Supplementary Information for

Theory-Assisted Development of a Robust and Z-Selective Olefin Metathesis Catalyst

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Table of contents

Analytical results

NMR and HRMS (ESI^+) spectra of complex 5a.

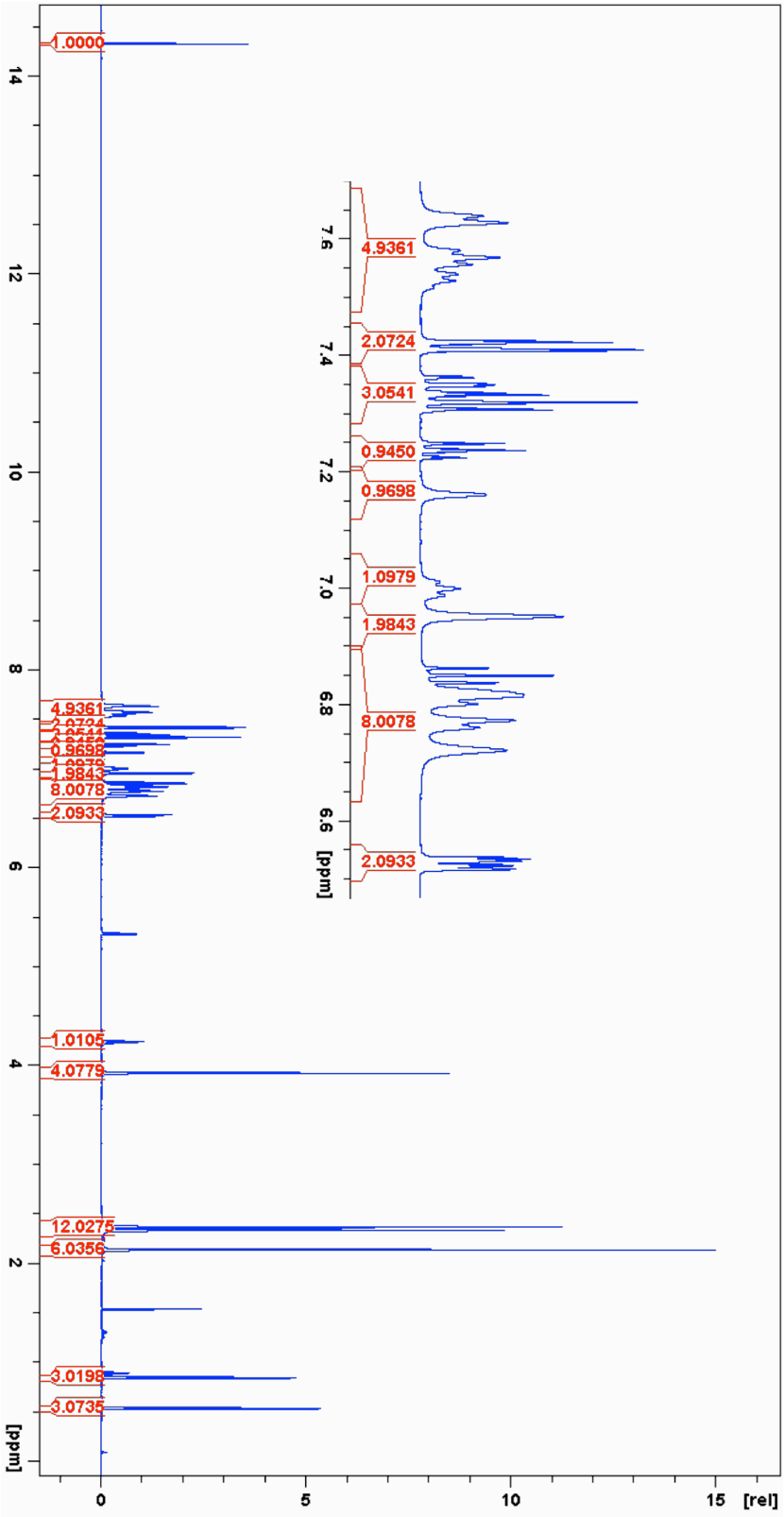

Figure S1. ^1H NMR (600.17 MHz, CD_2Cl_2) spectrum of complex 5a.

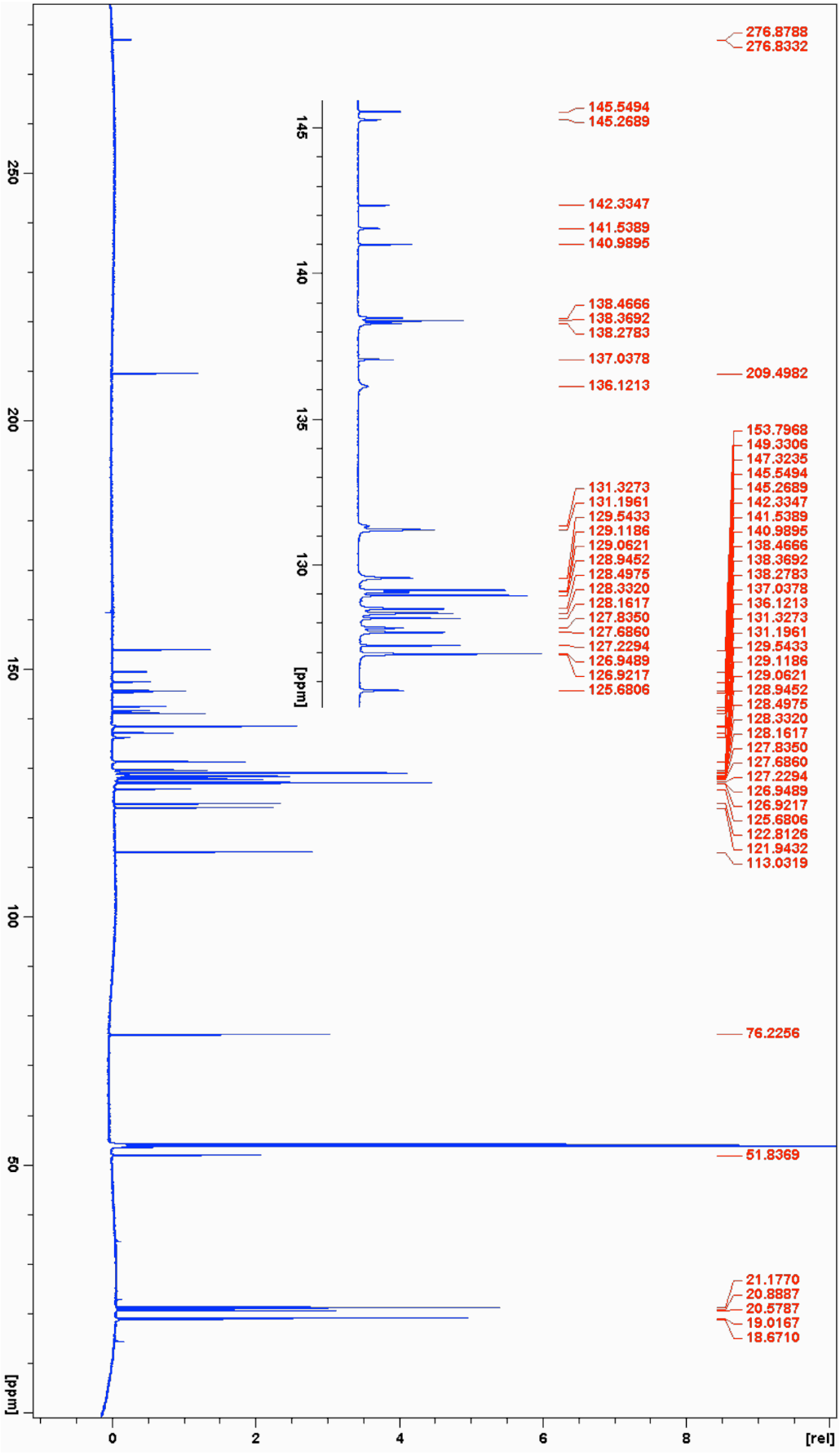

Figure S2. ^{13}C NMR (150.91 MHz, CD_2Cl_2) spectrum of complex **5a**.

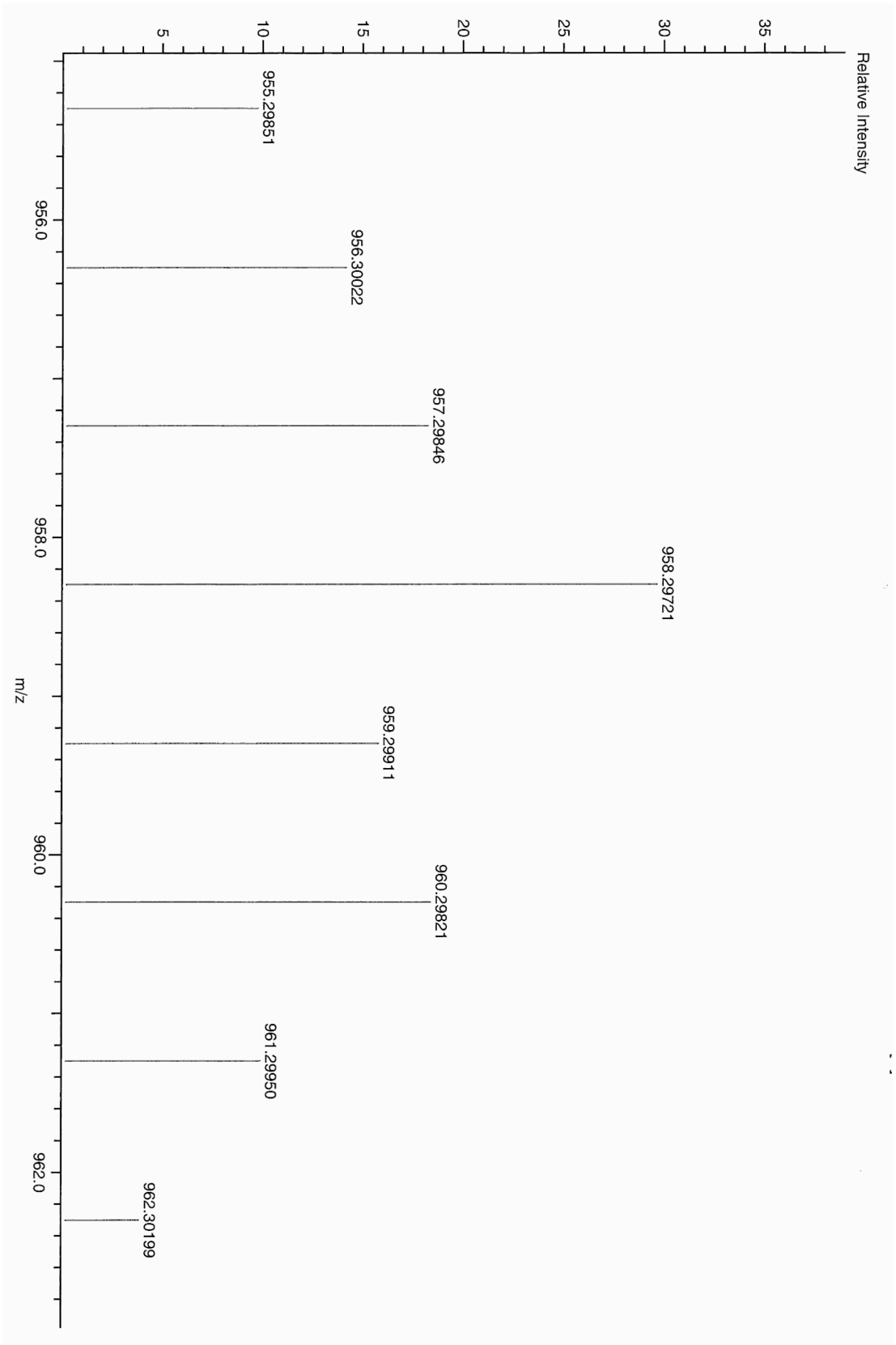

Figure S3. HRMS (ESI^+) spectrum of complex 5a, molecular ion $[M+Na]^+$ peaks.

X-ray crystallographic data for complex 5a

Table S1. Crystal data and structure refinement for complex 5a.

Empirical formula	$C_{57}\ H_{57}\ Cl_2\ N_3\ O_2\ Ru\ S$	
Formula weight	1020.08	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 12.4372(12) Å	α= 90°.
	b = 11.7065(11) Å	β= 95.4840(10)°.
	c = 34.327(3) Å	γ = 90°.
Volume	4975.0(8) $Å^3$	
Z	4	
Density (calculated)	1.362 Mg/m^3	
Absorption coefficient	0.510 mm^{-1}	
F(000)	2120	
Crystal colour/habit	Dark purple/Flat pinacoid prism	
Crystal size	0.449 x 0.292 x 0.228 mm^3	
Theta range for data collection	1.802 to 30.597°.	
Index ranges	–17<=h<=17, –16<=k<=16, – 49<=l<=49	
Reflections collected	81198	
Independent reflections	15194 [R(int) = 0.0582]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Numerical by face indexing	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	15194 / 0 / 606
Goodness-of-fit on F^2	1.138
Final R indices [I>2sigma(I)]	R1 = 0.0537, wR2 = 0.1330
R indices (all data)	R1 = 0.0605, wR2 = 0.1369
Extinction coefficient	n/a
Largest diff. peak and hole	1.746 and –1.650 e.$Å^{-3}$

Table S2. Bond lengths [Å] and angles [°] for complex 5a.

Ru(1)-C(27)	1.834(2)
Ru(1)-C(36)	1.991(2)
Ru(1)-N(1)	2.049(2)
Ru(1)-O(1)	2.2272(17)
Ru(1)-S(1)	2.3091(6)
S(1)-C(1)	1.787(2)
O(1)-C(25)	1.377(3)
O(1)-C(32)	1.475(3)
N(1)-C(35)	1.163(4)
C(1)-C(6)	1.420(3)
C(1)-C(2)	1.421(3)
Cl(1)-C(57)	1.733(4)
O(2)-C(35)	1.207(4)
N(2)-C(36)	1.357(3)
N(2)-C(37)	1.430(3)
N(2)-C(46)	1.466(3)
C(2)-C(3)	1.406(3)
C(2)-C(19)	1.492(3)
Cl(2)-C(57)	1.693(5)
N(3)-C(36)	1.349(3)
N(3)-C(48)	1.429(3)
N(3)-C(47)	1.476(3)
C(3)-C(4)	1.391(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.393(3)
C(4)-C(13)	1.485(3)
C(5)-C(6)	1.398(3)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.491(3)
C(7)-C(12)	1.397(3)
C(7)-C(8)	1.399(3)
C(8)-C(9)	1.392(3)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.389(4)
C(9)-H(9A)	0.9500
C(10)-C(11)	1.385(4)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.395(3)
C(11)-H(11A)	0.9500
C(12)-H(12A)	0.9500
C(13)-C(14)	1.397(4)
C(13)-C(18)	1.404(4)
C(14)-C(15)	1.393(4)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.381(5)
C(15)-H(15A)	0.9500
C(16)-C(17)	1.388(5)
C(16)-H(16A)	0.9500
C(17)-C(18)	1.389(4)
C(17)-H(17A)	0.9500
C(18)-H(18A)	0.9500
C(19)-C(24)	1.399(4)
C(19)-C(20)	1.401(4)
C(20)-C(21)	1.389(4)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.387(5)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.380(5)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.395(4)
C(23)-H(23A)	0.9500
C(24)-H(24A)	0.9500
C(25)-C(31)	1.387(3)
C(25)-C(26)	1.401(3)
C(26)-C(28)	1.405(3)
C(26)-C(27)	1.453(3)
C(27)-H(27)	0.94(3)
C(28)-C(29)	1.383(4)

C(28)-H(28A)	0.9500
C(29)-C(30)	1.382(5)
C(29)-H(29A)	0.9500
C(30)-C(31)	1.396(4)
C(30)-H(30A)	0.9500
C(31)-H(31A)	0.9500
C(32)-C(34)	1.515(4)
C(32)-C(33)	1.519(4)
C(32)-H(32A)	1.0000
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(37)-C(42)	1.398(3)
C(37)-C(38)	1.402(4)
C(38)-C(39)	1.389(4)
C(38)-C(45)	1.508(3)
C(39)-C(40)	1.392(4)
C(39)-H(39A)	0.9500
C(40)-C(41)	1.384(4)
C(40)-C(44)	1.510(4)
C(41)-C(42)	1.398(4)
C(41)-H(41A)	0.9500
C(42)-C(43)	1.502(4)
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-C(47)	1.524(4)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900
C(48)-C(49)	1.396(4)
C(48)-C(53)	1.399(3)
C(49)-C(50)	1.396(4)
C(49)-C(56)	1.502(4)
C(50)-C(51)	1.387(4)
C(50)-H(50A)	0.9500
C(51)-C(52)	1.397(4)
C(51)-C(55)	1.507(4)
C(52)-C(53)	1.390(4)
C(52)-H(52A)	0.9500
C(53)-C(54)	1.505(3)
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(55)-H(55A)	0.9800
C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800
C(56)-H(56A)	0.9800
C(56)-H(56B)	0.9800
C(56)-H(56C)	0.9800
C(57)-H(57A)	0.9900
C(57)-H(57B)	0.9900

C(27)-Ru(1)-C(36)	100.44(10)
C(27)-Ru(1)-N(1)	99.10(10)
C(36)-Ru(1)-N(1)	90.42(9)
C(27)-Ru(1)-O(1)	80.27(9)
C(36)-Ru(1)-O(1)	174.09(8)
N(1)-Ru(1)-O(1)	83.67(8)
C(27)-Ru(1)-S(1)	104.19(8)

C(36)-Ru(1)-S(1)	91.31(7)
N(1)-Ru(1)-S(1)	155.92(7)
O(1)-Ru(1)-S(1)	94.21(5)
C(1)-S(1)-Ru(1)	110.03(8)
C(25)-O(1)-C(32)	119.38(18)
C(25)-O(1)-Ru(1)	110.43(14)
C(32)-O(1)-Ru(1)	128.07(14)
C(35)-N(1)-Ru(1)	169.1(2)
C(6)-C(1)-C(2)	118.2(2)
C(6)-C(1)-S(1)	118.72(18)
C(2)-C(1)-S(1)	123.07(18)
C(36)-N(2)-C(37)	123.9(2)
C(36)-N(2)-C(46)	114.3(2)
C(37)-N(2)-C(46)	121.2(2)
C(3)-C(2)-C(1)	118.9(2)
C(3)-C(2)-C(19)	116.6(2)
C(1)-C(2)-C(19)	124.3(2)
C(36)-N(3)-C(48)	129.3(2)
C(36)-N(3)-C(47)	113.5(2)
C(48)-N(3)-C(47)	117.2(2)
C(4)-C(3)-C(2)	122.7(2)
C(4)-C(3)-H(3A)	118.7
C(2)-C(3)-H(3A)	118.7
C(3)-C(4)-C(5)	117.5(2)
C(3)-C(4)-C(13)	120.8(2)
C(5)-C(4)-C(13)	121.5(2)
C(4)-C(5)-C(6)	122.1(2)
C(4)-C(5)-H(5A)	119.0
C(6)-C(5)-H(5A)	119.0
C(5)-C(6)-C(1)	119.7(2)
C(5)-C(6)-C(7)	116.6(2)
C(1)-C(6)-C(7)	123.3(2)
C(12)-C(7)-C(8)	118.7(2)
C(12)-C(7)-C(6)	121.0(2)
C(8)-C(7)-C(6)	119.5(2)
C(9)-C(8)-C(7)	120.3(2)
C(9)-C(8)-H(8A)	119.8
C(7)-C(8)-H(8A)	119.8
C(10)-C(9)-C(8)	120.5(2)
C(10)-C(9)-H(9A)	119.8
C(8)-C(9)-H(9A)	119.8
C(11)-C(10)-C(9)	119.6(2)
C(11)-C(10)-H(10A)	120.2
C(9)-C(10)-H(10A)	120.2
C(10)-C(11)-C(12)	120.1(2)
C(10)-C(11)-H(11A)	119.9
C(12)-C(11)-H(11A)	119.9
C(11)-C(12)-C(7)	120.7(2)
C(11)-C(12)-H(12A)	119.7
C(7)-C(12)-H(12A)	119.7
C(14)-C(13)-C(18)	118.2(2)
C(14)-C(13)-C(4)	121.0(2)
C(18)-C(13)-C(4)	120.8(2)
C(15)-C(14)-C(13)	120.8(3)
C(15)-C(14)-H(14A)	119.6
C(13)-C(14)-H(14A)	119.6
C(16)-C(15)-C(14)	120.4(3)
C(16)-C(15)-H(15A)	119.8
C(14)-C(15)-H(15A)	119.8
C(15)-C(16)-C(17)	119.6(3)
C(15)-C(16)-H(16A)	120.2
C(17)-C(16)-H(16A)	120.2
C(16)-C(17)-C(18)	120.4(3)
C(16)-C(17)-H(17A)	119.8
C(18)-C(17)-H(17A)	119.8
C(17)-C(18)-C(13)	120.7(3)
C(17)-C(18)-H(18A)	119.7
C(13)-C(18)-H(18A)	119.7
C(24)-C(19)-C(20)	118.1(2)
C(24)-C(19)-C(2)	121.4(2)

C(20)-C(19)-C(2)	120.1(2)
C(21)-C(20)-C(19)	120.9(3)
C(21)-C(20)-H(20A)	119.5
C(19)-C(20)-H(20A)	119.5
C(22)-C(21)-C(20)	120.2(3)
C(22)-C(21)-H(21A)	119.9
C(20)-C(21)-H(21A)	119.9
C(23)-C(22)-C(21)	119.7(3)
C(23)-C(22)-H(22A)	120.2
C(21)-C(22)-H(22A)	120.2
C(22)-C(23)-C(24)	120.5(3)
C(22)-C(23)-H(23A)	119.7
C(24)-C(23)-H(23A)	119.7
C(23)-C(24)-C(19)	120.5(3)
C(23)-C(24)-H(24A)	119.7
C(19)-C(24)-H(24A)	119.7
O(1)-C(25)-C(31)	125.4(2)
O(1)-C(25)-C(26)	113.1(2)
C(31)-C(25)-C(26)	121.6(2)
C(25)-C(26)-C(28)	118.4(2)
C(25)-C(26)-C(27)	118.5(2)
C(28)-C(26)-C(27)	123.1(2)
C(26)-C(27)-Ru(1)	117.55(17)
C(26)-C(27)-H(27)	114(2)
Ru(1)-C(27)-H(27)	129(2)
C(29)-C(28)-C(26)	120.4(3)
C(29)-C(28)-H(28A)	119.8
C(26)-C(28)-H(28A)	119.8
C(30)-C(29)-C(28)	120.0(3)
C(30)-C(29)-H(29A)	120.0
C(28)-C(29)-H(29A)	120.0
C(29)-C(30)-C(31)	121.1(3)
C(29)-C(30)-H(30A)	119.4
C(31)-C(30)-H(30A)	119.4
C(25)-C(31)-C(30)	118.4(3)
C(25)-C(31)-H(31A)	120.8
C(30)-C(31)-H(31A)	120.8
O(1)-C(32)-C(34)	106.17(19)
O(1)-C(32)-C(33)	111.5(2)
C(34)-C(32)-C(33)	111.6(2)
O(1)-C(32)-H(32A)	109.2
C(34)-C(32)-H(32A)	109.2
C(33)-C(32)-H(32A)	109.2
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(32)-C(34)-H(34A)	109.5
C(32)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(32)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
N(1)-C(35)-O(2)	178.2(4)
N(3)-C(36)-N(2)	106.7(2)
N(3)-C(36)-Ru(1)	133.16(18)
N(2)-C(36)-Ru(1)	119.78(17)
C(42)-C(37)-C(38)	120.7(2)
C(42)-C(37)-N(2)	120.0(2)
C(38)-C(37)-N(2)	119.2(2)
C(39)-C(38)-C(37)	118.7(2)
C(39)-C(38)-C(45)	119.7(2)
C(37)-C(38)-C(45)	121.4(2)
C(38)-C(39)-C(40)	121.3(3)
C(38)-C(39)-H(39A)	119.3
C(40)-C(39)-H(39A)	119.3
C(41)-C(40)-C(39)	118.6(3)
C(41)-C(40)-C(44)	120.8(3)

C(39)-C(40)-C(44)	120.5(3)
C(40)-C(41)-C(42)	121.8(2)
C(40)-C(41)-H(41A)	119.1
C(42)-C(41)-H(41A)	119.1
C(41)-C(42)-C(37)	118.1(2)
C(41)-C(42)-C(43)	119.8(2)
C(37)-C(42)-C(43)	122.0(3)
C(42)-C(43)-H(43A)	109.5
C(42)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(42)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(40)-C(44)-H(44A)	109.5
C(40)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(40)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(38)-C(45)-H(45A)	109.5
C(38)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(38)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
N(2)-C(46)-C(47)	102.2(2)
N(2)-C(46)-H(46A)	111.3
C(47)-C(46)-H(46A)	111.3
N(2)-C(46)-H(46B)	111.3
C(47)-C(46)-H(46B)	111.3
H(46A)-C(46)-H(46B)	109.2
N(3)-C(47)-C(46)	103.0(2)
N(3)-C(47)-H(47A)	111.2
C(46)-C(47)-H(47A)	111.2
N(3)-C(47)-H(47B)	111.2
C(46)-C(47)-H(47B)	111.2
H(47A)-C(47)-H(47B)	109.1
C(49)-C(48)-C(53)	121.5(2)
C(49)-C(48)-N(3)	119.3(2)
C(53)-C(48)-N(3)	119.0(2)
C(48)-C(49)-C(50)	118.2(2)
C(48)-C(49)-C(56)	120.8(2)
C(50)-C(49)-C(56)	121.0(2)
C(51)-C(50)-C(49)	121.9(2)
C(51)-C(50)-H(50A)	119.1
C(49)-C(50)-H(50A)	119.1
C(50)-C(51)-C(52)	118.4(2)
C(50)-C(51)-C(55)	121.1(3)
C(52)-C(51)-C(55)	120.4(2)
C(53)-C(52)-C(51)	121.6(2)
C(53)-C(52)-H(52A)	119.2
C(51)-C(52)-H(52A)	119.2
C(52)-C(53)-C(48)	118.4(2)
C(52)-C(53)-C(54)	120.9(2)
C(48)-C(53)-C(54)	120.7(2)
C(53)-C(54)-H(54A)	109.5
C(53)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(53)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(51)-C(55)-H(55A)	109.5
C(51)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
C(51)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
C(49)-C(56)-H(56A)	109.5
C(49)-C(56)-H(56B)	109.5
H(56A)-C(56)-H(56B)	109.5

C(49)-C(56)-H(56C)	109.5
H(56A)-C(56)-H(56C)	109.5
H(56B)-C(56)-H(56C)	109.5
Cl(2)-C(57)-Cl(1)	115.6(3)
Cl(2)-C(57)-H(57A)	108.4
Cl(1)-C(57)-H(57A)	108.4
Cl(2)-C(57)-H(57B)	108.4
Cl(1)-C(57)-H(57B)	108.4
H(57A)-C(57)-H(57B)	107.4

Table S3. Torsion angles [°] for complex 5a.

Ru(1)-S(1)-C(1)-C(6)	-106.85(18)
Ru(1)-S(1)-C(1)-C(2)	73.2(2)
C(6)-C(1)-C(2)-C(3)	9.5(3)
S(1)-C(1)-C(2)-C(3)	-170.54(18)
C(6)-C(1)-C(2)-C(19)	-165.0(2)
S(1)-C(1)-C(2)-C(19)	14.9(3)
C(1)-C(2)-C(3)-C(4)	-2.1(4)
C(19)-C(2)-C(3)-C(4)	172.8(2)
C(2)-C(3)-C(4)-C(5)	-4.1(4)
C(2)-C(3)-C(4)-C(13)	-178.3(2)
C(3)-C(4)-C(5)-C(6)	2.8(4)
C(13)-C(4)-C(5)-C(6)	176.9(2)
C(4)-C(5)-C(6)-C(1)	4.7(4)
C(4)-C(5)-C(6)-C(7)	-168.8(2)
C(2)-C(1)-C(6)-C(5)	-10.8(3)
S(1)-C(1)-C(6)-C(5)	169.24(18)
C(2)-C(1)-C(6)-C(7)	162.2(2)
S(1)-C(1)-C(6)-C(7)	-17.8(3)
C(5)-C(6)-C(7)-C(12)	-45.1(3)
C(1)-C(6)-C(7)-C(12)	141.7(2)
C(5)-C(6)-C(7)-C(8)	124.6(2)
C(1)-C(6)-C(7)-C(8)	-48.6(3)
C(12)-C(7)-C(8)-C(9)	1.3(3)
C(6)-C(7)-C(8)-C(9)	-168.6(2)
C(7)-C(8)-C(9)-C(10)	0.1(4)
C(8)-C(9)-C(10)-C(11)	-1.2(4)
C(9)-C(10)-C(11)-C(12)	1.0(4)
C(10)-C(11)-C(12)-C(7)	0.5(4)
C(8)-C(7)-C(12)-C(11)	-1.6(4)
C(6)-C(7)-C(12)-C(11)	168.1(2)
C(3)-C(4)-C(13)-C(14)	138.9(3)
C(5)-C(4)-C(13)-C(14)	-35.1(3)
C(3)-C(4)-C(13)-C(18)	-38.7(3)
C(5)-C(4)-C(13)-C(18)	147.4(2)
C(18)-C(13)-C(14)-C(15)	1.0(4)
C(4)-C(13)-C(14)-C(15)	-176.6(2)
C(13)-C(14)-C(15)-C(16)	-0.6(4)
C(14)-C(15)-C(16)-C(17)	-0.5(4)
C(15)-C(16)-C(17)-C(18)	1.3(4)
C(16)-C(17)-C(18)-C(13)	-0.8(4)
C(14)-C(13)-C(18)-C(17)	-0.3(4)
C(4)-C(13)-C(18)-C(17)	177.3(2)
C(3)-C(2)-C(19)-C(24)	-137.9(2)
C(1)-C(2)-C(19)-C(24)	36.7(3)
C(3)-C(2)-C(19)-C(20)	35.1(3)
C(1)-C(2)-C(19)-C(20)	-150.3(2)
C(24)-C(19)-C(20)-C(21)	-0.4(4)
C(2)-C(19)-C(20)-C(21)	-173.7(2)
C(19)-C(20)-C(21)-C(22)	0.4(4)
C(20)-C(21)-C(22)-C(23)	-0.2(4)
C(21)-C(22)-C(23)-C(24)	0.1(4)
C(22)-C(23)-C(24)-C(19)	-0.1(4)
C(20)-C(19)-C(24)-C(23)	0.3(4)
C(2)-C(19)-C(24)-C(23)	173.4(2)
C(32)-O(1)-C(25)-C(31)	-16.2(4)
Ru(1)-O(1)-C(25)-C(31)	179.0(2)
C(32)-O(1)-C(25)-C(26)	165.0(2)
Ru(1)-O(1)-C(25)-C(26)	0.2(2)
O(1)-C(25)-C(26)-C(28)	-177.8(2)
C(31)-C(25)-C(26)-C(28)	3.4(4)
O(1)-C(25)-C(26)-C(27)	2.9(3)
C(31)-C(25)-C(26)-C(27)	-176.0(2)
C(25)-C(26)-C(27)-Ru(1)	-5.3(3)
C(28)-C(26)-C(27)-Ru(1)	175.4(2)
C(36)-Ru(1)-C(27)-C(26)	-170.15(18)
N(1)-Ru(1)-C(27)-C(26)	-78.02(19)
O(1)-Ru(1)-C(27)-C(26)	3.89(18)
S(1)-Ru(1)-C(27)-C(26)	95.81(18)

C(25)-C(26)-C(28)-C(29)	-0.9(4)
C(27)-C(26)-C(28)-C(29)	178.4(3)
C(26)-C(28)-C(29)-C(30)	-1.6(5)
C(28)-C(29)-C(30)-C(31)	1.8(5)
O(1)-C(25)-C(31)-C(30)	178.1(3)
C(26)-C(25)-C(31)-C(30)	-3.2(4)
C(29)-C(30)-C(31)-C(25)	0.6(5)
C(25)-O(1)-C(32)-C(34)	178.0(2)
Ru(1)-O(1)-C(32)-C(34)	-20.3(3)
C(25)-O(1)-C(32)-C(33)	-60.3(3)
Ru(1)-O(1)-C(32)-C(33)	101.5(2)
C(48)-N(3)-C(36)-N(2)	176.2(2)
C(47)-N(3)-C(36)-N(2)	-2.8(3)
C(48)-N(3)-C(36)-Ru(1)	-11.4(4)
C(47)-N(3)-C(36)-Ru(1)	169.6(2)
C(37)-N(2)-C(36)-N(3)	-172.2(2)
C(46)-N(2)-C(36)-N(3)	-0.7(3)
C(37)-N(2)-C(36)-Ru(1)	14.2(3)
C(46)-N(2)-C(36)-Ru(1)	-174.33(18)
C(36)-N(2)-C(37)-C(42)	-100.0(3)
C(46)-N(2)-C(37)-C(42)	89.1(3)
C(36)-N(2)-C(37)-C(38)	84.3(3)
C(46)-N(2)-C(37)-C(38)	-86.6(3)
C(42)-C(37)-C(38)-C(39)	8.9(4)
N(2)-C(37)-C(38)-C(39)	-175.4(2)
C(42)-C(37)-C(38)-C(45)	-167.7(2)
N(2)-C(37)-C(38)-C(45)	8.0(3)
C(37)-C(38)-C(39)-C(40)	-2.3(4)
C(45)-C(38)-C(39)-C(40)	174.4(2)
C(38)-C(39)-C(40)-C(41)	-3.8(4)
C(38)-C(39)-C(40)-C(44)	178.5(3)
C(39)-C(40)-C(41)-C(42)	3.4(4)
C(44)-C(40)-C(41)-C(42)	-178.9(3)
C(40)-C(41)-C(42)-C(37)	3.0(4)
C(40)-C(41)-C(42)-C(43)	-172.7(2)
C(38)-C(37)-C(42)-C(41)	-9.2(4)
N(2)-C(37)-C(42)-C(41)	175.1(2)
C(38)-C(37)-C(42)-C(43)	166.4(2)
N(2)-C(37)-C(42)-C(43)	-9.3(4)
C(36)-N(2)-C(46)-C(47)	3.6(3)
C(37)-N(2)-C(46)-C(47)	175.3(2)
C(36)-N(3)-C(47)-C(46)	4.9(3)
C(48)-N(3)-C(47)-C(46)	-174.2(2)
N(2)-C(46)-C(47)-N(3)	-4.7(3)
C(36)-N(3)-C(48)-C(49)	97.5(3)
C(47)-N(3)-C(48)-C(49)	-83.6(3)
C(36)-N(3)-C(48)-C(53)	-88.1(3)
C(47)-N(3)-C(48)-C(53)	90.8(3)
C(53)-C(48)-C(49)-C(50)	0.3(4)
N(3)-C(48)-C(49)-C(50)	174.5(2)
C(53)-C(48)-C(49)-C(56)	178.2(2)
N(3)-C(48)-C(49)-C(56)	-7.6(4)
C(48)-C(49)-C(50)-C(51)	-0.4(4)
C(56)-C(49)-C(50)-C(51)	-178.3(3)
C(49)-C(50)-C(51)-C(52)	0.4(4)
C(49)-C(50)-C(51)-C(55)	-177.8(3)
C(50)-C(51)-C(52)-C(53)	-0.3(4)
C(55)-C(51)-C(52)-C(53)	177.9(2)
C(51)-C(52)-C(53)-C(48)	0.2(4)
C(51)-C(52)-C(53)-C(54)	-177.8(2)
C(49)-C(48)-C(53)-C(52)	-0.2(4)
N(3)-C(48)-C(53)-C(52)	-174.5(2)
C(49)-C(48)-C(53)-C(54)	177.8(2)
N(3)-C(48)-C(53)-C(54)	3.6(3)

Complex decomposition in CD_2Cl_2 solution at room temperature

Decomposition of 3a and 5a in presence of air

In a glove box, a NMR tube was charged with 0.002 mmol of the complex and 0.7 mL of CD_2Cl_2 containing 1,3,5-Tri-tert-butylbenzene as an internal standard (0.001 M). The tube was closed with a plastic cap and wrapped with parafilm. A ^1H NMR spectrum of the solution was immediately recorded.

The plastic cap was then removed in the fume hood, and the solution was exposed to air for 10 minutes. The tube was again closed with the same plastic cap, wrapped with a new layer of parafilm, stored at room temperature (~20 °C), and shaken for some seconds from time to time. The decomposition of the catalyst was monitored by ^1H-NMR, by comparing the integral of the alkylidene proton with that of the tert-butyl groups (δ = 1.32 ppm (s, 27H) of the internal standard.

Table S4. Decomposition of complexes 3a and 5a in presence of air

Entry	Complex	Time, h	Decomposition, %	Ru–alkylidene species identified (%)[a]
1	**3a**	20	100	**3** (6)
2	**5a**	20	13	**5** (1)
		one week	49	**5** (2)[b]
		two weeks	79	**5** (2.5)[b]

[a]The estimated percentage of the identified alkylidene complex is given in parenthesis. [b]Three more peaks in the alkylidene region, originating from other, unidentified Ru complexes, were observed at 14.38 ppm, 13.63 ppm, and 13.53 ppm, respectively. The overall amount of these unidentified species was ca. 0.8 %.

Decomposition of 3a and 5a in presence of phenylphosphoric acid

In a glove box, a Young NMR tube was charged with 0.002 mmol of the complex and 0.7 mL of CD_2Cl_2 containing 1,3,5-Tri-tert-butylbenzene as an internal standard (0.001 M). The tube was closed and a ^{1}H-NMR spectrum of the solution was recorded.

Then, in the glove box, 0.002 mmol of phenylphosphoric acid was added to the solution. The tube was closed, shaken vigorously for some seconds from time to time and stored at room temperature (~20 °C). The decomposition of the catalyst was monitored by ^{1}H NMR, by comparing the integral of the alkylidene proton with that of the tert-butyl groups (δ = 1.32 ppm (s, 27H) of the internal standard.

Table S5. Decomposition of complexes 3a and 5a in presence of phenylphosphoric acid

Entry	Complex	Time, h	Decomposition, %	Ru–alkylidene species identified (%)[a]
1	**3a**	20	36	**3** (16)
		two weeks	46	**3** (21)
2	**5a**	20	2	**5** (0.5)
		two weeks	7	**5** (1)[a]

[a]The estimated percentage of the identified alkylidene complex is given in parenthesis. [b]Three more peaks in the alkylidene region, originating from other, unidentified Ru complexes, were observed at 14.75 ppm, 14.39 ppm, and 14.36 ppm, respectively. The overall amount of these unidentified species was ca. 0.7 %.

Experimental details of the catalytic tests

Homocoupling of terminal olefins in THF (4M in substrate) under argon (Table 3 of the main paper)

In a glove box, a 50 mL Schlenk flask equipped with a Young's tap was charged with the catalyst (5×10^{-3} mmol). Next, to remove the solvent (dichlorometane) present in the crystal lattice, the following procedure was performed twice: ~0.7 mL of THF was added to the Schlenk flask to dissolve the solid, followed by removal of the solvent under reduced pressure. Then, in a glove box, the substrate (2.0 mmol) and the solvent (THF) were added to the flask to obtain 0.5 mL of a 4 M solution, and the reaction mixture was stirred and heated in an oil bath at 40°C. Determination of conversions, yields, and Z-selectivities were done according to literature procedures.[1]

Homocoupling of neat 1-octene under argon (Table 3 of the main paper)

In a glove box, a 50 mL Schlenk flask equipped with a Young's tap was charged with the catalyst (6.4×10^{-4} mmol). Next, to remove the solvent (dichlorometane) present in the crystal lattice, the following procedure was performed twice: ~0.7 mL of THF was added to Schlenk flask to dissolve the solid, followed by removal of the solvent under reduced pressure. Finally, in a glove box, the substrate (6.4 mmol) was added to the flask and the reaction mixture was stirred and heated in an oil bath at 60°C. Determination of conversions, yields, and Z-selectivities were done according to literature procedures.[1]

Homocoupling of terminal olefins in air (neat substrate) (Table 4 of the main paper)

In the fume hood, a 1 mL vial equipped with a septum cap and a magnetic stirring bar was charged with the catalyst, and with 2 mmol of substrate (stored under air). The vial was closed, a syringe needle was inserted through the septum cap, and the reaction mixture was stirred at room temperature (20 °C) or heated in an oil bath. Determination of conversions, yields, and Z-selectivities were done according to literature procedures.[1]

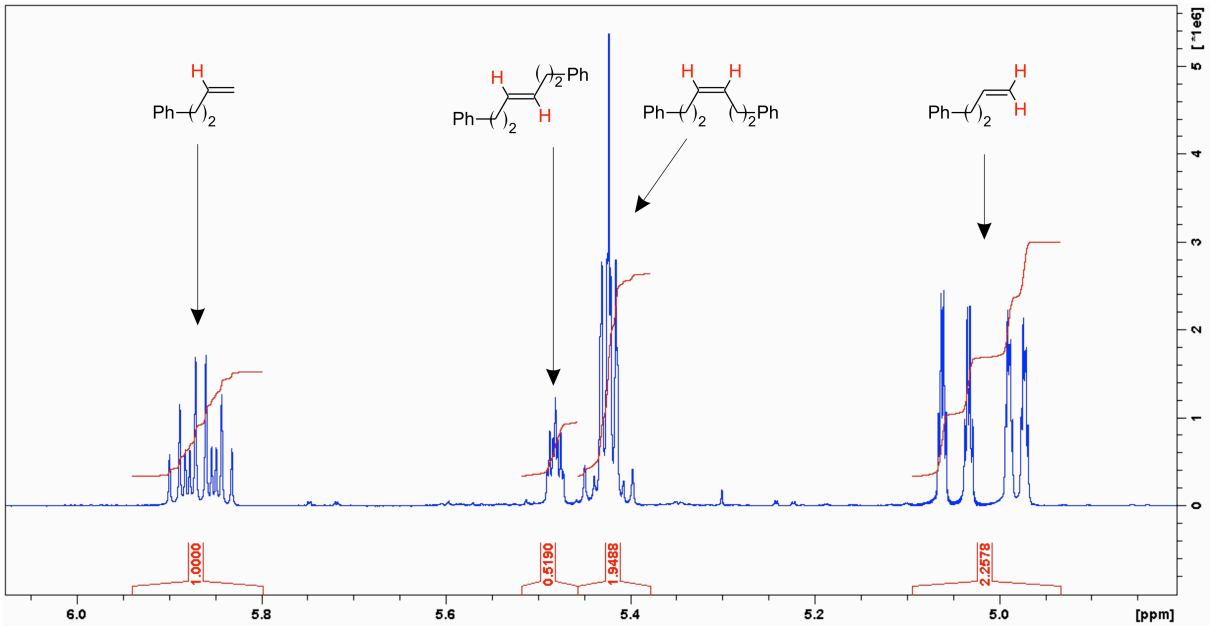

Figure S4. ^{1}H NMR spectrum (olefinic region) for the homocoupling of phenylbutene with 5a **in air at room temperature after 36 hours (Table 4, entry 4).**

Homocoupling of terminal olefins with catalyst 5a in presence of air and in solution (Table 5 of the main paper)

In the fume hood, a 50 mL Schlenk flask equipped with a Young's tap and a magnetic stirring bar was charged with the catalyst, and with 2 mmol of allylbenzene (stored under air). The solvent (stored under air) was added to the flask to obtain 0.5 mL of a 4 M solution. The Schlenk flask was closed and the reaction mixture was stirred and heated for four hours in an oil-bath at 40 ºC. Determination of conversions, yields, and Z-selectivities were done according to literature procedures.[1]

Homocoupling of terminal olefins with catalyst 5a in presence of air and in THF solution at different temperatures (Table 6 of the main paper)

In the fume hood, a 3 mL vial equipped with a skrew cap and a magnetic stirring bar was charged with the catalyst, and with 1 mmol of allylbenzene (stored under air). THF (stored under air) was added to the flask to obtain 0.25 mL of a 4 M solution. The Schlenk flask was closed and the reaction mixture was stirred and heated in an oil bath at different temperatures. Determination of conversions, yields, and Z-selectivities were done according to literature procedures.[1]

Allylbenzene homocoupling with 5a in air and in THF solution at different substrate concentrations (Table 7 of the main paper)

In the fume hood, a 3 mL vial equipped with a skrew cap and a magnetic stirring bar was charged with the catalyst, and with allylbenzene (stored under air), see Table S6. THF (stored under air) was added to the flask to obtain 0.5 mL of a solution. The vial was closed and the reaction mixture was

stirred and heated in an oil bath at 40 °C. Determination of conversions, yields, and Z-selectivities were done according to literature procedures.[1]

Table S6. Amounts of allylbenzene and catalyst 5a used in each entry of Table 7

Entry	substrate concentration, M	Allylbenzene, mmol	**5a**, mmol	cat. loading, mol %
1	4	2	0.05	0.25
2	2	1	0.05	0.5
3	1	0.5	0.05	1

Homocoupling of terminal olefins in presence of phenylphosphoric acid (Table 8 of the main paper)

In a glove box, a 3 mL vial equipped with a screw cap and a magnetic stirring bar was charged with the catalyst, phenylphosphoric acid, and the substrate (2 mmol). The vial was closed and the reaction mixture was stirred at room temperature (20 °C). Determination of conversions, yields, and Z-selectivities were done according to literature procedures.[1]

Thermal corrections to Gibbs free energy (ωB97XD, a.u.), single point energies in gas phase and in solution (PBE-D3(BJ), a.u.), and Cartesian coordinates (Å) of the investigated structures

3

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.549644
E (gas phase) = -2402.64003142
E(THF)= -2402.65115329
E(DCM)= -2402.65987511

Ru	0.50407	-0.01871	-0.24325
O	2.42603	-0.66542	-1.28882
N	-2.41521	0.20933	0.66822
N	-1.07492	1.70860	1.47925
C	-1.13754	0.62433	0.67490
C	-3.30390	1.02431	1.49949
H	-3.77352	0.40418	2.27824
H	-4.10759	1.45979	0.88648
C	-2.35500	2.08232	2.07300
H	-2.63029	3.10612	1.77683
H	-2.29345	2.04753	3.17146
C	-2.93675	-0.91958	-0.02798
C	-2.91678	-2.17101	0.60220
C	-3.40589	-3.26862	-0.10792
H	-3.38247	-4.25510	0.36251
C	-3.90366	-3.13962	-1.40762
C	-3.90509	-1.87467	-2.00101
H	-4.27554	-1.76156	-3.02321
C	-3.42592	-0.74820	-1.32903
C	0.12772	2.42527	1.77434
C	0.89794	2.04237	2.88727
C	2.12106	2.68094	3.09043
H	2.74255	2.36831	3.93356
C	2.56760	3.70169	2.24825
C	1.72541	4.13182	1.22303
H	2.03206	4.96792	0.58913
C	0.49079	3.52570	0.98010
C	-0.09270	-1.45143	-1.18092
H	-1.10126	-1.85800	-1.16289
C	0.82573	-2.14475	-2.06716
C	2.16579	-1.71355	-2.11968
C	3.08428	-2.32331	-2.96978
H	4.12068	-1.99379	-3.01816
C	2.65447	-3.38030	-3.77391
H	3.37296	-3.85942	-4.44151
C	1.33436	-3.82993	-3.73648
H	1.01876	-4.65872	-4.37114
C	0.42681	-3.21029	-2.88421
H	-0.61398	-3.53988	-2.83914
C	3.78196	-0.18876	-1.06671
H	4.24221	-0.07395	-2.06170
C	4.55277	-1.18380	-0.21370
H	4.60360	-2.17647	-0.68236
H	4.06179	-1.28706	0.76434
H	5.58121	-0.81976	-0.06863
C	3.66539	1.17804	-0.41525
H	3.05730	1.85640	-1.02866
H	4.67286	1.60448	-0.30050
H	3.21157	1.09754	0.58570
C	-2.30106	-2.33403	1.96542
H	-1.21740	-2.13454	1.92558
H	-2.45187	-3.35329	2.34506
H	-2.73219	-1.63266	2.69619
C	-4.44573	-4.33765	-2.14424
H	-5.51022	-4.49312	-1.90443
H	-3.90861	-5.25600	-1.86634
H	-4.36795	-4.20912	-3.23325
C	-3.35068	0.59296	-2.00653
H	-2.30008	0.89649	-2.14642
H	-3.83789	1.37995	-1.41049
H	-3.83810	0.56372	-2.99007
C	0.39603	1.04168	3.89342
H	-0.14201	1.57009	4.69942
H	1.22984	0.49152	4.34806
H	-0.27680	0.30247	3.44462
C	3.92887	4.31709	2.44102
H	4.69429	3.72868	1.90892
H	4.21336	4.34230	3.50293
H	3.96801	5.34297	2.04798
C	-0.44335	4.11768	-0.04064
H	-1.17662	3.39052	-0.40570
H	0.11094	4.48775	-0.91277
H	-0.97976	4.97054	0.40960
Cl	1.36114	-1.12336	1.66667
Cl	0.35955	1.60601	-1.95143

3a

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.871115
E (gas phase) = -3264.69419682
E(THF)= -3264.6937259
E(DCM)= -3264.70675554

Ru	-1.47270	0.03312	4.88150
Cl	-2.90894	0.03031	6.79512
S	0.54397	-0.10194	3.69178
O	-1.74220	-2.24193	5.12065
N	-2.12234	2.94764	4.17108
N	-0.70068	2.71960	5.79077
C	-2.96907	-2.54618	4.58655
C	-3.68088	-3.72284	4.80329
C	-4.90872	-3.89617	4.16003
C	-5.42508	-2.91736	3.31199
C	-4.70573	-1.74462	3.10728
C	-3.47844	-1.54094	3.74554
C	-2.73563	-0.29822	3.62259
C	-1.19664	-3.07010	6.19004
C	-0.56595	-4.32382	5.60380
C	-0.18671	-2.22979	6.95162
C	-1.42942	2.03770	4.87961
C	-3.03715	2.69820	3.10693
C	-4.39389	2.49921	3.39609
C	-4.88997	2.48984	4.81554
C	-5.25512	2.23463	2.32969
C	-4.79777	2.17741	1.01062
C	-5.73467	1.82552	-0.11557
C	-3.44400	2.41037	0.76277

C	-2.54285	2.66401	1.79766
C	-1.06954	2.81605	1.53557
C	-1.91009	4.32674	4.61666
C	-0.83410	4.17001	5.69271
C	0.20927	2.12388	6.71935
C	1.53329	1.88660	6.31786
C	2.08321	2.44655	5.03328
C	2.36986	1.18795	7.18684
C	1.93319	0.77022	8.44466
C	0.65319	1.13869	8.86129
C	-0.22044	1.83622	8.02529
C	-1.52947	2.34402	8.56764
C	2.82308	-0.05989	9.33181
C	0.91751	-1.78101	3.21466
C	0.15021	-2.49867	2.26267
C	0.43437	-3.84543	2.01530
C	1.49461	-4.51147	2.63026
C	2.31549	-3.76522	3.47425
C	2.04957	-2.42390	3.77027
C	3.06443	-1.75103	4.63615
C	3.38131	-2.27138	5.89629
C	4.46071	-1.77489	6.62560
C	5.24533	-0.74931	6.10300
C	4.92962	-0.21196	4.85427
C	3.84685	-0.70526	4.13078
C	1.74731	-5.95183	2.37807
C	0.67886	-6.85617	2.30317
C	0.90469	-8.21148	2.07570
C	2.20509	-8.68936	1.92083
C	3.27647	-7.80006	1.99361
C	3.04969	-6.44457	2.21905
C	-0.89347	-1.88362	1.39346
C	-2.10527	-2.53995	1.15465
C	-3.02533	-2.03884	0.23523
C	-2.74332	-0.87292	-0.46995
C	-1.53173	-0.21641	-0.25000
C	-0.61828	-0.71314	0.67237
H	2.86688	1.79498	4.62938
H	2.53036	3.43664	5.22833
H	1.31506	2.56493	4.25941
H	3.38612	0.95678	6.86474
H	2.64757	-1.13298	9.14985
H	3.88609	0.13567	9.13127
H	2.62671	0.13329	10.39656
H	0.31866	0.87963	9.86952
H	-2.25776	2.54502	7.77455
H	-1.35081	3.27387	9.13471
H	-1.98384	1.61354	9.24954
H	-1.13273	4.59509	6.66202
H	0.12768	4.62133	5.40121
H	-1.58800	4.95632	3.77409
H	-2.84830	4.74679	5.01154
H	-4.43754	1.65941	5.38139
H	-4.63069	3.41892	5.34636
H	-5.98193	2.37850	4.84735
H	-6.31354	2.05784	2.53915
H	-6.76150	2.15861	0.09270
H	-5.41172	2.27710	-1.06460
H	-3.07438	2.37540	-0.26448
H	-0.86507	2.88187	0.45859
H	-0.52111	1.94985	1.94257
H	-0.65723	3.71708	2.01492
H	-3.01785	0.33608	2.78557
H	-5.08580	-0.95700	2.45270
H	-1.28967	0.68751	-0.81197
H	-3.45931	-0.47828	-1.19384
H	-3.97039	-2.56270	0.08106
H	-2.34689	-3.44453	1.71682
H	0.33233	-0.20274	0.82819
H	2.78199	-3.08951	6.30119
H	6.09965	-0.36807	6.66578
H	5.53906	0.59116	4.43475
H	4.69443	-2.19966	7.60364
H	3.61564	-0.29797	3.14476
H	3.18351	-4.23687	3.93975
H	-0.66909	-1.38266	7.45664
H	0.59167	-1.84607	6.27508
H	0.29816	-2.86038	7.71184
H	4.29806	-8.16290	1.86508
H	2.38324	-9.75141	1.74312
H	3.89381	-5.75260	2.25086
H	-0.34120	-6.49223	2.44433
H	0.05898	-8.90009	2.02656
H	-0.26227	-4.99610	6.42061
H	0.32456	-4.06091	5.01959
H	-1.25104	-4.87441	4.94595
H	-0.15958	-4.37235	1.26590
H	-2.04127	-3.31615	6.85347
H	-3.30903	-4.50214	5.46486
H	-5.46785	-4.81736	4.33374
H	-6.38715	-3.06839	2.82054
H	-5.76371	0.73309	-0.26285

3a cation (entry 2, Table 1)

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.868958
E (gas phase) = -2804.41165931
E(THF)= -2804.45416949
E(DCM)= -2804.46778844

Ru	-0.61610	0.89090	0.75422
S	1.16201	0.70455	-0.63179
O	-1.24602	-1.28513	1.38868
N	-1.17680	3.76912	-0.22803
N	0.32144	3.49145	1.32324
C	-2.51836	-1.50167	0.91033
C	-3.33760	-2.57345	1.25159
C	-4.61608	-2.64439	0.69298
C	-5.07678	-1.67537	-0.19928
C	-4.24256	-0.62129	-0.54797
C	-2.95908	-0.51822	0.00689
C	-2.06789	0.57413	-0.31186
C	-0.58741	-2.33981	2.16186
C	-0.19030	-3.49320	1.26076
C	0.59452	-1.68960	2.84285
C	-0.51862	2.85593	0.48552
C	-2.19710	3.54335	-1.20412
C	-3.53025	3.46027	-0.77472
C	-3.88463	3.53890	0.68620
C	-4.51460	3.23315	-1.73473
C	-4.20079	3.10494	-3.09227
C	-5.28541	2.84160	-4.10310
C	-2.86522	3.21569	-3.47857
C	-1.84145	3.42773	-2.55192
C	-0.39985	3.47546	-2.97891
C	-0.73291	5.13855	0.07779
C	0.11190	4.94212	1.33933
C	0.96621	2.77763	2.37741
C	2.36846	2.79725	2.45655
C	3.18513	3.53384	1.43268
C	2.97536	2.09326	3.49141
C	2.23545	1.38413	4.44382
C	0.84678	1.38851	4.33995
C	0.18946	2.06130	3.30481
C	-1.31853	2.00618	3.21236
C	2.93541	0.60868	5.52609
C	1.53810	-1.00927	-0.97597

C	0.74296	-1.78316	-1.85134
C	1.07124	-3.12336	-2.07492
C	2.17595	-3.72852	-1.47235
C	2.97942	-2.93799	-0.64955
C	2.68777	-1.59369	-0.39509
C	3.66332	-0.85464	0.46063
C	4.35203	0.26158	-0.03008
C	5.36613	0.85537	0.71675
C	5.70137	0.35409	1.97432
C	5.01630	-0.74997	2.47785
C	4.01125	-1.35189	1.72300
C	2.48599	-5.16178	-1.70185
C	3.80623	-5.59210	-1.88819
C	4.09050	-6.93940	-2.09549
C	3.06032	-7.87848	-2.11810
C	1.74291	-7.46164	-1.93389
C	1.45834	-6.11408	-1.72830
C	-0.42808	-1.25026	-2.60300
C	-0.29693	-0.14728	-3.45780
C	-1.36776	0.27094	-4.23969
C	-2.59090	-0.39902	-4.18168
C	-2.72783	-1.50343	-3.34579
C	-1.65260	-1.92516	-2.56454
H	4.24765	3.28454	1.53571
H	3.08753	4.62541	1.54335
H	2.86405	3.26299	0.41553
H	4.06520	2.08525	3.55046
H	3.41439	-0.28659	5.09861
H	3.72650	1.20861	5.99840
H	2.23829	0.28066	6.30895
H	0.25188	0.85558	5.08593
H	-1.72940	1.23327	2.50346
H	-1.76697	2.96384	2.92002
H	-1.75216	1.69388	4.17159
H	-0.42182	5.23320	2.25931
H	1.06242	5.48744	1.30278
H	-0.14406	5.53852	-0.76163
H	-1.60012	5.79382	0.23251
H	-3.62124	2.59765	1.19657
H	-3.35062	4.35180	1.20009
H	-4.96134	3.70200	0.82228
H	-5.55762	3.15731	-1.41613
H	-6.09388	3.58292	-4.01927
H	-4.89769	2.87471	-5.13006
H	-2.60768	3.12742	-4.53614
H	-0.30984	3.36837	-4.06759
H	0.17258	2.66294	-2.50335
H	0.07940	4.42641	-2.70050
H	-2.32648	1.14173	-1.20428
H	-4.56455	0.14361	-1.25794
H	-3.67459	-2.04374	-3.29689
H	-3.42701	-0.06944	-4.80122
H	-1.23946	1.11461	-4.91913
H	0.66373	0.36353	-3.53090
H	-1.76946	-2.78824	-1.90520
H	4.11626	0.64383	-1.02473
H	6.50634	0.81231	2.55215
H	5.28223	-1.16167	3.45344
H	5.91372	1.70430	0.30280
H	3.49974	-2.23528	2.11024
H	3.86437	-3.37482	-0.18281
H	0.27012	-0.92721	3.56019
H	1.26164	-1.21767	2.10551
H	1.16767	-2.45271	3.38784
H	0.93150	-8.19135	-1.94558
H	3.28389	-8.93392	-2.28116
H	0.42523	-5.79782	-1.56708
H	4.61743	-4.86116	-1.89634
H	5.12323	-7.25669	-2.24901
H	0.19701	-4.31767	1.87728
H	0.59890	-3.18060	0.56712
H	-1.03861	-3.87738	0.67804
H	0.46365	-3.69745	-2.77695
H	-1.31208	-2.66468	2.92494
H	-3.01056	-3.35362	1.93588
H	-5.26033	-3.48209	0.96449
H	-6.07801	-1.75285	-0.62351
H	-5.73485	1.84881	-3.94306

3a cation (entry 3, Table 1)

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.55392
E (gas phase) = -1942.34228588
E(THF)= -1942.39830246
E(DCM)= -1942.40764955

C	-2.85783	-2.39328	8.50084
C	-4.02396	-2.69976	7.77665
C	-5.26391	-2.18666	8.21435
C	-5.33502	-1.36798	9.33813
C	-4.15857	-1.08093	10.03201
C	-2.92111	-1.58754	9.62678
C	-4.00216	-3.52677	6.60276
Ru	-5.55873	-3.87552	5.68636
Cl	-6.29101	-5.75770	6.79089
O	-6.32442	-2.57328	7.44120
C	-7.67671	-2.12277	7.77919
C	-7.89371	-0.74250	7.18576
C	-4.84694	-4.95796	4.19679
N	-5.76512	-5.16137	3.23573
C	-5.19443	-5.76283	2.02618
C	-3.82088	-6.21992	2.54066
N	-3.69965	-5.51048	3.82559
C	-7.01857	-4.49240	3.33827
C	-7.04096	-3.10765	3.60961
C	-8.28106	-2.46142	3.70378
C	-9.47874	-3.15401	3.56091
C	-9.41887	-4.53511	3.33553
C	-8.21459	-5.22489	3.22742
C	-5.77213	-2.29999	3.75532
C	-8.19280	-6.71656	3.04019
C	-10.80714	-2.45656	3.67240
C	-2.47841	-5.51023	4.57298
C	-2.23414	-6.53580	5.49678
C	-1.05000	-6.47396	6.23294
C	-0.12161	-5.44294	6.06016
C	-0.39971	-4.44631	5.12059
C	-1.57329	-4.46148	4.36496
C	-3.22690	-7.64554	5.71286
C	1.16186	-5.42860	6.84756
C	-1.89166	-3.33705	3.41482
C	-8.65191	-3.16777	7.28054
H	-5.99880	-1.22932	3.66106
H	-5.00603	-2.56538	3.01685
H	-5.22787	-2.26491	4.77088
H	-8.30285	-1.38380	3.88083
H	-11.40073	-2.88058	4.49667
H	-10.68661	-1.38057	3.85560
H	-11.39377	-2.58158	2.75007
H	-10.35154	-5.09913	3.25679
H	-7.40920	-7.17427	3.66147
H	-8.00560	-6.99049	1.98953
H	-9.15711	-7.15608	3.32468
H	-5.80355	-6.59783	1.66084
H	-5.11995	-5.00673	1.22815
H	-2.99535	-5.94361	1.87184
H	-3.77910	-7.30615	2.71045

H	-4.20071	-7.24969	6.03878
H	-3.39204	-8.22316	4.79005
H	-2.86829	-8.34458	6.47889
H	-0.84663	-7.25818	6.96612
H	1.00653	-5.79197	7.87326
H	1.90817	-6.08729	6.37569
H	0.31471	-3.63254	4.97355
H	-1.00219	-2.72612	3.21463
H	-2.66100	-2.67408	3.84518
H	-2.27563	-3.70131	2.45063
H	-3.02332	-3.92379	6.33148
H	-1.90614	-2.80456	8.15726
H	-8.45475	-4.14337	7.74125
H	-8.59583	-3.27926	6.18805
H	-9.67188	-2.84849	7.53902
H	-8.89007	-0.36877	7.46231
H	-7.83725	-0.78978	6.08810
H	-7.14573	-0.02107	7.54426
H	-7.72932	-2.09129	8.87641
H	-6.27463	-0.94671	9.68891
H	-4.21681	-0.44184	10.91457
H	-2.01952	-1.34888	10.19037
H	1.59508	-4.42021	6.89779

5a

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.879165
E (gas phase) = -2972.62914433
E(THF)= -2972.62541319
E(DCM)= -2972.63898833

C	2.41944	2.25881	3.81491
C	2.17352	3.24954	4.77423
C	2.99570	3.42528	5.89323
C	4.10332	2.58393	6.02851
C	4.39438	1.59901	5.08229
C	3.53695	1.44434	3.98928
N	1.06650	4.12582	4.58148
C	1.09014	5.30905	3.94636
N	-0.15051	5.83526	4.03919
C	-1.10903	4.97368	4.72509
C	-0.22892	3.80867	5.18712
C	-0.54727	7.07816	3.45220
C	-1.00241	7.09206	2.12420
C	-1.24340	8.32739	1.52349
C	-1.09120	9.52358	2.22534
C	-0.76306	9.46437	3.58132
C	-0.50228	8.25227	4.22201
Ru	2.56157	6.36112	3.08613
C	4.03368	5.37606	3.49114
C	5.34630	5.95693	3.25108
C	5.42317	7.17202	2.55008
C	6.64829	7.69145	2.13971
C	7.81810	7.03715	2.52828
C	7.77035	5.87665	3.30490
C	6.53723	5.33193	3.64432
O	4.20186	7.72818	2.28838
C	4.07924	9.14126	1.93478
C	2.59430	9.42345	1.79787
C	-1.31579	5.82204	1.37979
C	-1.26611	10.84801	1.53051
C	-0.26487	8.22207	5.70804
C	2.75489	4.55940	6.85298
C	5.61585	0.72600	5.21010
C	1.54205	2.13893	2.59977
S	1.92081	5.63167	0.94525
C	3.13902	6.23577	-0.21371
C	4.42217	5.64387	-0.30851
C	5.43618	6.31666	-0.99706
C	5.21765	7.53338	-1.64275
C	3.90465	8.00366	-1.69916
C	2.85907	7.36058	-1.02961
C	4.74987	4.28563	0.21530
C	5.99421	4.02916	0.80112
C	6.35520	2.74371	1.19757
C	5.48308	1.67836	0.99024
C	4.24911	1.91449	0.38441
C	3.88442	3.20281	0.00566
C	6.33758	8.27019	-2.28041
C	6.17447	8.94097	-3.50025
C	7.23129	9.64217	-4.07562
C	8.47385	9.68502	-3.44451
C	8.65094	9.01818	-2.23331
C	7.59326	8.31868	-1.65732
C	1.47860	7.86069	-1.30420
C	0.47704	6.96738	-1.70890
C	-0.76861	7.42839	-2.12617
C	-1.04453	8.79583	-2.14392
C	-0.06149	9.69517	-1.73715
C	1.18592	9.23052	-1.32503
N	2.55669	7.64381	4.65548
C	2.89168	8.39839	5.49980
O	3.18101	9.17840	6.34994
C	4.71120	10.05033	2.97937
H	6.42147	5.85214	-1.06330
H	3.67810	8.89668	-2.28533
H	0.69111	5.89756	-1.71941
H	-1.52698	6.71305	-2.45094
H	-2.01958	9.15737	-2.47594
H	-0.26294	10.76803	-1.74380
H	1.94980	9.94656	-1.01721
H	5.21389	8.89394	-4.01719
H	7.08506	10.15173	-5.02994
H	9.30159	10.23424	-3.89659
H	9.61870	9.04746	-1.72881
H	7.73531	7.81175	-0.70016
H	6.68963	4.85281	0.96435
H	7.32743	2.57875	1.66643
H	5.76720	0.66648	1.28714
H	3.56521	1.08467	0.19475
H	2.92194	3.37259	-0.47704
H	4.05152	4.36552	3.88852
H	6.47271	4.39359	4.19990
H	8.69416	5.38809	3.61732
H	8.78133	7.45005	2.22266
H	6.70219	8.59181	1.52933
H	4.57318	9.25035	0.95430
H	5.78690	9.88262	3.10997
H	4.22019	9.92128	3.95350
H	4.57024	11.09320	2.65771
H	2.09563	8.68602	1.15777
H	2.46044	10.41906	1.35060
H	2.10479	9.41620	2.78228
H	-1.54682	8.35168	0.47523
H	-0.69832	10.38874	4.16161
H	0.30785	9.09876	6.03927
H	0.28672	7.32763	6.01898
H	-1.23351	8.23873	6.23576
H	-1.61625	11.62659	2.22360
H	-1.97977	10.77401	0.69758
H	-0.30503	11.18486	1.10797
H	-1.13003	5.94495	0.30609
H	-2.38241	5.57322	1.51532
H	-0.71857	4.97009	1.72693
H	-1.90227	4.65660	4.02977
H	-1.58036	5.51184	5.56060
H	-0.13380	3.75603	6.28293

H	-0.58868	2.83122	4.83352
H	4.76900	2.72058	6.88470
H	3.75699	0.68202	3.23867
H	1.76688	1.22018	2.04292
H	1.70491	2.99908	1.92945
H	0.47419	2.12559	2.86569
H	6.19492	0.96796	6.11200
H	6.27457	0.85335	4.33652
H	5.33951	-0.33867	5.25875
H	2.85991	5.52696	6.33562
H	3.47187	4.53120	7.68389
H	1.74145	4.52970	7.28177

5a cation (entry 4, Table 1)

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.868958
E (gas phase) = -2804.41165931
E(THF)= -2804.45416949
E(DCM)= -2804.46778844

Ru	-0.61610	0.89090	0.75422
S	1.16201	0.70455	-0.63179
O	-1.24602	-1.28513	1.38868
N	-1.17680	3.76912	-0.22803
N	0.32144	3.49145	1.32324
C	-2.51836	-1.50167	0.91033
C	-3.33760	-2.57345	1.25159
C	-4.61608	-2.64439	0.69298
C	-5.07678	-1.67537	-0.19928
C	-4.24256	-0.62129	-0.54797
C	-2.95908	-0.51822	0.00689
C	-2.06789	0.57413	-0.31186
C	-0.58741	-2.33981	2.16186
C	-0.19030	-3.49320	1.26076
C	0.59452	-1.68960	2.84285
C	-0.51862	2.85593	0.48552
C	-2.19710	3.54335	-1.20412
C	-3.53025	3.46027	-0.77472
C	-3.88463	3.53890	0.68620
C	-4.51460	3.23315	-1.73473
C	-4.20079	3.10494	-3.09227
C	-5.28541	2.84160	-4.10310
C	-2.86522	3.21569	-3.47857
C	-1.84145	3.42773	-2.55192
C	-0.39985	3.47546	-2.97891
C	-0.73291	5.13855	0.07779
C	0.11190	4.94212	1.33933
C	0.96621	2.77763	2.37741
C	2.36846	2.79725	2.45655
C	3.18513	3.53384	1.43268
C	2.97536	2.09326	3.49141
C	2.23545	1.38413	4.44382
C	0.84678	1.38851	4.33995
C	0.18946	2.06130	3.30481
C	-1.31853	2.00618	3.21236
C	2.93541	0.60868	5.52609
C	1.53810	-1.00927	-0.97597
C	0.74296	-1.78316	-1.85134
C	1.07124	-3.12336	-2.07492
C	2.17595	-3.72852	-1.47235
C	2.97942	-2.93799	-0.64955
C	2.68777	-1.59369	-0.39509
C	3.66332	-0.85464	0.46063
C	4.35203	0.26158	-0.03008
C	5.36613	0.85537	0.71675
C	5.70137	0.35409	1.97432
C	5.01630	-0.74997	2.47785
C	4.01125	-1.35189	1.72300
C	2.48599	-5.16178	-1.70185
C	3.80623	-5.59210	-1.88819
C	4.09050	-6.93940	-2.09549
C	3.06032	-7.87848	-2.11810
C	1.74291	-7.46164	-1.93389
C	1.45834	-6.11408	-1.72830
C	-0.42808	-1.25026	-2.60300
C	-0.29693	-0.14728	-3.45780
C	-1.36776	0.27094	-4.23969
C	-2.59090	-0.39902	-4.18168
C	-2.72783	-1.50343	-3.34579
C	-1.65260	-1.92516	-2.56454
H	4.24765	3.28454	1.53571
H	3.08753	4.62541	1.54335
H	2.86405	3.26299	0.41553
H	4.06520	2.08525	3.55046
H	3.41439	-0.28659	5.09861
H	3.72650	1.20861	5.99840
H	2.23829	0.28066	6.30895
H	0.25188	0.85558	5.08593
H	-1.72940	1.23327	2.50346
H	-1.76697	2.96384	2.92002
H	-1.75216	1.69388	4.17159
H	-0.42182	5.23320	2.25931
H	1.06242	5.48744	1.30278
H	-0.14406	5.53852	-0.76163
H	-1.60012	5.79382	0.23251
H	-3.62124	2.59765	1.19657
H	-3.35062	4.35180	1.20009
H	-4.96134	3.70200	0.82228
H	-5.55762	3.15731	-1.41613
H	-6.09388	3.58292	-4.01927
H	-4.89769	2.87471	-5.13006
H	-2.60768	3.12742	-4.53614
H	-0.30984	3.36837	-4.06759
H	0.17258	2.66294	-2.50335
H	0.07940	4.42641	-2.70050
H	-2.32648	1.14173	-1.20428
H	-4.56455	0.14361	-1.25794
H	-3.67459	-2.04374	-3.29689
H	-3.42701	-0.06944	-4.80122
H	-1.23946	1.11461	-4.91913
H	0.66373	0.36353	-3.53090
H	-1.76946	-2.78824	-1.90520
H	4.11626	0.64383	-1.02473
H	6.50634	0.81231	2.55215
H	5.28223	-1.16167	3.45344
H	5.91372	1.70430	0.30280
H	3.49974	-2.23528	2.11024
H	3.86437	-3.37482	-0.18281
H	0.27012	-0.92721	3.56019
H	1.26164	-1.21767	2.10551
H	1.16767	-2.45271	3.38784
H	0.93150	-8.19135	-1.94558
H	3.28389	-8.93392	-2.28116
H	0.42523	-5.79782	-1.56708
H	4.61743	-4.86116	-1.89634
H	5.12323	-7.25669	-2.24901
H	0.19701	-4.31767	1.87728
H	0.59890	-3.18060	0.56712
H	-1.03861	-3.87738	0.67804
H	0.46365	-3.69745	-2.77695
H	-1.31208	-2.66468	2.92494
H	-3.01056	-3.35362	1.93588
H	-5.26033	-3.48209	0.96449
H	-6.07801	-1.75285	-0.62351
H	-5.73485	1.84881	-3.94306

5a cation (entry 5, Table 1)

```
Spin multiplicity: singlet
Thermal correction to Gibbs free
energy = 0.5621
E (gas phase) = -1650.27386201
E(THF)= -1650.33036143
E(DCM)= -1650.34051533

C     0.50790   -3.73653    1.01196
C    -0.20788   -2.79047    1.75001
C     0.12569   -2.46906    3.07678
C     1.22249   -3.10788    3.64390
C     1.98271   -4.04287    2.93130
C     1.60548   -4.34891    1.62598
N    -1.31709   -2.11505    1.14357
C    -1.28464   -0.88382    0.67285
N    -2.51765   -0.49536    0.31414
C    -3.49961   -1.57964    0.37571
C    -2.69872   -2.63728    1.17229
C    -2.43254    0.71215   -0.46459
C    -2.08346    0.66401   -1.83699
C    -1.96318    1.88173   -2.53084
C    -2.21746    3.10396   -1.92359
C    -2.60555    3.11761   -0.57126
C    -2.70897    1.95466    0.17704
Ru   -0.09010    0.56586    0.09944
C     0.71212   -0.43963   -1.18856
C     1.53039    0.22212   -2.17711
C     1.75438    1.60807   -2.04576
C     2.51248    2.29986   -2.98494
C     3.04386    1.59916   -4.06809
C     2.83440    0.22681   -4.22219
C     2.08210   -0.45626   -3.27748
O     1.15176    2.17765   -0.95255
C     1.69665    3.42394   -0.39693
C     0.70895    3.90141    0.64718
C    -2.01159   -0.62673   -2.61242
C    -2.07277    4.39820   -2.67405
C    -3.09283    1.98245    1.63220
C    -0.65527   -1.43643    3.84708
C     3.19386   -4.67158    3.56491
C     0.13278   -4.12088   -0.39689
N     1.17453    0.56264    1.61223
C     2.12648   -0.01594    2.05565
O     3.06996   -0.52119    2.53267
C     3.08804    3.18949    0.16169
H     0.61282   -1.52292   -1.29187
H     1.91137   -1.53062   -3.37470
H     3.26357   -0.30128   -5.07352
H     3.63738    2.14215   -4.80516
H     2.70053    3.36782   -2.89070
H     1.71809    4.14755   -1.22642
H     3.77889    2.80318   -0.59997
H     3.04483    2.47566    0.99551
H     3.49315    4.14205    0.53285
H    -0.29214    4.02917    0.21482
H     1.04311    4.87212    1.03889
H     0.65865    3.19385    1.48880
H    -1.68326    1.85134   -3.58610
H    -2.82332    4.07389   -0.08948
H    -3.30976    3.00669    1.95913
H    -2.28667    1.58469    2.26901
H    -3.98233    1.36322    1.81950
H    -2.99236    4.99768   -2.60393
H    -1.84922    4.23065   -3.73541
H    -1.25813    5.00220   -2.24385
H    -1.22134   -0.57722   -3.37379
H    -2.96676   -0.79080   -3.13531
H    -1.81833   -1.49778   -1.97504
H    -3.76569   -1.92895   -0.63441
H    -4.41748   -1.26911    0.89118
H    -3.04168   -2.72025    2.21457
H    -2.73641   -3.63585    0.71765
H     1.50856   -2.85769    4.66798
H     2.18367   -5.08308    1.05925
H     1.01314   -4.09293   -1.05642
H    -0.63361   -3.45871   -0.82242
H    -0.25980   -5.14906   -0.42968
H     2.96323   -5.05201    4.57075
H     3.99552   -3.92406    3.67105
H     3.58237   -5.50365    2.96265
H    -0.48878   -0.43232    3.42657
H    -0.34173   -1.41657    4.89846
H    -1.73779   -1.63532    3.82518
```

Cl anion

```
Spin multiplicity: singlet
Thermal correction to Gibbs free
energy = -0.015023
E (gas phase) = -460.10378555
E(THF)= -460.205683946
E(DCM)= -460.20854691
```

NCO anion

```
Spin multiplicity: singlet
Thermal correction to Gibbs free
energy = -0.006233
E (gas phase) = -168.02922798
E(THF)= -168.124146471
E(DCM)= -168.127231194

C     0.80471   -0.00095   -1.01709
O    -0.40220    0.00112   -0.91838
N     1.97541   -0.00317   -1.11247
```

SAr anion

```
Spin multiplicity: singlet
Thermal correction to Gibbs free
energy = 0.284282
E (gas phase) = -1322.15104779
E(THF)= -1322.21877236
E(DCM)= -1322.22462553

S    -0.82562    3.13394    0.90758
C    -0.40752    1.52081    0.45791
C    -1.25476    0.70669   -0.36913
C    -0.87357   -0.57503   -0.76038
H    -1.55763   -1.14040   -1.39969
C     0.34536   -1.15131   -0.38367
C     1.18045   -0.36939    0.42379
H     2.12287   -0.79086    0.78492
C     0.83604    0.91352    0.84377
C     1.82818    1.61072    1.71248
C     1.48650    2.09326    2.98428
H     0.44783    2.02761    3.30726
C     2.44898    2.65548    3.81613
H     2.15993    3.01911    4.80536
C     3.77628    2.76525    3.39356
H     4.52834    3.21501    4.04657
C     4.12799    2.30207    2.12902
H     5.15974    2.38890    1.77884
C     3.16068    1.72978    1.30051
H     3.43787    1.37610    0.30451
C     0.72485   -2.51635   -0.80428
C    -0.23919   -3.52562   -0.97706
H    -1.28691   -3.30002   -0.76878
```

C	0.11837	-4.80954	-1.38014
H	-0.65644	-5.57069	-1.50095
C	1.45523	-5.13197	-1.61356
H	1.73672	-6.14006	-1.92543
C	2.42678	-4.14593	-1.44183
H	3.47867	-4.37703	-1.62751
C	2.06654	-2.85952	-1.04949
H	2.83703	-2.09244	-0.94924
C	-2.57620	1.18360	-0.87068
C	-2.87059	1.13160	-2.23833
H	-2.09093	0.81207	-2.93392
C	-4.12893	1.49310	-2.72365
H	-4.32895	1.44985	-3.79732
C	-5.12144	1.91276	-1.84260
H	-6.10798	2.19810	-2.21634
C	-4.83984	1.97267	-0.47537
H	-5.60947	2.30499	0.22578
C	-3.58227	1.62073	0.00347
H	-3.35690	1.68972	1.06740

3 $TS2_E$

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.645461
E (gas phase) = -2597.54106084
E(THF)= -2597.55617673

Ru	1.54142	-0.63791	0.80344
C	3.38137	-0.75492	-0.08921
N	4.02177	-1.81223	-0.59274
C	5.29257	-1.44927	-1.23188
C	5.43527	0.03649	-0.87674
N	4.13110	0.33828	-0.28188
C	3.54616	-3.16185	-0.58761
C	3.81869	-3.96177	0.52964
C	3.32215	-5.26826	0.53838
C	2.58712	-5.78125	-0.53014
C	2.37107	-4.96418	-1.64363
C	2.84732	-3.65460	-1.70105
C	4.60679	-3.42755	1.69364
C	2.62507	-2.80676	-2.92366
C	2.03706	-7.18400	-0.49842
C	3.80600	1.62073	0.26979
C	4.24785	1.94847	1.56340
C	3.86458	3.18145	2.09325
C	3.08787	4.08771	1.36863
C	2.73168	3.75838	0.05865
C	3.08968	2.53775	-0.51872
C	5.15870	1.04296	2.34768
C	2.62147	5.37385	1.99763
C	2.74633	2.23314	-1.95074
C	0.84114	-2.30198	0.95577
C	-0.58418	-0.58809	1.91864
C	-0.10988	0.64088	1.49090
H	-0.34662	-0.89604	2.93400
C	-1.82736	-1.18748	1.29110
H	0.22353	-2.74306	0.16783
H	2.37662	-7.73093	0.39198
H	6.23633	0.21954	-0.14359
H	5.61830	0.67110	-1.75494
H	5.23009	-1.61598	-2.31785
H	6.11069	-2.06687	-0.83535
H	3.51935	-5.90003	1.40826
H	1.81246	-5.35775	-2.49708
H	4.17754	3.43541	3.10904
H	2.16351	4.47531	-0.53988
H	1.69552	5.20285	2.57121
H	4.99593	1.16919	3.42567
H	2.34865	-7.75246	-1.38802
H	0.93575	-7.17229	-0.48815
H	6.21183	1.29228	2.13207
H	4.98837	-0.01550	2.11867
H	2.40464	6.13881	1.23854
H	2.02234	1.40751	-2.02038
H	3.64342	1.93685	-2.51652
H	2.31449	3.11617	-2.44032
H	3.37197	5.77753	2.69231
H	1.91249	-3.28912	-3.60587
H	3.56624	-2.66147	-3.47946
H	2.22037	-1.82055	-2.65521
H	5.53969	-2.94583	1.36150
H	4.87230	-4.23573	2.38822
H	4.02696	-2.67076	2.24644
H	-0.55054	1.03215	0.57637
H	-1.92022	-2.25172	1.54912
H	-1.76266	-1.10055	0.19793
C	0.44743	1.70354	2.41531
H	1.28994	2.22274	1.93598
H	0.82153	1.24981	3.34032
H	1.02625	-2.91301	1.84494
C	-0.66444	2.69198	2.69468
C	-2.80811	4.44809	3.13784
C	-1.57031	2.46199	3.73447
C	-0.85224	3.80746	1.87328
C	-1.91554	4.68255	2.09328
C	-2.63212	3.33376	3.95778
H	-1.44678	1.58140	4.36935
H	-0.15493	3.98644	1.05016
H	-2.04711	5.55127	1.44491
H	-3.33278	3.13572	4.77081
H	-3.64189	5.13106	3.31119
C	-3.02295	-0.41660	1.81331
C	-5.13823	1.11200	2.84764
C	-3.61552	-0.75360	3.03358
C	-3.50309	0.69941	1.11943
C	-4.55154	1.45838	1.63110
C	-4.66760	0.00334	3.54824
H	-3.24982	-1.62207	3.58798
H	-3.04444	0.97746	0.16774
H	-4.90793	2.33012	1.07972
H	-5.12205	-0.27653	4.50080
H	-5.95974	1.70766	3.24996
Cl	2.47697	-0.84955	3.02216
Cl	0.49902	-0.40885	-1.36998

3 $TS2_Z$

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.64558
E (gas phase) = -2597.53986726
E(THF)= -2597.55468281

Ru	-1.65068	-1.57863	2.06881
C	-1.30016	-0.69829	0.24968
N	-1.10114	-1.27279	-0.93746
C	-1.00710	-0.29147	-2.02472
C	-0.95107	1.04219	-1.26616
N	-1.28246	0.63158	0.10083
C	-1.09541	-2.68514	-1.17188
C	0.10908	-3.38457	-0.99984
C	0.08770	-4.77106	-1.14722
C	-1.08560	-5.45849	-1.46920
C	-2.24924	-4.72101	-1.68834
C	-2.27864	-3.33025	-1.55449
C	1.38092	-2.66416	-0.64671
C	-3.54084	-2.56114	-1.83612

C	-1.08740	-6.96254	-1.55987
C	-1.32069	1.53441	1.21381
C	-0.12118	1.91555	1.83809
C	-0.20189	2.72946	2.96976
C	-1.42484	3.18161	3.46864
C	-2.59006	2.84563	2.77458
C	-2.56414	2.03526	1.63770
C	1.22285	1.51883	1.28965
C	-1.48997	3.98578	4.73990
C	-3.82546	1.73619	0.87551
C	-1.59551	-3.39959	2.01369
C	-2.13668	-2.69602	4.10066
C	-2.33660	-1.30339	4.09217
H	-2.47203	-4.00335	1.76542
H	-0.20131	-7.33195	-2.09727
H	0.05109	1.49848	-1.29159
H	-1.67671	1.77795	-1.63909
H	-1.89215	-0.36464	-2.67518
H	-0.11245	-0.47753	-2.63493
H	1.01533	-5.33075	-1.00078
H	-3.17019	-5.24052	-1.96496
H	0.72253	3.00825	3.48157
H	-3.55187	3.23258	3.12148
H	-2.35034	4.67034	4.73959
H	1.96648	1.45601	2.09434
H	-1.98289	-7.33544	-2.07622
H	-1.07063	-7.40922	-0.55258
H	1.57056	2.27413	0.56422
H	1.19612	0.53880	0.79870
H	-0.57578	4.57727	4.89048
H	-4.09539	0.67216	0.95360
H	-3.70484	1.97086	-0.19356
H	-4.66079	2.33570	1.26128
H	-1.60161	3.31530	5.60812
H	-4.41436	-3.22594	-1.81098
H	-3.50131	-2.10368	-2.83922
H	-3.70590	-1.77271	-1.08977
H	2.24706	-3.33149	-0.75022
H	1.34833	-2.29656	0.39143
H	1.54394	-1.79207	-1.29887
H	-3.36376	-0.98760	3.92847
C	-1.49187	-0.30107	4.85644
H	-1.35417	0.59508	4.23249
H	-0.48941	-0.69294	5.05780
H	-0.65535	-3.93455	2.15499
H	-3.03383	-3.28674	3.93698
C	-1.05679	-3.35191	4.93400
H	-0.10998	-2.81385	4.80343
H	-1.36879	-3.22009	5.98556
C	-0.85290	-4.82155	4.65623
C	-0.48316	-7.54434	4.07071
C	-1.88637	-5.74268	4.85843
C	0.37217	-5.28618	4.16753
C	0.55668	-6.63685	3.87532
C	-1.70617	-7.09297	4.56618
H	-2.84711	-5.40000	5.25202
H	1.18133	-4.57203	3.99580
H	1.51863	-6.98066	3.49010
H	-2.52440	-7.79720	4.72883
H	-0.34056	-8.60207	3.84162
C	-2.18727	0.09678	6.13972
C	-3.52002	0.81429	8.50743
C	-1.77845	-0.41846	7.37298
C	-3.27541	0.97736	6.10956
C	-3.93674	1.33495	7.28195
C	-2.43821	-0.06290	8.54936
H	-0.92439	-1.09915	7.41317
H	-3.60019	1.38922	5.15018
H	-4.78154	2.02535	7.23990
H	-2.10210	-0.47176	9.50430
H	-4.03642	1.09433	9.42735
Cl	0.69430	-1.48954	2.66848
Cl	-4.00700	-1.71036	1.53816

3a TS2$_E$

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.966806
E (gas phase) = -3459.59079134
E(THF)= -3459.58902974

Ru	1.34280	-0.59566	0.59003
C	-1.71637	1.16334	-1.88661
C	-1.12020	-0.11987	-1.90119
C	-1.96992	-1.23881	-2.08545
C	-3.35856	-1.07455	-2.10278
C	-3.95376	0.18112	-1.97618
C	-3.10991	1.28917	-1.90700
S	0.63640	-0.33114	-1.68927
C	3.31598	-0.71632	-0.07187
N	3.99121	-1.82388	-0.39849
C	5.42554	-1.57869	-0.59626
C	5.54260	-0.06451	-0.39564
N	4.16754	0.31563	-0.06316
C	3.47063	-3.14899	-0.56176
C	3.50467	-4.04295	0.52057
C	2.99327	-5.32705	0.32514
C	2.50507	-5.74644	-0.91354
C	2.56088	-4.85379	-1.98257
C	3.03085	-3.54846	-1.83158
C	4.10185	-3.65605	1.84526
C	3.04354	-2.60727	-3.00363
C	1.91995	-7.12316	-1.08720
C	3.82584	1.67192	0.24455
C	4.05941	2.17569	1.53426
C	3.67529	3.49251	1.80122
C	3.12106	4.31245	0.81839
C	2.98026	3.80117	-0.47292
C	3.34117	2.49215	-0.78912
C	4.76992	1.38216	2.59740
C	2.73521	5.73823	1.11971
C	3.24211	1.99507	-2.20432
C	0.55507	-2.21996	0.86896
C	-0.64738	-0.66621	1.80133
C	-0.27785	0.61133	1.31792
H	-0.31121	-0.90471	2.80742
C	-1.96883	-1.30316	1.39770
H	-0.06119	-2.69596	0.10405
H	0.84516	-7.11535	-0.84181
H	6.21948	0.20545	0.42778
H	5.87605	0.46494	-1.30118
H	5.72996	-1.90398	-1.60190
H	6.01120	-2.15028	0.13829
H	2.99486	-6.02524	1.16646
H	2.22245	-5.17733	-2.96809
H	3.82223	3.88576	2.81063
H	2.58038	4.43851	-1.26258
H	2.47228	5.86951	2.17923
H	4.31157	1.55163	3.58090
H	2.40557	-7.85601	-0.42662
H	2.01911	-7.47491	-2.12431
H	5.82379	1.70364	2.65527
H	4.73016	0.30408	2.40984
H	1.87593	6.05253	0.50847
H	2.34735	1.36672	-2.33454
H	4.11707	1.38920	-2.48329
H	3.17250	2.83989	-2.90178
H	3.56824	6.42391	0.89519

H	2.94521	-3.16144	-3.94704
H	3.96828	-2.01314	-3.05114
H	2.20245	-1.89951	-2.92621
H	5.19389	-3.52735	1.76039
H	3.92460	-4.44043	2.59353
H	3.67872	-2.71539	2.22558
H	-0.86691	0.98457	0.48501
H	-3.98816	-1.95538	-2.24540
H	-3.54162	2.29097	-1.85394
H	-1.94186	-2.38544	1.59015
H	-2.14138	-1.15413	0.32722
C	-0.95388	2.44637	-1.91846
C	0.15447	5.00970	-2.21911
C	-0.12567	2.74296	-3.00892
C	-1.19260	3.44345	-0.96719
C	-0.63794	4.71473	-1.11326
C	0.41656	4.01477	-3.16257
H	0.06601	1.97156	-3.75657
H	-1.82856	3.22979	-0.10501
H	-0.84420	5.47748	-0.36034
H	1.03896	4.23526	-4.03238
H	0.57069	6.01140	-2.34653
C	-1.46901	-2.62676	-2.30569
C	-0.75013	-5.27940	-2.88803
C	-1.90724	-3.68143	-1.49775
C	-0.65824	-2.92100	-3.40957
C	-0.31379	-4.23476	-3.70439
C	-1.54015	-4.99833	-1.77769
H	-2.54799	-3.46809	-0.63923
H	-0.31702	-2.10688	-4.05045
H	0.30038	-4.44692	-4.58214
H	-1.88717	-5.80656	-1.13092
H	-0.47295	-6.30974	-3.11884
C	0.33534	1.70346	2.17834
H	1.15088	2.19079	1.61957
H	0.79195	1.25741	3.07055
H	0.74445	-2.80415	1.77476
C	-5.42811	0.33618	-1.90373
C	-8.21317	0.64855	-1.70180
C	-6.18855	-0.52355	-1.09941
C	-6.08603	1.35570	-2.60435
C	-7.46660	1.50984	-2.50513
C	-7.56904	-0.36861	-0.99905
H	-5.68614	-1.30318	-0.52307
H	-5.50980	2.02335	-3.24837
H	-7.96347	2.30510	-3.06403
H	-8.14292	-1.04142	-0.35916
H	-9.29492	0.77092	-1.62295
C	-0.66111	2.77205	2.57721
C	-2.46721	4.79139	3.33334
C	-1.82358	2.46027	3.28980
C	-0.41482	4.11069	2.25940
C	-1.30544	5.11492	2.63394
C	-2.72070	3.46005	3.66113
H	-2.03720	1.42426	3.55890
H	0.48638	4.36000	1.69761
H	-1.09120	6.15476	2.37605
H	-3.62503	3.19000	4.20946
H	-3.17069	5.57366	3.62484
C	-3.10286	-0.68910	2.18745
C	-5.15879	0.50868	3.67577
C	-3.32653	-1.05875	3.51824
C	-3.92114	0.28728	1.61449
C	-4.94802	0.87709	2.34840
C	-4.34229	-0.45994	4.26094
H	-2.69492	-1.82240	3.98005
H	-3.74699	0.59112	0.58163
H	-5.58079	1.63173	1.87807
H	-4.50213	-0.75579	5.29959
H	-5.96011	0.97215	4.25452
Cl	2.30196	-0.81424	2.84751

3a TS2$_Z$

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.968013
E (gas phase) = -3459.59627648
E(THF)= -3459.59190529

Ru	0.52100	-0.23725	-1.30081
C	-1.82731	1.39913	1.71807
C	-1.92155	0.13582	1.08083
C	-1.97281	-1.01947	1.90090
C	-1.73096	-0.90886	3.27281
C	-1.45445	0.31655	3.87753
C	-1.56745	1.46375	3.09130
S	-1.80617	-0.01087	-0.69374
C	0.00177	-0.36173	-3.29485
N	-0.25201	-1.45723	-4.01758
C	-0.46958	-1.15996	-5.43876
C	-0.20158	0.34860	-5.51498
N	-0.00354	0.70136	-4.10755
C	-0.37204	-2.79557	-3.52102
C	0.75858	-3.62732	-3.52520
C	0.62576	-4.91589	-3.00504
C	-0.59537	-5.39439	-2.52622
C	-1.71105	-4.56226	-2.60786
C	-1.62533	-3.25752	-3.09560
C	2.07547	-3.15397	-4.07504
C	-2.84739	-2.38261	-3.12469
C	-0.70573	-6.76805	-1.91896
C	0.24997	2.04394	-3.67697
C	1.54748	2.57195	-3.75800
C	1.75991	3.86404	-3.26497
C	0.72008	4.63494	-2.74726
C	-0.57245	4.10586	-2.76218
C	-0.83577	2.82274	-3.23503
C	2.67648	1.83502	-4.42636
C	0.95677	6.02292	-2.21165
C	-2.24719	2.30833	-3.28867
C	0.71675	-1.88152	-0.53650
C	1.23508	-0.27176	0.94754
C	1.19326	0.99452	0.33391
H	-0.11531	-2.41337	-0.07631
H	0.06542	-7.44762	-2.30918
H	0.70224	0.58920	-6.09534
H	-1.04373	0.91427	-5.93936
H	-1.49848	-1.42472	-5.72742
H	0.21921	-1.74733	-6.06194
H	1.50380	-5.56687	-2.98478
H	-2.68111	-4.93201	-2.27158
H	2.77140	4.27798	-3.30258
H	-1.40366	4.70944	-2.39478
H	0.40145	6.77114	-2.79854
H	3.63060	2.04446	-3.92475
H	-1.69118	-7.21588	-2.11363
H	-0.58042	-6.71135	-0.82517
H	2.76520	2.16798	-5.47466
H	2.53664	0.74886	-4.40316
H	2.02198	6.29384	-2.23913
H	-2.44734	1.64367	-2.43389
H	-2.43837	1.73727	-4.20930
H	-2.95929	3.14307	-3.24525
H	0.60693	6.09822	-1.17052
H	-3.76053	-2.99264	-3.09503
H	-2.88849	-1.74798	-4.02168
H	-2.84952	-1.71325	-2.24921
H	2.82715	-3.95304	-4.02234

H	2.45159	-2.28423	-3.51523
H	1.98325	-2.85510	-5.13172
H	0.27792	1.55257	0.49705
H	-1.70853	-1.82191	3.87012
H	-1.47057	2.44555	3.55891
C	-2.02103	2.70085	1.01222
C	-2.56699	5.24668	-0.05422
C	-3.15190	2.91565	0.21246
C	-1.15847	3.77899	1.24769
C	-1.42692	5.03974	0.71779
C	-3.42491	4.17572	-0.31065
H	-3.83569	2.08712	0.02284
H	-0.26591	3.63679	1.85898
H	-0.73991	5.86223	0.92675
H	-4.32268	4.32580	-0.91390
H	-2.78730	6.23714	-0.45810
C	-2.24314	-2.39386	1.38874
C	-2.85676	-5.02768	0.62716
C	-1.41632	-3.46004	1.76521
C	-3.37957	-2.66691	0.61694
C	-3.68761	-3.97222	0.24794
C	-1.71487	-4.76581	1.37936
H	-0.51883	-3.26526	2.35607
H	-4.03205	-1.84487	0.31940
H	-4.58648	-4.16826	-0.34058
H	-1.04996	-5.57855	1.67883
H	-3.09866	-6.05077	0.33198
C	2.39730	1.88880	0.13154
H	2.38423	2.30531	-0.88519
H	3.33165	1.31960	0.21451
H	1.66511	-2.42083	-0.59400
H	0.35339	-0.54470	1.51154
C	2.51718	-0.90499	1.46503
H	3.16621	-1.21988	0.63728
H	3.07735	-0.12890	2.01205
C	-1.02174	0.38517	5.29482
C	-0.08689	0.46614	7.94737
C	-1.55578	-0.46876	6.26954
C	-0.01480	1.28356	5.67579
C	0.44855	1.32453	6.98844
C	-1.09258	-0.42857	7.58260
H	-2.35610	-1.16064	5.99962
H	0.42258	1.94312	4.92314
H	1.23998	2.02517	7.26186
H	-1.52606	-1.09715	8.32886
H	0.27698	0.49469	8.97588
C	2.20780	-2.03777	2.41611
C	1.49501	-4.10382	4.18416
C	1.61268	-1.75330	3.65195
C	2.44837	-3.37296	2.08431
C	2.09477	-4.39987	2.96113
C	1.25713	-2.77261	4.53049
H	1.41084	-0.71539	3.93015
H	2.91737	-3.61380	1.12736
H	2.28960	-5.43794	2.68445
H	0.78862	-2.52071	5.48446
H	1.21589	-4.90771	4.86773
C	2.35438	3.02726	1.12979
C	2.15909	5.16411	2.95274
C	2.37145	4.35184	0.68741
C	2.24421	2.78916	2.50615
C	2.15234	3.84544	3.40976
C	2.27395	5.41319	1.58670
H	2.44661	4.54870	-0.38349
H	2.21061	1.76228	2.87826
H	2.07288	3.64016	4.47954
H	2.28290	6.44039	1.21553
H	2.07797	5.99140	3.65990
Cl	2.87242	-0.41766	-1.99302

5a $TS2_E$

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.977171
E (gas phase) = -3167.52161975
E(THF)= -3167.52158177

C	-1.72183	1.10569	-2.02644
C	-1.12859	-0.17699	-1.97735
C	-1.98520	-1.30065	-2.08435
C	-3.37347	-1.12940	-2.08224
C	-3.96268	0.13361	-2.00856
C	-3.11367	1.24057	-2.01953
S	0.63261	-0.36651	-1.77620
Ru	1.35078	-0.54943	0.52216
C	3.28763	-0.65756	-0.21670
N	3.93691	-1.73185	-0.67689
C	5.36001	-1.46484	-0.92762
C	5.46574	0.04608	-0.69627
N	4.12939	0.37956	-0.19656
C	3.44607	-3.07680	-0.72809
C	3.49479	-3.86439	0.43335
C	3.01799	-5.17368	0.35732
C	2.54442	-5.71565	-0.83925
C	2.57376	-4.92078	-1.98422
C	3.00847	-3.59492	-1.95339
C	4.05071	-3.32440	1.72272
C	2.97927	-2.75022	-3.19639
C	1.99382	-7.11644	-0.88747
C	3.83192	1.66548	0.36020
C	4.18569	1.93036	1.69538
C	3.85350	3.17754	2.22128
C	3.22296	4.16022	1.45216
C	2.94449	3.88206	0.11410
C	3.25487	2.64482	-0.45947
C	4.96097	0.94683	2.53062
C	2.87358	5.49213	2.06418
C	2.99632	2.38739	-1.91622
C	0.61899	-2.18748	0.85651
C	-0.62911	-0.61043	1.76959
C	-0.27672	0.65697	1.26270
H	-0.28222	-0.83011	2.77578
C	-1.93851	-1.27659	1.38479
H	0.00545	-2.70714	0.11791
H	0.91774	-7.11148	-0.64760
H	6.22819	0.31345	0.04876
H	5.67571	0.60548	-1.62074
H	5.63067	-1.76138	-1.95044
H	5.97983	-2.04755	-0.22904
H	3.03318	-5.79165	1.25903
H	2.23760	-5.33975	-2.93413
H	4.09840	3.38832	3.26557
H	2.47419	4.64363	-0.51252
H	2.20104	5.36271	2.92618
H	4.64138	0.98266	3.58074
H	2.49283	-7.77332	-0.16045
H	2.10710	-7.55960	-1.88738
H	6.03550	1.19466	2.50029
H	4.82972	-0.08480	2.18420
H	2.37288	6.14937	1.33908
H	2.11136	1.74656	-2.05528
H	3.84694	1.87569	-2.39097
H	2.81918	3.33031	-2.44731
H	3.77622	6.00925	2.42484
H	2.77772	-3.36821	-4.08180
H	3.93013	-2.22133	-3.36144
H	2.18779	-1.98808	-3.11263
H	5.10911	-3.03727	1.61328

H	3.99664	-4.07948	2.51800
H	3.50056	-2.43213	2.05470
H	-0.86930	1.00922	0.42231
H	-4.00932	-2.01342	-2.16523
H	-3.53754	2.24723	-2.00954
H	-1.89819	-2.35201	1.60954
H	-2.11056	-1.15983	0.31031
C	-0.94375	2.37256	-2.16047
C	0.25039	4.87492	-2.60279
C	-0.24108	2.62874	-3.34505
C	-1.03209	3.38252	-1.19891
C	-0.43131	4.62299	-1.41497
C	0.34297	3.87128	-3.56849
H	-0.17198	1.84513	-4.10169
H	-1.58697	3.20606	-0.27505
H	-0.51644	5.39953	-0.65229
H	0.87374	4.05910	-4.50404
H	0.70504	5.85179	-2.77988
C	-1.49254	-2.69996	-2.24210
C	-0.78077	-5.37975	-2.69987
C	-1.92706	-3.71419	-1.38167
C	-0.69164	-3.04957	-3.33705
C	-0.35132	-4.37669	-3.57010
C	-1.56326	-5.04373	-1.59950
H	-2.56329	-3.45988	-0.53122
H	-0.35523	-2.26885	-4.02049
H	0.25396	-4.63240	-4.44233
H	-1.90759	-5.81898	-0.91216
H	-0.50625	-6.42051	-2.88242
C	0.32679	1.76329	2.11158
H	1.14742	2.24675	1.55996
H	0.76837	1.33511	3.01886
H	0.82771	-2.73347	1.78193
N	2.18900	-0.61333	2.43142
C	2.44969	-0.63234	3.58255
C	-5.43468	0.29681	-1.91062
C	-8.21425	0.62739	-1.66199
C	-6.17998	-0.52482	-1.05389
C	-6.10546	1.28721	-2.64037
C	-7.48311	1.45045	-2.51788
C	-7.55750	-0.36087	-0.93035
H	-5.66763	-1.28060	-0.45505
H	-5.54216	1.92432	-3.32545
H	-7.98995	2.22256	-3.09980
H	-8.11883	-1.00353	-0.24963
H	-9.29367	0.75696	-1.56496
C	-0.68817	2.82553	2.48018
C	-2.53980	4.82448	3.17313
C	-1.81247	2.51945	3.25369
C	-0.50447	4.14779	2.06551
C	-1.41917	5.14236	2.40748
C	-2.73111	3.50956	3.59582
H	-1.97925	1.49467	3.59224
H	0.36763	4.39164	1.45626
H	-1.25543	6.16956	2.07392
H	-3.60427	3.24503	4.19486
H	-3.26063	5.59902	3.44169
C	-3.07783	-0.64741	2.15528
C	-5.14334	0.58067	3.60372
C	-3.32657	-1.00788	3.48391
C	-3.87343	0.33743	1.56488
C	-4.90576	0.94159	2.27875
C	-4.34759	-0.39384	4.20709
H	-2.71228	-1.77726	3.95942
H	-3.67838	0.63499	0.53370
H	-5.52174	1.70146	1.79490
H	-4.52793	-0.68315	5.24419
H	-5.94940	1.05524	4.16665
O	2.74943	-0.64041	4.73728

5a $TS2_Z$

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.976298
E (gas phase) = -3167.52750727
E(THF)= -3167.52428206

C	-1.86064	1.43624	1.73163
C	-2.00418	0.17942	1.09058
C	-2.05931	-0.97968	1.90525
C	-1.78388	-0.88134	3.27223
C	-1.46600	0.33390	3.87708
C	-1.56834	1.48735	3.09884
S	-1.93036	0.04186	-0.68690
Ru	0.39509	-0.21860	-1.30689
C	-0.13758	-0.32810	-3.28726
N	-0.37720	-1.42611	-4.00829
C	-0.52320	-1.14318	-5.44035
C	-0.35777	0.38341	-5.50349
N	-0.14359	0.73414	-4.09712
C	-0.34516	-2.76467	-3.50423
C	0.86507	-3.47108	-3.50443
C	0.87826	-4.74519	-2.92804
C	-0.27292	-5.32233	-2.39428
C	-1.47339	-4.61174	-2.47471
C	-1.53433	-3.33173	-3.01997
C	2.12083	-2.91561	-4.12144
C	-2.82991	-2.57023	-3.04908
C	-0.23578	-6.67125	-1.72534
C	0.15771	2.06573	-3.66392
C	1.48217	2.52604	-3.70598
C	1.74192	3.81567	-3.22844
C	0.72631	4.64277	-2.75259
C	-0.58857	4.17088	-2.78546
C	-0.89980	2.89418	-3.24453
C	2.60456	1.71717	-4.29917
C	1.01483	6.02480	-2.22786
C	-2.32751	2.42699	-3.29101
C	0.58019	-1.88042	-0.58248
C	1.15729	-0.29148	0.92695
C	1.14548	0.97670	0.32332
H	-0.25066	-2.41075	-0.11761
H	-1.06638	-7.30842	-2.06437
H	0.50814	0.69369	-6.10740
H	-1.24978	0.89368	-5.89602
H	-1.50711	-1.48099	-5.79801
H	0.25059	-1.67820	-6.01087
H	1.82190	-5.29657	-2.89744
H	-2.38825	-5.05871	-2.08205
H	2.77312	4.17991	-3.24145
H	-1.39814	4.81493	-2.43892
H	0.46883	6.78745	-2.80437
H	3.50986	1.78914	-3.68129
H	-0.33535	-6.55764	-0.63375
H	0.70681	-7.19920	-1.92639
H	2.85168	2.10104	-5.30274
H	2.35559	0.65380	-4.37809
H	2.08671	6.26397	-2.27802
H	-2.53459	1.74943	-2.44733
H	-2.54977	1.88282	-4.22089
H	-3.01323	3.28136	-3.21839
H	0.69000	6.11198	-1.17940
H	-3.68064	-3.24734	-2.89477
H	-2.97704	-2.04401	-4.00399
H	-2.84262	-1.81387	-2.24711
H	3.00691	-3.17655	-3.52668
H	2.09595	-1.82251	-4.19591
H	2.26569	-3.33307	-5.13159

H	0.25509	1.56807	0.50647
H	-1.76650	-1.79772	3.86457
H	-1.43425	2.46398	3.56812
C	-2.02072	2.74665	1.03323
C	-2.48240	5.31151	-0.02746
C	-3.15632	3.00631	0.25386
C	-1.11153	3.78973	1.25202
C	-1.33827	5.05986	0.72486
C	-3.38748	4.27587	-0.26631
H	-3.87614	2.20594	0.07754
H	-0.21408	3.61307	1.84750
H	-0.61534	5.85429	0.92078
H	-4.28940	4.46171	-0.85321
H	-2.66989	6.30975	-0.42885
C	-2.35669	-2.34878	1.39191
C	-3.01289	-4.97640	0.63838
C	-1.54095	-3.42687	1.76032
C	-3.50182	-2.60749	0.62829
C	-3.83001	-3.90932	0.26186
C	-1.86118	-4.72899	1.38095
H	-0.63523	-3.24458	2.34189
H	-4.14554	-1.77750	0.33424
H	-4.73610	-4.09338	-0.31924
H	-1.20648	-5.55023	1.67977
H	-3.27363	-5.99709	0.35041
C	2.37983	1.81741	0.08241
H	2.35888	2.22640	-0.93688
H	3.29213	1.21089	0.15232
H	1.51904	-2.43315	-0.65832
H	0.27851	-0.54537	1.50451
C	2.43017	-0.97385	1.40443
H	3.05583	-1.29783	0.56295
H	3.02609	-0.22616	1.95315
N	2.37436	-0.36715	-1.93207
C	3.47792	-0.74240	-2.11390
C	-0.99652	0.38492	5.28343
C	0.00578	0.43008	7.91223
C	-1.52621	-0.46109	6.26736
C	0.04101	1.25716	5.64314
C	0.53754	1.28037	6.94406
C	-1.02965	-0.43869	7.56861
H	-2.34937	-1.13228	6.01443
H	0.47585	1.91014	4.88307
H	1.35193	1.96065	7.20096
H	-1.46033	-1.10055	8.32244
H	0.39562	0.44484	8.93144
C	2.11000	-2.11577	2.34115
C	1.38407	-4.19301	4.08933
C	1.54989	-1.83709	3.59447
C	2.30918	-3.45036	1.98111
C	1.94856	-4.48296	2.84825
C	1.18822	-2.86244	4.46345
H	1.38198	-0.79936	3.89502
H	2.75230	-3.68731	1.01092
H	2.11127	-5.52055	2.55000
H	0.74821	-2.61560	5.43210
H	1.10006	-5.00129	4.76562
C	2.40353	2.96247	1.07430
C	2.30821	5.10964	2.89201
C	2.44766	4.28402	0.62566
C	2.31792	2.73210	2.45372
C	2.27460	3.79336	3.35484
C	2.40028	5.35065	1.52291
H	2.50329	4.47536	-0.44731
H	2.26434	1.70788	2.83079
H	2.21182	3.59358	4.42673
H	2.43029	6.37589	1.14758
H	2.26553	5.94145	3.59716
O	4.59959	-1.09561	-2.32321

3(I)

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.549542
E (gas phase) = -2402.61549067
E(THF)= -2402.62841371
E(DCM)= -2402.63743054

Ru	-0.10778	-0.64518	1.28008
Cl	-1.27886	0.27955	3.07095
N	0.59996	2.02272	0.05343
N	1.92152	1.37668	1.65615
C	-3.20893	-1.95337	-1.13480
C	-4.28273	-2.84298	-1.10218
H	-4.85257	-3.01109	-2.01578
C	-4.62913	-3.48708	0.08285
H	-5.47135	-4.18145	0.09328
C	-3.91346	-3.23421	1.25240
H	-4.18828	-3.72683	2.18578
C	-2.86445	-2.32412	1.23320
H	-2.35062	-2.08378	2.16650
C	-2.48567	-1.66476	0.04751
C	-1.40299	-0.68342	0.00931
H	-1.41563	-0.05334	-0.87310
C	-2.07431	-1.98162	-3.26895
H	-1.89182	-1.18222	-4.00237
C	-0.74571	-2.43357	-2.68560
H	-0.20143	-1.59825	-2.22626
H	-0.11769	-2.85647	-3.48407
H	-0.88018	-3.20792	-1.91516
C	-2.82105	-3.11441	-3.96188
H	-2.98170	-3.96626	-3.28387
H	-2.22975	-3.47445	-4.81754
H	-3.79578	-2.76911	-4.33692
C	0.85868	1.01316	0.90600
C	-0.30506	1.98538	-1.04725
C	-1.59009	2.51820	-0.88895
C	-2.01979	3.09678	0.43147
H	-3.03057	3.52019	0.36399
H	-1.33872	3.89335	0.76850
H	-2.01840	2.31915	1.21234
C	-2.47662	2.41191	-1.96072
H	-3.49511	2.79046	-1.84347
C	-2.10827	1.79995	-3.16107
C	-3.12131	1.59084	-4.25375
H	-3.70480	0.68156	-4.03421
H	-2.64139	1.45937	-5.23412
H	-3.82543	2.43246	-4.32290
C	-0.80492	1.31700	-3.29274
H	-0.49947	0.84187	-4.22885
C	0.11168	1.38634	-2.24286
C	1.46879	0.74332	-2.35461
H	1.65575	0.39808	-3.38009
H	1.53697	-0.12891	-1.68368
H	2.28199	1.42981	-2.07490
C	1.55333	3.12862	0.16430
H	1.02023	4.08207	0.28502
H	2.16628	3.19620	-0.74906
C	2.37114	2.74271	1.39783
H	3.45590	2.76663	1.22161
H	2.15065	3.38323	2.26665
C	2.60809	0.54108	2.59338
C	3.63342	-0.29129	2.10404
C	4.03177	-0.25285	0.65329
H	3.20414	-0.57982	0.00999
H	4.88497	-0.91861	0.46811
H	4.32387	0.76465	0.34685
C	4.28797	-1.12551	3.00374

H	5.07149	-1.79097	2.63275
C	3.96708	-1.13370	4.36587
C	3.00230	-0.24147	4.82560
H	2.77006	-0.20343	5.89315
C	2.32056	0.62347	3.96175
C	1.38278	1.65337	4.53195
H	0.75600	1.21678	5.32129
H	0.70708	2.06727	3.77567
H	1.96592	2.47545	4.97992
C	4.65558	-2.09005	5.30406
H	4.51492	-1.79842	6.35418
H	5.73582	-2.14075	5.10163
H	4.25066	-3.10730	5.18108
Cl	1.30787	-2.30796	0.47531
O	-2.90161	-1.30045	-2.29750

3(II)

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 1.13431
E (gas phase) = -4805.27966749
E(THF)= -4805.27607732
E(DCM)= -4805.29388181

Ru	-0.23608	-0.18915	-1.79169
Cl	1.54649	-0.54061	-0.10493
Cl	-2.08625	0.01435	-3.28919
C	0.74921	1.18536	-2.45912
H	1.82053	1.16123	-2.21586
C	0.40490	-1.66900	-3.00140
C	1.38888	-3.10286	-4.57596
H	2.41088	-3.50291	-4.49812
H	1.12961	-3.04780	-5.64406
C	0.36992	-3.89716	-3.75838
H	-0.42700	-4.33796	-4.37544
H	0.83210	-4.70291	-3.16649
C	2.15741	-0.75861	-4.54899
C	3.45573	-0.58638	-4.04727
C	4.31365	0.27935	-4.72856
H	5.32676	0.42794	-4.34514
C	3.91792	0.93593	-5.89759
C	2.61896	0.73711	-6.36542
H	2.28421	1.26454	-7.26204
C	1.71289	-0.08848	-5.69659
C	-1.12136	-3.22682	-1.85241
C	-2.49521	-3.25456	-2.15285
C	-3.38332	-3.54150	-1.11722
H	-4.45565	-3.53061	-1.33020
C	-2.94221	-3.85473	0.17052
C	-1.57019	-3.93504	0.40055
H	-1.20591	-4.24532	1.38213
C	-0.64119	-3.63161	-0.59675
C	3.90583	-1.31161	-2.80841
H	3.33819	-0.98018	-1.92578
H	4.97295	-1.13758	-2.61679
H	3.74887	-2.39807	-2.89608
C	4.85661	1.88227	-6.60037
H	4.85034	2.87008	-6.11033
H	4.56682	2.03095	-7.65014
H	5.89249	1.51333	-6.57797
C	0.28762	-0.21107	-6.15698
H	0.00619	-1.25530	-6.36531
H	0.11998	0.37472	-7.07022
H	-0.40098	0.14966	-5.37512
C	-3.01583	-3.08192	-3.55416
H	-2.29288	-2.57832	-4.20448
H	-3.93153	-2.47595	-3.55819
H	-3.25911	-4.07127	-3.97836
C	-3.92537	-4.09737	1.28524
H	-4.20566	-3.14141	1.75827
H	-3.49369	-4.73603	2.06869
H	-4.84891	-4.56644	0.91514
C	0.82424	-3.81629	-0.31394
H	1.11038	-3.26743	0.58997
H	1.46297	-3.45346	-1.12818
H	1.03841	-4.88507	-0.14880
N	1.32359	-1.76489	-3.97327
N	-0.17965	-2.87574	-2.87182
Ru	0.38016	0.26028	1.92286
Cl	-1.41337	0.61090	0.21909
Cl	2.29413	0.09584	3.32986
C	-0.69218	-1.04910	2.59712
H	-1.76068	-0.86990	2.42363
C	-0.19414	1.72499	3.16682
C	-1.01034	3.09635	4.88068
H	-2.02339	3.51106	4.98335
H	-0.59064	2.97017	5.89110
C	-0.10702	3.93010	3.97027
H	0.71172	4.42360	4.51261
H	-0.66459	4.69867	3.41010
C	-1.92372	0.79358	4.71119
C	-3.24195	0.74031	4.23195
C	-4.12501	-0.15667	4.83307
H	-5.15416	-0.21095	4.46761
C	-3.72625	-0.97952	5.89128
C	-2.40519	-0.90605	6.33107
H	-2.07109	-1.56322	7.13766
C	-1.48120	-0.03264	5.75124
C	1.21857	3.28326	1.92335
C	2.61885	3.31453	2.03303
C	3.35684	3.55885	0.87445
H	4.44831	3.54861	0.93876
C	2.74433	3.81451	-0.35380
C	1.35259	3.89443	-0.39726
H	0.85614	4.15361	-1.33419
C	0.57081	3.64414	0.73084
C	-3.67490	1.61037	3.08263
H	-3.13205	1.34318	2.16197
H	-4.75021	1.50100	2.88919
H	-3.47083	2.67473	3.27800
C	-4.69417	-1.96152	6.49868
H	-4.88228	-2.79991	5.80794
H	-4.30635	-2.38221	7.43671
H	-5.66557	-1.48942	6.70901
C	-0.04528	-0.01566	6.19423
H	0.26736	0.98283	6.53782
H	0.11760	-0.72314	7.01790
H	0.62292	-0.28298	5.35975
C	3.32689	3.17576	3.35320
H	2.67918	2.74408	4.12348
H	4.20222	2.51926	3.25958
H	3.67664	4.16758	3.68670
C	3.56774	3.99142	-1.60234
H	3.84587	3.00737	-2.01608
H	3.00981	4.52871	-2.38186
H	4.50074	4.53685	-1.39641
C	-0.91796	3.84411	0.65655
H	-1.29039	3.49198	-0.31069
H	-1.46259	3.30423	1.44001
H	-1.14972	4.91922	0.75036
N	-1.05508	1.80059	4.19234
N	0.41641	2.92209	3.05344
C	-0.53362	-2.34785	3.25770
C	-0.59674	-4.85380	4.54570
C	-1.70663	-2.85830	3.84288
C	0.62953	-3.16300	3.29906
C	0.57662	-4.40853	3.94517
C	-1.75332	-4.07949	4.49960

H	-2.61001	-2.25060	3.77182
H	1.45724	-5.04705	3.97303
H	-2.68092	-4.42730	4.95593
H	-0.60300	-5.82693	5.04111
C	0.43175	2.33639	-3.31273
C	0.03689	4.23717	-5.34411
C	1.47166	2.73119	-4.16875
C	-0.79801	3.04276	-3.39741
C	-0.99360	3.94327	-4.45440
C	1.29314	3.66171	-5.18456
H	2.43986	2.24381	-4.04643
H	-1.95128	4.44359	-4.57936
H	2.11856	3.91605	-5.85075
H	-0.14652	4.95038	-6.15036
O	1.70417	-2.73152	2.62884
C	2.97659	-3.38612	2.74690
H	2.83260	-4.46572	2.55377
C	3.58150	-3.16901	4.12855
H	4.54417	-3.69847	4.19580
H	2.92956	-3.54216	4.93079
H	3.74624	-2.09494	4.29084
C	3.84416	-2.79718	1.64762
H	4.84460	-3.25407	1.68292
H	3.93196	-1.71043	1.78816
H	3.40661	-2.97997	0.65695
O	-1.68251	2.86678	-2.40107
C	-3.02795	3.35760	-2.52170
H	-3.35824	3.18158	-3.55980
C	-3.88066	2.52211	-1.58267
H	-3.79475	1.45826	-1.83558
H	-4.93190	2.83896	-1.66298
H	-3.55110	2.65893	-0.54162
C	-3.11112	4.84373	-2.17548
H	-4.12964	5.21102	-2.37461
H	-2.40685	5.45596	-2.75452
H	-2.89698	4.99894	-1.10814

3_{AC}(I)

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.38749
E (gas phase) = -1978.72808659
E(THF)= -1978.74362522
E(DCM)= -1978.75049549

C	2.68473	3.19331	0.58530
C	2.43729	3.07399	-0.78796
C	1.92288	4.13119	-1.54906
C	1.66511	5.33887	-0.89834
C	1.90718	5.50284	0.46837
C	2.41176	4.41982	1.19341
N	2.71959	1.83538	-1.43346
C	1.88865	0.79313	-1.60562
N	2.56469	-0.16304	-2.27432
C	3.94002	0.21017	-2.59553
C	4.04986	1.61867	-2.00615
C	2.05048	-1.43671	-2.67600
C	2.21889	-2.54291	-1.82713
C	1.67553	-3.76431	-2.22749
C	1.01256	-3.91169	-3.44647
C	0.94239	-2.81094	-4.30205
C	1.46858	-1.56862	-3.94814
C	3.03218	-2.46641	-0.56216
C	1.47749	-0.44684	-4.95273
C	0.37951	-5.22440	-3.82715
Ru	0.03099	0.54514	-1.04890
Cl	-0.97062	0.81890	-3.12347
C	1.58479	3.93643	-3.00274
C	1.64783	6.82559	1.14187
C	3.15221	2.00780	1.38614
C	-0.40912	2.06110	-0.22127
H	0.15563	2.96923	-0.02632
H	-1.44833	2.04983	0.15053
H	4.09381	0.18993	-3.68497
H	4.64288	-0.50111	-2.13603
H	4.81840	1.69610	-1.22237
H	4.26582	2.38508	-2.76584
H	0.46467	-2.91931	-5.27920
H	1.77826	-4.62664	-1.56371
H	2.58651	4.52769	2.26699
H	1.25126	6.17117	-1.47347
H	2.33675	-0.56683	-5.63461
H	0.56281	-0.45954	-5.55976
H	1.54098	0.53938	-4.47898
H	0.39117	-5.37653	-4.91599
H	0.89418	-6.07262	-3.35366
H	-0.67271	-5.25092	-3.50073
H	4.05481	-2.83199	-0.75742
H	3.09363	-1.44697	-0.16475
H	2.59393	-3.09702	0.22246
H	3.35235	2.29167	2.42769
H	2.38777	1.21374	1.38396
H	4.07398	1.57097	0.97191
H	0.82724	7.37043	0.65387
H	1.39014	6.69258	2.20216
H	2.54365	7.46609	1.09651
H	2.44589	3.56224	-3.57764
H	0.77417	3.19807	-3.11552
H	1.25830	4.87972	-3.45995
Cl	0.43310	-0.88273	0.73480

3_{AC}(II)

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.806783
E (gas phase) = -3957.52062558
E(THF)= -3957.53516616
E(DCM)= -3957.54854144

Ru	5.57379	13.24719	14.71516
Cl	7.24920	12.85781	16.45686
Cl	3.81259	13.83376	13.22128
C	6.68486	14.38127	13.88374
H	7.70330	14.56268	14.24100
C	6.07036	11.62713	13.64904
C	6.87784	10.06802	12.10328
H	7.90381	9.67578	12.05087
H	6.44660	10.02822	11.09139
C	6.01071	9.34077	13.13833
H	5.17318	8.79303	12.68377
H	6.58948	8.63540	13.75518
C	7.72503	12.43409	11.99868
C	9.01344	12.62349	12.52484
C	9.82474	13.59611	11.94335
H	10.82629	13.76162	12.34986
C	9.38769	14.36471	10.86006
C	8.11203	14.12898	10.34788
H	7.75806	14.71716	9.49742
C	7.26182	13.16477	10.89752
C	4.75083	10.20909	15.15414
C	3.34786	10.29460	15.08869
C	2.62376	10.09129	16.26364
H	1.53441	10.17260	16.22817
C	3.24962	9.77455	17.47214
C	4.63675	9.63155	17.48285
H	5.14533	9.36256	18.41202

C	5.40952	9.83534	16.33701
C	9.48708	11.82988	13.71179
H	8.92785	12.10727	14.61853
H	10.55387	12.00708	13.90244
H	9.34527	10.74823	13.56417
C	10.28774	15.41673	10.26499
H	10.58731	16.15373	11.02623
H	9.79198	15.95653	9.44657
H	11.21019	14.96689	9.86564
C	5.87671	12.95072	10.35420
H	5.71944	11.90490	10.04721
H	5.69849	13.58715	9.47725
H	5.11931	13.18856	11.11886
C	2.64394	10.56335	13.78754
H	2.98208	9.86754	13.00367
H	2.84309	11.58529	13.43064
H	1.55882	10.44125	13.90389
C	2.44558	9.61590	18.73640
H	2.25066	10.59984	19.19636
H	2.98031	9.00696	19.47926
H	1.47162	9.14529	18.53701
C	6.89475	9.59500	16.40480
H	7.30284	9.98432	17.34773
H	7.43852	10.08463	15.58820
H	7.10188	8.51235	16.36405
N	6.88216	11.44865	12.59706
N	5.51740	10.44296	13.96423
Ru	5.84764	13.54909	18.33348
Cl	4.34683	14.29772	16.54028
Cl	7.38684	12.49943	19.82433
C	4.56072	12.43285	18.89493
H	3.57164	12.41731	18.42558
C	5.40057	15.00954	19.61154
C	4.62026	16.43104	21.29090
H	3.64651	16.93958	21.33188
H	4.96515	16.27093	22.32413
C	5.65447	17.18466	20.44101
H	6.48323	17.58829	21.03909
H	5.20558	18.01206	19.86849
C	3.52708	14.17379	20.97672
C	2.28171	14.18129	20.33543
C	1.35120	13.20162	20.69152
H	0.38028	13.18907	20.18965
C	1.63638	12.23911	21.66057
C	2.87942	12.28223	22.29912
H	3.11370	11.53952	23.06638
C	3.84006	13.24059	21.97747
C	7.04594	16.35336	18.45517
C	8.40059	16.02326	18.64237
C	9.24489	16.08294	17.53520
H	10.29237	15.79658	17.65802
C	8.78321	16.47822	16.27705
C	7.45871	16.89576	16.15412
H	7.09148	17.24857	15.18712
C	6.57273	16.85787	17.23301
C	1.97437	15.18204	19.25528
H	2.55659	14.96478	18.34620
H	0.90955	15.15840	18.98871
H	2.22566	16.20809	19.56393
C	0.64101	11.16142	22.00466
H	0.98277	10.18323	21.62948
H	0.51516	11.06769	23.09376
H	-0.34390	11.36467	21.56193
C	5.18913	13.24260	22.64069
H	5.41047	14.21414	23.10920
H	5.24036	12.47428	23.42354
H	5.98271	13.04063	21.90264
C	8.92179	15.62686	19.99579
H	8.52201	14.64704	20.29736
H	10.01785	15.56074	19.98212
H	8.63493	16.36368	20.76227
C	9.69899	16.43398	15.08175
H	9.88485	15.38903	14.78208
H	9.26321	16.95471	14.21753
H	10.67546	16.88918	15.30589
C	5.17675	17.39988	17.07604
H	4.81456	17.25417	16.05017
H	4.45918	16.91218	17.74753
H	5.17037	18.48225	17.28968
N	4.49956	15.14665	20.59268
N	6.12624	16.13962	19.53524
H	6.35626	14.98364	13.03074
H	4.73357	11.68910	19.67871

$3a_{AC}$(I)

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.703119
E (gas phase) = -2840.78563508
E(THF)= -2840.79390142
E(DCM)= -2840.80466467

Ru	-0.05007	0.30389	-0.92331
C	2.40159	3.18136	0.62452
C	2.08407	3.06541	-0.73312
C	1.42218	4.08163	-1.43583
C	1.08566	5.24334	-0.74169
C	1.39807	5.40502	0.61232
C	2.05278	4.36671	1.27635
N	2.45446	1.88030	-1.43199
C	1.75382	0.73719	-1.55194
N	2.51063	-0.12336	-2.26815
C	3.78632	0.44104	-2.70313
C	3.77243	1.83005	-2.06548
C	2.19362	-1.46815	-2.63805
C	2.61657	-2.51833	-1.80524
C	2.35427	-3.82557	-2.20914
C	1.71921	-4.10868	-3.41921
C	1.34699	-3.04462	-4.23806
C	1.59172	-1.71679	-3.88080
C	3.41009	-2.27620	-0.54787
C	1.29387	-0.61754	-4.86566
C	1.49696	-5.53501	-3.84889
Cl	-1.22252	0.40655	-2.94256
C	1.01263	3.87571	-2.86942
C	1.04612	6.68181	1.33144
C	3.00960	2.03186	1.37895
C	-0.57985	1.77651	-0.05739
H	-0.11774	2.74227	0.12456
H	-1.59061	1.64003	0.36749
H	3.82845	0.47667	-3.80289
H	4.61903	-0.18513	-2.34930
H	4.56180	1.96257	-1.30898
H	3.87333	2.64167	-2.80134
H	0.86192	-3.24793	-5.19639
H	2.66435	-4.64869	-1.55977
H	2.28614	4.46864	2.33868
H	0.55414	6.03995	-1.26897
H	2.07596	-0.59307	-5.64347
H	0.33053	-0.79216	-5.36297
H	1.23804	0.36786	-4.38991
H	2.42611	-5.96802	-4.25409
H	1.18463	-6.16272	-3.00152
H	0.72832	-5.60542	-4.63140
H	3.32101	-1.24520	-0.18391
H	3.07465	-2.94249	0.25821
H	4.47793	-2.48219	-0.73184
H	3.38327	2.35638	2.35825

H	2.25075	1.24937	1.54881
H	3.83969	1.56533	0.82776
H	0.07054	7.06966	1.00387
H	1.00853	6.53295	2.41994
H	1.79588	7.46369	1.12859
H	1.86933	3.60721	-3.50676
H	0.28179	3.05391	-2.94598
H	0.55601	4.78476	-3.28262
S	0.65053	-1.08165	0.79106
C	-0.98395	-1.13851	1.51190
C	-3.64617	-0.95189	2.46816
C	-2.01010	-1.91367	0.93048
C	-1.29865	-0.29553	2.60336
C	-2.61421	-0.21446	3.05843
C	-3.31951	-1.80171	1.41145
H	-2.83913	0.45946	3.88804
H	-4.09305	-2.42534	0.95871
C	-5.04357	-0.84067	2.95902
C	-7.69029	-0.62543	3.88300
C	-5.32022	-0.76688	4.33091
C	-6.11674	-0.80489	2.05822
C	-7.42777	-0.69851	2.51574
C	-6.63118	-0.66012	4.78883
C	-0.27988	0.56256	3.27331
C	1.53730	2.19164	4.66403
C	-0.45442	1.95004	3.32025
C	0.82404	0.00232	3.92921
C	1.72243	0.80864	4.62094
C	0.44849	2.76011	4.00854
C	-1.76749	-2.87402	-0.18556
C	-1.45686	-4.75357	-2.23914
C	-0.98275	-4.01610	0.01153
C	-2.38174	-2.67874	-1.42542
C	-2.21834	-3.60866	-2.45123
C	-0.83609	-4.95318	-1.00550
H	0.96721	-1.07903	3.90312
H	2.57152	0.35423	5.13507
H	2.24119	2.82267	5.21062
H	0.29268	3.84032	4.03357
H	-1.31109	2.39931	2.81407
H	-0.49589	-4.17046	0.97618
H	-0.23322	-5.84761	-0.83377
H	-1.34122	-5.49001	-3.03624
H	-2.69034	-3.43126	-3.41895
H	-2.97545	-1.77906	-1.59740
H	-4.49863	-0.81619	5.04856
H	-6.82674	-0.61166	5.86173
H	-8.71775	-0.54192	4.24165
H	-8.24949	-0.66478	1.79791
H	-5.91843	-0.83979	0.98496

$3a_{AC}$(II)

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 1.442295
E (gas phase) = -5681.60236092
E(THF)= -5681.59167004
E(DCM)= -5681.61334102

Ru	-1.52026	0.13936	-3.07721
C	-2.59578	-1.27859	-2.79585
C	-2.96314	1.46632	-3.37762
C	-4.91299	2.74756	-3.50180
H	-5.58774	3.09711	-2.71009
H	-5.50079	2.61334	-4.42582
C	-3.70482	3.65942	-3.69536
H	-3.77036	4.28353	-4.59615
H	-3.53473	4.31464	-2.82480
C	-5.10188	0.36732	-2.75890
C	-5.63410	0.31748	-1.46272
C	-6.44323	-0.76577	-1.12402
H	-6.85507	-0.81725	-0.11176
C	-6.72229	-1.78771	-2.03333
C	-6.21525	-1.67999	-3.32865
H	-6.45039	-2.45474	-4.06284
C	-5.42119	-0.60038	-3.72400
C	-1.38921	3.02690	-4.48962
C	-1.33653	2.83899	-5.88156
C	-0.14712	3.13947	-6.54129
H	-0.08605	2.97187	-7.61944
C	0.96350	3.64182	-5.85915
C	0.84817	3.88427	-4.49193
H	1.69176	4.31900	-3.94955
C	-0.31805	3.58671	-3.78340
C	-5.37750	1.41540	-0.46983
H	-4.40789	1.89528	-0.64904
H	-5.37963	1.02881	0.55770
H	-6.16115	2.18979	-0.53375
C	-7.54953	-2.97350	-1.61047
H	-7.03586	-3.54360	-0.81954
H	-7.73709	-3.65667	-2.45019
H	-8.52199	-2.65661	-1.20335
C	-4.93845	-0.47749	-5.14386
H	-5.15818	0.52134	-5.55194
H	-5.43087	-1.21946	-5.78627
H	-3.84983	-0.62250	-5.22296
C	-2.52854	2.32392	-6.64030
H	-2.73083	1.28008	-6.36088
H	-2.34387	2.35542	-7.72219
H	-3.43216	2.91944	-6.43396
C	2.26044	3.89642	-6.58130
H	2.85064	2.96745	-6.64359
H	2.87274	4.64580	-6.05902
H	2.08948	4.24666	-7.60973
C	-0.40118	3.86746	-2.31361
H	-1.30384	4.43768	-2.05264
H	0.46772	4.44970	-1.98031
H	-0.43755	2.94056	-1.72264
N	-4.28401	1.47801	-3.12334
N	-2.61089	2.69394	-3.81404
Ru	1.21541	0.12502	-0.48601
C	1.94440	1.75625	-0.30089
C	2.95527	-0.81408	-1.13148
C	5.00169	-1.04114	-2.28634
H	5.28285	-0.58091	-3.24344
H	5.92305	-1.18433	-1.69804
C	4.19741	-2.31855	-2.45252
H	4.72782	-3.21605	-2.10338
H	3.87717	-2.49101	-3.49140
C	4.58704	1.09951	-1.17508
C	4.56821	2.16444	-2.08935
C	5.18953	3.35773	-1.71602
H	5.16673	4.20103	-2.41173
C	5.85211	3.49677	-0.49555
C	5.90035	2.39684	0.36090
H	6.45031	2.47746	1.30160
C	5.27032	1.19324	0.04652
C	2.26470	-3.25186	-1.30600
C	2.62852	-3.96142	-0.14581
C	2.14888	-5.25838	0.01614
H	2.43279	-5.82203	0.90818
C	1.34207	-5.86875	-0.94949
C	1.00482	-5.13953	-2.08643
H	0.36545	-5.59545	-2.84705
C	1.44649	-3.82667	-2.28936
C	3.88282	2.06074	-3.42419
H	2.79645	2.20322	-3.32528
H	4.26468	2.82345	-4.11671

H	4.01121	1.07417	-3.88924
C	6.48085	4.80800	-0.10350
H	5.73059	5.46981	0.35990
H	7.29122	4.66447	0.62554
H	6.89184	5.33677	-0.97569
C	5.30215	0.02065	0.98669
H	5.64600	-0.89629	0.48545
H	5.97136	0.20415	1.83749
H	4.29555	-0.18681	1.38155
C	3.56436	-3.34124	0.85474
H	3.13277	-2.42879	1.29115
H	3.79268	-4.03600	1.67358
H	4.51799	-3.05612	0.38252
C	0.79782	-7.25423	-0.72403
H	-0.10906	-7.20864	-0.09790
H	0.52449	-7.74103	-1.67080
H	1.52482	-7.89400	-0.20263
C	1.02627	-3.09977	-3.53634
H	-0.02414	-2.77925	-3.45185
H	1.60440	-2.18876	-3.72208
H	1.09454	-3.75627	-4.41537
N	4.07031	-0.17651	-1.55648
N	3.02111	-2.07227	-1.60716
S	0.75184	-0.13077	1.84438
C	1.93493	-0.64186	3.06913
C	3.94794	-1.59767	4.83340
C	2.90629	0.23949	3.60313
C	1.86979	-1.95561	3.60009
C	2.88593	-2.41585	4.44116
C	3.90700	-0.25872	4.44432
H	2.81438	-3.42956	4.84162
H	4.66940	0.43039	4.81423
S	-1.15112	0.66704	-0.71793
C	-2.26445	0.56619	0.68486
C	-3.99963	0.60540	2.93855
C	-2.53745	1.77018	1.37316
C	-2.88545	-0.62137	1.13332
C	-3.73954	-0.57231	2.24124
C	-3.38526	1.77102	2.48307
H	-4.18004	-1.50854	2.58839
H	-3.58090	2.72015	2.98596
C	-1.99829	3.10692	0.97931
C	-1.06339	5.70840	0.49292
C	-2.87891	4.11819	0.57632
C	-0.64406	3.41416	1.13539
C	-0.18138	4.70488	0.89328
C	-2.41522	5.41094	0.33165
H	-3.94290	3.89316	0.47366
H	0.03877	2.63275	1.47188
H	0.87954	4.92410	1.02931
H	-3.11627	6.19008	0.02460
C	-2.71614	-1.96789	0.52368
C	-2.47375	-4.56056	-0.51911
C	-3.85253	-2.70500	0.16431
C	-1.46005	-2.55923	0.38565
C	-1.34533	-3.84715	-0.12037
C	-3.73462	-3.98651	-0.36895
H	-4.83836	-2.25096	0.26951
H	-0.57531	-2.03215	0.73990
H	-0.36011	-4.29883	-0.17576
H	-4.63048	-4.53343	-0.67018
H	-2.37021	-5.56695	-0.93093
C	0.70270	-2.86302	3.38829
C	-1.47774	-4.63615	3.23533
C	-0.59496	-2.43489	3.70541
C	0.88353	-4.19446	3.00519
C	-0.19582	-5.07287	2.91646
C	-1.66976	-3.31437	3.63729
H	-0.76006	-1.40181	4.01407
H	1.88831	-4.54895	2.77613
H	-0.02887	-6.10362	2.59629
H	-2.66888	-2.96047	3.89713
H	-2.32697	-5.31755	3.16251
C	2.87415	1.71700	3.39715
C	2.85689	4.52835	3.23230
C	4.03405	2.42823	3.08066
C	1.70259	2.44449	3.65481
C	1.69765	3.83320	3.58284
C	4.02734	3.81894	2.98137
H	4.95952	1.88154	2.90985
H	0.78939	1.91091	3.91933
H	0.77560	4.37825	3.79205
H	4.94515	4.34574	2.71205
H	2.84580	5.61821	3.16637
C	5.04338	-2.12182	5.68763
C	7.12836	-3.12975	7.28635
C	5.58418	-3.39257	5.44718
C	5.56619	-1.36623	6.74622
C	6.59890	-1.86448	7.53673
C	6.61547	-3.89270	6.23838
H	5.20069	-3.98758	4.61544
H	5.14149	-0.38491	6.96729
H	6.98640	-1.26292	8.36126
H	7.02589	-4.88274	6.03028
H	7.93665	-3.52046	7.90709
C	-4.90279	0.61623	4.11642
C	-6.61604	0.63431	6.34543
C	-6.08310	-0.13951	4.12001
C	-4.59579	1.38095	5.24980
C	-5.44447	1.39001	6.35396
C	-6.93214	-0.13101	5.22386
H	-6.34718	-0.72744	3.23817
H	-3.66859	1.95713	5.27323
H	-5.18372	1.98527	7.23103
H	-7.85013	-0.72150	5.20523
H	-7.28043	0.64075	7.21129
H	-2.78147	-1.99742	-3.60153
H	-3.01562	-1.53820	-1.82673
H	2.21094	2.17236	0.67579
H	2.06892	2.43493	-1.15107
H	-0.69761	6.71990	0.30614
Cl	-1.24204	-0.57913	-5.34387
Cl	0.93028	0.33772	-2.94155

$3a_{AC}$(III)

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.385793
E (gas phase) = -1978.72807900
E(THF)= -1978.74376838
E(DCM)= -1978.75059431

C	2.41618	3.19359	0.61933
C	2.09626	3.06956	-0.73846
C	1.38258	4.05579	-1.43096
C	0.99540	5.19691	-0.72654
C	1.30250	5.36414	0.62669
C	2.00835	4.35206	1.28285
N	2.51166	1.90034	-1.43907
C	1.83834	0.74516	-1.57628
N	2.60318	-0.08967	-2.30868
C	3.88100	0.49170	-2.71252
C	3.81737	1.89416	-2.10219
C	2.27152	-1.43074	-2.68221
C	2.67191	-2.49086	-1.85162
C	2.30624	-3.78559	-2.21995
C	1.59430	-4.04490	-3.39226
C	1.29057	-2.97518	-4.23534

C	1.63394	-1.66189	-3.91223
C	3.54509	-2.27588	-0.64373
C	1.39632	-0.56083	-4.91156
C	1.15715	-5.44517	-3.73432
Ru	0.07736	0.21562	-0.91208
Cl	-1.07237	0.38574	-2.91991
C	0.97986	3.84589	-2.86589
C	0.89758	6.61820	1.35739
C	3.10454	2.07263	1.35076
C	-0.52370	1.63463	-0.01631
H	-0.08309	2.61000	0.17399
H	-1.52637	1.46592	0.41324
H	3.96062	0.50663	-3.80998
H	4.71321	-0.10919	-2.31574
H	4.61689	2.07881	-1.36889
H	3.86344	2.69251	-2.85822
H	0.77181	-3.16462	-5.17863
H	2.59049	-4.61631	-1.56889
H	2.23765	4.46051	2.34607
H	0.42624	5.97143	-1.24708
H	2.20352	-0.56370	-5.66385
H	0.44504	-0.71079	-5.43878
H	1.35682	0.42892	-4.44276
H	1.85690	-6.19416	-3.33662
H	0.16641	-5.65406	-3.29932
H	1.07783	-5.58854	-4.82142
H	3.45513	-1.26222	-0.23691
H	3.27900	-2.97526	0.15960
H	4.60005	-2.45608	-0.91255
H	3.34004	2.36321	2.38301
H	2.46099	1.17825	1.38091
H	4.04469	1.77841	0.85932
H	-0.03086	7.03985	0.94670
H	0.74428	6.42692	2.42890
H	1.67972	7.38948	1.26692
H	1.84668	3.62150	-3.50643
H	0.28451	2.99505	-2.95191
H	0.48461	4.73879	-3.26952
Cl	0.78201	-1.17719	0.80407

$3a_{AC}$(IV), $5a_{AC}$(IV)

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 1.022574
E (gas phase) = -3702.84784123
E(THF)= -3702.83680026
E(DCM)= -3702.85262541

C	5.21441	0.50250	2.52422
C	4.23000	1.17442	1.79026
C	3.22210	1.92531	2.41013
C	3.21678	1.98712	3.80313
C	4.18046	1.32731	4.57221
C	5.17424	0.59993	3.91709
N	4.25671	1.08364	0.36796
C	3.73849	0.10871	-0.40902
N	4.13901	0.35707	-1.67543
C	4.99509	1.53414	-1.80305
C	5.04874	2.06642	-0.37180
C	3.90900	-0.44880	-2.83418
C	4.82863	-1.46321	-3.14801
C	4.60166	-2.22824	-4.29109
C	3.52204	-1.97694	-5.13876
C	2.66900	-0.91892	-4.83110
C	2.84727	-0.13119	-3.69273
C	6.08060	-1.68055	-2.33821
C	1.95477	1.05952	-3.47260
C	3.30802	-2.78432	-6.39225
Ru	2.56715	-1.38656	0.11570
C	2.12776	2.55996	1.59721
C	4.11553	1.37311	6.07701
C	6.21024	-0.39505	1.84268
C	2.56199	-1.29077	1.89940
H	3.01569	-0.63903	2.63569
H	1.93556	-2.09536	2.30657
H	4.55164	2.25050	-2.51080
H	5.98461	1.24275	-2.18812
H	6.07161	2.11245	0.03207
H	4.60280	3.06798	-0.27100
H	1.83718	-0.68496	-5.49845
H	5.29556	-3.03879	-4.52865
H	5.92567	0.06528	4.50241
H	2.42882	2.55608	4.30424
H	2.12401	1.80399	-4.26766
H	0.89908	0.76486	-3.50818
H	2.12696	1.53784	-2.50131
H	3.66116	-2.23167	-7.27822
H	3.85042	-3.73938	-6.35535
H	2.24077	-3.00374	-6.54234
H	5.96603	-1.37558	-1.29029
H	6.37277	-2.73889	-2.34579
H	6.91393	-1.10057	-2.77067
H	7.00829	-0.69439	2.53408
H	5.70665	-1.31211	1.49167
H	6.67271	0.08305	0.96592
H	3.27202	0.76765	6.44643
H	5.03503	0.97989	6.53261
H	3.96500	2.40046	6.44124
H	2.52623	3.19132	0.78856
H	1.50706	1.78198	1.12307
H	1.48140	3.18545	2.22771
S	4.06077	-3.14111	-0.29041
C	2.97778	-4.32944	0.49493
C	1.01945	-5.90036	1.82626
C	1.94824	-4.96650	-0.23485
C	3.07045	-4.57347	1.88890
C	2.09054	-5.33488	2.52611
C	0.99017	-5.72854	0.44390
H	2.16387	-5.47050	3.60704
H	0.21538	-6.22643	-0.14130
C	-0.05897	-6.64869	2.52221
C	-2.12695	-8.02738	3.84384
C	-1.37626	-6.60785	2.03974
C	0.20116	-7.39820	3.67810
C	-0.82220	-8.07911	4.33278
C	-2.39919	-7.29055	2.69241
C	4.16936	-4.01947	2.73114
C	6.23085	-3.07588	4.39371
C	3.87847	-3.30545	3.90019
C	5.51251	-4.26177	2.41372
C	6.53280	-3.79856	3.23846
C	4.90008	-2.83069	4.72142
C	1.83361	-4.92822	-1.72012
C	1.50101	-5.15572	-4.50135
C	2.91958	-5.24498	-2.54572
C	0.58614	-4.70719	-2.31190
C	0.41770	-4.82810	-3.68986
C	2.75429	-5.35561	-3.92255
H	5.75398	-4.82987	1.51473
H	7.57278	-4.00553	2.97860
H	7.03312	-2.71096	5.03870
H	4.64912	-2.26488	5.62081
H	2.83801	-3.10787	4.16481
H	3.89801	-5.42595	-2.09980
H	3.61021	-5.61672	-4.54810
H	1.37034	-5.26096	-5.57998
H	-0.57084	-4.67290	-4.12877
H	-0.26237	-4.43995	-1.68137

H	-1.61406	-6.02499	1.14796
H	-3.41318	-7.23773	2.29218
H	-2.92783	-8.56246	4.35729
H	-0.59572	-8.66247	5.22736
H	1.22220	-7.46979	4.05791
S	0.65261	-0.24714	-0.60748
C	-0.67996	-1.43642	-0.49182
C	-2.56006	-3.56398	-0.59008
C	-1.06073	-2.11188	0.69573
C	-1.38852	-1.73152	-1.68348
C	-2.29092	-2.79340	-1.72467
C	-1.97750	-3.16868	0.60997
H	-2.80924	-3.00696	-2.66229
H	-2.24167	-3.70305	1.52397
C	-1.28371	-0.88853	-2.91203
C	-1.37358	0.65502	-5.25806
C	-0.82860	-1.41143	-4.12477
C	-1.77094	0.42548	-2.88629
C	-1.81375	1.19195	-4.04726
C	-0.87997	-0.64684	-5.29071
H	-0.41771	-2.42038	-4.15041
H	-2.12899	0.84125	-1.94247
H	-2.20079	2.21197	-4.00869
H	-0.52925	-1.07528	-6.23231
H	-1.41472	1.25138	-6.17143
C	-0.58634	-1.76030	2.06428
C	0.25447	-1.13299	4.67928
C	-0.43118	-0.42725	2.46881
C	-0.33774	-2.77001	3.00511
C	0.07647	-2.46180	4.29926
C	-0.00785	-0.11850	3.75848
H	-0.63066	0.37358	1.75725
H	-0.43518	-3.81660	2.71619
H	0.26939	-3.27060	5.00713
H	0.12017	0.92685	4.04559
H	0.59123	-0.88750	5.68833
C	-3.43099	-4.76441	-0.64494
C	-4.99842	-7.09703	-0.70854
C	-3.25821	-5.71633	-1.65903
C	-4.40468	-4.99924	0.33531
C	-5.18371	-6.15348	0.30166
C	-4.03335	-6.87352	-1.68918
H	-2.48658	-5.55992	-2.41612
H	-4.56166	-4.26006	1.12352
H	-5.94452	-6.31465	1.06816
H	-3.87483	-7.60965	-2.47932
H	-5.60511	-8.00394	-0.73143

$5a_{AC}$(I)

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.710881
E (gas phase) = -2548.71840569
E(THF)= -2548.72567741
E(DCM)= -2548.73672072

Ru	-0.08776	0.57776	-0.03541
S	-2.29240	0.31981	0.67993
C	-2.16733	0.25864	2.45545
C	-1.35170	1.15562	3.17975
C	-1.25787	1.04530	4.56851
C	-1.94958	0.06250	5.28107
C	-2.74163	-0.82680	4.55394
C	-2.85824	-0.74915	3.16289
C	-3.67709	-1.79763	2.48641
C	-3.33587	-3.14595	2.64547
C	-4.11228	-4.15215	2.07194
C	-5.24200	-3.82260	1.32621
C	-5.58791	-2.48143	1.15758
C	-4.81372	-1.47819	1.73430
H	-5.09440	-0.43137	1.60745
H	-6.47375	-2.21440	0.57801
H	-5.85320	-4.60786	0.87710
H	-3.83055	-5.19828	2.20866
H	-2.44591	-3.40486	3.22309
H	-3.27428	-1.62529	5.07530
C	-1.84228	-0.03478	6.75903
C	-2.96674	-0.32692	7.54326
C	-2.86560	-0.42112	8.92912
C	-1.63777	-0.22251	9.55873
C	-0.51201	0.07016	8.79026
C	-0.61357	0.16191	7.40437
H	0.27862	0.36912	6.80976
H	0.45578	0.22071	9.27242
H	-1.55851	-0.29503	10.64488
H	-3.75507	-0.64286	9.52196
H	-3.93745	-0.46025	7.06124
H	-0.64898	1.77444	5.10744
C	-0.54404	2.22854	2.52473
C	-1.14784	3.25919	1.78474
C	-0.38353	4.29799	1.26699
C	0.99647	4.33298	1.47620
C	1.60753	3.31933	2.20557
C	0.84290	2.27350	2.72428
H	1.32484	1.47828	3.29792
H	2.68833	3.32789	2.35300
H	1.59853	5.13577	1.04876
H	-0.86915	5.08616	0.69020
H	-2.22549	3.23484	1.61942
C	-0.64730	-0.03304	-1.81764
N	-0.68119	-1.25433	-2.37282
C	-1.16342	-1.24901	-3.75620
C	-1.55948	0.21401	-3.97204
N	-1.14512	0.84142	-2.71951
C	-1.15430	2.26561	-2.57687
C	-0.02560	2.98987	-3.00897
C	-0.00912	4.36506	-2.80380
C	-1.09131	5.03487	-2.22231
C	-2.22429	4.29993	-1.88724
C	-2.28683	2.91304	-2.06818
C	-3.57699	2.19223	-1.78120
H	-3.94421	2.42849	-0.77322
H	-3.47138	1.10264	-1.83917
H	-4.34479	2.50785	-2.50614
H	-3.09493	4.81245	-1.46872
C	-1.01528	6.51809	-1.97104
H	-1.96054	6.91108	-1.57140
H	-0.77993	7.06689	-2.89573
H	-0.21704	6.74760	-1.24710
H	0.88076	4.92924	-3.09323
C	1.12013	2.31796	-3.71910
H	2.04999	2.88401	-3.57470
H	0.92025	2.27201	-4.80320
H	1.28974	1.29766	-3.35431
H	-1.03808	0.67644	-4.82283
H	-2.64258	0.34487	-4.12147
H	-2.00883	-1.94263	-3.86909
H	-0.36218	-1.58015	-4.43553
C	-0.15026	-2.46150	-1.82897
C	1.22247	-2.71463	-1.96568
C	1.72447	-3.89979	-1.42929
C	0.89672	-4.81580	-0.77159
C	-0.46425	-4.52671	-0.65979
C	-1.01458	-3.35505	-1.18692
C	-2.47383	-3.03715	-1.01550
H	-3.02036	-3.89740	-0.60944
H	-2.94580	-2.75137	-1.96800
H	-2.60648	-2.19096	-0.32166

H	-1.12235	-5.22716	-0.13918
C	1.46519	-6.09639	-0.21663
H	2.44953	-5.92965	0.24473
H	1.59938	-6.84208	-1.01696
H	0.80131	-6.53633	0.54060
H	2.79448	-4.10739	-1.51363
C	2.13443	-1.69432	-2.59382
H	2.19077	-0.78913	-1.96679
H	1.77729	-1.37854	-3.58622
H	3.14962	-2.09495	-2.71316
C	0.63199	-0.87845	0.71395
H	0.70419	-1.90909	0.37579
H	1.04163	-0.67529	1.71797
N	1.49876	1.64804	-0.65961
C	2.28063	2.51757	-0.82622
O	3.07034	3.38153	-1.02823

$5a_{AC}$(II)

Spin multiplicity: singlet
Thermal correction to Gibbs free energy =1.466261
E (gas phase) = -5097.47060779
E(THF)= -5097.45983161
E(DCM)= -5097.48236743

Ru	-1.46382	0.23696	-2.86828
C	-2.43857	-1.25703	-2.63446
C	-2.97610	1.46942	-3.28340
C	-4.98324	2.62840	-3.59571
H	-5.64021	3.03947	-2.81739
H	-5.60292	2.38064	-4.47261
C	-3.81501	3.55896	-3.93334
H	-3.86938	3.95938	-4.95498
H	-3.73285	4.40461	-3.23269
C	-5.07388	0.30799	-2.66659
C	-5.61509	0.33081	-1.37424
C	-6.40322	-0.74760	-0.97507
H	-6.82652	-0.74324	0.03373
C	-6.64091	-1.83624	-1.81626
C	-6.10191	-1.81356	-3.10344
H	-6.29232	-2.65082	-3.77959
C	-5.33194	-0.74164	-3.56050
C	-1.39833	2.97927	-4.40689
C	-1.22013	2.66013	-5.76422
C	0.02942	2.89096	-6.33435
H	0.19398	2.60009	-7.37439
C	1.07496	3.46022	-5.60454
C	0.83608	3.83573	-4.28279
H	1.62687	4.32717	-3.71107
C	-0.39092	3.60045	-3.65787
C	-5.38232	1.49291	-0.44888
H	-4.41070	1.96706	-0.63866
H	-5.40119	1.17026	0.60079
H	-6.16742	2.25804	-0.57480
C	-7.45084	-3.00819	-1.32651
H	-7.57510	-3.76975	-2.10855
H	-8.45211	-2.69043	-0.99717
H	-6.96150	-3.48709	-0.46288
C	-4.81017	-0.70561	-4.97306
H	-5.18882	0.17986	-5.50899
H	-5.13267	-1.59430	-5.53130
H	-3.71108	-0.65900	-5.00441
C	-2.33873	2.10293	-6.60348
H	-3.00391	1.45369	-6.02109
H	-1.93725	1.50525	-7.43248
H	-2.94195	2.91953	-7.03549
C	2.43461	3.63294	-6.22692
H	3.01614	2.70267	-6.12165
H	3.00134	4.44206	-5.74381
H	2.36118	3.85602	-7.30096
C	-0.60608	4.00621	-2.22879
H	-1.56245	4.52926	-2.08772
H	0.19545	4.67560	-1.89091
H	-0.62684	3.13605	-1.55460
N	-4.30394	1.42289	-3.10961
N	-2.65829	2.67445	-3.79422
Ru	1.13201	0.19904	-0.39414
C	1.83655	1.84326	-0.24593
C	2.87357	-0.70719	-1.08428
C	4.88065	-0.85312	-2.32304
H	5.01628	-0.36513	-3.29819
H	5.86834	-0.94724	-1.84620
C	4.13942	-2.17572	-2.43074
H	4.69782	-3.02083	-1.99959
H	3.87353	-2.43216	-3.46539
C	4.54553	1.18158	-1.00181
C	4.54462	2.32067	-1.82412
C	5.23225	3.45250	-1.38570
H	5.21877	4.34855	-2.01200
C	5.95800	3.46288	-0.19388
C	5.98246	2.29809	0.56968
H	6.57397	2.27596	1.48809
C	5.27400	1.15514	0.19663
C	2.19026	-3.13568	-1.33575
C	2.55643	-3.83594	-0.17151
C	2.08950	-5.13824	-0.00242
H	2.37815	-5.69164	0.89427
C	1.28860	-5.76227	-0.96125
C	0.94837	-5.04319	-2.10521
H	0.31764	-5.51180	-2.86476
C	1.38152	-3.73051	-2.31818
C	3.83448	2.34816	-3.14646
H	2.74592	2.26444	-3.02218
H	4.03972	3.28824	-3.67447
H	4.13560	1.52019	-3.80183
C	6.67997	4.70577	0.25504
H	5.96418	5.44772	0.64500
H	7.40254	4.48648	1.05376
H	7.22127	5.17970	-0.57723
C	5.28900	-0.07862	1.05349
H	5.62690	-0.96042	0.48806
H	5.95613	0.03991	1.91746
H	4.27984	-0.30061	1.43199
C	3.47464	-3.20650	0.83772
H	3.02110	-2.30839	1.28086
H	3.71369	-3.90362	1.65109
H	4.42390	-2.89816	0.37354
C	0.75636	-7.15076	-0.72722
H	-0.14741	-7.10968	-0.09651
H	0.48245	-7.64384	-1.67053
H	1.49125	-7.78223	-0.20687
C	0.96330	-3.01298	-3.57008
H	0.14998	-2.30495	-3.35468
H	1.77548	-2.43341	-4.02569
H	0.59092	-3.72163	-4.32085
N	3.98928	-0.05047	-1.47673
N	2.92078	-1.93666	-1.64207
S	0.75375	-0.02442	1.96353
C	1.94535	-0.58138	3.15956
C	3.96577	-1.59087	4.88558
C	2.93058	0.27929	3.70074
C	1.87404	-1.90548	3.66333
C	2.89454	-2.39231	4.48404
C	3.93288	-0.24396	4.52458
H	2.81779	-3.41346	4.86416
H	4.70445	0.43073	4.90189
S	-1.21927	0.81228	-0.52714
C	-2.33072	0.65600	0.86960

C	-4.12466	0.65783	3.07345
C	-2.62259	1.84911	1.56880
C	-2.94827	-0.54354	1.28979
C	-3.83269	-0.51189	2.37440
C	-3.50248	1.83290	2.65276
H	-4.27303	-1.45487	2.70339
H	-3.71671	2.77427	3.16264
C	-2.06807	3.18491	1.19567
C	-1.09417	5.76375	0.67296
C	-2.93415	4.20405	0.78377
C	-0.70820	3.47304	1.34807
C	-0.22629	4.75256	1.08646
C	-2.45087	5.48608	0.52124
H	-4.00038	3.99054	0.67822
H	-0.03390	2.68463	1.68718
H	0.83850	4.95730	1.21516
H	-3.13988	6.27151	0.20340
C	-2.74140	-1.87842	0.66800
C	-2.41371	-4.43267	-0.44638
C	-1.46639	-2.42254	0.50715
C	-3.85259	-2.64903	0.30249
C	-3.69307	-3.91159	-0.26493
C	-1.30826	-3.68918	-0.03759
H	-0.59886	-1.87316	0.86946
H	-4.85302	-2.23557	0.42870
H	-4.57167	-4.48292	-0.57179
H	-0.30764	-4.10160	-0.11621
H	-2.27679	-5.42112	-0.89054
C	0.69580	-2.79786	3.44967
C	-1.50296	-4.54867	3.30154
C	-0.59248	-2.36399	3.79570
C	0.85813	-4.12373	3.03968
C	-0.23052	-4.99089	2.95352
C	-1.67632	-3.23250	3.72971
H	-0.74214	-1.33474	4.12435
H	1.85596	-4.48334	2.78876
H	-0.07843	-6.01721	2.61242
H	-2.66788	-2.87392	4.01138
H	-2.35933	-5.22130	3.23084
C	2.91798	1.75863	3.51076
C	2.95080	4.57003	3.36031
C	4.08903	2.45013	3.19503
C	1.76048	2.50514	3.77711
C	1.78015	3.89410	3.71136
C	4.10789	3.84116	3.10320
H	5.00254	1.88560	3.01832
H	0.83941	1.98677	4.04428
H	0.86886	4.45440	3.92767
H	5.03473	4.35227	2.83511
H	2.95919	5.66023	3.29990
C	5.06271	-2.14061	5.72159
C	7.14977	-3.19533	7.28705
C	5.59252	-3.41024	5.45261
C	5.59756	-1.41008	6.79168
C	6.63128	-1.93144	7.56574
C	6.62488	-3.93350	6.22736
H	5.19944	-3.98590	4.61176
H	5.18146	-0.43031	7.03488
H	7.02820	-1.34928	8.39965
H	7.02660	-4.92221	5.99714
H	7.95884	-3.60428	7.89487
C	-5.06438	0.64965	4.22260
C	-6.84681	0.63248	6.39660
C	-6.23926	-0.11339	4.18084
C	-4.79802	1.40358	5.37334
C	-5.68099	1.39520	6.45025
C	-7.12261	-0.12237	5.25743
H	-6.47148	-0.69313	3.28471
H	-3.87577	1.98510	5.43239
H	-5.45179	1.98224	7.34154
H	-8.03571	-0.71823	5.20358
H	-7.53811	0.62530	7.24113
H	-2.54673	-1.96621	-3.46225
H	-2.87298	-1.56211	-1.68653
H	2.14633	2.26606	0.71536
H	1.89690	2.52566	-1.10118
N	-1.15651	-0.30584	-4.81866
C	-0.82181	-0.56594	-5.91940
O	-0.51170	-0.81865	-7.04245
N	0.68101	0.31778	-2.55567
C	1.40258	0.16608	-3.51115
O	2.12911	0.01330	-4.41471
H	-0.71299	6.76645	0.46984

$5a_{AC}$(III)

Spin multiplicity: singlet
Thermal correction to Gibbs free energy = 0.403531
E (gas phase) = -1394.59361778
E(THF)= -1394.61163717
E(DCM)= -1394.61920248

Ru	0.03050	0.62525	-0.11391
C	-0.53746	0.00956	-1.87669
N	-0.54569	-1.21059	-2.43376
C	-1.07843	-1.21632	-3.79926
C	-1.41837	0.25873	-4.03872
N	-1.03938	0.87971	-2.77196
C	-1.16495	2.29122	-2.57284
C	-0.10175	3.13010	-2.95003
C	-0.22964	4.49718	-2.70835
C	-1.38269	5.03963	-2.13619
C	-2.44539	4.18466	-1.84286
C	-2.36756	2.80869	-2.06583
C	-3.57859	1.94495	-1.83330
H	-4.10553	2.23989	-0.91589
H	-3.32260	0.88306	-1.74272
H	-4.28510	2.06114	-2.67197
H	-3.36899	4.59721	-1.42866
C	-1.46857	6.51261	-1.83318
H	-2.51140	6.85858	-1.80484
H	-0.92610	7.10895	-2.58089
H	-1.01967	6.72864	-0.85026
H	0.59892	5.15756	-2.97693
C	1.11637	2.60499	-3.66291
H	2.01864	3.15397	-3.36173
H	0.99777	2.73524	-4.75176
H	1.29240	1.54191	-3.46061
H	-0.84227	0.70069	-4.86563
H	-2.48786	0.42397	-4.23760
H	-1.95908	-1.87306	-3.86026
H	-0.32201	-1.60077	-4.49973
C	-0.08136	-2.42815	-1.85607
C	1.26438	-2.78104	-2.01615
C	1.69643	-3.98071	-1.44878
C	0.82546	-4.81320	-0.74009
C	-0.50721	-4.41827	-0.59347
C	-0.98370	-3.22718	-1.14353
C	-2.39853	-2.76755	-0.91490
H	-2.97633	-3.52344	-0.36766
H	-2.92235	-2.56172	-1.86096
H	-2.40946	-1.83524	-0.32897
H	-1.19404	-5.04876	-0.02306
C	1.30925	-6.11773	-0.16194
H	2.37216	-6.06527	0.11323
H	1.19712	-6.93189	-0.89628
H	0.73516	-6.39805	0.73248
H	2.74623	-4.26658	-1.55269

C	2.22304	-1.85002	-2.70883
H	2.31665	-0.90780	-2.14590
H	1.88285	-1.58936	-3.72287
H	3.22041	-2.30048	-2.79308
C	0.61034	-0.84511	0.71015
H	0.67862	-1.87926	0.38138
H	0.95848	-0.63991	1.73785
N	1.70898	1.50141	-0.73643
C	2.81528	1.76580	-1.07010
O	3.90401	2.06867	-1.41775
N	-1.82181	0.85311	0.58771
C	-2.89470	0.61788	1.03659
O	-3.97630	0.42961	1.47379

Input file examples

Sample input file for a geometry optimization job (here, the 3aAC(III) complex). The initial geometry, the force constants and the wave function initial guess are read from the checkpoint file of the previous step.

```
%chk=prec_2Cl
%mem=27000MB
#P wB97XD/GenECP vshift=300
# IOp(1/7=67,1/8=5) opt=(Readfc,MaxCycle=180) Int=UltraFine
# guess=read geom=check SCF=(novaracc) SCFCyc=180 5d 7f Nosymm

prec_2Cl_geometry_optimization

0   1

1 0
S 10 1.00
0.20825000E+03 0.52300000E-03
0.18847100E+02 -0.44913000E-01
0.11781800E+02 0.25762600E+00
0.73619500E+01 -0.20913000E+00
0.42777100E+01 -0.51066200E+00
0.11910700E+01 0.80324700E+00
0.54856800E+00 0.49841400E+00
0.13869400E+00 0.33766000E-01
0.67651000E-01 -0.12094000E-01
0.30141000E-01 0.41970000E-02
S 10 1.00
0.20825000E+03 -0.17500000E-03
0.18847100E+02 0.14803000E-01
0.11781800E+02 -0.87527000E-01
0.73619500E+01 0.84282000E-01
0.42777100E+01 0.15491100E+00
0.11910700E+01 -0.33814100E+00
0.54856800E+00 -0.31600500E+00
0.13869400E+00 0.28352600E+00
0.67651000E-01 0.60927300E+00
0.30141000E-01 0.29320100E+00
S 10 1.00
0.20825000E+03 -0.18200000E-03
0.18847100E+02 0.52730000E-02
0.11781800E+02 -0.78557000E-01
0.73619500E+01 -0.13897000E-01
0.42777100E+01 0.54798700E+00
0.11910700E+01 -0.14980850E+01
0.54856800E+00 0.47950000E+00
0.13869400E+00 0.21402540E+01
0.67651000E-01 -0.14545610E+01
0.30141000E-01 -0.40922400E+00
S 10 1.00
0.20825000E+03 -0.63500000E-03
0.18847100E+02 0.51747000E-01
0.11781800E+02 -0.31718900E+00
0.73619500E+01 0.32984800E+00
0.42777100E+01 0.62705300E+00
0.11910700E+01 -0.34222090E+01
0.54856800E+00 0.38479480E+01
0.13869400E+00 -0.16239260E+01
0.67651000E-01 -0.60322300E+00
0.30141000E-01 0.12121780E+01
```

```
S 1 1.00
0.30141000E-01 0.10000000E+01
P 9 1.00
0.22775300E+02 -0.15440000E-02
0.14234000E+02 0.25771000E-01
0.59875500E+01 -0.18659800E+00
0.16392400E+01 0.44277400E+00
0.82788000E+00 0.47815100E+00
0.40901000E+00 0.20836900E+00
0.17187700E+00 0.24635000E-01
0.71271000E-01 -0.21900000E-03
0.29226000E-01 0.37000000E-03
P 9 1.00
0.22775300E+02 -0.14800000E-03
0.14234000E+02 -0.91740000E-02
0.59875500E+01 0.81374000E-01
0.16392400E+01 -0.23612500E+00
0.82788000E+00 -0.29433300E+00
0.40901000E+00 0.15098000E-01
0.17187700E+00 0.65608900E+00
0.71271000E-01 0.43894400E+00
0.29226000E-01 0.18168000E-01
P 9 1.00
0.22775300E+02 -0.63000000E-04
0.14234000E+02 -0.11461000E-01
0.59875500E+01 0.99993000E-01
0.16392400E+01 -0.30364100E+00
0.82788000E+00 -0.36388600E+00
0.40901000E+00 0.16593500E+00
0.17187700E+00 0.70054500E+00
0.71271000E-01 0.31894300E+00
0.29226000E-01 0.10008000E-01
P 9 1.00
0.22775300E+02 0.11030000E-02
0.14234000E+02 -0.22519000E-01
0.59875500E+01 0.18216100E+00
0.16392400E+01 -0.73133000E+00
0.82788000E+00 -0.49011700E+00
0.40901000E+00 0.15235390E+01
0.17187700E+00 -0.39182000E-01
0.71271000E-01 -0.86618300E+00
0.29226000E-01 -0.12690000E-01
P 1 1.00
0.29226000E-01 0.10000000E+01
D 8 1.00
0.25883800E+02 0.15230000E-02
0.75925500E+01 -0.18162000E-01
0.27129300E+01 0.10969100E+00
0.13970800E+01 0.29159700E+00
0.68256500E+00 0.36204400E+00
0.31937800E+00 0.29751400E+00
0.14178100E+00 0.16103700E+00
0.58017000E-01 0.38970000E-01
D 8 1.00
0.25883800E+02 -0.15510000E-02
0.75925500E+01 0.19035000E-01
0.27129300E+01 -0.12577400E+00
0.13970800E+01 -0.36328500E+00
0.68256500E+00 -0.27935100E+00
0.31937800E+00 0.24571200E+00
0.14178100E+00 0.54726100E+00
0.58017000E-01 0.28465700E+00
D 8 1.00
0.25883800E+02 0.26560000E-02
0.75925500E+01 -0.33760000E-01
0.27129300E+01 0.29292300E+00
0.13970800E+01 0.61737100E+00
0.68256500E+00 -0.36253000E+00
```

```
0.31937800E+00 -0.80315800E+00
0.14178100E+00 0.31546100E+00
0.58017000E-01 0.57512100E+00
D 1 1.00
0.58017000E-01 0.10000000E+01
F 1 1.00
0.16965000E+01 0.10000000E+01
F 1 1.00
0.47540000E+00 0.10000000E+01
****
2 0
S   8   1.00
  15330.0000000              0.0005080
   2299.0000000              0.0039290
    522.4000000              0.0202430
    147.3000000              0.0791810
     47.5500000              0.2306870
     16.7600000              0.4331180
      6.2070000              0.3502600
      0.6882000             -0.0081540
S   8   1.00
  15330.0000000             -0.0001150
   2299.0000000             -0.0008950
    522.4000000             -0.0046360
    147.3000000             -0.0187240
     47.5500000             -0.0584630
     16.7600000             -0.1364630
      6.2070000             -0.1757400
      0.6882000              0.6034180
S   1   1.00
      1.7520000              1.0000000
S   1   1.00
      0.2384000              1.0000000
P   3   1.00
     34.4600000              0.0159280
      7.7490000              0.0997400
      2.2800000              0.3104920
P   1   1.00
      0.7156000              1.0000000
P   1   1.00
      0.2140000              1.0000000
D   1   1.00
      2.3140000              1.0000000
D   1   1.00
      0.6450000              1.0000000
****
3 0
S   8   1.00
   9046.0000000              0.0007000
   1357.0000000              0.0053890
    309.3000000              0.0274060
     87.7300000              0.1032070
     28.5600000              0.2787230
     10.2100000              0.4485400
      3.8380000              0.2782380
      0.7466000              0.0154400
S   8   1.00
   9046.0000000             -0.0001530
   1357.0000000             -0.0012080
    309.3000000             -0.0059920
     87.7300000             -0.0245440
     28.5600000             -0.0674590
     10.2100000             -0.1580780
      3.8380000             -0.1218310
      0.7466000              0.5490030
S   1   1.00
      0.2248000              1.0000000
P   3   1.00
```

```
     13.5500000              0.0399190
      2.9170000              0.2171690
      0.7973000              0.5103190
P   1   1.00
      0.2185000              1.0000000
D   1   1.00
      0.8170000              1.0000000
****
4 0
S   8   1.00
   9046.0000000              0.0007000
   1357.0000000              0.0053890
    309.3000000              0.0274060
     87.7300000              0.1032070
     28.5600000              0.2787230
     10.2100000              0.4485400
      3.8380000              0.2782380
      0.7466000              0.0154400
S   8   1.00
   9046.0000000             -0.0001530
   1357.0000000             -0.0012080
    309.3000000             -0.0059920
     87.7300000             -0.0245440
     28.5600000             -0.0674590
     10.2100000             -0.1580780
      3.8380000             -0.1218310
      0.7466000              0.5490030
S   1   1.00
      0.2248000              1.0000000
P   3   1.00
     13.5500000              0.0399190
      2.9170000              0.2171690
      0.7973000              0.5103190
P   1   1.00
      0.2185000              1.0000000
D   1   1.00
      0.8170000              1.0000000
****
5 0
S   8   1.00
   8236.0000000              0.0005310
   1235.0000000              0.0041080
    280.8000000              0.0210870
     79.2700000              0.0818530
     25.5900000              0.2348170
      8.9970000              0.4344010
      3.3190000              0.3461290
      0.3643000             -0.0089830
S   8   1.00
   8236.0000000             -0.0001130
   1235.0000000             -0.0008780
    280.8000000             -0.0045400
     79.2700000             -0.0181330
     25.5900000             -0.0557600
      8.9970000             -0.1268950
      3.3190000             -0.1703520
      0.3643000              0.5986840
S   1   1.00
      0.9059000              1.0000000
S   1   1.00
      0.1285000              1.0000000
P   3   1.00
     18.7100000              0.0140310
      4.1330000              0.0868660
      1.2000000              0.2902160
P   1   1.00
      0.3827000              1.0000000
P   1   1.00
```

```
      0.1209000             1.0000000
D   1   1.00
      1.0970000             1.0000000
D   1   1.00
      0.3180000             1.0000000
****
6 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
7 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
8 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
9 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
```

```
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
10 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
11 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
12 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
```

```
13 0
S   8   1.00
   6665.0000000              0.0006920
   1000.0000000              0.0053290
    228.0000000              0.0270770
     64.7100000              0.1017180
     21.0600000              0.2747400
      7.4950000              0.4485640
      2.7970000              0.2850740
      0.5215000              0.0152040
S   8   1.00
   6665.0000000             -0.0001460
   1000.0000000             -0.0011540
    228.0000000             -0.0057250
     64.7100000             -0.0233120
     21.0600000             -0.0639550
      7.4950000             -0.1499810
      2.7970000             -0.1272620
      0.5215000              0.5445290
S   1   1.00
      0.1596000              1.0000000
P   3   1.00
      9.4390000              0.0381090
      2.0020000              0.2094800
      0.5456000              0.5085570
P   1   1.00
      0.1517000              1.0000000
D   1   1.00
      0.5500000              1.0000000
****
14 0
S   8   1.00
   6665.0000000              0.0006920
   1000.0000000              0.0053290
    228.0000000              0.0270770
     64.7100000              0.1017180
     21.0600000              0.2747400
      7.4950000              0.4485640
      2.7970000              0.2850740
      0.5215000              0.0152040
S   8   1.00
   6665.0000000             -0.0001460
   1000.0000000             -0.0011540
    228.0000000             -0.0057250
     64.7100000             -0.0233120
     21.0600000             -0.0639550
      7.4950000             -0.1499810
      2.7970000             -0.1272620
      0.5215000              0.5445290
S   1   1.00
      0.1596000              1.0000000
P   3   1.00
      9.4390000              0.0381090
      2.0020000              0.2094800
      0.5456000              0.5085570
P   1   1.00
      0.1517000              1.0000000
D   1   1.00
      0.5500000              1.0000000
****
15 0
S   3   1.00
     13.0100000              0.0196850
      1.9620000              0.1379770
      0.4446000              0.4781480
S   1   1.00
      0.1220000              1.0000000
P   1   1.00
```

```
      0.7270000             1.0000000
****
16 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
17 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
18 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
```

```
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
19 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
20 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
21 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
```

```
    228.0000000              0.0270770
     64.7100000              0.1017180
     21.0600000              0.2747400
      7.4950000              0.4485640
      2.7970000              0.2850740
      0.5215000              0.0152040
S   8   1.00
   6665.0000000             -0.0001460
   1000.0000000             -0.0011540
    228.0000000             -0.0057250
     64.7100000             -0.0233120
     21.0600000             -0.0639550
      7.4950000             -0.1499810
      2.7970000             -0.1272620
      0.5215000              0.5445290
S   1   1.00
      0.1596000              1.0000000
P   3   1.00
      9.4390000              0.0381090
      2.0020000              0.2094800
      0.5456000              0.5085570
P   1   1.00
      0.1517000              1.0000000
D   1   1.00
      0.5500000              1.0000000
****
22 0
S   8   1.00
   6665.0000000              0.0006920
   1000.0000000              0.0053290
    228.0000000              0.0270770
     64.7100000              0.1017180
     21.0600000              0.2747400
      7.4950000              0.4485640
      2.7970000              0.2850740
      0.5215000              0.0152040
S   8   1.00
   6665.0000000             -0.0001460
   1000.0000000             -0.0011540
    228.0000000             -0.0057250
     64.7100000             -0.0233120
     21.0600000             -0.0639550
      7.4950000             -0.1499810
      2.7970000             -0.1272620
      0.5215000              0.5445290
S   1   1.00
      0.1596000              1.0000000
P   3   1.00
      9.4390000              0.0381090
      2.0020000              0.2094800
      0.5456000              0.5085570
P   1   1.00
      0.1517000              1.0000000
D   1   1.00
      0.5500000              1.0000000
****
23 0
S   3   1.00
     13.0100000              0.0196850
      1.9620000              0.1379770
      0.4446000              0.4781480
S   1   1.00
      0.1220000              1.0000000
P   1   1.00
      0.7270000              1.0000000
****
24 0
S   8   1.00
```

```
   6665.0000000              0.0006920
   1000.0000000              0.0053290
    228.0000000              0.0270770
     64.7100000              0.1017180
     21.0600000              0.2747400
      7.4950000              0.4485640
      2.7970000              0.2850740
      0.5215000              0.0152040
S   8   1.00
   6665.0000000             -0.0001460
   1000.0000000             -0.0011540
    228.0000000             -0.0057250
     64.7100000             -0.0233120
     21.0600000             -0.0639550
      7.4950000             -0.1499810
      2.7970000             -0.1272620
      0.5215000              0.5445290
S   1   1.00
      0.1596000              1.0000000
P   3   1.00
      9.4390000              0.0381090
      2.0020000              0.2094800
      0.5456000              0.5085570
P   1   1.00
      0.1517000              1.0000000
D   1   1.00
      0.5500000              1.0000000
****
25 0
S   8   1.00
   6665.0000000              0.0006920
   1000.0000000              0.0053290
    228.0000000              0.0270770
     64.7100000              0.1017180
     21.0600000              0.2747400
      7.4950000              0.4485640
      2.7970000              0.2850740
      0.5215000              0.0152040
S   8   1.00
   6665.0000000             -0.0001460
   1000.0000000             -0.0011540
    228.0000000             -0.0057250
     64.7100000             -0.0233120
     21.0600000             -0.0639550
      7.4950000             -0.1499810
      2.7970000             -0.1272620
      0.5215000              0.5445290
S   1   1.00
      0.1596000              1.0000000
P   3   1.00
      9.4390000              0.0381090
      2.0020000              0.2094800
      0.5456000              0.5085570
P   1   1.00
      0.1517000              1.0000000
D   1   1.00
      0.5500000              1.0000000
****
26 0
S   3   1.00
     13.0100000              0.0196850
      1.9620000              0.1379770
      0.4446000              0.4781480
S   1   1.00
      0.1220000              1.0000000
P   1   1.00
      0.7270000              1.0000000
****
```

```
27 0
S   8   1.00
   6665.0000000              0.0006920
   1000.0000000              0.0053290
    228.0000000              0.0270770
     64.7100000              0.1017180
     21.0600000              0.2747400
      7.4950000              0.4485640
      2.7970000              0.2850740
      0.5215000              0.0152040
S   8   1.00
   6665.0000000             -0.0001460
   1000.0000000             -0.0011540
    228.0000000             -0.0057250
     64.7100000             -0.0233120
     21.0600000             -0.0639550
      7.4950000             -0.1499810
      2.7970000             -0.1272620
      0.5215000              0.5445290
S   1   1.00
      0.1596000              1.0000000
P   3   1.00
      9.4390000              0.0381090
      2.0020000              0.2094800
      0.5456000              0.5085570
P   1   1.00
      0.1517000              1.0000000
D   1   1.00
      0.5500000              1.0000000
****
28 0
S   8   1.00
   8236.0000000              0.0005310
   1235.0000000              0.0041080
    280.8000000              0.0210870
     79.2700000              0.0818530
     25.5900000              0.2348170
      8.9970000              0.4344010
      3.3190000              0.3461290
      0.3643000             -0.0089830
S   8   1.00
   8236.0000000             -0.0001130
   1235.0000000             -0.0008780
    280.8000000             -0.0045400
     79.2700000             -0.0181330
     25.5900000             -0.0557600
      8.9970000             -0.1268950
      3.3190000             -0.1703520
      0.3643000              0.5986840
S   1   1.00
      0.9059000              1.0000000
S   1   1.00
      0.1285000              1.0000000
P   3   1.00
     18.7100000              0.0140310
      4.1330000              0.0868660
      1.2000000              0.2902160
P   1   1.00
      0.3827000              1.0000000
P   1   1.00
      0.1209000              1.0000000
D   1   1.00
      1.0970000              1.0000000
D   1   1.00
      0.3180000              1.0000000
****
29 0
S   3   1.00
```

```
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
30 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
31 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
```

```
32 0
S   8   1.00
   6665.0000000              0.0006920
   1000.0000000              0.0053290
    228.0000000              0.0270770
     64.7100000              0.1017180
     21.0600000              0.2747400
      7.4950000              0.4485640
      2.7970000              0.2850740
      0.5215000              0.0152040
S   8   1.00
   6665.0000000             -0.0001460
   1000.0000000             -0.0011540
    228.0000000             -0.0057250
     64.7100000             -0.0233120
     21.0600000             -0.0639550
      7.4950000             -0.1499810
      2.7970000             -0.1272620
      0.5215000              0.5445290
S   1   1.00
      0.1596000              1.0000000
P   3   1.00
      9.4390000              0.0381090
      2.0020000              0.2094800
      0.5456000              0.5085570
P   1   1.00
      0.1517000              1.0000000
D   1   1.00
      0.5500000              1.0000000
****
33 0
S   3   1.00
     13.0100000              0.0196850
      1.9620000              0.1379770
      0.4446000              0.4781480
S   1   1.00
      0.1220000              1.0000000
P   1   1.00
      0.7270000              1.0000000
****
34 0
S   8   1.00
   6665.0000000              0.0006920
   1000.0000000              0.0053290
    228.0000000              0.0270770
     64.7100000              0.1017180
     21.0600000              0.2747400
      7.4950000              0.4485640
      2.7970000              0.2850740
      0.5215000              0.0152040
S   8   1.00
   6665.0000000             -0.0001460
   1000.0000000             -0.0011540
    228.0000000             -0.0057250
     64.7100000             -0.0233120
     21.0600000             -0.0639550
      7.4950000             -0.1499810
      2.7970000             -0.1272620
      0.5215000              0.5445290
S   1   1.00
      0.1596000              1.0000000
P   3   1.00
      9.4390000              0.0381090
      2.0020000              0.2094800
      0.5456000              0.5085570
P   1   1.00
      0.1517000              1.0000000
D   1   1.00
```

```
      0.5500000             1.0000000
****
35 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
36 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
37 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
38 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
```

```
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
39 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
40 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
41 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
42 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
```

```
    228.0000000              0.0270770
     64.7100000              0.1017180
     21.0600000              0.2747400
      7.4950000              0.4485640
      2.7970000              0.2850740
      0.5215000              0.0152040
S   8   1.00
   6665.0000000             -0.0001460
   1000.0000000             -0.0011540
    228.0000000             -0.0057250
     64.7100000             -0.0233120
     21.0600000             -0.0639550
      7.4950000             -0.1499810
      2.7970000             -0.1272620
      0.5215000              0.5445290
S   1   1.00
      0.1596000              1.0000000
P   3   1.00
      9.4390000              0.0381090
      2.0020000              0.2094800
      0.5456000              0.5085570
P   1   1.00
      0.1517000              1.0000000
D   1   1.00
      0.5500000              1.0000000
****
43 0
S   3   1.00
     13.0100000              0.0196850
      1.9620000              0.1379770
      0.4446000              0.4781480
S   1   1.00
      0.1220000              1.0000000
P   1   1.00
      0.7270000              1.0000000
****
44 0
S   3   1.00
     13.0100000              0.0196850
      1.9620000              0.1379770
      0.4446000              0.4781480
S   1   1.00
      0.1220000              1.0000000
P   1   1.00
      0.7270000              1.0000000
****
45 0
S   3   1.00
     13.0100000              0.0196850
      1.9620000              0.1379770
      0.4446000              0.4781480
S   1   1.00
      0.1220000              1.0000000
P   1   1.00
      0.7270000              1.0000000
****
46 0
S   8   1.00
   6665.0000000              0.0006920
   1000.0000000              0.0053290
    228.0000000              0.0270770
     64.7100000              0.1017180
     21.0600000              0.2747400
      7.4950000              0.4485640
      2.7970000              0.2850740
      0.5215000              0.0152040
S   8   1.00
   6665.0000000             -0.0001460
```

```
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
47 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
48 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
49 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
50 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
```

```
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
51 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
52 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
53 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
54 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
```

```
      0.5500000             1.0000000
****
55 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
56 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
57 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
58 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
59 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
```

```
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
60 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
61 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
62 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
63 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
64 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
```

```
      0.4446000              0.4781480
S   1   1.00
      0.1220000              1.0000000
P   1   1.00
      0.7270000              1.0000000
****
65 0
S   3   1.00
     13.0100000              0.0196850
      1.9620000              0.1379770
      0.4446000              0.4781480
S   1   1.00
      0.1220000              1.0000000
P   1   1.00
      0.7270000              1.0000000
****
66 0
S   8   1.00
   6665.0000000              0.0006920
   1000.0000000              0.0053290
    228.0000000              0.0270770
     64.7100000              0.1017180
     21.0600000              0.2747400
      7.4950000              0.4485640
      2.7970000              0.2850740
      0.5215000              0.0152040
S   8   1.00
   6665.0000000             -0.0001460
   1000.0000000             -0.0011540
    228.0000000             -0.0057250
     64.7100000             -0.0233120
     21.0600000             -0.0639550
      7.4950000             -0.1499810
      2.7970000             -0.1272620
      0.5215000              0.5445290
S   1   1.00
      0.1596000              1.0000000
P   3   1.00
      9.4390000              0.0381090
      2.0020000              0.2094800
      0.5456000              0.5085570
P   1   1.00
      0.1517000              1.0000000
D   1   1.00
      0.5500000              1.0000000
****
67 0
S   3   1.00
     13.0100000              0.0196850
      1.9620000              0.1379770
      0.4446000              0.4781480
S   1   1.00
      0.1220000              1.0000000
P   1   1.00
      0.7270000              1.0000000
****
68 0
S   3   1.00
     13.0100000              0.0196850
      1.9620000              0.1379770
      0.4446000              0.4781480
S   1   1.00
      0.1220000              1.0000000
P   1   1.00
      0.7270000              1.0000000
****
69 0
S   3   1.00
```

```
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
70 0
S   8   1.00
   6665.0000000             0.0006920
   1000.0000000             0.0053290
    228.0000000             0.0270770
     64.7100000             0.1017180
     21.0600000             0.2747400
      7.4950000             0.4485640
      2.7970000             0.2850740
      0.5215000             0.0152040
S   8   1.00
   6665.0000000            -0.0001460
   1000.0000000            -0.0011540
    228.0000000            -0.0057250
     64.7100000            -0.0233120
     21.0600000            -0.0639550
      7.4950000            -0.1499810
      2.7970000            -0.1272620
      0.5215000             0.5445290
S   1   1.00
      0.1596000             1.0000000
P   3   1.00
      9.4390000             0.0381090
      2.0020000             0.2094800
      0.5456000             0.5085570
P   1   1.00
      0.1517000             1.0000000
D   1   1.00
      0.5500000             1.0000000
****
71 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
72 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
73 0
S   3   1.00
     13.0100000             0.0196850
      1.9620000             0.1379770
      0.4446000             0.4781480
S   1   1.00
      0.1220000             1.0000000
P   1   1.00
      0.7270000             1.0000000
****
```

```
74 0
S   13   1.00
 456100.0000000              0.492970D-04
  68330.0000000              0.383029D-03
  15550.0000000              0.200854D-02
   4405.0000000              0.838558D-02
   1439.0000000              0.294703D-01
    520.4000000              0.878325D-01
    203.1000000              0.211473D+00
     83.9600000              0.365364D+00
     36.2000000              0.340884D+00
     15.8300000              0.102133D+00
      6.3340000              0.311675D-02
      2.6940000              0.105751D-02
      0.4313000              0.156136D-03
S   13   1.00
 456100.0000000             -0.138304D-04
  68330.0000000             -0.107279D-03
  15550.0000000             -0.565083D-03
   4405.0000000             -0.236135D-02
   1439.0000000             -0.845886D-02
    520.4000000             -0.259638D-01
    203.1000000             -0.686362D-01
     83.9600000             -0.141874D+00
     36.2000000             -0.199319D+00
     15.8300000             -0.195662D-01
      6.3340000              0.499741D+00
      2.6940000              0.563736D+00
      0.4313000             -0.835091D-02
S   13   1.00
 456100.0000000              0.418546D-05
  68330.0000000              0.324395D-04
  15550.0000000              0.171105D-03
   4405.0000000              0.714176D-03
   1439.0000000              0.256705D-02
    520.4000000              0.788552D-02
    203.1000000              0.210867D-01
     83.9600000              0.442264D-01
     36.2000000              0.651670D-01
     15.8300000              0.603012D-02
      6.3340000             -0.206495D+00
      2.6940000             -0.405871D+00
      0.4313000              0.725661D+00
S   1   1.00
      0.9768000              1.0000000
S   1   1.00
      0.1625000              1.0000000
P   7   1.00
    663.3000000              0.240448D-02
    156.8000000              0.192148D-01
     49.9800000              0.885097D-01
     18.4200000              0.256020D+00
      7.2400000              0.436927D+00
      2.9220000              0.350334D+00
      0.3818000             -0.458423D-02
P   7   1.00
    663.3000000             -0.652145D-03
    156.8000000             -0.519445D-02
     49.9800000             -0.246938D-01
     18.4200000             -0.728167D-01
      7.2400000             -0.134030D+00
      2.9220000             -0.947742D-01
      0.3818000              0.564667D+00
P   1   1.00
      1.0220000              1.0000000
P   1   1.00
      0.1301000              1.0000000
D   1   1.00
```

```
      1.0460000              1.0000000
D   1   1.00
      0.3440000              1.0000000
****
75 0
S   13   1.00
 456100.0000000              0.492970D-04
  68330.0000000              0.383029D-03
  15550.0000000              0.200854D-02
   4405.0000000              0.838558D-02
   1439.0000000              0.294703D-01
    520.4000000              0.878325D-01
    203.1000000              0.211473D+00
     83.9600000              0.365364D+00
     36.2000000              0.340884D+00
     15.8300000              0.102133D+00
      6.3340000              0.311675D-02
      2.6940000              0.105751D-02
      0.4313000              0.156136D-03
S   13   1.00
 456100.0000000             -0.138304D-04
  68330.0000000             -0.107279D-03
  15550.0000000             -0.565083D-03
   4405.0000000             -0.236135D-02
   1439.0000000             -0.845886D-02
    520.4000000             -0.259638D-01
    203.1000000             -0.686362D-01
     83.9600000             -0.141874D+00
     36.2000000             -0.199319D+00
     15.8300000             -0.195662D-01
      6.3340000              0.499741D+00
      2.6940000              0.563736D+00
      0.4313000             -0.835091D-02
S   13   1.00
 456100.0000000              0.418546D-05
  68330.0000000              0.324395D-04
  15550.0000000              0.171105D-03
   4405.0000000              0.714176D-03
   1439.0000000              0.256705D-02
    520.4000000              0.788552D-02
    203.1000000              0.210867D-01
     83.9600000              0.442264D-01
     36.2000000              0.651670D-01
     15.8300000              0.603012D-02
      6.3340000             -0.206495D+00
      2.6940000             -0.405871D+00
      0.4313000              0.725661D+00
S   1   1.00
      0.9768000              1.0000000
S   1   1.00
      0.1625000              1.0000000
P   7   1.00
    663.3000000              0.240448D-02
    156.8000000              0.192148D-01
     49.9800000              0.885097D-01
     18.4200000              0.256020D+00
      7.2400000              0.436927D+00
      2.9220000              0.350334D+00
      0.3818000             -0.458423D-02
P   7   1.00
    663.3000000             -0.652145D-03
    156.8000000             -0.519445D-02
     49.9800000             -0.246938D-01
     18.4200000             -0.728167D-01
      7.2400000             -0.134030D+00
      2.9220000             -0.947742D-01
      0.3818000              0.564667D+00
P   1   1.00
```

```
      1.0220000              1.0000000
P   1   1.00
      0.1301000              1.0000000
D   1   1.00
      1.0460000              1.0000000
D   1   1.00
      0.3440000              1.0000000
****

1 0
ECP28MDF 4 28
G-Komponente
1
2 1.000000 0.000000
S-G
2
2 11.500590 209.786493
2 5.068575 30.214307
P-G
4
2 10.532634 48.751244
2 10.192010 97.496529
2 4.734892 7.860188
2 4.509065 15.329751
D-G
4
2 8.877977 26.967506
2 8.766122 40.432303
2 3.170196 3.340758
2 3.228851 5.256352
F-G
2
2 7.820249 -8.847525
2 7.839647 -11.835518



---end---
```

Sample input file for a gas phase single point job (here, the 3aAC(III) complex). The geometry and the wave function initial guess are read from the checkpoint file of the previous step.

```
%chk=diCl_SP_gas
%mem=27000MB
#P PBEPBE/GenECP SP vshift=300 gfinput Int=UltraFine
#  geom=check guess=read SCF=(novaracc,Conver=5) SCFCyc=180 5d 7f
EmpiricalDispersion=GD3BJ
#  NoSymm

SP_gas_phase

0    1

H 0
S   3   1.00
     82.6400000              0.0020060
     12.4100000              0.0153430
      2.8240000              0.0755790
S   1   1.00
      0.7977000              1.0000000
S   1   1.00
      0.2581000              1.0000000
S   1   1.00
      0.0898900              1.0000000
P   1   1.00
```

```
      2.2920000              1.0000000
P   1   1.00
      0.8380000              1.0000000
P   1   1.00
      0.2920000              1.0000000
D   1   1.00
      2.0620000              1.0000000
D   1   1.00
      0.6620000              1.0000000
F   1   1.00
      1.3970000              1.0000000
****
C 0
S   9   1.00
  33980.0000000              0.0000910
   5089.0000000              0.0007040
   1157.0000000              0.0036930
    326.6000000              0.0153600
    106.1000000              0.0529290
     38.1100000              0.1470430
     14.7500000              0.3056310
      6.0350000              0.3993450
      2.5300000              0.2170510
S   9   1.00
  33980.0000000             -0.0000190
   5089.0000000             -0.0001510
   1157.0000000             -0.0007850
    326.6000000             -0.0033240
    106.1000000             -0.0115120
     38.1100000             -0.0341600
     14.7500000             -0.0771730
      6.0350000             -0.1414930
      2.5300000             -0.1180190
S   1   1.00
      0.7355000              1.0000000
S   1   1.00
      0.2905000              1.0000000
S   1   1.00
      0.1111000              1.0000000
P   3   1.00
     34.5100000              0.0053780
      7.9150000              0.0361320
      2.3680000              0.1424930
P   1   1.00
      0.8132000              1.0000000
P   1   1.00
      0.2890000              1.0000000
P   1   1.00
      0.1007000              1.0000000
D   1   1.00
      1.8480000              1.0000000
D   1   1.00
      0.6490000              1.0000000
D   1   1.00
      0.2280000              1.0000000
F   1   1.00
      1.4190000              1.0000000
F   1   1.00
      0.4850000              1.0000000
G   1   1.00
      1.0110000              1.0000000
****
Cl 0
S   13   1.00
 834900.0000000              0.231688D-04
 125000.0000000              0.180154D-03
  28430.0000000              0.947782D-03
   8033.0000000              0.400139D-02
```

```
   2608.0000000              0.144629D-01
    933.9000000              0.456586D-01
    360.0000000              0.123248D+00
    147.0000000              0.264369D+00
     62.8800000              0.382989D+00
     27.6000000              0.270934D+00
     11.0800000              0.471404D-01
      5.0750000             -0.371766D-02
      2.2780000              0.219158D-02
S   13   1.00
 834900.0000000             -0.649649D-05
 125000.0000000             -0.504895D-04
  28430.0000000             -0.266113D-03
   8033.0000000             -0.112499D-02
   2608.0000000             -0.410497D-02
    933.9000000             -0.131987D-01
    360.0000000             -0.375342D-01
    147.0000000             -0.897233D-01
     62.8800000             -0.167671D+00
     27.6000000             -0.174763D+00
     11.0800000              0.114909D+00
      5.0750000              0.563618D+00
      2.2780000              0.441606D+00
S   13   1.00
 834900.0000000              0.196645D-05
 125000.0000000              0.152620D-04
  28430.0000000              0.806086D-04
   8033.0000000              0.339960D-03
   2608.0000000              0.124551D-02
    933.9000000              0.399612D-02
    360.0000000              0.114751D-01
    147.0000000              0.275504D-01
     62.8800000              0.532917D-01
     27.6000000              0.571246D-01
     11.0800000             -0.395201D-01
      5.0750000             -0.264343D+00
      2.2780000             -0.349291D+00
S   1   1.00
      0.7775000              1.0000000
S   1   1.00
      0.3527000              1.0000000
S   1   1.00
      0.1431000              1.0000000
S   1   1.00
      0.0519000              1.0000000
P   8   1.00
   1703.0000000              0.474039D-03
    403.6000000              0.406412D-02
    130.3000000              0.213355D-01
     49.0500000              0.794611D-01
     20.2600000              0.208927D+00
      8.7870000              0.364945D+00
      3.9190000              0.371725D+00
      1.7650000              0.146292D+00
P   8   1.00
   1703.0000000             -0.128266D-03
    403.6000000             -0.109356D-02
    130.3000000             -0.583429D-02
     49.0500000             -0.219258D-01
     20.2600000             -0.601385D-01
      8.7870000             -0.106929D+00
      3.9190000             -0.122454D+00
      1.7650000              0.383619D-01
P   1   1.00
      0.7207000              1.0000000
P   1   1.00
      0.2839000              1.0000000
P   1   1.00
```

```
      0.1060000             1.0000000
P   1   1.00
      0.0376000             1.0000000
D   1   1.00
      0.2540000             1.0000000
D   1   1.00
      0.6280000             1.0000000
D   1   1.00
      1.5510000             1.0000000
D   1   1.00
      0.0952000             1.0000000
F   1   1.00
      0.4230000             1.0000000
F   1   1.00
      1.0890000             1.0000000
F   1   1.00
      0.2170000             1.0000000
G   1   1.00
      0.8270000             1.0000000
G   1   1.00
      0.3780000             1.0000000
****
N 0
S   9   1.00
  45840.0000000             0.0000920
   6868.0000000             0.0007170
   1563.0000000             0.0037490
    442.4000000             0.0155320
    144.3000000             0.0531460
     52.1800000             0.1467870
     20.3400000             0.3046630
      8.3810000             0.3976840
      3.5290000             0.2176410
S   9   1.00
  45840.0000000            -0.0000200
   6868.0000000            -0.0001590
   1563.0000000            -0.0008240
    442.4000000            -0.0034780
    144.3000000            -0.0119660
     52.1800000            -0.0353880
     20.3400000            -0.0800770
      8.3810000            -0.1467220
      3.5290000            -0.1163600
S   1   1.00
      1.0540000             1.0000000
S   1   1.00
      0.4118000             1.0000000
S   1   1.00
      0.1552000             1.0000000
S   1   1.00
      0.0546400             1.0000000
P   3   1.00
     49.3300000             0.0055330
     11.3700000             0.0379620
      3.4350000             0.1490280
P   1   1.00
      1.1820000             1.0000000
P   1   1.00
      0.4173000             1.0000000
P   1   1.00
      0.1428000             1.0000000
P   1   1.00
      0.0440200             1.0000000
D   1   1.00
      2.8370000             1.0000000
D   1   1.00
      0.9680000             1.0000000
D   1   1.00
```

```
      0.3350000              1.0000000
D   1   1.00
      0.1110000              1.0000000
F   1   1.00
      2.0270000              1.0000000
F   1   1.00
      0.6850000              1.0000000
F   1   1.00
      0.2450000              1.0000000
G   1   1.00
      1.4270000              1.0000000
G   1   1.00
      0.5590000              1.0000000
****
Ru 0
S 14 1.00
0.72698900E+04 0.11000000E-04
0.10878400E+04 0.78000000E-04
0.24178700E+03 0.31100000E-03
0.35452500E+02 0.87340000E-02
0.22141500E+02 -0.63604000E-01
0.13829200E+02 0.18571500E+00
0.51321300E+01 -0.45449000E+00
0.31705900E+01 -0.25634200E+00
0.14948700E+01 0.53304500E+00
0.80053000E+00 0.63997200E+00
0.41163800E+00 0.21527300E+00
0.14241700E+00 0.11261000E-01
0.63563000E-01 -0.95000000E-04
0.28296000E-01 0.11070000E-02
S 14 1.00
0.72698900E+04 -0.40000000E-05
0.10878400E+04 -0.25000000E-04
0.24178700E+03 -0.10600000E-03
0.35452500E+02 -0.24970000E-02
0.22141500E+02 0.18842000E-01
0.13829200E+02 -0.57581000E-01
0.51321300E+01 0.16045800E+00
0.31705900E+01 0.69126000E-01
0.14948700E+01 -0.20397900E+00
0.80053000E+00 -0.32049800E+00
0.41163800E+00 -0.17465600E+00
0.14241700E+00 0.33269600E+00
0.63563000E-01 0.63032100E+00
0.28296000E-01 0.24640700E+00
S 14 1.00
0.72698900E+04 -0.70000000E-05
0.10878400E+04 -0.65000000E-04
0.24178700E+03 -0.17400000E-03
0.35452500E+02 -0.83680000E-02
0.22141500E+02 0.51785000E-01
0.13829200E+02 -0.14177100E+00
0.51321300E+01 0.41442700E+00
0.31705900E+01 0.78473000E-01
0.14948700E+01 -0.44468800E+00
0.80053000E+00 -0.14550350E+01
0.41163800E+00 0.12722320E+01
0.14241700E+00 0.14072450E+01
0.63563000E-01 -0.99964400E+00
0.28296000E-01 -0.46140700E+00
S 14 1.00
0.72698900E+04 -0.12000000E-04
0.10878400E+04 -0.84000000E-04
0.24178700E+03 -0.36200000E-03
0.35452500E+02 -0.76580000E-02
0.22141500E+02 0.58439000E-01
0.13829200E+02 -0.18623700E+00
0.51321300E+01 0.57496600E+00
```

```
0.31705900E+01 0.40155200E+00
0.14948700E+01 -0.21997860E+01
0.80053000E+00 -0.43552200E+00
0.41163800E+00 0.34276070E+01
0.14241700E+00 -0.24454790E+01
0.63563000E-01 -0.14994300E+00
0.28296000E-01 0.10823060E+01
S 14 1.00
0.72698900E+04 -0.16000000E-04
0.10878400E+04 -0.18100000E-03
0.24178700E+03 -0.33200000E-03
0.35452500E+02 -0.25429000E-01
0.22141500E+02 0.14439700E+00
0.13829200E+02 -0.38364400E+00
0.51321300E+01 0.13902860E+01
0.31705900E+01 0.12715400E+00
0.14948700E+01 -0.68551520E+01
0.80053000E+00 0.96961050E+01
0.41163800E+00 -0.47399940E+01
0.14241700E+00 -0.92146600E+00
0.63563000E-01 0.30543570E+01
0.28296000E-01 -0.18558670E+01
S 1 1.00
0.28296000E-01 0.10000000E+01
P 11 1.00
0.17430700E+03 0.10300000E-03
0.11504000E+02 0.53994000E-01
0.71917600E+01 -0.16101200E+00
0.35749800E+01 -0.12903800E+00
0.21307800E+01 0.31476300E+00
0.10892200E+01 0.50414100E+00
0.55863700E+00 0.32527100E+00
0.27047700E+00 0.78702000E-01
0.12389600E+00 0.37630000E-02
0.55823000E-01 0.12860000E-02
0.24842000E-01 -0.21500000E-03
P 11 1.00
0.17430700E+03 -0.33000000E-04
0.11504000E+02 -0.15713000E-01
0.71917600E+01 0.48772000E-01
0.35749800E+01 0.35193000E-01
0.21307800E+01 -0.10322300E+00
0.10892200E+01 -0.18111500E+00
0.55863700E+00 -0.12438800E+00
0.27047700E+00 0.11202800E+00
0.12389600E+00 0.42251100E+00
0.55823000E-01 0.47723100E+00
0.24842000E-01 0.15682000E+00
P 11 1.00
0.17430700E+03 -0.61000000E-04
0.11504000E+02 -0.28785000E-01
0.71917600E+01 0.89305000E-01
0.35749800E+01 0.70717000E-01
0.21307800E+01 -0.20474700E+00
0.10892200E+01 -0.37151100E+00
0.55863700E+00 -0.14363500E+00
0.27047700E+00 0.46222100E+00
0.12389600E+00 0.58558100E+00
0.55823000E-01 0.15074900E+00
0.24842000E-01 0.45640000E-02
P 11 1.00
0.17430700E+03 0.11200000E-03
0.11504000E+02 0.49262000E-01
0.71917600E+01 -0.15382000E+00
0.35749800E+01 -0.17315200E+00
0.21307800E+01 0.53097500E+00
0.10892200E+01 0.81762600E+00
0.55863700E+00 -0.78673200E+00
```

```
0.27047700E+00 -0.10474860E+01
0.12389600E+00 0.75490800E+00
0.55823000E-01 0.46325100E+00
0.24842000E-01 0.55220000E-02
P 11 1.00
0.17430700E+03 -0.25000000E-03
0.11504000E+02 -0.62992000E-01
0.71917600E+01 0.19162100E+00
0.35749800E+01 0.65282900E+00
0.21307800E+01 -0.21533740E+01
0.10892200E+01 0.40944200E+00
0.55863700E+00 0.24570950E+01
0.27047700E+00 -0.22868480E+01
0.12389600E+00 0.77769000E-01
0.55823000E-01 0.76560400E+00
0.24842000E-01 -0.22730000E-02
P 1 1.00
0.24842000E-01 0.10000000E+01
D 10 1.00
0.75375100E+02 0.18000000E-03
0.19890100E+02 0.20840000E-02
0.78792400E+01 -0.18671000E-01
0.29083400E+01 0.78054000E-01
0.16388300E+01 0.22632800E+00
0.87573000E+00 0.31710000E+00
0.45048300E+00 0.30503600E+00
0.22277000E+00 0.21515000E+00
0.10534200E+00 0.99758000E-01
0.46455000E-01 0.19451000E-01
D 10 1.00
0.75375100E+02 -0.20300000E-03
0.19890100E+02 -0.20860000E-02
0.78792400E+01 0.19428000E-01
0.29083400E+01 -0.87106000E-01
0.16388300E+01 -0.28641300E+00
0.87573000E+00 -0.33190800E+00
0.45048300E+00 -0.21210000E-02
0.22277000E+00 0.40235500E+00
0.10534200E+00 0.45433200E+00
0.46455000E-01 0.16126800E+00
D 10 1.00
0.75375100E+02 -0.35500000E-03
0.19890100E+02 -0.31930000E-02
0.78792400E+01 0.31956000E-01
0.29083400E+01 -0.18559900E+00
0.16388300E+01 -0.58318500E+00
0.87573000E+00 -0.72766000E-01
0.45048300E+00 0.79870700E+00
0.22277000E+00 0.30163600E+00
0.10534200E+00 -0.54096800E+00
0.46455000E-01 -0.35606000E+00
D 10 1.00
0.75375100E+02 -0.18200000E-03
0.19890100E+02 -0.72830000E-02
0.78792400E+01 0.61663000E-01
0.29083400E+01 -0.44416800E+00
0.16388300E+01 -0.79983900E+00
0.87573000E+00 0.13061620E+01
0.45048300E+00 0.34708800E+00
0.22277000E+00 -0.12223020E+01
0.10534200E+00 0.17440000E+00
0.46455000E-01 0.62628100E+00
D 1 1.00
0.46455000E-01 0.10000000E+01
F 1 1.00
0.28980000E+01 0.10000000E+01
F 1 1.00
0.95880000E+00 0.10000000E+01
```

```
F 1 1.00
0.31720000E+00 0.10000000E+01
G 1 1.00
0.17100000E+01 0.10000000E+01
G 1 1.00
0.57780000E+00 0.10000000E+01
H 1 1.00
0.11646000E+01 0.10000000E+01
****

Ru 0
ECP28MDF 4 28
G-Komponente
1
2 1.000000 0.000000
S-G
2
2 11.500590 209.786493
2 5.068575 30.214307
P-G
4
2 10.532634 48.751244
2 10.192010 97.496529
2 4.734892 7.860188
2 4.509065 15.329751
D-G
4
2 8.877977 26.967506
2 8.766122 40.432303
2 3.170196 3.340758
2 3.228851 5.256352
F-G
2
2 7.820249 -8.847525
2 7.839647 -11.835518



 ---end---
```

Sample input file for a single point calculation in dichloromethane (here, the 3aAC(III) complex). The geometry and the wave function initial guess are read from the checkpoint file of the previous step.

```
%chk=diCl_SP_DCM
%mem=27000MB
#P PBEPBE/GenECP SP vshift=300 gfinput Int=UltraFine
#  geom=check guess=read SCF=(novaracc,Conver=5) SCFCyc=180 5d 7f
# EmpiricalDispersion=GD3BJ
#  NoSymm
#  SCRF=(pcm,solvent=Dichloromethane,read)

SP_PCM_DCM

0    1

H 0
S   3   1.00
     82.6400000              0.0020060
     12.4100000              0.0153430
      2.8240000              0.0755790
S   1   1.00
      0.7977000              1.0000000
S   1   1.00
      0.2581000              1.0000000
```

```
S   1   1.00
      0.0898900             1.0000000
P   1   1.00
      2.2920000             1.0000000
P   1   1.00
      0.8380000             1.0000000
P   1   1.00
      0.2920000             1.0000000
D   1   1.00
      2.0620000             1.0000000
D   1   1.00
      0.6620000             1.0000000
F   1   1.00
      1.3970000             1.0000000
****
C 0
S   9   1.00
  33980.0000000             0.0000910
   5089.0000000             0.0007040
   1157.0000000             0.0036930
    326.6000000             0.0153600
    106.1000000             0.0529290
     38.1100000             0.1470430
     14.7500000             0.3056310
      6.0350000             0.3993450
      2.5300000             0.2170510
S   9   1.00
  33980.0000000            -0.0000190
   5089.0000000            -0.0001510
   1157.0000000            -0.0007850
    326.6000000            -0.0033240
    106.1000000            -0.0115120
     38.1100000            -0.0341600
     14.7500000            -0.0771730
      6.0350000            -0.1414930
      2.5300000            -0.1180190
S   1   1.00
      0.7355000             1.0000000
S   1   1.00
      0.2905000             1.0000000
S   1   1.00
      0.1111000             1.0000000
P   3   1.00
     34.5100000             0.0053780
      7.9150000             0.0361320
      2.3680000             0.1424930
P   1   1.00
      0.8132000             1.0000000
P   1   1.00
      0.2890000             1.0000000
P   1   1.00
      0.1007000             1.0000000
D   1   1.00
      1.8480000             1.0000000
D   1   1.00
      0.6490000             1.0000000
D   1   1.00
      0.2280000             1.0000000
F   1   1.00
      1.4190000             1.0000000
F   1   1.00
      0.4850000             1.0000000
G   1   1.00
      1.0110000             1.0000000
****
Cl 0
S   13   1.00
 834900.0000000             0.231688D-04
```

```
 125000.0000000              0.180154D-03
  28430.0000000              0.947782D-03
   8033.0000000              0.400139D-02
   2608.0000000              0.144629D-01
    933.9000000              0.456586D-01
    360.0000000              0.123248D+00
    147.0000000              0.264369D+00
     62.8800000              0.382989D+00
     27.6000000              0.270934D+00
     11.0800000              0.471404D-01
      5.0750000             -0.371766D-02
      2.2780000              0.219158D-02
S   13   1.00
 834900.0000000             -0.649649D-05
 125000.0000000             -0.504895D-04
  28430.0000000             -0.266113D-03
   8033.0000000             -0.112499D-02
   2608.0000000             -0.410497D-02
    933.9000000             -0.131987D-01
    360.0000000             -0.375342D-01
    147.0000000             -0.897233D-01
     62.8800000             -0.167671D+00
     27.6000000             -0.174763D+00
     11.0800000              0.114909D+00
      5.0750000              0.563618D+00
      2.2780000              0.441606D+00
S   13   1.00
 834900.0000000              0.196645D-05
 125000.0000000              0.152620D-04
  28430.0000000              0.806086D-04
   8033.0000000              0.339960D-03
   2608.0000000              0.124551D-02
    933.9000000              0.399612D-02
    360.0000000              0.114751D-01
    147.0000000              0.275504D-01
     62.8800000              0.532917D-01
     27.6000000              0.571246D-01
     11.0800000             -0.395201D-01
      5.0750000             -0.264343D+00
      2.2780000             -0.349291D+00
S   1   1.00
      0.7775000              1.0000000
S   1   1.00
      0.3527000              1.0000000
S   1   1.00
      0.1431000              1.0000000
S   1   1.00
      0.0519000              1.0000000
P   8   1.00
   1703.0000000              0.474039D-03
    403.6000000              0.406412D-02
    130.3000000              0.213355D-01
     49.0500000              0.794611D-01
     20.2600000              0.208927D+00
      8.7870000              0.364945D+00
      3.9190000              0.371725D+00
      1.7650000              0.146292D+00
P   8   1.00
   1703.0000000             -0.128266D-03
    403.6000000             -0.109356D-02
    130.3000000             -0.583429D-02
     49.0500000             -0.219258D-01
     20.2600000             -0.601385D-01
      8.7870000             -0.106929D+00
      3.9190000             -0.122454D+00
      1.7650000              0.383619D-01
P   1   1.00
      0.7207000              1.0000000
```

```
P   1   1.00
      0.2839000             1.0000000
P   1   1.00
      0.1060000             1.0000000
P   1   1.00
      0.0376000             1.0000000
D   1   1.00
      0.2540000             1.0000000
D   1   1.00
      0.6280000             1.0000000
D   1   1.00
      1.5510000             1.0000000
D   1   1.00
      0.0952000             1.0000000
F   1   1.00
      0.4230000             1.0000000
F   1   1.00
      1.0890000             1.0000000
F   1   1.00
      0.2170000             1.0000000
G   1   1.00
      0.8270000             1.0000000
G   1   1.00
      0.3780000             1.0000000
****
N 0
S   9   1.00
  45840.0000000             0.0000920
   6868.0000000             0.0007170
   1563.0000000             0.0037490
    442.4000000             0.0155320
    144.3000000             0.0531460
     52.1800000             0.1467870
     20.3400000             0.3046630
      8.3810000             0.3976840
      3.5290000             0.2176410
S   9   1.00
  45840.0000000            -0.0000200
   6868.0000000            -0.0001590
   1563.0000000            -0.0008240
    442.4000000            -0.0034780
    144.3000000            -0.0119660
     52.1800000            -0.0353880
     20.3400000            -0.0800770
      8.3810000            -0.1467220
      3.5290000            -0.1163600
S   1   1.00
      1.0540000             1.0000000
S   1   1.00
      0.4118000             1.0000000
S   1   1.00
      0.1552000             1.0000000
S   1   1.00
      0.0546400             1.0000000
P   3   1.00
     49.3300000             0.0055330
     11.3700000             0.0379620
      3.4350000             0.1490280
P   1   1.00
      1.1820000             1.0000000
P   1   1.00
      0.4173000             1.0000000
P   1   1.00
      0.1428000             1.0000000
P   1   1.00
      0.0440200             1.0000000
D   1   1.00
      2.8370000             1.0000000
```

```
D   1   1.00
      0.9680000              1.0000000
D   1   1.00
      0.3350000              1.0000000
D   1   1.00
      0.1110000              1.0000000
F   1   1.00
      2.0270000              1.0000000
F   1   1.00
      0.6850000              1.0000000
F   1   1.00
      0.2450000              1.0000000
G   1   1.00
      1.4270000              1.0000000
G   1   1.00
      0.5590000              1.0000000
****
Ru 0
S 14 1.00
0.72698900E+04 0.11000000E-04
0.10878400E+04 0.78000000E-04
0.24178700E+03 0.31100000E-03
0.35452500E+02 0.87340000E-02
0.22141500E+02 -0.63604000E-01
0.13829200E+02 0.18571500E+00
0.51321300E+01 -0.45449000E+00
0.31705900E+01 -0.25634200E+00
0.14948700E+01 0.53304500E+00
0.80053000E+00 0.63997200E+00
0.41163800E+00 0.21527300E+00
0.14241700E+00 0.11261000E-01
0.63563000E-01 -0.95000000E-04
0.28296000E-01 0.11070000E-02
S 14 1.00
0.72698900E+04 -0.40000000E-05
0.10878400E+04 -0.25000000E-04
0.24178700E+03 -0.10600000E-03
0.35452500E+02 -0.24970000E-02
0.22141500E+02 0.18842000E-01
0.13829200E+02 -0.57581000E-01
0.51321300E+01 0.16045800E+00
0.31705900E+01 0.69126000E-01
0.14948700E+01 -0.20397900E+00
0.80053000E+00 -0.32049800E+00
0.41163800E+00 -0.17465600E+00
0.14241700E+00 0.33269600E+00
0.63563000E-01 0.63032100E+00
0.28296000E-01 0.24640700E+00
S 14 1.00
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G 1 1.00
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P-G
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2 10.192010 97.496529
2 4.734892 7.860188
2 4.509065 15.329751
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2 8.766122 40.432303
2 3.170196 3.340758
2 3.228851 5.256352
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radii=UAHF
pcmdoc
Dis
Rep
Cav


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References

1. G. Occhipinti, F. R. Hansen, K. W. Törnroos and V. R. Jensen, *J. Am. Chem. Soc.*, 2013, **135**, 3331-3334.