Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supplementary Information for

Rational Design of Fe Catalyts for Olefin Aziridination through DFT-based Mechanistic Analysis

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Scheme S1. Simplified mechanistic scheme of nitrene transfers by [$\mathbf{1_{Cl}(NCCH_3)}$]$(ClO_4)_2$.

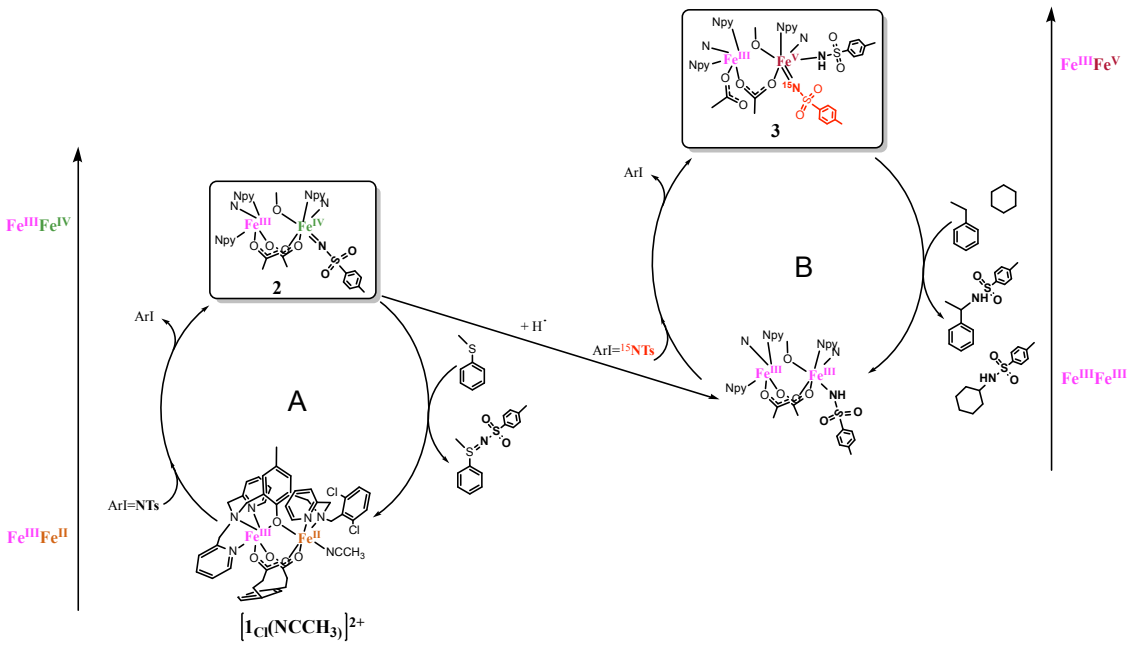

Table S1. Crystal data and data collection parameters for **4(Py)**

	II
Formula	$C_{35.61}\ H_{35.61}\ Cl_4\ Fe\ N_4\ O_{3.11}$
T, (K)	150(2)
Formula weight	767.08
Crystal system	Monoclinic
Space group	P 2_1/c
a, Å	27.042(3)
b, Å	10.5667(9)
c, Å	28.273(3)
α , deg	90
β, deg	118.213(14)
γ, deg	90
V, Å^3	7119.0(15)
Radiation (λ, Å)	Mo Kα (0.71073)
Z	8
dcalcd, g.cm^{-3}	1.431
F(000)	3169
μ, mm^{-1}	0.766
No. of unique data	14374
No. of parameters, refined	937
GOF on F^2	0.975
R1 [I > 2σ(I)]	0.0877
R1 (all data)	0.1563
wR2 (all data)	0.2240

a $R1 = \frac{\sum ||Fo| - |Fc||}{\sum |Fo|}$; b $wR2 = \sqrt{\frac{\sum \left[w\left(Fo^2 - Fc^2\right)^2\right]}{\sum \left[w\left(Fo^2\right)^2\right]}}$

Table S2. Atomic coordinates and equivalent isotropic displacement parameters (A^2) for **4(Py)**.U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	Occ	Mult	x	y	z	U(eq)
Fe(1)	1	1	0.08338(4)	0.71844(9)	0.22535(4)	0.0183(2)
Cl(1)	1	1	0.35941(7)	1.0491(2)	0.34018(8)	0.0426(5)
Cl(2)	1	1	0.17118(7)	1.04296(15)	0.36027(6)	0.0236(3)
Cl(3)	1	1	-0.02059(8)	0.69480(18)	-0.05460(7)	0.0355(4)
Cl(4)	1	1	-0.08249(7)	0.56808(18)	0.09414(7)	0.0311(4)
O(1)	1	1	0.13426(17)	0.8510(4)	0.27723(18)	0.0219(10)
O(2)	1	1	0.03919(18)	0.5858(4)	0.16933(17)	0.0211(10)
N(1)	1	1	0.1364(2)	0.7480(5)	0.1844(2)	0.0201(12)
N(2)	1	1	0.0343(2)	0.8590(5)	0.1623(2)	0.0193(11)
N(3)	1	1	0.0287(2)	0.7152(5)	0.2620(2)	0.0193(11)
N(4)	1	1	0.1319(2)	0.5682(5)	0.2838(2)	0.0230(12)
C(1)	1	1	0.1961(3)	0.7453(7)	0.2244(3)	0.0269(16)
C(2)	1	1	0.2161(2)	0.8505(6)	0.2649(2)	0.0188(13)
C(3)	1	1	0.2691(3)	0.9017(7)	0.2804(3)	0.0245(15)
C(4)	1	1	0.2923(3)	0.9917(7)	0.3204(3)	0.0266(15)
C(5)	1	1	0.2614(3)	1.0376(6)	0.3444(2)	0.0208(14)
C(6)	1	1	0.2099(3)	0.9886(6)	0.3295(3)	0.0207(14)
C(7)	1	1	0.1832(2)	0.8939(6)	0.2891(2)	0.0156(12)
C(8)	1	1	0.1268(3)	0.6410(7)	0.1461(3)	0.0249(15)
C(9)	1	1	0.0666(3)	0.6334(6)	0.1030(3)	0.0214(14)
C(10)	1	1	0.0528(3)	0.6588(6)	0.0501(3)	0.0258(15)
C(11)	1	1	-0.0028(3)	0.6572(6)	0.0113(2)	0.0230(14)
C(12)	1	1	-0.0449(3)	0.6292(6)	0.0246(3)	0.0235(14)
C(13)	1	1	-0.0303(3)	0.6026(6)	0.0769(3)	0.0211(14)
C(14)	1	1	0.0264(3)	0.6050(6)	0.1193(2)	0.0179(13)
C(15)	1	1	0.1199(3)	0.8696(6)	0.1557(3)	0.0217(14)
C(16)	1	1	0.0581(3)	0.8972(6)	0.1325(2)	0.0186(13)
C(17)	1	1	0.0282(3)	0.9624(7)	0.0850(3)	0.0294(16)
C(18)	1	1	-0.0277(3)	0.9872(7)	0.0684(3)	0.0351(18)
C(19)	1	1	-0.0534(3)	0.9483(7)	0.0977(3)	0.0292(16)
C(20)	1	1	-0.0200(3)	0.8855(6)	0.1454(3)	0.0256(15)
C(21)	1	1	0.0370(3)	0.7923(6)	0.3031(3)	0.0240(14)
C(22)	1	1	0.0042(3)	0.7845(7)	0.3288(3)	0.0269(15)
C(23)	1	1	-0.0375(3)	0.6955(6)	0.3128(3)	0.0253(15)
C(24)	1	1	-0.0467(3)	0.6168(7)	0.2703(3)	0.0271(16)
C(25)	1	1	-0.0127(3)	0.6293(6)	0.2462(3)	0.0223(14)
C(26)	1	1	0.1617(3)	0.5936(7)	0.3358(3)	0.0289(16)
C(27)	1	1	0.1872(3)	0.5021(7)	0.3754(3)	0.0373(19)
C(28)	1	1	0.1790(3)	0.3782(7)	0.3609(3)	0.0345(18)
C(29)	1	1	0.1477(4)	0.3500(8)	0.3076(3)	0.045(2)

C(30)	1	1	0.1243(3)	0.4462(7)	0.2706(3)	0.0368(19)
Fe(2)	1	1	0.34832(4)	0.65618(9)	0.55475(4)	0.0217(2)
Cl(31)	1	1	0.31414(9)	0.5248(2)	0.28400(7)	0.0466(5)
Cl(32)	1	1	0.33082(8)	0.27781(18)	0.45731(8)	0.0368(4)
Cl(33)	1	1	0.19866(8)	1.24377(19)	0.51537(9)	0.0433(5)
Cl(34)	1	1	0.28251(9)	0.8632(2)	0.65888(8)	0.0472(5)
O(31)	1	1	0.35472(19)	0.5251(4)	0.50664(17)	0.0248(10)
O(32)	1	1	0.34541(19)	0.8001(4)	0.60083(18)	0.0252(10)
N(31)	1	1	0.3272(2)	0.7961(5)	0.4870(2)	0.0235(12)
N(32)	1	1	0.2549(2)	0.6630(5)	0.5139(2)	0.0212(12)
N(33)	1	1	0.3550(2)	0.5056(6)	0.6109(2)	0.0265(13)
N(34)	1	1	0.4418(2)	0.6765(5)	0.5982(2)	0.0261(13)
C(31)	1	1	0.3621(3)	0.7661(6)	0.4606(3)	0.0269(15)
C(32)	1	1	0.3482(3)	0.6425(7)	0.4307(3)	0.0252(15)
C(33)	1	1	0.3375(3)	0.6388(7)	0.3777(3)	0.0304(16)
C(34)	1	1	0.3262(3)	0.5264(7)	0.3503(3)	0.0295(17)
C(35)	1	1	0.3246(3)	0.4141(7)	0.3745(3)	0.0296(16)
C(36)	1	1	0.3347(3)	0.4183(7)	0.4271(3)	0.0250(15)
C(37)	1	1	0.3462(3)	0.5294(7)	0.4571(3)	0.0250(15)
C(38)	1	1	0.3431(3)	0.9233(6)	0.5110(3)	0.0218(14)
C(39)	1	1	0.3085(3)	0.9658(7)	0.5367(3)	0.0266(15)
C(40)	1	1	0.2722(3)	1.0702(7)	0.5163(3)	0.0275(16)
C(41)	1	1	0.2413(3)	1.1100(7)	0.5399(3)	0.0313(17)
C(42)	1	1	0.2437(3)	1.0474(7)	0.5842(3)	0.0338(17)
C(43)	1	1	0.2789(3)	0.9446(7)	0.6036(3)	0.0307(17)
C(44)	1	1	0.3128(3)	0.8975(7)	0.5819(3)	0.0242(15)
C(45)	1	1	0.2669(3)	0.7903(7)	0.4481(3)	0.0228(14)
C(46)	1	1	0.2303(3)	0.7469(6)	0.4730(3)	0.0205(14)
C(47)	1	1	0.1762(3)	0.7878(7)	0.4543(3)	0.0285(16)
C(48)	1	1	0.1449(3)	0.7402(7)	0.4764(3)	0.0331(17)
C(49)	1	1	0.1690(3)	0.6538(8)	0.5177(3)	0.0333(17)
C(50)	1	1	0.2237(3)	0.6191(7)	0.5350(3)	0.0283(16)
C(51)	1	1	0.3536(3)	0.3854(7)	0.5981(3)	0.0311(17)
C(52)	1	1	0.3586(3)	0.2860(8)	0.6339(3)	0.0374(18)
C(53)	1	1	0.3667(3)	0.3172(9)	0.6840(3)	0.043(2)
C(54)	1	1	0.3689(3)	0.4435(9)	0.6976(3)	0.043(2)
C(55)	1	1	0.3631(3)	0.5352(8)	0.6602(3)	0.0327(17)
C(56)	1	1	0.4740(3)	0.5869(7)	0.5939(3)	0.0349(18)
C(57)	1	1	0.5326(3)	0.5894(8)	0.6222(4)	0.046(2)
C(58)	1	1	0.5583(3)	0.6879(8)	0.6562(4)	0.045(2)
C(59)	1	1	0.5264(3)	0.7823(9)	0.6612(3)	0.042(2)
C(60)	1	1	0.4693(3)	0.7717(8)	0.6325(3)	0.0357(18)
O(61)	1	1	0.1486(4)	0.3116(10)	0.6658(4)	0.098(3)
C(61)	1	1	0.1994(6)	0.2705(15)	0.7137(5)	0.093(4)
C(62)	1	1	0.2481(4)	0.2835(12)	0.7022(4)	0.068(3)
C(63)	1	1	0.2232(4)	0.3595(11)	0.6517(4)	0.061(3)
C(64)	1	1	0.1616(4)	0.3207(12)	0.6244(5)	0.071(3)

O(62)	0.566(11)	0.4520(9)	0.629(2)	0.7951(8)	0.108(4)
C(65)	0.566(11)	0.4934(16)	0.670(4)	0.7804(15)	0.103(4)
C(66)	0.566(11)	0.4915(12)	0.822(3)	0.7841(13)	0.106(5)
C(67)	0.566(11)	0.4318(10)	0.846(3)	0.7615(11)	0.098(4)
C(68)	0.566(11)	0.4158(11)	0.738(2)	0.7880(11)	0.097(4)
O(62B)	0.434(11)	0.4875(11)	0.562(3)	0.7999(10)	0.108(4)
C(65B)	0.434(11)	0.494(2)	0.647(5)	0.7623(18)	0.101(5)
C(66B)	0.434(11)	0.4718(17)	0.772(4)	0.7628(16)	0.101(4)
C(67B)	0.434(11)	0.4771(15)	0.770(4)	0.8240(15)	0.106(4)
C(68B)	0.434(11)	0.4938(16)	0.640(4)	0.8454(16)	0.110(5)
C(71)	1 1	0.5137(5)	0.6988(12)	0.4834(5)	0.075(3)
C(72)	1 1	0.5226(4)	0.8182(11)	0.5153(5)	0.070(3)
C(73)	0.778(11)	0.4984(5)	0.9434(13)	0.4829(5)	0.058(3)
O(71B)	0.222(11)	0.4938(15)	0.704(4)	0.4297(15)	0.084(6)
C(74B)	0.222(11)	0.523(2)	0.818(5)	0.4213(16)	0.083(7)
C(73B)	0.222(11)	0.528(2)	0.891(5)	0.476(2)	0.070(5)

Table S3. Bond lengths [A] and angles [deg] for **4(Py)**.

Fe(1)-O(1)	2.024(4)	C(26)-N(4)-C(30)	116.0(6)
Fe(1)-O(2)	2.028(4)	C(26)-N(4)-Fe(1)	121.1(5)
Fe(1)-N(3)	2.170(5)	C(30)-N(4)-Fe(1)	121.7(4)
Fe(1)-N(2)	2.215(5)	N(1)-C(1)-C(2)	116.1(5)
Fe(1)-N(4)	2.219(5)	N(1)-C(1)-H(1A)	97(4)
Fe(1)-N(1)	2.250(5)	C(2)-C(1)-H(1A)	109(4)
Cl(1)-C(4)	1.736(7)	N(1)-C(1)-H(1B)	109(5)
Cl(2)-C(6)	1.744(7)	C(2)-C(1)-H(1B)	109(5)
Cl(3)-C(11)	1.737(6)	H(1A)-C(1)-H(1B)	117(6)
Cl(4)-C(13)	1.734(7)	C(3)-C(2)-C(7)	120.3(6)
O(1)-C(7)	1.284(7)	C(3)-C(2)-C(1)	118.2(6)
O(2)-C(14)	1.304(8)	C(7)-C(2)-C(1)	121.4(5)
N(1)-C(1)	1.470(8)	C(4)-C(3)-C(2)	121.8(6)
N(1)-C(15)	1.472(9)	C(4)-C(3)-H(3)	119.1
N(1)-C(8)	1.501(8)	C(2)-C(3)-H(3)	119.1
N(2)-C(20)	1.341(8)	C(3)-C(4)-C(5)	119.7(6)
N(2)-C(16)	1.344(8)	C(3)-C(4)-Cl(1)	120.5(5)
N(3)-C(25)	1.342(8)	C(5)-C(4)-Cl(1)	119.8(5)
N(3)-C(21)	1.349(9)	C(6)-C(5)-C(4)	118.8(6)
N(4)-C(26)	1.328(9)	C(6)-C(5)-H(5)	120.6
N(4)-C(30)	1.330(9)	C(4)-C(5)-H(5)	120.6
C(1)-C(2)	1.500(9)	C(5)-C(6)-C(7)	124.9(6)
C(1)-H(1A)	1.12(8)	C(5)-C(6)-Cl(2)	119.4(5)
C(1)-H(1B)	0.90(9)	C(7)-C(6)-Cl(2)	115.7(5)
C(2)-C(3)	1.395(9)	O(1)-C(7)-C(2)	124.0(5)
C(2)-C(7)	1.430(9)	O(1)-C(7)-C(6)	121.6(6)
C(3)-C(4)	1.379(10)	C(2)-C(7)-C(6)	114.4(5)
C(3)-H(3)	0.9500	N(1)-C(8)-C(9)	112.1(5)
C(4)-C(5)	1.390(10)	N(1)-C(8)-H(8A)	109.2
C(5)-C(6)	1.355(9)	C(9)-C(8)-H(8A)	109.2
C(5)-H(5)	0.9500	N(1)-C(8)-H(8B)	109.2
C(6)-C(7)	1.431(9)	C(9)-C(8)-H(8B)	109.2
C(8)-C(9)	1.504(9)	H(8A)-C(8)-H(8B)	107.9
C(8)-H(8A)	0.9900	C(10)-C(9)-C(14)	122.7(6)
C(8)-H(8B)	0.9900	C(10)-C(9)-C(8)	120.0(6)
C(9)-C(10)	1.386(10)	C(14)-C(9)-C(8)	117.2(6)
C(9)-C(14)	1.399(9)	C(11)-C(10)-C(9)	119.5(6)
C(10)-C(11)	1.381(9)	C(11)-C(10)-H(10)	120.3
C(10)-H(10)	0.9500	C(9)-C(10)-H(10)	120.3
C(11)-C(12)	1.388(10)	C(10)-C(11)-C(12)	120.9(6)
C(12)-C(13)	1.369(9)	C(10)-C(11)-Cl(3)	119.6(5)
C(12)-H(12)	0.9500	C(12)-C(11)-Cl(3)	119.5(5)
C(13)-C(14)	1.432(9)	C(13)-C(12)-C(11)	118.8(6)
C(15)-C(16)	1.507(9)	C(13)-C(12)-H(12)	120.6

C(15)-H(15A)	0.9900	C(11)-C(12)-H(12)	120.6
C(15)-H(15B)	0.9900	C(12)-C(13)-C(14)	123.2(6)
C(16)-C(17)	1.381(9)	C(12)-C(13)-Cl(4)	119.3(5)
C(17)-C(18)	1.380(10)	C(14)-C(13)-Cl(4)	117.5(5)
C(17)-H(17)	0.9500	O(2)-C(14)-C(9)	122.7(6)
C(18)-C(19)	1.373(11)	O(2)-C(14)-C(13)	122.3(6)
C(18)-H(18)	0.9500	C(9)-C(14)-C(13)	114.9(6)
C(19)-C(20)	1.385(10)	N(1)-C(15)-C(16)	113.2(5)
C(19)-H(19)	0.9500	N(1)-C(15)-H(15A)	108.9
C(20)-H(20)	0.9500	C(16)-C(15)-H(15A)	108.9
C(21)-C(22)	1.391(10)	N(1)-C(15)-H(15B)	108.9
C(21)-H(21)	0.9500	C(16)-C(15)-H(15B)	108.9
C(22)-C(23)	1.369(10)	H(15A)-C(15)-H(15B)	107.8
C(22)-H(22)	0.9500	N(2)-C(16)-C(17)	121.8(6)
C(23)-C(24)	1.383(10)	N(2)-C(16)-C(15)	115.6(5)
C(23)-H(23)	0.9500	C(17)-C(16)-C(15)	122.6(6)
C(24)-C(25)	1.388(10)	C(18)-C(17)-C(16)	118.0(7)
C(24)-H(24)	0.9500	C(18)-C(17)-H(17)	121.0
C(25)-H(25)	0.9500	C(16)-C(17)-H(17)	121.0
C(26)-C(27)	1.390(10)	C(19)-C(18)-C(17)	121.5(7)
C(26)-H(26)	0.9500	C(19)-C(18)-H(18)	119.2
C(27)-C(28)	1.359(11)	C(17)-C(18)-H(18)	119.2
C(27)-H(27)	0.9500	C(18)-C(19)-C(20)	116.7(6)
C(28)-C(29)	1.368(11)	C(18)-C(19)-H(19)	121.6
C(28)-H(28)	0.9500	C(20)-C(19)-H(19)	121.6
C(29)-C(30)	1.379(11)	N(2)-C(20)-C(19)	123.1(7)
C(29)-H(29)	0.9500	N(2)-C(20)-H(20)	118.4
C(30)-H(30)	0.9500	C(19)-C(20)-H(20)	118.4
		N(3)-C(21)-C(22)	121.9(6)
O(1)-Fe(1)-O(2)	172.69(18)	N(3)-C(21)-H(21)	119.1
O(1)-Fe(1)-N(3)	92.79(18)	C(22)-C(21)-H(21)	119.1
O(2)-Fe(1)-N(3)	94.51(19)	C(23)-C(22)-C(21)	119.7(7)
O(1)-Fe(1)-N(2)	93.57(18)	C(23)-C(22)-H(22)	120.1
O(2)-Fe(1)-N(2)	85.84(18)	C(21)-C(22)-H(22)	120.1
N(3)-Fe(1)-N(2)	96.28(19)	C(22)-C(23)-C(24)	118.9(6)
O(1)-Fe(1)-N(4)	89.73(18)	C(22)-C(23)-H(23)	120.6
O(2)-Fe(1)-N(4)	90.57(19)	C(24)-C(23)-H(23)	120.6
N(3)-Fe(1)-N(4)	86.0(2)	C(23)-C(24)-C(25)	118.8(6)
N(2)-Fe(1)-N(4)	175.9(2)	C(23)-C(24)-H(24)	120.6
O(1)-Fe(1)-N(1)	84.04(18)	C(25)-C(24)-H(24)	120.6
O(2)-Fe(1)-N(1)	88.73(18)	N(3)-C(25)-C(24)	122.9(6)
N(3)-Fe(1)-N(1)	172.5(2)	N(3)-C(25)-H(25)	118.6
N(2)-Fe(1)-N(1)	77.23(19)	C(24)-C(25)-H(25)	118.6
N(4)-Fe(1)-N(1)	100.7(2)	N(4)-C(26)-C(27)	124.2(7)
C(7)-O(1)-Fe(1)	134.2(4)	N(4)-C(26)-H(26)	117.9
C(14)-O(2)-Fe(1)	119.7(4)	C(27)-C(26)-H(26)	117.9
C(1)-N(1)-C(15)	112.2(5)	C(28)-C(27)-C(26)	118.6(7)

C(1)-N(1)-C(8)	107.0(5)	C(28)-C(27)-H(27)	120.7
C(15)-N(1)-C(8)	110.8(5)	C(26)-C(27)-H(27)	120.7
C(1)-N(1)-Fe(1)	109.7(4)	C(27)-C(28)-C(29)	118.1(7)
C(15)-N(1)-Fe(1)	107.7(4)	C(27)-C(28)-H(28)	121.0
C(8)-N(1)-Fe(1)	109.3(4)	C(29)-C(28)-H(28)	121.0
C(20)-N(2)-C(16)	118.8(6)	C(28)-C(29)-C(30)	119.8(7)
C(20)-N(2)-Fe(1)	124.5(4)	C(28)-C(29)-H(29)	120.1
C(16)-N(2)-Fe(1)	115.0(4)	C(30)-C(29)-H(29)	120.1
C(25)-N(3)-C(21)	117.9(5)	N(4)-C(30)-C(29)	123.2(7)
C(25)-N(3)-Fe(1)	120.1(4)	N(4)-C(30)-H(30)	118.4
C(21)-N(3)-Fe(1)	121.9(4)	C(29)-C(30)-H(30)	118.4

Fe(2)-O(31)	2.005(5)	C(39)-C(38)-H(38A)	109.1
Fe(2)-O(32)	2.028(5)	N(31)-C(38)-H(38B)	109.1
Fe(2)-N(33)	2.193(6)	C(39)-C(38)-H(38B)	109.1
Fe(2)-N(32)	2.226(5)	H(38A)-C(38)-H(38B)	107.8
Fe(2)-N(34)	2.237(5)	C(40)-C(39)-C(44)	120.8(6)
Fe(2)-N(31)	2.269(6)	C(40)-C(39)-C(38)	120.7(6)
Cl(31)-C(34)	1.745(7)	C(44)-C(39)-C(38)	118.6(6)
Cl(32)-C(36)	1.740(7)	C(41)-C(40)-C(39)	120.9(7)
Cl(33)-C(41)	1.747(8)	C(41)-C(40)-H(40)	119.5
Cl(34)-C(43)	1.745(8)	C(39)-C(40)-H(40)	119.5
O(31)-C(37)	1.310(8)	C(40)-C(41)-C(42)	121.1(7)
O(32)-C(44)	1.295(8)	C(40)-C(41)-Cl(33)	120.0(6)
N(31)-C(38)	1.475(9)	C(42)-C(41)-Cl(33)	118.9(6)
N(31)-C(45)	1.476(8)	C(43)-C(42)-C(41)	117.7(7)
N(31)-C(31)	1.489(9)	C(43)-C(42)-H(42)	121.2
N(32)-C(50)	1.329(9)	C(41)-C(42)-H(42)	121.2
N(32)-C(46)	1.356(8)	C(42)-C(43)-C(44)	124.9(7)
N(33)-C(51)	1.315(10)	C(42)-C(43)-Cl(34)	118.9(6)
N(33)-C(55)	1.342(9)	C(44)-C(43)-Cl(34)	116.3(6)
N(34)-C(56)	1.332(10)	O(32)-C(44)-C(43)	123.7(6)
N(34)-C(60)	1.350(9)	O(32)-C(44)-C(39)	121.7(6)
C(31)-C(32)	1.504(10)	C(43)-C(44)-C(39)	114.7(6)
C(31)-H(31A)	0.9900	N(31)-C(45)-C(46)	113.3(5)
C(31)-H(31B)	0.9900	N(31)-C(45)-H(45A)	108.9
C(32)-C(33)	1.385(10)	C(46)-C(45)-H(45A)	108.9
C(32)-C(37)	1.422(10)	N(31)-C(45)-H(45B)	108.9
C(33)-C(34)	1.371(11)	C(46)-C(45)-H(45B)	108.9
C(33)-H(33)	0.9500	H(45A)-C(45)-H(45B)	107.7
C(34)-C(35)	1.381(11)	N(32)-C(46)-C(47)	122.7(6)
C(35)-C(36)	1.380(10)	N(32)-C(46)-C(45)	115.1(5)
C(35)-H(35)	0.9500	C(47)-C(46)-C(45)	122.1(6)
C(36)-C(37)	1.394(10)	C(48)-C(47)-C(46)	119.2(6)
C(38)-C(39)	1.500(10)	C(48)-C(47)-H(47)	120.4
C(38)-H(38A)	0.9900	C(46)-C(47)-H(47)	120.4
C(38)-H(38B)	0.9900	C(47)-C(48)-C(49)	119.1(6)

C(39)-C(40)	1.405(10)	C(47)-C(48)-H(48)	120.5
C(39)-C(44)	1.423(10)	C(49)-C(48)-H(48)	120.5
C(40)-C(41)	1.360(10)	C(50)-C(49)-C(48)	118.5(7)
C(40)-H(40)	0.9500	C(50)-C(49)-H(49)	120.8
C(41)-C(42)	1.391(11)	C(48)-C(49)-H(49)	120.8
C(42)-C(43)	1.376(11)	N(32)-C(50)-C(49)	123.7(6)
C(42)-H(42)	0.9500	N(32)-C(50)-H(50)	118.1
C(43)-C(44)	1.414(10)	C(49)-C(50)-H(50)	118.1
C(45)-C(46)	1.531(9)	N(33)-C(51)-C(52)	122.6(7)
C(45)-H(45A)	0.9900	N(33)-C(51)-H(51)	118.7
C(45)-H(45B)	0.9900	C(52)-C(51)-H(51)	118.7
C(46)-C(47)	1.371(9)	C(53)-C(52)-C(51)	118.3(8)
C(47)-C(48)	1.364(10)	C(53)-C(52)-H(52)	120.9
C(47)-H(47)	0.9500	C(51)-C(52)-H(52)	120.9
C(48)-C(49)	1.380(10)	C(52)-C(53)-C(54)	119.1(7)
C(48)-H(48)	0.9500	C(52)-C(53)-H(53)	120.5
C(49)-C(50)	1.371(10)	C(54)-C(53)-H(53)	120.5
C(49)-H(49)	0.9500	C(53)-C(54)-C(55)	119.1(7)
C(50)-H(50)	0.9500	C(53)-C(54)-H(54)	120.4
C(51)-C(52)	1.420(11)	C(55)-C(54)-H(54)	120.4
C(51)-H(51)	0.9500	N(33)-C(55)-C(54)	122.2(8)
C(52)-C(53)	1.368(12)	N(33)-C(55)-H(55)	118.9
C(52)-H(52)	0.9500	C(54)-C(55)-H(55)	118.9
C(53)-C(54)	1.382(13)	N(34)-C(56)-C(57)	123.3(7)
C(53)-H(53)	0.9500	N(34)-C(56)-H(56)	118.4
C(54)-C(55)	1.390(11)	C(57)-C(56)-H(56)	118.4
C(54)-H(54)	0.9500	C(58)-C(57)-C(56)	118.7(8)
C(55)-H(55)	0.9500	C(58)-C(57)-H(57)	120.7
C(56)-C(57)	1.398(10)	C(56)-C(57)-H(57)	120.7
C(56)-H(56)	0.9500	C(57)-C(58)-C(59)	119.6(7)
C(57)-C(58)	1.364(12)	C(57)-C(58)-H(58)	120.2
C(57)-H(57)	0.9500	C(59)-C(58)-H(58)	120.2
C(58)-C(59)	1.369(13)	C(58)-C(59)-C(60)	117.9(8)
C(58)-H(58)	0.9500	C(58)-C(59)-H(59)	121.0
C(59)-C(60)	1.370(10)	C(60)-C(59)-H(59)	121.0
C(59)-H(59)	0.9500	N(34)-C(60)-C(59)	124.8(8)
C(60)-H(60)	0.9500	N(34)-C(60)-H(60)	117.6
O(61)-C(64)	1.378(15)	C(59)-C(60)-H(60)	117.6
O(61)-C(61)	1.466(16)	C(64)-O(61)-C(61)	107.6(8)
C(61)-C(62)	1.504(17)	O(61)-C(61)-C(62)	107.9(10)
C(61)-H(61A)	0.9900	O(61)-C(61)-H(61A)	110.1
C(61)-H(61B)	0.9900	C(62)-C(61)-H(61A)	110.1
C(62)-C(63)	1.492(15)	O(61)-C(61)-H(61B)	110.1
C(62)-H(62A)	0.9900	C(62)-C(61)-H(61B)	110.1
C(62)-H(62B)	0.9900	H(61A)-C(61)-H(61B)	108.4
C(63)-C(64)	1.522(14)	C(63)-C(62)-C(61)	102.1(10)
C(63)-H(63A)	0.9900	C(63)-C(62)-H(62A)	111.4

C(63)-H(63B)	0.9900	C(61)-C(62)-H(62A)	111.4
C(64)-H(64A)	0.9900	C(63)-C(62)-H(62B)	111.4
C(64)-H(64B)	0.9900	C(61)-C(62)-H(62B)	111.4
O(62)-C(65)	1.43(4)	H(62A)-C(62)-H(62B)	109.2
O(62)-C(68)	1.46(3)	C(62)-C(63)-C(64)	103.5(10)
C(65)-C(66)	1.60(5)	C(62)-C(63)-H(63A)	111.1
C(65)-H(65C)	0.9900	C(64)-C(63)-H(63A)	111.1
C(65)-H(65D)	0.9900	C(62)-C(63)-H(63B)	111.1
C(66)-C(67)	1.45(4)	C(64)-C(63)-H(63B)	111.1
C(66)-H(66C)	0.9900	H(63A)-C(63)-H(63B)	109.0
C(66)-H(66D)	0.9900	O(61)-C(64)-C(63)	104.1(9)
C(67)-C(68)	1.54(4)	O(61)-C(64)-H(64A)	110.9
C(67)-H(67C)	0.9900	C(63)-C(64)-H(64A)	110.9
C(67)-H(67D)	0.9900	O(61)-C(64)-H(64B)	110.9
C(68)-H(68C)	0.9900	C(63)-C(64)-H(64B)	110.9
C(68)-H(68D)	0.9900	H(64A)-C(64)-H(64B)	109.0
O(62B)-C(65B)	1.46(5)	C(65)-O(62)-C(68)	107(2)
O(62B)-C(68B)	1.47(4)	O(62)-C(65)-C(66)	103(3)
C(65B)-C(66B)	1.45(7)	O(62)-C(65)-H(65C)	111.1
C(65B)-H(65A)	0.9900	C(66)-C(65)-H(65C)	111.1
C(65B)-H(65B)	0.9900	O(62)-C(65)-H(65D)	111.1
C(66B)-C(67B)	1.67(5)	C(66)-C(65)-H(65D)	111.1
C(66B)-H(66A)	0.9900	H(65C)-C(65)-H(65D)	109.1
C(66B)-H(66B)	0.9900	C(67)-C(66)-C(65)	102(2)
C(67B)-C(68B)	1.48(5)	C(67)-C(66)-H(66C)	111.3
C(67B)-H(67A)	0.9900	C(65)-C(66)-H(66C)	111.3
C(67B)-H(67B)	0.9900	C(67)-C(66)-H(66D)	111.3
C(68B)-H(68A)	0.9900	C(65)-C(66)-H(66D)	111.3
C(68B)-H(68B)	0.9900	H(66C)-C(66)-H(66D)	109.2
C(71)-O(71B)	1.35(4)	C(66)-C(67)-C(68)	99(2)
C(71)-C(72)	1.504(16)	C(66)-C(67)-H(67C)	111.9
C(71)-H(71A)	0.9800	C(68)-C(67)-H(67C)	111.9
C(71)-H(71B)	0.9800	C(66)-C(67)-H(67D)	111.9
C(71)-H(71C)	0.9800	C(68)-C(67)-H(67D)	111.9
C(71)-H(71D)	0.9900	H(67C)-C(67)-H(67D)	109.6
C(71)-H(71E)	0.9900	O(62)-C(68)-C(67)	109.2(19)
C(72)-C(73B)	1.41(6)	O(62)-C(68)-H(68C)	109.8
C(72)-C(73)	1.566(18)	C(67)-C(68)-H(68C)	109.8
C(72)-H(72A)	0.9900	O(62)-C(68)-H(68D)	109.8
C(72)-H(72B)	0.9900	C(67)-C(68)-H(68D)	109.8
C(72)-H(72C)	0.9900	H(68C)-C(68)-H(68D)	108.3
C(72)-H(72D)	0.9900	C(65B)-O(62B)-C(68B)	107(3)
C(73)-C(73)#1	1.51(3)	C(66B)-C(65B)-O(62B)	111(3)
C(73)-H(73A)	0.9900	C(66B)-C(65B)-H(65A)	109.4
C(73)-H(73B)	0.9900	O(62B)-C(65B)-H(65A)	109.4
O(71B)-C(74B)	1.53(5)	C(66B)-C(65B)-H(65B)	109.4
C(74B)-C(73B)	1.68(7)	O(62B)-C(65B)-H(65B)	109.4

C(74B)-H(74A)	0.9900
C(74B)-H(74B)	0.9900
C(73B)-H(73C)	0.9900
C(73B)-H(73D)	0.9900
O(31)-Fe(2)-O(32)	174.65(19)
O(31)-Fe(2)-N(33)	89.2(2)
O(32)-Fe(2)-N(33)	95.4(2)
O(31)-Fe(2)-N(32)	96.35(19)
O(32)-Fe(2)-N(32)	86.01(19)
N(33)-Fe(2)-N(32)	94.8(2)
O(31)-Fe(2)-N(34)	90.1(2)
O(32)-Fe(2)-N(34)	87.2(2)
N(33)-Fe(2)-N(34)	89.2(2)
N(32)-Fe(2)-N(34)	172.4(2)
O(31)-Fe(2)-N(31)	86.86(19)
O(32)-Fe(2)-N(31)	89.02(19)
N(33)-Fe(2)-N(31)	170.2(2)
N(32)-Fe(2)-N(31)	76.69(19)
N(34)-Fe(2)-N(31)	99.7(2)
C(37)-O(31)-Fe(2)	132.4(4)
C(44)-O(32)-Fe(2)	123.8(4)
C(38)-N(31)-C(45)	111.0(5)
C(38)-N(31)-C(31)	108.0(5)
C(45)-N(31)-C(31)	110.9(5)
C(38)-N(31)-Fe(2)	107.7(4)
C(45)-N(31)-Fe(2)	110.6(4)
C(31)-N(31)-Fe(2)	108.6(4)
C(50)-N(32)-C(46)	116.8(6)
C(50)-N(32)-Fe(2)	124.2(4)
C(46)-N(32)-Fe(2)	116.3(4)
C(51)-N(33)-C(55)	118.6(6)
C(51)-N(33)-Fe(2)	121.4(5)
C(55)-N(33)-Fe(2)	119.9(5)
C(56)-N(34)-C(60)	115.7(6)
C(56)-N(34)-Fe(2)	120.0(5)
C(60)-N(34)-Fe(2)	124.2(5)
N(31)-C(31)-C(32)	114.6(5)
N(31)-C(31)-H(31A)	108.6
C(32)-C(31)-H(31A)	108.6
N(31)-C(31)-H(31B)	108.6
C(32)-C(31)-H(31B)	108.6
H(31A)-C(31)-H(31B)	107.6
C(33)-C(32)-C(37)	120.2(6)
C(33)-C(32)-C(31)	120.0(6)
C(37)-C(32)-C(31)	119.8(6)
C(34)-C(33)-C(32)	120.8(7)

H(65A)-C(65B)-H(65B)	108.0
C(65B)-C(66B)-C(67B)	99(4)
C(65B)-C(66B)-H(66A)	111.9
C(67B)-C(66B)-H(66A)	111.9
C(65B)-C(66B)-H(66B)	111.9
C(67B)-C(66B)-H(66B)	111.9
H(66A)-C(66B)-H(66B)	109.6
C(68B)-C(67B)-C(66B)	107(3)
C(68B)-C(67B)-H(67A)	110.3
C(66B)-C(67B)-H(67A)	110.3
C(68B)-C(67B)-H(67B)	110.3
C(66B)-C(67B)-H(67B)	110.3
H(67A)-C(67B)-H(67B)	108.5
O(62B)-C(68B)-C(67B)	106(3)
O(62B)-C(68B)-H(68A)	110.5
C(67B)-C(68B)-H(68A)	110.5
O(62B)-C(68B)-H(68B)	110.5
C(67B)-C(68B)-H(68B)	110.5
H(68A)-C(68B)-H(68B)	108.7
O(71B)-C(71)-C(72)	120(2)
C(72)-C(71)-H(71A)	109.5
C(72)-C(71)-H(71B)	109.5
H(71A)-C(71)-H(71B)	109.5
C(72)-C(71)-H(71C)	109.5
H(71A)-C(71)-H(71C)	109.5
H(71B)-C(71)-H(71C)	109.5
O(71B)-C(71)-H(71D)	107.2
C(72)-C(71)-H(71D)	107.2
O(71B)-C(71)-H(71E)	107.2
C(72)-C(71)-H(71E)	107.2
H(71D)-C(71)-H(71E)	106.8
C(73B)-C(72)-C(71)	92(2)
C(71)-C(72)-C(73)	117.0(10)
C(71)-C(72)-H(72A)	108.0
C(73)-C(72)-H(72A)	108.0
C(71)-C(72)-H(72B)	108.0
C(73)-C(72)-H(72B)	108.0
H(72A)-C(72)-H(72B)	107.3
C(73B)-C(72)-H(72C)	113.3
C(71)-C(72)-H(72C)	113.3
C(73B)-C(72)-H(72D)	113.3
C(71)-C(72)-H(72D)	113.3
H(72C)-C(72)-H(72D)	110.6
C(73)#1-C(73)-C(72)	114.4(14)
C(73)#1-C(73)-H(73A)	108.7
C(72)-C(73)-H(73A)	108.7
C(73)#1-C(73)-H(73B)	108.7

C(34)-C(33)-H(33)	119.6	C(72)-C(73)-H(73B)	108.7
C(32)-C(33)-H(33)	119.6	H(73A)-C(73)-H(73B)	107.6
C(33)-C(34)-C(35)	121.0(6)	C(71)-O(71B)-C(74B)	104(3)
C(33)-C(34)-Cl(31)	119.7(6)	O(71B)-C(74B)-C(73B)	92(3)
C(35)-C(34)-Cl(31)	119.4(6)	O(71B)-C(74B)-H(74A)	113.3
C(36)-C(35)-C(34)	118.0(7)	C(73B)-C(74B)-H(74A)	113.3
C(36)-C(35)-H(35)	121.0	O(71B)-C(74B)-H(74B)	113.3
C(34)-C(35)-H(35)	121.0	C(73B)-C(74B)-H(74B)	113.3
C(35)-C(36)-C(37)	123.7(7)	H(74A)-C(74B)-H(74B)	110.7
C(35)-C(36)-Cl(32)	118.3(6)	C(72)-C(73B)-C(74B)	119(4)
C(37)-C(36)-Cl(32)	117.9(5)	C(72)-C(73B)-H(73C)	107.5
O(31)-C(37)-C(36)	119.8(6)	C(74B)-C(73B)-H(73C)	107.6
O(31)-C(37)-C(32)	124.0(6)	C(72)-C(73B)-H(73D)	107.6
C(36)-C(37)-C(32)	116.2(6)	C(74B)-C(73B)-H(73D)	107.6
N(31)-C(38)-C(39)	112.5(5)	H(73C)-C(73B)-H(73D)	107.0
N(31)-C(38)-H(38A)	109.1		

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z+1

Table S4. Anisotropic displacement parameters (A^2) for **4(Py)**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Fe(1)	0.0074(4)	0.0195(5)	0.0223(5)	-0.0018(4)	0.0024(4)	-0.0018(4
Cl(1)	0.0168(9)	0.0590(13)	0.0442(11)	-0.0148(10)	0.0081(8)	-0.0200(8)
Cl(2)	0.0205(8)	0.0221(8)	0.0249(8)	0.0000(7)	0.0080(7)	0.0010(6)
Cl(3)	0.0442(11)	0.0368(11)	0.0258(9)	0.0009(7)	0.0169(8)	-0.0010(8)
Cl(4)	0.0131(8)	0.0443(11)	0.0298(9)	0.0064(8)	0.0053(7)	-0.0054(7)
O(1)	0.008(2)	0.020(2)	0.038(3)	-0.001(2)	0.0103(19)	0.0007(17)
O(2)	0.013(2)	0.021(2)	0.024(2)	-0.0005(19)	0.0036(19)	-0.0043(18)
N(1)	0.009(3)	0.021(3)	0.026(3)	-0.008(2)	0.005(2)	-0.004(2)
N(2)	0.003(2)	0.024(3)	0.026(3)	-0.003(2)	0.002(2)	0.000(2)
N(3)	0.011(3)	0.021(3)	0.022(3)	0.002(2)	0.005(2)	-0.004(2)
N(4)	0.007(3)	0.025(3)	0.022(3)	-0.001(2)	-0.006(2)	0.006(2)
C(1)	0.010(3)	0.035(4)	0.034(4)	-0.010(3)	0.010(3)	0.000(3)
C(2)	0.009(3)	0.023(3)	0.017(3)	-0.004(3)	0.000(2)	-0.001(2)
C(3)	0.011(3)	0.032(4)	0.024(3)	-0.002(3)	0.003(3)	0.005(3)
C(4)	0.014(3)	0.033(4)	0.024(3)	-0.003(3)	0.001(3)	-0.008(3)
C(5)	0.012(3)	0.024(4)	0.018(3)	0.002(3)	0.000(3)	-0.004(3)
C(6)	0.014(3)	0.020(3)	0.022(3)	0.004(3)	0.003(3)	0.003(3)
C(7)	0.007(3)	0.015(3)	0.015(3)	0.000(2)	-0.003(2)	0.002(2)
C(8)	0.011(3)	0.028(4)	0.031(4)	-0.009(3)	0.006(3)	-0.003(3)
C(9)	0.013(3)	0.013(3)	0.032(4)	-0.011(3)	0.006(3)	-0.004(2)
C(10)	0.025(4)	0.023(4)	0.036(4)	-0.013(3)	0.020(3)	-0.007(3)
C(11)	0.029(4)	0.019(3)	0.017(3)	-0.003(3)	0.007(3)	-0.002(3)
C(12)	0.025(4)	0.023(4)	0.020(3)	0.000(3)	0.008(3)	0.002(3)
C(13)	0.016(3)	0.020(3)	0.023(3)	-0.001(3)	0.005(3)	0.001(3)
C(14)	0.016(3)	0.017(3)	0.019(3)	-0.001(3)	0.007(3)	0.002(2)
C(15)	0.009(3)	0.025(4)	0.028(3)	-0.001(3)	0.006(3)	-0.004(3)
C(16)	0.013(3)	0.017(3)	0.022(3)	-0.006(3)	0.006(3)	-0.003(2)
C(17)	0.021(4)	0.029(4)	0.030(4)	0.005(3)	0.005(3)	-0.005(3)
C(18)	0.024(4)	0.037(4)	0.031(4)	0.004(3)	0.002(3)	0.007(3)
C(19)	0.008(3)	0.036(4)	0.030(4)	0.004(3)	-0.002(3)	0.003(3)
C(20)	0.016(3)	0.022(4)	0.038(4)	0.001(3)	0.012(3)	0.002(3)
C(21)	0.018(3)	0.024(4)	0.026(3)	0.004(3)	0.006(3)	0.001(3)
C(22)	0.025(4)	0.027(4)	0.031(4)	0.004(3)	0.015(3)	0.006(3)
C(23)	0.018(3)	0.029(4)	0.033(4)	0.008(3)	0.015(3)	0.007(3)
C(24)	0.012(3)	0.032(4)	0.027(4)	0.004(3)	0.001(3)	-0.006(3)
C(25)	0.018(3)	0.022(4)	0.022(3)	0.001(3)	0.005(3)	-0.004(3)
C(26)	0.024(4)	0.020(4)	0.026(4)	-0.004(3)	-0.002(3)	-0.004(3)
C(27)	0.031(4)	0.036(5)	0.021(4)	0.006(3)	-0.008(3)	0.004(3)
C(28)	0.029(4)	0.023(4)	0.031(4)	0.005(3)	-0.003(3)	0.000(3)

C(29)	0.043(5)	0.023(4)	0.035(4)	-0.003(3)	-0.009(4)	-0.003(4)
C(30)	0.024(4)	0.028(4)	0.027(4)	0.000(3)	-0.013(3)	-0.002(3)
Fe(2)	0.0104(5)	0.0283(5)	0.0199(5)	0.0015(4)	0.0016(4)	-0.0015(4)
Cl(31)	0.0514(13)	0.0609(14)	0.0265(9)	0.0079(9)	0.0177(9)	0.0264(10)
Cl(32)	0.0402(11)	0.0291(10)	0.0366(10)	-0.0035(8)	0.0146(9)	-0.0082(8)
Cl(33)	0.0325(11)	0.0390(11)	0.0504(12)	-0.0047(9)	0.0131(9)	0.0069(8)
Cl(34)	0.0488(13)	0.0656(15)	0.0386(11)	0.0080(10)	0.0301(10)	0.0051(10)
O(31)	0.020(2)	0.027(3)	0.022(2)	0.0029(19)	0.005(2)	0.0024(19)
O(32)	0.018(2)	0.028(3)	0.027(2)	0.000(2)	0.008(2)	-0.001(2)
N(31)	0.017(3)	0.023(3)	0.032(3)	0.002(2)	0.013(2)	-0.002(2)
N(32)	0.016(3)	0.023(3)	0.015(3)	0.000(2)	0.000(2)	-0.003(2)
N(33)	0.014(3)	0.033(4)	0.021(3)	0.006(2)	-0.001(2)	-0.002(2)
N(34)	0.015(3)	0.029(3)	0.024(3)	0.002(2)	0.000(2)	-0.005(2)
C(31)	0.018(4)	0.025(4)	0.035(4)	0.003(3)	0.011(3)	0.000(3)
C(32)	0.019(4)	0.028(4)	0.029(4)	0.002(3)	0.012(3)	0.001(3)
C(33)	0.029(4)	0.032(4)	0.032(4)	0.012(3)	0.016(3)	0.012(3)
C(34)	0.018(4)	0.047(5)	0.015(3)	0.006(3)	0.001(3)	0.015(3)
C(35)	0.017(4)	0.035(4)	0.027(4)	-0.005(3)	0.003(3)	0.002(3)
C(36)	0.009(3)	0.034(4)	0.030(4)	-0.003(3)	0.008(3)	-0.003(3)
C(37)	0.009(3)	0.031(4)	0.031(4)	0.000(3)	0.007(3)	-0.005(3)
C(38)	0.009(3)	0.027(4)	0.025(3)	0.004(3)	0.005(3)	-0.001(3)
C(39)	0.017(3)	0.034(4)	0.027(4)	-0.007(3)	0.010(3)	-0.008(3)
C(40)	0.017(4)	0.027(4)	0.030(4)	-0.004(3)	0.004(3)	-0.009(3)
C(41)	0.013(4)	0.034(4)	0.042(4)	-0.013(3)	0.009(3)	-0.010(3)
C(42)	0.020(4)	0.042(5)	0.035(4)	-0.009(4)	0.010(3)	-0.003(3)
C(43)	0.024(4)	0.041(5)	0.022(3)	-0.010(3)	0.006(3)	-0.012(3)
C(44)	0.014(3)	0.034(4)	0.018(3)	-0.005(3)	0.002(3)	-0.007(3)
C(45)	0.013(3)	0.029(4)	0.019(3)	-0.001(3)	0.002(3)	-0.002(3)
C(46)	0.013(3)	0.022(4)	0.020(3)	0.000(3)	0.002(3)	0.001(2)
C(47)	0.018(4)	0.034(4)	0.024(3)	0.008(3)	0.002(3)	0.005(3)
C(48)	0.008(3)	0.050(5)	0.032(4)	0.009(3)	0.002(3)	0.005(3)
C(49)	0.013(3)	0.048(5)	0.032(4)	0.003(4)	0.004(3)	-0.003(3)
C(50)	0.014(3)	0.036(4)	0.022(3)	0.009(3)	-0.003(3)	-0.005(3)
C(51)	0.021(4)	0.038(5)	0.025(4)	0.007(3)	0.003(3)	-0.002(3)
C(52)	0.031(4)	0.034(4)	0.040(4)	0.008(4)	0.011(4)	-0.003(3)
C(53)	0.038(5)	0.053(6)	0.032(4)	0.023(4)	0.012(4)	0.005(4)
C(54)	0.033(5)	0.066(6)	0.020(4)	0.009(4)	0.006(3)	-0.003(4)
C(55)	0.019(4)	0.044(5)	0.027(4)	-0.003(3)	0.004(3)	-0.005(3)
C(56)	0.018(4)	0.028(4)	0.047(5)	-0.001(3)	0.005(3)	0.001(3)
C(57)	0.012(4)	0.047(5)	0.057(5)	0.001(4)	-0.001(4)	0.001(3)
C(58)	0.017(4)	0.049(5)	0.055(5)	0.002(4)	0.005(4)	-0.007(4)
C(59)	0.023(4)	0.055(5)	0.037(4)	-0.011(4)	0.003(3)	-0.020(4)
C(60)	0.019(4)	0.047(5)	0.030(4)	-0.017(4)	0.002(3)	-0.016(3)
O(61)	0.065(5)	0.139(7)	0.106(6)	-0.036(5)	0.053(5)	-0.018(4)
C(61)	0.083(10)	0.139(12)	0.077(8)	-0.030(8)	0.055(8)	-0.034(8)
C(62)	0.045(6)	0.088(8)	0.060(6)	-0.015(6)	0.016(5)	-0.015(6)
C(63)	0.029(5)	0.073(7)	0.060(6)	-0.014(5)	0.005(4)	-0.001(5)

C(64)	0.036(6)	0.086(8)	0.083(8)	-0.029(6)	0.021(5)	0.006(5)
O(62)	0.089(7)	0.120(9)	0.122(8)	-0.016(7)	0.056(7)	-0.029(6)
C(65)	0.083(7)	0.117(9)	0.120(9)	-0.018(8)	0.057(7)	-0.028(7)
C(66)	0.084(8)	0.119(9)	0.120(9)	-0.023(8)	0.053(7)	-0.026(7)
C(67)	0.075(8)	0.115(10)	0.119(9)	-0.029(8)	0.059(7)	-0.026(7)
C(68)	0.081(8)	0.116(9)	0.118(9)	-0.026(8)	0.066(7)	-0.022(7)
O(62B)	0.093(8)	0.121(9)	0.119(8)	-0.016(8)	0.057(7)	-0.027(7)
C(65B)	0.083(8)	0.116(10)	0.118(10)	-0.017(9)	0.059(8)	-0.031(8)
C(66B)	0.083(8)	0.114(9)	0.119(9)	-0.022(8)	0.057(7)	-0.027(7)
C(67B)	0.087(8)	0.120(9)	0.120(8)	-0.024(7)	0.058(7)	-0.025(7)
C(68B)	0.093(9)	0.121(10)	0.119(9)	-0.019(8)	0.052(8)	-0.030(8)
C(71)	0.045(5)	0.092(7)	0.075(6)	-0.021(5)	0.017(5)	0.000(5)
C(72)	0.039(5)	0.081(6)	0.072(5)	-0.014(5)	0.012(4)	-0.012(4)
C(73)	0.037(6)	0.077(7)	0.062(6)	-0.016(5)	0.025(5)	-0.015(5)
O(71B)	0.058(9)	0.094(10)	0.074(9)	-0.018(9)	0.009(8)	-0.001(8)
C(74B)	0.056(9)	0.090(10)	0.076(10)	-0.015(9)	0.009(9)	-0.008(9)
C(73B)	0.045(7)	0.082(8)	0.071(8)	-0.013(7)	0.019(7)	-0.009(7)

Table S5. Mössbauer parameters of **4(Solvent)** in solid and in solution.

	δ (mm s^{-1})	ΔE_Q (mm s^{-1})
4(Py)$_2$ solid	1.14	2.70
4(Py)$_2$ pyridine solution	1.14	2.70
4(OH$_2$) solid	1.07	2.07

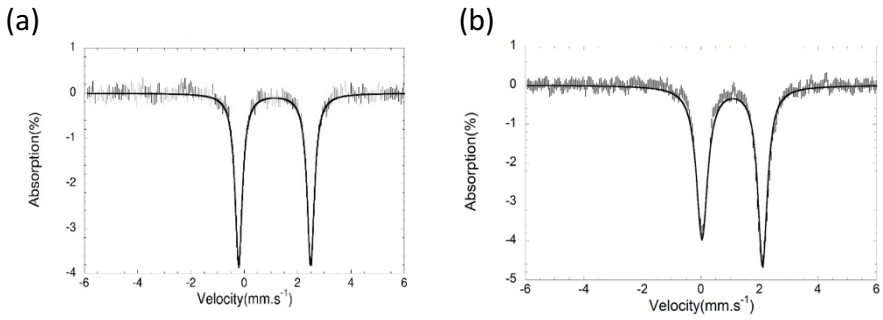

Figure S1. Mössbauer spectra of **4(Py)$_2$** in pyridine solution (a) and **4(OH$_2$)** in the solid state (b).

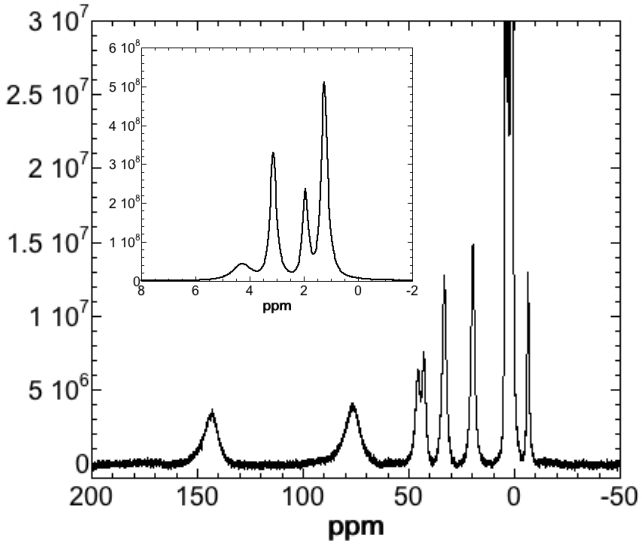

Figure S2. ^{1}H-NMR spectrum of **4(Py)$_2$** in pyridine solution.

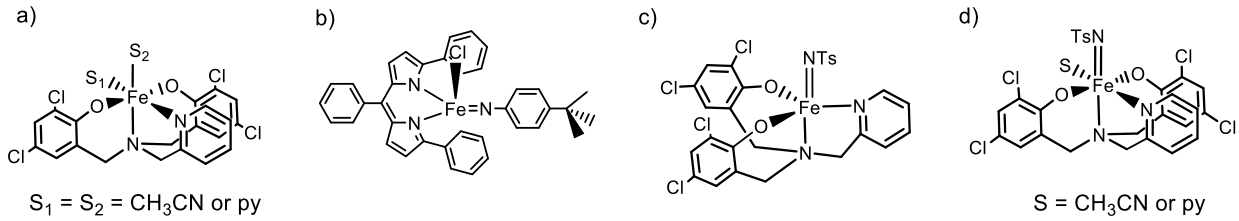

Figure S3. Schematic view of the complexes used in computations: a) Fe^{II} with two solvent molecules (acetonitrile or pyridine); b) Fe^{IV} complex from Betley et al.[21]; c) Fe^{IV} without solvent **5**; d) Fe^{IV} with one solvent molecule coordinated S=CH_3CN noted **5(NCCH$_3$)** and S=pyridine noted **5(Py)**.

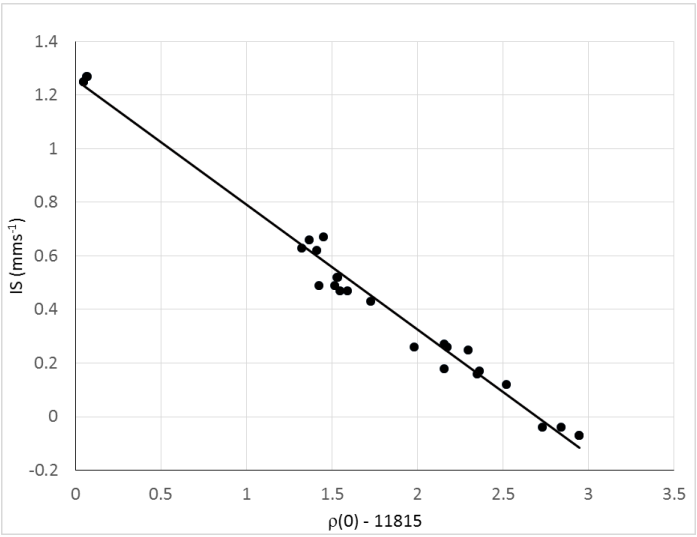

Figure S4. Experimental IS (mms^{-1}) *vs* ρ(0) calculated as described in the computation details. The full line represents the linear correlation obtained from the equation IS = -0.467 (ρ(0) – 11816.7), with R^2 = 0.99.

Table S6. DFT modelling of Fe^{II} complexes: Fe-ligand distances (Å) and calculated Mössbauer parameters (δ_c and $|\Delta E_Q|_c$, mm. s^{-1}), compared to the experimental data (δ_{exp} and $|\Delta E_Q|_{exp}$, mm. s^{-1}). Geometry optimizations at Orca B3LYP/BS1 level.

Solv	dFe-O1	dFe-O2	dFe-N_{Py}	dFe-N	dFe-N_{solv}	δ_c	$\|\Delta E_Q\|_c$	δ_{exp}	$\|\Delta E_Q\|_{exp}$
No	1.89	1.91	2.15	2.19	-	1.06	1.67		
4(NCCH$_3$)	1.93	1.98	2.16	2.25	2.95; 2.38	1.23	1.92	1.07	2.07
4(py)	2.00	2.04	2.25	2.29	2.26; 2.18	1.25	2.62	1.14	2.70
4(py) exp. *	2.015	2.028						1.14	2.70

* this work.

Table S7. DFT modelling of Fe^{II} complex: coordination energies (kcal mol^{-1}).

	ΔE	ΔH	ΔG
4(py)	-42.8	-40.9	-14.7
4($NCCH_3$)	-16.7	-15.5	6.3

Table S8. DFT modelling of Fe^{IV} dipyrromethene complex: geometry optimized with Orca (B3LYP/BS1 level) for the three spin states, with the resulting energetic ordering, group spin densities (ρ_{Fe}, ρ_{nit} and ρ_{Cl}) and MB parameters (δ and $|\Delta E_Q|$, mm. s^{-1}), compared to experimental data.[21] Nit represents the nitrene group: NC_6H_4-*p*-^{t}Bu.

	dFe-N(nit)	dFe-Cl	ΔE	ΔH	ΔG	ρ_{Fe}	ρ_{nit}	ρ_{Cl}	δ	$\|\Delta E_Q\|$
S = 1	1.81	2.25	0.0	0.0	0.0	3.32	-1.48	0.07	0.44	1.96
S = 2	1.79	2.28	-8.7	-9.0	-7.2	3.99	-0.36	0.18	0.31	2.14
S = 3	1.90	2.27	-0.8	-1.4	-0.3	4.05	1.55	0.16	0.48	2.29
Exp [21]	1.77	2.21							0.29	2.29

Table S9. DFT modelling of the Fe^{IV} dipyrromethene complex: influence of the choice of the functional for describing the electronic configuration of the quintet state. Comparison with experimental data for Fe-ligand distances and MB parameters (mm. s^{-1}).[21] Geometry optimizations with ADF and TZ2P basis sets. Nit represents the nitrene group: NC_6H_4-*p*-^{t}Bu.

	dFe-N(nit)	dFe-Cl	ρ_{Fe}	ρ_{nit}	ρ_{Cl}	δ	$\|\Delta E_Q\|$
B3LYP	1.80	2.26	3.89	-0.32	0.21	0.33	2.143
B3LYP*	1.79	2.26	3.82	-0.27	0.22	0.33	2.183
OPBE	1.74	2.22	3.59	-0.04	0.22	0.27	2.291
Exp.	1.77	2.21				0.29	2.29

Table S10. DFT modelling of Fe^{IV}=NTs complexes (**5**, **5(NCCH$_3$)** and **5(Py)** from geometry optimizations with Orca (B3LYP/BS1) : Fe-ligand distances (Å), relative energetic spin ordering (kcal mol^{-1}) and group spin densities of Fe, NTs and average of both phenolate ligands (Oph), for the three possible spin states. Three possible structures were examined: with no solvent coordinated, or with one molecule of acetonitrile or one molecule of pyridine. Spin densities on solvent molecules were in a range 0-0.07.

	dFe-N(Ts)	dFe-N(Solv)	ΔE	ΔH	ΔG	ρ_{Fe}	ρ_{nit}	ρ_{Cl}
^{3}**5**	1.83		0.00	0.00	0.00	1.54	0.40	0.05
^{5}**5**	2.01		-2.10	-1.70	-2.70	3.95	-0.55	0.23
^{7}**5**	2.26		-3.80	-3.60	-5.90	4.11	1.22	0.24
^{3}**5(NCCH$_3$)**	1.75	3.21	0.00	0.00	0.00	1.26	0.76	-0.01
^{5}**5(NCCH$_3$)**	1.86	3.12	-8.30	-9.00	-11.20	4.03	-0.61	0.22
^{7}**5(NCCH$_3$)**	2.01	3.33	-4.80	-6.00	-7.20	4.14	1.18	0.26
^{3}**5(Py)**	1.79	2.10	0.00	0.00	0.00	1.18	0.87	-0.01
^{5}**5(Py)**	1.91	2.34	-10.00	-10.80	-13.60	4.11	-0.72	0.22
^{7}**5(Py)**	2.00	2.30	-1.20	-3.20	-4.00	4.13	1.21	0.24

Table S11. DFT modelling of **5**: coordination energies (kcal mol^{-1}) with acetonitrile or pyridine for the quintet state.

Solvant	ΔE	ΔH	ΔG
MeCN	-7.7	-7.8	3
py	-25.5	-24.7	-12.5

Table S12. DFT modelling of Fe^{IV}=NTs complex **5** without solvent with ADF on the quintet state: influence of the functional (OPBE, B3LYP* or B3LYP) and of the initial geometry on the Fe-N(Ts) optimized distance (dFe-N(Ts), Å) and on the group spin densities.

Functional	Init. geom.*	dFe-N(Ts)	ΔE	ρ_{Fe}	ρ_{nit}	ρ_{Cl}
B3LYP	Fe^{IV}	1.84	0.00	3.83	-0.42	0.23
B3LYP	Fe^{III}	1.92	-3.80	4.04	-0.64	0.24
B3LYP*	Fe^{IV}	1.78	0.00	3.47	-0.07	0.22
B3LYP*	Fe^{III}	1.91	-1.20	3.97	-0.59	0.24
OPBE	Fe^{IV}	1.74	0.00	3.10	0.30	0.22
OPBE	Fe^{III}	1.72	-2.20	3.17	0.38	0.17

* Fe^{IV} geometry: d_{init} (Fe-N_{Ts}) = 1.76 Å; Fe^{III} geometry: d_{init} (Fe-N_{Ts}) = 1.92 Å.

Table S13. Computed EA and BDE (kcal mol^{-1}) of the complex Fe^{IV}=NR without or with coordinated solvent (acetonitrile or pyridine), and influence of the nitrene nature. NTs: R = $SO_2C_6H_4$-*p*-CH_3; Ns: R = SO_2Ph-p-NO_2; Pys: N-SO_2py-*p*-CH_3: the phenyl ring of NTs is replaced by pyridine. Fe^{IV} complexes and their reduced species were all considered in the high spin state (resp. S=2 and S = 5/2).

Ligand	solvent	Nitrene	EA ΔE	EA ΔH	EA ΔG	BDE ΔE
$L^{(Cl,py)}$	-	NTs	120.1	122.1	120.5	105.5
	CH_3CN	NTs	114.5	115.3	113.6	106.6
	py	NTs	108.3	109.2	109.5	98.8
	-	Ns	124.9	126.1	125.9	
	-	Pys	121.9	123.4	123.4	
$L^{(tBu,py)}$	-	NTs	106.6	107.3	106.9	
$L^{(NO2,py)}$	-	NTs	122.3	124.8	122.6	
$L^{(NO2,py)}$	-	Ns	127.1	128.3	129.1	

Table S14. Electronic energies (Eh), enthalpy and free enthalpy (kcal mol^{-1}) of the critical points in the styrene aziridination pathway for S=1 channel, with attack on the C_β carbon of styrene.

	E	ΔE	ΔH	ΔG
5' + styr	-5278.81018	0	0.00	0
Re	-5278.80263	0.17	4.03	19.98
TS1	-5278.79185	11.50	11.33	25.54
Int	-5278.83213	-13.77	-11.66	4.71
TS2	-5278.80576	2.78	3.31	19.40
Pdt	-5278.84243	-20.24	-18.45	-1.99

Table S15. Selected distances (Å): Fe-N, N being the nitrogen from the nitrene group NSO_2Ph, and both N(nitrene) – carbon distances from the double bond which will form the aziridine cycle, imaginary frequency of both TS (ν_{im}), together with group spin densities and Mülliken charges (Fe, NSO_2Ph, styrene) of the critical points (Re, TS1, Int, TS2, Pdt) in the styrene aziridination pathway for S=1 channel, with attack on the C_β carbon of styrene.

	Re	TS1	Int	TS2	Prod
$dFe\text{-}N_t$	1.87	1.88	2.04	2.78	3.13
$dN\text{-}C_{prox}$		2.19	1.47	1.48	1.46
$dN\text{-}C_{dist}$		2.92	2.52	2.20	1.47
ν_{im}		i289		i370	
spin densities					
Fe	3.01	3.03	0.94	-0.01	1.94
NSO_2Ph	-1.16	-0.80	0.00	0.29	-0.01
styrene	0.00	-0.36	0.99	0.07	0.00
Charges					
Fe	1.00	1.01	0.94	-0.22	0.87
NSO_2Ph	-0.34	-0.48	-0.50	-0.20	-0.21
styrene	0.01	0.21	0.15	0.32	0.35

Table S16. Electronic energies (Eh) and energy differences (kcal mol^{-1}) of the critical points in the styrene aziridination pathway for the S=2 channel, with attack on the C_α carbon of styrene.

	E	ΔE	ΔH	ΔG
5' + styr.	-5278.82063	0.00	0.00	0.00
Re	-5278.81854	1.31	1.29	18.60
TS1	-5278.79595	15.49	15.81	31.65
Int	-5278.81928	0.85	1.61	17.78
TS2	-5278.81058	6.31	7.50	23.07
Pdt	-5278.85797	-23.43	-20.50	-5.92

Table S17. Selected distances (Å): Fe-N, N being the nitrene group NSO_2Ph, and both N (nitrene) – carbon distances from the double bond which will form the aziridine cycle, imaginary frequency of both TS (ν_{im}), together with group spin densities and Mülliken charges (Fe, NSO_2Ph, styrene) of the critical points (Re, TS1, Int, TS2, Pdt) in the styrene aziridination pathway for S=2 channel, with attack on the C_α carbon of styrene.

	Re	TS1	Int	TS2	Pdt
dFe-N	1.97	2.02	2.08	2.09	2.51
dN-C_{prox}		2.12	1.48	1.50	1.48
dN-C_{dist}		2.64	2.47	2.08	1.52
ν_{im}		i311		i588	
spin densities					
Fe	4.13	4.10	4.17	3.98	3.75
NSO_2Ph	-0.79	-0.27	0.18	0.15	0.01
styrene	0.00	-0.38	-0.96	-0.52	0.01
Charges					
Fe	1.13	1.10	1.14	1.08	0.98
NSO_2Ph	-0.49	-0.57	-0.59	-0.48	-0.34
styrene	0.00	0.25	0.19	0.32	0.41

Table S18. Electronic energies (Eh) and energy differences (kcal mol^{-1}) of the critical points in the styrene aziridination pathway for the S=2 channel, with attack on the C_β carbon of styrene.

	E	ΔE	ΔH	ΔG
5' + styr.	-5278.82063	0	0.00	0
Re	-5278.81254	5.08	5.25	22.77
TS1	-5278.81026	6.51	6.93	22.95
Int	-5278.84567	-15.71	-13.63	2.34
TS2	-5278.83838	-11.14	-9.25	5.79
Pdt	-5278.85797	-23.43	-20.50	-5.92

Table S19. Selected distances (Å): Fe-N, N being the nitrogen from the nitrene group NSO_2Ph, and both N (nitrene) – carbon distances from the double bond which will form the aziridine cycle, imaginary frequency of both TS (ν_{im}), together with group spin densities and Mülliken charges (Fe, NSO_2Ph, styrene) of the critical points (Re, TS1, Int, TS2, Pdt) in the styrene aziridination pathway for S=2 channel, with attack on the C_β carbon of styrene.

	Re	TS1	Int	TS2	Pdt
dFe-N	1.97	1.92	2.05	2.15	2.51
dN-C_{prox}		2.30	1.48	1.47	1.48
dN-C_{dist}		2.87	2.44	2.10	1.52
ν_{im}		i218		i351	
spin densities					
Fe	4.13	4.12	4.16	3.90	3.75
NSO_2Ph	-0.79	-0.44	0.17	0.03	0.01
Styrene	0.00	-0.27	-0.93	-0.23	0.01
Charges					
Fe	1.13	1.14	1.13	1.03	0.98
NSO_2Ph	-0.49	-0.61	-0.58	-0.03	-0.34
Styrene	0.00	0.20	0.18	0.00	0.41

Table S20. Electronic energies (Eh) and energy differences (kcal mol^{-1}) of the critical points in the first step of styrene aziridination pathway for the S=2 channel, with attack on the C_β carbon of styrene, from optimizations in solvent (COSMO with acetonitrile).

	E	ΔE	ΔH	ΔG
5' + styr.	-5278.82175	0.00	0.00	0.00
Re	-5278.81936	1.50	1.31	20.11
TS1	-5278.81310	5.43	5.77	22.50
Int	-5278.85639	-21.74	-19.75	-2.18
Pdt	-5278.87979	-36.42	-34.16	-16.49

Table S21. Selected distances (Å): Fe-N, N being the nitrene group NSO_2Ph, and both N (nitrene) – carbon distances from the double bond which will form the aziridine cycle, imaginary frequency of TS (ν_{im}), together with group spin densities and Mülliken charges (Fe, NSO_2Ph, styrene) of the critical points (Re, TS1, Int) in the styrene aziridination pathway for S=2 channel, with attack on the Cβ carbon of styrene, from optimizations in solvent (COSMO with acetonitrile).

	Re	TS1	Int
dFe-N	1.97	1.93	2.00
dN-C_{prox}		2.42	1.47
dN-C_{dist}		2.95	2.41
ν_{im}		i139	
spin densities			
Fe	4.13	4.13	4.11
NSO_2Ph	-0.78	-0.46	0.16
Styrene	0.00	-0.26	-0.83
Charges			
Fe	1.13	1.13	1.12
NSO_2Ph	-0.56	-0.69	-0.73
Styrene	0.02	0.24	0.31

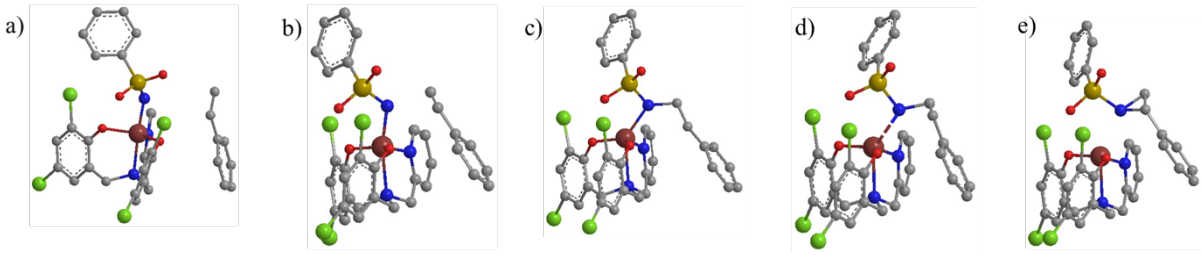

Figure S5. Structures of the critical points along the aziridination pathway: a) Re; b) TS1; c) Int; d) TS2, e) Pdt.

Cartesian coordinates of geometry optimized species

^{5}4

C	1.931392	6.912770	13.770439
C	2.287779	6.773684	12.399465
C	2.509360	5.456978	11.928680
C	2.383894	4.339212	12.746924
C	2.034263	4.517250	14.084075
C	1.811328	5.791875	14.595660
O	2.407376	7.811522	11.590667
Fe	3.368582	9.343358	12.132546
Cl	2.971337	5.239332	10.254365
Cl	1.880397	3.115229	15.135103
C	1.647374	8.286083	14.324050
N	2.817675	9.205896	14.246163
C	2.430707	10.587645	14.654448
C	3.554796	11.573179	14.471129
C	4.019074	11.831169	13.150665
C	5.136873	12.691168	13.028903
C	5.748976	13.282176	14.129125
C	5.247881	13.018939	15.402847
C	4.157354	12.172701	15.577281
O	3.476173	11.252465	12.096441
Cl	6.025478	13.742773	16.806102
Cl	5.801230	12.968134	11.431877
N	5.322255	9.071819	12.995642
C	6.446949	9.422831	12.350037
C	7.589611	9.849488	13.015634
C	7.556779	9.923522	14.408372
C	6.393586	9.557433	15.081158
C	5.288016	9.138550	14.343898
C	3.990446	8.711041	14.995170
H	1.299096	8.207293	15.365097
H	2.564132	3.348269	12.347147
H	1.535520	5.914109	15.638747
H	6.326507	9.628827	16.161503
H	8.420525	10.276474	14.963648
H	8.469807	10.139384	12.452661
H	6.608096	13.928588	13.993226
H	6.409091	9.375250	11.266470
H	3.944166	7.616815	14.983695
H	3.963957	9.035857	16.044420
H	2.099855	10.580396	15.704168
H	1.574487	10.864681	14.030055

^{5}4.(CH_3CN)

C	1.333688	7.153855	13.851649
C	1.956669	6.844451	12.609586
C	1.877626	5.494782	12.181658
C	1.250377	4.502743	12.926495
C	0.672275	4.844685	14.147419
C	0.711556	6.157701	14.607401
O	2.564013	7.743992	11.875881
Fe	3.560491	9.306111	12.422857
N	4.533857	9.567461	10.271550
C	4.431770	10.699801	10.028419
C	4.246676	12.123355	9.798456
Cl	2.605385	5.071700	10.641546
Cl	-0.116667	3.601987	15.113051
C	1.292752	8.583743	14.325845
N	2.629334	9.220049	14.466430
C	2.454710	10.623726	14.935277
C	3.762560	11.351811	15.072432
C	4.509023	11.586686	13.884184
C	5.768113	12.214602	14.048686
C	6.263803	12.595645	15.290196
C	5.491122	12.353612	16.425001
C	4.246223	11.739049	16.320711
O	4.073989	11.192130	12.714832
Cl	6.112251	12.810665	18.008620
Cl	6.764920	12.469380	12.621594
N	5.244762	8.653647	13.612190
C	6.506971	8.804087	13.182127
C	7.580115	8.943219	14.054766
C	7.324679	8.937222	15.426544
C	6.014914	8.782295	15.873432
C	4.991749	8.647042	14.936228
C	3.544486	8.456308	15.336743
H	0.752616	8.634838	15.284717
H	1.220046	3.482411	12.562717
H	0.245762	6.410368	15.555168
H	5.778316	8.803785	16.931977
H	8.132901	9.068050	16.139968
H	8.583616	9.077109	13.665925
H	7.238065	13.063206	15.371181
H	6.637147	8.833501	12.105049
H	3.292493	7.396428	15.223090
H	3.408292	8.718108	16.395853
H	1.921148	10.620532	15.899133
H	1.821224	11.118552	14.191737
H	0.746251	9.204989	13.606790
H	3.661324	11.546975	17.215241
H	4.982287	12.675734	10.388981
H	4.349654	12.363403	8.735823
H	3.245009	12.390106	10.150281
N	1.268783	10.624343	11.118501
C	1.141512	9.715239	10.405551
C	1.006318	8.570010	9.512594
H	0.671575	8.895771	8.522667
H	1.970655	8.060610	9.446327
H	0.283397	7.861354	9.926733

^{5}4.(Py)

Fe	2.014960	6.875104	13.773204
Cl	4.658121	5.530287	6.983733
Cl	2.900464	2.838246	11.369318

Cl	-1.711076	12.911872	12.668274
Cl	-1.283517	8.902562	16.315665
O	2.906928	5.509212	12.619868
O	1.309530	8.383953	14.945971
N	2.370709	8.384458	12.086019
N	0.011725	7.008507	12.750749
N	1.451870	5.348292	15.225354
N	3.969455	7.118030	14.888062
C	3.679546	8.047710	11.468428
H	4.400853	8.021403	12.293169
H	3.991729	8.855857	10.786604
C	3.685611	6.741565	10.714188
C	4.091200	6.724998	9.377848
H	4.375714	7.651962	8.888737
C	4.139504	5.529448	8.667331
C	3.775313	4.329044	9.274215
H	3.807197	3.395230	8.725242
C	3.362111	4.351081	10.600272
C	3.295364	5.539623	11.374997
C	2.454351	9.723548	12.727621
H	2.763584	10.469902	11.977428
H	3.246129	9.656854	13.481452
C	1.155137	10.153854	13.354744
C	0.437626	11.225837	12.825002
H	0.832428	11.776748	11.976505
C	-0.795633	11.576910	13.365531
C	-1.325553	10.872740	14.445796
H	-2.289305	11.139360	14.863623
C	-0.599348	9.813506	14.975837
C	0.659240	9.406955	14.462229
C	1.254516	8.311263	11.125068
H	1.493073	7.520223	10.407579
H	1.147956	9.247807	10.558058
C	-0.051307	7.959243	11.800415
C	-1.258616	8.558177	11.438314
H	-1.269640	9.341957	10.688218
C	-2.426511	8.169353	12.087766
H	-3.373455	8.639625	11.839435
C	-2.357596	7.184759	13.074018
H	-3.240280	6.863620	13.616503
C	-1.115307	6.636396	13.373777
H	-1.001288	5.886957	14.150299
C	1.703640	4.047893	14.986827
H	2.167345	3.833026	14.028972
C	1.390121	3.051478	15.907805
H	1.608672	2.014430	15.673417
C	0.796748	3.412261	17.117837
H	0.539573	2.656737	17.855176
C	0.538957	4.761591	17.363339
H	0.078178	5.089068	18.289984
C	0.881654	5.699460	16.393211
H	0.702025	6.762591	16.519376
C	4.985606	6.269460	14.651043
H	4.803370	5.544474	13.864571
C	6.180274	6.312211	15.365386
H	6.972337	5.606715	15.134730
C	6.330571	7.269234	16.369367
H	7.250828	7.330089	16.943751
C	5.273421	8.142973	16.624032
H	5.341178	8.899580	17.399503
C	4.111568	8.032689	15.863405
H	3.247415	8.670675	16.019087

FeIV dipyrro (Betley) S=1 (Orca/B3LYP)

Fe	-0.091411	-0.723228	0.586067
N	0.039740	-0.243150	2.535879
C	1.266820	-0.110215	3.194630
C	1.013541	-0.009066	4.598866
C	-0.357612	-0.024973	4.768292
C	-0.932702	-0.178300	3.475089
C	-2.368066	-0.195304	3.166171
H	-0.909357	0.026678	5.697391
H	1.767788	0.064665	5.368632
C	2.516448	0.012853	2.558996
N	1.813990	-0.283967	0.187632
C	2.388842	-0.049069	-1.016399
C	3.726839	0.394995	-0.839905
C	3.968766	0.408975	0.523264
C	2.762579	-0.000485	1.170098
H	4.881074	0.698033	1.024757
H	4.415953	0.639106	-1.637437
C	1.679515	-0.204596	-2.293468
C	3.704734	0.242832	3.431111
C	4.766221	-0.674559	3.425142
C	5.883342	-0.468946	4.234132
C	5.960513	0.662247	5.049406
C	4.913285	1.586047	5.053643
C	3.790939	1.376642	4.252684
H	4.701654	-1.552193	2.789348
H	6.693127	-1.193389	4.227687
H	6.833045	0.824060	5.676454
H	4.971099	2.473341	5.678247
H	2.978472	2.096486	4.246872
C	1.800954	0.791768	-3.278111
C	1.117562	0.681709	-4.487679
C	0.305803	-0.427850	-4.736197
C	0.193128	-1.430742	-3.771475
C	0.876774	-1.325558	-2.561614
H	2.415778	1.664228	-3.075039
H	1.212014	1.466697	-5.233569
H	-0.233336	-0.509964	-5.675749
H	-0.433414	-2.298478	-3.955875
H	0.792703	-2.114915	-1.823337
N	-1.225318	0.185595	-0.486548
C	-2.918693	-1.050106	2.196740
C	-4.279936	-1.002734	1.902570
C	-5.118512	-0.113989	2.578286
C	-4.586476	0.722363	3.562963
C	-3.225068	0.681114	3.855780
H	-2.289353	-1.783668	1.707506
H	-4.687032	-1.673381	1.150396
H	-6.179631	-0.078348	2.346577
H	-5.231606	1.414552	4.097561
H	-2.808220	1.350975	4.602317

C	-1.993980	0.047108	-1.568712
C	-2.077097	1.109103	-2.514026
C	-2.832801	0.953986	-3.658189
C	-3.549690	-0.232432	-3.925166
C	-3.474972	-1.269404	-2.975649
C	-2.717667	-1.152253	-1.822849
H	-1.512415	2.015638	-2.326999
H	-2.861144	1.770079	-4.373183
C	-4.344700	-0.358757	-5.227523
H	-4.007551	-2.197907	-3.145073
H	-2.627822	-1.968789	-1.115496
C	-5.103147	-1.693283	-5.323944
C	-5.373845	0.790739	-5.318890
C	-3.364648	-0.269801	-6.420309
H	-5.662666	-1.729932	-6.264937
H	-4.421483	-2.551022	-5.311660
H	-5.821502	-1.811453	-4.504879
H	-3.913508	-0.344883	-7.366587
H	-2.813749	0.676257	-6.424845
H	-2.633825	-1.085507	-6.383150
H	-5.942651	0.710757	-6.252594
H	-6.080788	0.748903	-4.482815
H	-4.893479	1.774237	-5.304583
Cl	-0.437446	-2.940364	0.375463

FeIV dipyrro (Betley) S=2 (Orca/B3LYP)

Fe	-0.062282	-0.714661	0.592591
N	0.038701	-0.187705	2.521101
C	1.264868	-0.087525	3.189286
C	0.995237	0.019714	4.588532
C	-0.378979	0.032547	4.744706
C	-0.945467	-0.106823	3.448663
C	-2.371800	-0.127000	3.110491
H	-0.937921	0.093029	5.668755
H	1.742449	0.080483	5.366149
C	2.523534	0.010679	2.563007
N	1.838941	-0.250080	0.178790
C	2.421894	-0.000816	-1.016957
C	3.763775	0.423627	-0.821917
C	3.996170	0.411752	0.542716
C	2.782942	0.001682	1.177056
H	4.906161	0.687027	1.055987
H	4.461354	0.672696	-1.610330
C	1.718088	-0.156351	-2.295395
C	3.708891	0.206376	3.446886
C	4.748584	-0.735616	3.440221
C	5.863656	-0.562954	4.259635
C	5.960362	0.559134	5.085329
C	4.935068	1.507320	5.089709
C	3.814385	1.331153	4.278627
H	4.668164	-1.605996	2.796350
H	6.656477	-1.305827	4.253062
H	6.831418	0.695261	5.720399
H	5.009045	2.387857	5.722018
H	3.019795	2.070661	4.271603
C	1.838345	0.839079	-3.280450
C	1.144327	0.731033	-4.483590
C	0.328527	-0.377484	-4.725944
C	0.223973	-1.383031	-3.763593
C	0.914845	-1.278181	-2.558044
H	2.453805	1.711722	-3.080314
H	1.231671	1.517323	-5.228787
H	-0.221456	-0.455952	-5.659633
H	-0.405648	-2.249062	-3.944181
H	0.835044	-2.068884	-1.819648
N	-1.146483	0.160428	-0.527888
C	-2.889420	-0.976458	2.118252
C	-4.241040	-0.930791	1.783095
C	-5.101729	-0.052701	2.443996
C	-4.603356	0.775124	3.453836
C	-3.251369	0.737879	3.785895
H	-2.246710	-1.710686	1.645382
H	-4.621684	-1.592751	1.010209
H	-6.155521	-0.018156	2.181156
H	-5.267519	1.458568	3.976024
H	-2.859153	1.402959	4.549902
C	-1.960497	0.031305	-1.568446
C	-2.119339	1.102906	-2.502181
C	-2.898253	0.945202	-3.629305
C	-3.582429	-0.262686	-3.895288
C	-3.453730	-1.312754	-2.962941
C	-2.666139	-1.184137	-1.833378
H	-1.577665	2.023282	-2.311119
H	-2.973813	1.768224	-4.333386
C	-4.396178	-0.399582	-5.184682
H	-3.964512	-2.253158	-3.135413
H	-2.533975	-2.008837	-1.140313
C	-5.124026	-1.751098	-5.281349
C	-5.453699	0.725228	-5.254835
C	-3.434318	-0.278971	-6.390216
H	-5.698208	-1.792654	-6.213412
H	-4.422207	-2.592378	-5.288234
H	-5.825116	-1.894079	-4.451361
H	-3.993355	-0.361824	-7.329972
H	-2.906814	0.680258	-6.394521
H	-2.683575	-1.077074	-6.367160
H	-6.032427	0.637511	-6.181812
H	-6.148763	0.660923	-4.410211
H	-4.997231	1.719816	-5.239651
Cl	-0.271968	-2.979232	0.468631

FeIV dipyrro (Betley) S=3 (Orca/B3LYP)

Fe	0.010483	-0.747649	0.568014
N	0.071466	-0.182400	2.489203
C	1.286250	-0.103415	3.183335
C	0.989115	0.015501	4.575584
C	-0.388245	0.057846	4.702572
C	-0.929157	-0.075144	3.395678
C	-2.345793	-0.059127	3.018525
H	-0.964189	0.137506	5.614698
H	1.719871	0.064856	5.369449
C	2.560497	-0.022941	2.584384
N	1.920413	-0.281952	0.190920
C	2.520013	-0.026944	-0.994174

C	3.858548	0.396959	-0.779511
C	4.071652	0.377175	0.589247
C	2.848681	-0.034145	1.203993
H	4.974324	0.650769	1.116334
H	4.566395	0.655146	-1.555853
C	1.807356	-0.168600	-2.269655
C	3.729793	0.161091	3.491508
C	4.762298	-0.788889	3.500032
C	5.863886	-0.627745	4.339738
C	5.954844	0.491139	5.170397
C	4.937380	1.447687	5.159245
C	3.829802	1.282885	4.328074
H	4.686565	-1.656591	2.851991
H	6.650761	-1.376911	4.344866
H	6.815583	0.618488	5.821150
H	5.007465	2.326086	5.794948
H	3.042029	2.029388	4.308638
C	1.894669	0.845989	-3.238108
C	1.160838	0.758636	-4.418945
C	0.340546	-0.348152	-4.656763
C	0.273830	-1.375119	-3.714408
C	1.002855	-1.289978	-2.529668
H	2.510986	1.718262	-3.039088
H	1.219009	1.560453	-5.150238
H	-0.241514	-0.408476	-5.572229
H	-0.356144	-2.241030	-3.892703
H	0.953217	-2.097411	-1.806551
N	-1.140674	0.230791	-0.589169
C	-2.850385	-0.880858	1.997016
C	-4.186112	-0.792375	1.610955
C	-5.046204	0.099935	2.253046
C	-4.563130	0.898605	3.293520
C	-3.225566	0.820596	3.673773
H	-2.214108	-1.631928	1.541288
H	-4.553187	-1.429598	0.811339
H	-6.087844	0.168520	1.951497
H	-5.227465	1.592711	3.801235
H	-2.843838	1.465909	4.459714
C	-1.967078	0.070646	-1.597001
C	-2.256830	1.159779	-2.492570
C	-3.056445	0.968399	-3.595897
C	-3.640843	-0.287990	-3.891563
C	-3.390073	-1.351913	-2.999319
C	-2.584102	-1.196674	-1.888498
H	-1.798229	2.120636	-2.284040
H	-3.233365	1.807127	-4.262867
C	-4.485243	-0.446995	-5.157544
H	-3.822315	-2.327838	-3.189570
H	-2.361369	-2.031072	-1.231542
C	-5.045921	-1.870331	-5.316446
C	-5.674236	0.539961	-5.110601
C	-3.604014	-0.133139	-6.389211
H	-5.638348	-1.931138	-6.236046
H	-4.246751	-2.616525	-5.386756
H	-5.700184	-2.144841	-4.481370
H	-4.191010	-0.231989	-7.310175
H	-3.202390	0.884729	-6.354440
H	-2.757559	-0.827170	-6.448127
H	-6.281590	0.441762	-6.018243
H	-6.314924	0.335132	-4.245693
H	-5.339400	1.579937	-5.042576
Cl	-0.270921	-3.000232	0.443445

FeIV dipyrro (Betley) : S=2 (ADF/B3LYP)

Fe	-0.170961	-0.647779	0.500196
N	-0.050835	-0.117510	2.443403
C	1.179748	-0.028935	3.097749
C	0.928947	0.051254	4.497299
C	-0.437867	0.056698	4.669529
C	-1.015902	-0.054524	3.381364
C	-2.445322	-0.054380	3.055283
H	-0.986177	0.099140	5.595983
H	1.682954	0.099092	5.263875
C	2.426025	0.093384	2.463530
N	1.741476	-0.151036	0.086059
C	2.325328	0.101542	-1.100076
C	3.662252	0.527679	-0.903985
C	3.890220	0.518266	0.455390
C	2.680524	0.104810	1.083319
H	4.795547	0.793025	0.969387
H	4.358171	0.776035	-1.688101
C	1.624964	-0.050565	-2.379932
C	3.610994	0.295223	3.345453
C	4.604532	-0.682612	3.408747
C	5.713429	-0.500467	4.226296
C	5.843086	0.662721	4.978902
C	4.859089	1.644570	4.911634
C	3.746733	1.461497	4.099295
H	4.498637	-1.582613	2.817178
H	6.476170	-1.267126	4.274950
H	6.707955	0.803636	5.614556
H	4.958061	2.553961	5.490544
H	2.978527	2.221310	4.039303
C	1.715720	0.959338	-3.344333
C	1.017414	0.854480	-4.539824
C	0.219895	-0.258723	-4.789652
C	0.143107	-1.276625	-3.846376
C	0.846055	-1.179228	-2.652911
H	2.311664	1.838804	-3.137238
H	1.085244	1.648783	-5.272200
H	-0.338292	-0.329195	-5.713799
H	-0.474060	-2.145853	-4.030882
H	0.787014	-1.976684	-1.925342
N	-1.255386	0.244414	-0.622996
C	-2.988511	-0.934514	2.113326
C	-4.330386	-0.855515	1.766252
C	-5.156955	0.083016	2.374291
C	-4.635210	0.937430	3.341781
C	-3.290059	0.872015	3.679164
H	-2.371986	-1.709234	1.680197
H	-4.731973	-1.534688	1.025561
H	-6.202896	0.144714	2.102511
H	-5.275029	1.665308	3.824117
H	-2.878436	1.560518	4.405519

C	-2.055936	0.087918	-1.664266
C	-2.202271	1.132598	-2.622961
C	-2.961705	0.945354	-3.750969
C	-3.633657	-0.267629	-3.998780
C	-3.512022	-1.293339	-3.046096
C	-2.747040	-1.133110	-1.911859
H	-1.667084	2.055572	-2.447027
H	-3.027258	1.749849	-4.470628
C	-4.438468	-0.428525	-5.289746
H	-4.007726	-2.240407	-3.200878
H	-2.617643	-1.938992	-1.201485
C	-5.140982	-1.791180	-5.380041
C	-5.514433	0.676322	-5.357677
C	-3.477367	-0.296657	-6.491717
H	-5.704675	-1.847560	-6.312759
H	-4.426783	-2.616612	-5.376186
H	-5.844964	-1.934967	-4.558259
H	-4.032029	-0.398683	-7.427006
H	-2.973057	0.669922	-6.503368
H	-2.715166	-1.077434	-6.458124
H	-6.108886	0.563602	-6.266629
H	-6.183193	0.612598	-4.497440
H	-5.075345	1.673780	-5.367888
Cl	-0.381033	-2.895714	0.354351

FeIV dipyrro (Betley) : S=2 (ADF/B3LYP*)

Fe	-0.174535	-0.630984	0.502886
N	-0.054478	-0.102967	2.446335
C	1.177353	-0.020081	3.100738
C	0.929400	0.052760	4.502674
C	-0.438134	0.060369	4.677196
C	-1.019422	-0.042993	3.388060
C	-2.450417	-0.047361	3.067403
H	-0.984743	0.096370	5.607392
H	1.686509	0.093417	5.269658
C	2.424055	0.101728	2.465553
N	1.736817	-0.130041	0.084775
C	2.327313	0.117351	-1.102000
C	3.666960	0.537620	-0.902137
C	3.891816	0.527380	0.458846
C	2.677278	0.120204	1.084095
H	4.799711	0.796688	0.975521
H	4.369288	0.779633	-1.685375
C	1.641213	-0.046393	-2.388853
C	3.611406	0.292352	3.348961
C	4.591479	-0.700435	3.422340
C	5.702034	-0.528638	4.242261
C	5.847419	0.638444	4.987656
C	4.877166	1.634588	4.911224
C	3.762849	1.462184	4.096893
H	4.473461	-1.606109	2.838034
H	6.454558	-1.307518	4.298374
H	6.714535	0.771445	5.625358
H	4.988293	2.548106	5.485055
H	3.006384	2.235868	4.028913
C	1.729373	0.963888	-3.355356
C	1.061229	0.839411	-4.567384
C	0.298947	-0.295764	-4.833409
C	0.222306	-1.312547	-3.886618
C	0.892359	-1.194152	-2.674603
H	2.300270	1.859684	-3.137226
H	1.126755	1.634848	-5.301737
H	-0.230857	-0.385473	-5.774971
H	-0.365738	-2.201301	-4.085938
H	0.835829	-1.993231	-1.944895
N	-1.264946	0.223123	-0.634884
C	-2.997433	-0.945058	2.142299
C	-4.346215	-0.883006	1.812825
C	-5.173133	0.059882	2.416253
C	-4.645475	0.936306	3.362179
C	-3.295343	0.884498	3.686177
H	-2.375594	-1.719626	1.709446
H	-4.753506	-1.579713	1.088764
H	-6.224981	0.108589	2.156712
H	-5.285327	1.670493	3.839341
H	-2.879496	1.588612	4.398095
C	-2.070017	0.073887	-1.677733
C	-2.226399	1.128785	-2.625602
C	-2.994538	0.952359	-3.751807
C	-3.662856	-0.261678	-4.010046
C	-3.533508	-1.296488	-3.066953
C	-2.762499	-1.145661	-1.933711
H	-1.694589	2.054617	-2.441401
H	-3.069355	1.767069	-4.462407
C	-4.468886	-0.418250	-5.302013
H	-4.029828	-2.244308	-3.229897
H	-2.631887	-1.960581	-1.230667
C	-5.167830	-1.783275	-5.397971
C	-5.547644	0.685060	-5.367101
C	-3.506661	-0.279076	-6.503757
H	-5.731610	-1.837545	-6.332995
H	-4.451016	-2.608977	-5.397352
H	-5.873644	-1.934044	-4.576408
H	-4.061226	-0.377941	-7.441672
H	-3.002387	0.689794	-6.510442
H	-2.741481	-1.059705	-6.473881
H	-6.139424	0.576119	-6.280577
H	-6.221871	0.615719	-4.509121
H	-5.110373	1.685545	-5.370114
Cl	-0.355510	-2.885073	0.374900

FeIV dipyrro (Betley) : S=2 (ADF/OPBE)

Fe	-0.193405	-0.624325	0.524370
N	-0.045668	-0.158111	2.448461
C	1.174078	-0.068250	3.100478
C	0.935353	0.020606	4.498896
C	-0.431825	0.035385	4.673274
C	-1.011068	-0.084782	3.387346
C	-2.424754	-0.071086	3.049489
H	-0.985805	0.083653	5.601832
H	1.705869	0.066857	5.256748
C	2.410308	0.059065	2.456178
N	1.679374	-0.157920	0.103110
C	2.230083	0.128797	-1.092038

C	3.568134	0.555757	-0.920114
C	3.829975	0.515609	0.434316
C	2.638119	0.081081	1.074851
H	4.742915	0.784203	0.949448
H	4.244051	0.820856	-1.723216
C	1.494756	-0.015949	-2.339342
C	3.592831	0.273196	3.314183
C	4.621592	-0.667221	3.318170
C	5.734517	-0.471504	4.125073
C	5.827498	0.666193	4.920216
C	4.806265	1.611342	4.906357
C	3.689282	1.416637	4.105369
H	4.529414	-1.546636	2.685400
H	6.532089	-1.211946	4.136287
H	6.700591	0.817798	5.552260
H	4.883179	2.506970	5.520063
H	2.879422	2.141499	4.077911
C	1.550268	0.994491	-3.303992
C	0.819940	0.875443	-4.477155
C	0.031111	-0.250068	-4.700052
C	-0.010946	-1.265741	-3.752461
C	0.723062	-1.155538	-2.581360
H	2.145333	1.883736	-3.107571
H	0.851670	1.674831	-5.215502
H	-0.569594	-0.322447	-5.601350
H	-0.642602	-2.135758	-3.908747
H	0.691909	-1.943223	-1.835462
N	-1.160726	0.258638	-0.616548
C	-2.945883	-0.893744	2.045664
C	-4.276248	-0.784932	1.670449
C	-5.113563	0.118072	2.316474
C	-4.613225	0.909807	3.346812
C	-3.277109	0.821925	3.708993
H	-2.320251	-1.659710	1.598239
H	-4.663850	-1.418430	0.876414
H	-6.158962	0.200006	2.025395
H	-5.266435	1.613298	3.859224
H	-2.871245	1.471895	4.480244
C	-1.912839	0.072008	-1.695550
C	-1.977601	1.069550	-2.701600
C	-2.749741	0.874545	-3.822581
C	-3.481430	-0.307551	-4.016637
C	-3.398058	-1.306293	-3.035431
C	-2.640570	-1.128288	-1.898286
H	-1.373161	1.961699	-2.569464
H	-2.768151	1.648572	-4.584295
C	-4.333335	-0.453139	-5.263082
H	-3.933509	-2.242495	-3.161844
H	-2.541683	-1.905957	-1.146526
C	-5.105816	-1.766486	-5.294208
C	-5.344463	0.698465	-5.296791
C	-3.428232	-0.393273	-6.497475
H	-5.714198	-1.803087	-6.204823
H	-4.428411	-2.628174	-5.306327
H	-5.777812	-1.847533	-4.432034
H	-4.040925	-0.471299	-7.404049
H	-2.868954	0.546371	-6.540697
H	-2.716765	-1.226200	-6.481624
H	-5.996502	0.589985	-6.171648
H	-5.957262	0.680945	-4.388522
H	-4.847161	1.671171	-5.356083
Cl	-0.423940	-2.825122	0.336351

5 S=1 (Orca/B3LYP)

Fe	-0.059345	0.416113	-0.701781
O	1.157400	-0.992234	-0.840264
O	-1.326002	-0.650453	0.184083
N	0.756939	1.094814	1.132317
N	1.336994	1.651430	-1.441875
C	1.793932	0.157061	1.654452
H	1.260256	-0.750090	1.947970
H	2.243849	0.590505	2.559166
C	2.852137	-0.179988	0.645486
C	4.199831	0.057586	0.908053
H	4.502470	0.518945	1.843030
C	5.160301	-0.299336	-0.035146
C	4.792960	-0.891168	-1.242239
H	5.540710	-1.158415	-1.979479
C	3.443799	-1.117522	-1.500790
C	2.435764	-0.780204	-0.568807
C	-0.363504	1.240836	2.111905
H	0.003978	1.761594	3.007406
H	-1.109457	1.874890	1.621182
C	-0.963469	-0.080709	2.494733
C	-1.099055	-0.433080	3.837860
H	-0.737739	0.235239	4.613354
C	-1.706069	-1.635904	4.184268
C	-2.177359	-2.504034	3.200092
H	-2.650591	-3.441395	3.467444
C	-2.023077	-2.156928	1.863146
C	-1.412853	-0.941430	1.461986
C	1.322622	2.429907	0.822947
H	2.030277	2.748468	1.599271
H	0.486912	3.137976	0.807643
C	1.959210	2.431132	-0.537877
C	3.068771	3.192393	-0.885443
H	3.563379	3.800832	-0.135714
C	3.538006	3.136611	-2.197616
H	4.412182	3.710965	-2.488873
C	2.880097	2.328741	-3.123523
H	3.218410	2.252233	-4.150593
C	1.777021	1.591735	-2.708811
H	1.222955	0.926705	-3.359967
Cl	6.857939	0.019424	0.289343
Cl	2.973492	-1.796797	-3.040045
Cl	-1.878478	-2.070901	5.878339
Cl	-2.622702	-3.240075	0.627155
N	-0.789324	0.197426	-2.367753
S	-1.766853	1.479958	-2.228155
O	-1.642887	2.552374	-3.224644
O	-1.370259	1.921258	-0.781684
C	-3.459508	0.932253	-2.215570
C	-3.791966	-0.264782	-1.575028
C	-5.121989	-0.671570	-1.576896

C	-6.117835	0.094070	-2.202716
C	-5.747895	1.284111	-2.844840
C	-4.421623	1.710404	-2.860439
C	-7.559402	-0.349093	-2.168092
H	-3.024787	-0.856570	-1.089786
H	-5.388608	-1.603528	-1.084821
H	-6.506847	1.880405	-3.344826
H	-4.125774	2.620501	-3.370449
H	-8.142177	0.116591	-2.969238
H	-8.029317	-0.073361	-1.214599
H	-7.644825	-1.436500	-2.268512

5 S=2 (Orca/B3LYP)

Fe	-0.262506	-0.063037	-0.634838
O	1.002689	-1.470943	-0.389207
O	-1.223033	-0.311899	0.973711
N	1.159976	1.338333	0.481072
N	1.269917	0.607481	-2.239833
C	2.146753	0.519182	1.243237
H	1.567458	-0.072054	1.957611
H	2.798266	1.194901	1.816944
C	2.978499	-0.379598	0.370475
C	4.365023	-0.245758	0.323437
H	4.860569	0.511448	0.922961
C	5.114893	-1.075606	-0.505971
C	4.499512	-2.046542	-1.294045
H	5.083701	-2.683339	-1.947720
C	3.115521	-2.179500	-1.241555
C	2.316895	-1.363111	-0.409932
C	0.306820	2.152619	1.392879
H	0.924739	2.936405	1.855551
H	-0.435039	2.636058	0.749193
C	-0.393737	1.373618	2.479751
C	-0.339743	1.854418	3.789577
H	0.268665	2.723109	4.020622
C	-1.074539	1.241148	4.800051
C	-1.881007	0.138374	4.525993
H	-2.461819	-0.335985	5.307975
C	-1.924037	-0.351191	3.226367
C	-1.176848	0.228910	2.172590
C	1.803583	2.216329	-0.519888
H	2.681754	2.715287	-0.086963
H	1.069035	2.984755	-0.782412
C	2.174828	1.488991	-1.792731
C	3.345158	1.749733	-2.502344
H	4.076963	2.448316	-2.109639
C	3.563483	1.076516	-3.703928
H	4.475187	1.249904	-4.267867
C	2.605981	0.173814	-4.165986
H	2.742815	-0.372085	-5.092947
C	1.467481	-0.039446	-3.393646
H	0.695567	-0.746394	-3.677330
Cl	6.860348	-0.882133	-0.581312
Cl	2.326251	-3.354542	-2.266286
Cl	-0.990508	1.866018	6.439482
Cl	-2.939335	-1.728482	2.863070
N	-1.358957	1.512527	-1.215053
S	-2.212495	0.783688	-2.357950
O	-1.581585	-0.629607	-2.227109
O	-2.205515	1.381518	-3.697048
C	-3.907337	0.591958	-1.847766
C	-4.935412	0.993827	-2.697251
C	-6.255801	0.843677	-2.272017
C	-6.554160	0.300158	-1.016991
C	-5.493446	-0.095398	-0.184073
C	-4.171440	0.049913	-0.584255
C	-7.982148	0.148526	-0.554925
H	-4.698100	1.410552	-3.669780
H	-7.066103	1.152389	-2.927369
H	-5.705641	-0.521467	0.793386
H	-3.359799	-0.253659	0.068590
H	-8.194037	0.813170	0.292327
H	-8.183461	-0.875549	-0.218909
H	-8.689732	0.389174	-1.354235

5 S=3 (Orca/B3LYP)

Fe	-0.203680	-0.233591	-0.633472
O	1.154873	-1.552401	-0.297547
O	-1.332943	-0.335994	0.883627
N	1.072593	1.293961	0.439937
N	1.184700	0.469005	-2.240480
C	2.110697	0.585303	1.245496
H	1.569089	-0.033206	1.966710
H	2.692081	1.328949	1.810942
C	3.025610	-0.262245	0.407775
C	4.392812	0.001846	0.343447
H	4.818409	0.821105	0.914470
C	5.210986	-0.777408	-0.469613
C	4.684070	-1.826740	-1.221486
H	5.321367	-2.424696	-1.862163
C	3.320269	-2.090975	-1.148061
C	2.452091	-1.328897	-0.333161
C	0.170751	2.094037	1.317345
H	0.742898	2.921510	1.762750
H	-0.589084	2.519835	0.653783
C	-0.498983	1.308553	2.416537
C	-0.434175	1.772381	3.730964
H	0.166156	2.644956	3.968210
C	-1.148558	1.131313	4.739904
C	-1.945849	0.023447	4.458301
H	-2.508239	-0.471375	5.241068
C	-2.003672	-0.443530	3.150397
C	-1.275517	0.162909	2.099842
C	1.669329	2.167592	-0.595555
H	2.528125	2.721243	-0.191549
H	0.898789	2.890532	-0.882275
C	2.062547	1.402715	-1.838078
C	3.221433	1.666972	-2.563801
H	3.930927	2.405838	-2.206114
C	3.461202	0.944183	-3.731585
H	4.366464	1.120034	-4.304965
C	2.533823	-0.011029	-4.147989
H	2.688014	-0.596154	-5.047724
C	1.403926	-0.224305	-3.365518

H	0.654332	-0.966811	-3.616699
Cl	6.929933	-0.420922	-0.571998
Cl	2.640252	-3.371487	-2.125256
Cl	-1.051348	1.728983	6.388605
Cl	-3.008331	-1.826897	2.777320
N	-1.372635	1.531672	-1.411892
S	-2.148037	0.509524	-2.410505
O	-1.557689	-0.883387	-2.092214
O	-2.088327	0.885400	-3.829648
C	-3.826528	0.462163	-1.841417
C	-4.793435	1.166416	-2.562579
C	-6.104003	1.171258	-2.094417
C	-6.454494	0.496644	-0.914909
C	-5.455941	-0.190357	-0.207986
C	-4.140632	-0.217644	-0.659667
C	-7.882311	0.488135	-0.429490
H	-4.516400	1.682960	-3.475226
H	-6.868457	1.707194	-2.650955
H	-5.707901	-0.710946	0.712187
H	-3.373794	-0.741712	-0.101634
H	-7.932444	0.458096	0.663935
H	-8.415117	-0.395835	-0.804785
H	-8.429007	1.371300	-0.775399

5.(CH_3CN) S=1 (Orca/B3LYP)

Fe	-5.266036	-0.749483	-1.429399
O	-5.106648	-2.616249	-1.563775
C	-4.616006	-3.267236	-2.604172
C	-3.397488	-2.890104	-3.217154
C	-2.681132	-1.694928	-2.658383
N	-3.536648	-0.468900	-2.686236
C	-3.929512	-0.170464	-4.098196
C	-4.899242	0.967224	-4.201586
C	-2.798682	0.668103	-2.080067
C	-7.051896	1.875356	-3.567870
C	-6.125029	0.813213	-3.518686
C	-3.748672	1.688406	-1.517335
N	-4.884779	1.179818	-0.999604
N	-6.308625	-0.927661	-0.035631
S	-7.942298	-1.076716	0.112570
C	-7.985993	-2.287776	1.426341
C	-7.941726	-3.641468	1.087953
C	-7.859458	-4.589013	2.104986
C	-7.824477	-4.203431	3.453965
C	-7.874897	-2.836276	3.762841
C	-7.953368	-1.873422	2.757178
C	-4.617575	2.126371	-4.919157
C	-5.563662	3.149797	-4.959476
C	-6.781402	3.035922	-4.290665
C	-3.477128	3.050871	-1.468057
C	-4.403303	3.901240	-0.865541
C	-5.567462	3.361617	-0.321477
C	-5.780591	1.990386	-0.407678
C	-5.273318	-4.410248	-3.114294
C	-4.752960	-5.146128	-4.174614
C	-3.552053	-4.739381	-4.754554
C	-2.873904	-3.617051	-4.285639
O	-6.375534	-0.294756	-2.827053
C	-7.761958	-5.240733	4.548169
Cl	-8.530569	1.739495	-2.661689
Cl	-5.204718	4.623448	-5.846087
Cl	-2.890624	-5.654457	-6.100487
Cl	-6.774967	-4.918172	-2.381220
O	-8.593660	-1.667545	-1.060076
O	-8.432855	0.215099	0.643676
H	-4.386177	-1.084054	-4.486812
H	-3.021673	0.033135	-4.683749
H	-3.670272	2.238563	-5.437103
H	-7.504929	3.842078	-4.315569
H	-1.757135	-1.504703	-3.223034
H	-2.417631	-1.858101	-1.609773
H	-1.940705	-3.313329	-4.749518
H	-5.280558	-6.017078	-4.544776
H	-2.110003	1.121312	-2.805122
H	-2.215045	0.266311	-1.245717
H	-2.563439	3.434591	-1.909755
H	-4.219216	4.970790	-0.828629
H	-6.316583	3.987385	0.150549
H	-6.678572	1.520287	-0.021536
H	-7.990515	-0.814420	2.990103
H	-7.853281	-2.524001	4.804171
H	-7.819683	-5.645187	1.849209
H	-7.955468	-3.932229	0.043356
H	-7.114805	-6.079421	4.268631
H	-8.758110	-5.654780	4.753107
H	-7.385361	-4.814264	5.483587
N	-2.875628	-1.076190	0.682838
C	-3.581374	-1.901986	1.095142
C	-4.475837	-2.950395	1.567164
H	-3.905843	-3.740359	2.066485
H	-5.215305	-2.536296	2.257241
H	-5.003501	-3.357495	0.699296

5.(CH_3CN) S=2 (Orca/B3LYP)

Fe	-5.415920	-0.703269	-1.390606
O	-5.099051	-2.583489	-1.442760
C	-4.575660	-3.295302	-2.426851
C	-3.377151	-2.905154	-3.071753
C	-2.681246	-1.659813	-2.596440
N	-3.534574	-0.438033	-2.692011
C	-3.969295	-0.231562	-4.109671
C	-4.910402	0.927358	-4.265630
C	-2.784593	0.732662	-2.186171
C	-7.018552	1.954277	-3.661787
C	-6.155316	0.840192	-3.599468
C	-3.709134	1.801688	-1.663997
N	-4.790759	1.347486	-1.009068
N	-6.456032	-0.690467	0.152577
S	-8.003989	-0.777430	0.586406
C	-8.074969	-2.220134	1.636872
C	-8.040459	-3.480099	1.034556
C	-7.954797	-4.611807	1.839169
C	-7.909048	-4.505385	3.238545
C	-7.952813	-3.228850	3.814563

C	-8.032635	-2.082039	3.022831
C	-4.569151	2.062857	-4.996855
C	-5.457086	3.134971	-5.054567
C	-6.680210	3.094358	-4.387362
C	-3.452199	3.163973	-1.786112
C	-4.342530	4.069233	-1.210775
C	-5.452789	3.587513	-0.517648
C	-5.647041	2.212795	-0.440663
C	-5.180347	-4.498829	-2.852063
C	-4.637896	-5.280970	-3.867128
C	-3.461812	-4.860654	-4.484924
C	-2.832253	-3.681171	-4.094570
O	-6.457757	-0.240775	-2.892231
C	-7.842888	-5.742625	4.100017
Cl	-8.502068	1.909339	-2.750206
Cl	-5.013033	4.580147	-5.952002
Cl	-2.767756	-5.832075	-5.773696
Cl	-6.653214	-5.024901	-2.067499
O	-8.840538	-1.043094	-0.593924
O	-8.260459	0.408459	1.430566
H	-4.456996	-1.157960	-4.421331
H	-3.075878	-0.089332	-4.735317
H	-3.611126	2.121406	-5.504069
H	-7.356824	3.940185	-4.417148
H	-1.760752	-1.503935	-3.178590
H	-2.407335	-1.756766	-1.542464
H	-1.914881	-3.369972	-4.584264
H	-5.129003	-6.197333	-4.172086
H	-2.115105	1.134950	-2.959065
H	-2.174438	0.388885	-1.344804
H	-2.583057	3.504671	-2.339213
H	-4.173652	5.137471	-1.309482
H	-6.170643	4.258545	-0.059257
H	-6.499739	1.775168	0.067442
H	-8.062899	-1.091667	3.464533
H	-7.923875	-3.130389	4.897053
H	-7.918191	-5.594280	1.374951
H	-8.063453	-3.564157	-0.046257
H	-7.200514	-6.508641	3.651605
H	-8.838965	-6.187818	4.223920
H	-7.458340	-5.515319	5.099486
N	-3.072063	-0.914509	0.661117
C	-3.713182	-1.757353	1.139648
C	-4.533986	-2.827842	1.691080
H	-3.905343	-3.569201	2.194320
H	-5.263520	-2.424400	2.398102
H	-5.076321	-3.294861	0.864033

5.(CH_3CN) S=3 (Orca/B3LYP)

Fe	-5.411085	-0.898383	-1.674228
O	-4.943890	-2.713697	-1.833803
C	-4.348275	-3.337704	-2.838525
C	-3.159628	-2.821370	-3.405458
C	-2.554580	-1.587588	-2.791251
N	-3.469071	-0.405513	-2.798022
C	-3.840182	-0.058528	-4.205467
C	-4.825367	1.071985	-4.297139
C	-2.824481	0.731152	-2.104461
C	-7.011593	1.955051	-3.743920
C	-6.105114	0.874671	-3.727314
C	-3.841798	1.684401	-1.531135
N	-4.943590	1.114911	-1.008030
N	-6.359537	-1.191642	0.074446
S	-7.962004	-1.291199	0.262267
C	-8.127025	-2.383690	1.666879
C	-8.244949	-3.756613	1.443835
C	-8.253751	-4.621757	2.535910
C	-8.148628	-4.135174	3.846898
C	-8.033201	-2.750809	4.040747
C	-8.019736	-1.871218	2.960133
C	-4.489836	2.287886	-4.890215
C	-5.417867	3.326404	-4.904914
C	-6.678850	3.173481	-4.331064
C	-3.649109	3.062204	-1.494798
C	-4.624223	3.864056	-0.904678
C	-5.759330	3.264640	-0.360674
C	-5.889161	1.882280	-0.435509
C	-4.869136	-4.537144	-3.365101
C	-4.249681	-5.200894	-4.420317
C	-3.087418	-4.659627	-4.967153
C	-2.541249	-3.478628	-4.468808
O	-6.407024	-0.277035	-3.139854
C	-8.189926	-5.078719	5.023928
Cl	-8.548688	1.764856	-2.945100
Cl	-4.981116	4.868943	-5.626553
Cl	-2.300492	-5.481916	-6.305780
Cl	-6.327977	-5.192939	-2.662184
O	-8.609527	-1.956129	-0.880147
O	-8.410689	0.063080	0.669931
H	-4.262854	-0.966494	-4.643883
H	-2.922855	0.189362	-4.760006
H	-3.505697	2.432057	-5.324902
H	-7.389403	3.991490	-4.325946
H	-1.625942	-1.327265	-3.320880
H	-2.310551	-1.774437	-1.742269
H	-1.631805	-3.076312	-4.903946
H	-4.672476	-6.118778	-4.811047
H	-2.131296	1.258362	-2.774379
H	-2.254735	0.316703	-1.267074
H	-2.761481	3.494936	-1.944392
H	-4.503412	4.943076	-0.882295
H	-6.548094	3.851726	0.096425
H	-6.767126	1.370155	-0.054334
H	-7.932771	-0.799924	3.107901
H	-7.955289	-2.358837	5.051964
H	-8.345215	-5.692344	2.369336
H	-8.328134	-4.129036	0.428194
H	-7.711596	-6.035276	4.787384
H	-9.226042	-5.296791	5.315256
H	-7.687723	-4.651325	5.898026
N	-2.946476	-1.227366	0.539448
C	-3.612882	-2.093222	0.933346
C	-4.452126	-3.192266	1.395643
H	-3.844272	-3.947020	1.905050

H	-5.223681	-2.814285	2.071194
H	-4.944782	-3.634039	0.524423

5.(py) S=1 (Orca/B3LYP)

C	-3.983527	-0.320848	-0.323622
C	-3.751477	0.013295	-1.659302
C	-4.565379	0.926280	-2.325452
C	-5.621016	1.521835	-1.635659
C	-5.869068	1.218212	-0.290332
C	-5.033264	0.292906	0.353575
S	-2.396090	-0.768906	-2.526456
O	-2.082715	0.082308	-3.702145
C	-7.021921	1.856155	0.446578
N	-1.098152	-0.761886	-1.553964
Fe	-0.178024	0.358935	-0.512855
N	1.144285	0.734632	-1.989039
C	2.010573	1.744499	-1.764046
C	3.053304	2.015361	-2.641520
C	3.208594	1.214240	-3.772965
C	2.314585	0.167824	-3.989785
C	1.292921	-0.048625	-3.071238
C	1.736507	2.546660	-0.519424
N	1.193721	1.667545	0.540526
C	0.464225	2.466043	1.568358
C	-0.129799	1.589993	2.639204
C	0.157577	1.842126	3.981842
C	-0.402827	1.046862	4.975842
C	-1.245286	-0.014075	4.646629
C	-1.515291	-0.270906	3.307315
C	-0.973791	0.513262	2.257660
Cl	-0.041782	1.376600	6.664698
Cl	-2.585858	-1.592177	2.898243
O	-1.320718	0.282528	1.010774
O	0.855697	-1.093742	0.171604
C	2.143733	-1.121329	-0.101395
C	2.986581	-0.090500	0.378029
C	4.348831	-0.063115	0.095981
C	4.900322	-1.084172	-0.675916
C	4.110635	-2.125378	-1.162747
C	2.745657	-2.134510	-0.881917
C	2.307489	0.930528	1.232356
Cl	6.616940	-1.048050	-1.064263
Cl	1.736917	-3.391102	-1.552700
O	-2.769681	-2.170133	-2.756167
H	1.843482	0.430602	2.084404
H	3.020989	1.673899	1.616149
H	4.976698	0.740370	0.469303
H	4.545366	-2.910961	-1.769687
H	1.155555	3.191134	2.021971
H	-0.305703	3.034687	1.040263
H	0.817006	2.661177	4.252492
H	-1.680184	-0.637300	5.419022
H	2.642237	3.066737	-0.179629
H	0.979907	3.307889	-0.739631
H	3.743736	2.823926	-2.424971
H	4.025626	1.397069	-4.464268
H	2.407245	-0.488665	-4.847640
H	0.573686	-0.852343	-3.162738
H	-4.352815	1.177757	-3.358702
H	-6.257861	2.240499	-2.146766
H	-5.199776	0.050771	1.400389
H	-3.324981	-1.009689	0.191008
H	-6.771359	2.045366	1.496324
H	-7.904033	1.202283	0.438376
H	-7.315909	2.805977	-0.013012
N	-1.334492	1.987691	-1.167809
C	-1.204675	2.512068	-2.402163
C	-1.969996	3.585586	-2.844731
C	-2.924246	4.135783	-1.993008
C	-3.091111	3.568819	-0.731388
C	-2.290265	2.496433	-0.360866
H	-0.486675	2.041765	-3.054869
H	-1.820936	3.963119	-3.850568
H	-3.538712	4.971975	-2.313658
H	-3.846052	3.928360	-0.041526
H	-2.409933	1.988759	0.584460

5.(py) S=2 (Orca/B3LYP)

C	-4.011691	-0.366621	-0.624109
C	-3.845959	0.046620	-1.947311
C	-4.709296	0.978452	-2.520875
C	-5.748439	1.503446	-1.754272
C	-5.934462	1.111624	-0.421541
C	-5.048899	0.174688	0.130796
S	-2.505514	-0.633791	-2.920424
O	-2.208908	0.362742	-3.974633
C	-7.071938	1.672080	0.397250
N	-1.219314	-0.751928	-1.973407
Fe	-0.220279	0.111302	-0.590726
N	1.255416	0.854916	-2.057826
C	2.210594	1.679535	-1.590684
C	3.405397	1.873322	-2.278996
C	3.611825	1.188052	-3.474631
C	2.613983	0.340098	-3.954627
C	1.447593	0.192923	-3.211933
C	1.873333	2.399124	-0.306988
N	1.213736	1.505270	0.662884
C	0.425194	2.300600	1.637789
C	-0.295072	1.465399	2.667028
C	-0.167236	1.789035	4.019032
C	-0.875348	1.078374	4.983546
C	-1.719348	0.030777	4.619714
C	-1.837899	-0.297299	3.274242
C	-1.131500	0.392704	2.258338
Cl	-0.704546	1.504037	6.679961
Cl	-2.903182	-1.604944	2.806950
O	-1.284437	0.048889	0.999083
O	1.095391	-1.262519	-0.234627
C	2.400637	-1.143669	-0.279992
C	3.064554	-0.171404	0.510196
C	4.447168	-0.008204	0.446271
C	5.193218	-0.800177	-0.421765
C	4.578768	-1.761662	-1.224316
C	3.199371	-1.925347	-1.149099

C	2.211860	0.676415	1.404425
Cl	6.934490	-0.570214	-0.531353
Cl	2.411501	-3.088555	-2.186598
O	-2.875571	-2.004812	-3.309370
H	1.638371	0.044868	2.087484
H	2.842308	1.344808	2.011480
H	4.939234	0.741197	1.058750
H	5.162482	-2.368919	-1.906114
H	1.091299	3.008504	2.156073
H	-0.288519	2.892020	1.057099
H	0.484212	2.603193	4.321085
H	-2.272033	-0.524549	5.368164
H	2.773336	2.862551	0.123010
H	1.166420	3.203879	-0.539555
H	4.170123	2.521641	-1.864433
H	4.545532	1.305381	-4.016534
H	2.739682	-0.219807	-4.874576
H	0.641845	-0.469228	-3.506729
H	-4.546980	1.300955	-3.543414
H	-6.420220	2.236669	-2.194856
H	-5.161280	-0.131709	1.167555
H	-3.314103	-1.062198	-0.172707
H	-6.818722	1.708327	1.462198
H	-7.970882	1.049138	0.298453
H	-7.341671	2.683297	0.073095
N	-1.383452	2.059600	-1.149393
C	-2.386139	2.454757	-0.340930
C	-3.235471	3.507953	-0.658604
C	-3.055622	4.173860	-1.870543
C	-2.036718	3.751390	-2.721237
C	-1.228593	2.688790	-2.325442
H	-2.507291	1.881812	0.567730
H	-4.031904	3.777603	0.025728
H	-3.707985	4.995121	-2.153221
H	-1.872361	4.219354	-3.685965
H	-0.444840	2.311180	-2.968217

5.(py) S=3 (Orca/B3LYP)

C	-4.750181	-1.183691	-2.186269
C	-4.449936	0.176044	-2.087923
C	-5.418582	1.099243	-1.696840
C	-6.704286	0.649476	-1.401539
C	-7.034219	-0.708940	-1.491979
C	-6.039211	-1.615293	-1.887465
S	-2.784088	0.733260	-2.406041
O	-2.865142	2.179789	-2.706717
C	-8.435173	-1.186701	-1.197609
N	-1.977634	0.518190	-1.036872
Fe	-0.252074	0.918162	-0.102240
N	1.113369	1.055370	-1.890062
C	2.375007	1.449070	-1.628913
C	3.427581	1.172443	-2.496739
C	3.166355	0.457544	-3.664101
C	1.859744	0.053035	-3.929970
C	0.857954	0.363883	-3.015090
C	2.554607	2.233758	-0.353387
N	1.777876	1.652435	0.756852
C	1.520776	2.696300	1.787133
C	0.798491	2.183005	3.003734
C	1.317114	2.428934	4.275846
C	0.626113	2.004092	5.406640
C	-0.584581	1.323168	5.289381
C	-1.093662	1.069412	4.020605
C	-0.423882	1.481571	2.841954
Cl	1.288181	2.324756	7.003582
Cl	-2.611807	0.220156	3.860053
O	-0.937429	1.224056	1.660798
O	0.449982	-0.860414	0.034408
C	1.678238	-1.253430	-0.219383
C	2.782338	-0.615233	0.401762
C	4.089871	-1.003715	0.115710
C	4.321906	-2.020160	-0.806562
C	3.263827	-2.664142	-1.447021
C	1.960015	-2.278446	-1.151688
C	2.491492	0.492590	1.372264
Cl	5.974857	-2.483510	-1.193392
Cl	0.625413	-3.034109	-1.987682
O	-2.220534	-0.174134	-3.434206
H	1.848684	0.128908	2.177273
H	3.427121	0.853806	1.826207
H	4.925653	-0.505903	0.597616
H	3.448899	-3.446540	-2.173545
H	2.476873	3.146314	2.096791
H	0.930461	3.474211	1.291768
H	2.259282	2.956852	4.385601
H	-1.122407	0.989956	6.169027
H	3.620659	2.313350	-0.094560
H	2.179537	3.251432	-0.513084
H	4.435692	1.480786	-2.240042
H	3.974818	0.208942	-4.345237
H	1.611165	-0.517565	-4.817915
H	-0.168352	0.048268	-3.170974
H	-5.161841	2.151226	-1.634972
H	-7.465126	1.363990	-1.096595
H	-6.279274	-2.673213	-1.961616
H	-3.982640	-1.883923	-2.497858
H	-8.428092	-2.158280	-0.691455
H	-9.013294	-1.307256	-2.123662
H	-8.975240	-0.475979	-0.563689
N	-0.796737	3.101112	-0.584909
C	-0.446718	3.747314	-1.708150
C	-1.041402	4.937671	-2.110166
C	-2.063265	5.472906	-1.328463
C	-2.444237	4.796032	-0.171011
C	-1.788896	3.616197	0.165430
H	0.321138	3.274384	-2.308161
H	-0.721037	5.417105	-3.029120
H	-2.558956	6.394131	-1.620839
H	-3.241456	5.167374	0.464565
H	-2.054453	3.039288	1.043552

^{5}5 avec ADF/B3LYP initFeIII

Fe	-0.220678	0.277742	-0.014893

O	0.919197	-1.228158	0.142775
O	-1.113312	0.623590	1.620303
N	1.497349	1.595730	0.872211
N	0.999434	0.962037	-1.771770
C	2.508840	0.652340	1.452454
H	1.994150	0.082440	2.224911
H	3.304752	1.233593	1.932587
C	3.083949	-0.290228	0.436499
C	4.425773	-0.242032	0.079723
H	5.093939	0.462085	0.556406
C	4.905567	-1.084207	-0.912053
C	4.061918	-1.982357	-1.552411
H	4.435214	-2.624902	-2.335714
C	2.724680	-2.038650	-1.187965
C	2.203447	-1.208779	-0.175785
C	0.942398	2.482034	1.942120
H	1.720972	3.173241	2.285906
H	0.146553	3.067064	1.474609
C	0.384697	1.715916	3.104382
C	0.861161	1.909890	4.395563
H	1.653888	2.620550	4.585697
C	0.314900	1.187866	5.446928
C	-0.698457	0.263812	5.222405
H	-1.114618	-0.304144	6.041218
C	-1.170792	0.068581	3.932954
C	-0.648115	0.793776	2.842803
C	2.081217	2.424254	-0.202442
H	3.087080	2.768296	0.062303
H	1.449552	3.308376	-0.319524
C	2.093751	1.692779	-1.518140
C	3.145652	1.771489	-2.416946
H	4.026905	2.348692	-2.173012
C	3.060721	1.062259	-3.607522
H	3.879953	1.086149	-4.314909
C	1.924525	0.308047	-3.865991
H	1.828153	-0.274852	-4.771128
C	0.910054	0.281728	-2.922438
H	0.017956	-0.313921	-3.061658
Cl	6.594826	-0.993990	-1.388803
Cl	1.640690	-3.110693	-2.033295
Cl	0.915074	1.434624	7.078839
Cl	-2.430286	-1.101596	3.639556
N	-1.797924	0.253834	-1.117276
S	-2.560905	-1.037768	-1.674683
O	-2.564009	-2.097387	-0.681836
O	-1.986166	-1.276139	-3.000005
C	-4.257516	-0.553432	-1.912991
C	-4.653201	0.031226	-3.110614
C	-5.980496	0.400977	-3.280255
C	-6.921201	0.195062	-2.268533
C	-6.496792	-0.389324	-1.073170
C	-5.174474	-0.766948	-0.888881
C	-8.367601	0.552944	-2.473547
H	-3.931141	0.175626	-3.901987
H	-6.290733	0.848575	-4.216418
H	-7.212131	-0.559460	-0.278027
H	-4.852464	-1.234526	0.031105
H	-8.826605	0.889324	-1.543672
H	-8.926121	-0.318480	-2.824167
H	-8.480965	1.342895	-3.215567

^{5}5 avec ADF/B3LYP initFeIV

Fe	0.020960	-1.448423	-0.257543
O	1.902282	-1.811906	-0.143475
O	-0.519366	-2.026049	1.440568
N	0.222336	0.586038	0.568486
N	0.661582	-0.177833	-2.034894
C	1.570311	0.642018	1.229360
H	1.560270	-0.119472	2.008021
H	1.681965	1.617879	1.714237
C	2.721282	0.385315	0.296558
C	3.663127	1.376720	0.048041
H	3.577668	2.342441	0.527365
C	4.708982	1.138140	-0.831079
C	4.836909	-0.092231	-1.461505
H	5.646173	-0.275397	-2.152209
C	3.902389	-1.083904	-1.208281
C	2.820618	-0.884424	-0.325649
C	-0.877696	0.793360	1.564178
H	-0.895658	1.847271	1.863007
H	-1.807823	0.575721	1.035394
C	-0.779352	-0.075875	2.783900
C	-0.857983	0.490871	4.050958
H	-0.944002	1.562603	4.165665
C	-0.831231	-0.318756	5.176773
C	-0.725715	-1.698435	5.053401
H	-0.704454	-2.328981	5.929812
C	-0.636711	-2.265666	3.792218
C	-0.651429	-1.472258	2.623962
C	0.086593	1.583145	-0.517821
H	0.463420	2.559645	-0.195847
H	-0.979778	1.684554	-0.737948
C	0.768271	1.127433	-1.781375
C	1.439751	1.984661	-2.641578
H	1.545004	3.032781	-2.396814
C	2.001385	1.458838	-3.796843
H	2.552571	2.098342	-4.473533
C	1.865460	0.101782	-4.063939
H	2.299520	-0.344713	-4.947362
C	1.186577	-0.686414	-3.149334
H	1.085799	-1.755447	-3.279872
Cl	5.871717	2.411194	-1.170545
Cl	4.023334	-2.611950	-2.049214
Cl	-0.927157	0.405720	6.773142
Cl	-0.493820	-3.996086	3.635281
N	-1.554424	-1.687733	-1.170656
S	-3.120183	-1.726676	-0.881563
O	-3.403071	-1.881308	0.534225
O	-3.676934	-2.651324	-1.856390
C	-3.697843	-0.084583	-1.321057
C	-3.648037	0.327301	-2.650148
C	-4.127955	1.582243	-2.996231
C	-4.661929	2.443458	-2.032771

C	-4.689356	2.015853	-0.704631
C	-4.217706	0.758410	-0.344846
C	-5.254013	3.770537	-2.423591
H	-3.256340	-0.339474	-3.406419
H	-4.106574	1.890966	-4.034337
H	-5.108587	2.663269	0.056442
H	-4.276916	0.415928	0.679086
H	-5.061199	4.532126	-1.667553
H	-6.337768	3.679392	-2.530606
H	-4.855650	4.123422	-3.374598

^{5}5 avec ADF/B3LYP* initFeIII

Fe	-0.221909	0.263509	-0.032971
O	0.934825	-1.237954	0.090666
O	-1.096790	0.539569	1.630957
N	1.472093	1.608570	0.840432
N	0.989361	0.969119	-1.800893
C	2.515514	0.683591	1.394049
H	2.033552	0.115717	2.192837
H	3.316787	1.283892	1.846654
C	3.090206	-0.268964	0.384791
C	4.441778	-0.235928	0.055572
H	5.099909	0.489085	0.519596
C	4.949939	-1.132286	-0.874839
C	4.124139	-2.069810	-1.484280
H	4.522056	-2.762208	-2.214087
C	2.775825	-2.106487	-1.154784
C	2.224026	-1.219762	-0.204951
C	0.916499	2.469779	1.932722
H	1.691952	3.167431	2.278354
H	0.109316	3.057026	1.481835
C	0.382194	1.688473	3.097461
C	0.850987	1.912705	4.388998
H	1.630572	2.643547	4.568393
C	0.314004	1.200022	5.452904
C	-0.686912	0.256714	5.242632
H	-1.099463	-0.302087	6.072255
C	-1.152510	0.030829	3.954821
C	-0.634703	0.741520	2.848795
C	2.022598	2.467486	-0.228635
H	3.023776	2.835308	0.032199
H	1.366860	3.339843	-0.324201
C	2.043696	1.760094	-1.557855
C	3.059511	1.933702	-2.488773
H	3.907700	2.567148	-2.257706
C	2.978085	1.258846	-3.700501
H	3.765379	1.364685	-4.438559
C	1.884987	0.436131	-3.944877
H	1.791592	-0.119636	-4.869759
C	0.906654	0.314696	-2.968724
H	0.042790	-0.327681	-3.102861
Cl	6.655330	-1.075785	-1.298857
Cl	1.721761	-3.245273	-1.951948
Cl	0.907100	1.484992	7.082191
Cl	-2.401528	-1.156620	3.681425
N	-1.800828	0.270557	-1.114492
S	-2.581315	-1.004578	-1.680525
O	-2.583819	-2.083338	-0.703693
O	-2.014815	-1.229440	-3.016299
C	-4.279882	-0.515694	-1.909136
C	-4.670508	0.116580	-3.086312
C	-6.000814	0.478953	-3.255274
C	-6.952170	0.217424	-2.264312
C	-6.533172	-0.413505	-1.089303
C	-5.207094	-0.783605	-0.905506
C	-8.400261	0.567131	-2.472679
H	-3.941316	0.302444	-3.865153
H	-6.306408	0.964036	-4.176553
H	-7.256526	-0.627129	-0.309320
H	-4.889541	-1.288841	-0.001678
H	-8.878128	0.852344	-1.533201
H	-8.945188	-0.292996	-2.875173
H	-8.513106	1.392452	-3.178333

^{5}5 avec ADF/B3LYP* initFeIV

Fe	0.003471	-1.391522	-0.287808
O	1.874762	-1.768029	-0.106412
O	-0.546582	-1.985340	1.388969
N	0.213937	0.658938	0.571751
N	0.640959	-0.158967	-2.000104
C	1.571333	0.729477	1.209750
H	1.565128	0.001823	2.024118
H	1.697754	1.725662	1.654349
C	2.719820	0.430251	0.284406
C	3.688983	1.396339	0.030193
H	3.611064	2.378041	0.482394
C	4.756471	1.109990	-0.810499
C	4.879994	-0.143743	-1.397832
H	5.709818	-0.366052	-2.055371
C	3.917047	-1.109562	-1.143071
C	2.811735	-0.860067	-0.299270
C	-0.865494	0.860712	1.586146
H	-0.858450	1.906526	1.921980
H	-1.811878	0.681757	1.067027
C	-0.763194	-0.048270	2.777721
C	-0.835269	0.486632	4.061178
H	-0.916342	1.558062	4.200209
C	-0.809507	-0.349758	5.168462
C	-0.710741	-1.727885	5.011274
H	-0.689950	-2.381416	5.873484
C	-0.629642	-2.264998	3.735163
C	-0.647152	-1.443226	2.583223
C	0.059155	1.640314	-0.521833
H	0.447156	2.624223	-0.227832
H	-1.013018	1.746071	-0.724035
C	0.714784	1.158628	-1.789716
C	1.325207	2.004993	-2.707014
H	1.401651	3.066261	-2.502368
C	1.858139	1.458271	-3.866946
H	2.362619	2.092487	-4.586957
C	1.750950	0.088835	-4.086584
H	2.158565	-0.374282	-4.976493
C	1.131430	-0.690345	-3.122494

H	1.044967	-1.766063	-3.222575
Cl	5.958305	2.347771	-1.148663
Cl	4.041376	-2.671690	-1.919826
Cl	-0.899227	0.337705	6.782446
Cl	-0.503152	-3.992431	3.534476
N	-1.504267	-1.659661	-1.198423
S	-3.075146	-1.726042	-0.853708
O	-3.346671	-1.863378	0.568523
O	-3.639070	-2.677535	-1.802041
C	-3.677690	-0.095388	-1.314636
C	-3.644262	0.303836	-2.649601
C	-4.153970	1.545653	-3.006508
C	-4.703163	2.406457	-2.049204
C	-4.718408	1.989963	-0.715520
C	-4.216161	0.746326	-0.344765
C	-5.317480	3.720588	-2.450948
H	-3.241133	-0.363627	-3.402107
H	-4.143785	1.844777	-4.049810
H	-5.151081	2.636181	0.042135
H	-4.266179	0.409816	0.683988
H	-5.128858	4.495344	-1.704473
H	-6.402946	3.616211	-2.549298
H	-4.930100	4.067950	-3.410629

^{5}5 avec ADF/OPBE initFeIII

Fe	-0.291544	0.416761	-0.058806
O	0.716779	-1.170190	0.314726
O	-1.418988	1.033515	1.368679
N	1.342623	1.634378	0.851317
N	0.941025	0.901709	-1.724212
C	2.240869	0.695830	1.587321
H	1.616421	0.128701	2.284947
H	2.986163	1.272046	2.155362
C	2.871208	-0.225701	0.610242
C	4.201269	-0.118061	0.237381
H	4.863914	0.582368	0.736669
C	4.659999	-0.866564	-0.836716
C	3.815137	-1.732010	-1.520780
H	4.172784	-2.283228	-2.382924
C	2.493476	-1.854863	-1.121947
C	1.982840	-1.116476	-0.029784
C	0.771610	2.641604	1.781222
H	1.561084	3.329414	2.120544
H	0.007410	3.192702	1.218873
C	0.165161	1.910043	2.918245
C	0.738458	1.927862	4.176883
H	1.557158	2.603858	4.407215
C	0.286714	1.029633	5.135047
C	-0.703530	0.104205	4.830646
H	-1.023087	-0.619545	5.573363
C	-1.271347	0.096018	3.563156
C	-0.876507	1.023306	2.569949
C	2.097448	2.321747	-0.207398
H	3.113789	2.572868	0.127729
H	1.566954	3.254713	-0.442119
C	2.117251	1.493533	-1.446640
C	3.216003	1.379221	-2.277714
H	4.165315	1.821129	-1.991701
C	3.091472	0.626440	-3.437123
H	3.953060	0.481818	-4.084442
C	1.869222	0.047367	-3.740414
H	1.734375	-0.561544	-4.629975
C	0.814170	0.197968	-2.855139
H	-0.143750	-0.285583	-3.007105
Cl	6.280474	-0.653596	-1.397881
Cl	1.412802	-2.846847	-2.000515
Cl	0.997945	1.030304	6.708562
Cl	-2.443665	-1.087766	3.167982
N	-1.579658	-0.060627	-1.101420
S	-2.279217	-1.448329	-1.534100
O	-2.281164	-2.439476	-0.473570
O	-1.817605	-1.821664	-2.869334
C	-3.904495	-0.763861	-1.701678
C	-4.239241	-0.096602	-2.876382
C	-5.470383	0.532782	-2.967760
C	-6.373461	0.500971	-1.902641
C	-6.010408	-0.171048	-0.732950
C	-4.776381	-0.794200	-0.619240
C	-7.720990	1.135595	-2.035079
H	-3.530497	-0.079558	-3.699409
H	-5.740574	1.058437	-3.882094
H	-6.706845	-0.201760	0.103031
H	-4.474362	-1.301160	0.292860
H	-8.119394	1.434308	-1.060180
H	-8.421057	0.418111	-2.483983
H	-7.681131	2.017936	-2.682494

^{5}5 avec ADF/OPBE initFeIV

Fe	-0.078630	-1.459945	-0.315140
O	1.800224	-1.800405	0.019819
O	-0.705328	-2.087422	1.306005
N	0.121249	0.539404	0.563333
N	0.656386	-0.337374	-1.924284
C	1.388754	0.601544	1.331248
H	1.361891	-0.217064	2.058219
H	1.440760	1.556379	1.876152
C	2.554935	0.418562	0.430873
C	3.432533	1.456969	0.157835
H	3.316065	2.421048	0.643953
C	4.428325	1.274150	-0.788608
C	4.584391	0.051941	-1.430860
H	5.358786	-0.084070	-2.177571
C	3.724112	-0.989472	-1.128094
C	2.673181	-0.847416	-0.192213
C	-1.046379	0.729218	1.444877
H	-1.137823	1.790076	1.724787
H	-1.925957	0.428596	0.869056
C	-0.911520	-0.119808	2.656959
C	-0.875234	0.458374	3.915438
H	-0.986927	1.532448	4.031950
C	-0.681321	-0.337913	5.035018
C	-0.513679	-1.710370	4.906945
H	-0.360235	-2.333255	5.781776

C	-0.528013	-2.283160	3.645877
C	-0.723072	-1.507302	2.479312
C	0.115605	1.508076	-0.532195
H	0.508333	2.483757	-0.208563
H	-0.924974	1.622833	-0.868063
C	0.895179	0.957991	-1.682493
C	1.765460	1.694491	-2.469993
H	1.994655	2.724322	-2.212404
C	2.386421	1.063882	-3.537411
H	3.116302	1.603497	-4.137273
C	2.078794	-0.260523	-3.819573
H	2.548500	-0.785924	-4.645930
C	1.205851	-0.933254	-2.981916
H	0.970969	-1.985225	-3.108529
Cl	5.460330	2.590893	-1.220197
Cl	3.890880	-2.489505	-1.950798
Cl	-0.627568	0.385559	6.601889
Cl	-0.291824	-3.973941	3.483778
N	-1.554247	-1.688310	-1.206180
S	-3.117522	-1.684070	-0.836926
O	-3.392688	-1.798539	0.587756
O	-3.765983	-2.579988	-1.783307
C	-3.576887	-0.018805	-1.288000
C	-3.442233	0.390286	-2.611957
C	-3.874546	1.655017	-2.982296
C	-4.436259	2.528310	-2.046504
C	-4.532790	2.109491	-0.719004
C	-4.117865	0.839770	-0.337058
C	-5.005362	3.846580	-2.466985
H	-3.026454	-0.298111	-3.342772
H	-3.802830	1.963650	-4.024034
H	-4.973640	2.776397	0.020685
H	-4.238226	0.491162	0.685147
H	-4.835816	4.616420	-1.706258
H	-6.090378	3.743123	-2.601964
H	-4.578496	4.188478	-3.414957

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Fe	-0.716508	-1.146536	0.331713
O	1.127513	-1.659858	-0.215902
O	-0.790626	-2.098075	2.042659
N	0.209415	0.618721	1.508422
N	-0.393866	0.507914	-1.170977
C	1.678720	0.429322	1.619202
H	1.824991	-0.485717	2.197786
H	2.110915	1.262557	2.198456
C	2.383616	0.305852	0.296957
C	3.345789	1.239374	-0.081467
H	3.576095	2.074892	0.573281
C	4.002650	1.109676	-1.301805
C	3.711306	0.051830	-2.159162
H	4.209833	-0.042631	-3.116867
C	2.750309	-0.877077	-1.774755
C	2.049572	-0.801082	-0.541194
C	-0.437391	0.620852	2.852107
H	-0.180372	1.554579	3.380007
H	-1.514567	0.612328	2.657292
C	-0.049397	-0.551961	3.709723
C	0.499134	-0.340263	4.973998
H	0.673509	0.673006	5.324265
C	0.820999	-1.421229	5.788456
C	0.611164	-2.727593	5.352422
H	0.865871	-3.572517	5.981652
C	0.073923	-2.935442	4.087585
C	-0.282406	-1.869754	3.212622
C	-0.138554	1.860103	0.801058
H	0.483575	2.702866	1.143872
H	-1.182425	2.079300	1.047367
C	-0.059073	1.712252	-0.698833
C	0.262333	2.765060	-1.554978
H	0.548739	3.730058	-1.147433
C	0.223832	2.543764	-2.930041
H	0.473589	3.346038	-3.619298
C	-0.128278	1.282293	-3.409844
H	-0.170805	1.071533	-4.472805
C	-0.425052	0.283762	-2.488053
H	-0.702697	-0.722986	-2.778971
Cl	5.209854	2.311892	-1.782541
Cl	2.335645	-2.173292	-2.884679
Cl	1.511765	-1.138243	7.393901
Cl	-0.178760	-4.581243	3.537201
N	-2.146453	-1.856103	-0.720091
S	-3.248824	-0.826050	-0.324434
O	-2.623397	0.139124	0.704843
O	-4.591841	-1.315589	0.049916
C	-3.509406	0.242208	-1.764125
C	-3.672334	-0.346776	-3.019863
C	-3.782184	0.456182	-4.152548
C	-3.725614	1.854361	-4.056594
C	-3.567418	2.425916	-2.788607
C	-3.465324	1.630257	-1.647432
C	-3.845830	2.720236	-5.288241
H	-3.668880	-1.429512	-3.100341
H	-3.895521	-0.006972	-5.131223
H	-3.507392	3.508907	-2.695654
H	-3.317434	2.068254	-0.666623
H	-3.323550	3.675102	-5.157994
H	-4.895511	2.952624	-5.517236
H	-3.425953	2.222925	-6.170407

5.H

C	-4.205914	0.073201	-0.582327
C	-3.940459	0.556593	-1.868520
C	-4.966089	0.901409	-2.743746
C	-6.288576	0.756070	-2.320331
C	-6.589100	0.274026	-1.041680
C	-5.529102	-0.064835	-0.183112
S	-2.244872	0.761552	-2.375477
O	-2.220566	1.172988	-3.786143
C	-8.018395	0.114371	-0.585161
Fe	-0.232456	-0.004361	-0.616483
O	-1.596763	-0.600012	-2.048766
O	1.013314	-1.450641	-0.409128
C	2.325092	-1.346089	-0.421473

C	2.985289	-0.394575	0.399220
C	4.371654	-0.252996	0.360800
C	5.124368	-1.042812	-0.503870
C	4.512101	-1.982100	-1.332537
C	3.129042	-2.124848	-1.285240
C	2.140936	0.470760	1.291547
N	1.191170	1.337098	0.528487
C	1.903368	2.201356	-0.436655
C	2.197057	1.489683	-1.737608
N	1.222436	0.679641	-2.178987
C	1.353291	0.045704	-3.351966
C	2.486282	0.200042	-4.144711
C	3.512880	1.026044	-3.686843
C	3.366443	1.686816	-2.467919
Cl	6.869786	-0.839067	-0.571923
Cl	2.346651	-3.264301	-2.355142
O	-1.251961	-0.183741	0.971868
C	-1.173583	0.293408	2.192708
C	-0.348863	1.398559	2.530707
C	-0.260089	1.836191	3.853196
C	-1.001400	1.211846	4.852140
C	-1.845051	0.143671	4.552289
C	-1.922653	-0.300168	3.237588
C	0.366183	2.170574	1.450952
Cl	-0.877408	1.777928	6.510966
Cl	-2.982814	-1.634778	2.844334
N	-1.476339	1.702320	-1.331440
H	1.530692	-0.144600	1.957531
H	2.780378	1.112051	1.916092
H	4.863687	0.479407	0.993343
H	5.099380	-2.588492	-2.011931
H	1.007358	2.932289	1.918965
H	-0.367143	2.681491	0.817748
H	0.380296	2.676037	4.104091
H	-2.428226	-0.339549	5.327116
H	2.826277	2.602847	0.004395
H	1.247598	3.052308	-0.654345
H	4.153426	2.322627	-2.075775
H	4.422786	1.148059	-4.266846
H	2.566817	-0.335068	-5.084339
H	0.530826	-0.603428	-3.631883
H	-4.727088	1.266083	-3.736781
H	-7.097861	1.018676	-2.996856
H	-5.743280	-0.445112	0.812791
H	-3.393800	-0.193447	0.085807
H	-8.218132	0.718452	0.308537
H	-8.235102	-0.928631	-0.323185
H	-8.724366	0.419979	-1.363500
H	-1.298189	2.616522	-1.743711

5.(CH_3CN) red

Fe	-6.094492	-0.761749	-1.583805
O	-5.582401	-2.667207	-1.498202
C	-4.989326	-3.405178	-2.401632
C	-3.705514	-3.074736	-2.915696
C	-3.033510	-1.848904	-2.368196
N	-3.801797	-0.606945	-2.612462
C	-4.007528	-0.394108	-4.068189
C	-4.736665	0.889117	-4.342960
C	-3.109084	0.536179	-2.000217
C	-6.719807	2.235470	-4.042738
C	-6.079886	0.978034	-3.882809
C	-4.066668	1.595245	-1.519279
N	-5.186146	1.149937	-0.917115
N	-7.477076	-0.708726	-0.426586
S	-8.221402	-0.681620	0.950023
C	-7.888010	-2.286626	1.714126
C	-7.651968	-3.403412	0.910949
C	-7.371207	-4.631343	1.505063
C	-7.326922	-4.767521	2.900337
C	-7.567272	-3.634308	3.687673
C	-7.846208	-2.397468	3.103269
C	-4.102510	1.970573	-4.951565
C	-4.780545	3.177140	-5.094901
C	-6.088379	3.323452	-4.636761
C	-3.780265	2.954914	-1.621100
C	-4.672285	3.875111	-1.076762
C	-5.809440	3.407795	-0.420772
C	-6.035905	2.035891	-0.364255
C	-5.578870	-4.593448	-2.906342
C	-4.953332	-5.401325	-3.851088
C	-3.697874	-5.031485	-4.325904
C	-3.074077	-3.875472	-3.865357
O	-6.669723	-0.036345	-3.310235
C	-7.022126	-6.105687	3.531964
Cl	-8.342534	2.426660	-3.416542
Cl	-3.963262	4.558578	-5.839740
Cl	-2.890646	-6.045084	-5.528545
Cl	-7.162748	-5.064648	-2.316499
O	-9.693386	-0.578266	0.836867
O	-7.579328	0.304301	1.881882
H	-4.582912	-1.247381	-4.435968
H	-3.029948	-0.393313	-4.581292
H	-3.074887	1.879643	-5.291115
H	-6.607754	4.270103	-4.730007
H	-2.021358	-1.757565	-2.799712
H	-2.922977	-1.939208	-1.283187
H	-2.094730	-3.597781	-4.243548
H	-5.443163	-6.298346	-4.211327
H	-2.369456	0.975829	-2.687100
H	-2.567138	0.172691	-1.120969
H	-2.886822	3.277593	-2.145436
H	-4.481298	4.941122	-1.167510
H	-6.527978	4.086303	0.026246
H	-6.898038	1.608791	0.132999
H	-8.003774	-1.512103	3.711015
H	-7.526973	-3.720480	4.772270
H	-7.167228	-5.491134	0.870192
H	-7.632691	-3.292358	-0.166171
H	-6.086106	-6.528657	3.145231
H	-7.813573	-6.837576	3.321721
H	-6.928543	-6.021872	4.620428
N	-2.380998	-0.597512	1.091846

C	-3.438294	-0.990376	1.373638
C	-4.766407	-1.495371	1.694636
H	-4.745301	-2.074326	2.623147
H	-5.482390	-0.672278	1.808780
H	-5.116639	-2.146296	0.886901

5.(CH_3CN)-H

C	1.385118	-2.183826	-1.170001
N	1.108565	-1.108292	-0.409824
C	2.000503	-0.678916	0.500160
C	3.223807	-1.319622	0.677576
C	3.521661	-2.431556	-0.107877
C	2.590797	-2.867578	-1.050555
Fe	-0.948005	-0.410946	-0.213165
N	-1.384057	-0.502466	-2.129236
S	-1.976939	-1.735656	-3.038327
O	-2.068476	-1.284891	-4.439232
C	1.605778	0.560514	1.261173
N	0.157182	0.590508	1.546811
C	-0.292227	2.010259	1.698279
C	-1.754411	2.128121	2.026618
C	-2.198211	2.794616	3.168177
C	-3.564468	2.896545	3.421754
C	-4.501484	2.329366	2.558259
C	-4.053231	1.657562	1.425149
C	-2.677144	1.547605	1.126543
Cl	-4.119380	3.741371	4.860004
Cl	-5.199948	0.910682	0.338429
O	-2.264979	0.921372	0.042379
O	-1.354738	-1.904416	0.877345
C	-0.456405	-2.439415	1.694753
C	-0.076734	-3.793805	1.585766
C	0.889488	-4.353158	2.417830
C	1.499993	-3.549656	3.378748
C	1.158685	-2.206125	3.511723
C	0.194092	-1.648872	2.673404
Cl	-0.802774	-4.766886	0.332241
C	-0.175577	-0.195221	2.774383
Cl	2.738393	-4.238260	4.418683
O	-1.182643	-2.934516	-2.710143
C	-3.637699	-1.985364	-2.426011
C	-3.815106	-2.642847	-1.205014
C	-5.093096	-2.720744	-0.664109
C	-6.196343	-2.149829	-1.317925
C	-5.989884	-1.513033	-2.547215
C	-4.714768	-1.422865	-3.106764
C	-7.565769	-2.198768	-0.686841
H	-1.252520	-0.089960	2.925864
H	0.331725	0.263087	3.636601
H	1.651435	-1.592726	4.259401
H	1.166753	-5.394684	2.306545
H	0.306451	2.496856	2.482675
H	-0.072368	2.496486	0.742671
H	-1.484070	3.234224	3.857405
H	-5.562391	2.401109	2.766634
H	2.193068	0.654208	2.185546
H	1.827117	1.424277	0.626098
H	3.916276	-0.964095	1.433649
H	4.462562	-2.957462	0.025038
H	2.775941	-3.737863	-1.670560
H	0.603239	-2.500434	-1.856275
H	-4.550117	-0.927617	-4.057685
H	-6.836084	-1.076004	-3.071485
H	-5.237204	-3.223365	0.289070
H	-2.965323	-3.069224	-0.684534
H	-7.620556	-1.517575	0.172434
H	-7.801932	-3.204028	-0.319021
H	-8.345411	-1.903533	-1.396144
H	-1.869846	0.354601	-2.400644
N	0.836872	1.910346	-1.601122
C	0.944659	1.300105	-2.583287
C	1.093060	0.519826	-3.806903
H	1.675498	1.078828	-4.546168
H	1.608541	-0.417463	-3.573969
H	0.109652	0.265397	-4.213296

5.(py) red

C	-4.055572	-0.248389	-0.592787
C	-3.848403	0.043613	-1.943824
C	-4.711779	0.909269	-2.611210
C	-5.783759	1.483358	-1.925556
C	-6.008686	1.203505	-0.572405
C	-5.126474	0.331702	0.082645
S	-2.457042	-0.715017	-2.822735
O	-2.099384	0.269557	-3.893027
C	-7.172531	1.821376	0.167057
N	-1.322558	-0.851300	-1.751928
Fe	-0.280918	0.012302	-0.535307
N	1.193577	0.770999	-2.035105
C	2.187476	1.568742	-1.612617
C	3.368042	1.711043	-2.339655
C	3.513992	0.995524	-3.526385
C	2.471308	0.178301	-3.962399
C	1.321050	0.088466	-3.183036
C	1.904382	2.332631	-0.338891
N	1.277163	1.490221	0.687478
C	0.514883	2.324289	1.640062
C	-0.166743	1.539486	2.732480
C	0.061864	1.884024	4.065174
C	-0.610737	1.226404	5.089839
C	-1.524532	0.214068	4.805147
C	-1.742353	-0.134197	3.478180
C	-1.072523	0.490684	2.386701
Cl	-0.310501	1.681420	6.773393
Cl	-2.912378	-1.390691	3.113077
O	-1.321868	0.133587	1.165142
O	1.153278	-1.351930	-0.116576
C	2.433173	-1.188433	-0.214521
C	3.117624	-0.177991	0.525031
C	4.491950	0.017773	0.408504
C	5.229282	-0.772345	-0.466926
C	4.612618	-1.768095	-1.223801
C	3.243402	-1.967035	-1.091081

C	2.281065	0.680973	1.423367
Cl	6.970961	-0.499625	-0.644265
Cl	2.461964	-3.190819	-2.071817
O	-2.967771	-2.016519	-3.314677
H	1.718468	0.056020	2.121534
H	2.927729	1.353801	2.014400
H	4.981337	0.798441	0.984239
H	5.186257	-2.375185	-1.914728
H	1.184978	3.069988	2.104836
H	-0.226039	2.872235	1.050715
H	0.766046	2.676261	4.302882
H	-2.056649	-0.296944	5.599108
H	2.825570	2.811494	0.032854
H	1.191228	3.129970	-0.579009
H	4.168570	2.335797	-1.956863
H	4.436732	1.066905	-4.095893
H	2.548674	-0.399912	-4.876908
H	0.469445	-0.530614	-3.442379
H	-4.515293	1.148737	-3.651157
H	-6.449043	2.172135	-2.444641
H	-5.264796	0.115549	1.140443
H	-3.349020	-0.880304	-0.066691
H	-6.878278	2.161199	1.167901
H	-7.992357	1.102155	0.303148
H	-7.579861	2.681798	-0.376505
N	-1.417979	2.088929	-1.079064
C	-2.422466	2.504885	-0.286820
C	-3.323876	3.494334	-0.665480
C	-3.194220	4.069425	-1.929111
C	-2.175147	3.621627	-2.765087
C	-1.317143	2.624175	-2.304149
H	-2.502310	1.994152	0.664113
H	-4.124951	3.778326	0.008375
H	-3.890274	4.834678	-2.263292
H	-2.053795	4.010934	-3.770949
H	-0.538831	2.218793	-2.935726

5.(py)-H

C	-0.443859	3.985561	-1.516614
N	-0.940796	3.065792	-0.674250
C	-2.102281	3.332127	-0.049181
C	-2.791463	4.529107	-0.229109
C	-2.263131	5.488126	-1.092918
C	-1.065464	5.209525	-1.752094
Fe	-0.268311	0.745687	-0.535021
O	0.648507	-0.925107	-0.498051
C	1.944035	-1.129249	-0.585817
C	2.829125	-0.516358	0.334999
C	4.208425	-0.692810	0.236537
C	4.728387	-1.469360	-0.794759
C	3.890602	-2.079990	-1.728078
C	2.513487	-1.909188	-1.620214
C	2.217351	0.350198	1.394122
N	1.480738	1.521976	0.828696
C	0.908222	2.337710	1.932558
C	0.035589	1.549750	2.874496
C	0.290247	1.605663	4.246053
C	-0.527778	0.924558	5.141519
C	-1.605859	0.169812	4.684818
C	-1.851661	0.107082	3.317718
C	-1.048117	0.784964	2.367280
Cl	-0.197004	1.010852	6.865916
Cl	-3.206088	-0.841681	2.747871
O	-1.325767	0.710002	1.082588
Cl	6.471515	-1.661821	-0.944716
Cl	1.455309	-2.619766	-2.807145
N	-1.590274	0.672300	-1.984237
S	-2.394833	-0.602064	-2.648827
O	-1.850607	-1.829401	-2.063464
C	-4.064926	-0.372017	-2.037099
C	-4.257965	-0.218176	-0.661032
C	-5.550544	-0.056086	-0.174288
C	-6.656926	-0.051145	-1.039603
C	-6.432744	-0.203639	-2.412855
C	-5.141412	-0.365365	-2.919282
C	-8.056582	0.092351	-0.492667
O	-2.441976	-0.440119	-4.114721
N	1.324959	1.380028	-1.953220
C	2.480588	1.808925	-1.413664
C	3.675011	1.781725	-2.129209
C	3.665425	1.283936	-3.431087
C	2.463073	0.842319	-3.983704
C	1.309904	0.900379	-3.208389
C	2.370926	2.349669	-0.007301
H	1.490910	-0.218383	1.979020
H	2.992917	0.717242	2.083977
H	4.874512	-0.216753	0.949558
H	4.301591	-2.674720	-2.535374
H	1.725387	2.801571	2.506640
H	0.337798	3.141403	1.457936
H	1.129022	2.186186	4.617408
H	-2.242763	-0.366802	5.377924
H	3.367829	2.446395	0.446140
H	1.934971	3.354317	-0.052429
H	4.596924	2.107116	-1.658782
H	4.588687	1.227777	-4.000014
H	2.417106	0.431367	-4.986050
H	0.348691	0.540694	-3.560740
H	-4.959660	-0.478384	-3.982813
H	-7.278887	-0.195703	-3.096095
H	-5.703011	0.065954	0.895737
H	-3.409079	-0.213639	0.013796
H	-8.096697	0.828922	0.317975
H	-8.417454	-0.859724	-0.081140
H	-8.761877	0.402254	-1.270787
H	-2.470780	2.540823	0.594062
H	-3.726487	4.695368	0.295618
H	-2.777751	6.430648	-1.256020
H	-0.621527	5.919083	-2.442853
H	0.474683	3.714185	-2.026133
H	-1.914990	1.531758	-2.422704

(L^{Cl}, NNs)

C	-0.258292	-0.269140	-0.639771

C	0.750884	-1.199380	-0.370190
C	0.811630	-1.911721	0.829261
C	-0.162328	-1.681497	1.796845
C	-1.167578	-0.755409	1.523618
C	-1.235285	-0.045845	0.325721
S	1.978141	-1.542745	-1.620536
O	3.101681	-2.287277	-1.036739
N	-2.203591	-0.518806	2.546885
Fe	1.585201	-0.560078	-4.146209
O	2.346538	-0.168992	-2.210800
O	2.252933	0.708379	-5.415485
C	2.833816	0.399608	-6.557937
C	2.208775	-0.489251	-7.470553
C	2.835795	-0.849329	-8.662433
C	4.099479	-0.346189	-8.959291
C	4.749909	0.521602	-8.082639
C	4.116970	0.884074	-6.898000
C	0.862351	-1.045999	-7.103345
N	0.890034	-1.860058	-5.851020
C	1.837780	-2.994333	-5.948714
C	3.263038	-2.578942	-5.666049
N	3.420236	-1.723248	-4.641887
C	4.647650	-1.337391	-4.267085
C	5.789073	-1.797324	-4.914913
C	5.637223	-2.671794	-5.991114
C	4.357480	-3.074698	-6.369830
Cl	4.899902	-0.828375	-10.447562
Cl	4.941792	1.931601	-5.768262
O	-0.205365	-0.022420	-3.835145
C	-1.339857	-0.217018	-4.475871
C	-1.527312	-1.294927	-5.380025
C	-2.732871	-1.430094	-6.069134
C	-3.770310	-0.524636	-5.858888
C	-3.630338	0.525980	-4.953614
C	-2.426409	0.665878	-4.273382
C	-0.472465	-2.364488	-5.514126
Cl	-5.276999	-0.711849	-6.738136
Cl	-2.235424	1.973141	-3.126995
N	1.200765	-2.331620	-2.805129
H	0.147962	-0.236767	-6.928305
H	0.472332	-1.667887	-7.922608
H	2.347625	-1.530571	-9.352401
H	5.737512	0.904085	-8.311727
H	-0.787769	-3.087068	-6.281111
H	-0.367514	-2.896276	-4.562886
H	-2.870800	-2.252713	-6.763470
H	-4.439735	1.225602	-4.782724
H	1.761233	-3.481319	-6.930497
H	1.544364	-3.721236	-5.184448
H	4.205149	-3.740491	-7.212775
H	6.504896	-3.030990	-6.536239
H	6.767710	-1.458046	-4.594329
H	4.691625	-0.635867	-3.441131
H	1.615331	-2.619825	0.997453
H	-0.155897	-2.201340	2.746357
H	-2.036972	0.662607	0.159430
H	-0.287404	0.261465	-1.584567
O	-3.080471	0.301786	2.286488
O	-2.122737	-1.158345	3.594013

(L^{Cl}, NNs) red

C	-0.720616	-1.143882	0.297490
C	0.582835	-1.493349	-0.066003
C	1.359946	-2.304612	0.770079
C	0.830968	-2.782748	1.961553
C	-0.483806	-2.444195	2.297587
C	-1.266036	-1.625121	1.482177
S	1.256195	-1.009668	-1.680340
O	2.192727	0.090604	-1.375361
N	-1.063830	-2.980642	3.524462
Fe	0.422227	-2.528224	-3.675122
O	-0.007278	-0.575285	-2.445689
O	0.226593	-4.338067	-4.446630
C	-0.878635	-5.028511	-4.402022
C	-2.129096	-4.479955	-4.815960
C	-3.309130	-5.214689	-4.723051
C	-3.286899	-6.510685	-4.215672
C	-2.093081	-7.090692	-3.794535
C	-0.918480	-6.351697	-3.889662
C	-2.140602	-3.086214	-5.379494
N	-1.701945	-2.037615	-4.420812
C	-2.590312	-1.951710	-3.250867
C	-2.280588	-2.999993	-2.209989
N	-0.994012	-3.348235	-2.114578
C	-0.600255	-4.229488	-1.189041
C	-1.493571	-4.792946	-0.284184
C	-2.838353	-4.429336	-0.366080
C	-3.241713	-3.524324	-1.345722
Cl	-4.793315	-7.427836	-4.085047
Cl	0.575758	-7.056655	-3.297503
O	1.081107	-1.586170	-5.245434
C	0.513008	-1.154258	-6.330159
C	-0.840304	-0.705916	-6.363119
C	-1.421930	-0.248063	-7.544959
C	-0.679782	-0.208291	-8.720982
C	0.647114	-0.632475	-8.740410
C	1.220825	-1.098061	-7.563115
C	-1.630517	-0.702108	-5.083464
Cl	-1.427720	0.380120	-10.212328
Cl	2.886442	-1.642287	-7.590468
N	1.785780	-2.314511	-2.335902
H	-1.455618	-3.027697	-6.228702
H	-3.150225	-2.839174	-5.747895
H	-4.249138	-4.772131	-5.039622
H	-2.075228	-8.093702	-3.384397
H	-2.652272	-0.343394	-5.290121
H	-1.165428	-0.036262	-4.349988
H	-2.456913	0.081068	-7.546316
H	1.226152	-0.608311	-9.656223
H	-3.649213	-2.004402	-3.550974
H	-2.412449	-0.974894	-2.789622
H	-4.283134	-3.234593	-1.449003
H	-3.565994	-4.850766	0.321751
H	-1.142146	-5.497544	0.461762

H	0.458754	-4.462060	-1.192302
H	2.359252	-2.584991	0.453683
H	1.400332	-3.423410	2.623552
H	-2.281065	-1.393369	1.779677
H	-1.299307	-0.522671	-0.375707
O	-2.235961	-2.692799	3.787899
O	-0.356230	-3.700480	4.235679

(L^{Cl}, NSO2pyMe)

C	-0.076270	-0.050321	-0.624309
C	0.757430	-1.149509	-0.410649
N	0.625608	-2.034334	0.567986
C	-0.374845	-1.835708	1.429063
C	-1.287187	-0.772516	1.339646
C	-1.121077	0.125800	0.278176
S	2.085515	-1.498776	-1.580921
O	3.227961	-2.163835	-0.952272
C	-2.398800	-0.614439	2.342763
Fe	1.629928	-0.522476	-4.096312
O	2.416564	-0.119591	-2.205586
O	2.264957	0.725298	-5.412748
C	2.819276	0.394850	-6.560993
C	2.174883	-0.510800	-7.443941
C	2.774540	-0.892485	-8.643046
C	4.030560	-0.394561	-8.978315
C	4.700301	0.489092	-8.132873
C	4.094034	0.873009	-6.941089
C	0.838896	-1.063405	-7.034566
N	0.901489	-1.856849	-5.771778
C	1.852347	-2.987351	-5.873834
C	3.282287	-2.563766	-5.628809
N	3.461480	-1.689758	-4.624427
C	4.696220	-1.299125	-4.280968
C	5.824070	-1.772017	-4.943259
C	5.649533	-2.665077	-6.000588
C	4.362030	-3.072836	-6.346073
Cl	4.797257	-0.903664	-10.476510
Cl	4.944788	1.942861	-5.850955
O	-0.156060	0.012896	-3.762210
C	-1.301149	-0.197814	-4.374181
C	-1.506467	-1.296254	-5.250296
C	-2.727374	-1.451829	-5.907815
C	-3.763535	-0.546067	-5.695139
C	-3.605895	0.527161	-4.820237
C	-2.386816	0.686642	-4.172076
C	-0.448321	-2.362184	-5.390960
Cl	-5.291724	-0.759991	-6.533738
Cl	-2.175945	2.028055	-3.065864
N	1.350580	-2.333591	-2.767307
H	0.128570	-0.251936	-6.853625
H	0.428677	-1.697775	-7.834543
H	2.271255	-1.587037	-9.308512
H	5.682348	0.867327	-8.391072
H	-0.779851	-3.100724	-6.136020
H	-0.314358	-2.876247	-4.433552
H	-2.877134	-2.290600	-6.580136
H	-4.412731	1.229801	-4.649463
H	1.757663	-3.488523	-6.847069
H	1.579942	-3.704247	-5.092685
H	4.191790	-3.753735	-7.173418
H	6.505689	-3.035473	-6.556417
H	6.809416	-1.429244	-4.647836
H	4.756643	-0.584308	-3.467481
H	-0.465204	-2.566005	2.231558
H	-1.808396	0.957773	0.148295
H	-3.373873	-0.554296	1.845240
H	-2.273972	0.306591	2.925413
H	-2.425590	-1.454476	3.043290
H	0.069851	0.614092	-1.465042

(L^{Cl}, NSO2pyMe) red

C	-0.710376	-1.102739	0.244575
C	0.595588	-1.506358	-0.057381
N	1.326656	-2.270865	0.751197
C	0.759919	-2.691647	1.886140
C	-0.550844	-2.395888	2.274773
C	-1.286506	-1.563237	1.421291
S	1.338849	-1.063755	-1.668398
O	2.287438	0.026086	-1.366681
C	-1.145201	-2.966645	3.536483
Fe	0.461743	-2.545611	-3.660727
O	0.085236	-0.606984	-2.454485
O	0.209192	-4.374340	-4.414614
C	-0.907067	-5.040040	-4.370373
C	-2.146010	-4.472391	-4.797533
C	-3.341490	-5.181865	-4.705527
C	-3.349534	-6.471069	-4.181801
C	-2.170271	-7.070785	-3.746629
C	-0.979820	-6.358655	-3.844246
C	-2.126127	-3.079874	-5.362179
N	-1.677105	-2.046863	-4.393553
C	-2.554739	-1.978065	-3.215737
C	-2.239972	-3.047484	-2.197470
N	-0.944064	-3.350491	-2.076379
C	-0.537273	-4.232839	-1.158069
C	-1.433687	-4.855725	-0.294887
C	-2.790279	-4.551569	-0.413011
C	-3.203307	-3.633503	-1.376451
Cl	-4.877229	-7.355385	-4.046146
Cl	0.495844	-7.090890	-3.238038
O	1.100327	-1.635295	-5.270307
C	0.517204	-1.168511	-6.329311
C	-0.829893	-0.695304	-6.327619
C	-1.425968	-0.203797	-7.488470
C	-0.707314	-0.151581	-8.678461
C	0.611288	-0.597586	-8.733303
C	1.199423	-1.097162	-7.577559
C	-1.599660	-0.702896	-5.035078
Cl	-1.475429	0.480802	-10.142961
Cl	2.855141	-1.669550	-7.652022
N	1.840516	-2.369593	-2.347727
H	-1.431901	-3.032267	-6.204369
H	-3.127838	-2.813405	-5.739695
H	-4.270142	-4.722483	-5.031936

H	-2.175745	-8.069087	-3.324639
H	-2.620104	-0.328166	-5.221187
H	-1.115336	-0.054634	-4.298130
H	-2.455098	0.142495	-7.462321
H	1.172775	-0.564223	-9.659752
H	-3.617310	-2.018303	-3.505942
H	-2.364885	-1.011281	-2.737936
H	-4.252879	-3.387251	-1.506812
H	-3.521510	-5.030904	0.232584
H	-1.074175	-5.566267	0.441660
H	0.532348	-4.411275	-1.130621
H	1.383395	-3.318431	2.525632
H	-1.242196	-0.470649	-0.455074
H	-1.945581	-3.683736	3.308898
H	-1.582803	-2.183463	4.168295
H	-0.388116	-3.492009	4.128690
H	-2.309929	-1.292150	1.675265

(L^{tBu}, NTs)

Fe	-0.134628	-1.430578	0.009812
O	1.709489	-1.716329	0.146265
O	-0.971567	-1.786090	1.635902
N	0.147305	0.716758	0.851968
N	-0.032603	-0.083619	-1.787170
C	1.536655	0.738430	1.401949
H	1.572743	-0.023898	2.183376
H	1.712968	1.716463	1.875619
C	2.576987	0.472408	0.352231
C	3.468393	1.466981	-0.053740
H	3.385369	2.448130	0.403304
C	4.430771	1.215062	-1.030206
C	4.502179	-0.093790	-1.539794
H	5.268101	-0.307396	-2.275107
C	3.650878	-1.132404	-1.158253
C	2.633494	-0.816790	-0.218369
C	-0.862451	0.965042	1.926895
H	-0.779869	2.010283	2.262760
H	-1.843221	0.842070	1.449522
C	-0.726383	0.045690	3.103505
C	-0.557716	0.558277	4.391676
H	-0.504872	1.635629	4.512307
C	-0.463828	-0.288156	5.494643
C	-0.528766	-1.671187	5.248965
H	-0.444403	-2.337668	6.098115
C	-0.683738	-2.239929	3.984074
C	-0.794569	-1.344650	2.885096
C	0.001434	1.726999	-0.209170
H	0.579694	2.632837	0.019372
H	-1.055833	2.016918	-0.249317
C	0.373460	1.178207	-1.560152
C	1.009818	1.934954	-2.541166
H	1.357849	2.936102	-2.310198
C	1.206190	1.372720	-3.800091
H	1.715882	1.934945	-4.577052
C	0.740329	0.081004	-4.046242
H	0.862649	-0.389878	-5.015660
C	0.133703	-0.618719	-3.008688
H	-0.225873	-1.635740	-3.117362
C	5.388607	2.289358	-1.560760
C	3.806240	-2.556915	-1.715764
C	-0.288433	0.221119	6.931074
C	-0.684920	-3.760746	3.773655
N	-0.869074	-2.736855	-1.195302
S	-0.877848	-4.341677	-1.009170
O	-2.221402	-4.673764	-0.491568
O	0.322182	-4.816653	-0.296847
C	-0.756046	-4.980487	-2.677767
C	0.337875	-5.760846	-3.041086
C	0.431631	-6.234670	-4.351258
C	-0.553017	-5.938705	-5.299436
C	-1.649944	-5.153814	-4.904441
C	-1.758373	-4.675168	-3.603837
C	-0.449180	-6.443807	-6.717845
H	1.097980	-5.986065	-2.301539
H	1.283890	-6.845397	-4.638821
H	-2.428315	-4.921790	-5.627926
H	-2.609486	-4.073964	-3.300237
H	-0.351114	-5.613830	-7.429377
H	-1.344552	-7.008557	-7.004789
H	0.417935	-7.098838	-6.846853
C	3.937574	-3.564941	-0.550071
C	5.060534	-2.693809	-2.598007
C	2.582636	-2.927488	-2.577650
C	6.849836	1.858137	-1.307359
C	5.162790	3.651899	-0.884411
C	5.161833	2.463017	-3.079309
C	1.022210	-0.343505	7.522505
C	-1.482551	-0.249311	7.790984
C	-0.221550	1.756144	6.999022
C	-1.961497	-4.206178	3.024954
C	-0.642346	-4.527099	5.108781
C	0.575634	-4.149924	2.967168
H	-1.953485	-5.294858	2.896138
H	-2.036357	-3.755996	2.036535
H	-2.855670	-3.937932	3.601751
H	-0.665945	-5.603017	4.903660
H	-1.504514	-4.290580	5.744141
H	0.272701	-4.322161	5.677233
H	0.575405	-5.226286	2.761229
H	1.481254	-3.906330	3.536573
H	0.622402	-3.638093	2.007076
H	1.160474	0.006321	8.553359
H	1.886077	-0.018819	6.931099
H	1.019849	-1.438127	7.537082
H	-1.374621	0.101858	8.824909
H	-1.557923	-1.341407	7.813600
H	-2.425263	0.142261	7.392055
H	-0.091619	2.075589	8.039253
H	-1.140432	2.219042	6.620902
H	0.623975	2.149497	6.422744
H	7.546799	2.617584	-1.682910
H	7.084606	0.912498	-1.806774
H	7.033068	1.723976	-0.235447

H	5.854476	4.393667	-1.299190
H	5.337252	3.600963	0.196231
H	4.142722	4.019229	-1.049042
H	5.844759	3.217835	-3.488608
H	4.133441	2.786593	-3.280204
H	5.328603	1.526805	-3.622307
H	4.100397	-4.573211	-0.950489
H	3.036488	-3.584718	0.064177
H	4.794764	-3.309538	0.084429
H	5.149418	-3.732367	-2.935301
H	5.975539	-2.442384	-2.049251
H	5.009947	-2.061791	-3.492957
H	2.686392	-3.947257	-2.965503
H	2.489178	-2.247316	-3.431794
H	1.664051	-2.887242	-1.993346

(L^{tBu}, NTs) red

Fe	0.714143	-1.758308	-0.618188
O	2.477196	-1.600769	0.211402
O	-0.757881	-2.077921	0.618036
N	0.416617	0.570047	0.205720
N	1.133227	-0.373734	-2.330439
C	1.582777	0.867097	1.073553
H	1.524870	0.168588	1.911352
H	1.481852	1.892173	1.475112
C	2.898593	0.719895	0.366948
C	3.702722	1.827643	0.095184
H	3.339730	2.807396	0.394429
C	4.925290	1.689272	-0.559350
C	5.334509	0.380380	-0.874526
H	6.295695	0.256456	-1.360320
C	4.584370	-0.764015	-0.603967
C	3.298326	-0.586704	-0.006803
C	-0.851129	0.660484	0.971911
H	-1.012733	1.699413	1.312661
H	-1.651861	0.404034	0.267572
C	-0.887107	-0.274090	2.144063
C	-0.978585	0.204651	3.451930
H	-1.011521	1.280746	3.599200
C	-1.019226	-0.667109	4.539223
C	-0.963963	-2.043675	4.254155
H	-0.989424	-2.731466	5.091660
C	-0.871337	-2.574856	2.967880
C	-0.828268	-1.660585	1.871315
C	0.384863	1.462266	-0.952872
H	0.684748	2.490169	-0.689358
H	-0.653548	1.510649	-1.305626
C	1.224640	0.947393	-2.095007
C	1.976651	1.791384	-2.909378
H	2.055692	2.845788	-2.663944
C	2.643300	1.249638	-4.005845
H	3.254309	1.883397	-4.643530
C	2.516021	-0.113067	-4.266057
H	3.008237	-0.579468	-5.113098
C	1.756870	-0.898303	-3.400658
H	1.632715	-1.966707	-3.553973
C	5.816061	2.877069	-0.943252
C	5.114268	-2.172262	-0.919446
C	-1.110142	-0.196141	5.996215
C	-0.822903	-4.090141	2.718072
N	0.691450	-3.240256	-1.645879
S	0.704274	-4.382235	-2.707679
O	1.534609	-5.543523	-2.306121
O	0.945466	-3.867337	-4.092336
C	-0.996814	-4.988504	-2.725593
C	-1.783662	-4.879551	-3.868191
C	-3.109177	-5.322971	-3.839925
C	-3.662217	-5.872046	-2.679088
C	-2.849293	-5.976796	-1.538431
C	-1.528895	-5.542391	-1.557336
C	-5.102387	-6.326458	-2.638321
H	-1.346394	-4.447829	-4.762315
H	-3.724727	-5.238006	-4.734318
H	-3.262163	-6.397051	-0.623096
H	-0.906685	-5.617555	-0.672326
H	-5.710839	-5.676235	-1.994725
H	-5.193375	-7.345185	-2.239810
H	-5.552071	-6.316044	-3.637577
C	5.095414	-3.026137	0.369304
C	6.563634	-2.139994	-1.438652
C	4.242325	-2.854104	-1.994926
C	7.190796	2.751645	-0.250222
C	5.196890	4.224364	-0.535044
C	6.019262	2.890463	-2.474961
C	0.131771	-0.680757	6.777308
C	-2.381800	-0.777708	6.653089
C	-1.175457	1.336427	6.108876
C	-2.044511	-4.504518	1.867026
C	-0.864488	-4.894600	4.030361
C	0.478228	-4.473889	1.974529
H	-2.010649	-5.582218	1.656512
H	-2.050770	-3.964066	0.919265
H	-2.978896	-4.292725	2.403107
H	-0.836274	-5.965679	3.797481
H	-1.780294	-4.703430	4.603623
H	-0.003693	-4.671905	4.672824
H	0.560633	-5.566601	1.904089
H	1.357956	-4.101899	2.513046
H	0.500004	-4.070565	0.962567
H	0.080166	-0.364394	7.828171
H	1.047200	-0.269031	6.337167
H	0.217206	-1.772221	6.756964
H	-2.460822	-0.458532	7.701507
H	-2.377692	-1.872401	6.633119
H	-3.278621	-0.439254	6.121158
H	-1.246889	1.631032	7.163255
H	-2.050804	1.740558	5.587319
H	-0.280280	1.809326	5.688815
H	7.846135	3.589594	-0.525243
H	7.696225	1.821814	-0.530544
H	7.072725	2.749790	0.839515
H	5.858843	5.046764	-0.833589
H	5.050054	4.289126	0.549093

H	4.225481	4.383792	-1.018150
H	6.656160	3.732265	-2.779376
H	5.054602	2.982047	-2.987052
H	6.490314	1.965626	-2.823230
H	5.469480	-4.035437	0.154260
H	4.079475	-3.105017	0.758931
H	5.737576	-2.578928	1.139589
H	6.907037	-3.167074	-1.608890
H	7.248323	-1.670749	-0.720681
H	6.645316	-1.603902	-2.392335
H	4.629737	-3.855349	-2.220602
H	4.251359	-2.270776	-2.923645
H	3.209818	-2.969267	-1.666232

(L^{NO2}, NTs)

C	-4.761149	-0.755815	-0.600235
C	-4.143503	-0.528477	-1.833995
C	-4.850055	-0.013797	-2.920556
C	-6.205403	0.269728	-2.767217
C	-6.855849	0.053615	-1.544490
C	-6.114011	-0.457194	-0.468428
S	-2.404497	-0.863432	-1.992656
O	-2.044644	-0.864723	-3.430762
C	-8.329874	0.337229	-1.392846
N	-1.653081	0.478944	-1.441373
Fe	-0.154774	0.483978	-0.307633
N	1.148989	1.188294	-1.901229
C	2.297485	1.809270	-1.571682
C	3.371001	1.873796	-2.453438
C	3.245529	1.277333	-3.708725
C	2.048228	0.649408	-4.047990
C	1.016352	0.619968	-3.114687
C	2.308717	2.466307	-0.213027
N	1.587204	1.659284	0.791530
C	1.023381	2.546755	1.851020
C	0.272741	1.791688	2.911949
C	0.597305	1.890106	4.254186
C	-0.174255	1.217178	5.207278
C	-1.263613	0.437300	4.840257
C	-1.567654	0.312039	3.492045
C	-0.830064	0.994814	2.488724
N	0.175555	1.337804	6.620060
N	-2.694011	-0.549511	3.125610
O	-1.165054	0.961637	1.230283
O	0.886889	-1.084070	-0.065310
C	2.169539	-1.143364	-0.319300
C	3.073217	-0.309308	0.403072
C	4.436228	-0.370894	0.168756
C	4.937344	-1.259593	-0.786010
C	4.094637	-2.090160	-1.513685
C	2.726751	-2.007320	-1.295912
C	2.486198	0.637027	1.409256
N	6.373348	-1.291958	-1.045936
N	1.864957	-2.813160	-2.166019
O	-2.093700	-2.019568	-1.143217
H	1.883208	0.084501	2.133695
H	3.289286	1.149536	1.959139
H	5.129332	0.264513	0.708017
H	4.491629	-2.775062	-2.251394
H	1.831567	3.132771	2.312783
H	0.346574	3.243541	1.343405
H	1.437167	2.488054	4.589184
H	-1.859135	-0.071065	5.587098
H	3.338200	2.675971	0.108571
H	1.792186	3.429928	-0.296705
H	4.291160	2.364162	-2.152722
H	4.076280	1.298196	-4.407790
H	1.910840	0.169819	-5.010649
H	0.073532	0.124013	-3.319594
H	-4.343081	0.147282	-3.865665
H	-6.768384	0.663348	-3.609775
H	-6.604417	-0.627285	0.486752
H	-4.194555	-1.154008	0.235325
H	-8.558166	0.745739	-0.402435
H	-8.918777	-0.582470	-1.508028
H	-8.680915	1.049027	-2.146850
O	6.784245	-2.080608	-1.896622
O	7.084244	-0.515752	-0.402914
O	-0.522043	0.736380	7.435787
O	1.151111	2.036046	6.905218
O	-2.648028	-1.118454	2.036726
O	-3.604219	-0.663021	3.947093
O	0.797756	-2.320378	-2.521727
O	2.296047	-3.909857	-2.518746

(L^{NO2}, NTs) red

C	-3.942177	0.082486	-0.536634
C	-3.343331	-0.591576	-1.607052
C	-2.985849	0.107609	-2.756321
C	-3.205831	1.486463	-2.826910
C	-3.789349	2.181933	-1.762088
C	-4.159825	1.455259	-0.616702
S	-2.976707	-2.359243	-1.447534
O	-2.444590	-2.758305	-2.776964
C	-4.028925	3.671218	-1.836106
N	-1.873824	-2.396867	-0.314950
Fe	-0.392889	-1.572130	0.282552
N	0.011001	-0.763461	-1.775418
C	0.170590	0.559471	-1.901761
C	0.629169	1.133235	-3.084923
C	0.918417	0.294022	-4.160586
C	0.731593	-1.081465	-4.024802
C	0.271938	-1.576897	-2.807065
C	-0.259244	1.369616	-0.705217
N	-0.034370	0.651602	0.564873
C	-1.000115	1.159309	1.582081
C	-0.754479	0.679519	2.986941
C	-0.730149	1.588308	4.022178
C	-0.584969	1.155899	5.350466
C	-0.445856	-0.195773	5.642426
C	-0.430050	-1.117365	4.607946
C	-0.601301	-0.737831	3.229017
N	-0.570817	2.126397	6.419352
N	-0.217677	-2.513711	4.983398

O	-0.640722	-1.578772	2.274358
O	1.600075	-1.900970	0.280993
C	2.427185	-1.090337	-0.268021
C	2.399191	0.319671	0.048988
C	3.289385	1.200551	-0.525317
C	4.252900	0.743421	-1.438211
C	4.327546	-0.601551	-1.777803
C	3.420956	-1.491691	-1.222028
C	1.373776	0.800932	1.038316
N	5.159126	1.687483	-2.052962
N	3.489576	-2.870271	-1.698048
O	-4.240167	-2.987826	-1.012573
H	1.457185	0.225544	1.962071
H	1.558793	1.858556	1.280579
H	3.255052	2.258652	-0.291624
H	5.067161	-0.951457	-2.484947
H	-0.979369	2.260237	1.580728
H	-1.992462	0.850247	1.233925
H	-0.831092	2.651100	3.832575
H	-0.337157	-0.531271	6.664609
H	0.238461	2.351186	-0.694716
H	-1.335680	1.547574	-0.798645
H	0.768549	2.207761	-3.152480
H	1.289815	0.710605	-5.092849
H	0.941509	-1.764789	-4.840412
H	0.098919	-2.630832	-2.638393
H	-2.528039	-0.434710	-3.576488
H	-2.913090	2.030329	-3.722825
H	-4.623406	1.976471	0.218982
H	-4.231362	-0.478047	0.347486
H	-3.612609	4.190027	-0.963321
H	-5.101786	3.903311	-1.863547
H	-3.573766	4.103917	-2.733286
O	5.994649	1.259399	-2.857037
O	5.046244	2.882063	-1.746338
O	-0.437030	1.720038	7.579505
O	-0.693762	3.322420	6.118546
O	0.270469	-3.276212	4.155012
O	-0.519606	-2.839032	6.139882
O	2.457516	-3.538471	-1.708850
O	4.585735	-3.276951	-2.101187

(L^{NO2}, NNs)

C	-5.361199	-0.900214	-0.571338
C	-4.460624	-0.688141	-1.649999
C	-4.979023	-0.030763	-2.809764
C	-6.304522	0.360285	-2.869901
C	-7.153724	0.110583	-1.787499
C	-6.697155	-0.527790	-0.642856
O	-3.208060	-1.044603	-1.623148
Fe	-1.714084	0.148350	-1.892665
O	-0.667846	-0.735955	-3.210962
C	-0.691429	-0.865872	-4.503809
C	-1.404752	0.058540	-5.329692
C	-1.453349	-0.132764	-6.701148
C	-0.763756	-1.194910	-7.293385
C	0.008363	-2.064739	-6.537741
C	0.028810	-1.903803	-5.159365
C	-1.976917	1.319301	-4.729464
N	-2.892909	1.118557	-3.570395
C	-4.032105	0.228859	-3.947272
N	-0.835351	-1.373167	-8.741756
O	-1.522867	-0.571640	-9.377683
N	0.876636	-2.818233	-4.392199
O	1.881082	-3.250946	-4.960028
N	-8.541281	0.559277	-1.850831
O	-8.900287	1.149420	-2.872511
N	-4.901947	-1.481851	0.692189
O	-5.736190	-2.081269	1.369714
N	-0.241037	1.870500	-2.102163
S	0.515342	1.295844	-0.777205
O	-0.317166	0.069487	-0.343260
C	2.056706	0.630672	-1.374938
C	2.111034	-0.694482	-1.816492
C	3.302985	-1.175605	-2.353763
C	4.396462	-0.315345	-2.418539
C	4.351598	1.004461	-1.968693
C	3.159033	1.489226	-1.442645
N	5.663542	-0.819251	-2.988106
O	0.739817	2.297257	0.269127
N	-2.907879	1.654026	-0.823091
C	-3.716138	2.396948	-1.600531
C	-4.772774	3.122764	-1.058596
C	-4.981527	3.077117	0.320186
C	-4.125645	2.317517	1.117693
C	-3.096030	1.610403	0.504887
C	-3.356411	2.433403	-3.067696
O	-0.207112	-2.309452	-9.233269
O	0.551590	-3.095713	-3.238626
O	-9.261652	0.333185	-0.879033
O	-3.728814	-1.303419	1.018017
H	-3.589159	-0.708363	-4.295756
H	-4.572753	0.681739	-4.790610
H	-6.701866	0.869535	-3.740583
H	-7.362312	-0.715694	0.189548
H	-2.506334	1.878532	-5.514418
H	-1.158067	1.943246	-4.357058
H	-2.004668	0.547169	-7.340501
H	0.579035	-2.854271	-7.008618
H	-4.199504	2.803739	-3.666225
H	-2.522824	3.133240	-3.186915
H	-5.426151	3.697842	-1.706583
H	-5.806968	3.625176	0.764375
H	-4.256568	2.257482	2.192338
H	-2.412014	0.981971	1.062257
H	3.082662	2.507504	-1.077439
H	5.237395	1.622781	-2.038610
H	3.380218	-2.190287	-2.725639
H	1.243029	-1.336184	-1.757035
O	5.690469	-1.989359	-3.356938
O	6.604931	-0.030859	-3.053417

(L^{NO2}, NNs) red

C	-3.994751	0.059658	-0.512735

C	-3.324596	-0.524564	-1.635026
C	-3.075456	0.357320	-2.746460
C	-3.492932	1.671537	-2.725857
C	-4.167897	2.181252	-1.607276
C	-4.427795	1.376887	-0.504728
O	-2.953672	-1.756153	-1.680268
Fe	-1.058424	-2.276801	-1.963533
O	-0.965592	-3.477786	-3.563372
C	-1.283830	-3.348168	-4.797293
C	-0.938524	-2.160177	-5.533045
C	-1.226712	-2.038213	-6.876473
C	-1.853145	-3.088532	-7.564132
C	-2.205634	-4.259913	-6.903826
C	-1.950516	-4.374727	-5.546540
C	-0.209775	-1.070847	-4.801324
N	-0.920795	-0.575598	-3.589358
C	-2.325015	-0.199406	-3.922516
N	-2.145305	-2.945922	-8.974322
O	-1.828638	-1.884097	-9.525889
N	-2.405515	-5.602600	-4.895281
O	-2.486218	-6.616648	-5.600473
N	-4.568389	3.572694	-1.586931
O	-4.295742	4.266550	-2.574632
N	-4.209387	-0.703982	0.714974
O	-5.178705	-0.388454	1.414196
N	-0.230320	-3.329743	-0.727014
S	1.283685	-3.465869	-0.295506
O	1.738962	-4.866107	-0.211655
C	2.177580	-2.758942	-1.709152
C	2.254746	-3.484633	-2.905524
C	2.868523	-2.921588	-4.018493
C	3.386852	-1.626530	-3.917539
C	3.318346	-0.890962	-2.732400
C	2.710345	-1.468450	-1.621337
N	4.001584	-1.012537	-5.094632
O	1.617616	-2.569111	0.840874
N	-0.449261	-0.437256	-0.876605
C	-0.392250	0.721318	-1.551826
C	-0.475357	1.952013	-0.907080
C	-0.626874	1.967786	0.479793
C	-0.671120	0.760593	1.175529
C	-0.577766	-0.430872	0.460032
C	-0.178671	0.574692	-3.037242
O	-2.696475	-3.887161	-9.554943
O	-2.709634	-5.554004	-3.708041
O	-5.152144	3.997964	-0.584644
O	-3.400620	-1.582582	1.002640
H	-2.817401	-1.103687	-4.287311
H	-2.317994	0.536267	-4.742008
H	-3.294164	2.332869	-3.561558
H	-4.941715	1.773883	0.360062
H	-0.028174	-0.231934	-5.491303
H	0.761237	-1.438351	-4.456823
H	-0.968658	-1.138680	-7.423824
H	-2.685584	-5.070386	-7.435200
H	-0.434282	1.505174	-3.565239
H	0.887677	0.384166	-3.204054
H	-0.450138	2.871680	-1.483148
H	-0.716252	2.913303	1.007417
H	-0.788899	0.731862	2.253215
H	-0.602566	-1.403560	0.932968
H	2.642206	-0.943374	-0.675383
H	3.743718	0.104753	-2.699699
H	2.942171	-3.453666	-4.958855
H	1.825554	-4.479240	-2.951111
O	4.074780	-1.684686	-6.125187
O	4.405377	0.149828	-4.994390

^{5}5’ (gas phase)

N	6.161146	-0.238273	-1.148380
Fe	5.765207	1.572000	-0.709703
O	7.351106	2.622173	-0.735972
O	5.487491	1.384028	1.177347
N	4.502205	3.430853	-0.673830
N	5.518219	2.095593	-2.862603
C	5.371961	4.617930	-0.387344
H	5.722616	4.486362	0.640626
H	4.744723	5.522174	-0.405189
C	6.562997	4.802773	-1.294056
C	6.764915	6.013951	-1.958339
H	6.021019	6.802727	-1.894650
C	7.931804	6.221537	-2.691301
C	8.912095	5.233479	-2.771280
H	9.819586	5.396842	-3.341175
C	8.708004	4.023417	-2.113253
C	7.537858	3.770262	-1.358579
C	3.471598	3.269561	0.407809
H	2.761715	4.108729	0.352454
H	2.928397	2.349666	0.165114
C	4.033949	3.183421	1.804195
C	3.542446	4.022540	2.807694
H	2.800850	4.778928	2.568131
C	3.990600	3.884080	4.118431
C	4.934141	2.911709	4.449074
H	5.285168	2.802884	5.468831
C	5.428152	2.081385	3.448436
C	5.003633	2.188821	2.099605
C	3.809320	3.549801	-1.979968
H	3.445773	4.575715	-2.136725
H	2.934372	2.890241	-1.942710
C	4.667859	3.096821	-3.137264
C	4.536668	3.611346	-4.427061
H	3.847464	4.427927	-4.620374
C	5.308830	3.061959	-5.449896
H	5.227778	3.446619	-6.462683
C	6.188717	2.019931	-5.155131
H	6.807801	1.567125	-5.922300
C	6.267003	1.566537	-3.841445
H	6.931230	0.761815	-3.543476
Cl	8.173513	7.749430	-3.529622
Cl	9.925845	2.772890	-2.227613
Cl	3.362931	4.945151	5.373008
Cl	6.608520	0.857396	3.864523
S	4.690920	-0.844483	-1.431559

O	4.482764	-1.442593	-2.755898
O	3.879449	0.411291	-1.100734
C	4.290859	-2.088445	-0.209499
C	4.599336	-1.847684	1.133873
C	4.270477	-2.821047	2.076603
C	3.647996	-4.008350	1.677827
C	3.351328	-4.233215	0.331213
C	3.673752	-3.270269	-0.626322
H	3.397793	-4.762726	2.419268
H	5.089561	-0.924664	1.428863
H	4.506111	-2.651483	3.123422
H	2.872258	-5.158570	0.023496
H	3.461983	-3.425090	-1.678704

^{3}5’ (gas phase)

N	5.078583	-0.338563	1.178785
Fe	4.694772	1.257833	0.323123
O	6.478403	1.696063	-0.002351
O	4.592697	2.237124	1.905358
N	3.942872	2.877443	-0.833981
N	4.623870	0.345701	-1.494232
C	5.030864	3.799283	-1.286955
H	5.357844	4.333955	-0.390424
H	4.602826	4.543888	-1.974395
C	6.221234	3.128360	-1.917450
C	6.710421	3.573357	-3.147397
H	6.179503	4.343539	-3.699695
C	7.895121	3.047469	-3.656777
C	8.606501	2.077647	-2.951633
H	9.529748	1.669542	-3.346729
C	8.109714	1.626543	-1.731655
C	6.909525	2.134357	-1.173719
C	2.949286	3.621565	0.014862
H	2.420782	4.357536	-0.608627
H	2.226095	2.871099	0.353586
C	3.588913	4.305368	1.191525
C	3.361399	5.662363	1.434206
H	2.744463	6.242442	0.754137
C	3.917242	6.269426	2.555998
C	4.715298	5.540657	3.438389
H	5.153821	6.014669	4.309018
C	4.954767	4.193603	3.186864
C	4.392638	3.528078	2.064930
C	3.235210	2.246875	-1.978018
H	3.083538	2.965913	-2.794738
H	2.246165	1.939532	-1.617987
C	3.965800	1.019308	-2.457632
C	3.937212	0.559315	-3.772455
H	3.404280	1.122473	-4.532261
C	4.616590	-0.616913	-4.089551
H	4.615622	-0.990047	-5.109762
C	5.308854	-1.295460	-3.086445
H	5.861724	-2.205018	-3.295105
C	5.294900	-0.779296	-1.794339
H	5.818265	-1.241844	-0.964508
Cl	8.502010	3.608537	-5.210078
Cl	8.991577	0.390953	-0.862603
Cl	3.621057	7.976502	2.862161
Cl	5.955551	3.287993	4.292736
S	3.528523	-0.623728	1.569049
O	2.849510	0.490324	0.723149
O	3.190232	-0.702021	2.990803
C	2.999593	-2.173467	0.826012
C	3.355634	-3.361365	1.474149
C	2.968634	-4.579128	0.916586
C	2.226346	-4.605584	-0.268494
C	1.868245	-3.412430	-0.900107
C	2.258193	-2.186224	-0.357063
H	3.913064	-3.327969	2.404943
H	3.239207	-5.507421	1.411988
H	1.279284	-3.434189	-1.813225
H	1.978665	-1.249298	-0.825194
H	1.921318	-5.557469	-0.695036

^{5}5’ (solvent)

N	6.125419	-0.157391	-1.137217
Fe	5.656036	1.609255	-0.745055
O	7.309242	2.576526	-0.693520
O	5.412752	1.376980	1.150829
N	4.475112	3.454440	-0.678655
N	5.455682	2.124163	-2.856119
C	5.373233	4.627010	-0.395648
H	5.712610	4.503263	0.636807
H	4.766939	5.540813	-0.435503
C	6.580903	4.770382	-1.289090
C	6.822805	5.969722	-1.960118
H	6.093531	6.772644	-1.918589
C	8.010765	6.139680	-2.670132
C	8.973661	5.133770	-2.724280
H	9.895935	5.271123	-3.277174
C	8.722536	3.937135	-2.057842
C	7.532957	3.716325	-1.327821
C	3.439920	3.330642	0.406636
H	2.767930	4.196711	0.354136
H	2.855438	2.437212	0.163586
C	4.009279	3.216050	1.797668
C	3.547591	4.060405	2.810220
H	2.821872	4.833718	2.578499
C	4.010095	3.902316	4.114388
C	4.938598	2.913088	4.434321
H	5.300609	2.791869	5.448967
C	5.400119	2.081589	3.418873
C	4.959240	2.199023	2.077323
C	3.767755	3.608350	-1.982484
H	3.447878	4.647474	-2.124465
H	2.863333	2.991519	-1.940803
C	4.606373	3.128865	-3.137887
C	4.470770	3.628723	-4.432571
H	3.781109	4.442974	-4.630105
C	5.236478	3.066087	-5.453150
H	5.149799	3.438356	-6.469547
C	6.118747	2.025988	-5.151171
H	6.734285	1.565059	-5.916083

C	6.202198	1.584260	-3.835290
H	6.867903	0.781140	-3.538139
Cl	8.306805	7.658487	-3.516615
Cl	9.922194	2.656243	-2.123639
Cl	3.417289	4.971561	5.386394
Cl	6.569370	0.831091	3.814756
S	4.672444	-0.809880	-1.422770
O	4.518973	-1.420599	-2.755139
O	3.780508	0.394800	-1.130116
C	4.320767	-2.079998	-0.214082
C	4.539512	-1.807425	1.142066
C	4.247598	-2.799572	2.077721
C	3.748186	-4.038760	1.659572
C	3.538589	-4.294613	0.301534
C	3.825816	-3.312726	-0.649330
H	3.525243	-4.806961	2.394859
H	4.933213	-0.843265	1.450152
H	4.412017	-2.607640	3.134193
H	3.153478	-5.257446	-0.021446
H	3.672373	-3.497625	-1.706701

Re S=1, Cβ

C	-0.736232	0.053943	-0.013486
N	3.018302	-0.167780	0.335743
Fe	3.633847	1.578605	0.063798
O	5.402851	0.971425	-0.388884
O	2.728924	2.300791	1.558682
N	4.164195	3.616214	-0.597386
N	2.942700	1.526749	-1.962707
C	5.661663	3.739505	-0.639536
H	6.007154	3.539770	0.380025
H	5.920111	4.780115	-0.886132
C	6.317931	2.800354	-1.610684
C	7.113787	3.273269	-2.655024
H	7.247282	4.341279	-2.802422
C	7.754772	2.369377	-3.499682
C	7.609198	0.994997	-3.314503
H	8.106620	0.292042	-3.973025
C	6.808587	0.530178	-2.274276
C	6.141693	1.410831	-1.386525
C	3.620467	4.628327	0.369273
H	3.989202	5.625673	0.087427
H	2.533693	4.616557	0.239678
C	3.928589	4.342869	1.811304
C	4.602917	5.262711	2.613769
H	5.028081	6.163697	2.181548
C	4.702924	5.029129	3.983931
C	4.106261	3.911227	4.563302
H	4.158416	3.749603	5.633800
C	3.433027	2.992548	3.757267
C	3.364888	3.162891	2.354677
C	3.564057	3.872324	-1.941821
H	4.217045	4.518964	-2.540539
H	2.624554	4.417292	-1.790875
C	3.226324	2.612864	-2.703563
C	3.114191	2.598023	-4.094744
H	3.365309	3.484182	-4.669696
C	2.679746	1.432675	-4.722471
H	2.587067	1.396472	-5.804410
C	2.374438	0.313965	-3.945103
H	2.036863	-0.613300	-4.396116
C	2.530969	0.397926	-2.566000
H	2.341262	-0.436997	-1.899359
Cl	8.755954	2.965077	-4.819249
Cl	6.615418	-1.196884	-2.059841
Cl	5.565668	6.175391	5.000654
Cl	2.618314	1.652977	4.510933
S	3.354860	-0.930914	1.799515
O	2.045973	-1.072851	2.463301
O	4.493780	-0.310196	2.490218
C	3.878138	-2.551213	1.236896
C	5.229163	-2.764724	0.949289
C	5.633834	-4.030984	0.525449
C	4.697194	-5.060621	0.395767
C	3.349319	-4.832421	0.690283
C	2.930042	-3.570626	1.111819
H	5.939390	-1.952821	1.060521
H	6.681100	-4.213804	0.301166
H	2.626489	-5.638564	0.597648
H	1.892907	-3.373820	1.362367
H	5.019173	-6.045943	0.068515
C	-0.947745	2.585874	-1.731576
C	-1.147371	3.808041	-2.371466
C	-0.898628	5.008854	-1.698191
C	-0.445953	4.971806	-0.376440
C	-0.241835	3.746360	0.261052
C	-0.497307	2.529241	-0.399061
C	-0.266088	1.263354	0.320808
H	-0.484531	-0.813705	0.588525
H	-1.385572	-0.113444	-0.870405
H	0.352340	1.346609	1.212999
H	-1.128341	1.662740	-2.275786
H	-1.496407	3.825114	-3.401340
H	-1.060034	5.961022	-2.197321
H	-0.260590	5.898013	0.162831
H	0.109722	3.719944	1.289158

TS1 S=1, Cβ

C	-0.268861	0.024757	0.458132
N	1.864071	-0.110855	-0.033679
Fe	2.733918	1.560086	0.003095
O	4.265710	1.076607	-1.120292
O	2.350581	1.860066	1.832045
N	3.341506	3.703889	-0.147683
N	1.752680	2.150001	-1.823658
C	4.794419	3.776550	-0.516608
H	5.330798	3.250868	0.280285
H	5.107630	4.831547	-0.492442
C	5.120339	3.180242	-1.855651
C	5.733836	3.951274	-2.844772
H	5.948648	5.000773	-2.663519
C	6.087193	3.370282	-4.059499

C	5.829741	2.021396	-4.300245
H	6.099854	1.566550	-5.246525
C	5.211362	1.260024	-3.312870
C	4.839185	1.799916	-2.052284
C	3.140879	4.407223	1.160751
H	3.522808	5.436131	1.078277
H	2.058506	4.458122	1.321047
C	3.760039	3.708617	2.335637
C	4.688168	4.338091	3.163992
H	5.077799	5.319509	2.910213
C	5.092129	3.706484	4.338508
C	4.550692	2.477466	4.710463
H	4.842073	2.004771	5.641342
C	3.622724	1.852072	3.877595
C	3.236941	2.429383	2.644128
C	2.478828	4.361639	-1.170278
H	2.990418	5.221163	-1.623368
H	1.594256	4.746654	-0.648677
C	1.991738	3.409533	-2.234412
C	1.724030	3.815472	-3.543069
H	1.937860	4.834744	-3.849831
C	1.199190	2.889489	-4.441712
H	0.986920	3.181238	-5.466477
C	0.972965	1.579595	-4.014176
H	0.587333	0.822691	-4.689109
C	1.279136	1.246243	-2.699188
H	1.175974	0.238696	-2.307881
Cl	6.858370	4.344783	-5.307578
Cl	4.869707	-0.425832	-3.654179
Cl	6.275164	4.483712	5.382892
Cl	2.886788	0.366719	4.412058
S	2.571530	-1.255493	1.000219
O	1.615609	-1.723715	2.020511
O	3.895482	-0.740000	1.393582
C	2.846333	-2.642143	-0.115149
C	3.928294	-2.597552	-0.997810
C	4.156838	-3.688641	-1.836805
C	3.315135	-4.804156	-1.787332
C	2.240803	-4.836822	-0.894118
C	2.000204	-3.751717	-0.049563
H	4.571108	-1.724649	-1.022452
H	4.996966	-3.668445	-2.525757
H	1.595478	-5.710187	-0.847116
H	1.188756	-3.765932	0.670494
H	3.501157	-5.652631	-2.441048
C	-1.111174	2.969582	0.353761
C	-1.402949	4.331089	0.392111
C	-1.320407	5.039836	1.597026
C	-0.947402	4.368778	2.766651
C	-0.653630	3.008598	2.728721
C	-0.721248	2.277214	1.522193
C	-0.398324	0.859530	1.544504
H	-0.242184	-1.043342	0.621578
H	-0.534149	0.349317	-0.542175
H	-0.180956	0.433291	2.519960
H	-1.198652	2.435326	-0.587481
H	-1.712820	4.840800	-0.517294
H	-1.556546	6.100422	1.625100
H	-0.885708	4.908401	3.708179
H	-0.349032	2.493089	3.635651

Int S=1, Cβ

C	0.115087	0.833710	0.397473
N	1.459724	0.572340	-0.124387
Fe	3.247868	1.525902	-0.321703
O	5.054800	1.844768	-0.772459
O	3.537561	1.512592	1.518407
N	2.729073	3.492140	-0.403739
N	2.886564	1.617271	-2.312504
C	3.916859	4.407256	-0.562513
H	4.435543	4.368709	0.399373
H	3.539214	5.431080	-0.694348
C	4.882895	4.057972	-1.655949
C	5.304970	5.018360	-2.577314
H	4.857067	6.008103	-2.582328
C	6.323573	4.712909	-3.476471
C	6.931997	3.457596	-3.465564
H	7.727064	3.221334	-4.163628
C	6.497286	2.499842	-2.553575
C	5.462228	2.763504	-1.620924
C	2.015712	3.874667	0.865795
H	1.642172	4.903620	0.763839
H	1.151817	3.210027	0.953746
C	2.882658	3.761476	2.091488
C	2.940544	4.820295	3.002820
H	2.402755	5.742193	2.801251
C	3.676597	4.690556	4.175466
C	4.371360	3.512465	4.451285
H	4.950581	3.410810	5.361917
C	4.324438	2.464590	3.538124
C	3.579216	2.546284	2.330570
C	1.792342	3.615867	-1.558165
H	1.707270	4.661674	-1.881649
H	0.802509	3.297718	-1.212639
C	2.225968	2.724993	-2.694837
C	1.957723	2.986738	-4.037096
H	1.427446	3.890876	-4.319941
C	2.402944	2.081064	-4.999257
H	2.211261	2.263803	-6.052681
C	3.123864	0.957058	-4.593880
H	3.517588	0.247870	-5.314180
C	3.356241	0.765704	-3.235411
H	3.950428	-0.055241	-2.852713
Cl	6.851009	5.921760	-4.643542
Cl	7.243279	0.914641	-2.563967
Cl	3.740377	6.025859	5.321211
Cl	5.198349	0.994163	3.890997
S	2.140746	-0.859975	0.207250
O	1.956250	-1.378399	1.567383
O	3.536972	-0.539906	-0.303290

C	1.460005	-2.137878	-0.867082
C	2.069498	-2.455296	-2.082448
C	1.503548	-3.439443	-2.894587
C	0.334247	-4.092296	-2.497008
C	-0.260912	-3.778842	-1.272209
C	0.305792	-2.808667	-0.444905
H	2.991706	-1.963524	-2.365087
H	1.982709	-3.703532	-3.833599
H	-1.157722	-4.301426	-0.950861
H	-0.119303	-2.594819	0.530155
H	-0.103978	-4.856475	-3.133419
C	-2.295704	2.073656	1.796769
C	-3.373493	2.648381	2.457839
C	-3.302727	2.930535	3.828664
C	-2.130190	2.624147	4.536157
C	-1.048444	2.049500	3.887467
C	-1.090316	1.755902	2.491254
C	0.039227	1.178591	1.860602
H	-0.531294	-0.035512	0.174120
H	-0.314535	1.641879	-0.213681
H	0.903019	0.919730	2.464178
H	-2.380118	1.854103	0.735668
H	-4.281662	2.877634	1.905140
H	-4.149763	3.380011	4.339639
H	-2.067665	2.837761	5.600295
H	-0.141830	1.815147	4.439897

TS2 S=1, Cβ

N	0.605173	0.400106	0.300530
C	2.405667	-0.857764	0.265100
C	2.058304	0.548648	0.556568
Fe	-1.781197	-0.195613	-1.000564
O	-3.750549	-0.601039	-1.109830
O	-0.976910	-1.912919	-0.925722
N	-1.600459	-0.058030	-3.054958
N	-2.210537	1.774357	-1.157981
C	-2.832682	-0.568013	-3.756185
H	-2.886427	-1.631902	-3.509863
H	-2.674837	-0.478625	-4.841640
C	-4.109666	0.110671	-3.353676
C	-4.914557	0.751529	-4.296220
H	-4.596682	0.818700	-5.333315
C	-6.138976	1.291738	-3.910207
C	-6.574229	1.199544	-2.586356
H	-7.528707	1.618873	-2.288293
C	-5.765211	0.569390	-1.648039
C	-4.505966	-0.009360	-1.985663
C	-0.407948	-0.857485	-3.494670
H	-0.226284	-0.674483	-4.564566
H	0.445273	-0.458186	-2.931130
C	-0.535026	-2.333274	-3.240172
C	-0.312286	-3.253114	-4.266877
H	-0.121378	-2.906853	-5.278802
C	-0.321800	-4.617121	-3.991248
C	-0.553251	-5.079879	-2.694580
H	-0.562868	-6.142586	-2.479829
C	-0.782608	-4.161851	-1.675928
C	-0.788176	-2.756879	-1.903838
C	-1.357100	1.379215	-3.364321
H	-1.616454	1.609715	-4.406531
H	-0.280971	1.558770	-3.246248
C	-2.092465	2.277945	-2.404111
C	-2.567686	3.546051	-2.730916
H	-2.466357	3.918746	-3.745475
C	-3.193357	4.304903	-1.742159
H	-3.581678	5.292564	-1.974191
C	-3.333223	3.769004	-0.461204
H	-3.833966	4.317270	0.329778
C	-2.835860	2.494005	-0.209133
H	-2.934678	2.009158	0.755203
Cl	-7.152584	2.105859	-5.102171
Cl	-6.309496	0.472752	0.016318
Cl	-0.033195	-5.775572	-5.288938
Cl	-1.048982	-4.748501	-0.048638
S	-0.285828	0.022078	1.604092
O	0.204411	-1.089962	2.437072
O	-1.688143	-0.086045	1.051610
C	-0.307562	1.461058	2.704443
C	-0.251608	2.755215	2.178282
C	-0.287024	3.847219	3.046989
C	-0.381836	3.643392	4.426609
C	-0.433693	2.345862	4.941897
C	-0.391178	1.246432	4.082376
H	-0.169388	2.899951	1.105656
H	-0.237029	4.856585	2.646919
H	-0.502233	2.187082	6.014686
H	-0.414331	0.231275	4.464054
H	-0.409453	4.496163	5.099839
C	3.319920	-0.576026	-2.044345
C	3.803626	-1.155018	-3.208736
C	3.856869	-2.550805	-3.335912
C	3.423424	-3.370288	-2.285068
C	2.938238	-2.800998	-1.117538
C	2.876776	-1.387575	-0.962822
H	2.316747	0.856327	1.578254
H	2.473729	1.281482	-0.139753
H	2.122975	-1.563084	1.041519
H	3.287907	0.505589	-1.955669
H	4.144113	-0.524186	-4.025588
H	4.232108	-2.997411	-4.252559
H	3.454012	-4.450687	-2.389700
H	2.582062	-3.430775	-0.306993

Prod S=1, Cβ

N	1.814313	0.105200	0.186906
C	2.666592	-0.151665	1.353638
C	2.618149	1.207621	0.708716
Fe	-1.723884	0.461628	-2.245543
O	-2.997757	0.440566	-0.798351
O	-0.375720	-0.591213	-3.142543
N	-3.173452	0.132080	-3.641770
N	-1.753400	2.413520	-3.202571
C	-4.147226	-0.883956	-3.125166
H	-3.548718	-1.773628	-2.900061

H	-4.842163	-1.158932	-3.933034
C	-4.940257	-0.435298	-1.921422
C	-6.317156	-0.678421	-1.894987
H	-6.801180	-1.139852	-2.751329
C	-7.072192	-0.346196	-0.774991
C	-6.468206	0.247071	0.332783
H	-7.051015	0.515474	1.206598
C	-5.102691	0.502159	0.298098
C	-4.277068	0.174784	-0.814684
C	-2.559844	-0.349355	-4.926917
H	-3.362355	-0.484423	-5.667692
H	-1.919117	0.469616	-5.274686
C	-1.750895	-1.610503	-4.813712
C	-2.028461	-2.706057	-5.634555
H	-2.886647	-2.686396	-6.300807
C	-1.192828	-3.818484	-5.615038
C	-0.072386	-3.848656	-4.784548
H	0.583012	-4.712192	-4.770296
C	0.194144	-2.758405	-3.963294
C	-0.634696	-1.603554	-3.929153
C	-3.843108	1.436656	-3.901361
H	-4.517749	1.636416	-3.061877
H	-4.461557	1.386838	-4.809525
C	-2.832041	2.555991	-3.995843
C	-3.005851	3.680713	-4.803343
H	-3.882570	3.765977	-5.438676
C	-2.034599	4.682289	-4.779725
H	-2.146043	5.567356	-5.400075
C	-0.916538	4.527001	-3.959024
H	-0.135707	5.279871	-3.919914
C	-0.815758	3.371255	-3.187684
H	0.032582	3.187722	-2.534478
Cl	-8.807020	-0.663314	-0.756662
Cl	-4.358021	1.270061	1.693011
Cl	-1.545405	-5.201503	-6.652535
Cl	1.609462	-2.812373	-2.926414
S	0.119478	0.067776	0.257435
O	-0.276902	-1.331844	0.259051
O	-0.279707	0.994574	-0.840618
C	-0.405735	0.827863	1.793192
C	-0.611105	2.209534	1.854736
C	-0.999433	2.778513	3.067958
C	-1.181665	1.972307	4.195040
C	-0.984675	0.591047	4.115515
C	-0.594141	0.007238	2.910034
H	-0.504299	2.813643	0.960452
H	-1.175323	3.848738	3.128150
H	-1.148304	-0.035254	4.987743
H	-0.470454	-1.067058	2.820058
H	-1.491526	2.420472	5.135137
C	4.539620	-1.485989	2.320622
C	5.630443	-2.347344	2.197502
C	5.991971	-2.841123	0.941999
C	5.255787	-2.471885	-0.186661
C	4.166397	-1.608023	-0.067028
C	3.804964	-1.106130	1.189773
H	2.120475	2.002222	1.263426
H	3.417029	1.524095	0.042395
H	2.166465	-0.193647	2.322236
H	4.257123	-1.106476	3.300810
H	6.192665	-2.636324	3.081746
H	6.837926	-3.516629	0.845063
H	5.523419	-2.864057	-1.164253
H	3.577295	-1.336427	-0.938052

Re S=2, Cα

C	-0.675128	0.042932	2.030299
N	4.207755	0.180889	-0.800005
C	-0.809916	0.820544	3.116214
Fe	4.506274	-0.925216	0.787482
O	6.268894	-0.928738	1.481644
O	4.199546	-2.655310	0.116609
N	3.602144	-1.667936	2.733885
N	4.076284	0.925564	1.952803
C	4.750374	-2.231151	3.521231
H	5.134324	-3.070696	2.934406
H	4.357086	-2.642900	4.462840
C	5.872464	-1.266572	3.818427
C	6.246396	-1.010840	5.140251
H	5.687273	-1.452934	5.959630
C	7.348802	-0.204207	5.412856
C	8.096674	0.356947	4.378691
H	8.954771	0.984394	4.590778
C	7.722395	0.106717	3.061444
C	6.609632	-0.706574	2.739228
C	2.588899	-2.742857	2.440804
H	2.085210	-3.018726	3.378761
H	1.839237	-2.280114	1.788024
C	3.146356	-3.981571	1.790187
C	2.849845	-5.246011	2.303658
H	2.262128	-5.343078	3.211484
C	3.298851	-6.386663	1.642544
C	4.050436	-6.287390	0.471637
H	4.403052	-7.176654	-0.038018
C	4.352142	-5.027067	-0.036082
C	3.909504	-3.844118	0.603914
C	2.924688	-0.569787	3.463818
H	2.924391	-0.763820	4.545496
H	1.875537	-0.543013	3.143382
C	3.521130	0.784455	3.166375
C	3.430803	1.855308	4.058255
H	2.982086	1.709623	5.036195
C	3.931656	3.096332	3.672574
H	3.878105	3.943042	4.351233
C	4.511156	3.234423	2.409366
H	4.919801	4.181827	2.074002
C	4.568858	2.120710	1.579115
H	5.010025	2.158054	0.588529
Cl	7.804513	0.114190	7.081881
Cl	8.644873	0.827234	1.761077
Cl	2.919220	-7.976045	2.293497
Cl	5.302087	-4.895849	-1.494851
S	2.767917	0.083445	-1.553460

O	1.727193	0.045514	-0.490801
O	2.818958	-0.986337	-2.560810
C	2.548858	1.634371	-2.433168
C	3.029549	1.741309	-3.740673
C	2.888349	2.953298	-4.417517
C	2.271448	4.040072	-3.791689
C	1.788024	3.917855	-2.486208
C	1.924903	2.711041	-1.798569
H	2.160928	4.980922	-4.324470
H	3.491225	0.882626	-4.216892
H	3.255105	3.046279	-5.436089
H	1.296702	4.759708	-2.005500
H	1.539196	2.593405	-0.791305
C	-2.112389	-1.927755	2.726524
C	-2.593357	-3.211918	2.485097
C	-2.204976	-3.907773	1.334536
C	-1.335256	-3.304105	0.425072
C	-0.854952	-2.015119	0.663997
C	-1.229373	-1.307462	1.822118
H	-0.361948	1.809938	3.151016
H	-1.376311	0.519273	3.994312
H	-0.084277	0.417682	1.194945
H	-2.433588	-1.398315	3.619763
H	-3.277476	-3.672612	3.193615
H	-2.582203	-4.910200	1.149520
H	-1.029513	-3.833257	-0.473654
H	-0.178784	-1.545257	-0.046397

TS1 S=2, Cα

C	-0.073611	-0.005244	0.023488
N	2.037767	0.112879	0.023499
C	-0.288776	1.356955	-0.063025
Fe	3.353743	-1.213851	0.778970
O	5.223146	-0.830773	1.020790
O	2.619473	-2.799258	0.021931
N	3.653453	-2.753685	2.705134
N	3.047172	-0.022365	2.700548
C	5.112621	-3.049060	2.785549
H	5.387048	-3.506340	1.829459
H	5.284095	-3.804323	3.570506
C	5.985934	-1.851126	3.043664
C	6.817730	-1.812137	4.164419
H	6.799169	-2.625488	4.884143
C	7.685731	-0.739834	4.354252
C	7.742989	0.299575	3.428070
H	8.423010	1.131926	3.568529
C	6.911105	0.257527	2.312606
C	6.002609	-0.806104	2.080712
C	2.898680	-4.025295	2.490340
H	3.051918	-4.692180	3.355053
H	1.838738	-3.749718	2.460540
C	3.254947	-4.747198	1.220270
C	3.686901	-6.073813	1.225131
H	3.839559	-6.597538	2.164263
C	3.911242	-6.728961	0.015863
C	3.705183	-6.078688	-1.200190
H	3.876939	-6.592792	-2.138921
C	3.277595	-4.752136	-1.200897
C	3.049792	-4.048926	0.006060
C	3.156437	-2.109539	3.935043
H	3.669996	-2.495684	4.828537
H	2.095327	-2.368644	4.039506
C	3.236440	-0.602254	3.897721
C	3.392410	0.151226	5.064356
H	3.554057	-0.351415	6.013286
C	3.347683	1.540184	4.985243
H	3.474526	2.145840	5.878402
C	3.145390	2.138058	3.740292
H	3.107702	3.216880	3.629037
C	3.005297	1.320279	2.623793
H	2.842541	1.719223	1.628730
Cl	8.723902	-0.694016	5.775355
Cl	7.004319	1.572836	1.155788
Cl	4.456662	-8.402803	0.020428
Cl	3.000719	-3.943523	-2.722393
S	2.576498	0.209872	-1.511825
O	1.612346	-0.179419	-2.553604
O	3.865947	-0.561118	-1.358576
C	3.067801	1.900151	-1.889696
C	4.191590	2.440561	-1.257703
C	4.549811	3.760772	-1.530531
C	3.794603	4.525805	-2.425249
C	2.681509	3.968959	-3.059207
C	2.312491	2.647963	-2.795043
H	4.081075	5.552928	-2.636073
H	4.786342	1.829147	-0.586612
H	5.425962	4.188721	-1.050650
H	2.104244	4.558009	-3.766970
H	1.467471	2.187400	-3.296263
C	-0.537430	-0.271229	2.503113
C	-0.891638	-1.076115	3.584722
C	-1.099160	-2.448267	3.403829
C	-0.935892	-3.009402	2.134422
C	-0.573056	-2.203335	1.054346
C	-0.381904	-0.820850	1.218628
H	-0.203980	1.865552	-1.017028
H	-0.471382	1.975615	0.810049
H	-0.042552	-0.559388	-0.908826
H	-0.378640	0.791487	2.661161
H	-1.016334	-0.631645	4.569063
H	-1.391608	-3.072133	4.244765
H	-1.096713	-4.073609	1.982063
H	-0.430895	-2.643728	0.071639

Int S=2, Cα

C	0.497110	0.103724	0.051582
N	1.969550	0.002181	-0.076890
C	0.056257	1.509530	0.322382
Fe	3.491089	-1.131228	0.780133
O	5.356632	-0.747118	1.027048
O	3.067018	-2.811349	0.020107
N	3.670495	-2.466763	2.799588
N	3.202850	0.260978	2.568721
C	5.120494	-2.770647	2.997548
H	5.436024	-3.335440	2.114775
H	5.225255	-3.438943	3.867598
C	6.012908	-1.571173	3.170858
C	6.806869	-1.436987	4.311753
H	6.738403	-2.167493	5.112592
C	7.702185	-0.375421	4.418544
C	7.824602	0.559863	3.391974
H	8.524955	1.383322	3.472049
C	7.030545	0.424477	2.256908
C	6.100761	-0.635006	2.105507
C	2.909464	-3.748347	2.650352
H	2.960077	-4.307758	3.598317
H	1.864347	-3.466234	2.482891
C	3.382683	-4.625241	1.523614
C	3.721028	-5.962372	1.738267
H	3.704634	-6.377502	2.741728
C	4.071714	-6.768656	0.657607
C	4.092296	-6.258410	-0.640198
H	4.367125	-6.887868	-1.478781
C	3.760911	-4.922154	-0.851431
C	3.400608	-4.070442	0.221125
C	3.106833	-1.723465	3.944920
H	3.528064	-2.079349	4.897112
H	2.028853	-1.927576	3.970697
C	3.276609	-0.230140	3.816141
C	3.408937	0.603986	4.929420
H	3.471690	0.172763	5.923967
C	3.471881	1.981393	4.737851

H	3.582450	2.649520	5.587417
C	3.402863	2.487002	3.438195
H	3.458727	3.552356	3.240176
C	3.273114	1.590273	2.382981
H	3.220985	1.926191	1.353102
Cl	8.692410	-0.208854	5.864269
Cl	7.190235	1.607358	0.972523
Cl	4.495752	-8.454689	0.931040
Cl	3.781423	-4.280124	-2.473798
S	2.615363	0.221557	-1.557918
O	1.764191	-0.242580	-2.662362
O	3.969616	-0.385417	-1.323564
C	2.923406	1.972226	-1.847396
C	4.091285	2.552595	-1.342849
C	4.307385	3.917755	-1.541152
C	3.368497	4.685577	-2.235992
C	2.210963	4.089646	-2.744293
C	1.982676	2.725888	-2.553817
H	3.544539	5.746810	-2.391732
H	4.824687	1.936564	-0.831748
H	5.216825	4.377296	-1.163146
H	1.488862	4.684027	-3.297704
H	1.101549	2.242588	-2.962497
C	-0.338142	-0.559630	2.389757
C	-0.846132	-1.505653	3.286032
C	-1.047439	-2.825277	2.873330
C	-0.727623	-3.194815	1.562473
C	-0.212780	-2.249944	0.673143
C	-0.018428	-0.919540	1.074562
H	-0.952856	1.825239	0.073505
H	0.704981	2.206159	0.841630
H	0.056391	-0.204060	-0.909513
H	-0.208939	0.472354	2.705223
H	-1.104199	-1.205717	4.299215
H	-1.459255	-3.557902	3.563013
H	-0.885709	-4.217633	1.229744
H	0.042439	-2.541688	-0.342230

TS2 S=2, Cα

N	0.005326	0.038106	-0.042554
C	2.088378	0.043313	-0.019249
C	1.066697	1.099785	-0.011627
Fe	-1.583488	-0.255563	1.276000
O	-2.653591	-1.884610	1.298327
O	-2.474420	1.398108	0.878057
N	-2.165701	0.221258	3.501026
N	-0.133132	-1.452230	2.604277
C	-3.418957	-0.560235	3.742741
H	-4.153411	-0.181922	3.024715
H	-3.795199	-0.316904	4.749395
C	-3.301711	-2.057060	3.605047
C	-3.626066	-2.871739	4.693410
H	-3.886358	-2.421748	5.647389
C	-3.639318	-4.256761	4.558801
C	-3.344179	-4.850631	3.333257
H	-3.364570	-5.928392	3.218507
C	-3.021823	-4.038074	2.251314
C	-2.975033	-2.620667	2.335965
C	-2.439013	1.680421	3.693878
H	-2.672081	1.864990	4.755397
H	-1.501643	2.199705	3.464739
C	-3.545252	2.238213	2.838398
C	-4.586473	2.969569	3.415034
H	-4.642933	3.080016	4.494197
C	-5.546857	3.568856	2.604915
C	-5.484363	3.448279	1.217032
H	-6.231414	3.915634	0.585638
C	-4.450179	2.712222	0.645596
C	-3.453249	2.078770	1.431384
C	-1.085215	-0.175345	4.424512
H	-1.472801	-0.361091	5.438125
H	-0.389903	0.670987	4.494955
C	-0.301407	-1.369169	3.934344
C	0.278494	-2.289560	4.811785
H	0.110651	-2.197135	5.880636
C	1.048367	-3.326282	4.292034
H	1.502259	-4.058862	4.953587
C	1.211144	-3.418075	2.908308
H	1.789347	-4.218138	2.457565
C	0.596265	-2.464183	2.103768
H	0.676438	-2.500575	1.022403
Cl	-4.038639	-5.270802	5.943592
Cl	-2.663987	-4.809261	0.712867
Cl	-6.855632	4.493578	3.337907
Cl	-4.366790	2.571109	-1.095799
S	-0.618720	-0.315585	-1.595734
O	-0.274596	0.743621	-2.554267
O	-2.014088	-0.658697	-1.271163
C	0.165497	-1.831229	-2.160783
C	-0.278956	-3.048378	-1.636411
C	0.322222	-4.227754	-2.079848
C	1.338754	-4.183353	-3.038783
C	1.756393	-2.958817	-3.567726
C	1.167977	-1.770076	-3.131488
H	1.797314	-5.106003	-3.384679
H	-1.092464	-3.071133	-0.917297
H	-0.016363	-5.181182	-1.683823
H	2.532325	-2.928193	-4.327768
H	1.457576	-0.810928	-3.548915
C	1.766932	1.921501	2.304970
C	1.698219	2.867362	3.332974
C	0.843326	3.965531	3.218138
C	0.053490	4.111627	2.072922
C	0.120155	3.164853	1.051096
C	0.979200	2.059737	1.155381
H	2.454447	-0.346805	-0.961120
H	2.327174	-0.503078	0.884075
H	1.043318	1.665426	-0.946112
H	2.459683	1.090154	2.394282
H	2.327660	2.754375	4.212302
H	0.798306	4.707854	4.010961
H	-0.612315	4.964524	1.973513
H	-0.503219	3.272386	0.168327

Prod S=2, Cα

C	0.022421	0.879336	-0.612525
N	1.339532	0.289765	-0.145334
C	1.047473	1.735477	0.021169
Fe	1.201220	-1.876246	1.114963
O	2.965431	-2.539365	1.684037
O	-0.017838	-2.260410	-0.361474
N	0.109523	-3.424133	2.385071
N	1.099844	-0.876353	3.095076
C	1.072582	-4.545473	2.580128
H	1.316542	-4.910710	1.576829
H	0.566068	-5.367868	3.112749
C	2.335751	-4.184004	3.322982
C	2.644549	-4.871905	4.500006
H	1.947564	-5.606828	4.892947
C	3.844777	-4.638880	5.163717
C	4.762860	-3.723596	4.654727
H	5.705994	-3.543442	5.157942
C	4.452622	-3.037639	3.485404
C	3.235329	-3.218686	2.772113
C	-1.108550	-3.903547	1.662284
H	-1.603231	-4.687820	2.258924
H	-1.785985	-3.042402	1.611708
C	-0.870546	-4.404631	0.262895
C	-1.248916	-5.698734	-0.101520
H	-1.614251	-6.391568	0.651401
C	-1.181351	-6.094684	-1.434281
C	-0.762424	-5.201260	-2.419187
H	-0.728720	-5.500354	-3.460675
C	-0.384475	-3.912985	-2.051557
C	-0.389081	-3.473980	-0.701449
C	-0.290026	-2.796105	3.661617
H	-0.361354	-3.534261	4.474118
H	-1.295301	-2.379450	3.520043
C	0.610238	-1.651901	4.081470
C	0.860171	-1.371385	5.428253
H	0.460970	-2.025177	6.197823
C	1.638339	-0.266307	5.759947
H	1.849906	-0.035435	6.800252
C	2.160296	0.524954	4.734212
H	2.789598	1.383611	4.944569
C	1.873971	0.173887	3.420029
H	2.284558	0.734882	2.585755
Cl	4.212273	-5.507151	6.653203
Cl	5.642728	-1.896935	2.868965
Cl	-1.652195	-7.732366	-1.888313
Cl	0.088661	-2.783509	-3.307101
S	2.504821	-0.055967	-1.438186
O	2.038271	0.565851	-2.684961
O	2.762817	-1.488272	-1.326515
C	3.947876	0.843255	-0.870026
C	4.668878	0.336763	0.215152
C	5.797258	1.037452	0.644390
C	6.195977	2.206168	-0.011215
C	5.471322	2.686462	-1.105479
C	4.335044	2.004661	-1.544047
H	7.080799	2.739494	0.326292
H	4.368568	-0.587832	0.700894
H	6.368878	0.659394	1.486587
H	5.792541	3.586711	-1.622006
H	3.765690	2.346713	-2.402067
C	-1.555501	0.751266	1.376137
C	-2.780276	0.368464	1.928835
C	-3.728302	-0.291725	1.143912
C	-3.444454	-0.567619	-0.196895
C	-2.219403	-0.191253	-0.744070
C	-1.258686	0.468530	0.036265
H	1.591073	2.429456	-0.615928
H	0.951453	2.053450	1.055419
H	-0.026682	0.958369	-1.695882
H	-0.838560	1.275782	2.000696
H	-2.998554	0.603282	2.967792
H	-4.685475	-0.580524	1.570658
H	-4.175626	-1.080488	-0.815787
H	-1.990654	-0.428701	-1.778903

Re S=2, Cβ

C	-0.546055	1.660342	-2.442817
N	4.654317	-0.539661	0.940324
Fe	5.021400	1.286624	0.312278
O	6.799683	1.691679	-0.205496
O	4.705059	2.309864	1.859772
N	4.140611	2.997995	-0.866303
N	4.677683	0.440977	-1.726236
C	5.286491	3.909908	-1.198960
H	5.651723	4.294786	-0.242126
H	4.893305	4.766636	-1.766248
C	6.431629	3.282715	-1.957397
C	6.832576	3.818250	-3.184024
H	6.275199	4.637951	-3.627596
C	7.958272	3.317438	-3.833775
C	8.703267	2.280389	-3.274482
H	9.579757	1.890643	-3.779232
C	8.301330	1.741870	-2.055361
C	7.164833	2.220397	-1.360648
C	3.125311	3.716845	-0.015865
H	2.623895	4.477532	-0.631672
H	2.378437	2.963494	0.257192
C	3.681575	4.363872	1.225230
C	3.397657	5.699726	1.517111
H	2.820011	6.300060	0.820869
C	3.844692	6.259799	2.711369
C	4.580254	5.505483	3.625362
H	4.931074	5.944845	4.552058
C	4.867843	4.175585	3.331773
C	4.428551	3.569016	2.130391
C	3.461347	2.499219	-2.086587
H	3.429861	3.280639	-2.858701
H	2.422227	2.265933	-1.823137
C	4.092741	1.240598	-2.631164
C	4.013740	0.883043	-3.978848
H	3.540981	1.552644	-4.690974
C	4.558432	-0.332698	-4.385722

H	4.514374	-0.629777	-5.429832
C	5.169733	-1.156733	-3.438238
H	5.613119	-2.107362	-3.715559
C	5.212925	-0.729810	-2.115474
H	5.675559	-1.320781	-1.331740
Cl	8.447188	3.998507	-5.380207
Cl	9.219468	0.423674	-1.361849
Cl	3.482262	7.942581	3.073227
Cl	5.796005	3.228602	4.468128
S	3.105383	-0.786276	1.383680
O	2.267280	0.060603	0.485506
O	2.985522	-0.635993	2.841274
C	2.711714	-2.492476	0.985307
C	2.940809	-3.479280	1.947667
C	2.663463	-4.809865	1.632686
C	2.163116	-5.143928	0.371153
C	1.933257	-4.146888	-0.580618
C	2.207136	-2.812459	-0.277517
H	3.313799	-3.200511	2.927696
H	2.832416	-5.584711	2.375380
H	1.532002	-4.406798	-1.556596
H	2.016358	-2.023726	-0.997667
H	1.945352	-6.181486	0.132154
C	-1.632688	3.664100	-0.392846
C	-2.004379	4.564053	0.602423
C	-1.543102	4.398987	1.913302
C	-0.710899	3.321187	2.219782
C	-0.340401	2.416367	1.223382
C	-0.788223	2.575687	-0.101800
C	-0.350425	1.599686	-1.116328
H	-0.186196	0.869183	-3.094984
H	-1.078222	2.475635	-2.927325
H	0.204443	0.752904	-0.714084
H	-2.011351	3.800773	-1.402319
H	-2.660561	5.395964	0.358038
H	-1.834941	5.104089	2.687265
H	-0.348410	3.180723	3.234742
H	0.309461	1.579286	1.466129

TS1 S=2, Cβ

C	0.548687	-0.213606	-0.259991
N	2.744805	0.029891	0.376148
Fe	3.653045	1.706363	0.121871
O	5.536445	1.564260	0.035902
O	2.995283	2.734299	1.567229
N	3.841882	3.846050	-0.969516
N	3.436582	1.343693	-2.093642
C	5.288587	4.220825	-0.904188
H	5.522555	4.335534	0.158690
H	5.422340	5.206361	-1.378672
C	6.242961	3.231279	-1.520836
C	7.090451	3.614522	-2.562379
H	7.023318	4.615235	-2.979216
C	8.037455	2.720175	-3.056516
C	8.158324	1.439813	-2.519497
H	8.898690	0.745691	-2.900374
C	7.310624	1.058412	-1.482272
C	6.331647	1.932572	-0.953084
C	3.024911	4.873624	-0.246581
H	3.112298	5.838957	-0.770839
H	1.981914	4.547547	-0.323349
C	3.389472	5.053243	1.202461
C	3.707916	6.313192	1.713999
H	3.757928	7.174763	1.054590
C	3.951718	6.464582	3.076783
C	3.883731	5.372810	3.941838
H	4.076211	5.492949	5.001827
C	3.570508	4.115664	3.429902
C	3.317643	3.920893	2.050163
C	3.365700	3.749331	-2.362851
H	3.839462	4.508827	-3.002672
H	2.288078	3.957061	-2.359359
C	3.553824	2.371539	-2.951744
C	3.749345	2.167257	-4.319143
H	3.850684	3.019822	-4.983986
C	3.824298	0.863652	-4.804010
H	3.984254	0.680976	-5.863027
C	3.701606	-0.200213	-3.908559
H	3.760668	-1.231105	-4.241846
C	3.514999	0.082915	-2.559468
H	3.418608	-0.691686	-1.805599
Cl	9.096271	3.209879	-4.374428
Cl	7.464536	-0.552553	-0.814244
Cl	4.351201	8.054211	3.718869
Cl	3.479720	2.749046	4.508381
S	2.923885	-0.802670	1.780852
O	1.691488	-0.809680	2.588466
O	4.193690	-0.325897	2.365430
C	3.204552	-2.510561	1.266322
C	4.414052	-2.841064	0.645379
C	4.633167	-4.157831	0.241919
C	3.655532	-5.134206	0.462799
C	2.457620	-4.795349	1.094690
C	2.227101	-3.478230	1.502378
H	5.173366	-2.078846	0.498053
H	5.571917	-4.425048	-0.236528
H	1.704071	-5.556443	1.280177
H	1.313497	-3.199049	2.017098
H	3.833668	-6.160158	0.150667
C	-0.376135	2.407724	-1.536343
C	-0.701220	3.674281	-2.016642
C	-0.981981	4.717907	-1.125523
C	-0.938190	4.480095	0.251631
C	-0.616874	3.212323	0.732859
C	-0.323549	2.150386	-0.148489
C	-0.010424	0.838174	0.405770
H	0.587703	-1.189415	0.205909
H	0.761099	-0.180738	-1.323791
H	-0.179800	0.715615	1.472649
H	-0.189565	1.601349	-2.240122
H	-0.757483	3.845992	-3.089091
H	-1.245357	5.702536	-1.502872
H	-1.158187	5.282421	0.950864
H	-0.577655	3.031301	1.803751

Int S=2, Cβ

C	-0.022330	0.067268	0.356357
N	1.444087	-0.079152	0.262819
Fe	2.878233	1.388127	0.295568
O	4.584292	1.241162	-0.558837
O	2.680827	1.936276	2.102552
N	3.134798	3.811153	-0.015501
N	2.074325	1.908572	-1.758502
C	4.592905	4.060226	-0.214356
H	5.089800	3.702931	0.693289
H	4.765301	5.147090	-0.276395
C	5.193431	3.387109	-1.419674
C	5.825710	4.142951	-2.409128
H	5.839285	5.226841	-2.340626
C	6.455991	3.509345	-3.477314
C	6.471806	2.118863	-3.570641
H	6.966984	1.623327	-4.397812
C	5.839361	1.368321	-2.583584
C	5.177924	1.967976	-1.482669
C	2.658780	4.555548	1.191985
H	2.762106	5.638501	1.015487
H	1.589412	4.333026	1.283814
C	3.362548	4.179350	2.466356
C	3.989513	5.134593	3.267541
H	4.033015	6.172930	2.952162
C	4.551896	4.750901	4.483279
C	4.495714	3.425255	4.912764
H	4.933321	3.131179	5.859878
C	3.873143	2.472670	4.108418
C	3.296448	2.822925	2.864280
C	2.337301	4.247066	-1.179994
H	2.758218	5.154830	-1.637656
H	1.334444	4.506297	-0.818076
C	2.164373	3.167150	-2.219941
C	2.011389	3.465513	-3.576221
H	2.100259	4.493245	-3.914880
C	1.757253	2.431422	-4.472598
H	1.641781	2.639495	-5.532696
C	1.664154	1.125158	-3.988414
H	1.475104	0.286871	-4.650924
C	1.835364	0.907778	-2.625643
H	1.786540	-0.083577	-2.187227
Cl	7.242678	4.470557	-4.724095
Cl	5.868950	-0.379679	-2.714573
Cl	5.342971	5.954656	5.494460
Cl	3.790051	0.816760	4.648530
S	2.196402	-1.272121	1.089855
O	1.481491	-1.707585	2.297747
O	3.573392	-0.692084	1.170242
C	2.322231	-2.711403	0.017593
C	3.266511	-2.710303	-1.014147
C	3.333811	-3.811184	-1.868364
C	2.468835	-4.895645	-1.689575
C	1.536649	-4.887002	-0.649139
C	1.459021	-3.791601	0.213756
H	3.947282	-1.872024	-1.124625
H	4.069777	-3.825840	-2.667902
H	0.874395	-5.736061	-0.502268
H	0.758431	-3.775914	1.042132
H	2.528963	-5.752206	-2.356059
C	-1.479020	2.498585	-0.973223
C	-2.112494	3.613896	-1.504759
C	-2.338538	4.754769	-0.720668
C	-1.919324	4.761470	0.618637
C	-1.285901	3.653423	1.161434
C	-1.038185	2.477741	0.385048
C	-0.374529	1.381596	0.986903
H	-0.428353	-0.742300	0.979512
H	-0.464734	-0.041663	-0.641576
H	-0.039885	1.496922	2.014888
H	-1.313069	1.631221	-1.604552
H	-2.438949	3.599262	-2.542013
H	-2.838320	5.621558	-1.144089
H	-2.096975	5.636980	1.238472
H	-0.975597	3.659799	2.203927

TS2 S=2, Cβ

C	-0.499497	0.680485	1.063350
C	-0.105113	-0.121224	-0.110420
N	1.316103	0.046382	0.228390
Fe	2.764876	1.630557	0.057142
O	4.575643	1.240852	-0.513599
O	2.179291	2.251833	1.839882
N	3.076919	3.904359	-0.443610
N	2.149454	1.838381	-2.110190
C	4.555509	4.108452	-0.492240
H	4.926173	3.855662	0.506328
H	4.763088	5.178568	-0.658786
C	5.282408	3.293830	-1.531784
C	6.024080	3.940711	-2.523794
H	6.023773	5.025701	-2.578796
C	6.779098	3.204125	-3.431796
C	6.818718	1.813473	-3.354461
H	7.414961	1.234829	-4.050764
C	6.079455	1.171499	-2.365900
C	5.275807	1.871649	-1.427301
C	2.479666	4.772223	0.619586
H	2.653422	5.830707	0.363764
H	1.398627	4.592865	0.583479
C	2.973266	4.497493	2.012951
C	3.550764	5.511578	2.780433
H	3.731114	6.490523	2.345079
C	3.879744	5.272838	4.111734
C	3.627300	4.031234	4.694928
H	3.874884	3.847051	5.734236
C	3.054933	3.022943	3.925066
C	2.723719	3.205999	2.555645
C	2.435145	4.217332	-1.735512
H	2.911257	5.078421	-2.228567
H	1.398310	4.507270	-1.521231
C	2.380738	3.036234	-2.678604
C	2.477988	3.187873	-4.064235
H	2.679770	4.167118	-4.487660
C	2.332520	2.069078	-4.880262

H	2.411783	2.162704	-5.959776
C	2.101455	0.826039	-4.288059
H	1.996172	-0.075226	-4.883189
C	2.027460	0.757581	-2.900742
H	1.877507	-0.187292	-2.387429
Cl	7.698113	4.032643	-4.687278
Cl	6.157704	-0.581883	-2.278585
Cl	4.609818	6.555157	5.078127
Cl	2.712985	1.474989	4.671747
S	1.988199	-1.217839	1.130187
O	1.058248	-1.688620	2.170220
O	3.331898	-0.726291	1.454815
C	2.147909	-2.550634	-0.068034
C	3.162322	-2.469830	-1.028434
C	3.274621	-3.489777	-1.973533
C	2.388591	-4.572525	-1.951103
C	1.388941	-4.645328	-0.978148
C	1.262657	-3.630657	-0.026065
H	3.858247	-1.635934	-1.020299
H	4.062125	-3.442475	-2.720767
H	0.711895	-5.494989	-0.952530
H	0.511802	-3.679603	0.755740
H	2.484882	-5.366093	-2.687586
C	-1.215510	2.762454	-0.124869
C	-1.673718	4.073620	-0.062176
C	-1.813832	4.714276	1.176237
C	-1.490039	4.033920	2.357637
C	-1.032202	2.724903	2.302482
C	-0.891530	2.053933	1.060473
H	-0.450614	-1.160184	-0.098457
H	-0.324087	0.321631	-1.084436
H	-0.404037	0.174640	2.018053
H	-1.118457	2.277064	-1.091082
H	-1.933673	4.599795	-0.977151
H	-2.173316	5.738870	1.219785
H	-1.588145	4.532618	3.317569
H	-0.757309	2.200527	3.212916

Prod S=2, Cβ

C	0.022421	0.879336	-0.612525
N	1.339532	0.289765	-0.145334
C	1.047473	1.735477	0.021169
Fe	1.201220	-1.876246	1.114963
O	2.965431	-2.539365	1.684037
O	-0.017838	-2.260410	-0.361474
N	0.109523	-3.424133	2.385071
N	1.099844	-0.876353	3.095076
C	1.072582	-4.545473	2.580128
H	1.316542	-4.910710	1.576829
H	0.566068	-5.367868	3.112749
C	2.335751	-4.184004	3.322982
C	2.644549	-4.871905	4.500006
H	1.947564	-5.606828	4.892947
C	3.844777	-4.638880	5.163717
C	4.762860	-3.723596	4.654727
H	5.705994	-3.543442	5.157942
C	4.452622	-3.037639	3.485404
C	3.235329	-3.218686	2.772113
C	-1.108550	-3.903547	1.662284
H	-1.603231	-4.687820	2.258924
H	-1.785985	-3.042402	1.611708
C	-0.870546	-4.404631	0.262895
C	-1.248916	-5.698734	-0.101520
H	-1.614251	-6.391568	0.651401
C	-1.181351	-6.094684	-1.434281
C	-0.762424	-5.201260	-2.419187
H	-0.728720	-5.500354	-3.460675
C	-0.384475	-3.912985	-2.051557
C	-0.389081	-3.473980	-0.701449
C	-0.290026	-2.796105	3.661617
H	-0.361354	-3.534261	4.474118
H	-1.295301	-2.379450	3.520043
C	0.610238	-1.651901	4.081470
C	0.860171	-1.371385	5.428253
H	0.460970	-2.025177	6.197823
C	1.638339	-0.266307	5.759947
H	1.849906	-0.035435	6.800252
C	2.160296	0.524954	4.734212
H	2.789598	1.383611	4.944569
C	1.873971	0.173887	3.420029
H	2.284558	0.734882	2.585755
Cl	4.212273	-5.507151	6.653203
Cl	5.642728	-1.896935	2.868965
Cl	-1.652195	-7.732366	-1.888313
Cl	0.088661	-2.783509	-3.307101
S	2.504821	-0.055967	-1.438186
O	2.038271	0.565851	-2.684961
O	2.762817	-1.488272	-1.326515
C	3.947876	0.843255	-0.870026
C	4.668878	0.336763	0.215152
C	5.797258	1.037452	0.644390
C	6.195977	2.206168	-0.011215
C	5.471322	2.686462	-1.105479
C	4.335044	2.004661	-1.544047
H	7.080799	2.739494	0.326292
H	4.368568	-0.587832	0.700894
H	6.368878	0.659394	1.486587
H	5.792541	3.586711	-1.622006
H	3.765690	2.346713	-2.402067
C	-1.555501	0.751266	1.376137
C	-2.780276	0.368464	1.928835
C	-3.728302	-0.291725	1.143912
C	-3.444454	-0.567619	-0.196895
C	-2.219403	-0.191253	-0.744070
C	-1.258686	0.468530	0.036265
H	1.591073	2.429456	-0.615928
H	0.951453	2.053450	1.055419
H	-0.026682	0.958369	-1.695882
H	-0.838560	1.275782	2.000696
H	-2.998554	0.603282	2.967792
H	-4.685475	-0.580524	1.570658
H	-4.175626	-1.080488	-0.815787
H	-1.990654	-0.428701	-1.778903

Re S=2, Cβ, solvent optimization

C	-0.546055	1.660342	-2.442817
N	4.654317	-0.539661	0.940324
Fe	5.021400	1.286624	0.312278
O	6.799683	1.691679	-0.205496
O	4.705059	2.309864	1.859772
N	4.140611	2.997995	-0.866303
N	4.677683	0.440977	-1.726236
C	5.286491	3.909908	-1.198960
H	5.651723	4.294786	-0.242126
H	4.893305	4.766636	-1.766248
C	6.431629	3.282715	-1.957397
C	6.832576	3.818250	-3.184024
H	6.275199	4.637951	-3.627596
C	7.958272	3.317438	-3.833775
C	8.703267	2.280389	-3.274482
H	9.579757	1.890643	-3.779232
C	8.301330	1.741870	-2.055361
C	7.164833	2.220397	-1.360648
C	3.125311	3.716845	-0.015865
H	2.623895	4.477532	-0.631672
H	2.378437	2.963494	0.257192
C	3.681575	4.363872	1.225230
C	3.397657	5.699726	1.517111
H	2.820011	6.300060	0.820869
C	3.844692	6.259799	2.711369
C	4.580254	5.505483	3.625362
H	4.931074	5.944845	4.552058
C	4.867843	4.175585	3.331773
C	4.428551	3.569016	2.130391
C	3.461347	2.499219	-2.086587
H	3.429861	3.280639	-2.858701
H	2.422227	2.265933	-1.823137
C	4.092741	1.240598	-2.631164
C	4.013740	0.883043	-3.978848
H	3.540981	1.552644	-4.690974
C	4.558432	-0.332698	-4.385722
H	4.514374	-0.629777	-5.429832
C	5.169733	-1.156733	-3.438238
H	5.613119	-2.107362	-3.715559
C	5.212925	-0.729810	-2.115474
H	5.675559	-1.320781	-1.331740
Cl	8.447188	3.998507	-5.380207
Cl	9.219468	0.423674	-1.361849
Cl	3.482262	7.942581	3.073227
Cl	5.796005	3.228602	4.468128
S	3.105383	-0.786276	1.383680
O	2.267280	0.060603	0.485506
O	2.985522	-0.635993	2.841274
C	2.711714	-2.492476	0.985307
C	2.940809	-3.479280	1.947667
C	2.663463	-4.809865	1.632686
C	2.163116	-5.143928	0.371153
C	1.933257	-4.146888	-0.580618
C	2.207136	-2.812459	-0.277517
H	3.313799	-3.200511	2.927696
H	2.832416	-5.584711	2.375380
H	1.532002	-4.406798	-1.556596
H	2.016358	-2.023726	-0.997667
H	1.945352	-6.181486	0.132154
C	-1.632688	3.664100	-0.392846
C	-2.004379	4.564053	0.602423
C	-1.543102	4.398987	1.913302
C	-0.710899	3.321187	2.219782
C	-0.340401	2.416367	1.223382
C	-0.788223	2.575687	-0.101800
C	-0.350425	1.599686	-1.116328
H	-0.186196	0.869183	-3.094984
H	-1.078222	2.475635	-2.927325
H	0.204443	0.752904	-0.714084
H	-2.011351	3.800773	-1.402319
H	-2.660561	5.395964	0.358038
H	-1.834941	5.104089	2.687265
H	-0.348410	3.180723	3.234742
H	0.309461	1.579286	1.466129

TS1 S=2, Cβ, solvent optimization

C	0.583296	-0.284270	-0.190376
N	2.893189	0.051761	0.439907
Fe	3.720477	1.755868	0.086350
O	5.612866	1.628878	0.099401
O	3.154227	2.717113	1.631203
N	3.862052	3.860385	-0.933612
N	3.486148	1.375312	-2.071051
C	5.302773	4.272002	-0.877285
H	5.543699	4.402282	0.182088
H	5.409963	5.251143	-1.364345
C	6.274941	3.292450	-1.486146
C	7.111283	3.678527	-2.535244
H	7.018393	4.670640	-2.966020
C	8.073529	2.792783	-3.017647
C	8.223976	1.519523	-2.472549
H	8.973168	0.833435	-2.850975
C	7.383176	1.139994	-1.428756
C	6.394009	2.002404	-0.906421
C	3.024501	4.867208	-0.199839
H	3.077758	5.830587	-0.725554
H	1.990231	4.510790	-0.262361
C	3.400100	5.058961	1.245799
C	3.652472	6.334785	1.753326
H	3.642080	7.194066	1.089763
C	3.907181	6.500912	3.113211
C	3.919155	5.412768	3.984456
H	4.119799	5.545299	5.041640
C	3.672845	4.142995	3.468768
C	3.407355	3.923345	2.095599
C	3.381054	3.785452	-2.334673
H	3.874021	4.538682	-2.961902
H	2.310807	4.024762	-2.335931
C	3.536127	2.409667	-2.931572
C	3.636189	2.213358	-4.309837
H	3.678086	3.069774	-4.975258
C	3.680422	0.912554	-4.806468
H	3.759454	0.736490	-5.875122

C	3.626302	-0.158368	-3.910576
H	3.659400	-1.186432	-4.255027
C	3.535075	0.115173	-2.551516
H	3.490565	-0.669138	-1.804381
Cl	9.126433	3.289657	-4.343897
Cl	7.559415	-0.465015	-0.736019
Cl	4.223383	8.117577	3.750243
Cl	3.685051	2.764140	4.555671
S	3.103814	-0.813395	1.796224
O	1.955592	-0.733581	2.725797
O	4.445386	-0.470417	2.331490
C	3.202224	-2.532232	1.259333
C	4.280556	-2.928199	0.458422
C	4.368492	-4.256232	0.041245
C	3.387728	-5.179867	0.423885
C	2.319227	-4.775831	1.227560
C	2.222294	-3.446104	1.651499
H	5.039979	-2.206275	0.171575
H	5.201892	-4.572881	-0.579973
H	1.560598	-5.492767	1.529491
H	1.403365	-3.120886	2.284444
H	3.460424	-6.213529	0.096638
C	-0.265802	2.288181	-1.601013
C	-0.596031	3.527890	-2.143952
C	-0.953022	4.594396	-1.307233
C	-0.982192	4.408220	0.078997
C	-0.655064	3.166988	0.623421
C	-0.283937	2.084079	-0.202565
C	0.036749	0.803374	0.419086
H	0.649817	-1.228227	0.335719
H	0.802662	-0.310255	-1.252520
H	-0.150437	0.739091	1.488821
H	-0.014127	1.466918	-2.265812
H	-0.588382	3.663033	-3.222393
H	-1.214000	5.558610	-1.734885
H	-1.262912	5.228761	0.733763
H	-0.680144	3.024327	1.700904

Int S=2, Cβ, solvent optimization

C	1.190899	0.225367	0.550024
N	2.619802	0.180827	0.904260
Fe	3.688123	1.810053	0.440697
O	5.569091	1.542031	0.229819
O	3.460838	2.757617	2.094135
N	3.837847	3.875634	-0.561142
N	3.346449	1.419517	-1.698393
C	5.292700	4.228758	-0.665316
H	5.648611	4.357079	0.361487
H	5.377989	5.202490	-1.166991
C	6.170602	3.221005	-1.364072
C	6.941975	3.604823	-2.462906
H	6.841497	4.605218	-2.872388
C	7.852032	2.708935	-3.020622
C	8.018201	1.428789	-2.497236
H	8.731289	0.735579	-2.928765
C	7.242196	1.051803	-1.403799
C	6.296537	1.918837	-0.810238
C	3.138320	4.919039	0.260337
H	3.174445	5.878438	-0.273392
H	2.087845	4.613227	0.310663
C	3.689720	5.097906	1.651873
C	4.029221	6.371636	2.113559
H	3.952463	7.226449	1.448712
C	4.456459	6.543592	3.428343
C	4.558247	5.461515	4.301081
H	4.892626	5.596489	5.323508
C	4.225973	4.194378	3.830565
C	3.784830	3.967127	2.504097
C	3.199424	3.828206	-1.900971
H	3.611577	4.603858	-2.558573
H	2.134320	4.054176	-1.772178
C	3.308981	2.467537	-2.541659
C	3.296414	2.295802	-3.926561
H	3.270014	3.163173	-4.578399
C	3.320367	1.003878	-4.447491
H	3.312277	0.845819	-5.521754
C	3.362538	-0.081742	-3.568750
H	3.387543	-1.103351	-3.932538
C	3.379758	0.170172	-2.202243
H	3.420210	-0.632398	-1.473740
Cl	8.820393	3.202779	-4.411349
Cl	7.455923	-0.559087	-0.733089
Cl	4.879796	8.158412	4.004349
Cl	4.348158	2.822188	4.921965
S	3.110728	-0.939236	1.990989
O	2.108857	-1.124776	3.066014
O	4.489081	-0.577263	2.370169
C	3.188770	-2.500403	1.097904
C	4.298284	-2.757336	0.283593
C	4.348288	-3.949473	-0.440471
C	3.299225	-4.871553	-0.350033
C	2.198302	-4.605317	0.468481
C	2.136825	-3.414800	1.198489
H	5.111814	-2.040047	0.231165
H	5.207460	-4.161927	-1.070777
H	1.387255	-5.324285	0.544272
H	1.293159	-3.204793	1.847516
H	3.343498	-5.798901	-0.914609
C	-0.303399	1.601760	-1.814404
C	-1.071115	2.231760	-2.785885
C	-1.562825	3.528775	-2.578081
C	-1.278667	4.194687	-1.376006
C	-0.512608	3.574528	-0.398543
C	0.002517	2.256299	-0.585942
C	0.785224	1.666557	0.445651
H	0.582922	-0.255240	1.331821
H	1.008013	-0.324989	-0.381478
H	0.950983	2.252451	1.347330
H	0.073422	0.601927	-2.003078
H	-1.289211	1.713397	-3.715793
H	-2.161273	4.014894	-3.343414
H	-1.663306	5.196567	-1.205237
H	-0.315572	4.086627	0.540467

Prod S=2, Cβ, solvent optimization

C	0.059727	0.728471	-0.898812
N	1.417581	1.320787	-0.636211
C	0.844748	1.354351	-1.998581
Fe	1.458307	-2.351587	1.616967
O	3.247859	-3.136029	1.640267
O	0.082022	-2.445668	0.193034
N	0.650692	-4.166994	2.675124
N	0.613758	-1.485678	3.406591
C	1.512104	-5.354097	2.423096
H	1.474187	-5.531780	1.342810
H	1.081572	-6.241265	2.912733
C	2.951252	-5.194400	2.862804
C	3.523916	-6.182593	3.668698
H	2.911894	-7.006844	4.023468
C	4.873894	-6.124998	4.007615
C	5.681728	-5.084222	3.555400
H	6.733396	-5.035959	3.815134
C	5.103559	-4.096993	2.763860
C	3.732129	-4.095522	2.387977
C	-0.732515	-4.388024	2.157593
H	-1.187009	-5.237313	2.689663
H	-1.308125	-3.492321	2.420138
C	-0.822181	-4.621473	0.667729
C	-1.366806	-5.816219	0.191117
H	-1.668334	-6.587799	0.893359
C	-1.534470	-6.015937	-1.177280
C	-1.164469	-5.034612	-2.093089
H	-1.292581	-5.186085	-3.159104
C	-0.618557	-3.847889	-1.611058
C	-0.420557	-3.585856	-0.229360
C	0.589557	-3.823339	4.111570
H	1.587967	-3.981124	4.535574
H	-0.097077	-4.487272	4.656985
C	0.204652	-2.375123	4.336803
C	-0.486721	-1.970440	5.479609
H	-0.811386	-2.710119	6.204804
C	-0.750194	-0.614021	5.669438
H	-1.286397	-0.279008	6.552564
C	-0.322843	0.302042	4.706454
H	-0.510173	1.365241	4.813324
C	0.351223	-0.177764	3.588166
H	0.697787	0.488421	2.805102
Cl	5.577586	-7.389525	5.026577
Cl	6.120851	-2.776359	2.187052
Cl	-2.227285	-7.533819	-1.764995
Cl	-0.151705	-2.613452	-2.780167
S	2.649893	0.198708	-0.304818
O	2.885364	-0.740699	-1.410855
O	2.292391	-0.356806	1.032052
C	4.072523	1.253014	-0.101918
C	4.162124	2.068167	1.031889
C	5.279024	2.890220	1.174564
C	6.281728	2.890101	0.197498
C	6.175725	2.067352	-0.926967
C	5.063168	1.237742	-1.086414
H	7.149363	3.533068	0.315981
H	3.382305	2.055997	1.785945
H	5.367819	3.528443	2.048716
H	6.957323	2.066863	-1.680894
H	4.969147	0.588945	-1.950440
C	-1.293824	2.750369	-0.175210
C	-2.392637	3.294198	0.490967
C	-3.305762	2.458173	1.143426
C	-3.109996	1.075130	1.131187
C	-2.008637	0.529726	0.466273
C	-1.094537	1.361646	-0.197073
H	1.275377	0.682495	-2.737637
H	0.618110	2.358211	-2.347405
H	0.030739	-0.359620	-0.917380
H	-0.588762	3.411724	-0.671899
H	-2.537781	4.371453	0.499990
H	-4.162380	2.884557	1.659187
H	-3.811905	0.419677	1.640355
H	-1.843824	-0.545075	0.465315

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