SUPPORTING INFORMATION

A Non–Classical Hydrogen Bond in the Molybdenum Arene Complex [h⁶-$C_6H_5C_6H_3$(Ph)OH]Mo(PMe_3)$_3$: Evidence that Hydrogen Bonding Facilitates Oxidative Addition of the O–H Bond

Tony Hascall, Mu-Hyun Baik, Brian M. Bridgewater, Jun Ho Shin, David G. Churchill, Richard A. Friesner* and Gerard Parkin*

Department of Chemistry,

Columbia University,

New York,

New York 10027.

Received xxxx xx, 2002.

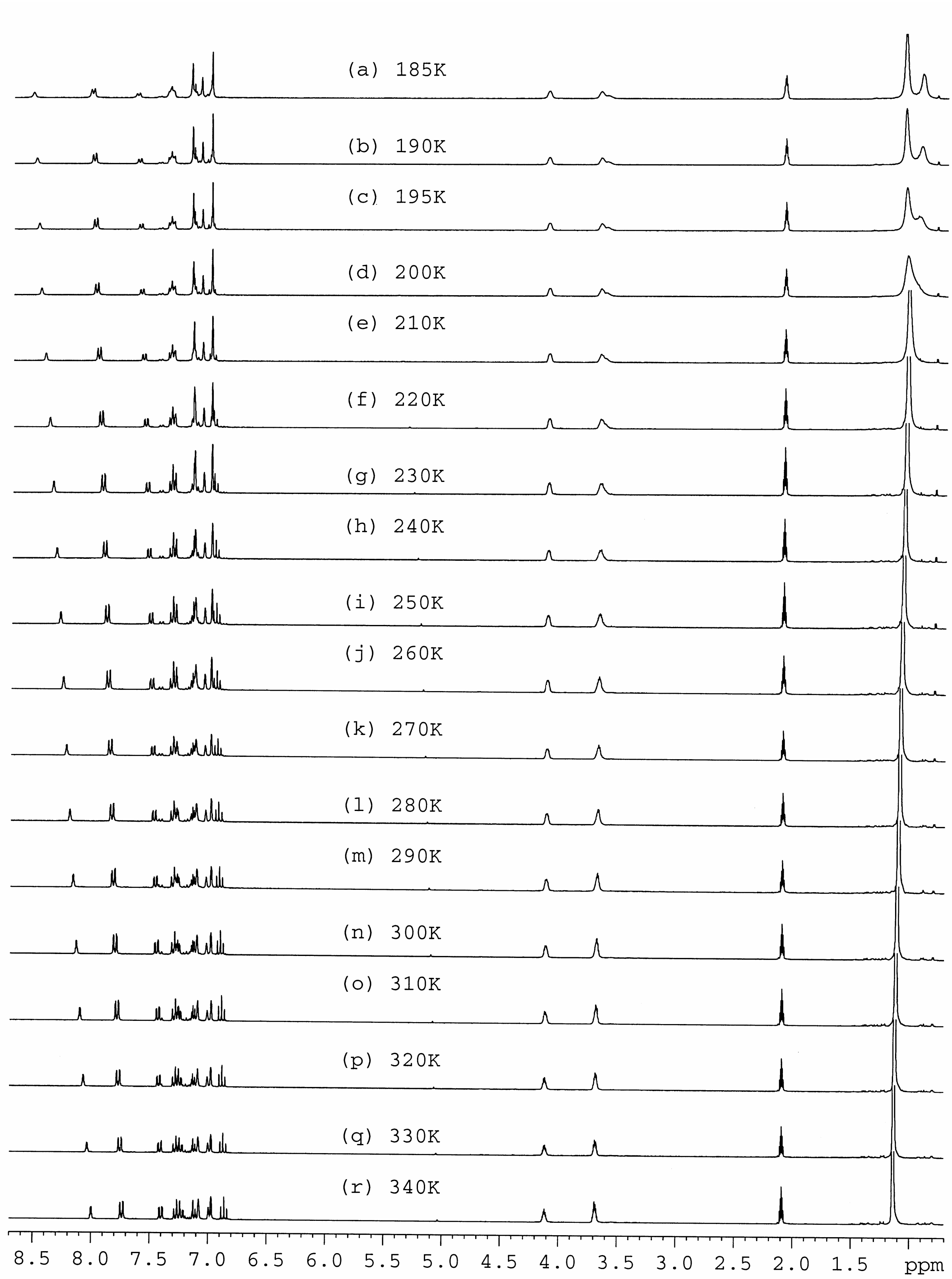
Synthesis of [h^{6},h^{1}-$C_6H_5C_6H_3$(Ph)O]Mo(PMe_3)$_2$H

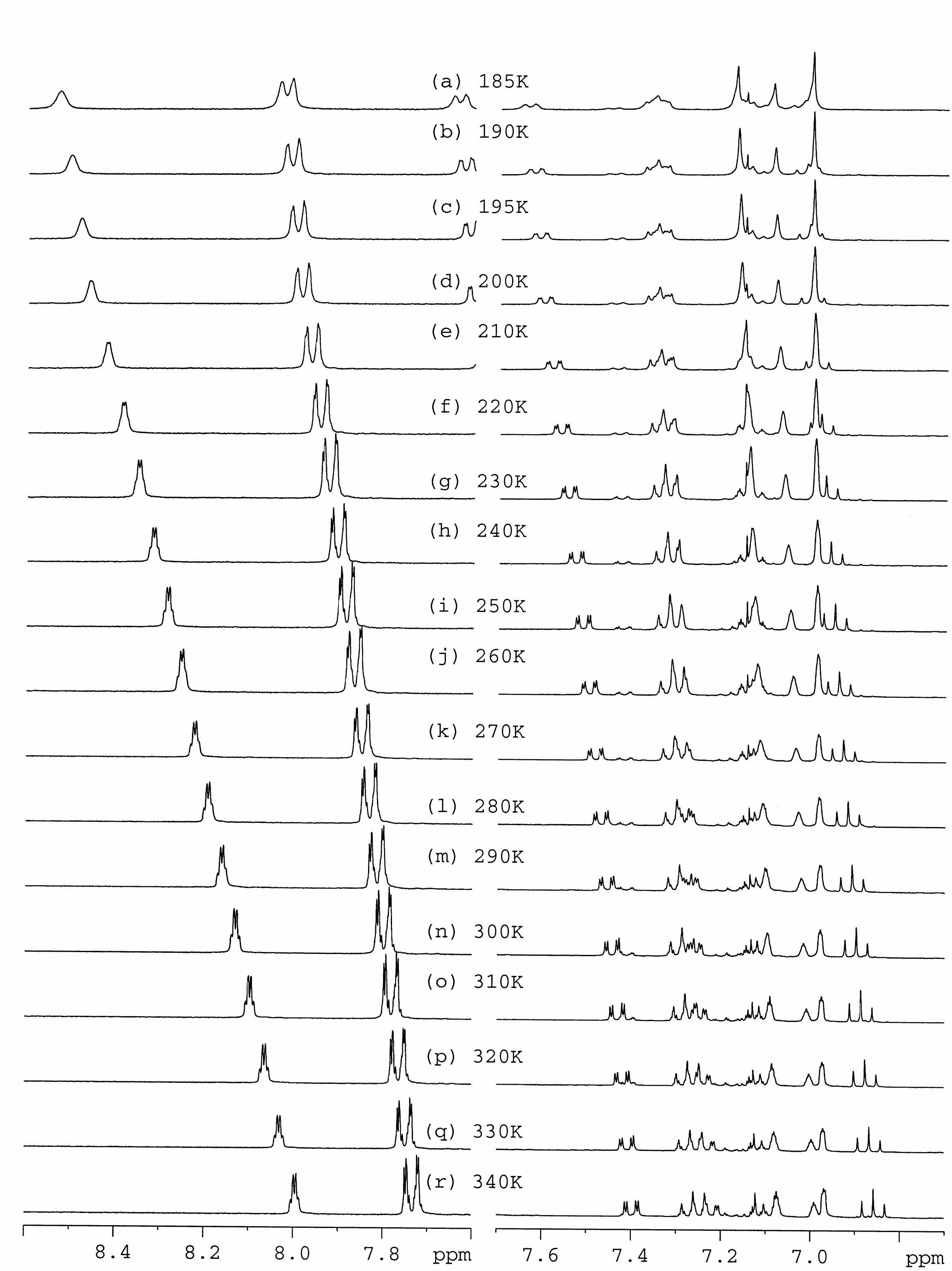
A mixture of Mo(PMe_3)$_6$ (0.34 g, 0.62 mmol) and 2,6-diphenylphenol (0.15 g, 0.61 mmol) in benzene (5 mL) was heated at 80°C for 2 days giving a red solution, after which the volatile components were removed *in vacuo*. The residue was extracted into diethyl ether (10 mL) and filtered. The solvent was removed from the filtrate *in vacuo* to give [η^6,η^1-$C_6H_5C_6H_3$(Ph)O]Mo(PMe_3)$_2$H as a red solid (0.22 g, 73%). ^{1}H NMR (C_6D_6): -4.00 [t, $^2J_{P-H}$ = 58, 1 H, Mo-$\underline{H}$], 1.11 [d, $^2J_{P-H}$ = 7, 18 H of 2 P(C$\underline{H}_3$)$_3$], 2.62 [t, $^3J_{H-H}$ = 5, 1 H of $OC_6H_3(C_6H_5)(\eta^6\text{-}C_6\underline{H}_5)$], 4.13 [m, 2 H of $OC_6H_3(C_6H_5)(\eta^6\text{-}C_6\underline{H}_5)$], 4.73 [t, $^3J_{H-H}$ = 5, 2 H of $OC_6H_3(C_6H_5)(\eta^6\text{-}C_6\underline{H}_5)$], 6.62 [t, $^3J_{H-H}$ = 7, 1 H of $OC_6\underline{H}_3(C_6H_5)(\eta^6\text{-}C_6H_5)$], 7.17 [t, $^3J_{H-H}$ = 8, 1 H of $OC_6H_3(C_6\underline{H}_5)(\eta^6\text{-}C_6H_5)$], 7.22 [d, $^3J_{H-H}$ = 7, 1 H of $OC_6\underline{H}_3(C_6H_5)(\eta^6\text{-}C_6H_5)$], 7.31 [t, $^3J_{H-H}$ = 8, 2 H of $OC_6H_3(C_6\underline{H}_5)(\eta^6\text{-}C_6H_5)$], 7.35 [d, $^3J_{H-H}$ = 7, 1 H of $OC_6\underline{H}_3(C_6H_5)(\eta^6\text{-}C_6H_5)$], 7.86 [d, $^3J_{H-H}$ = 8, 2 H of $OC_6H_3(C_6\underline{H}_5)(\eta^6\text{-}C_6H_5)$]. ^{13}C NMR ($C_6D_6$): 21.9 [dq, $^1J_{P-C}$ = 24, $^1J_{C-H}$ = 128, 6 C of 2 P($\underline{C}H_3$)$_3$], 76.5 [d, $^1J_{C-H}$ = 168, 1 C of $OC_6H_3(C_6H_5)(\eta^6\text{-}\underline{C}_6H_5)$], 77.0 [d, $^1J_{C-H}$ = 171, 2 C of $OC_6H_3(C_6H_5)(\eta^6\text{-}\underline{C}_6H_5)$], 82.3 [d, $^1J_{C-H}$ = 175, 2 C of $OC_6H_3(C_6H_5)(\eta^6\text{-}\underline{C}_6H_5)$], 112.1 [d, $^1J_{C-H}$ = 160, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 118.5 [s, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 124.3 [d, $^1J_{C-H}$ = 155, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 125.5 [d, $^1J_{C-H}$ = 154, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 127.5 [overlapped with solvent, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 128.8 [overlapped with solvent, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 130.1 [d, $^1J_{C-H}$ = 158, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 131.7 [s, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 142.1 [s, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 172.1 [s, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 1C of $OC_6H_3(C_6H_5)(\eta^6\text{-}\underline{C}_6H_5)$ [not located]. ^{31}P NMR (C_6D_6): 9.1 [s]. Analysis calcd. for $C_{24}H_{32}OP_2Mo$: C, 58.3%; H, 6.5%. Found: C, 58.3%; H, 6.1%. IR data (KBr, cm^{-1}): 2966 (m), 2901 (m), 1735 (w) [ν_{Mo-H}], 1586 (w), 1560 (w), 1498 (w), 1449 (w), 1405 (s), 1284 (s), 1257 (m), 1070 (w), 939 (s), 847 (m), 785 (w), 751 (m), 704 (m).

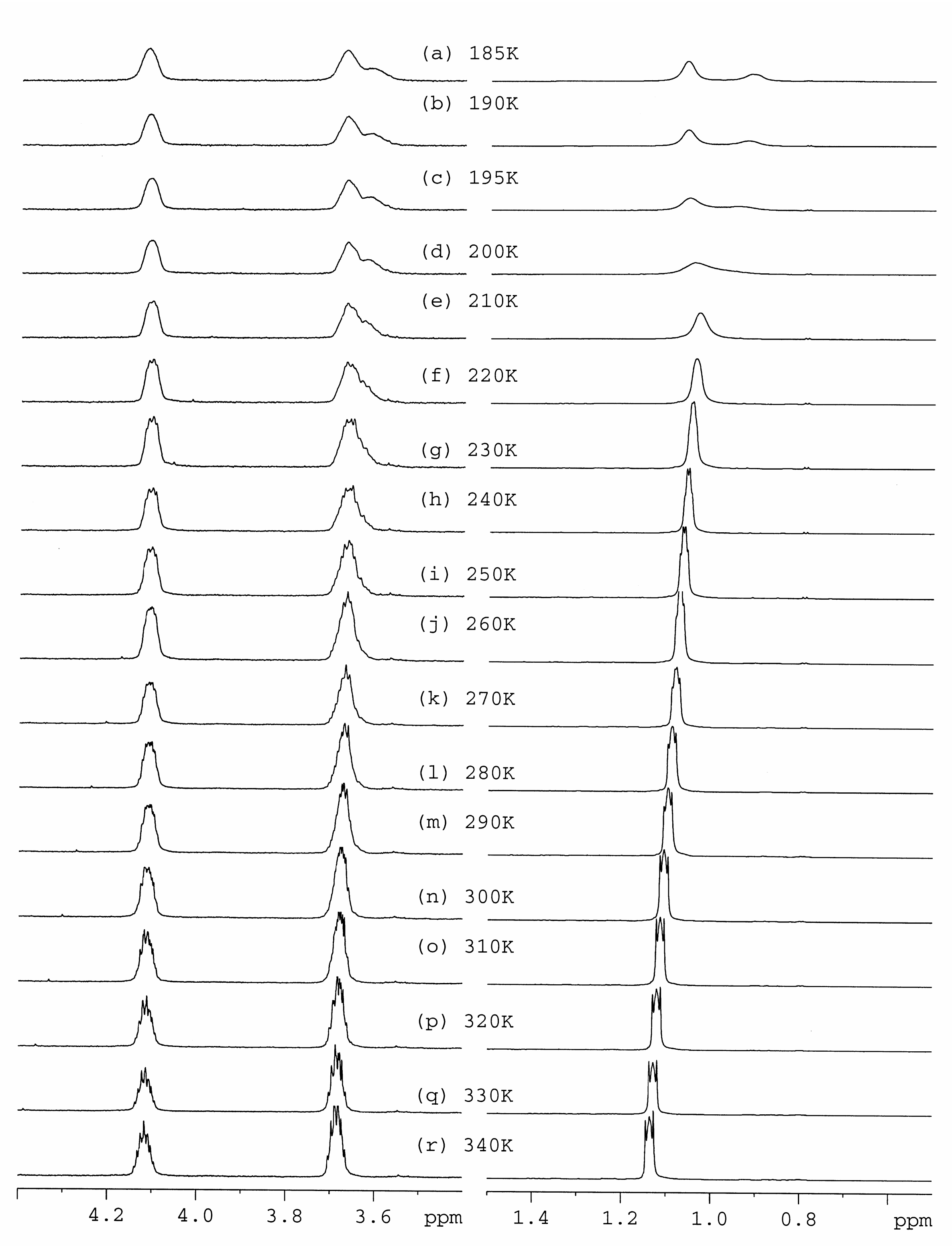
Synthesis of [h^{6}-$C_6H_5C_6H_3$(Ph)OH]Mo(PMe_3)$_3$

A mixture of Mo(PMe_3)$_6$ (0.41 g, 0.74 mmol) and 2,6-diphenylphenol (0.18 g, 0.73 mmol) in benzene (5 mL) was stirred at 70°C for 1 hour. The volatile components were removed under reduced pressure and the residue was washed twice with diethyl ether (5 mL and 2 mL) giving $[\eta^6\text{-}C_6H_5C_6H_3(Ph)OH]Mo(PMe_3)_3$ as an orange solid (0.16 g, 38%). ^{1}H NMR (C_6D_6): 1.09 [m, 27 H of 3 $P(C\underline{H}_3)_3$], 3.70 [m, 3 H of $HOC_6H_3(C_6H_5)(\eta^6\text{-}C_6\underline{H}_5)$], 4.18 [m, 2 H of $HOC_6H_3(C_6H_5)(\eta^6\text{-}C_6\underline{H}_5)$], 6.93 [t, $^3J_{H\text{-}H}$ = 8, 1 H of $HOC_6\underline{H}_3(C_6H_5)(\eta^6\text{-}C_6H_5)$], 7.13 [m, 1 H of $HOC_6H_3(C_6\underline{H}_5)(\eta^6\text{-}C_6H_5)$], 7.31 [m, 2 H of $HOC_6H_3(C_6\underline{H}_5)(\eta^6\text{-}C_6H_5)$], 7.33 [m, 1 H of $HOC_6\underline{H}_3(C_6H_5)(\eta^6\text{-}C_6H_5)$], 7.53 [dd, $^3J_{H\text{-}H}$ = 8, $^4J_{H-H}$ = 2, 1 H of $HOC_6\underline{H}_3(C_6H_5)(\eta^6\text{-}C_6H_5)$], 7.88 [dd, $^3J_{H\text{-}H}$ = 8, $^4J_{H\text{-}H}$ = 1, 2 H of $HOC_6H_3(C_6\underline{H}_5)(\eta^6\text{-}C_6H_5)$], 8.24 [m, 1 H of $\underline{H}OC_6H_3(C_6H_5)(\eta^6\text{-}C_6H_5)$]. ^{13}C NMR ($C_6D_6$): 27.0 [q, $^1J_{C\text{-}H}$ = 127, 9 C of 3 $P(\underline{C}H_3)_3$], 68.9 [d, $^1J_{C\text{-}H}$ = 167, $HOC_6H_3(C_6H_5)(\eta^6\text{-}\underline{C}_6H_5)$], 74.6 [d, $^1J_{C\text{-}H}$ = 162, $HOC_6H_3(C_6H_5)(\eta^6\text{-}\underline{C}_6H_5)$], 76.7 [d, $^1J_{C\text{-}H}$ = 161, $HOC_6H_3(C_6H_5)(\eta^6\text{-}\underline{C}_6H_5)$], 78.4 [s, $HOC_6H_3(C_6H_5)(\eta^6\text{-}\underline{C}_6H_5)$], 119.9 [d, $^1J_{C\text{-}H}$ = 159, $HO\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 126.7 [d, $^1J_{C\text{-}H}$ = 159, $HO\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 129.4 [s, $HO\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 129.9 [d, $^1J_{C\text{-}H}$ = 159, $HO\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 130.6 [d, $^1J_{C\text{-}H}$ = 150, $HO\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 140.2 [s, $HO\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 150.3 [s, $HO\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], [two additional peaks are obscured by the solvent resonance]. ^{31}P NMR (C_6D_6): -1.1 [s]. Analysis calcd. for $C_{27}H_{41}OP_3Mo$: C, 56.8%; H, 7.2%. Found: C, 57.4%; H, 6.6%. IR data (KBr, cm^{-1}): 2964 (m), 2903 (m), 1498 (w), 1460 (w), 1422 (m), 1272 (w), 1244 (w), 937 (s), 756 (m), 700 (m). Removal of the volatile components from the diethyl ether filtrate gave a red solid (80 mg) consisting of $[\eta^6,\eta^1\text{-}C_6H_5C_6H_3(Ph)O]Mo(PMe_3)_2H$, contaminated by a small amount of $[\eta^6\text{-}C_6H_5C_6H_3(Ph)OH]Mo(PMe_3)_3$.

Variable temperature ^{1}H NMR spectra of in d8–toluene are shown below.


(a) 185K
(b) 190K
(c) 195K
(d) 200K
(e) 210K
(f) 220K
(g) 230K
(h) 240K
(i) 250K
(j) 260K
(k) 270K
(l) 280K
(m) 290K
(n) 300K
(o) 310K
(p) 320K
(q) 330K
(r) 340K
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm


(a) 185K
(b) 190K
(c) 195K
(d) 200K
(e) 210K
(f) 220K
(g) 230K
(h) 240K
(i) 250K
(j) 260K
(k) 270K
(l) 280K
(m) 290K
(n) 300K
(o) 310K
(p) 320K
(q) 330K
(r) 340K
8.4
8.2
8.0
7.8
ppm
7.6
7.4
7.2
7.0
ppm



Synthesis of [h^6,h^1-$C_6H_5C_6H_3$(Ph)O]W(PMe_3)$_2$H

A solution of $W(PMe_3)_4(\eta^2\text{-}CH_2PMe_2)H$ (0.30 g, 0.53 mmol) and 2,6-diphenylphenol (0.13 g, 0.53 mmol) in benzene (5 mL) was stirred at 80°C for 2 hours, resulting in the formation of a dark red solution. After this period, the volatile components were removed *in vacuo* and the residue was extracted into diethyl ether (5 mL) and filtered. The solvent was removed from the filtrate *in vacuo* to give $[\eta^6,\eta^1\text{-}C_6H_5C_6H_3(Ph)O]W(PMe_3)_2H$ as a red solid (0.23 g, 74%). ^1H NMR (C_6D_6): -2.42 [t, $^2J_{P\text{-}H}$ = 50, 1 H, W-$\underline{H}$], 1.26 [d, $^2J_{P\text{-}H}$ = 8, 18 H of 2 $P(C\underline{H}_3)_3$], 2.42 [t, $^3J_{H\text{-}H}$ = 6, 1 H of $OC_6H_3(C_6H_5)(\eta^6\text{-}C_6\underline{H}_5)$], 4.06 [m, 2 H of $OC_6H_3(C_6H_5)(\eta^6\text{-}C_6\underline{H}_5)$], 4.43 [m, 2 H of $OC_6H_3(C_6H_5)(\eta^6\text{-}C_6\underline{H}_5)$], 6.59 [t, $^3J_{H\text{-}H}$ = 7, 1 H of $OC_6\underline{H}_3(C_6H_5)(\eta^6\text{-}C_6H_5)$], 7.17 [m, 1 H of $OC_6\underline{H}_3(C_6H_5)(\eta^6\text{-}C_6H_5)$], 7.18 [m, 1 H of $OC_6H_3(C_6\underline{H}_5)(\eta^6\text{-}C_6H_5)$], 7.23 [dd, $^3J_{H\text{-}H}$ = 7, $^4J_{H\text{-}H}$ = 2, 1 H of $OC_6\underline{H}_3(C_6H_5)(\eta^6\text{-}C_6H_5)$], 7.30 [t, $^3J_{H\text{-}H}$ = 8, 2 H of $OC_6H_3(C_6\underline{H}_5)(\eta^6\text{-}C_6H_5)$], 7.75 [d, $^3J_{H\text{-}H}$ = 8, 2 H of $OC_6H_3(C_6\underline{H}_5)(\eta^6\text{-}C_6H_5)$]. ^{13}C NMR (C_6D_6): 22.5 [dq, $^1J_{P\text{-}C}$ = 27, $^1J_{C\text{-}H}$ = 128, 6 C of 2 $P(\underline{C}H_3)_3$], 68.1 [d, $^1J_{C\text{-}H}$ = 174, 2 C of $OC_6H_3(C_6H_5)(\eta^6\text{-}\underline{C}_6H_5)$], 77.8 [d, $^1J_{C\text{-}H}$ = 165, 1 C of $OC_6H_3(C_6H_5)(\eta^6\text{-}\underline{C}_6H_5)$], 83.9 [d, $^1J_{C\text{-}H}$ = 165, 2 C of $OC_6H_3(C_6H_5)(\eta^6\text{-}\underline{C}_6H_5)$], 112.9 [d, $^1J_{C\text{-}H}$ = 160, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 116.1 [s, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 124.5 [dd, $^1J_{C\text{-}H}$ = 155, $^2J_{C\text{-}H}$ = 9, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 125.7 [dt, $^1J_{C\text{-}H}$ = 159, $^2J_{C\text{-}H}$ = 8, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 127.5 [dd, $^1J_{C\text{-}H}$ = 157, $^2J_{C\text{-}H}$ = 8, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 128.9 [dd, $^1J_{C\text{-}H}$ = 153, $^2J_{C\text{-}H}$ = 9, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 129.7 [s, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 130.2 [dt, $^1J_{C\text{-}H}$ = 158, $^2J_{C\text{-}H}$ = 7, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 131.5 [s, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 142.0 [s, $O\underline{C}_6H_3(\underline{C}_6H_5)(\eta^6\text{-}C_6H_5)$], 1C of $OC_6H_3(C_6H_5)(\eta^6\text{-}\underline{C}_6H_5)$ [not located]. ^{31}P NMR (C_6D_6): –18.1 [s, $^1J_{W\text{-}P}$ = 317]. Analysis calcd. for $C_{24}H_{32}OP_2W$: C, 49.5%; H, 5.5%. Found: C, 50.0%; H, 4.8%. IR data (KBr, cm^{-1}): 3066 (w), 2968 (w), 2902 (w), 1792 (w) [$\nu_{W\text{-}H}$], 1586 (w), 1498 (w), 1450 (w), 1406 (s), 1281 (m), 1254 (m), 1069 (w), 1011 (w), 939 (s), 848 (m), 797 (w), 754 (m), 704 (m), 667 (m), 598 (w).

X-ray Structure Determination

X-ray diffraction data were collected on a Bruker P4 diffractometer equipped with a

SMART CCD detector. The structures were solved using direct methods and standard difference map techniques, and were refined by full-matrix least-squares procedures on F^2 with SHELXTL (Version 6.10). The crystallographic data for $[\eta^6\text{-}C_6H_5C_6H_3(Ph)OH]Mo(PMe_3)_3$ (CCDC 193308), $[\eta^6,\eta^1\text{-}C_6H_5C_6H_3(Ph)O]Mo(PMe_3)_2H$ (CCDC 193307) and $[\eta^6,\eta^1\text{-}C_6H_5C_6H_3(Ph)O]W(PMe_3)_2H$ (CCDC 193309) have been deposited with the Cambridge Crystallographic Data Centre. The M–H and O–H hydrogen atoms were located in a difference map and refined isotropically.

Computational Details and Discussion

All calculations were carried out using DFT as implemented in the Jaguar 4.1 suite[S1] of *ab initio* quantum chemistry programs. Geometry optimizations were performed with the B3LYP[S2] functional and the 6-31G** basis set for C, H, O and P, while Mo was represented using the Los Alamos LACVP** basis set[S3] that includes relativistic effective core potentials. The energies of the optimized structures were reevaluated by additional single point calculations on each optimized geometry using Dunning's correlation consistent triple-ζ basis set[S4] cc-pVTZ(-f) that includes a double set of polarization functions. For Mo a modified version of LACVP**, designated as LACV3P**, was used, where the exponents were decontracted to match the effective core potential with the triple-ζ quality basis. Cartesian coordinates for the derived structures are listed in Table S1, while the computed electronic energy surface for various mechanisms for oxidative addition of the O–H bond are illustrated in Figure S1.

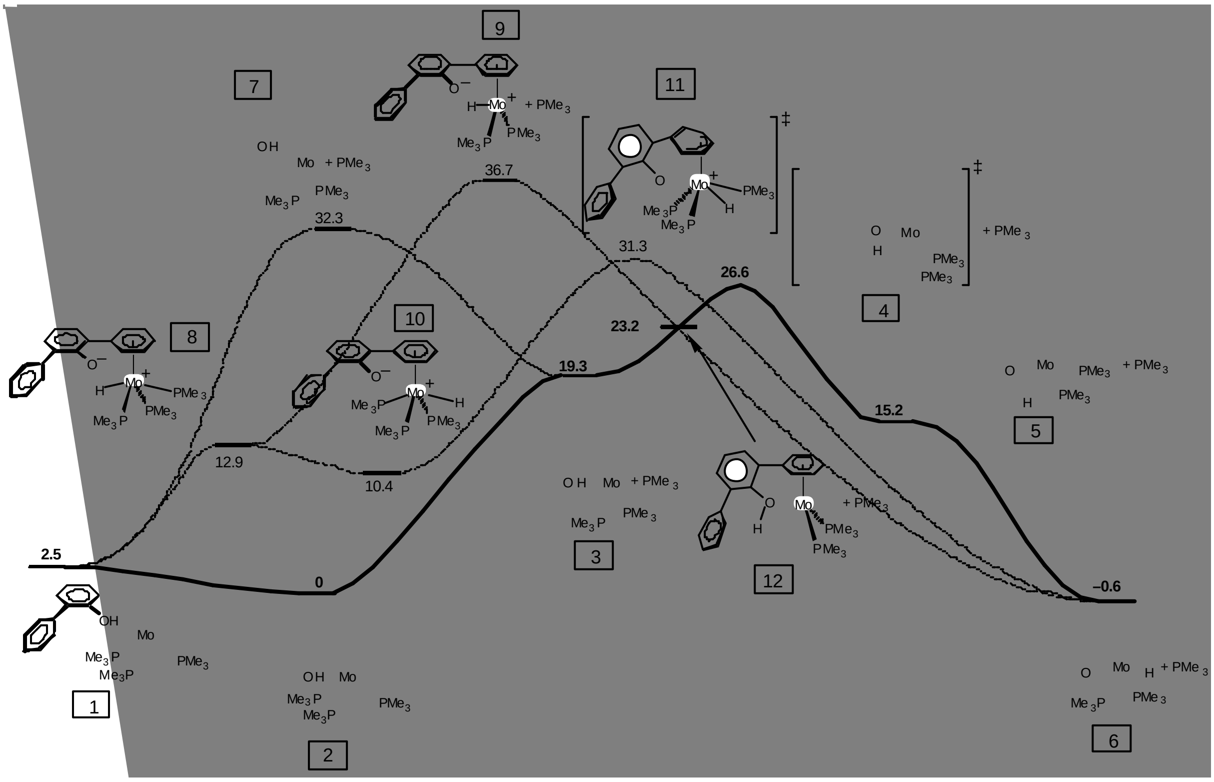


Figure S1. Computed electronic energy surface for various mechanisms for oxidative addition of the O–H bond. All structures are labeled for ease of discussion.

The transition state structures **4** and **11** (Figure S1), corresponding to the dissociative and associative pathways, respectively, were located by first sampling the direct reaction path between the reactants and products utilizing the linear transit method, followed by a quadratic synchronous transit (QST) search using the highest energy structure from the linear transit run as the starting guess of the transition state. The main reaction coordinate for the dissociative pathway was identified as the composite movement of the O–H group and the Mo center by calculations on the computationally simpler model $[\eta^6\text{-}C_6H_5C_6H_4O]Mo(PH_3)_2H$, for which the imaginary frequency of 435i cm^{-1} was the only physically meaningful imaginary frequency in the model. The reaction coordinate for the associative pathway leading to the transition state structure

11, consists of the Mo–O vector coupled to a hapticity change of the aryl ligand from η^6 to η^4, as indicated in Figure S1. Surprisingly, the Mo–P bond between the metal center and the leaving group is not involved and stays intact at a bond length of 2.434 Å. Thus, the main reaction coordinate contains two fairly independent components: (i) formation of the Mo–O bond promoted by ring-slippage of the aryl ligand and (ii) subsequent cleavage of the Mo–P.

One of the most salient features of the reaction energy profile (Figure S1) is that the hydrogen bond is much stronger in **3**, {[η^6-$C_6H_5C_6H_3$(Ph)OH]Mo(PMe_3)$_2$}, than in **2**, [η^6-$C_6H_5C_6H_3$(Ph)OH]Mo(PMe_3)$_3$, as indicated by comparison with the corresponding non-hydrogen bonded structures **7** and **1**, respectively. This observation is counterintuitive in the sense that the more electron rich metal center in **2** would be expected to form the stronger metal-hydrogen bond. Nevertheless, analysis of the frontier orbitals are fully consistent with the relative energetics found, as illustrated in Figure S2 for the most important orbitals. As expected for a d^6-Mo(0) center, there are 3 occupied MOs that are dominated by metal-centered d-orbitals. The HOMO of **7** is a complex combination of d-orbitals that can be described as Mo-$d_{x^2-z^2}$, whereas the most important orbital for the hydrogen bond interaction in **1** is (HOMO-1), mostly a Mo-$d_{x^2-y^2}$ orbital. Surprisingly, the HOMO of **7** is substantially higher in energy than any of the filled metal-based orbitals of **1** with an orbital energy of -2.617 eV. Upon formation of the hydrogen bond, all occupied metal-dominated orbitals become stabilized, but the stabilization is greater for {[η^6-$C_6H_5C_6H_3$(Ph)OH]Mo(PMe_3)$_2$} than for [η^6-$C_6H_5C_6H_3$(Ph)OH]Mo(PMe_3)$_3$, consistent with a stronger hydrogen bond.

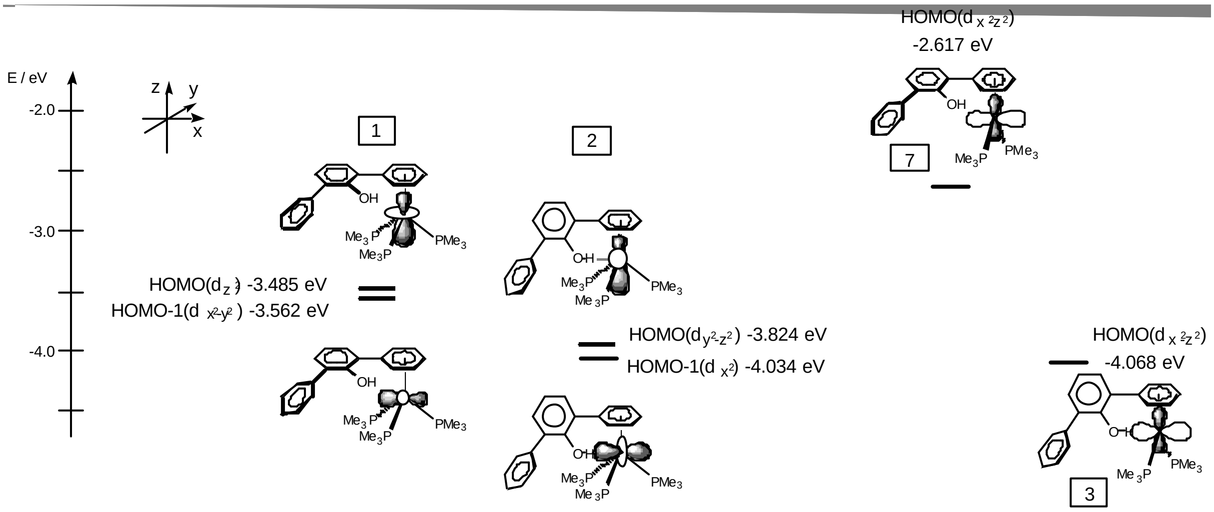
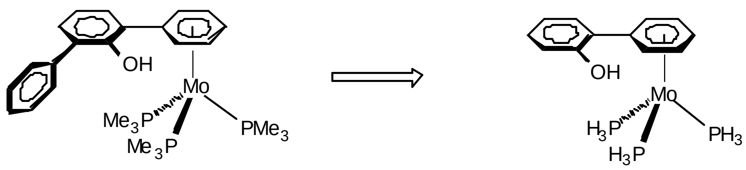


Figure S2. Cartoon representations of the most important MOs promoting the hydrogen bond interaction. The HOMOs of **1** and **2**, which are not significantly involved, are also shown.

Vibrational frequency calculations are prohibitively expensive for the full system. Thus, they were carried on a truncated model shown below, in which the phenyl group and methyl groups were replaced with hydrogens, while the rest of the molecule was left at the optimized coordinates of the respective structure.



The C–H (substitute for the phenyl group) and P–H bond lengths were set to 1.087 Å and 1.427 Å, respectively. Bond angles were not modified. This approach assumes that the truncation does not affect the potential energy surface with respect to the main structural distortion vector of interest, Mo•••(HO) coordinate. Testing this truncated models for convergence to local mininum for equilibrium and intermediate structures or a local maximum for transition states is at least a reasonable approach. Owing to the fact that the rest of the molecule is frozen at the optimized geometry of the full model, a number of meaningless imaginary frequencies are expected since the PH_3 geometries are not optimized. These frequencies correspond to vibrations that are connected directly to the newly introduced hydrogen atoms. For example, axial rotations of the PH_3 ligand often gave rise to imaginary frequencies (between 80-300 cm^{-1}). Likewise, bending modes associated witrh the Mo–P–H bonds also gave imaginary frequencies (e.g. 41 cm^{-1} in truncated model of **3**). These artificial frequencies are marked in Table 2 by parentheses.

Table S1. Cartesian coordinates (in Å) of all optimized geometries.

==

1

==
=

Mo	0.015245054	0.021494230	-0.001728379
P	-0.005143711	0.051969553	2.469104304
P	2.474096627	0.031725805	-0.115908237
P	0.015619482	-2.436870869	-0.071836501
C	1.014957729	1.338579128	3.354909621
H	0.804492365	1.356962561	4.430648843
H	0.795850045	2.310675112	2.912167833
H	2.078854217	1.130083496	3.210261763
C	0.453366922	-1.405936791	3.549269586
H	1.496252605	-1.680759666	3.368534496
H	-0.173722440	-2.269584146	3.312297503
H	0.332128392	-1.169493283	4.612648938
C	-1.661133240	0.433744300	3.247028749
H	-1.596093732	0.484170678	4.339744102
H	-2.382156049	-0.339834302	2.967552284
H	-2.028787341	1.392045969	2.871279440
C	3.603881533	-0.712447851	1.178835824
H	3.365897831	-1.766577451	1.333041457
H	3.460914410	-0.192534762	2.130272244
H	4.657799994	-0.624886853	0.891105080
C	3.313634178	1.689901120	-0.241841705
H	4.398427422	1.586637976	-0.358508218
H	3.104391679	2.264449107	0.664394632
H	2.911693836	2.252153936	-1.086866537
C	3.217896394	-0.777375607	-1.626232540
H	2.770651484	-0.334497906	-2.520657865
H	2.985554344	-1.845942631	-1.630401652
H	4.306058286	-0.651931444	-1.668696425
C	1.363422779	-3.547580461	0.603344385
H	1.109723348	-4.605294213	0.469237497
H	1.514841954	-3.353718936	1.667637679

H	2.303295141	-3.350087018	0.081331700
C	-1.449567566	-3.319724225	0.679455340
H	-2.369108450	-2.914618346	0.247804569
H	-1.481683154	-3.140829040	1.757405594
H	-1.416033630	-4.400654952	0.501050574
C	-0.072479437	-3.191865709	-1.780341044
H	-0.099735622	-4.286568046	-1.739140532
H	0.796058066	-2.876824501	-2.364741470
H	-0.970547864	-2.838987417	-2.294236305
C	-0.311259064	2.230193282	-0.915088795
C	-1.362138150	1.921159572	-0.000474015
H	-1.568255991	2.607080242	0.809217451
C	-2.197155336	0.775562523	-0.181008614
H	-3.012758429	0.590147307	0.508186678
C	-1.936256374	-0.132924270	-1.236076244
H	-2.573276579	-1.001157939	-1.370700605
C	-0.873848386	0.130087869	-2.156768528
H	-0.670740801	-0.550206767	-2.975121226
C	-0.042146647	1.253203934	-1.949437649
H	0.786314334	1.417289576	-2.628491171
C	0.728086400	4.299973320	0.201927312
C	0.426261832	3.518361508	-0.939059473
C	0.878693587	4.020751195	-2.177001756
H	0.607526154	3.485847176	-3.080605016
C	1.638787315	5.184066154	-2.284311256
H	1.963780277	5.531685449	-3.260521082
C	1.989402146	5.885095763	-1.134584006
H	2.622199132	6.765891456	-1.191076113
C	1.546182985	5.446353667	0.122729957
C	1.971066852	6.172324751	1.353840122
C	1.828580962	7.567805458	1.453126517
H	1.357174042	8.108122564	0.637141545
C	2.275316739	8.255152226	2.582188585
H	2.154974120	9.333627160	2.637449011
C	2.865991909	7.562093941	3.643072230
H	3.209458137	8.098274921	4.523084831
C	3.012985392	6.175761351	3.562229478
H	3.480884854	5.627207515	4.375109650
C	2.573820034	5.488158504	2.428927771
H	2.728510653	4.414904220	2.359074046
O	0.208918005	3.905488079	1.408170791
H	0.434938475	4.577461144	2.068851619

==

2

==

Mo	0.431335901	1.235238902	-0.933873085
P	-1.306770509	1.913373625	0.733322291
P	-0.895637451	-0.552564315	-2.047710587
P	-0.423591987	2.914837552	-2.557048712
O	-0.168966120	-1.154010617	1.647075366
H	-0.113177281	-0.465856997	0.931003760
C	-2.829842802	0.873178210	1.060243370
H	-3.393737690	1.258151970	1.917045414

H	-2.532313727	-0.157575601	1.272530764
H	-3.479189196	0.880194381	0.180528155
C	-2.167490051	3.575201018	0.639033703
H	-2.707708217	3.685417462	-0.306567388
H	-1.424262103	4.375821877	0.710300180
H	-2.880848555	3.687985927	1.462647919
C	-0.717962478	2.070110628	2.501266259
H	-1.522243340	2.436335331	3.146376005
H	0.121257832	2.769500761	2.554392533
H	-0.389940627	1.092848368	2.863559966
C	-2.761944470	-0.645548204	-2.164479853
H	-3.174490161	0.308358229	-2.498907419
H	-3.175935289	-0.868434339	-1.180352411
H	-3.077424565	-1.431490717	-2.858227246
C	-0.618691021	-2.310515606	-1.492628878
H	-1.148267812	-3.019093150	-2.139576698
H	-0.978812150	-2.426628750	-0.469528852
H	0.447294794	-2.548344932	-1.499487064
C	-0.492161000	-0.775067684	-3.851913545
H	0.589649959	-0.855878200	-3.972747232
H	-0.828859810	0.091881736	-4.421775933
H	-0.970463667	-1.671116102	-4.265381241
C	-2.171868759	2.956231802	-3.223379800
H	-2.339632625	3.824946843	-3.867579693
H	-2.889044368	2.980016839	-2.400452685
H	-2.363680301	2.052781529	-3.807549396
C	-0.240999556	4.722804417	-2.112303106
H	0.781571380	4.905879270	-1.770950250
H	-0.918933653	4.986519670	-1.299918886
H	-0.451399696	5.370270088	-2.970998172
C	0.479834510	2.980340829	-4.192866993
H	0.072452615	3.762966027	-4.842955122
H	0.406000217	2.016415380	-4.702146992
H	1.539615722	3.186646541	-4.018267181
C	2.055315202	-0.180449979	0.084337889
C	1.966321939	1.059772990	0.793652254
H	1.789222381	1.032800654	1.861775197
C	2.214978190	2.309765029	0.156098646
H	2.198389848	3.230735251	0.727496774
C	2.437600768	2.333076249	-1.243344268
H	2.605324128	3.281403793	-1.743821753
C	2.519266964	1.114695431	-1.989442756
H	2.722804885	1.129997211	-3.053748306
C	2.287050235	-0.114996703	-1.329458913
H	2.335684520	-1.041592400	-1.891860255
C	0.963797982	-1.906868808	1.586380695
C	2.060341431	-1.484133966	0.801775822
C	3.189535588	-2.313324508	0.719834310
H	4.029692286	-1.991090243	0.109289790
C	3.253548076	-3.514643377	1.424352330
H	4.136350052	-4.144822408	1.354670648
C	2.175223808	-3.898988542	2.222923207
H	2.214158745	-4.837593601	2.769235235
C	1.009533497	-3.117944992	2.314331184

C	-0.121363853	-3.572590952	3.172750910
C	0.141493592	-4.074295880	4.462222849
H	1.163873928	-4.074855592	4.832967653
C	-0.889389482	-4.546880444	5.276814924
H	-0.659617736	-4.923350921	6.271713843
C	-2.210489225	-4.527322642	4.819413240
H	-3.015209852	-4.891914504	5.452303503
C	-2.488055308	-4.030447041	3.539903313
H	-3.511380703	-4.012664613	3.170821035
C	-1.457653276	-3.556909492	2.727833372
H	-1.685271045	-3.173309673	1.738719348

==

3

==

Mo	0.351179920	1.118633466	-0.727164367
P	-1.424841411	1.945202835	0.782256651
P	-1.003171726	-0.459233573	-2.086226849
O	-0.008047341	-1.191768448	1.773730075
H	0.011693789	-0.453758330	1.106326428
C	-2.857867096	0.886531844	1.322483937
H	-3.512527600	1.420622942	2.020093560
H	-2.476449593	-0.014831632	1.810285976
H	-3.444348622	0.587010364	0.449251275
C	-2.338571833	3.424131579	0.108084340
H	-2.835295219	3.158332345	-0.829563654
H	-1.627991080	4.229730523	-0.097655585
H	-3.090955955	3.786004405	0.817308313
C	-0.905895121	2.597420907	2.444979739
H	-1.750614031	3.030507160	2.991247466
H	-0.131860907	3.358627523	2.319578768
H	-0.488586146	1.775272105	3.033217838
C	-2.362643096	0.264019297	-3.137727269
H	-1.943331044	1.019469792	-3.809439611
H	-3.101369933	0.752741422	-2.495828329
H	-2.864904500	-0.502172136	-3.738608023
C	-1.919969167	-1.818356152	-1.211839892
H	-2.444337966	-2.465628423	-1.923341585
H	-2.642361626	-1.394910987	-0.511138064
H	-1.205882638	-2.415738383	-0.639799400
C	-0.115578458	-1.471496600	-3.370995467
H	0.606021531	-2.126230068	-2.875260583
H	0.432432297	-0.808959762	-4.046745179
H	-0.809137588	-2.086703905	-3.954474282
C	2.073441731	-0.123011890	0.090589378
C	1.943725536	1.080641093	0.880700565
H	1.803220742	0.989417745	1.952313194
C	2.025638419	2.368313420	0.284499169
H	1.916357665	3.257579768	0.895310697
C	2.109783771	2.481958937	-1.131645024
H	2.088329762	3.460617116	-1.600596767
C	2.318048618	1.308854323	-1.930503804
H	2.429983616	1.394500571	-3.005908652

C	2.314467426	0.035387670	-1.317705396
H	2.413194247	-0.854136717	-1.929693059
C	1.106598436	-1.942892291	1.567675414
C	2.146655831	-1.467090635	0.732645696
C	3.267064527	-2.284182034	0.526773927
H	4.066471774	-1.918995829	-0.112734953
C	3.374948961	-3.529531775	1.145464036
H	4.250570750	-4.150017625	0.978876005
C	2.351244673	-3.970755714	1.982589414
H	2.423307390	-4.944231961	2.459488908
C	1.198273689	-3.200541739	2.205360816
C	0.124487175	-3.715561553	3.101233910
C	0.463216585	-4.328387944	4.320596651
H	1.507225423	-4.371805039	4.618598893
C	-0.518572582	-4.857333760	5.160441293
H	-0.229946582	-5.319058992	6.101130693
C	-1.865471362	-4.784708058	4.798924620
H	-2.631989072	-5.193449262	5.451795986
C	-2.218161870	-4.177315299	3.590260064
H	-3.263096749	-4.117197215	3.296395634
C	-1.236874209	-3.646791046	2.753345322
H	-1.521412225	-3.173470537	1.821043598

==

4

==

Mo	0.065680407	-0.036018707	2.073198537
P	2.507260328	0.057836449	1.691126435
P	0.064740015	-2.413451512	2.712783916
O	-0.327314567	-0.593692773	-0.383118373
H	0.335995495	0.105894337	-0.509881774
C	3.345082157	-1.119044139	0.501381429
H	4.422445861	-0.934624128	0.422351998
H	2.896584355	-1.017386692	-0.492080027
H	3.184567603	-2.149881931	0.831352738
C	3.609681472	-0.149915760	3.175586939
H	3.443310265	-1.130531923	3.625269799
H	3.341251282	0.608945711	3.915130496
H	4.670086183	-0.045822783	2.917992799
C	3.208566978	1.658195079	1.030698831
H	4.298786940	1.614468558	0.930174074
H	2.949401288	2.477955176	1.706633221
H	2.770536389	1.879777591	0.052148763
C	1.518186106	-3.279289217	3.500987333
H	1.751990527	-2.799136428	4.456257701
H	2.397054303	-3.202268467	2.854590799
H	1.307263283	-4.339829094	3.680300726
C	-0.249649932	-3.587458353	1.294376573
H	-0.301997047	-4.630211447	1.626588868
H	0.548129489	-3.484516715	0.553235507
H	-1.194989198	-3.318739195	0.813061082
C	-1.265493559	-3.001688329	3.880816715
H	-2.243682175	-2.693602030	3.502081646
H	-1.121304206	-2.543574893	4.863508723

H	-1.253323125	-4.091226154	3.993888168
C	-1.729418122	1.057041851	1.417016258
C	-0.682253396	2.048124131	1.493782041
H	-0.432127657	2.651755249	0.628087254
C	0.063504440	2.163608309	2.702694672
H	0.900944982	2.853451308	2.739430134
C	-0.259752375	1.393449430	3.863015195
H	0.299575487	1.512943227	4.783417979
C	-1.350000807	0.479917952	3.786923016
H	-1.598800752	-0.124877476	4.652429866
C	-2.137915797	0.355733266	2.599874537
H	-2.951804853	-0.358249893	2.547228954
C	-1.581421941	-0.107126207	-0.793525530
C	-2.320557971	0.697639867	0.093255885
C	-3.594286164	1.124664146	-0.301631421
H	-4.175165703	1.740509557	0.378991396
C	-4.108042978	0.762607837	-1.548359679
H	-5.100412036	1.090368810	-1.844172875
C	-3.350545187	-0.022484147	-2.415173771
H	-3.757403697	-0.315152097	-3.378649110
C	-2.068250771	-0.478160922	-2.059387637
C	-1.278099330	-1.298783291	-3.018430768
C	-1.215697121	-0.921527176	-4.372154115
H	-1.714902611	-0.011449183	-4.694134244
C	-0.504763173	-1.685210365	-5.298369852
H	-0.464527734	-1.369964158	-6.337807090
C	0.158565184	-2.844529514	-4.888374865
H	0.713640765	-3.441064599	-5.606807713
C	0.102926241	-3.231087863	-3.545873410
H	0.610373758	-4.134333366	-3.217659979
C	-0.604927476	-2.467248375	-2.619545347
H	-0.646850789	-2.778767060	-1.582492408

==

5

==

Mo	0.185981524	-0.043493606	1.773798578
P	2.590684257	0.454010515	2.008852497
P	0.602178475	-2.465111022	1.961804168
O	-0.925893382	-0.909573590	0.104355521
H	1.202139171	0.180799965	0.405389893
C	3.804218381	-0.689274525	1.205806861
H	4.821222445	-0.292317581	1.288944076
H	3.538456894	-0.798424440	0.152080056
H	3.775082970	-1.675083298	1.675316732
C	3.368431120	0.616165941	3.697420419
H	3.279033775	-0.336111902	4.228124224
H	2.842381081	1.376976033	4.280638549
H	4.426253202	0.892596729	3.635177258
C	3.113664178	2.057288159	1.238281532
H	4.188990988	2.221868151	1.361244499
H	2.574632286	2.890990652	1.695176780
H	2.864571768	2.032719585	0.175537509
C	1.644251646	-3.168606677	3.328142957

H	1.247121946	-2.830241519	4.289437316
H	2.676150713	-2.816398832	3.246559553
H	1.646589001	-4.263750154	3.307777418
C	1.254447295	-3.342860522	0.466823726
H	1.211052945	-4.432113608	0.577031086
H	2.286955385	-3.042537521	0.274896235
H	0.643125813	-3.030999670	-0.383268846
C	-0.977457417	-3.397474337	2.231670907
H	-1.683056760	-3.078432329	1.461894003
H	-1.392900265	-3.144832094	3.211339240
H	-0.829116482	-4.481267299	2.171886676
C	-1.678378263	1.226098434	1.473873136
C	-0.697439188	2.178850663	1.830955486
H	-0.443219592	2.990705221	1.160353743
C	0.048762775	1.939918730	3.012022385
H	0.871849219	2.605514790	3.252994764
C	-0.260806259	0.861019169	3.914789449
H	0.307779911	0.734339410	4.828322714
C	-1.418213596	0.075745063	3.671895948
H	-1.737093201	-0.672119549	4.390445123
C	-2.098200910	0.236660912	2.465529435
H	-2.907981522	-0.433895104	2.202111674
C	-1.774346191	-0.120020123	-0.537335652
C	-2.211497304	1.078813686	0.096561462
C	-3.054554174	1.983235536	-0.545587217
H	-3.371557461	2.886167164	-0.028292369
C	-3.501288881	1.711718167	-1.842237783
H	-4.167140478	2.401263234	-2.352272462
C	-3.096402536	0.531307058	-2.468732894
H	-3.459286478	0.310965529	-3.469610986
C	-2.244303824	-0.402104096	-1.854299404
C	-1.818335233	-1.613886868	-2.598702801
C	-1.488443641	-1.532627410	-3.964323414
H	-1.499756908	-0.562565415	-4.453205720
C	-1.123519571	-2.667793781	-4.690123206
H	-0.867670552	-2.573526543	-5.742399145
C	-1.075289210	-3.916727318	-4.066401958
H	-0.788680388	-4.801348247	-4.628634684
C	-1.395421971	-4.014586655	-2.709056221
H	-1.365669707	-4.981182425	-2.212112512
C	-1.759785760	-2.878843337	-1.985209808
H	-2.010023675	-2.960854010	-0.934444460

==

6

==

Mo	1.403579114	-0.798494997	0.231436008
P	1.936630091	1.377000714	1.253073644
P	1.361924939	-0.029207909	-2.106613719
O	-0.589879484	0.151916285	0.246991175
C	1.373979424	1.527188082	3.015385350
H	1.578321472	2.521562239	3.427059448
H	1.878804389	0.775618733	3.628597129
H	0.298591584	1.334532648	3.052756208

C	3.710065372	1.878572181	1.391882356	C	1.875281670	-2.105420265	2.196418560
H	4.141498230	1.954903202	0.390483985	H	2.312462541	-1.799595164	3.140557882
H	4.258460183	1.104364684	1.935462790	C	0.480167708	-1.991101267	1.980238308
H	3.823429100	2.836429255	1.910693603	H	-0.167793511	-1.583250441	2.745862900
C	1.163391070	2.900390522	0.537695374	C	-1.654522341	-0.630484885	0.263968187
H	1.313792586	3.773589922	1.181990770	C	-1.505803666	-2.037743118	0.444170523
H	0.095341311	2.712473293	0.408922603	C	-2.591724068	-2.906648532	0.345605022
H	1.595077438	3.111885326	-0.444635287	H	-2.437035834	-3.974870416	0.482397281
C	1.561282899	-1.362548230	-3.383055001	C	-3.869773430	-2.401440996	0.095748027
H	0.740458285	-2.077086938	-3.292773926	H	-4.723733693	-3.068433088	0.027291299
H	2.501449711	-1.892617574	-3.212264226	C	-4.040007347	-1.021195081	-0.036695951
H	1.562187970	-0.951056655	-4.398196716	H	-5.038401287	-0.621252301	-0.197004622
C	2.667022351	1.144904777	-2.708519350	C	-2.971369161	-0.116284028	0.051703553
H	3.649254918	0.699800902	-2.533388247	C	-3.220783628	1.339856015	-0.102021219
H	2.614840993	2.082761558	-2.151809366	C	-2.636951418	2.279098281	0.768745959
H	2.552118978	1.361607330	-3.775907419	H	-1.969341088	1.924598075	1.546248382
C	-0.187443100	0.788634714	-2.692802095	C	-2.914279453	3.640947577	0.650058188
H	-0.102134572	1.093854672	-3.741101083	H	-2.457497031	4.344776225	1.341757073
H	-0.402627833	1.654860884	-2.066544676	C	-3.778480317	4.102232875	-0.348029722
H	-1.022235664	0.095169608	-2.579105006	H	-3.991383593	5.163636475	-0.442007342
C	-0.109648196	-2.462977047	0.738615585	C	-4.362805566	3.184090510	-1.223662512
C	0.707097820	-3.017544486	-0.264988237	H	-5.030680791	3.528680189	-2.009187028
H	0.262216588	-3.368752903	-1.188159140	C	-4.085349157	1.820740902	-1.101938242
C	2.124677725	-2.954307663	-0.114116498	H	-4.530018407	1.115721754	-1.799217016
H	2.774891857	-3.299780284	-0.908282884	H	3.041329615	-0.552819152	-0.250045197
C	2.694959770	-2.551153591	1.146587676				
H	3.772497863	-2.543278190	1.263557056				

==

7

==

Mo	-0.0701074707	0.0876071996	0.0270874074
P	0.3008896802	-0.0351973372	2.4706313366
P	2.2405715783	-0.5177115887	-0.6616753198
C	1.8736536126	0.6763350612	3.2179154074
H	1.8904249160	0.5711663966	4.3156180802
H	1.9181980418	1.7431374604	2.9539850706
H	2.7557815392	0.1731546990	2.7954047933
C	0.3137661666	-1.7640089417	3.2278460420
H	1.1300235323	-2.3555639094	2.7866366166
H	-0.6381554735	-2.2687778890	3.0001296178
H	0.4442148569	-1.7302279382	4.3223161707
C	-0.9470913201	0.7904650445	3.6146914789
H	-0.7100169449	0.6191251808	4.6776758443
H	-1.9527602333	0.3985895830	3.4012063957
H	-0.9474902449	1.8710845858	3.4128307443
C	3.1806443447	-1.9821423535	0.0727279351
H	2.6032925734	-2.9058021432	-0.0924201865
H	3.2914072236	-1.8407712549	1.1585740679
H	4.1807963217	-2.1045989203	-0.3760250155
C	3.5103422493	0.8462221424	-0.4205902448
H	4.4984599524	0.5600472387	-0.8181554080
H	3.6046351442	1.0759759420	0.6502139135
H	3.1564438342	1.7536092222	-0.9304942333
C	2.5303287381	-0.8999129166	-2.4845654456
H	2.1718129101	-0.0615214972	-3.0987546172
H	1.9573592087	-1.7972041052	-2.7633206952
H	3.5973079195	-1.0723840116	-2.7019695618
C	-0.4090000090	2.2760000230	-0.6990000010
C	-1.4129999880	1.9019999500	0.2619999950
H	-1.5570000410	2.5260000230	1.1410000320
C	-2.2960000040	0.7860000130	0.0370000000
H	-3.0780000690	0.5609999900	0.7639999990
C	-2.1150000100	-0.0489999990	-1.1050000190
H	-2.7839999200	-0.8970000150	-1.2699999810
C	-1.0970000030	0.2689999940	-2.0729999540
H	-0.9530000090	-0.3549999890	-2.9549999240
C	-0.2169999930	1.3609999420	-1.8209999800
H	0.5820000170	1.5599999430	-2.5350000860
C	0.7580000160	4.2490000720	0.5139999990
C	0.3720000090	3.5469999310	-0.6690000300
C	0.7919999960	4.1250000000	-1.8999999760
H	0.4589999910	3.6610000130	-2.8310000900
C	1.5959999560	5.2729997630	-1.9639999870
H	1.8930000070	5.6770000460	-2.9360001090
C	2.0290000440	5.8860001560	-0.7799999710
H	2.7009999750	6.7480001450	-0.8090000150
C	1.6250000000	5.3759999280	0.4749999940
C	2.1400001050	6.0050001140	1.7350000140
C	2.0859999660	7.4089999200	1.9210000040
H	1.6100000140	8.0260000230	1.1529999970
C	2.6240000720	8.0089998250	3.0720000270
H	2.5710000990	9.0950002670	3.1909999850

C	3.2219998840	7.2189998630	4.0729999540
H	3.6380000110	7.6869997980	4.9699997900
C	3.2839999200	5.8229999540	3.9079999920
H	3.7579998970	5.1989998820	4.6710000040
C	2.7520000930	5.2230000500	2.7520000930
H	2.8480000500	4.1420001980	2.6150000100
O	0.2669999900	3.7880001070	1.7259999510
H	0.5730000140	4.4070000650	2.4219999310

==

8

==

Mo	-0.150030743	0.143971287	0.065925023
P	2.014950613	0.625654851	-1.066633888
P	-1.830269596	1.368713814	-1.234459586
P	-0.455049908	-1.780183695	-1.514559530
C	2.588418934	2.370610969	-0.892881132
H	3.608954708	2.488665902	-1.273012722
H	2.536939852	2.648821738	0.166115217
H	1.917027339	3.026444077	-1.454952864
C	2.333226797	0.373156083	-2.888789986
H	1.593878788	0.930410213	-3.470815924
H	2.265283547	-0.683742759	-3.160624152
H	3.332344788	0.733172661	-3.156038236
C	3.494742731	-0.274146173	-0.382965102
H	4.410832240	0.026531271	-0.901805886
H	3.366040283	-1.355488059	-0.482224367
H	3.602558785	-0.031859050	0.677084561
C	-1.360173467	2.104382256	-2.877694451
H	-1.051423739	1.319714603	-3.572424453
H	-0.512842722	2.778821197	-2.724890635
H	-2.188892049	2.668966500	-3.319418506
C	-2.463996235	2.894911963	-0.390072171
H	-3.106167090	3.475135808	-1.061025374
H	-1.621490425	3.507471651	-0.062427202
H	-3.040523745	2.620098276	0.496227790
C	-3.472342374	0.595169208	-1.678464773
H	-3.947665947	0.221375463	-0.766524982
H	-3.340854636	-0.247109642	-2.362178594
H	-4.140503460	1.323439667	-2.150631069
C	-0.709870460	-1.566021213	-3.344318759
H	-0.788673910	-2.540869971	-3.837249633
H	0.121165444	-1.012153111	-3.782757282
H	-1.628957765	-1.007625579	-3.532689032
C	0.893126101	-3.063056064	-1.534262324
H	1.070015632	-3.417334562	-0.515139711
H	1.823192770	-2.623624505	-1.902728802
H	0.628299089	-3.915536914	-2.168850936
C	-1.911741592	-2.883984203	-1.155097008
H	-1.970366428	-3.710704087	-1.871130356
H	-2.834166404	-2.301058567	-1.205323833
H	-1.829120634	-3.298490195	-0.147643722
C	-0.161491500	1.208588542	2.371107199
C	1.014586041	0.420782097	2.088621119

H	1.968689125	0.913414675	2.215990547
C	0.921770489	-0.991086375	1.894135203
H	1.828336090	-1.585542000	1.856481368
C	-0.331044252	-1.612525590	1.761372935
H	-0.392140467	-2.685670662	1.607502175
C	-1.504017781	-0.818733015	1.746443107
H	-2.477880023	-1.275154073	1.609806813
C	-1.403485200	0.580046620	2.011233854
H	-2.318768548	1.153148622	2.060423357
C	1.110689831	3.376445681	2.755392312
C	-0.109021030	2.570279690	2.869878982
C	-1.267227158	3.121651619	3.474148862
H	-2.146627789	2.496109175	3.607173207
C	-1.300994192	4.417067960	3.947699802
H	-2.195555219	4.812844819	4.418880807
C	-0.150166495	5.221995653	3.814358597
H	-0.192402818	6.254489799	4.154004458
C	1.027501043	4.755370071	3.250508490
C	2.206841614	5.655841087	3.171739114
C	2.470657582	6.574248414	4.207134505
H	1.842314253	6.565592683	5.093342439
C	3.534818386	7.473823148	4.130887953
H	3.712685309	8.166894247	4.949669437
C	4.375905344	7.473903158	3.015377191
H	5.208798348	8.169678926	2.953429184
C	4.138089480	6.559272913	1.984516577
H	4.786851553	6.545167494	1.111541351
C	3.074982311	5.659909281	2.061789995
H	2.906636789	4.945263467	1.267475323
O	2.179413996	2.930074026	2.244004764
H	0.103074284	1.804247189	-0.196366815

==============================

9

==============================

Mo	-0.346450649	-0.271532351	0.470839131
P	-2.026787746	-0.102436711	-1.275911463
P	1.694057333	0.256608740	-0.809850190
C	-2.267205516	-1.656886410	-2.271886994
H	-3.049900632	-1.527541597	-3.026909567
H	-2.548444801	-2.481643617	-1.610465268
H	-1.333616914	-1.923328935	-2.776083101
C	-1.847848735	1.154812388	-2.627820603
H	-0.929348166	0.964459271	-3.189154892
H	-1.773294207	2.149992528	-2.181465890
H	-2.698710763	1.130829832	-3.317133725
C	-3.770262489	0.249833604	-0.743452782
H	-4.456647420	0.278548092	-1.596255862
H	-3.798687627	1.216122913	-0.232668634
H	-4.103837370	-0.519235178	-0.041528763
C	1.814678077	1.936599473	-1.556939203
H	1.777953885	2.639518952	-0.720397843
H	0.973597038	2.125928855	-2.227065530
H	2.755507008	2.058438069	-2.103800843

C	2.049675534	-0.867009150	-2.252767501
H	3.001657075	-0.606277017	-2.727425747
H	1.252024008	-0.788170542	-2.997248923
H	2.104380542	-1.907285702	-1.915607222
C	3.295535918	0.187686524	0.111102221
H	3.411129371	-0.782742379	0.602344463
H	3.268784236	0.983409702	0.860137790
H	4.140659748	0.348302131	-0.566887724
C	-0.313078679	1.135880205	2.516490266
C	0.788621873	0.234416245	2.497734513
H	1.779099193	0.650958175	2.602752515
C	0.595430981	-1.172413378	2.381328910
H	1.450224497	-1.836899587	2.441341210
C	-0.729917095	-1.705947213	2.335166555
H	-0.878443584	-2.781529997	2.278391798
C	-1.838199941	-0.849089152	2.261858702
H	-2.843161123	-1.251547500	2.200872637
C	-1.612410483	0.557369299	2.206049777
H	-2.456856903	1.223839235	2.093098082
C	1.069439067	3.249810062	2.328972481
C	-0.160028697	2.567304075	2.731180226
C	-1.228591523	3.284223534	3.310057841
H	-2.126753278	2.748450422	3.610834488
C	-1.140386891	4.643860514	3.550896602
H	-1.963881076	5.182125033	4.009981907
C	0.043021436	5.318123891	3.200996655
H	0.098172633	6.390604985	3.372030542
C	1.136819150	4.681224185	2.621859240
C	2.360282171	5.470598215	2.320879723
C	2.734251839	6.544933603	3.155034075
H	2.158567291	6.741545743	4.054933512
C	3.840649989	7.344203668	2.867665180
H	4.099961689	8.161922282	3.535887000
C	4.620676516	7.086837680	1.737278761
H	5.485620337	7.705164453	1.511715070
C	4.278138155	6.015010963	0.908638277
H	4.878465086	5.797526753	0.028053750
C	3.171193799	5.215719422	1.195990815
H	2.926335342	4.375721671	0.561526135
O	2.010452866	2.636128650	1.733360866
H	-0.419859087	1.379939479	0.190846048

==============================

10

==============================

Mo	-0.246025814	0.174015122	0.027102329
O	2.266225142	2.814388575	2.365702429
P	-0.873080235	2.366068692	-1.001312336
P	-0.656400611	-1.470442581	-1.717595457
P	2.073766720	0.591018870	-0.985837146
C	-2.707503059	2.622969741	-1.111378449
H	-2.945315759	3.629634807	-1.471113124
H	-3.147649173	2.482030104	-0.121090827
H	-3.144341320	1.882297861	-1.786182553

C	-0.424875547	2.811021523	-2.756043167
H	-0.737363823	2.012793684	-3.434143354
H	0.654758309	2.945639077	-2.855022591
H	-0.913985139	3.744078496	-3.055424696
C	-0.400904105	3.941191121	-0.144161051
H	-0.731797402	4.806957801	-0.727592574
H	0.677572775	3.993159250	0.008143138
H	-0.868605791	3.972362552	0.841863040
C	-0.931154445	-0.998047108	-3.497489523
H	-0.050726350	-0.494098714	-3.900232417
H	-1.775415757	-0.304462238	-3.547888432
H	-1.155384519	-1.873521773	-4.117049728
C	-2.201304800	-2.469842054	-1.455829476
H	-2.318001054	-3.233802877	-2.231546530
H	-3.066680920	-1.802908319	-1.471307905
H	-2.167140057	-2.959904624	-0.479307048
C	0.554559728	-2.873693194	-1.924001341
H	0.652698181	-3.398151550	-0.969086943
H	1.542141128	-2.498363791	-2.200740957
H	0.222676378	-3.585850268	-2.687276690
C	2.410753334	0.379643697	-2.804670128
H	3.450234536	0.643073351	-3.025848754
H	1.754162617	1.028719945	-3.387236200
H	2.241377986	-0.652397835	-3.119015150
C	2.833115702	2.254710132	-0.711251387
H	2.747426293	2.509545670	0.351860667
H	2.306776679	3.011267581	-1.298415498
H	3.884605017	2.249277400	-1.018039119
C	3.437526271	-0.473963161	-0.309717317
H	4.382607285	-0.243787997	-0.811808824
H	3.202965114	-1.531785064	-0.453697052
H	3.559836308	-0.281811859	0.758570923
C	-0.135357627	1.185494475	2.391065377
C	0.998089213	0.371024838	2.115764628
H	1.968269475	0.822594559	2.275438910
C	0.867155902	-1.006271455	1.743821945
H	1.756834571	-1.614849901	1.633351625
C	-0.404140626	-1.611850938	1.643876689
H	-0.500669062	-2.673805182	1.444415379
C	-1.542937436	-0.791655284	1.748259928
H	-2.531435582	-1.211303943	1.594502875
C	-1.405462835	0.606444519	1.998549826
H	-2.305435022	1.203310302	2.061137535
C	1.204695899	3.292088516	2.873164074
C	-0.043959336	2.527637928	2.946927448
C	-1.193349280	3.103540978	3.539678801
H	-2.095443815	2.505278395	3.642297444
C	-1.194831186	4.396400205	4.029004884
H	-2.085128901	4.814907919	4.488552280
C	-0.018606108	5.164284305	3.925581977
H	-0.037836410	6.196193670	4.268604591
C	1.157210664	4.665859345	3.379017466
C	2.353409485	5.545900441	3.307411113
C	2.605018966	6.490998664	4.322324565

H	1.961903916	6.510760161	5.197639545
C	3.672924772	7.385359765	4.239093777
H	3.838438046	8.100483767	5.041304902
C	4.532268294	7.354501534	3.137960781
H	5.366434212	8.048067285	3.070158553
C	4.310521705	6.411016006	2.130602534
H	4.974336343	6.370468457	1.269880091
C	3.243814209	5.516464055	2.215163066
H	3.091646909	4.777670880	1.440396393
H	-1.834775593	0.183918287	-0.588903048

==============================

11

==============================

Mo	0.011518000	0.024323000	-0.074362000
O	0.166871000	-0.075554000	3.028668000
P	2.413314000	-0.022102000	0.631738000
P	0.089199000	-1.032342000	-2.265173000
P	-0.458902000	-2.261307000	0.999491000
C	3.143014000	1.688490000	0.568057000
H	4.224142000	1.665194000	0.740500000
H	2.678216000	2.299930000	1.346422000
H	2.941522000	2.146991000	-0.403418000
C	3.623050000	-0.899409000	-0.478610000
H	3.497022000	-0.558839000	-1.509323000
H	3.438734000	-1.977307000	-0.448042000
H	4.655458000	-0.711437000	-0.165518000
C	3.113552000	-0.525090000	2.274754000
H	4.204515000	-0.425168000	2.262876000
H	2.861692000	-1.556030000	2.514405000
H	2.669820000	0.113404000	3.037785000
C	1.224927000	-2.461379000	-2.650302000
H	1.098613000	-3.264010000	-1.923655000
H	2.260729000	-2.122427000	-2.597767000
H	1.033784000	-2.856482000	-3.654147000
C	0.591613000	0.075638000	-3.674142000
H	0.528335000	-0.446927000	-4.634127000
H	1.618295000	0.414821000	-3.515515000
H	-0.052540000	0.958436000	-3.709850000
C	-1.493186000	-1.712333000	-2.990463000
H	-2.221690000	-0.906887000	-3.117817000
H	-1.928547000	-2.463343000	-2.329748000
H	-1.310828000	-2.165982000	-3.970303000
C	-1.005784000	-3.755149000	0.029649000
H	-1.247701000	-4.566107000	0.724360000
H	-0.229134000	-4.111747000	-0.649025000
H	-1.900360000	-3.524965000	-0.554064000
C	0.745889000	-3.065693000	2.149302000
H	0.917320000	-2.364046000	2.967787000
H	1.686379000	-3.287813000	1.638301000
H	0.331014000	-3.996808000	2.549889000
C	-1.906723000	-2.128624000	2.148605000
H	-2.105245000	-3.095307000	2.623438000
H	-2.799236000	-1.810212000	1.604341000

H	-1.642709000	-1.388852000	2.905660000
C	-1.218580000	1.908456000	1.590685000
C	-2.221580000	1.033463000	1.187250000
H	-2.842370000	0.569343000	1.946174000
C	-2.349421000	0.609537000	-0.173617000
H	-3.125764000	-0.096611000	-0.446865000
C	-1.671373000	1.334151000	-1.193067000
H	-1.901907000	1.190427000	-2.241478000
C	-0.672030000	2.251455000	-0.813150000
H	-0.084026000	2.764105000	-1.566965000
C	-0.336932000	2.389035000	0.553306000
H	0.492751000	3.027982000	0.833493000
C	-0.270910000	0.937191000	3.689766000
C	-0.906701000	2.060577000	3.034181000
C	-1.221381000	3.236078000	3.722340000
H	-1.614950000	4.084510000	3.164713000
C	-1.039294000	3.327816000	5.102198000
H	-1.268132000	4.244801000	5.636571000
C	-0.603204000	2.189168000	5.789971000
H	-0.535266000	2.217561000	6.875968000
C	-0.260420000	0.999296000	5.139503000
C	0.032821000	-0.210850000	5.948492000
C	-0.815750000	-0.553550000	7.020064000
H	-1.687849000	0.064986000	7.213847000
C	-0.575243000	-1.679646000	7.809635000
H	-1.252778000	-1.919591000	8.625741000
C	0.518690000	-2.506264000	7.540427000
H	0.705330000	-3.387821000	8.148413000
C	1.368974000	-2.185673000	6.477617000
H	2.229883000	-2.814928000	6.262703000
C	1.129847000	-1.055597000	5.694289000
H	1.795416000	-0.813913000	4.876684000
H	1.202261000	0.605712000	-1.116763000

==============================

12

==============================

Mo	0.008628320	-0.129232168	2.082493964
P	2.398363421	0.166053914	1.542898384
P	0.233344766	-2.493680699	2.716862547
O	-0.562213867	-0.780432284	-0.213326582
H	-0.117566321	-1.310660872	-0.890308037
C	3.292884098	-0.978019849	0.362207460
H	4.335386467	-0.681699559	0.196777776
H	2.774247782	-0.977005373	-0.602338095
H	3.274158515	-1.999841684	0.752726537
C	3.613493081	0.170147030	2.953337834
H	3.584831166	-0.793672723	3.466954290
H	3.313269145	0.939422639	3.670138254
H	4.637848738	0.369096937	2.617282943
C	2.861720384	1.786431804	0.743485638
H	3.942834306	1.873129005	0.585844972
H	2.527023290	2.614708163	1.373565964

H	2.351925525	1.871295913	-0.220527503
C	1.759720071	-3.148809166	3.565808830
H	1.918640414	-2.594571224	4.495333668
H	2.634457203	-2.998220688	2.926954618
H	1.672207139	-4.216613653	3.796662964
C	0.104950414	-3.744856202	1.329707023
H	0.158496119	-4.778036151	1.691272545
H	0.914979336	-3.579628968	0.612425797
H	-0.847211692	-3.600160232	0.810977563
C	-1.048837924	-3.221773109	3.860813058
H	-2.046009919	-3.036499839	3.451929662
H	-0.987522810	-2.732907172	4.837246231
H	-0.911511571	-4.300175713	3.996704995
C	-1.732689068	1.059207449	1.454152052
C	-0.701576888	2.028486506	1.709517323
H	-0.370866907	2.691454412	0.918482079
C	-0.008577475	1.978330803	2.958940215
H	0.837393234	2.640629241	3.120044830
C	-0.411747669	1.095737578	4.004786608
H	0.089697421	1.104331316	4.965398497
C	-1.498509285	0.202846697	3.752909100
H	-1.808525541	-0.487539342	4.530464466
C	-2.219966310	0.224536268	2.520841595
H	-3.038324700	-0.464315753	2.345338406
C	-1.613613290	-0.073603826	-0.769703693
C	-2.240365085	0.872447097	0.060731177
C	-3.294845388	1.619783570	-0.473485994
H	-3.787502970	2.349243218	0.163029385
C	-3.708395006	1.440798724	-1.796885379
H	-4.530538579	2.026333207	-2.197388307
C	-3.064428741	0.503362249	-2.601837567
H	-3.384243569	0.350579255	-3.628904465
C	-2.009856906	-0.280403752	-2.104049200
C	-1.311058759	-1.265333766	-2.976291985
C	-0.800873508	-0.869806779	-4.226328744
H	-0.909011765	0.165889291	-4.535783926
C	-0.146843711	-1.783213583	-5.053614780
H	0.245199763	-1.454730286	-6.012218149
C	0.018212183	-3.110875134	-4.646999170
H	0.532966842	-3.819335966	-5.289515423
C	-0.485610001	-3.520643795	-3.410843039
H	-0.374749504	-4.552570184	-3.089772432
C	-1.146081445	-2.608074750	-2.583642361
H	-1.569938786	-2.945722484	-1.641578459

Table S2. Vibrational frequencies of truncted models.

==============================

Truncated model of 1

==============================

(-282.28)	(-265.60)	(-251.06)	(-54.03)	(-23.07)	19.13	60.64
63.86	72.06	96.14	101.82	130.62	189.94	210.25
254.52	279.88	289.25	299.64	303.03	314.25	336.57
346.14	354.79	365.90	403.07	411.20	419.87	427.20
437.98	451.80	456.58	512.13	516.85	568.98	574.82
624.96	633.32	643.67	724.66	757.63	773.45	808.69
837.35	848.24	866.84	912.35	926.04	939.75	962.18
979.94	986.03	998.97	1008.53	1017.33	1022.22	1029.60
1076.10	1089.38	1092.79	1094.00	1098.54	1101.98	1102.71
1105.31	1135.07	1186.45	1198.00	1208.59	1227.39	1300.56
1321.92	1330.46	1367.32	1391.59	1427.83	1460.86	1495.34
1503.78	1524.11	1545.25	1569.77	1638.35	1658.05	2329.55
2332.35	2336.63	2340.64	2343.48	2347.47	2350.75	2351.40
2358.38	3178.99	3189.66	3192.70	3202.63	3208.18	3214.91
3220.30	3226.52	3258.27	3753.02			

==============================

Truncated model of 2

==============================

49.53	66.63	85.26	105.18	118.24	119.22	126.31
138.18	153.03	168.05	192.75	198.11	213.22	227.79
251.03	265.43	276.64	279.03	317.40	335.49	357.94
363.81	421.88	460.81	497.64	510.57	523.73	526.78

535.95	538.43	540.79	554.81	564.89	569.91	623.07
625.04	640.35	714.79	729.36	755.22	769.73	798.32
822.69	841.59	868.84	897.21	914.09	924.58	945.56
975.38	989.86	1007.63	1016.73	1044.77	1052.49	1055.87
1057.65	1082.41	1129.46	1131.24	1133.57	1135.83	1138.05
1141.09	1143.58	1152.32	1154.07	1181.46	1224.12	1279.43
1296.07	1309.24	1323.77	1400.23	1418.73	1435.71	1471.56
1497.00	1507.82	1515.92	1540.87	1621.64	1647.54	2342.76
2344.71	2347.22	2349.47	2350.34	2352.35	2355.25	2357.47
2362.57	3170.67	3180.81	3191.33	3192.71	3198.43	3202.75
3211.79	3218.54	3224.16	3245.63			

==============================

Truncated model of 3

==============================

(-168.00)	(-114.06)	(-40.96)	-4.68[1]	42.59	67.94	84.70
98.87	130.02	192.52	225.38	260.76	282.59	290.33
301.10	316.03	329.55	357.84	370.68	409.88	426.97
440.53	456.70	462.19	508.29	526.30	565.80	575.23
597.74	632.19	642.46	647.46	734.91	767.29	788.23
827.52	849.74	859.45	893.71	897.10	916.68	932.29
947.77	969.43	976.73	1004.01	1010.91	1016.37	1033.37
1069.42	1073.28	1076.66	1084.05	1108.15	1112.82	1151.46
1186.90	1190.03	1221.48	1238.39	1302.57	1326.77	1332.91
1360.13	1419.87	1436.34	1465.11	1491.89	1506.40	1530.19
1539.54	1552.53	1640.21	1664.14	2345.32	2346.95	2352.24
2357.09	2370.54	2380.24	3177.48	3187.13	3193.43	3200.75

3202.24	3205.10	3211.74	3212.81	3217.31	3224.49	

[1]:numerical noise

==============================

Truncated model of 4

==============================

-435.01	(-235.47)	(-158.65)	(-44.54)	(-17.22)	39.58	54.25
90.85	99.45	127.43	195.25	237.39	264.66	288.95
294.38	308.44	330.34	346.24	369.76	378.96	400.58
425.13	436.38	450.93	457.53	495.33	531.46	565.94
580.88	633.73	639.19	660.81	731.83	760.29	792.83
804.41	809.64	824.77	842.95	907.63	909.43	918.08
961.92	981.44	983.61	991.93	1015.59	1025.86	1039.76
1052.68	1072.16	1085.56	1086.59	1099.25	1101.16	1141.44
1163.29	1176.04	1184.56	1225.24	1263.13	1311.89	1328.14
1336.36	1346.71	1428.64	1447.30	1486.05	1501.65	1509.38
1523.31	1538.44	1638.33	1652.92	2333.99	2342.77	2346.02
2353.60	2355.31	2358.55	3183.85	3185.28	3195.71	3196.09
3205.97	3207.95	3215.46	3217.40	3224.19	3674.23	

==============================

Truncated Model of 5

==============================

(-136.31)	(-86.54)	43.57	78.18	90.06	100.86	129.26
154.14	173.75	218.39	244.58	253.91	286.28	310.09
327.06	328.06	357.34	367.58	407.99	437.94	455.26
477.09	488.00	498.65	514.73	530.44	573.32	582.07
596.03	628.17	651.62	678.26	739.50	768.74	773.24

816.02	874.24	875.34	876.53	883.05	955.24	958.80
961.70	975.15	990.45	997.60	1000.36	1003.45	1009.72
1034.60	1064.18	1091.15	1094.18	1104.28	1111.63	1114.02
1152.01	1193.36	1200.24	1218.55	1255.72	1317.97	1342.04
1360.26	1370.42	1404.96	1465.38	1504.97	1510.34	1518.83
1526.80	1571.83	1616.96	1651.75	1748.23	2346.36	2353.85
2369.26	2373.40	2374.57	2391.62	3169.04	3175.68	3191.60
3201.24	3207.23	3210.65	3223.42	3232.39	3238.97	

===============================

Truncated model of 6

===============================

(-123.96)	(-103.22)	33.15	76.89	90.16	92.89	100.39
126.48	187.87	217.14	240.62	271.67	284.08	308.22
330.38	346.42	362.11	382.37	421.14	432.04	458.27
467.46	472.05	496.63	515.11	567.92	581.20	589.65
629.05	642.31	672.66	739.20	752.55	766.39	774.48
833.65	858.03	870.60	876.77	880.75	915.97	933.64
951.07	961.34	968.76	981.51	997.06	1000.88	1019.61
1035.66	1066.36	1089.28	1095.55	1096.51	1112.33	1115.36
1153.25	1183.29	1206.86	1218.42	1253.74	1320.24	1340.65
1358.32	1377.24	1414.22	1456.58	1504.48	1513.41	1523.21
1529.78	1569.55	1614.16	1652.25	1818.28	2350.49	2358.83
2367.79	2372.20	2392.05	2397.38	3167.66	3173.52	3197.51
3207.87	3210.89	3221.30	3229.48	3237.39	3242.61	

===============================

Truncated Truncated model of 7

==============================

(-220.55)	(-177.32)	(-31.74)	22.87	46.18	52.45	91.97
101.43	153.65	208.24	246.31	256.43	282.12	293.67
296.09	314.99	320.03	359.64	363.23	392.93	428.86
430.25	442.36	451.79	464.27	514.86	526.39	567.62
580.43	621.76	631.41	640.79	718.68	762.10	789.59
829.91	844.29	863.84	876.75	924.84	945.52	951.16
959.97	971.91	976.63	984.45	1016.09	1017.74	1025.72
1059.89	1071.55	1075.91	1079.97	1110.48	1111.40	1130.34
1187.63	1188.62	1201.38	1229.65	1275.19	1288.80	1302.07
1350.51	1381.47	1405.83	1437.44	1481.36	1488.12	1503.74
1517.22	1547.08	1601.68	1620.56	2337.60	2343.05	2345.15
2355.38	2369.36	2371.39	3115.83	3128.57	3132.98	3142.61
3147.83	3152.36	3165.66	3194.70	3195.84	3606.85	

==============================

Truncated Model of 8

==============================

41.55	61.98	66.55	102.26	117.66	120.49	130.35
140.73	156.44	195.26	207.00	218.73	230.27	257.90
262.17	269.60	277.58	289.47	296.89	308.98	355.45
376.55	424.66	442.54	502.08	529.74	532.13	537.66
545.08	550.83	562.04	579.52	599.96	602.06	606.28
619.35	660.01	685.16	718.94	752.06	765.88	816.87
843.63	846.39	854.03	878.45	921.46	929.77	953.33
975.96	978.15	983.99	1006.85	1038.79	1041.59	1049.28

1050.94	1057.09	1081.07	1131.58	1136.62	1137.15	1139.84
1141.19	1144.25	1148.65	1152.09	1161.51	1175.90	1200.15
1278.41	1296.70	1347.64	1383.09	1404.36	1429.98	1480.84
1498.82	1523.14	1539.30	1570.70	1581.47	1641.92	1833.18
2348.87	2350.91	2356.08	2359.93	2361.77	2362.78	2366.47
2370.10	2380.70	3158.60	3163.15	3186.36	3190.07	3197.30
3209.56	3215.05	3243.67	3244.31			

==============================

Truncated Model of 9

==============================

26.40	60.96	70.50	114.48	121.57	126.74	152.30
196.08	227.04	261.79	269.29	286.58	290.36	299.25
310.21	315.18	338.57	364.85	391.81	442.91	486.11
522.39	526.82	531.06	556.26	570.81	578.96	588.01
599.16	610.78	650.39	699.81	714.01	748.72	766.29
767.48	812.60	845.65	850.54	861.35	919.60	930.64
936.30	963.83	973.31	981.54	1004.27	1017.31	1025.14
1040.19	1049.43	1068.46	1106.57	1117.35	1135.00	1138.22
1150.36	1152.43	1165.14	1175.01	1198.29	1280.67	1301.99
1341.04	1383.64	1398.24	1429.57	1477.74	1490.28	1509.53
1540.43	1558.38	1574.40	1633.03	1911.35	2349.08	2354.80
2361.69	2370.55	2371.86	2385.19	3153.94	3163.48	3180.42
3188.38	3198.34	3212.85	3217.33	3242.98	3273.17	

==============================

Truncated Model of 10

==============================

40.25	63.68	66.54	101.29	113.10	120.85	135.98
149.13	154.57	195.11	213.39	225.49	231.74	238.71
245.41	254.78	279.23	289.34	311.67	322.44	354.14
384.92	421.73	441.26	516.50	531.36	532.68	538.90
546.14	552.00	559.09	575.00	594.29	597.97	605.91
614.73	672.14	705.26	732.07	751.42	764.45	827.03
843.67	847.49	851.31	894.71	919.10	928.52	964.89
969.64	975.24	983.01	1007.24	1036.02	1038.52	1049.88
1051.29	1055.21	1078.12	1131.13	1134.26	1137.35	1139.90
1144.99	1146.39	1149.22	1151.49	1169.20	1176.36	1201.20
1281.95	1296.48	1344.50	1389.87	1402.72	1429.11	1481.86
1504.23	1526.33	1541.30	1566.80	1578.22	1637.54	1831.47
2345.89	2354.07	2357.01	2363.95	2365.30	2366.52	2374.95
2376.12	2377.98	3159.81	3164.59	3188.35	3197.70	3200.06
3211.68	3221.33	3233.40	3240.13			

==============================

Truncated model of 11

==============================

-81.18	30.45	59.39	75.38	102.55	103.86	117.53
128.33	130.08	162.33	185.57	192.25	207.15	228.05
247.31	249.13	257.45	273.81	292.92	302.55	332.54
358.70	413.42	475.24	494.08	516.95	530.64	539.47
543.11	558.10	565.90	577.54	587.71	604.55	613.26
618.96	672.17	701.09	726.08	736.85	748.44	818.40
831.45	853.71	866.10	884.99	912.89	931.30	951.65

956.07 982.58 990.37 1015.17 1026.94 1042.09 1049.04

1056.37 1061.17 1086.69 1125.59 1128.26 1130.92 1132.45

1144.22 1146.13 1158.82 1159.12 1173.09 1174.68 1200.94

1283.28 1305.93 1318.07 1361.55 1382.66 1430.74 1485.89

1490.33 1512.38 1533.11 1574.13 1586.46 1633.06 1873.35

2342.10 2352.44 2360.79 2362.85 2367.75 2369.95 2374.02

2376.38 2385.97 3149.14 3153.40 3182.84 3194.92 3203.25

3207.45 3218.56 3222.55 3229.

==============================

Truncated model of 12

==============================

49.67 77.96 80.75 102.20 105.79 123.26 141.68

180.89 206.43 234.06 242.61 266.24 279.75 288.07

295.78 317.76 348.64 368.72 401.60 437.36 461.36

467.22 492.61 499.20 522.45 530.20 542.49 559.07

575.11 625.94 626.86 656.09 725.95 749.53 760.85

780.40 787.99 795.79 833.45 849.96 896.27 901.53

942.34 979.47 981.04 1000.82 1018.82 1027.58 1031.91

1053.35 1059.76 1114.04 1117.10 1124.38 1130.40 1134.42

1141.75 1146.51 1180.88 1195.77 1251.38 1290.88 1293.58

1314.45 1354.95 1400.57 1420.54 1466.18 1480.57 1481.65

1505.67 1533.65 1629.49 1648.37 2332.16 2333.28 2344.61

2347.11 2351.40 2353.35 3177.66 3178.78 3188.39 3189.60

3195.84 3207.22 3211.04 3211.99 3217.46 3779.64

References

(S1) Jaguar 4.1 Schrödinger , Inc., Portland, Oregon, 2001.

(S2) (a) Slater, J. C. *Quantum Theory of Molecules and Solids, Vol. 4: The Self-Consistent Field for Molecules and Solids;* McGraw-Hill: New York, 1974.
(b) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.
(c) Becke, A. D. *Phys. Rev. A* **1988**, *38*, 3098.
(d) Lee, C. T.; Yang, W. T.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.
(e) Vosko, S. H.; Wilk, L.; Nusair, M. *Can. J. Phys.* **1980**, *58*, 1200.

(S3) (a) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 270.
(b) Wadt, W. R. ; Hay, P. J. *J. Chem. Phys.* **1985**, *82*, 284.
(c) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299.

(S4) Dunning, T. H. *J. Chem. Phys.* **1989**, *90*, 1007.