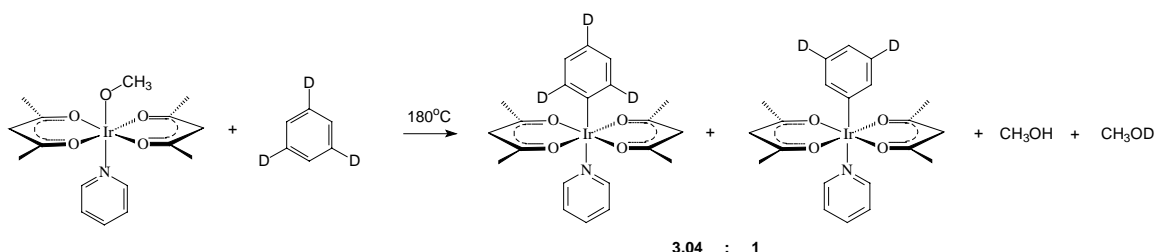


Supporting information:

Experimental:

For synthetic details, see reference 1.

Deuterium kinetic isotope effect on benzene CH activation by (acac-O,O)₂Ir(OCH₃)(Py) **1**: Three 5 mL Schlenk tubes were charged with 10 mg of **1**, and 0.5 mL of 1,3,5-trideuterobenzene under an atmosphere of argon. The tubes were then placed in a temperature controlled oil-bath maintained at 180 °C until the reaction had reached 5 % completion. The tubes were then cooled and methyl lithium was added. The gas phase was then analyzed via GCMS. The molar ratio of the liberated methane isotopologues was determined using a deconvolution spreadsheet calibrated with known mixtures of methane isotopologues. The liquid phase was analyzed to ensure that deuterium scrambling was minimized in the starting materials. Control experiments without added **1**, and with **1** but without heating were also carried out, each in triplicate, to account for background generation of methane from reactions with methyl lithium.



Theoretical:

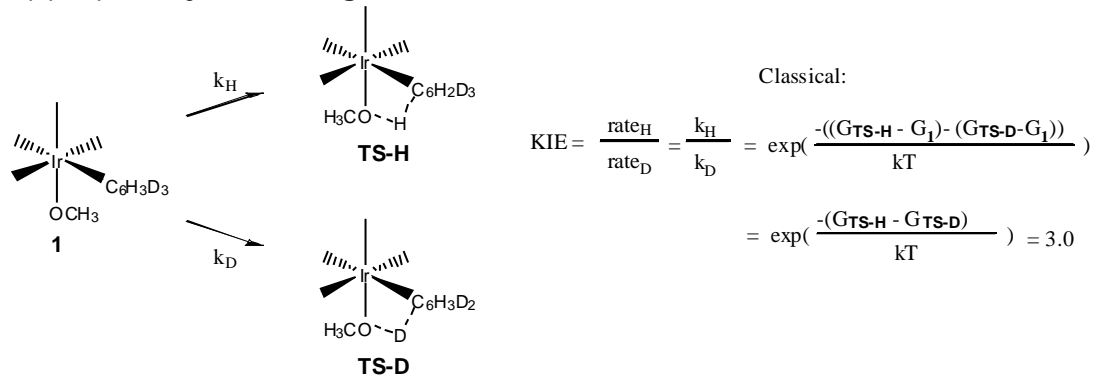
All calculations were performed using the hybrid DFT functional B3LYP as implemented by the Jaguar 6.0 and Jaguar 6.5 program packages.¹ This DFT functional utilizes the Becke three-parameter functional² (B3) combined with the correlation functional of Lee, Yang, and Par³ (LYP), and is known to produce good descriptions of reaction profiles for transition metal containing compounds.^{4,5} The metals were described by the Wadt and Hay⁶ core-valence (relativistic) effective core potential (treating the valence electrons explicitly) using the LACVP basis set with the valence double- ζ contraction of the basis functions, LACVP**. All electrons were used for all other elements using a modified variant of Pople's⁷ 6-31G** basis set, where the six d functions have been reduced to five.

All geometries were optimized and evaluated for the correct number of imaginary frequencies through vibrational frequency calculations using the analytic Hessian. Zero imaginary frequencies correspond to a local minimum, while one imaginary frequency corresponds to a transition structure.

To reduce computational time the methyl groups on the acac ligands were replaced with hydrogens. Control calculations show that relative energies of intermediates and transition structures change less than 0.1 kcal/mol when methyl groups are included.

The deuterium kinetic isotope effect calculated for the reaction of 1,3,5-trideuterobenzene with (acac-O,O)₂Ir(III)(OCH₃)(Pyr) assumes that generation of MeOH and MeOD involve the same intermediates up until the arene complex (acac-O,O)₂Ir(III)(OCH₃)(C₆H₃D₃) (below, **1**). Using transition state theory, the kinetic isotope effect is then where G_{TS-H} and G_{TS-D} contain the mass dependent quantities (zero point

energy and vibrational enthalpy and entropy at 473K) evaluated using the appropriately mass-weighted Hessians.



The tunneling was evaluated to 1.05 according to the method by Skodje and Thrular⁸ (imaginary frequency of TS-H = -822.00 cm⁻¹, TS-D = -646.32 cm⁻¹. Multiplying the classical KIE of 3.0 with the tunneling correction of 1.05 yields a total KIE of 3.2.

TS1 Localized Orbitals

1	Orbital Energy	-19.169436	Occupation	1.000000
	S			
O6	1.00			
2	Orbital Energy	-19.168783	Occupation	1.000000
	S			
O2	-1.00			
3	Orbital Energy	-19.168680	Occupation	1.000000
	S			
O9	1.00			
4	Orbital Energy	-19.164889	Occupation	1.000000
	S			
O10	-1.00			
5	Orbital Energy	-19.124253	Occupation	1.000000
	S			
O30	-1.00			
6	Orbital Energy	-10.266372	Occupation	1.000000
	S			
C3	0.05			
	S			
C5	-0.99			
7	Orbital Energy	-10.264919	Occupation	1.000000
	S			
C3	0.99			
	S			
C5	0.05			
8	Orbital Energy	-10.264228	Occupation	1.000000
	S			
C11	-0.20			
	S			
C12	-0.97			

9 Orbital Energy -10.262767 Occupation 1.000000
 S
 C11 -0.97
 S
 C12 0.20
 10 Orbital Energy -10.200299 Occupation 1.000000
 S
 C20 0.99
 11 Orbital Energy -10.200027 Occupation 1.000000
 S
 C31 1.00
 12 Orbital Energy -10.194649 Occupation 1.000000
 S
 C21 0.06
 S
 C22 0.99
 13 Orbital Energy -10.191706 Occupation 1.000000
 S
 C18 0.99
 S
 C19 0.12
 14 Orbital Energy -10.190469 Occupation 1.000000
 S
 C21 -0.99
 S
 C22 0.06
 15 Orbital Energy -10.189644 Occupation 1.000000
 S
 C18 0.13
 S
 C19 -0.99
 16 Orbital Energy -10.182280 Occupation 1.000000
 S
 C17 -0.99
 17 Orbital Energy -10.175585 Occupation 1.000000
 S
 C4 1.00
 18 Orbital Energy -10.172442 Occupation 1.000000
 S
 C13 -1.00
 19 Orbital Energy -3.700915 Occupation 1.000000
 S
 Ir1 1.01
 20 Orbital Energy -2.109924 Occupation 1.000000
 X Y Z
 Ir1 0.15 -0.82 -0.56
 21 Orbital Energy -2.105316 Occupation 1.000000
 X Y

Ir1 -0.99 -0.16
 22 Orbital Energy -2.097537 Occupation 1.000000
 X Y Z
 Ir1 0.06 -0.56 0.83
 23 Orbital Energy -0.257913 Occupation 1.000000
 XX YY ZZ XY XZ YZ YY ZZ XY XZ YZ
 Ir1 0.06 0.25 -0.31 0.53 -0.38 0.45 0.08 -0.08 0.16 -0.13 0.15
 S S S
 C22 -0.01 0.01 0.05
 24 Orbital Energy -0.263057 Occupation 1.000000
 XX YY ZZ XY XZ YZ XX ZZ XZ YZ
 Ir1 -0.36 0.14 0.23 0.08 0.59 0.48 -0.11 0.08 0.18 0.16
 Z Z
 C12 0.06 0.06
 25 Orbital Energy -0.262872 Occupation 1.000000
 XX ZZ XY XZ YZ XX ZZ XY XZ YZ
 Ir1 -0.28 0.29 0.61 0.13 -0.45 -0.07 0.09 0.20 0.05 -0.15
 Y Y
 C3 0.07 0.06
 S S
 H29 -0.02 0.05
 26 Orbital Energy -0.550957 Occupation 1.000000
 S S S X X XX YY ZZ XY XZ
 Ir1 0.10 -0.06 -0.10 0.13 -0.09 -0.19 0.10 0.09 -0.06 -0.10
 S S X Z S X Z
 C5 -0.02 0.04 0.02 -0.07 0.11 -0.06 -0.07
 S S X Y Z S X Y
 O6 0.12 -0.24 0.48 0.10 0.08 -0.34 0.33 0.05
 S S
 H7 -0.03 -0.05
 27 Orbital Energy -0.546049 Occupation 1.000000
 S S S Z Z XX YY ZZ XZ YZ
 Ir1 0.10 -0.06 -0.09 0.13 -0.10 0.08 0.09 -0.17 0.11 -0.06
 S S X Y Z S X Z
 O2 0.12 -0.24 -0.21 0.09 0.44 -0.35 -0.20 0.28
 S S X Z S Z
 C3 -0.02 0.04 -0.07 -0.03 0.11 -0.09
 S S
 H28 -0.03 -0.06
 28 Orbital Energy -0.549494 Occupation 1.000000
 S S S X X XX YY ZZ XY XZ
 Ir1 0.10 -0.06 -0.09 -0.13 0.09 -0.19 0.11 0.08 -0.06 -0.10
 S S X Y Z S X Y Z
 O9 0.12 -0.24 -0.46 -0.12 -0.13 -0.34 -0.30 -0.14 -0.08
 S S X Y S X
 C12 -0.02 0.04 0.02 -0.07 0.10 0.08
 S S
 H15 -0.03 -0.05

29 Orbital Energy -0.538797 Occupation 1.000000
 S S S Y Y XX YY ZZ
 Ir1 0.10 -0.06 -0.11 0.13 -0.08 0.11 -0.21 0.10
 S S X Y Z S X Y
 O10 0.12 -0.24 0.01 0.49 -0.06 -0.34 0.06 0.33
 S S X Y S X Y
 C11 -0.02 0.04 0.07 0.00 0.11 0.06 -0.07
 S S
 H14 -0.03 -0.06
 Y Y
 C17 0.03 0.06
 30 Orbital Energy -0.486659 Occupation 1.000000
 S S S X Z X Z XX YY ZZ XZ YZ
 Ir1 -0.10 0.06 0.13 -0.04 0.13 0.06 -0.12 -0.09 -0.13 0.22 -0.13 0.07
 XZ
 Ir1 -0.05
 S S
 H29 0.04 -0.10
 S S X Y Z S Y Z
 O30 -0.10 0.19 -0.06 0.25 0.43 0.25 0.17 0.32
 S S S
 C31 0.01 -0.01 -0.06
 S S
 H32 0.03 0.06
 31 Orbital Energy -0.450744 Occupation 1.000000
 S S S Y Y XX YY ZZ YZ XX YY
 Ir1 -0.12 0.07 0.10 0.14 -0.13 -0.12 0.25 -0.13 -0.07 -0.06 0.08
 S S Y S Y
 O10 0.01 -0.02 0.05 -0.06 0.05
 S S Y Z S Y Z
 C17 -0.11 0.20 0.33 -0.16 0.27 0.26 -0.14
 Y Z Y Z
 C18 0.00 0.02 -0.06 0.06
 S S S
 C19 -0.01 0.02 -0.06
 S S S
 C20 0.00 0.00 0.08
 S S S
 C21 -0.01 0.02 -0.06
 Y Z Y Z
 C22 0.00 0.04 -0.07 0.06
 S
 H29 0.21
 S S S
 O30 0.01 -0.03 -0.09
 32 Orbital Energy -0.610931 Occupation 1.000000
 S S Y Z S Y
 C5 -0.08 0.15 -0.25 -0.15 0.07 -0.10

S S X Y Z S X Y Z
 O6 -0.09 0.19 0.12 -0.30 0.38 0.15 0.06 -0.22 0.20
 33 Orbital Energy -0.619961 Occupation 1.000000
 S S X Y Z S Y
 C5 0.08 -0.15 0.10 -0.10 0.27 -0.06 -0.09
 S S Y Z S Y
 O6 0.09 -0.20 -0.47 -0.15 -0.15 -0.29
 34 Orbital Energy -0.615501 Occupation 1.000000
 S S X Y Z S X Y Z
 O2 -0.09 0.19 0.24 -0.29 0.32 0.14 0.13 -0.21 0.16
 S S X Y Z S Y
 C3 -0.08 0.15 -0.10 -0.26 -0.13 0.07 -0.11
 35 Orbital Energy -0.616442 Occupation 1.000000
 S S X Y Z S Y
 O2 0.09 -0.19 -0.12 -0.47 -0.10 -0.14 -0.29
 S S X Y Z S Y
 C3 0.08 -0.15 0.17 -0.11 0.23 -0.07 -0.10
 36 Orbital Energy -0.611759 Occupation 1.000000
 Z Z
 Ir1 0.02 -0.05
 S S X Y Z S X Y Z
 O9 0.09 -0.19 0.29 -0.26 -0.31 -0.14 0.15 -0.13 -0.22
 S S X Y Z S Z
 C12 0.08 -0.15 -0.09 0.14 -0.25 -0.06 -0.10
 37 Orbital Energy -0.499347 Occupation 1.000000
 XX
 Ir1 0.07
 S S X S X
 C4 0.01 -0.02 -0.02 -0.13 -0.06
 S S X Z S X
 C5 -0.02 0.06 -0.06 -0.07 0.11 -0.05
 S S X Y Z S X Z
 O6 0.15 -0.34 -0.33 0.06 0.36 -0.41 -0.22 0.23
 S S
 H7 0.03 0.05
 38 Orbital Energy -0.614772 Occupation 1.000000
 S S X Y Z S Y Z
 O9 0.09 -0.19 0.05 -0.18 0.46 -0.15 -0.08 0.28
 S S X Y Z S Z
 C12 0.08 -0.15 -0.21 0.19 0.11 -0.06 0.09
 39 Orbital Energy -0.495337 Occupation 1.000000
 XZ
 Ir1 -0.06
 S S X Y Z S X
 O2 0.15 -0.34 0.49 0.06 -0.05 -0.41 0.31
 S S X Z S X
 C3 -0.02 0.06 -0.02 -0.09 0.10 0.06
 S S X S X

C4 0.01 -0.02 0.03 -0.13 0.07
 S S
 H28 0.03 0.06
 40 Orbital Energy -0.497578 Occupation 1.000000
 Y Y XX
 Ir1 -0.02 0.05 0.06
 S S X Y S X Y
 O9 0.15 -0.34 0.14 0.48 -0.41 0.10 0.31
 S S X Y S Y
 C12 -0.02 0.06 0.09 -0.04 0.10 0.06
 S S Y S Y
 C13 0.01 -0.02 0.03 -0.13 0.07
 S S
 H15 0.03 0.05
 S S S
 C17 0.00 0.00 0.07
 X X
 C18 -0.02 -0.06
 S S
 H23 0.00 -0.06
 41 Orbital Energy -0.562033 Occupation 1.000000
 S S X Y S X Y
 C17 0.11 -0.22 0.31 0.20 -0.16 0.09 0.05
 S S X Y S X Y
 C18 0.11 -0.22 -0.30 -0.23 -0.17 -0.08 -0.07
 S S
 H23 0.02 0.06
 S S
 H24 -0.02 -0.06
 S S
 H27 -0.02 -0.06
 42 Orbital Energy -0.459487 Occupation 1.000000
 S S S Z Z
 Ir1 0.02 -0.02 -0.06 0.01 0.05
 S S Y Z S Y Z
 C17 0.01 -0.02 -0.04 0.02 -0.12 -0.09 0.07
 S S
 H29 0.13 0.20
 S S Y Z S Y Z
 O30 -0.11 0.23 -0.52 0.10 0.29 -0.35 0.08
 S S
 H33 0.03 0.10
 43 Orbital Energy -0.613313 Occupation 1.000000
 S S X Y Z S X Y Z
 O10 0.09 -0.19 0.36 -0.17 -0.29 -0.14 0.19 -0.08 -0.21
 S S X Y Z S Z
 C11 0.08 -0.15 -0.14 0.09 -0.26 -0.07 -0.10
 44 Orbital Energy -0.495048 Occupation 1.000000

S S X Z S Z
 C17 0.09 -0.19 -0.20 -0.32 -0.12 -0.14
 Z Z
 C18 -0.08 -0.06
 Z
 C20 0.06
 S S X Y Z S X Y Z
 C22 0.10 -0.20 0.30 -0.18 -0.02 -0.17 0.10 -0.07 -0.06
 S S
 H27 0.02 0.06
 S S
 H29 0.07 0.10
 S S S
 O30 0.01 -0.02 -0.05
 45 Orbital Energy -0.613824 Occupation 1.000000
 S S X Y Z S Z
 O10 0.09 -0.20 0.13 -0.07 0.47 -0.14 0.29
 S S X Y Z S Z
 C11 0.08 -0.15 -0.25 0.13 0.11 -0.06 0.10
 46 Orbital Energy -0.495342 Occupation 1.000000
 YY
 Ir1 0.08
 S S X Y Z S X Y Z
 O10 0.15 -0.34 -0.41 -0.25 -0.09 -0.41 -0.26 -0.18 -0.06
 S S X Y S
 C11 -0.02 0.06 0.06 -0.08 0.11
 S S X S X
 C13 0.01 -0.03 -0.03 -0.13 -0.05
 S S
 H14 0.03 0.06
 47 Orbital Energy -0.656009 Occupation 1.000000
 S S X Y Z S X Y Z
 O30 -0.10 0.22 0.41 0.13 -0.13 0.16 0.23 0.07 -0.05
 S S X Y Z S X
 C31 -0.09 0.17 -0.29 -0.08 0.12 0.09 -0.08
 48 Orbital Energy -0.447080 Occupation 1.000000
 X Z X Z Z YY ZZ
 Ir1 0.02 0.01 -0.06 -0.01 -0.06 0.06 -0.09
 S S S
 C17 0.00 0.01 0.05
 S S
 H29 -0.05 -0.07
 S S X Y Z S X Y Z
 O30 -0.15 0.33 -0.36 0.11 -0.32 0.40 -0.25 0.08 -0.23
 S S S
 C31 0.01 -0.04 -0.06
 S S
 H34 0.03 0.09

49 Orbital Energy -0.416119 Occupation 1.000000
 S S S Y Y YY ZZ
 Ir1 0.04 -0.03 -0.08 -0.03 0.08 -0.11 0.06
 S S X Y Z S X Y Z
 C17 -0.08 0.15 0.24 -0.19 -0.22 0.13 0.10 -0.11 -0.14
 Y Z Z
 C18 -0.07 -0.12 -0.07
 Z
 C19 0.05
 Z Z
 C20 0.09 0.08
 S S X Z S Z
 C22 -0.07 0.13 -0.11 -0.28 0.08 -0.16
 S S
 H29 0.10 0.10
 S S S
 O30 0.01 -0.02 -0.05
 50 Orbital Energy -0.592124 Occupation 1.000000
 S S X Z S Z
 C4 0.11 -0.22 -0.19 0.31 -0.18 0.09
 S S X Y Z S X Z
 C5 0.12 -0.24 0.24 -0.09 -0.27 -0.17 0.05 -0.06
 S S
 H7 0.03 0.09
 S S
 H8 0.03 0.07
 51 Orbital Energy -0.594203 Occupation 1.000000
 X
 O2 0.05
 S S X Y S X
 C3 0.12 -0.24 -0.37 -0.08 -0.18 -0.08
 S S X S X
 C4 0.11 -0.22 0.36 -0.18 0.10
 S S
 H8 0.03 0.07
 S S
 H28 0.04 0.09
 52 Orbital Energy -0.594992 Occupation 1.000000
 Y
 O9 -0.05
 S S X Y S Y
 C12 -0.12 0.24 0.10 0.36 0.17 0.08
 S S Y S Y
 C13 -0.11 0.22 -0.35 0.18 -0.10
 S S
 H15 -0.04 -0.09
 S S
 H16 -0.03 -0.07

53 Orbital Energy -0.594294 Occupation 1.000000
 X
 O10 0.05
 S S X Y Z S X
 C11 -0.12 0.24 -0.31 -0.19 -0.10 0.18 -0.07
 S S X Y S X
 C13 -0.11 0.22 0.33 0.14 0.18 0.09
 S S
 H14 -0.04 -0.09
 S S
 H16 -0.03 -0.07
 54 Orbital Energy -0.575596 Occupation 1.000000
 S S S
 C19 0.00 0.01 0.05
 S S Y Z S Y
 C21 0.11 -0.22 -0.34 0.17 -0.15 -0.09
 S S Y Z S Y Z
 C22 0.11 -0.22 0.33 -0.18 -0.17 0.09 -0.05
 S S
 H25 -0.02 -0.06
 S S
 H26 0.03 0.07
 S S
 H27 0.03 0.07
 55 Orbital Energy -0.498702 Occupation 1.000000
 S S S
 C17 -0.01 0.03 0.05
 S S S
 C21 -0.01 0.03 0.07
 S S X Y S X Y
 C22 0.11 -0.21 -0.32 -0.21 -0.17 -0.12 -0.06
 S S
 H27 -0.33 -0.24
 56 Orbital Energy -0.451998 Occupation 1.000000
 S S Y Z S Z
 C18 0.09 -0.17 0.12 -0.32 -0.13 -0.16
 S S X Y Z S X Y Z
 C19 0.09 -0.17 0.07 -0.35 -0.12 -0.12 0.06 -0.14 -0.13
 Y Z Y Z
 C20 -0.06 -0.12 -0.06 -0.07
 Y Z Y Z
 C22 0.05 0.08 0.05 0.06
 S S
 H24 0.02 0.05
 57 Orbital Energy -0.297706 Occupation 1.000000
 Y Y
 Ir1 -0.01 0.05
 Y Y

O2 0.10 0.10
X Y Z Y
C3 0.07 -0.22 0.06 -0.12
S S X Y Z S X Y Z
C4 -0.03 0.07 0.06 -0.42 0.07 0.06 0.05 -0.31 0.08
Y Z Y
C5 -0.23 0.12 -0.13
Y Y
O6 0.10 0.10
58 Orbital Energy -0.491572 Occupation 1.000000
S S X Y Z S X Z
C18 0.11 -0.22 0.33 -0.13 0.16 -0.18 0.13 0.05
S S S
C19 -0.01 0.03 0.07
S S
H23 -0.33 -0.22
59 Orbital Energy -0.445539 Occupation 1.000000
S S X Y Z S Y Z
C18 0.08 -0.17 -0.07 0.32 0.08 -0.11 0.12 0.10
S S X Y Z S Z
C19 0.09 -0.17 -0.07 -0.09 0.36 -0.13 0.20
Y Z Z
C20 0.06 0.11 0.08
Z Z
C21 -0.05 -0.05
Z Z
C22 -0.09 -0.08
S S
H24 0.02 0.05
60 Orbital Energy -0.286149 Occupation 1.000000
Z Z
O9 -0.10 -0.10
Z Z
O10 -0.10 -0.10
X Z Z
C11 -0.10 0.23 0.12
X Y Z Z
C12 -0.06 0.06 0.24 0.13
X Z X Z
C13 -0.11 0.43 -0.09 0.32
61 Orbital Energy -0.573153 Occupation 1.000000
S S X Y Z S X Y
C19 -0.11 0.22 0.31 -0.14 0.16 0.15 0.07 -0.05
S S X Y Z S X
C20 -0.11 0.22 -0.33 0.11 -0.15 0.17 -0.10
S S
H23 0.02 0.05
S S

H24 -0.03 -0.07
 S S
 H25 -0.03 -0.07
 S S
 H26 0.02 0.05
 62 Orbital Energy -0.459146 Occupation 1.000000
 Z
 C17 0.05
 Z Z
 C18 0.07 0.07
 S S X Y Z S Y Z
 C20 0.09 -0.17 -0.16 -0.25 -0.17 -0.13 -0.10 -0.12
 S S X Z S X Z
 C21 0.09 -0.17 0.28 -0.25 -0.13 0.09 -0.17
 Y Z Y Z
 C22 -0.07 -0.12 -0.05 -0.06
 S S
 H25 0.02 0.05
 S S
 H26 0.02 0.05
 63 Orbital Energy -0.449101 Occupation 1.000000
 Z Z
 C18 -0.06 -0.06
 S S X Z S X Z
 C20 0.08 -0.17 -0.26 0.22 -0.13 -0.09 0.13
 S S X Y Z S Y Z
 C21 0.08 -0.17 0.14 0.26 0.23 -0.11 0.13 0.15
 Y Z Z
 C22 0.06 0.14 0.09
 64 Orbital Energy -0.460328 Occupation 1.000000
 X
 O30 0.05
 S S X Y Z S X Y Z
 C31 0.10 -0.19 -0.28 0.15 -0.24 -0.17 -0.11 0.06 -0.09
 S S
 H32 0.02 0.07
 S S
 H33 0.02 0.07
 S S
 H34 -0.33 -0.26
 65 Orbital Energy -0.520917 Occupation 1.000000
 S S S
 C4 -0.01 0.03 0.10
 S S X Y S X
 C5 0.11 -0.22 -0.38 -0.08 -0.19 -0.11
 S S
 H7 -0.33 -0.25
 66 Orbital Energy -0.458905 Occupation 1.000000

S S Y S Y
 C31 0.10 -0.20 -0.39 -0.17 -0.16
 S S
 H32 0.02 0.06
 S S
 H33 -0.33 -0.25
 S S
 H34 0.02 0.07
 67 Orbital Energy -0.519767 Occupation 1.000000
 S S X Y Z S Z
 C3 0.11 -0.22 0.18 -0.07 -0.34 -0.19 -0.12
 S S S
 C4 -0.01 0.03 0.10
 S S
 H28 -0.33 -0.25
 68 Orbital Energy -0.518654 Occupation 1.000000
 S S X Y Z S X
 C12 -0.11 0.22 -0.36 -0.12 -0.10 0.18 -0.12
 S S S
 C13 0.01 -0.03 -0.10
 S S
 H15 0.33 0.25
 69 Orbital Energy -0.518146 Occupation 1.000000
 S S Y S Y
 C11 -0.11 0.22 0.39 0.19 0.12
 S S S
 C13 0.01 -0.03 -0.10
 S S
 H14 0.33 0.25
 70 Orbital Energy -0.503208 Occupation 1.000000
 S S S
 C3 -0.01 0.03 0.06
 S S X Y Z S X Z
 C4 0.11 -0.21 -0.16 -0.13 -0.31 -0.16 -0.05 -0.10
 S S S
 C5 -0.01 0.03 0.06
 S S
 H8 -0.33 -0.25
 71 Orbital Energy -0.463510 Occupation 1.000000
 S S Y Z S Y Z
 C31 0.10 -0.20 0.16 0.36 -0.16 0.06 0.14
 S S
 H32 -0.33 -0.26
 S S
 H33 0.02 0.06
 S S
 H34 0.02 0.06
 72 Orbital Energy -0.501000 Occupation 1.000000

```

    S   S   S
C11   0.01 -0.03 -0.06
    S   S   S
C12   0.01 -0.03 -0.06
    S   S   X   Y   Z   S   X   Y
C13   -0.11 0.21 -0.28 0.22 -0.12 0.16 -0.09 0.07
    S   S
H16   0.33 0.25
    73 Orbital Energy  -0.502786 Occupation  1.000000
    S   S   S
C17   -0.01 0.01 0.05
    S   S   S
C19   -0.01 0.02 0.05
    S   S   S
C20   0.01 -0.03 -0.07
    S   S   X   Y   Z   S   X
C21   -0.11 0.21 0.33 -0.12 0.15 0.18 0.10
    S   S   S
C22   0.01 -0.03 -0.07
    S   S
H26   0.33 0.26
    74 Orbital Energy  -0.500493 Occupation  1.000000
    S   S   S
C17   -0.01 0.02 0.05
    S   S   S
C18   0.01 -0.03 -0.07
    S   S   X   Y   S   X   Y
C19   -0.11 0.21 -0.31 -0.22 0.18 -0.09 -0.07
    S   S   S
C20   0.01 -0.03 -0.07
    S   S   S
C21   -0.01 0.02 0.05
    S   S
H24   0.33 0.26
    75 Orbital Energy  -0.507041 Occupation  1.000000
    S   S   S
C19   0.01 -0.03 -0.06
    S   S   Y   Z   S   Y   Z
C20   -0.11 0.21 -0.34 0.18 0.17 -0.11 0.06
    S   S   S
C21   0.01 -0.03 -0.06
    S   S
H25   0.33 0.25
    76 Orbital Energy  -0.060372 Occupation  0.000000
    S   S   S   Y   Y   XX   YY   ZZ   XY   YZ   XX   YY
Ir1   0.05 -0.04 -0.13 -0.05 0.12 0.20 -0.45 0.24 0.07 0.09 0.05 -0.14
    ZZ
Ir1   0.09

```

S S S
 C4 0.00 0.01 0.06
 Y Y
 C5 -0.05 -0.07
 X
 O9 -0.06
 S S Y S Y
 O10 -0.02 0.05 -0.15 0.13 -0.11
 X X
 C11 -0.04 -0.08
 S S S
 C13 0.00 -0.01 -0.06
 S S
 H14 0.04 0.10
 S S X Y Z S X Y Z
 C17 -0.01 0.03 0.04 -0.02 -0.19 0.09 0.06 -0.09 -0.16
 X Y Z X Y Z
 C18 -0.06 0.09 0.19 -0.08 0.14 0.17
 S S Y Z S Y Z
 C19 0.00 0.01 0.05 0.06 0.05 0.07 0.07
 X Y Z X Y Z
 C20 0.07 -0.13 -0.24 0.07 -0.15 -0.26
 S S Y Z S Y Z
 C21 0.00 0.01 0.05 0.06 0.05 0.06 0.07
 S S Y Z S Y Z
 C22 0.00 -0.01 0.09 0.20 -0.06 0.13 0.20
 S S
 H29 0.14 0.28
 S S Y Z S Y Z
 O30 0.03 -0.06 0.08 -0.14 -0.18 0.07 -0.12
 X X
 C31 -0.03 -0.06
 S S
 H34 0.02 0.07
 77 Orbital Energy -0.049899 Occupation 0.000000
 XX ZZ XY
 Ir1 0.05 -0.07 -0.14
 Y Z Y Z
 O2 -0.25 0.07 -0.25 0.06
 X Y Z X Y Z
 C3 -0.05 0.33 -0.09 -0.05 0.33 -0.10
 X Y Z X Y Z
 C5 0.06 -0.33 0.10 0.05 -0.33 0.10
 Y Z Y Z
 O6 0.24 -0.07 0.24 -0.08
 Z Z
 O9 -0.11 -0.11
 Z Z

O10 0.11 0.11
Z Z
C11 -0.15 -0.15
X Z Z
C12 -0.05 0.15 0.15
S S S
C21 0.00 0.00 -0.05
X Y X Y
C22 0.01 0.00 0.07 -0.06
78 Orbital Energy -0.045529 Occupation 0.000000
XX YY ZZ XY XZ YZ
Ir1 -0.06 0.11 -0.05 -0.11 0.13 0.15
Y Y
O2 -0.11 -0.11
Y Y
C3 0.14 0.14
Y Z Y Z
C5 -0.13 0.05 -0.14 0.05
Y Y
O6 0.10 0.11
X Z X Z
O9 -0.07 0.25 -0.08 0.24
X Z X Z
O10 0.08 -0.25 0.08 -0.25
X Z X Z
C11 -0.10 0.33 -0.09 0.33
X Z X Z
C12 0.10 -0.33 0.10 -0.33
S S S
C18 0.00 0.00 0.07
S S S
C19 0.00 0.00 -0.05
S S S
C21 0.00 0.00 -0.06
Y Y
C22 -0.01 -0.07
S S
H29 -0.02 -0.07
79 Orbital Energy -0.003678 Occupation 0.000000
X X XX ZZ XY XZ
Ir1 -0.01 0.07 0.13 -0.13 0.08 0.07
S S S
C5 0.00 0.00 0.06
S S S
O6 0.01 -0.02 -0.10
X X
C17 0.01 -0.07
S S X Y Z S X Y Z

C18 0.00 0.00 0.08 -0.15 -0.26 -0.08 0.08 -0.19 -0.34
 X Y Z X Y Z
 C19 -0.07 0.14 0.26 -0.09 0.19 0.33
 X Y Z X Y Z
 C21 0.07 -0.14 -0.26 0.10 -0.19 -0.34
 S S X Y Z S X Y Z
 C22 0.00 0.00 -0.07 0.15 0.26 0.07 -0.10 0.19 0.34
 S S S
 O30 -0.01 0.01 0.05
 S S X S X
 C31 0.00 0.00 0.02 0.05 0.05
 S S
 H34 0.00 -0.08
 80 Orbital Energy -0.002493 Occupation 0.000000
 Z Z Z XX ZZ XY XZ YZ XX ZZ XZ
 Ir1 -0.01 0.02 -0.07 -0.58 0.54 -0.18 -0.45 0.12 -0.16 0.15 -0.12
 S S X Z S X Z
 O2 0.03 -0.07 -0.10 0.16 -0.21 -0.09 0.10
 S S X S X
 C3 -0.01 0.03 -0.03 0.10 -0.13
 X Z X Z
 C4 -0.05 0.02 -0.08 0.05
 S S X Z S X Z
 C5 0.01 -0.04 0.00 0.03 -0.06 -0.09 0.10
 S S X S X
 O6 -0.03 0.07 -0.19 0.19 -0.13
 S S
 H7 0.05 0.20
 S S X Y Z S X Y
 O9 -0.03 0.07 0.17 0.07 0.05 0.22 0.12 0.07
 S S S
 C11 0.00 0.01 0.06
 Y Y
 C12 0.04 0.14
 S S Y S Y
 C13 0.01 -0.01 0.02 -0.16 0.06
 S S
 H15 0.04 0.17
 Z Z
 C18 -0.06 -0.09
 Z Z
 C19 0.05 0.07
 Z Z
 C21 -0.06 -0.09
 Y Z Y Z
 C22 0.03 0.05 0.06 0.07
 S S
 H28 -0.05 -0.18

	S	S	Y	Z	S	Y	Z
O30	0.03	-0.07	-0.10	-0.19	-0.20	-0.09	-0.16
	S	S	X	S	X		
C31	-0.01	0.01	-0.04	0.06	-0.06		
	S	S					
H32	-0.04	-0.11					
	S	S					
H33	0.02	0.05					

Ir(2NH3)(2CH3)(OH)(CH4)

Gas phase Energy: -413.99169826054 hartrees

Zero Point Energy: 132.855 kcal/mol

Coordinates:

Ir1	-0.4700089074	0.2624058305	-0.0904949614
C2	-0.3396997614	-2.2765096271	0.0295245189
H3	0.4397475453	-3.0286625699	0.1958008707
H4	-1.1992804377	-2.4764211713	0.6647636354
H5	0.2728327881	-1.3629758675	0.3622413890
O6	-0.2169922333	0.0696211177	-2.1055318901
H7	0.7406176225	0.0379493313	-2.2429899230
H8	-0.6102711994	-2.2496770177	-1.0226977655
N9	-0.7943188978	2.1740526727	-0.7393657435
H10	-0.1169796831	2.8690339167	-0.4288330757
H11	-1.7457311666	2.5182599207	-0.6194406941
H12	-0.6305275994	1.9319461503	-1.7375261736
N13	-0.8410179113	0.5422890123	2.0312500036
H14	-0.1537338911	0.0568008027	2.6051064143
H15	-1.7672809652	0.1910123592	2.2734989988
H16	-0.8024076249	1.5224656807	2.3021847218
C17	-2.5848759131	-0.1115450805	-0.3457326829
H18	-2.7750543863	-0.6270811029	-1.2959735646
H19	-3.1958495387	0.8109738058	-0.3645407176
H20	-3.0250440039	-0.7378892063	0.4520501560
C21	1.6463541227	0.7459680245	0.1687021102
H22	2.2740135775	0.3971278250	-0.6686223152
H23	2.1090554064	0.3288462342	1.0791780153
H24	1.8132390206	1.8377177283	0.2310871938

Orbital coefficients:

1	Orbital Energy	1.000000	Occupation	1.000000
	S			
O6	-1.00			
2	Orbital Energy	2.000000	Occupation	1.000000
	S			
N13	-1.00			
3	Orbital Energy	3.000000	Occupation	1.000000
	S			
N9	-1.00			

4	Orbital Energy	4.000000	Occupation	1.000000
	S			
C2	-1.00			
5	Orbital Energy	5.000000	Occupation	1.000000
	S			
C21	-1.00			
6	Orbital Energy	6.000000	Occupation	1.000000
	S			
C17	-1.00			
7	Orbital Energy	7.000000	Occupation	1.000000
	S			
Ir1	1.01			
8	Orbital Energy	8.000000	Occupation	1.000000
	X Y Z			
Ir1	-.15 .90 -.42			
9	Orbital Energy	9.000000	Occupation	1.000000
	X Y Z			
Ir1	.29 -.36 -.88			
10	Orbital Energy	10.000000	Occupation	1.000000
	X Y Z			
Ir1	-.95 -.25 -.21			
11	Orbital Energy	34.598300	Occupation	1.000000
	XX ZZ XY XZ YZ XX ZZ XZ			
Ir1	-.22 .23 .06 .79 .10 -.08 .08 .29			
	S S			
H7	.02 .06			
	S S			
H14	-.02 -.06			
	S S			
H15	.02 .07			
	S S			
H18	-.02 -.05			
	S S			
H22	.02 .06			
12	Orbital Energy	33.822998	Occupation	1.000000
	Y Y YY ZZ XY YZ YY ZZ XY YZ			
Ir1	-.02 .08 .19 -.19 -.21 .78 .08 -.09 -.07 .28			
	S S			
H12	.03 .11			
	S S			
H16	-.03 -.06			
13	Orbital Energy	32.898855	Occupation	1.000000
	XX YY XY XZ YZ XX YY XY YZ			
Ir1	.24 -.27 -.74 .11 -.15 .09 -.10 -.27 -.06			
	S S Y S Y			
C2	.01 -.01 -.04 -.07 -.07			
	S S			
H5	.05 .08			

```

      S  S
H10   .02 .08
      S  S
H11  -.02 -.07
      S  S
H19  -.02 -.06
      S  S
H24   .02 .06
  14 Orbital Energy 25.858774 Occupation 1.000000
      S  S  S  X  Z  X  Z  Z  XX  YY  ZZ  XZ
Ir1  -.11 .07 .14 -.03 .14 .06 -.12 .07 -.12 -.16 .28 -.08
      YZ  ZZ
Ir1   .06 .06
      S  S  Z  S  Z
O6   -.09 .20 .49 .21 .35
      S  S
H7   -.01 -.09
      S  S
H12   .00 -.05
      Z  Z
N13   .04 .05
  15 Orbital Energy 22.216891 Occupation 1.000000
      S  S  S  Y  Y  XX  YY  ZZ  XY  YZ
Ir1   .13 -.08 -.09 .14 -.06 .13 -.26 .12 .07 .08
      S  S  X  Y  Z  S  Y  Z
N9   .11 -.23 -.05 .40 -.23 -.33 .29 -.17
      S  S
H10   .02 .06
      S  S
H11   .02 .06
      S  S
H12   .00 .06
  16 Orbital Energy 22.715900 Occupation 1.000000
      S  S  S  Z  Z  XX  YY  ZZ  XZ
Ir1  -.10 .06 .07 -.14 .11 -.09 -.08 .17 -.06
      S  S  X  Z  S  X  Z
N13  -.12 .25 .09 -.46 .35 .06 -.34
      S  S
H14  -.02 -.06
      S  S
H15  -.01 -.06
      S  S
H16  -.02 -.06
  17 Orbital Energy 31.335049 Occupation 1.000000
      S  S  S  X  X  X  XX  YY  ZZ  XY  XZ  XX
Ir1   .13 -.09 -.16 -.18 .24 -.08 -.31 .16 .15 -.10 -.08 -.10
      ZZ
Ir1   .05

```

```

      S  S  X  Y  Z  S  X
C17   .11 -0.20 -0.38 -0.07 -0.06 -0.27 -0.23
      S  S
H18   .01 .07
      S  S
H19   .02 .07
      S  S
H20   .02 .08
      X  X
C21   -0.05 -0.06
      18 Orbital Energy  31.148336 Occupation  1.000000
      S  S  S  X  X  X  XX  YY  ZZ  XY  XZ  XX
Ir1   .13 -0.08 -0.16 .18 -0.25 .08 -0.29 .14 .15 -0.11 -0.06 -0.09
      ZZ
Ir1   .05
      X  X
C17   .05 .06
      S  S  X  Y  Z  S  X  Y
C21   .11 -0.20 .37 .09 .05 -0.27 .23 .06
      S  S
H22   .02 .07
      S  S
H23   .02 .07
      S  S
H24   .02 .07
      19 Orbital Energy  28.685383 Occupation  1.000000
      S  S  S  X  Y  X  Y  Y  ZZ
Ir1   -0.02 .01 .05 -0.01 .03 .06 -0.10 -0.06 .06
      S  S
H5    .00 -0.08
      S  S  X  Y  Z  S  X  Y  Z
O6    .12 -0.27 .17 -0.46 .18 -0.34 .11 -0.34 .13
      S  S
H7    .03 .06
      S  S  Z  S  Z
N9    -0.02 .03 -0.03 .16 -0.07
      S  S
H12   -0.03 -0.15
      20 Orbital Energy  28.636192 Occupation  1.000000
      Y  Z  Y  Z  Y  Z  ZZ
Ir1   .03 .00 -0.08 .02 -0.07 -0.07 -0.07
      S  S  X  Y  Z  S  X  Y  Z
O6    -0.14 .31 -0.24 -0.41 -0.18 .38 -0.16 -0.31 -0.13
      S  S
H7    -0.04 -0.08
      S  S  S
N9    -0.01 .02 .08
      S  S

```

H12 -.02 -.07
 S S S
 C17 .01 .00 -.05
 21 Orbital Energy 20.178278 Occupation 1.000000
 S S S Z Z
 Ir1 -.02 .01 .05 .01 -.07
 S S X Z S X
 O6 .09 -.20 -.45 .07 -.12 -.23
 S S
 H7 -.32 -.18
 22 Orbital Energy 18.341769 Occupation 1.000000
 S S X Y Z S Z
 N9 .10 -.21 -.07 .06 .44 -.23 .26
 S S
 H12 -.30 -.11
 23 Orbital Energy 20.205077 Occupation 1.000000
 S S S Y Y XX YY ZZ YY
 Ir1 .07 -.04 -.08 -.10 .08 .07 -.13 .06 -.09
 S S X Y S X Y
 C2 .09 -.16 -.15 -.33 -.16 -.07 -.14
 S S
 H3 .03 .07
 S S
 H4 .02 .06
 S S
 H5 -.33 -.17
 S S Y S Y
 N9 -.01 .01 -.02 .07 -.06
 24 Orbital Energy 17.382510 Occupation 1.000000
 S S X Y Z S X Y
 N9 .10 -.21 .40 -.15 -.06 -.19 .21 -.09
 S S
 H11 -.32 -.15
 25 Orbital Energy 17.113345 Occupation 1.000000
 S S X Y Z S X Y Z
 N9 .10 -.21 -.28 -.29 -.15 -.18 -.14 -.16 -.08
 S S
 H10 -.32 -.15
 26 Orbital Energy 16.804102 Occupation 1.000000
 S S X Y Z S X Y Z
 N13 .10 -.21 .40 .14 -.10 -.18 .21 .07 -.07
 S S
 H15 -.32 -.15
 27 Orbital Energy 16.560842 Occupation 1.000000
 S S X Y Z S X Y Z
 N13 .10 -.21 -.28 .23 -.24 -.18 -.14 .12 -.14
 S S
 H14 -.32 -.16

28 Orbital Energy 16.487403 Occupation 1.000000
 S S Y Z S Y Z
 N13 .10 -.21 -.41 -.12 -.17 -.22 -.07
 S S
 H16 -.32 -.16
 29 Orbital Energy 21.132408 Occupation 1.000000
 S S X Z S X Z
 C2 -.10 .20 -.27 -.29 .20 -.13 -.13
 S S
 H4 -.02 -.06
 S S
 H5 -.03 -.06
 S S
 H8 .32 .19
 30 Orbital Energy 26.075465 Occupation 1.000000
 S S X Y Z S Y Z
 C17 .10 -.19 .05 .17 .33 -.17 .08 .15
 S S
 H18 -.32 -.25
 S S
 H19 .02 .07
 S S
 H20 .02 .07
 31 Orbital Energy 25.166525 Occupation 1.000000
 S S X Y S X Y
 C17 .09 -.18 .19 -.32 -.12 .09 -.13
 S S
 H18 .02 .05
 S S
 H19 -.32 -.30
 S S
 H20 .02 .07
 32 Orbital Energy 25.228119 Occupation 1.000000
 S S X Y Z S X Y Z
 C17 .09 -.18 .14 .21 -.27 -.13 .07 .08 -.11
 S S
 H18 .02 .06
 S S
 H19 .02 .07
 S S
 H20 -.32 -.30
 33 Orbital Energy 24.276967 Occupation 1.000000
 S S Y S Y
 C21 -.09 .18 .37 .13 .15
 S S
 H22 -.02 -.06
 S S
 H23 -.02 -.07

```

      S  S
H24   .32 .30
      34 Orbital Energy  24.339388 Occupation 1.000000
      S  S  X  Y  Z  S  X  Z
C21   .10 -.18 -.20 .12 .28 -.15 -.10 .12
      S  S
H22   -.32 -.28
      S  S
H23   .02 .07
      S  S
H24   .02 .07
      35 Orbital Energy  24.562533 Occupation 1.000000
      S  S  X  Y  Z  S  X  Y  Z
C21   .10 -.18 -.13 .15 -.31 -.13 -.07 .06 -.13
      S  S
H22   .02 .06
      S  S
H23   -.32 -.29
      S  S
H24   .02 .07
      36 Orbital Energy  21.131012 Occupation 1.000000
      S  S  X  Y  Z  S  X  Z
C2   .10 -.19 .16 .10 -.34 -.17 .05 -.14
      S  S
H3   .02 .06
      S  S
H4   -.33 -.25
      S  S
H5   .02 .05
      37 Orbital Energy  21.097580 Occupation 1.000000
      S  S  X  Y  Z  S  X  Y
C2   -.10 .19 .29 -.24 -.10 .16 .12 -.10
      S  S
H3   .32 .24
      S  S
H4   -.02 -.06
      38 Orbital Energy   .000000 Occupation .000000
      X  Z  X  Z  XX  YY  ZZ  XY  XZ  YZ
C2   .00 -.01 -.05 -.08 -.06 .11 -.05 .19 -.32 .13
      X  Z
H3   -.07 -.21
      X  Z
H4   -.13 -.14
      X  Z
H5   -.09 -.09
      S  X  Y  Z
H8   -.07 -.11 -.13 -.16
      XX  ZZ  XZ  YZ

```



```

N9      .15 -.12 -.25 -.10
      X  Z
H10     .10 -.15
      X  Y  Z
H11     .06 -.06 .10
      X
H12     .20
      XX YY XY YZ
N13     .08 -.09 .16 .06
      X  Y  Z
H14     .07 .07 .05
      Z
H15     -.05
      X  Z
H16     .12 .05
      YY ZZ
C17     -.06 .07
      Y
H18     .05
      YZ
C21     .06
39 Orbital Energy .000000 Occupation .000000
      XX YY XZ
C2      -.10 .08 .07
      Y
H3      -.08
      X
H4      .06
      XX YY ZZ XZ YZ
N9      -.17 .08 .10 .14 .10
      X  Z
H10     -.10 .13
      Y
H11     .10
      X  Y
H12     -.13 -.05
      XX YY XY XZ YZ
N13     .31 -.33 .18 .18 .16
      X  Y
H14     .18 .27
      S  Y  Z
H15     .07 .09 -.19
      S  X  Z
H16     -.06 .19 .17
      YY ZZ YZ
C21     .08 -.09 .05
      Y
H22     -.07

```

X
H23 .05

TS: Ir(2NH3)(2CH3)(OH-H-CH3)

Gas phase Energy: -413.96411164184 hartrees

Zero Point Energy: 130.028 kcal/mol

Imaginary frequency: -1218.28 cm⁻¹

Coordinates:

Ir1	-.4925044620	.2051437669	-.0505116855
C2	-.1380467919	-2.0592201914	.1540740074
H3	-.6492507561	-2.8285914309	-.4402784589
H4	.8920581289	-2.3635434940	.3563394375
H5	-.0492226341	-1.3324895378	-.9878409328
O6	.0354526049	-.4308645753	-1.9812306770
H7	.9919647953	-.2794430481	-2.0344407931
H8	-.6921103538	-2.0339154951	1.0942974549
N9	-.7694376920	2.2355930453	-.5937072400
H10	-.0961685290	2.8810985726	-.1802120666
H11	-1.7165746340	2.5803069473	-.4353611001
H12	-.6182577463	2.2376869279	-1.6033064098
N13	-1.0263292288	.5544381726	1.9756938073
H14	-.3535539093	.1006543112	2.5924932211
H15	-1.9509945897	.1636973987	2.1610950415
H16	-1.0502420307	1.5372542785	2.2456195694
C17	-2.5820672369	-.1547340182	-.4867855933
H18	-2.7133618111	-.8045135258	-1.3628217789
H19	-3.1530182080	.7685243044	-.7056830209
H20	-3.1251114414	-.6463696230	.3430279947
C21	1.5918300284	.6107793355	.4158483607
H22	2.2914146291	.2505819183	-.3601126930
H23	1.9296536994	.1276984867	1.3492291784
H24	1.8224794944	1.6870743598	.5385361842

Orbital coefficients:

1	Orbital Energy	1.000000	Occupation	1.000000
	S			
O6	-1.00			
2	Orbital Energy	2.000000	Occupation	1.000000
	S			
N13	-1.00			
3	Orbital Energy	3.000000	Occupation	1.000000
	S			
N9	-1.00			
4	Orbital Energy	4.000000	Occupation	1.000000
	S			
C2	-1.00			
5	Orbital Energy	5.000000	Occupation	1.000000
	S			

C21 -1.00
 6 Orbital Energy 6.000000 Occupation 1.000000
 S

C17 -1.00
 7 Orbital Energy 7.000000 Occupation 1.000000
 S

Ir1 1.01
 8 Orbital Energy 8.000000 Occupation 1.000000
 X Y Z

Ir1 -0.27 0.79 0.55
 9 Orbital Energy 9.000000 Occupation 1.000000
 X Y Z

Ir1 0.11 0.60 -0.79
 10 Orbital Energy 10.000000 Occupation 1.000000
 X Y Z

Ir1 0.96 0.16 0.25
 11 Orbital Energy 33.065211 Occupation 1.000000
 XX YY ZZ XY XZ YZ XX ZZ XY XZ YZ

Ir1 -0.25 -0.09 0.34 0.46 0.23 -0.55 -0.08 0.13 0.18 0.09 -0.21
 S S

H5 -0.04 0.05
 S S

H11 0.02 0.06
 S S

H12 -0.02 -0.06
 S S

H14 -0.02 -0.07
 S S

H16 0.02 0.06
 12 Orbital Energy 33.593593 Occupation 1.000000
 XX YY XY XZ YZ XX YY XY XZ YZ

Ir1 -0.26 0.29 0.51 0.18 0.54 -0.10 0.12 0.19 0.07 0.20
 S S

H10 -0.02 -0.07
 S S

H15 0.02 0.05
 S S

H24 -0.02 -0.05
 13 Orbital Energy 34.851450 Occupation 1.000000
 XX YY ZZ XY XZ YZ XX ZZ XY XZ

Ir1 -0.16 -0.09 0.25 -0.38 0.68 0.13 -0.06 0.09 -0.14 0.25
 S S

H10 0.02 0.05
 S S

H11 -0.02 -0.06
 S S

H15 0.02 0.07
 S S

H20 0.02 0.06
 S S
 H23 -0.02 -0.06
 14 Orbital Energy 24.506180 Occupation 1.000000
 S S S X Y Z X Y Z Z XX YY
 Ir1 0.10 -0.06 -0.15 0.04 -0.03 -0.13 -0.08 0.07 0.13 -0.05 0.08 0.13
 ZZ XZ YZ ZZ
 Ir1 -0.21 0.09 -0.07 -0.05
 S S
 H5 -0.06 0.10
 S S X Y Z S X Y Z
 O6 0.09 -0.19 0.11 -0.25 -0.43 -0.22 0.06 -0.17 -0.31
 S S
 H7 0.01 0.08
 15 Orbital Energy 22.338644 Occupation 1.000000
 S S S Y Y XX YY ZZ YZ
 Ir1 0.11 -0.06 -0.08 0.14 -0.08 0.11 -0.20 0.09 0.06
 S S X Y Z S Y Z
 N9 0.12 -0.25 -0.05 0.44 -0.17 -0.36 0.32 -0.13
 S S
 H10 0.02 0.06
 S S
 H11 0.02 0.06
 S S
 H12 0.01 0.06
 16 Orbital Energy 22.014161 Occupation 1.000000
 S S S Z Z XX YY ZZ XZ YZ
 Ir1 0.11 -0.06 -0.06 0.14 -0.09 0.09 0.09 -0.18 0.09 -0.06
 S S X Y Z S X Z
 N13 0.12 -0.25 -0.12 0.06 0.45 -0.35 -0.09 0.33
 S S
 H14 0.01 0.06
 S S
 H15 0.01 0.06
 S S
 H16 0.02 0.06
 17 Orbital Energy 31.956493 Occupation 1.000000
 S S S X X X XX YY ZZ XY XZ XX
 Ir1 0.13 -0.08 -0.16 -0.18 0.25 -0.08 -0.29 0.16 0.13 -0.10 -0.12 -0.09
 S S X Y Z S X Z
 C17 0.11 -0.21 -0.37 -0.07 -0.08 -0.27 -0.23 -0.06
 S S
 H18 0.01 0.06
 S S
 H19 0.02 0.07
 S S
 H20 0.02 0.08
 X X

C21 -0.05 -0.06
 18 Orbital Energy 31.763728 Occupation 1.000000
 S S S X Z X Z X XX YY ZZ XY
 Ir1 0.13 -0.08 -0.15 0.18 0.04 -0.25 -0.06 0.08 -0.28 0.15 0.14 -0.09
 XZ XX
 Ir1 -0.11 -0.08
 X X
 C17 0.05 0.06
 S S X Y Z S X Z
 C21 0.11 -0.21 0.37 0.07 0.08 -0.28 0.24 0.05
 S S
 H22 0.02 0.07
 S S
 H23 0.01 0.07
 S S
 H24 0.02 0.08
 19 Orbital Energy 25.309829 Occupation 1.000000
 S S S Y Z Y Z Y
 Ir1 -0.02 0.02 0.10 -0.02 -0.01 -0.01 -0.06 0.06
 S S Y S Y
 C2 -0.02 0.03 0.03 0.13 0.06
 S S
 H5 -0.13 -0.20
 S S Y Z S Y Z
 O6 0.11 -0.23 0.52 -0.10 -0.28 0.36 -0.07
 20 Orbital Energy 25.642136 Occupation 1.000000
 S S S Y Y Y XX YY ZZ XY YZ XX
 Ir1 0.11 -0.07 -0.12 -0.14 0.17 -0.05 0.11 -0.23 0.12 0.05 0.08 0.07
 YY
 Ir1 -0.11
 S S Y Z S Y Z
 C2 0.10 -0.18 -0.34 0.18 -0.24 -0.19 0.12
 S S
 H3 0.03 0.08
 S S
 H4 0.02 0.07
 S S
 H5 -0.22 -0.07
 S S Y Z S Y Z
 O6 -0.02 0.04 -0.05 0.04 0.10 -0.06 0.06
 S S
 H8 0.01 0.06
 S S Y S Y
 N9 -0.01 0.02 -0.03 0.07 -0.05
 21 Orbital Energy 25.070592 Occupation 1.000000
 X Z X Z Z YY ZZ
 Ir1 -0.02 0.00 0.06 0.00 0.08 -0.06 0.08
 S S S

C2 0.01 -0.01 -0.05
 S S
 H5 0.06 0.08
 S S X Y Z S X Y Z
 O6 0.15 -0.34 0.28 -0.15 0.36 -0.42 0.19 -0.10 0.26
 S S
 H7 0.06 0.08
 22 Orbital Energy 18.079583 Occupation 1.000000
 S S X Y Z S X
 O6 0.10 -0.21 -0.45 -0.09 0.06 -0.14 -0.23
 S S
 H7 -0.31 -0.16
 23 Orbital Energy 17.769723 Occupation 1.000000
 S S X Z S Z
 N9 0.10 -0.21 -0.07 0.43 -0.19 0.24
 S S
 H12 -0.32 -0.14
 24 Orbital Energy 16.771075 Occupation 1.000000
 S S X Y Z S X Y Z
 N13 0.10 -0.21 0.40 0.17 -0.08 -0.19 0.21 0.09 -0.06
 S S
 H15 -0.32 -0.15
 25 Orbital Energy 16.743574 Occupation 1.000000
 S S X Y Z S X Y Z
 N13 0.10 -0.21 -0.29 0.20 -0.26 -0.18 -0.15 0.10 -0.15
 S S
 H14 -0.32 -0.15
 26 Orbital Energy 17.682161 Occupation 1.000000
 S S X Y Z S X Y
 N9 0.10 -0.21 0.40 -0.15 -0.08 -0.18 0.21 -0.09
 S S
 H11 -0.32 -0.16
 27 Orbital Energy 17.635095 Occupation 1.000000
 S S X Y Z S X Y Z
 N9 0.10 -0.21 -0.28 -0.27 -0.18 -0.18 -0.14 -0.15 -0.09
 S S
 H10 -0.32 -0.16
 28 Orbital Energy 16.574897 Occupation 1.000000
 S S Y Z S Y Z
 N13 -0.10 0.20 0.42 0.10 0.17 0.22 0.06
 S S
 H16 0.32 0.16
 29 Orbital Energy 21.777761 Occupation 1.000000
 S S X Z S X Z
 C2 0.10 -0.19 0.19 -0.33 -0.13 0.07 -0.15
 S S
 H4 0.02 0.06
 S S

H5 0.05 0.06
 S S
 H8 -0.32 -0.24
 30 Orbital Energy 25.975276 Occupation 1.000000
 S S Y Z S Y Z
 C17 -0.10 0.19 -0.22 -0.30 0.16 -0.10 -0.14
 S S
 H18 0.32 0.26
 S S
 H19 -0.02 -0.07
 S S
 H20 -0.01 -0.07
 31 Orbital Energy 24.446850 Occupation 1.000000
 S S X Y Z S X Z
 C21 -0.09 0.18 0.22 -0.12 -0.27 0.14 0.10 -0.11
 S S
 H22 0.32 0.29
 S S
 H23 -0.02 -0.06
 S S
 H24 -0.02 -0.07
 32 Orbital Energy 25.618576 Occupation 1.000000
 S S X Y Z S X Y Z
 C17 0.09 -0.18 0.17 0.16 -0.29 -0.13 0.08 0.06 -0.12
 S S
 H18 0.02 0.06
 S S
 H19 0.02 0.07
 S S
 H20 -0.33 -0.30
 33 Orbital Energy 25.192235 Occupation 1.000000
 S S X Y Z S X Y
 C17 0.09 -0.18 0.17 -0.32 0.07 -0.13 0.08 -0.13
 S S
 H18 0.02 0.06
 S S
 H19 -0.33 -0.31
 S S
 H20 0.02 0.07
 34 Orbital Energy 24.318340 Occupation 1.000000
 S S X Y Z S X Y Z
 C21 0.10 -0.18 -0.10 0.17 -0.32 -0.13 -0.05 0.06 -0.14
 S S
 H22 0.02 0.06
 S S
 H23 -0.32 -0.29
 S S
 H24 0.02 0.07

35 Orbital Energy 24.571066 Occupation 1.000000
 S S X Y S Y
 C21 0.09 -0.18 -0.06 -0.36 -0.13 -0.14
 S S
 H22 0.02 0.07
 S S
 H23 0.02 0.07
 S S
 H24 -0.33 -0.31
 36 Orbital Energy 22.515371 Occupation 1.000000
 S S X Y Z S X Y
 C2 0.10 -0.19 -0.36 0.10 -0.06 -0.17 -0.15 0.05
 S S
 H3 0.02 0.06
 S S
 H4 -0.32 -0.25
 S S
 H8 0.02 0.05
 37 Orbital Energy 22.216400 Occupation 1.000000
 Y Y YY
 Ir1 0.02 -0.05 0.07
 S S X Y Z S X Y Z
 C2 0.10 -0.19 0.17 0.25 0.22 -0.17 0.07 0.11 0.09
 S S
 H3 -0.32 -0.25
 S S
 H4 0.02 0.06
 38 Orbital Energy 0.000000 Occupation 0.000000
 XX ZZ XZ YZ
 N9 0.11 -0.08 -0.12 -0.07
 X Z
 H10 0.09 -0.07
 Y
 H11 -0.05
 X
 H12 0.11
 X X XX YY XY
 N13 -0.01 -0.07 0.14 -0.11 -0.50
 S Y Z
 H14 0.08 -0.05 -0.20
 S X Y Z
 H15 -0.05 -0.18 0.25 0.05
 X
 H16 -0.34
 YY ZZ
 C17 -0.07 0.07
 39 Orbital Energy 0.000000 Occupation 0.000000
 XX YY ZZ XZ YZ

N9 -0.15 0.05 0.10 0.12 0.09
 X Z
 H10 -0.10 0.10
 Y
 H11 0.08
 X Y
 H12 -0.12 -0.06
 XX YY XY
 N13 0.15 -0.13 -0.13
 Y Z
 H14 0.06 -0.07
 Y
 H15 0.14
 X
 H16 -0.09
 Y Y YY ZZ XZ YZ
 C17 -0.01 -0.07 0.36 -0.35 0.07 0.06
 Y Z
 H18 -0.24 0.15
 S X Y Z
 H19 0.05 0.14 -0.07 0.13
 X Y
 H20 -0.08 -0.22
 YY ZZ XY
 C21 -0.17 0.18 0.09
 Y Z
 H22 0.12 -0.06
 X Y
 H23 -0.08 0.11
 X Y
 H24 0.08 0.06

Ir(2NH3)(2CH3)(CH3)(H2O)

Gas phase Energy: -414.00493681908 hartrees

Zero Point Energy: 132.582 kcal/mol

Coordinates:

Ir1	-.4824351012	.1571166408	.0091024514
C2	-.1850735077	-1.8444321699	.4985964876
H3	-1.1239611980	-2.4012842137	.6391133424
H4	.3760843202	-2.3813330685	-.2880671791
H5	-.3078460941	-1.0191498770	-2.2611109394
O6	.1913136164	-.2239145411	-2.0195458719
H7	1.1036724373	-.5108418491	-1.8490748094
H8	.4204267699	-1.9765086714	1.4127643134
N9	-.7618286997	2.2948194251	-.6718808383
H10	-.1545099663	2.9611737310	-.1990192377
H11	-1.7263791336	2.6124262253	-.6011215698

H12	-.5131803427	2.3070687578	-1.6594437535
N13	-1.0852618764	.4215091340	1.9736733876
H14	-.6501879035	-.3090839061	2.5394514175
H15	-2.0974361852	.3115308622	2.0547251251
H16	-.8211311108	1.3161362701	2.3832864704
C17	-2.5354175109	-.2586986451	-.5450839911
H18	-2.6353049775	-1.0118934180	-1.3484214528
H19	-3.1033622017	.6232488773	-.9004730323
H20	-3.1288751082	-.6755484193	.2915861541
C21	1.5811807375	.5957506550	.5272578958
H22	2.3143761966	.2346999168	-.2247296381
H23	1.9050543732	.1244922730	1.4703477793
H24	1.8049846163	1.6749984982	.6348808535

Orbital coefficients:

1 Orbital Energy	1.000000	Occupation	1.000000
S			
O6	-.99		
2 Orbital Energy	2.000000	Occupation	1.000000
S			
N13	-1.00		
3 Orbital Energy	3.000000	Occupation	1.000000
S			
N9	-1.00		
4 Orbital Energy	4.000000	Occupation	1.000000
S			
C2	-1.00		
5 Orbital Energy	5.000000	Occupation	1.000000
S			
C21	-1.00		
6 Orbital Energy	6.000000	Occupation	1.000000
S			
C17	-1.00		
7 Orbital Energy	7.000000	Occupation	1.000000
S			
Ir1	1.01		
8 Orbital Energy	8.000000	Occupation	1.000000
X Y Z			
Ir1	-.31 .09 .95		
9 Orbital Energy	9.000000	Occupation	1.000000
X Y Z			
Ir1	.17 -.97 .15		
10 Orbital Energy	10.000000	Occupation	1.000000
X Y Z			
Ir1	.94 .21 .28		
11 Orbital Energy	33.748382	Occupation	1.000000
XX YY ZZ XY XZ YZ XX ZZ XY XZ YZ			
Ir1	.31 .13 -.44 -.35 -.44 .40 .12 -.16 -.13 -.17 .16		

```

      S  S
H4   -.02 -.06
      S  S
H14  .03 .09
      S  S
H15  -.02 -.06
    12 Orbital Energy 33.827692 Occupation 1.000000
      XX YY ZZ XZ YZ XX YY XZ YZ
Ir1  -.29 .22 .07 .46 .61 -.12 .09 .18 .24
      S  S
H15  .02 .07
      S  S
H16  -.03 -.08
      S  S
H22  .02 .05
    13 Orbital Energy 35.578024 Occupation 1.000000
      XX YY ZZ XY XZ YZ XX YY ZZ XY XZ YZ
Ir1  .13 -.28 .15 -.69 .30 -.18 .05 -.11 .06 -.26 .11 -.07
      S  S
H3   .02 .07
      S  S
H8   -.02 -.06
      S  S
H10  .02 .06
      S  S
H11  -.02 -.06
      S  S
H19  -.02 -.07
      S  S
H23  -.02 -.05
      S  S
H24  .02 .07
    14 Orbital Energy 20.907758 Occupation 1.000000
      S S S Y Z Y Z XX YY ZZ XZ
Ir1  .08 -.04 -.10 -.03 -.11 .05 .08 .06 .06 -.12 .07
      S  S
H5   .01 .07
      S S X Y Z S X Y Z
O6   .11 -.25 .18 -.13 -.48 -.30 .12 -.08 -.33
      S  S
H7   .01 .08
    15 Orbital Energy 22.028698 Occupation 1.000000
      S S S Z Z XX YY ZZ XZ YZ
Ir1  .12 -.07 -.06 .14 -.07 .09 .11 -.20 .12 -.06
      S S X Z S X Z
N13  .12 -.25 -.14 .45 -.35 -.10 .33
      S  S
H14  .01 .05

```

```

      S S
H15   .01 .06
      S S
H16   .02 .06
      16 Orbital Energy 29.584504 Occupation 1.000000
      S S S Y Y Y XX YY ZZ XY YZ XX
Ir1   .15 -.10 -.15 -.15 .17 -.06 .19 -.36 .17 .09 .16 .08
      YY
Ir1   -.11
      S S X Y Z S Y
C2    .11 -.20 .06 -.37 .09 -.25 -.22
      S S
H3    .01 .07
      S S
H4    .02 .07
      S S
H8    .02 .07
      S S Y S Y
N9    -.01 .03 -.04 .06 -.05
      17 Orbital Energy 31.592582 Occupation 1.000000
      S S S X Z X Z X XX YY ZZ XY
Ir1   -.13 .09 .15 .17 .05 -.23 -.06 .09 .26 -.13 -.13 .10
      XZ XX
Ir1   .13 .08
      S S X Y Z S X Y Z
C17   -.11 .21 .37 .08 .10 .29 .24 .06 .06
      S S
H18   -.02 -.07
      S S
H19   -.02 -.08
      S S
H20   -.01 -.07
      X X
C21   .04 .06
      18 Orbital Energy 31.484078 Occupation 1.000000
      S S S X Y Z X Y Z X XX YY
Ir1   -.13 .08 .15 -.17 -.03 -.05 .24 .05 .06 -.08 .26 -.13
      ZZ XY XZ XX
Ir1   -.13 .10 .13 .08
      X X
C17   -.04 -.06
      S S X Y Z S X Z
C21   -.11 .21 -.37 -.08 -.09 .29 -.24 -.06
      S S
H22   -.02 -.07
      S S
H23   -.01 -.06
      S S

```

H24 -.02 -.07
 19 Orbital Energy 24.508487 Occupation 1.000000
 S S S Y Y XX YY YZ
 Ir1 .08 -.04 -.08 .13 -.12 .07 -.12 .06
 S S X Y Z S Y Z
 N9 .12 -.26 -.05 .44 -.18 -.37 .33 -.14
 S S
 H10 .01 .06
 S S
 H11 .01 .06
 S S
 H12 .01 .06
 20 Orbital Energy 21.767576 Occupation 1.000000
 Z Z Z
 Ir1 .01 -.01 .05
 S S Y Z S Y Z
 O6 .14 -.31 -.39 .35 -.37 -.27 .26
 21 Orbital Energy 15.895347 Occupation 1.000000
 S S X Y S X Y
 O6 .10 -.22 -.45 .14 -.15 -.23 .08
 S S
 H7 -.31 -.13
 22 Orbital Energy 15.806413 Occupation 1.000000
 S S
 H5 -.31 -.13
 S S X Y Z S X Y Z
 O6 .10 -.22 .23 .38 .15 -.15 .11 .21 .07
 23 Orbital Energy 17.431210 Occupation 1.000000
 S S X Y Z S X Y Z
 N13 .10 -.21 -.19 .31 -.24 -.18 -.09 .16 -.14
 S S
 H14 -.32 -.15
 24 Orbital Energy 17.304925 Occupation 1.000000
 S S X S X
 N13 .10 -.21 .43 -.19 .23
 S S
 H15 -.32 -.15
 25 Orbital Energy 16.767805 Occupation 1.000000
 S S X Y Z S X Y Z
 N13 .10 -.21 -.11 -.39 -.17 -.18 -.05 -.20 -.09
 S S
 H16 -.32 -.16
 26 Orbital Energy 18.880547 Occupation 1.000000
 S S X Z S X Z
 N9 .10 -.20 -.11 .42 -.18 -.05 .22
 S S
 H12 -.32 -.16
 27 Orbital Energy 18.492581 Occupation 1.000000

	S	S	X	Y	S	X	Y		
N9	.10	-.20	.41	-.14	-.17	.21	-.09		
	S	S							
H10	.03	.05							
	S	S							
H11	-.32	-.16							
	28 Orbital Energy 18.444299 Occupation 1.000000								
	S	S	X	Y	Z	S	X	Y	Z
N9	.10	-.20	-.25	-.28	-.20	-.17	-.12	-.16	-.10
	S	S							
H10	-.32	-.16							
	S	S							
H11	.03	.05							
	29 Orbital Energy 23.428622 Occupation 1.000000								
	S	S	X	Y	Z	S	X	Y	Z
C2	.09	-.18	-.19	.16	.27	-.13	-.07	.07	.12
	S	S							
H3	.02	.06							
	S	S							
H4	-.33	-.30							
	S	S							
H8	.01	.06							
	30 Orbital Energy 24.128938 Occupation 1.000000								
	S	S	X	Z	S	X	Z		
C2	.10	-.18	-.20	-.31	-.14	-.08	-.14		
	S	S							
H3	.02	.07							
	S	S							
H4	.02	.06							
	S	S							
H8	-.32	-.29							
	31 Orbital Energy 24.443444 Occupation 1.000000								
	S	S	X	Y	S	X	Y		
C2	.10	-.19	.33	.18	-.16	.13	.09		
	S	S							
H3	-.32	-.27							
	S	S							
H4	.02	.07							
	S	S							
H8	.02	.07							
	32 Orbital Energy 24.838177 Occupation 1.000000								
	S	S	X	Y	Z	S	X	Z	
C21	.09	-.18	-.23	.12	.26	-.13	-.10	.11	
	S	S							
H22	-.32	-.31							
	S	S							
H23	.02	.06							
	S	S							

H24 .02 .07
 33 Orbital Energy 25.660739 Occupation 1.000000
 S S X Y Z S X Z
 C17 .09 -.18 .19 .13 -.29 -.13 .09 -.12
 S S
 H18 .01 .06
 S S
 H19 .02 .07
 S S
 H20 -.32 -.30
 34 Orbital Energy 25.400070 Occupation 1.000000
 S S X Y Z S X Y Z
 C21 .10 -.18 -.10 .16 -.32 -.14 -.06 .06 -.14
 S S
 H22 .01 .07
 S S
 H23 -.32 -.29
 S S
 H24 .02 .07
 35 Orbital Energy 25.422153 Occupation 1.000000
 S S Y Z S Y Z
 C17 .09 -.18 .25 .27 -.13 .10 .12
 S S
 H18 -.32 -.29
 S S
 H19 .02 .07
 S S
 H20 .01 .06
 36 Orbital Energy 25.541372 Occupation 1.000000
 S S X Y Z S X Y
 C17 .09 -.18 .17 -.30 .12 -.13 .08 -.12
 S S
 H18 .02 .07
 S S
 H19 -.32 -.31
 S S
 H20 .02 .07
 37 Orbital Energy 25.085577 Occupation 1.000000
 S S X Y S Y
 C21 .09 -.18 -.06 -.36 -.13 -.15
 S S
 H22 .02 .07
 S S
 H23 .02 .07
 S S
 H24 -.32 -.31
 38 Orbital Energy .000000 Occupation .000000
 XX ZZ XZ

N9 .10 -.11 -.30
 X Y Z
 H10 .06 .10 -.10
 Z
 H11 .17
 X Z
 H12 .21 .06
 Y Y XX YY XY XZ
 N13 -.01 -.06 -.10 .11 .42 -.07
 S X Y Z
 H14 -.06 -.16 -.13 .10
 Y Z
 H15 -.30 .05
 S X Y Z
 H16 .06 .14 -.08 -.12
 YY ZZ YZ
 C21 -.06 .06 .05
 39 Orbital Energy .000000 Occupation .000000
 XX ZZ
 C2 .07 -.07
 X
 H8 .05
 XX ZZ XY XZ YZ
 N9 -.15 .13 -.07 .15 .08
 X Z
 H10 -.08 .12
 Y Z
 H11 .09 -.06
 X Y
 H12 -.14 -.06
 XX YY XY
 N13 -.07 .07 .22
 X Y
 H14 -.09 -.06
 Y
 H15 -.16
 X Y Z
 H16 .07 -.05 -.06
 Y Y YY ZZ XZ YZ
 C17 .01 .05 -.25 .22 -.08 .11
 Y Z
 H18 .16 -.09
 X Z
 H19 -.12 -.05
 Y
 H20 .18
 Y Y YY ZZ XY XZ
 C21 .00 -.06 .26 -.26 -.09 .08

	X	Y	Z
H22	.10	-.15	.06
	X	Y	Z
H23	.10	-.17	-.08
	X	Y	Z
H24	-.10	-.09	-.06

-
- ¹ Jaguar 6.0, Schrodinger, Inc., Portland, Oregon, 2004, Jaguar 6.5, Schrodinger, Inc., Portland, Oregon, 2005.
 - ² Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.
 - ³ Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.
 - ⁴ Baker, J.; Muir, M.; Andzelm, J.; Scheiner, A. In *Chemical Applications of Density-Functional Theory*; Laird, B. B., Ross, R. B., Ziegler, T., Eds.; ACS Symposium Series 629; American Chemical Society: Washington, DC, 1996.
 - ⁵ Niu, S.; Hall, B. M. *Chem. Rev.* **2000**, *100*, 353.
 - ⁶ (a) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299. b) Goddard, W. A., III *Phys. Rev.* **1968**, *174*, 659. (b) Melius, C. F.; Olafson, B. O.; Goddard, W. A., III *Chem. Phys. Lett.* **1974**, *28*, 457.
 - ⁷ (a) Hariharan, P. C.; Pople, J. A. *Chem. Phys. Lett.* **1972**, *16*, 217. (b) Francl, M. M.; Pietro, W. J.; Hehre, W. J.; Binkley, J. S.; Gordon, M. S.; DeFrees, D. J.; Pople, J. A. *J. Chem. Phys.* **1982**, *77*, 3654.
 - ⁸ Skodje, R. T.; Truhlar, D. G. *J. Phys. Chem.* **1981**, *85*, 624.