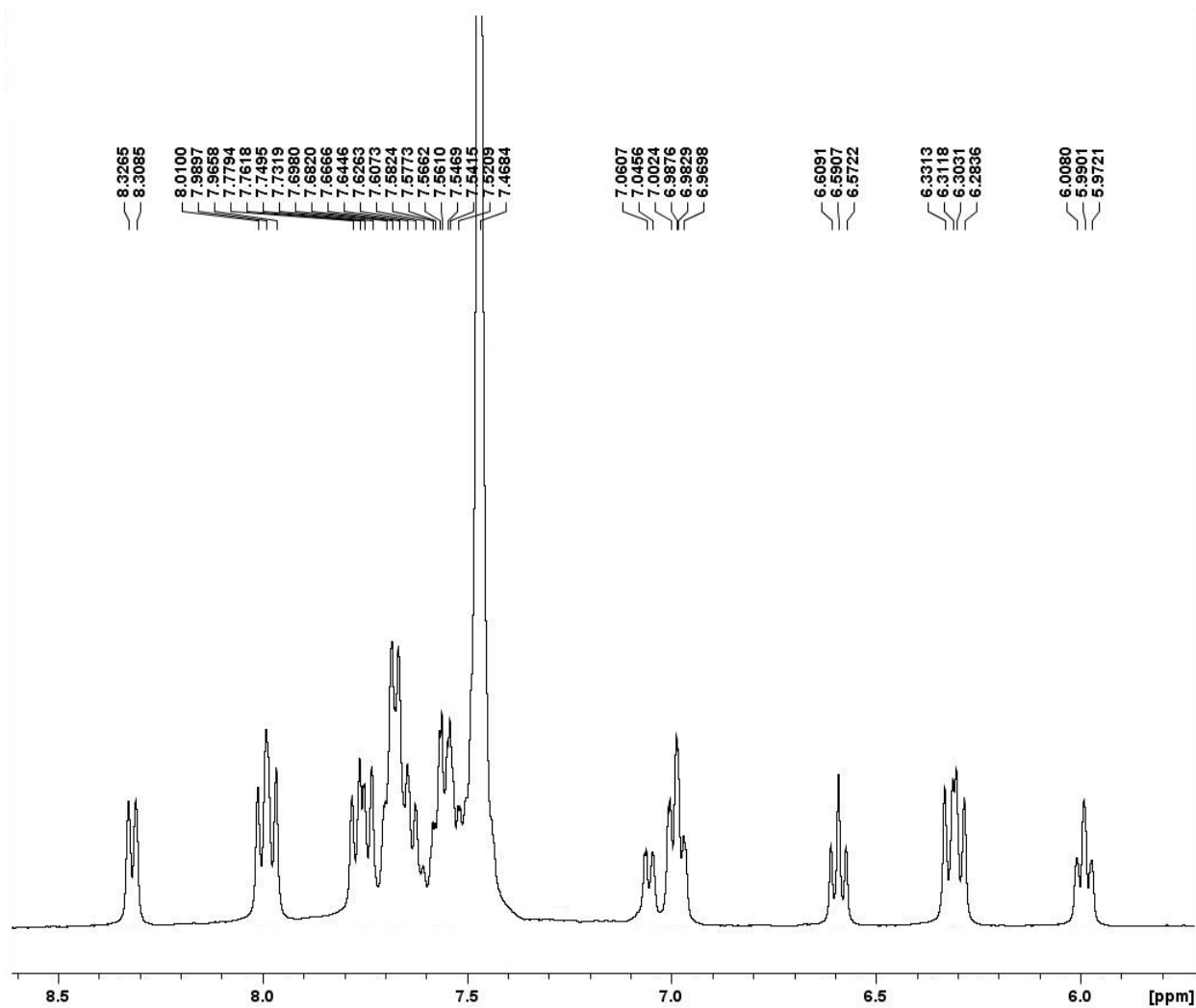


Fig. S6. Aromatic region of the ^1H NMR spectrum of $[\text{HO}_3(\text{CO})_7(\text{SbPh}_3)\{\mu_3\text{-Ph}_2\text{PCH}_2(\text{Ph})\text{C}_6\text{H}_4\}]$ (2) in CD_2Cl_2 .

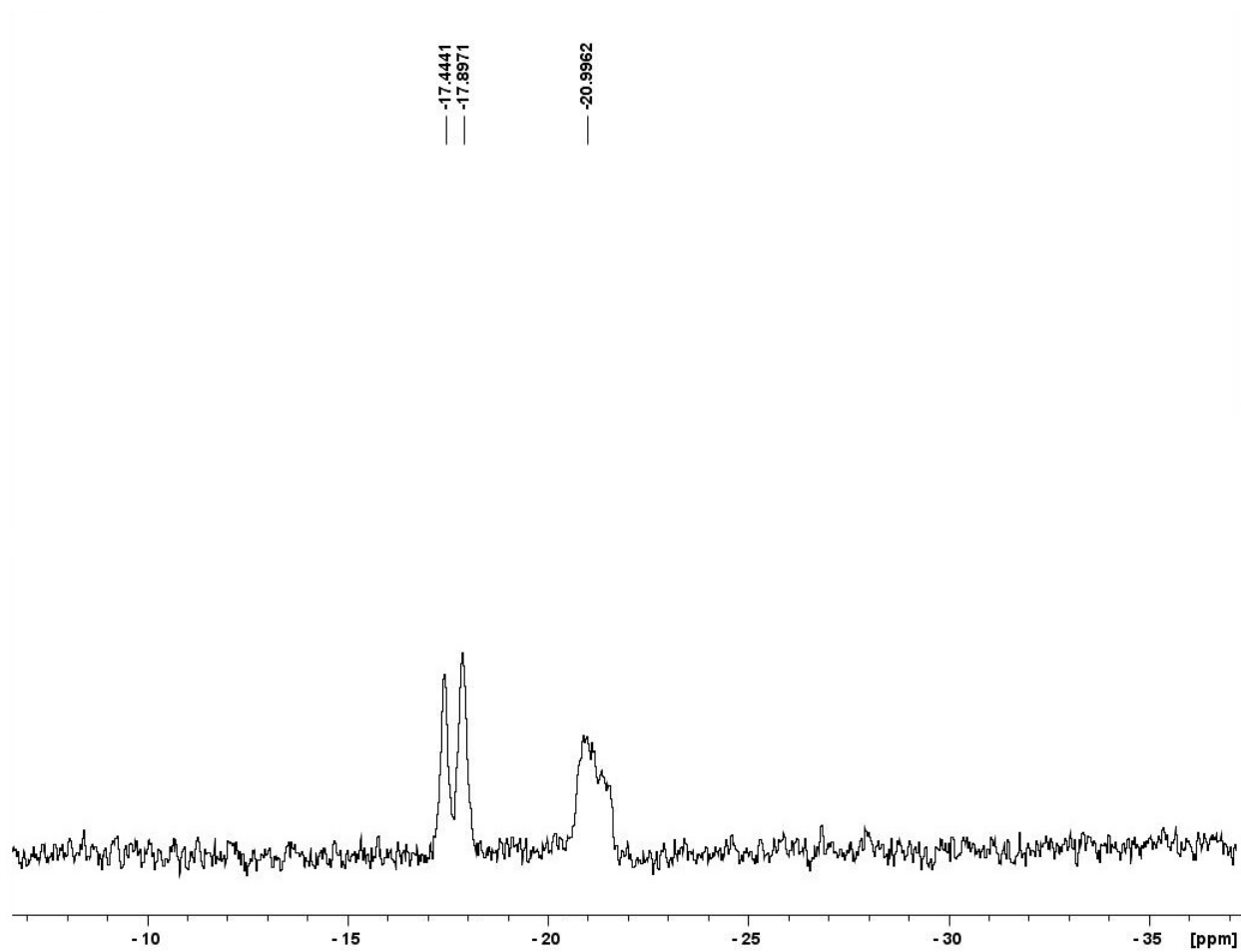


Fig. S7. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\text{HOs}_3(\text{CO})_7(\text{SbPh}_3)\{\mu_3\text{-Ph}_2\text{PCH}_2(\text{Ph})\text{C}_6\text{H}_4\}]$ (**2**) in CD_2Cl_2 .

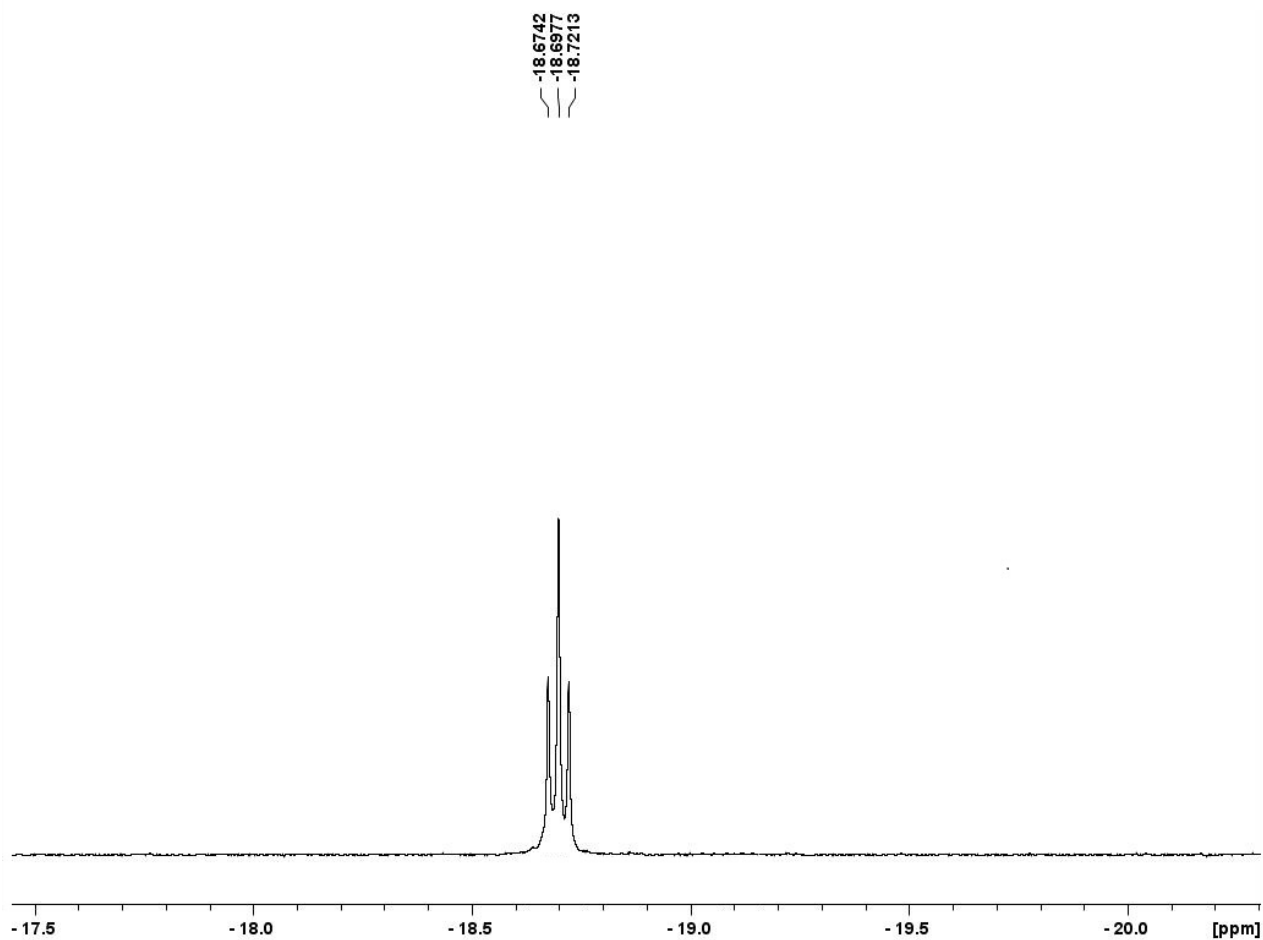


Fig. S8. Hydride region of the ^1H NMR spectrum of $[\text{HOs}_3(\text{CO})_7(\text{SbPh}_3)(\mu, \eta^2\text{-C}_6\text{H}_4)(\mu\text{-SbPh}_2)(\mu\text{-dppm})]$ (**3**) in CDCl_3 .

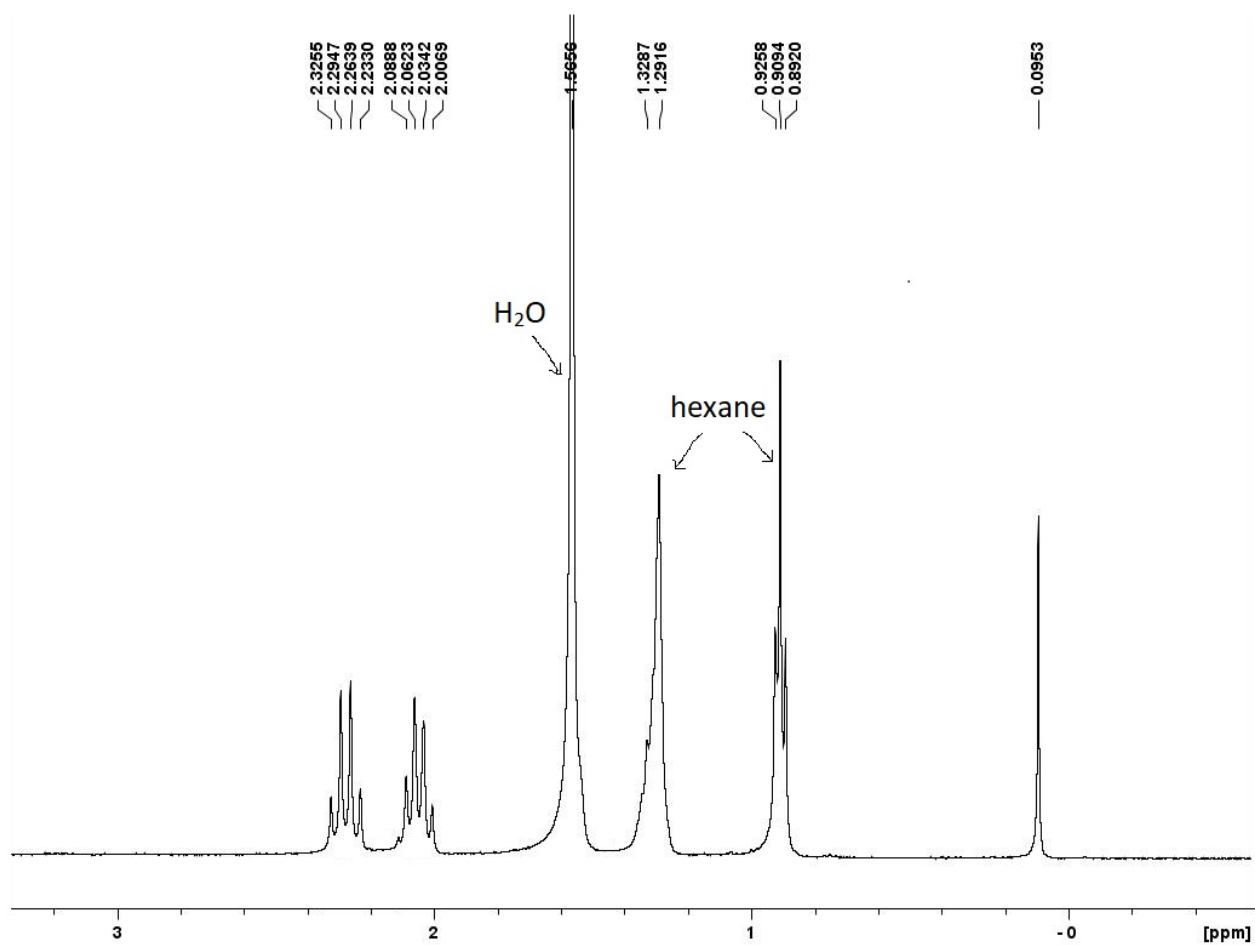


Fig. S9. Aliphatic region of the ^1H NMR spectrum of $[\text{HOs}_3(\text{CO})_7(\text{SbPh}_3)(\mu, \eta^2\text{-C}_6\text{H}_4)(\mu\text{-SbPh}_2)(\mu\text{-dppm})]$ (**3**) in CDCl_3 .

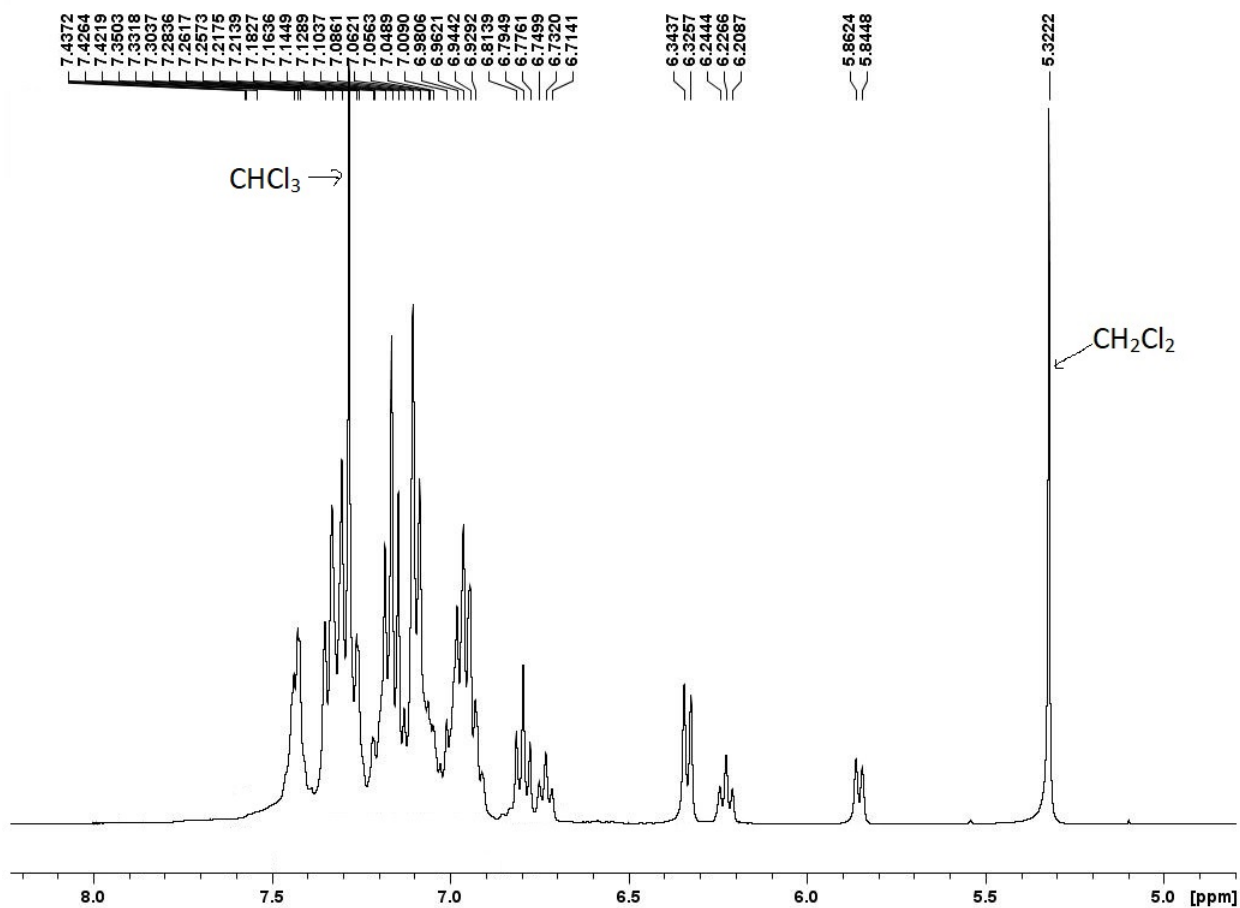


Fig. S10. Aromatic region of the ^1H NMR spectrum of $[\text{HO}_3(\text{CO})_7(\text{SbPh}_3)(\mu,\eta^2\text{-C}_6\text{H}_4)(\mu\text{-SbPh}_2)(\mu\text{-dppm})]$ (**3**) in CDCl_3 .

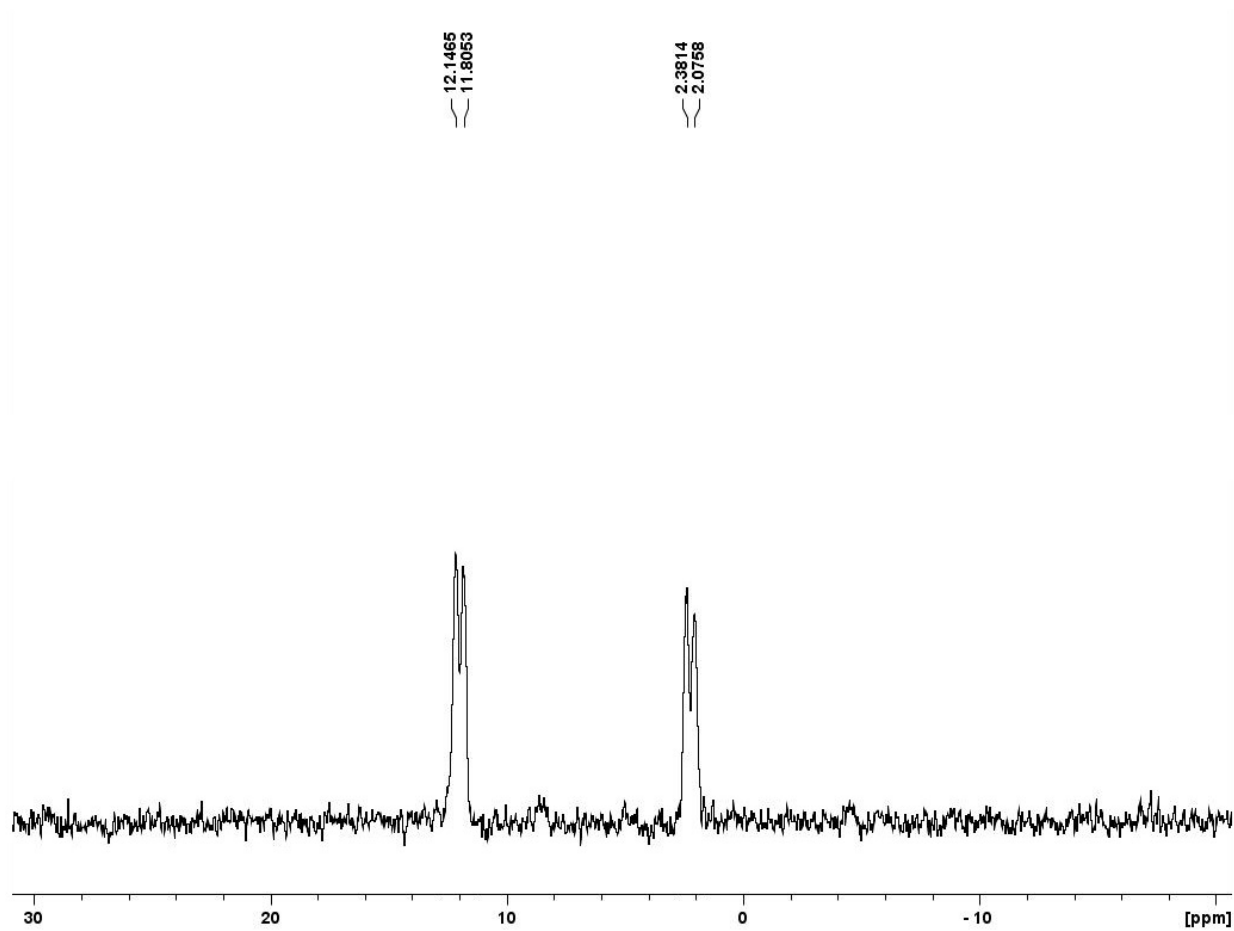


Fig. S11. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\text{HOs}_3(\text{CO})_7(\text{SbPh}_3)(\mu,\eta^2\text{-C}_6\text{H}_4)(\mu\text{-SbPh}_2)(\mu\text{-dppm})]$ (**3**) in CDCl_3 .

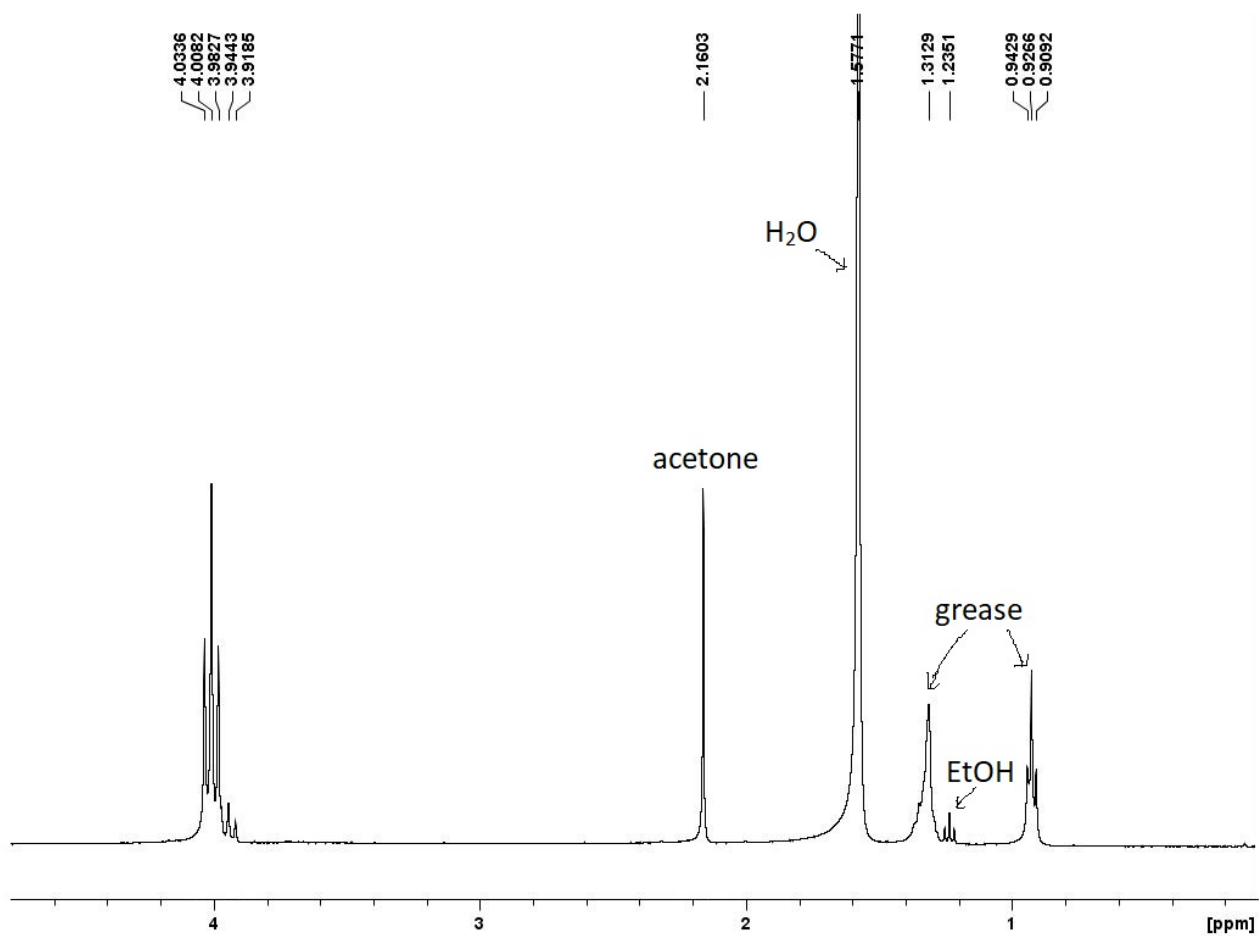


Fig. S12. Aliphatic region of the ¹H NMR spectrum of [Os₃(CO)₈(η¹-Ph)(SbPh₃)(μ-SbPh₂)(μ-dppm)] (**4**) in CD₂Cl₂.

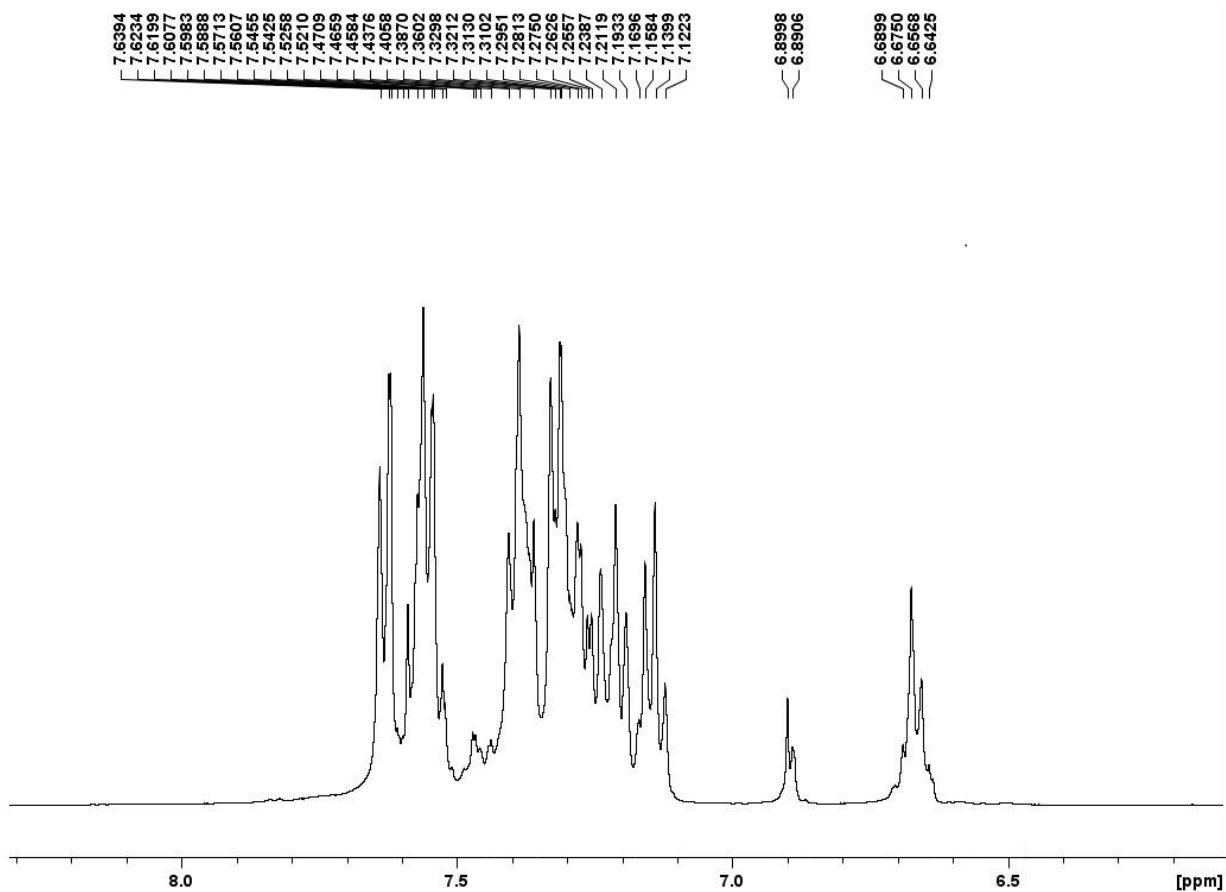


Fig. S13. Aromatic region of the ^1H NMR spectrum of $[\text{Os}_3(\text{CO})_8(\eta^1\text{-Ph})(\text{SbPh}_3)(\mu\text{-SbPh}_2)(\mu\text{-dppm})]$ (**4**) in CD_2Cl_2 .

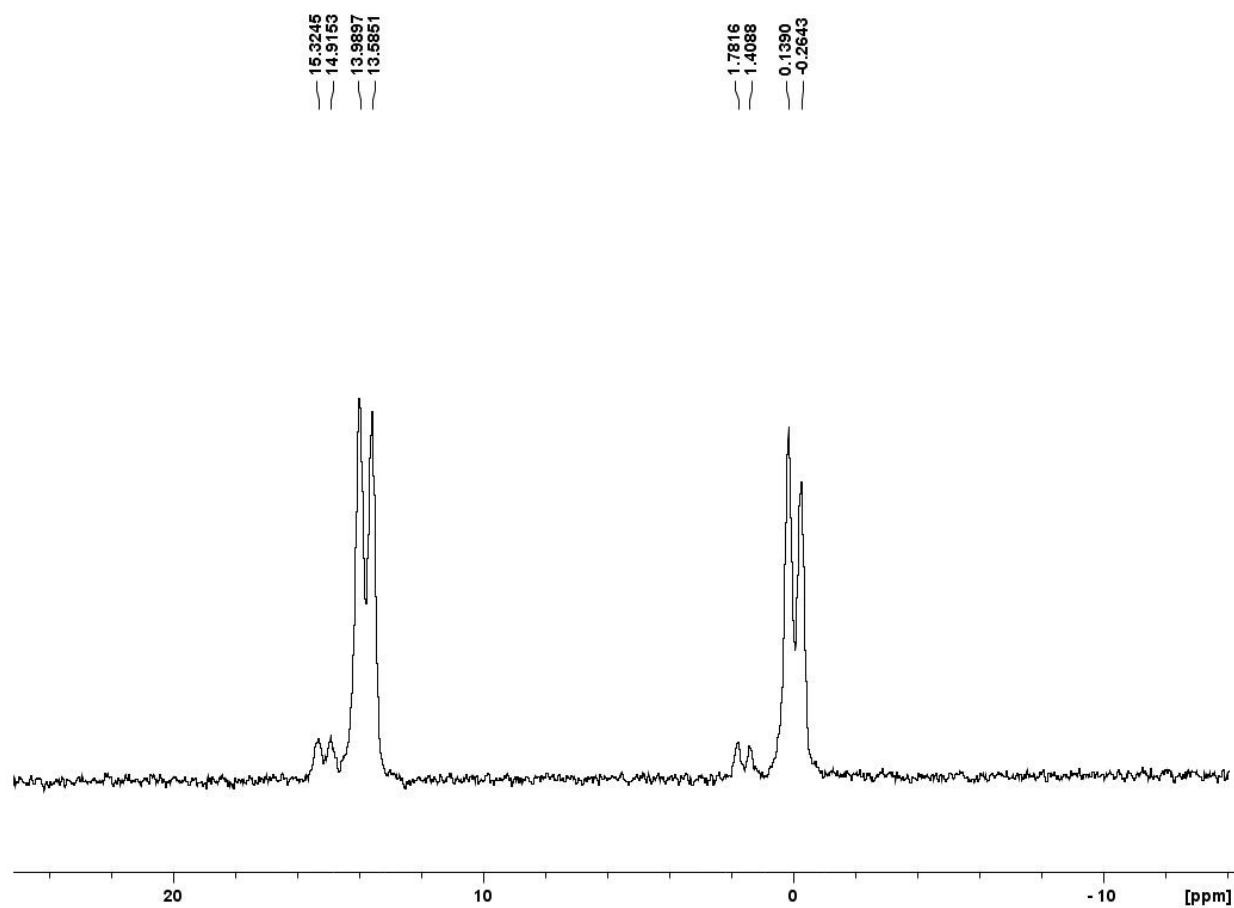


Fig. S14. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\text{Os}_3(\text{CO})_8(\eta^1\text{-Ph})(\text{SbPh}_3)(\mu\text{-SbPh}_2)(\mu\text{-dppm})]$ (**4**) in CD_2Cl_2 .

Table S1. Selected bond distances (Å) and angles (°) for clusters **1-4**

Cluster 1

Bond Distances

Os(1)–Os(2) 2.8807(2), Os(1)–Os(3) 2.9153(2), Os(2)–Os(3) 2.8648(2), Os(1)–P(1) 2.3363(9), Os(2)–P(2) 2.3234(9), Os(3)–Sb(1) 2.5921(3)

Bond Angles

Os(2)–Os(1)–Os(3) 59.240(5), Os(1)–Os(2)–Os(3) 60.982(5), Os(1)–Os(3)–Os(2) 59.779(5), Sb(1)–Os(3)–Os(1) 93.868(8), Sb(1)–Os(3)–Os(2) 153.206(9), P(1)–Os(1)–Os(2) 88.54(2), P(1)–Os(1)–Os(3) 147.54(2), P(2)–Os(2)–Os(1) 94.12(2), P(2)–Os(2)–Os(3) 153.06(2)

Cluster 2

Bond Distances

Os(1)–Os(2) 2.8249(3), Os(1)–Os(3) 2.7720(3), Os(2)–Os(3) 2.8101(3), Os(1)–P(1) 2.3290(12), Os(2)–P(2) 2.3314(12), Os(3)–Sb(1) 2.6343(4), Os(1)–C(10) 2.232(4), Os(3)–C(10) 2.399(4)

Bond Angles

Os(2)–Os(1)–Os(3) 60.266(7), Os(1)–Os(2)–Os(3) 58.935(7), Os(1)–Os(3)–Os(2) 60.799(6), Sb(1)–Os(3)–Os(1) 109.604(9), Sb(1)–Os(3)–Os(2) 169.035(10), Sb(1)–Os(3)–C(10) 93.54(10), P(1)–Os(1)–Os(2) 90.71(3), P(1)–Os(1)–Os(3) 131.53(3), P(2)–Os(2)–Os(1) 77.51(3), P(2)–Os(2)–Os(3) 85.60(3), C(10)–Os(1)–Os(3) 56.06(11), Os(1)–C(10)–Os(3) 73.42(13)

Cluster 3

Bond Distances

Os(1)–Os(2) 3.1729(4), Os(2)–Os(3) 2.9725(4), Os(1)–P(1) 2.335(2), Os(2)–P(2) 2.3328(19), Os(1)–Sb(1) 2.6400(6), Os(3)–Sb(1) 2.7081(5), Os(3)–Sb(2) 2.6137(6), Os(1)–C(8) 2.134(7), Os(2)–C(9) 2.128(7)

Bond Angles

Os(2)–Os(1)–Os(3) 88.959(11), P(1)–Os(1)–Os(2) 87.45(5), P(1)–Os(1)–C(8) 85.7(2), P(1)–Os(1)–Sb(1) 163.05(5), Sb(1)–Os(1)–Os(2) 78.881(14), Sb(1)–Os(1)–C(8) 79.5(2), P(2)–Os(2)–Os(1) 89.72(5), P(2)–Os(2)–Os(3) 176.04(6), P(2)–Os(2)–C(9) 82.9(2), C(9)–Os(2)–Os(3) 93.2(2), C(9)–Os(2)–Os(1) 66.1(2), Sb(2)–Os(3)–Os(2) 176.300(19), Sb(1)–Os(3)–Sb(2) 100.789(18), Sb(1)–Os(3)–Os(2) 81.559(13), Os(1)–Sb(1)–Os(3) 107.319(19)

Cluster 4

Bond Distances

Os(1)–Os(2) 3.0211(3), Os(2)–Os(3) 3.0024(3), Os(1)–P(1) 2.3177(11), Os(2)–P(2) 2.3096(12), Os(1)–Sb(1) 2.6479(3), Os(3)–Sb(1) 2.6695(4), Os(3)–Sb(2) 2.6468(4), Os(1)–C(9) 2.143(5)

Bond Angles

Os(2)–Os(1)–Os(3) 92.473(7), P(1)–Os(1)–Os(2) 94.12(3), P(1)–Os(1)–C(9) 93.11(12), P(1)–Os(1)–Sb(1) 167.76(3), Sb(1)–Os(1)–Os(2) 75.271(9), Sb(1)–Os(1)–C(9) 97.26(12), P(2)–Os(2)–Os(1) 85.14(3), P(2)–Os(2)–Os(3) 176.03(3), Sb(2)–Os(3)–Os(2) 95.815(9), Sb(1)–Os(3)–Sb(2) 167.637(11), Sb(1)–Os(3)–Os(2) 75.292(8), Os(1)–Sb(1)–Os(3) 109.790(11), C(9)–Os(1)–Os(2) 172.35(12)

Computational Details

M06 geometries for the optimized structures A-D

Coordinates: A

Os	26.06520000	8.07750000	9.03760000
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Coordinates: **A_alt**

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C	23.35180000	8.27910000	4.61200000
H	22.91650000	9.10770000	4.05400000
C	22.66550000	7.07360000	4.72350000
H	21.69050000	6.95330000	4.25220000
C	23.22650000	6.02290000	5.44610000
H	22.69370000	5.07720000	5.54370000
C	24.46730000	6.17590000	6.05500000
H	24.87180000	5.34890000	6.64070000
C	30.45680000	6.83980000	6.28900000
C	31.25760000	7.94060000	6.58850000
H	31.20640000	8.39750000	7.57490000
C	32.13240000	8.45660000	5.63310000
H	32.74720000	9.32130000	5.88030000
C	32.22080000	7.86590000	4.37810000
H	32.90730000	8.26730000	3.63300000
C	31.43980000	6.74930000	4.07730000
H	31.51840000	6.27300000	3.10020000
C	30.56450000	6.23960000	5.02680000
H	29.97040000	5.35400000	4.78950000
C	29.80210000	4.38090000	7.53610000
C	31.16720000	4.12510000	7.72450000
H	31.87610000	4.95600000	7.75270000
C	31.62590000	2.82300000	7.87500000
H	32.69000000	2.63940000	8.02050000
C	30.72630000	1.75820000	7.84340000
H	31.08530000	0.73660000	7.96380000
C	29.36980000	2.00470000	7.66390000
H	28.65990000	1.17850000	7.64550000
C	28.90620000	3.31040000	7.51360000
H	27.83460000	3.47610000	7.39900000
C	26.83870000	4.10210000	13.81690000
C	28.22730000	3.95190000	13.80600000
H	28.85660000	4.63780000	13.23540000
C	28.82480000	2.92050000	14.52770000
H	29.90910000	2.81270000	14.51740000
C	28.03870000	2.03430000	15.25820000
H	28.50830000	1.22720000	15.82040000
C	26.65350000	2.18210000	15.27810000
H	26.03730000	1.49500000	15.85800000
C	26.05460000	3.21720000	14.56570000
H	24.96890000	3.33670000	14.60300000
C	24.67520000	6.37420000	14.46110000
C	25.30450000	6.99950000	15.54380000
H	26.38530000	7.16180000	15.54190000
C	24.56160000	7.42220000	16.64220000
H	25.06240000	7.90940000	17.47870000

C	23.18260000	7.22610000	16.66800000
H	22.59990000	7.56080000	17.52610000
C	22.55110000	6.59880000	15.59890000
H	21.47270000	6.43990000	15.61720000
C	23.29440000	6.17040000	14.49950000
H	22.78730000	5.67250000	13.67070000
C	24.37730000	4.75090000	11.67230000
C	24.44100000	3.38470000	11.39660000
H	25.24360000	2.77550000	11.81790000
C	23.49030000	2.79920000	10.56260000
H	23.54350000	1.73200000	10.34690000
C	22.48200000	3.57590000	9.99710000
H	21.74490000	3.11600000	9.33870000
C	22.41560000	4.94160000	10.26780000
H	21.63480000	5.55760000	9.82160000
C	23.36200000	5.52840000	11.10410000
H	23.31250000	6.60540000	11.29190000

Coordinates: **B**

Os	10.00500000	9.44020000	9.89590000
Os	12.09740000	11.35370000	10.56800000
Os	10.31290000	11.88000000	8.39480000
Sb	8.18770000	12.02250000	6.73830000
P	11.56090000	7.67980000	10.19590000
P	13.15040000	9.91920000	8.99990000
C	8.57540000	8.28970000	9.37270000
C	9.46830000	9.59230000	11.72570000
C	13.27330000	12.87090000	10.31060000
C	12.93030000	10.41950000	12.02050000
C	10.79710000	12.24670000	11.70210000
C	11.54740000	12.77270000	7.30230000
C	9.94090000	13.50610000	9.22080000
O	7.73800000	7.53640000	9.10170000
O	9.11950000	9.70800000	12.82240000
O	13.97780000	13.77030000	10.14500000
O	13.43240000	9.81870000	12.87440000
O	10.03380000	12.76350000	12.39210000
O	12.33970000	13.30250000	6.63750000
O	9.70800000	14.52190000	9.72430000
C	13.26730000	8.20080000	9.66920000
H	13.89520000	8.26490000	10.56940000
H	13.71960000	7.48240000	8.96930000
C	12.14400000	9.65760000	7.50670000
C	10.75700000	9.54220000	7.78210000
C	9.95890000	9.13280000	6.68040000
H	8.88300000	8.99240000	6.82160000
C	10.49000000	8.87650000	5.42330000
H	9.83210000	8.57100000	4.60820000

C	11.85990000	9.03720000	5.19540000
H	12.27490000	8.86020000	4.20240000
C	12.69390000	9.42130000	6.23880000
H	13.76770000	9.53030000	6.07710000
C	14.84860000	10.26140000	8.41070000
C	15.92550000	9.40350000	8.65310000
H	15.77440000	8.46100000	9.17920000
C	17.20890000	9.74560000	8.23200000
H	18.04010000	9.07030000	8.43350000
C	17.42670000	10.94280000	7.55860000
H	18.43110000	11.20990000	7.23100000
C	16.35870000	11.80290000	7.30870000
H	16.52130000	12.74530000	6.78700000
C	15.08000000	11.46910000	7.73800000
H	14.25490000	12.15740000	7.54640000
C	11.80520000	6.92920000	11.84720000
C	10.71290000	6.82500000	12.71330000
H	9.74150000	7.21540000	12.41060000
C	10.85150000	6.21760000	13.95760000
H	9.99190000	6.15320000	14.62350000
C	12.08550000	5.70810000	14.34950000
H	12.19990000	5.24560000	15.32940000
C	13.17420000	5.78630000	13.48440000
H	14.14040000	5.38010000	13.78200000
C	13.03340000	6.38560000	12.23770000
H	13.89290000	6.42130000	11.56720000
C	11.23270000	6.20760000	9.14510000
C	11.55810000	6.21760000	7.78470000
H	12.09220000	7.06290000	7.34740000
C	11.19450000	5.15600000	6.96340000
H	11.45560000	5.18470000	5.90510000
C	10.49910000	4.07060000	7.48960000
H	10.21280000	3.23890000	6.84640000
C	10.17220000	4.05180000	8.84250000
H	9.63080000	3.20540000	9.26420000
C	10.53510000	5.11320000	9.66630000
H	10.27310000	5.08740000	10.72520000
C	6.64980000	10.55020000	6.92860000
C	6.32200000	9.67690000	5.88750000
H	6.81440000	9.77060000	4.91570000
C	5.36600000	8.68220000	6.08430000
H	5.11650000	8.00130000	5.27050000
C	4.73010000	8.55980000	7.31690000
H	3.98330000	7.78090000	7.46890000
C	5.05290000	9.42580000	8.35900000
H	4.56630000	9.32220000	9.32860000
C	6.01910000	10.41020000	8.17050000
H	6.28760000	11.06590000	9.00370000
C	8.54310000	12.01380000	4.62950000
C	9.84350000	11.82990000	4.15380000

H	10.66670000	11.67420000	4.85540000
C	10.09710000	11.83260000	2.78370000
H	11.11500000	11.68720000	2.42050000
C	9.05160000	12.02460000	1.88470000
H	9.24870000	12.02690000	0.81270000
C	7.75360000	12.22300000	2.35270000
H	6.93800000	12.38340000	1.64760000
C	7.49920000	12.22230000	3.72160000
H	6.48110000	12.39100000	4.08230000
C	7.02050000	13.80900000	6.84620000
C	7.69310000	15.03230000	6.75520000
H	8.78170000	15.05980000	6.65260000
C	6.98070000	16.22750000	6.78740000
H	7.51070000	17.17730000	6.71890000
C	5.59340000	16.20690000	6.91110000
H	5.03580000	17.14280000	6.93990000
C	4.91810000	14.99230000	6.99700000
H	3.83230000	14.97580000	7.09060000
C	5.62860000	13.79370000	6.96360000
H	5.09150000	12.84480000	7.02850000
H	9.06670000	10.95150000	9.52930000

Coordinates: **C**

Os	10.40810000	15.99680000	7.87420000
Os	12.59910000	15.59510000	5.48510000
Os	10.30270000	15.43860000	3.53600000
Sb	8.85760000	15.09720000	5.87550000
Sb	8.21730000	15.10960000	1.89610000
P	12.26650000	16.35820000	9.29630000
P	14.31750000	15.47840000	7.12840000
C	9.21930000	15.41400000	9.23280000
C	9.78050000	17.83910000	7.94420000
C	13.63370000	14.69610000	4.19290000
C	12.92600000	17.37690000	4.77470000
C	9.99620000	17.31240000	4.01510000
C	11.60980000	15.92110000	2.22730000
C	10.83480000	13.55430000	3.45630000
O	8.50840000	15.05080000	10.06850000
O	9.42010000	18.93450000	8.02380000
O	14.26630000	14.16190000	3.38260000
O	13.07690000	18.46000000	4.39570000
O	9.82970000	18.40400000	4.34150000
O	12.42700000	16.23710000	1.47480000
O	11.15510000	12.45280000	3.35910000
C	11.14880000	13.96370000	7.60690000
C	12.00130000	13.76990000	6.49620000
C	12.48440000	12.47470000	6.23930000
H	13.14900000	12.29560000	5.38690000

C	12.16060000	11.39430000	7.06140000
H	12.55810000	10.40210000	6.83760000
C	11.34850000	11.59650000	8.17450000
H	11.08250000	10.76130000	8.82530000
C	10.83910000	12.87090000	8.43310000
H	10.17090000	12.99780000	9.29150000
C	13.69450000	15.28180000	8.85760000
H	14.49910000	15.35580000	9.60280000
H	13.28310000	14.26460000	8.88540000
C	11.92510000	15.93410000	11.03470000
C	11.19010000	16.84430000	11.80560000
H	10.94740000	17.82920000	11.39930000
C	10.75630000	16.49620000	13.07880000
H	10.18540000	17.21190000	13.66940000
C	11.03950000	15.23150000	13.59190000
H	10.69180000	14.95580000	14.58700000
C	11.75920000	14.31900000	12.82770000
H	11.97710000	13.32640000	13.22070000
C	12.20090000	14.66580000	11.55290000
H	12.74480000	13.92930000	10.95960000
C	13.02870000	18.02070000	9.35490000
C	12.92820000	18.85460000	8.23720000
H	12.31380000	18.55260000	7.38790000
C	13.63060000	20.05560000	8.18730000
H	13.55500000	20.68380000	7.30010000
C	14.42420000	20.44030000	9.26340000
H	14.97570000	21.37950000	9.22640000
C	14.51500000	19.62420000	10.39030000
H	15.13100000	19.92700000	11.23710000
C	13.82670000	18.41700000	10.43510000
H	13.91040000	17.77520000	11.31470000
C	15.43000000	14.02480000	6.96390000
C	15.26920000	12.85230000	7.70670000
H	14.50150000	12.77290000	8.47540000
C	16.07320000	11.74340000	7.45750000
H	15.92430000	10.83450000	8.04030000
C	17.04570000	11.79030000	6.46450000
H	17.66820000	10.91850000	6.26510000
C	17.22110000	12.95790000	5.72520000
H	17.98270000	13.00880000	4.94790000
C	16.42130000	14.06670000	5.97520000
H	16.57510000	14.97640000	5.39180000
C	15.55160000	16.84180000	7.21410000
C	16.24930000	17.14200000	8.38890000
H	16.05610000	16.58990000	9.30830000
C	17.18880000	18.16670000	8.41220000
H	17.70540000	18.40090000	9.34320000
C	17.46520000	18.89070000	7.25540000
H	18.19930000	19.69580000	7.27670000
C	16.80370000	18.57770000	6.07230000

H	17.01940000	19.12850000	5.15730000
C	15.85300000	17.56150000	6.05420000
H	15.33900000	17.32330000	5.12350000
C	6.94500000	16.10040000	5.71820000
C	6.86860000	17.46900000	6.00730000
H	7.75040000	18.01230000	6.34990000
C	5.66820000	18.16390000	5.86660000
H	5.63080000	19.22800000	6.10190000
C	4.52380000	17.49810000	5.43330000
H	3.58320000	18.03820000	5.32340000
C	4.58660000	16.13790000	5.14340000
H	3.69580000	15.60780000	4.80330000
C	5.78690000	15.44240000	5.28510000
H	5.80840000	14.37480000	5.05280000
C	8.12760000	13.14000000	6.36680000
C	7.04110000	13.02920000	7.24080000
H	6.52330000	13.92400000	7.59410000
C	6.60710000	11.77700000	7.67110000
H	5.75800000	11.70410000	8.35100000
C	7.26120000	10.62470000	7.24080000
H	6.92580000	9.64590000	7.58470000
C	8.35320000	10.72900000	6.38290000
H	8.89210000	9.83620000	6.06340000
C	8.78500000	11.98050000	5.94970000
H	9.66800000	12.03840000	5.31230000
C	7.05280000	16.80190000	1.31270000
C	6.59630000	17.67890000	2.30260000
H	6.84120000	17.51240000	3.35560000
C	5.81290000	18.77580000	1.95430000
H	5.45760000	19.45160000	2.73270000
C	5.48710000	19.00480000	0.61970000
H	4.87740000	19.86650000	0.34790000
C	5.94040000	18.13470000	-0.36880000
H	5.68740000	18.31500000	-1.41370000
C	6.72060000	17.03260000	-0.02530000
H	7.07230000	16.35410000	-0.80560000
C	6.64940000	13.76790000	2.45920000
C	6.98740000	12.58790000	3.12680000
H	8.03260000	12.34990000	3.33930000
C	5.99340000	11.70990000	3.55290000
H	6.26970000	10.80950000	4.10260000
C	4.65610000	12.00030000	3.29380000
H	3.87640000	11.31730000	3.63080000
C	4.31350000	13.16460000	2.60820000
H	3.26640000	13.39070000	2.40400000
C	5.30600000	14.05330000	2.19880000
H	5.02710000	14.97890000	1.68870000
C	8.67350000	14.26300000	-0.01640000
C	7.68690000	13.57810000	-0.73470000
H	6.68580000	13.45450000	-0.31390000

C	7.97680000	13.04250000	-1.98700000
H	7.20380000	12.50930000	-2.54040000
C	9.25360000	13.18240000	-2.52640000
H	9.48000000	12.75930000	-3.50500000
C	10.24100000	13.85780000	-1.81500000
H	11.24160000	13.96620000	-2.23300000
C	9.95240000	14.39740000	-0.56290000
H	10.73700000	14.92430000	-0.01700000
H	11.52390000	16.61190000	6.58270000

Coordinates: **D**

Os	2.81130000	3.04470000	4.47040000
Os	5.52120000	3.17770000	5.95710000
Os	5.23510000	0.15000000	6.71220000
Sb	3.44210000	0.44260000	4.70560000
Sb	6.97970000	0.49910000	8.73720000
P	2.33060000	5.32530000	4.72550000
P	5.39490000	5.46400000	5.37270000
C	1.75380000	2.65390000	6.06250000
C	3.82000000	3.36790000	2.83980000
C	4.32710000	3.51000000	7.45610000
C	7.26110000	3.38700000	6.69820000
C	6.18710000	2.57670000	4.21940000
C	3.82500000	0.57700000	8.01420000
C	4.99780000	-1.72800000	6.86650000
C	6.63920000	-0.05350000	5.35210000
O	1.07250000	2.40350000	6.95760000
O	4.36460000	3.56470000	1.83890000
O	3.65880000	3.79950000	8.36400000
O	8.34190000	3.64130000	7.04080000
O	6.62500000	2.22500000	3.20880000
O	3.03090000	0.74360000	8.83090000
O	4.85140000	-2.87430000	6.91800000
O	7.45660000	-0.24920000	4.56750000
C	1.08410000	2.59270000	3.28230000
C	-0.23160000	2.76460000	3.75490000
H	-0.40640000	3.18190000	4.75000000
C	-1.35120000	2.41160000	3.00190000
H	-2.34580000	2.55620000	3.42800000
C	-1.20840000	1.87420000	1.72610000
H	-2.08200000	1.59530000	1.13670000
C	0.07700000	1.70630000	1.21820000
H	0.22370000	1.28950000	0.22000000
C	6.45630000	6.33000000	7.83330000
H	6.06180000	5.39780000	8.24620000
C	1.19110000	2.05640000	1.98140000
H	2.17570000	1.88530000	1.53730000
C	3.73040000	6.25930000	5.52790000

H	3.77480000	7.31780000	5.22830000
H	3.54600000	6.25730000	6.61300000
C	0.91240000	5.71410000	5.82510000
C	1.03300000	5.63470000	7.21680000
H	1.98850000	5.39510000	7.68640000
C	-0.07970000	5.81550000	8.03170000
H	0.03210000	5.74770000	9.11330000
C	-1.32840000	6.06250000	7.46850000
H	-2.19980000	6.19760000	8.10860000
C	-1.46110000	6.12600000	6.08420000
H	-2.43630000	6.30830000	5.63320000
C	-0.34900000	5.95250000	5.26600000
H	-0.46540000	5.99750000	4.18230000
C	1.93930000	6.35210000	3.25440000
C	1.78060000	5.76040000	2.00090000
H	1.83430000	4.67610000	1.90610000
C	1.53370000	6.54830000	0.87760000
H	1.41370000	6.07230000	-0.09500000
C	1.43800000	7.92980000	1.00070000
H	1.25000000	8.54560000	0.12140000
C	1.56470000	8.52750000	2.25540000
H	1.46990000	9.60810000	2.36010000
C	1.80450000	7.74240000	3.37650000
H	1.88170000	8.21600000	4.35780000
C	6.33440000	6.60910000	6.46740000
C	6.86870000	7.80040000	5.96500000
H	6.78130000	8.02900000	4.90160000
C	7.51710000	8.69450000	6.81150000
H	7.93450000	9.61610000	6.40630000
C	7.63210000	8.41090000	8.16960000
H	8.14200000	9.10980000	8.83240000
C	7.09900000	7.22950000	8.67770000
H	7.19150000	6.99130000	9.73740000
C	6.01150000	5.90250000	3.71100000
C	5.30100000	6.70100000	2.81250000
H	4.33950000	7.13110000	3.08680000
C	5.80560000	6.94820000	1.53770000
H	5.22360000	7.55380000	0.84290000
C	7.03360000	6.41880000	1.15840000
H	7.42440000	6.60390000	0.15830000
C	7.76860000	5.65380000	2.06360000
H	8.73690000	5.24480000	1.77770000
C	7.26080000	5.39730000	3.33030000
H	7.83880000	4.79220000	4.03240000
C	1.70120000	-0.75030000	5.12740000
C	1.51160000	-1.44070000	6.32570000
H	2.28780000	-1.44510000	7.09290000
C	0.32580000	-2.13560000	6.56160000
H	0.19040000	-2.66940000	7.50250000
C	-0.68050000	-2.14210000	5.60050000

H	-1.60970000	-2.68060000	5.78760000
C	-0.49990000	-1.45600000	4.40150000
H	-1.28590000	-1.44640000	3.64580000
C	0.68440000	-0.76420000	4.16410000
H	0.80250000	-0.21790000	3.22480000
C	4.19440000	-0.67420000	3.03500000
C	4.25560000	-2.06910000	3.13400000
H	3.87870000	-2.57680000	4.02600000
C	4.79670000	-2.82200000	2.09560000
H	4.84080000	-3.90810000	2.17990000
C	5.28080000	-2.18790000	0.95270000
H	5.70700000	-2.77790000	0.14120000
C	5.22120000	-0.80150000	0.84880000
H	5.60080000	-0.30080000	-0.04190000
C	4.67960000	-0.04480000	1.88700000
H	4.65170000	1.04150000	1.79470000
C	6.69790000	-0.88480000	10.34560000
C	6.64110000	-0.46220000	11.67640000
H	6.72510000	0.59880000	11.92010000
C	6.47540000	-1.39440000	12.69920000
H	6.42800000	-1.05880000	13.73520000
C	6.37220000	-2.74990000	12.39910000
H	6.24190000	-3.47740000	13.20010000
C	6.43420000	-3.17810000	11.07490000
H	6.35430000	-4.23850000	10.83660000
C	6.59470000	-2.24890000	10.05070000
H	6.64050000	-2.59710000	9.01600000
C	9.07000000	0.23920000	8.39920000
C	9.88180000	-0.27040000	9.41820000
H	9.44700000	-0.56010000	10.37780000
C	11.25160000	-0.41250000	9.21140000
H	11.88120000	-0.81100000	10.00680000
C	11.81450000	-0.04850000	7.99030000
H	12.88650000	-0.16260000	7.83030000
C	11.01020000	0.45960000	6.97360000
H	11.44750000	0.74560000	6.01750000
C	9.64000000	0.60500000	7.17610000
H	9.02190000	1.00990000	6.37370000
C	6.97370000	2.31450000	9.86920000
C	5.76660000	2.79230000	10.38960000
H	4.83190000	2.25210000	10.22560000
C	5.73690000	3.98210000	11.11290000
H	4.78900000	4.35040000	11.50480000
C	6.91420000	4.69770000	11.32010000
H	6.89270000	5.62560000	11.89330000
C	8.11890000	4.22780000	10.80090000
H	9.03910000	4.79180000	10.95430000
C	8.15110000	3.03700000	10.07820000
H	9.09490000	2.68290000	9.65960000

Coordinates: **Species D_alt1**

Os	2.69700000	3.01520000	4.24720000
Os	5.44780000	3.18130000	5.93530000
Os	5.10360000	0.18760000	6.77370000
Sb	3.36270000	0.47510000	4.72140000
Sb	6.93360000	0.45730000	8.73800000
P	2.24350000	5.30220000	4.70930000
P	5.31210000	5.46580000	5.35280000
C	1.36030000	2.73980000	2.95680000
C	3.93480000	3.37370000	2.80860000
C	4.42230000	3.63440000	7.52490000
C	7.21140000	3.34280000	6.62830000
C	6.18710000	2.52490000	4.24110000
C	3.76150000	0.77290000	8.08570000
C	4.71150000	-1.65640000	7.00880000
C	6.48060000	-0.15530000	5.41100000
O	0.60190000	2.60940000	2.08780000
O	4.55670000	3.56520000	1.84860000
O	3.89500000	4.02010000	8.48410000
O	8.31130000	3.55700000	6.93200000
O	6.70920000	2.15710000	3.28000000
O	3.02580000	1.03910000	8.92960000
O	4.45590000	-2.77870000	7.11580000
O	7.27290000	-0.40810000	4.61810000
C	1.13790000	2.48050000	5.75510000
C	1.16690000	2.82210000	7.11610000
H	2.01920000	3.35830000	7.52230000
C	0.12690000	2.53130000	8.00060000
H	0.22180000	2.82840000	9.04700000
C	-1.01600000	1.87790000	7.55430000
H	-1.83280000	1.64880000	8.23970000
C	-1.09110000	1.52260000	6.21080000
H	-1.96950000	1.00140000	5.82520000
C	6.53370000	6.28140000	7.78440000
H	6.27950000	5.29740000	8.18280000
C	-0.03890000	1.81400000	5.34660000
H	-0.15630000	1.48260000	4.31270000
C	3.63010000	6.20070000	5.56100000
H	3.62700000	7.28330000	5.35560000
H	3.47070000	6.07890000	6.64320000
C	0.78550000	5.67810000	5.75300000
C	0.83880000	6.28470000	7.00800000
H	1.78690000	6.60900000	7.43750000
C	-0.32820000	6.47970000	7.74460000
H	-0.27110000	6.95050000	8.72580000
C	-1.55370000	6.06860000	7.23470000
H	-2.46370000	6.21180000	7.81660000
C	-1.61640000	5.47040000	5.97660000

H	-2.57110000	5.13470000	5.57330000
C	-0.45520000	5.27520000	5.24230000
H	-0.51100000	4.79330000	4.26360000
C	1.90420000	6.41950000	3.28250000
C	2.01950000	5.97840000	1.96460000
H	2.26880000	4.94000000	1.75690000
C	1.84150000	6.86480000	0.90370000
H	1.93970000	6.50290000	-0.11920000
C	1.54990000	8.20110000	1.15290000
H	1.41810000	8.89720000	0.32470000
C	1.41250000	8.64870000	2.46740000
H	1.16760000	9.69140000	2.66870000
C	1.57860000	7.76150000	3.52390000
H	1.45220000	8.11360000	4.55030000
C	6.24130000	6.61760000	6.45800000
C	6.60230000	7.88660000	5.98750000
H	6.39080000	8.16290000	4.95320000
C	7.24000000	8.79770000	6.82200000
H	7.51940000	9.77830000	6.43730000
C	7.52600000	8.45380000	8.14080000
H	8.03010000	9.16500000	8.79470000
C	7.17110000	7.19610000	8.61790000
H	7.39860000	6.90830000	9.64430000
C	5.91790000	5.96030000	3.70550000
C	5.22160000	6.82700000	2.86090000
H	4.26450000	7.25060000	3.16320000
C	5.73690000	7.15180000	1.60810000
H	5.16630000	7.80990000	0.95270000
C	6.96010000	6.63120000	1.20060000
H	7.35910000	6.87880000	0.21740000
C	7.67930000	5.79560000	2.05440000
H	8.64310000	5.39330000	1.74510000
C	7.16160000	5.46260000	3.29920000
H	7.72700000	4.80600000	3.96380000
C	1.68870000	-0.83040000	5.04810000
C	1.27070000	-1.19200000	6.32860000
H	1.83280000	-0.86880000	7.20720000
C	0.11470000	-1.94810000	6.50720000
H	-0.20630000	-2.21470000	7.51420000
C	-0.63300000	-2.34760000	5.40290000
H	-1.54040000	-2.93540000	5.54160000
C	-0.22200000	-1.99230000	4.11960000
H	-0.80590000	-2.30100000	3.25210000
C	0.93470000	-1.23700000	3.94230000
H	1.24070000	-0.95410000	2.93100000
C	4.25100000	-0.66360000	3.12260000
C	4.37430000	-2.05140000	3.26640000
H	3.94840000	-2.55660000	4.13700000
C	5.03250000	-2.80500000	2.29900000
H	5.12300000	-3.88460000	2.42170000

C	5.57500000	-2.17960000	1.17760000
H	6.09690000	-2.76840000	0.42310000
C	5.44550000	-0.80340000	1.02070000
H	5.86470000	-0.30860000	0.14450000
C	4.78310000	-0.04800000	1.98820000
H	4.70420000	1.03100000	1.85430000
C	6.65200000	-0.87420000	10.39000000
C	6.74910000	-0.42620000	11.71070000
H	6.95920000	0.62440000	11.92120000
C	6.57620000	-1.31940000	12.76620000
H	6.64860000	-0.96320000	13.79390000
C	6.31060000	-2.66150000	12.50920000
H	6.17310000	-3.35830000	13.33580000
C	6.21980000	-3.11570000	11.19540000
H	6.01240000	-4.16570000	10.99060000
C	6.38840000	-2.22510000	10.13860000
H	6.31480000	-2.59450000	9.11320000
C	8.98560000	0.07060000	8.30100000
C	9.79980000	-0.53230000	9.26540000
H	9.38200000	-0.83780000	10.22760000
C	11.14960000	-0.74860000	9.00060000
H	11.78070000	-1.22070000	9.75340000
C	11.69090000	-0.36360000	7.77620000
H	12.74740000	-0.53540000	7.57070000
C	10.88460000	0.23830000	6.81360000
H	11.30480000	0.54070000	5.85500000
C	9.53400000	0.45640000	7.07380000
H	8.91350000	0.93260000	6.31280000
C	7.11330000	2.28230000	9.83880000
C	5.96980000	2.84940000	10.41070000
H	4.99330000	2.37330000	10.29700000
C	6.06090000	4.03850000	11.12960000
H	5.16120000	4.47700000	11.56090000
C	7.29760000	4.66100000	11.28670000
H	7.37120000	5.58660000	11.85920000
C	8.43980000	4.10120000	10.71740000
H	9.40660000	4.59080000	10.83470000
C	8.35020000	2.91290000	9.99540000
H	9.24710000	2.48550000	9.54270000

Coordinates: **D_alt2**

Os	2.91860000	2.97030000	4.77150000
Os	5.63150000	3.34300000	6.20780000
Os	5.65540000	0.33760000	7.01600000
Sb	3.55160000	0.39360000	5.20980000
Sb	5.53200000	-2.22860000	7.71090000
P	2.39980000	5.25410000	4.72160000
P	5.46420000	5.54790000	5.38190000

C	1.87010000	2.74740000	6.39850000
C	3.95480000	3.06840000	3.12440000
C	4.39490000	3.81300000	7.63750000
C	7.29730000	3.63130000	7.09170000
C	6.41410000	2.65510000	4.55390000
C	4.34750000	0.98910000	8.32610000
C	7.12610000	0.73280000	8.18560000
C	6.81090000	-0.11310000	5.49630000
O	1.19960000	2.57730000	7.32120000
O	4.51290000	3.10620000	2.11330000
O	3.73660000	4.18890000	8.51760000
O	8.31410000	3.89290000	7.57930000
O	6.93170000	2.27490000	3.59220000
O	3.57920000	1.32450000	9.11570000
O	8.00940000	0.95660000	8.89260000
O	7.48240000	-0.43040000	4.61780000
C	1.21740000	2.33630000	3.62920000
C	-0.10780000	2.60980000	4.02200000
H	-0.29960000	3.20060000	4.92190000
C	-1.21200000	2.13500000	3.31430000
H	-2.21620000	2.37070000	3.67190000
C	-1.04100000	1.35720000	2.17170000
H	-1.90250000	0.97930000	1.62060000
C	0.25530000	1.07600000	1.74780000
H	0.42770000	0.46320000	0.86050000
C	6.44850000	6.71350000	7.74580000
H	6.09200000	5.80830000	8.23970000
C	1.35370000	1.56040000	2.45900000
H	2.34720000	1.28820000	2.09130000
C	3.77650000	6.31170000	5.40370000
H	3.81010000	7.32250000	4.96880000
H	3.57540000	6.44490000	6.47840000
C	0.96440000	5.77310000	5.74490000
C	1.05750000	5.82840000	7.13970000
H	2.00150000	5.62300000	7.64670000
C	-0.06480000	6.11290000	7.91060000
H	0.02690000	6.15170000	8.99550000
C	-1.29680000	6.33220000	7.30050000
H	-2.17560000	6.55220000	7.90610000
C	-1.40300000	6.26090000	5.91440000
H	-2.36530000	6.42090000	5.42840000
C	-0.28070000	5.98250000	5.14020000
H	-0.37540000	5.92110000	4.05540000
C	2.01040000	6.07360000	3.12450000
C	1.84910000	5.31680000	1.96280000
H	1.89180000	4.22900000	2.01830000
C	1.61720000	5.94670000	0.74100000
H	1.50060000	5.34390000	-0.15880000
C	1.53410000	7.33330000	0.67390000
H	1.36120000	7.82470000	-0.28350000

C	1.65560000	8.09550000	1.83640000
H	1.56880000	9.18080000	1.79200000
C	1.88340000	7.46820000	3.05490000
H	1.95840000	8.07060000	3.96290000
C	6.33460000	6.84460000	6.35830000
C	6.80660000	8.00960000	5.74340000
H	6.72290000	8.12560000	4.66140000
C	7.39010000	9.01880000	6.50320000
H	7.76130000	9.91840000	6.01250000
C	7.50210000	8.87820000	7.88430000
H	7.96380000	9.66730000	8.47730000
C	7.02780000	7.72590000	8.50470000
H	7.11640000	7.60580000	9.58390000
C	6.12730000	5.80920000	3.70190000
C	5.38000000	6.35810000	2.65860000
H	4.35560000	6.68960000	2.81760000
C	5.93060000	6.47720000	1.38450000
H	5.32540000	6.89120000	0.57820000
C	7.23700000	6.06630000	1.14780000
H	7.66580000	6.15310000	0.14980000
C	8.00280000	5.55070000	2.19310000
H	9.03170000	5.23860000	2.01790000
C	7.45250000	5.42320000	3.46140000
H	8.05840000	5.01710000	4.27520000
C	1.81770000	-0.61580000	5.99900000
C	1.80010000	-1.12410000	7.29830000
H	2.69640000	-1.06800000	7.92080000
C	0.64970000	-1.70440000	7.82700000
H	0.66310000	-2.10190000	8.84310000
C	-0.50660000	-1.77590000	7.05640000
H	-1.41020000	-2.22720000	7.46670000
C	-0.50930000	-1.25590000	5.76390000
H	-1.41470000	-1.28710000	5.15660000
C	0.64260000	-0.67690000	5.23760000
H	0.61390000	-0.26030000	4.22910000
C	3.85280000	-0.72370000	3.38800000
C	2.95960000	-1.72530000	2.99290000
H	2.14780000	-2.03330000	3.65440000
C	3.08780000	-2.33620000	1.74720000
H	2.37630000	-3.10810000	1.44960000
C	4.11090000	-1.95740000	0.88170000
H	4.20750000	-2.43200000	-0.09480000
C	5.00790000	-0.96540000	1.26850000
H	5.81210000	-0.65870000	0.59990000
C	4.87910000	-0.35000000	2.51220000
H	5.58560000	0.43700000	2.77880000
C	4.07140000	-3.57520000	6.93520000
C	3.20570000	-4.26760000	7.78540000
H	3.30360000	-4.17420000	8.86950000
C	2.19270000	-5.05940000	7.25050000

H	1.50840000	-5.58640000	7.91540000
C	2.04760000	-5.16810000	5.87000000
H	1.24880000	-5.78120000	5.45350000
C	2.92210000	-4.49570000	5.01970000
H	2.81430000	-4.58020000	3.93790000
C	3.92950000	-3.69390000	5.54980000
H	4.59050000	-3.14450000	4.87200000
C	7.31700000	-3.31050000	7.27100000
C	7.27110000	-4.66050000	6.91010000
H	6.31090000	-5.17510000	6.82720000
C	8.45180000	-5.35170000	6.64720000
H	8.41280000	-6.40280000	6.36130000
C	9.67840000	-4.69940000	6.74420000
H	10.60050000	-5.24110000	6.53400000
C	9.72940000	-3.35490000	7.10390000
H	10.68860000	-2.84290000	7.17810000
C	8.55160000	-2.66070000	7.36590000
H	8.60100000	-1.60440000	7.64200000
C	5.32010000	-2.64350000	9.79490000
C	4.51020000	-1.83130000	10.59500000
H	4.01100000	-0.95510000	10.17600000
C	4.33460000	-2.13180000	11.94410000
H	3.70360000	-1.49370000	12.56240000
C	4.96710000	-3.24170000	12.49840000
H	4.83200000	-3.47320000	13.55470000
C	5.77280000	-4.05520000	11.70530000
H	6.26920000	-4.92290000	12.13980000
C	5.94840000	-3.76000000	10.35570000
H	6.58240000	-4.40300000	9.74040000