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ELECTRONIC SUPPLEMENTARY INFORMATION

σ-Hole interactions in organometallic catalysts: the case of methyltrioxorhenium(VII)

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S.1. Synthesis and Characterization

S.1.1. Synthesis of methyltrioxorhenium·1,4-diazabicyclo[2.2.2]octane adduct (3b). 0.05 mmol of 1,4-diazabicyclo[2.2.2]octane (**2b**) were added to a solution of CH_3ReO_3 (**1**, 0.1 mmol) in dichloromethane (2 mL) inside a clear borosilicate vial. White crystals of **3b** suitable for single crystal X-Ray diffraction were obtained in 24 hours by slow evaporation of the solvent. FT-IR (selected bands, cm^{-1}) 2962, 1644, 1469, 1358, 1325, 1056, 1001, 897, 839, 549. ^{13}C NMR (400 MHz, $CDCl_3$): δ 46.14 (N<u>C</u>), 23.97 (<u>C</u>H_3). ^{13}C NMR (400 MHz, $CDCl_3$) of a 1:5 solution of **3b** and **2b**: δ 45.98 (N<u>C</u>), 21.14 (<u>C</u>H_3).

S.1.2. Synthesis of methyltrioxorhenium·[4,4'-bipyridine] 1,1'-dioxide adducts (3c). 0.05 mmol of was [4,4'-bipyridine] 1,1'-dioxide (**2c**) were added to a solution of CH_3ReO_3 (**1**, 0.1 mmol) in dichloromethane (2 mL) inside a clear borosilicate vial. White crystals of **3c** suitable for single crystal X-Ray diffraction were obtained in 24 hours by slow evaporation of the solvent. FT-IR (selected bands, cm^{-1}) 2985, 2899, 1611, 1470, 1432, 1358, 1206, 995, 927, 570. ^{13}C NMR (400 MHz, $CDCl_3$): δ 140.8 (N<u>C</u>), 134.2 (NCC<u>C</u>), 123.4 (NC<u>C</u>), 29.7 (<u>C</u>H_3).

S.1.3. Synthesis of methyltrioxorhenium·pyrazine *N*-oxide adduct (3d). 0.1 mmol of pyrazine *N*-oxide were added to a solution of CH_3ReO_3 (0.1 mmol) in dichloromethane (2 mL) inside a clear borosilicate vial. White crystals of **3d** suitable for single crystal X-Ray diffraction were obtained in 24 hours by slow evaporation of the solvent. FT-IR (selected bands, cm^{-1}) 3114, 3090, 3035, 2389, 1610, 1462, 1443, 1312, 1200, 964, 926, 539. ^{13}C NMR (400 MHz, $CDCl_3$): 147.53 (N<u>C</u>), 134.33 (N<u>C</u>), 19.48 (<u>C</u>H_3).

S.1.4. Synthesis of 1,2-di(pyridine-4-yl)ethane·1,2-diiodotetrafluoroethane adduct. 0.1 mmol of 1,2-di(pyridine-4-yl)ethane were added to a solution of 1,2-diiodotetrafluoroethane (0.1 mmol in acetone (2 mL) inside a clear borosilicate vial. White crystals (elongated blocks) of the title adduct suitable for single crystal X-Ray diffraction were obtained in 24 hours by slow evaporation of the solvent. FT-IR (selected bands, cm^{-1}) 2935, 1601, 1561, 1420, 1217, 1115, 1084, 999, 816, 697, 539. ^{19}F NMR (400 MHz, $CDCl_3$-d_6): δ s -52.57 (C<u>F</u>$_{2)}$ ^{13}C NMR (400 MHz, $CDCl_3$-d_6): 149.92 (N<u>C</u>), 149.41(NCC<u>C</u>), 123.78 (NC<u>C</u>), 94.91 (tt, $^1J_{C\text{-}F}$ 310 Hz, $^2J_{C\text{-}F}$ 40 Hz, <u>C</u>F_2), 35.70 (<u>C</u>H_2).

Table S.1. ^{13}C NMR chemical shifts (δ, ppm) of MTO in different nucleophilic solvents

Solvents	^{13}C NMR
Chloroform	19.04
Ethylene carbonate[a]	19.48
Acetone	19.56
Acetonitrile	21.34
N,N-Dimethylformamide[a]	21.49
Dimethylsulphoxide	25.38
Pyridine	26.07

[a] Non-deuterated solvent was used.

S.1.5. Matere, halogen, and hydrogen bonds: competitive co-crystallization experiments

Any competitive co-crystallization experiment was performed in two different solvents (acetone and dichloromethane or methanol and methanol/dichloromethane 1:1). The outcomes of these experiments were established by SC-XRD analyses carried out on the first crystals formed in each experiment. In each experiment three compounds were present in the solution (specifically, **1** i.e. the MaB donor, the HaB or HB donor, and **2a**,**c** i.e. the Lewis base). Their molar ratio was established in order to have equimolar amounts of MaB donor sites (**1** was assumed as a monodentate MaB donor), HaB or HB donor sites, and basic sites. All experiments were performed by using 0.03 mmol of **1**.

The tables below summarize the results obtained for the two investigated Lewis bases (i.e., 1,2-di(pyridin-4-yl)ethane (**2a**) and [4,4'-bipyridine]1,1'-dioxide (**2c**)).

Table S.2. Competitive co-crystallization experiments involving MTO (1), 1,2-di(pyridin-4-yl)ethane (2a), and four different HaB or HB donors in two different solvents.

HaB or HB donor	Formed adduct (prevailing interaction)	
	Acetone	Dichloromethane
1,2-Diiodotetrafluoroethane	**3a** (MaB)	**3a**(MaB)
1,4-Diodotetraflurobenzene	**3a** (MaB)	**3a** (MaB)
1,4-Dihydroxybenzene	**3a** (MaB)	**3a** (MaB)
4-Cyanophenol	**3a** (MaB)	**3a** (MaB)

Table S.3. Competitive co-crystallization experiments involving MTO (1), 4,4'-bipyridine-1,1'-dioxide (2c), and two HB donors in two different solvents.

HB donor	Formed adduct (prevailing interaction)	
	Methanol	Methanol/dichloromethane 1:1
Pyromellitic acid	**3c** (MaB)	**3c** (MaB)
Tartaric acid	**2c·Tartaric acid** (HB)	**2c·Tartaric acid** (HB)

Table S.4. Nc values for adduct which formed/might be formed in competitive co-crystallization experiments.

Adduct (Refcode)	Nc value
3a (this paper)	0.67
2a·1,2-Diiodotetrafluoroethane (this paper)	0.76
2a·1,4-Diodotetraflurobenzene (MEKWOO)	0.75
2a·1,4-Dihydroxybenzene (MEKWUU)	0.63
2a·4-Cyanophenol (KIHYEG)	0.64
3c (this paper)	0.63
2c·Pyromellitic acid (HOPKIH)	0.57
2c·Tartaric acid (KIMBEQ)	0.54

S.2. Crystallographic Details.

Table S.5. Crystal data and structure refinement for **3a**.

Identification code	**3a**
Empirical formula	$C_{14}H_{18}N_2O_6Re_2$
Formula weight	682.70
Temperature/K	296 K
Crystal system	triclinic
Space group	P-1
a/Å	6.02510(10)
b/Å	6.7106(2)
c/Å	11.4878(3)
α/°	79.5150(10)
β/°	76.4570(10)
γ/°	77.5250(10)
Volume/Å^3	436.655(19)
Z	1
ρ_{calc}g/cm^3	2.596
μ/mm^{-1}	13.880
F(000)	314.0
Crystal size/mm^3	0.06 × 0.04 × 0.02
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.826 to 61.13
Index ranges	-8 ≤ h ≤ 8, -9 ≤ k ≤ 9, -16 ≤ l ≤ 16
Reflections collected	9026
Independent reflections	2684 [R_{int} = 0.0364, R_{sigma} = 0.0300]
Data/restraints/parameters	2684/0/111
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0179, wR_2 = 0.0429
Final R indexes [all data]	R_1 = 0.0200, wR_2 = 0.0438
Largest diff. peak/hole / e Å^{-3}	0.72/-0.80
CCDC number	2174961

Table S.6. Crystal data and structure refinement for **3b**.

Identification code	**3b**
Empirical formula	$C_8H_{18}N_2O_6Re_2$
Formula weight	610.64
Temperature/K	296 K
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.7251(9)
b/Å	9.6283(9)
c/Å	31.118(3)
α/°	90
β/°	96.230(5)
γ/°	90
Volume/Å^3	2896.5(5)
Z	8
ρ_{calc}g/cm^3	2.801
μ/mm^{-1}	16.720
F(000)	2224.0
Crystal size/mm^3	0.06 × 0.04 × 0.03
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.634 to 52.132
Index ranges	-11 ≤ h ≤ 11, -11 ≤ k ≤ 11, -37 ≤ l ≤ 37
Reflections collected	32530
Independent reflections	5361 [R_{int} = 0.1058, R_{sigma} = 0.0662]
Data/restraints/parameters	5361/0/323
Goodness-of-fit on F^2	1.076
Final R indexes [I>=2σ (I)]	R_1 = 0.0528, wR_2 = 0.0950
Final R indexes [all data]	R_1 = 0.0851, wR_2 = 0.1043
Largest diff. peak/hole / e Å^{-3}	2.21/-2.74
CCDC number	2174970

Table S.7. Crystal data and structure refinement for **3c**.

Identification code	**3c**
Empirical formula	$C_{12}H_{14}N_2O_8Re_2$
Formula weight	686.65
Temperature/K	296 K
Crystal system	monoclinic
Space group	C2/c
a/Å	19.6709(19)
b/Å	8.1455(7)
c/Å	10.5288(9)
α/°	90
β/°	103.923(7)
γ/°	90
Volume/Å^3	1637.5(3)
Z	4
ρ_{calc}g/cm^3	2.785
μ/mm^{-1}	14.815
F(000)	1256.0
Crystal size/mm^3	0.06 × 0.04 × 0.02
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	7.04 to 69.43
Index ranges	-31 ≤ h ≤ 30, -12 ≤ k ≤ 12, -14 ≤ l ≤ 16
Reflections collected	18664
Independent reflections	3291 [R_{int} = 0.0479, R_{sigma} = 0.0303]
Data/restraints/parameters	3291/0/110
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0224, wR_2 = 0.0522
Final R indexes [all data]	R_1 = 0.0340, wR_2 = 0.0561
Largest diff. peak/hole / e Å^{-3}	0.83/-1.16
CCDC number	2174969

Table S.8. Crystal data and structure refinement for **3d**.

Identification code	**3d**
Empirical formula	$C_5H_7N_2O_4Re$
Formula weight	345.33
Temperature/K	100 K
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.0455(5)
b/Å	10.9263(6)
c/Å	8.6505(5)
α/°	90
β/°	110.156(2)
γ/°	90
Volume/Å^3	802.60(8)
Z	4
ρ_{calc}g/cm^3	2.858
μ/mm^{-1}	15.116
F(000)	632.0
Crystal size/mm^3	0.06 × 0.04 × 0.03
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.076 to 61.28
Index ranges	-12 ≤ h ≤ 12, -15 ≤ k ≤ 15, -12 ≤ l ≤ 12
Reflections collected	16559
Independent reflections	2464 [R_{int} = 0.0393, R_{sigma} = 0.0276]
Data/restraints/parameters	2464/0/110
Goodness-of-fit on F^2	1.048
Final R indexes [I>=2σ (I)]	R_1 = 0.0234, wR_2 = 0.0656
Final R indexes [all data]	R_1 = 0.0245, wR_2 = 0.0664
Largest diff. peak/hole / e Å^{-3}	2.14/-1.83
CCDC number	2174971

Table S.9. Crystal data and structure refinement for adduct **2a·1,2-diiodotetrafluoroethane**.

Identification code	**2a·1,2-diiodotetrafluoroethane**
Empirical formula	$C_{13}H_{12}F_4I_2N_2$
Formula weight	526.05
Temperature/K	296 K
Crystal system	triclinic
Space group	P-1
a/Å	6.6506(7)
b/Å	7.5300(8)
c/Å	9.1546(10)
α/°	94.188(6)
β/°	96.753(7)
γ/°	105.647(7)
Volume/Å^3	435.76(8)
Z	1
ρ_{calc}g/cm^3	2.005
μ/mm^{-1}	3.640
F(000)	246.0
Crystal size/mm^3	0.06 × 0.04 × 0.03
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.652 to 57.11
Index ranges	-8 ≤ h ≤ 8, -10 ≤ k ≤ 10, -12 ≤ l ≤ 12
Reflections collected	7820
Independent reflections	2153 [R_{int} = 0.0233, R_{sigma} = 0.0226]
Data/restraints/parameters	2153/261/208
Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0350, wR_2 = 0.0950
Final R indexes [all data]	R_1 = 0.0540, wR_2 = 0.1055
Largest diff. peak/hole / e Å^{-3}	1.04/-0.43
CCDC number	2208886

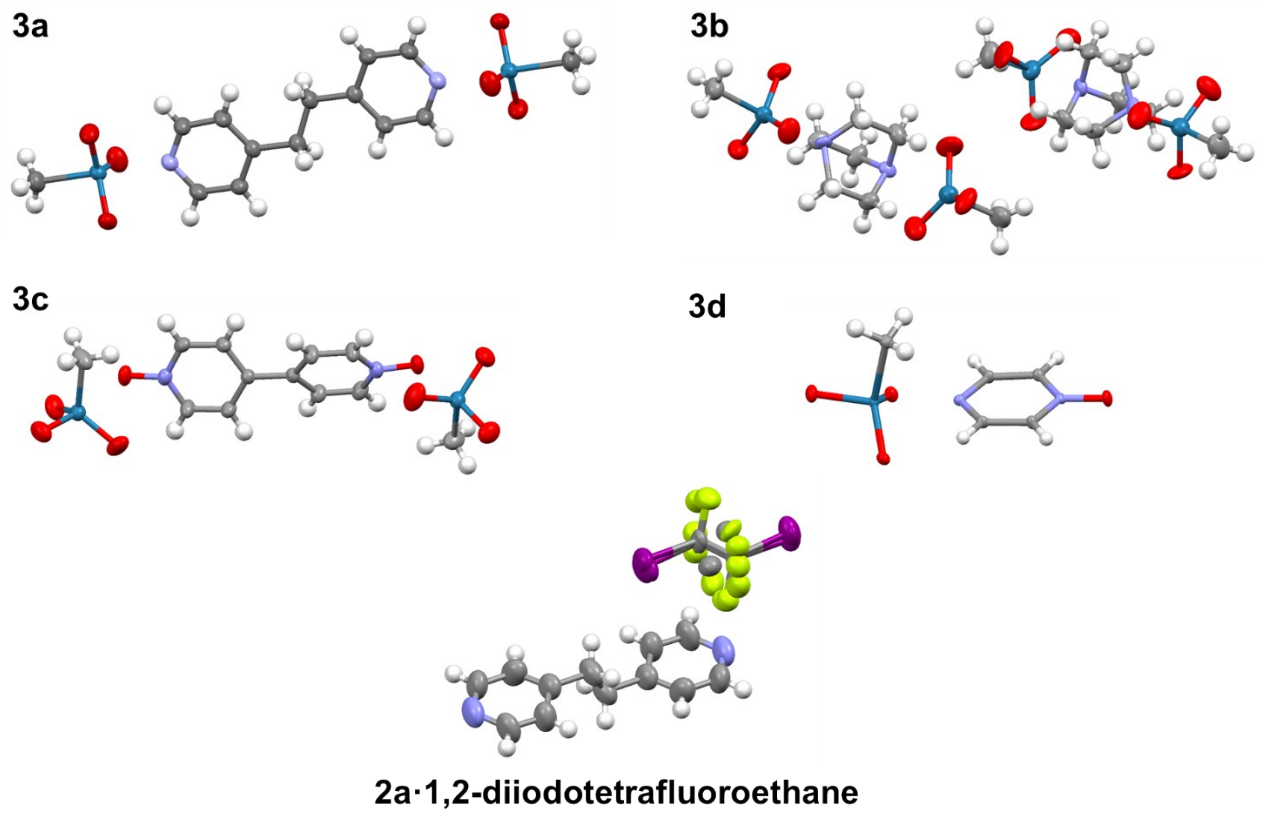

Figure S1: ADPs for each crystal structure reported in this work. Colour code: whitish, hydrogen; grey, carbon; indigo, nitrogen; red, oxygen; navy, rhenium; purple, iodine; yellow, fluorine.

S.3. CSD Surveys

Table S.6. Hits in the Cambridge Structural Database (CSD) containing methyltrioxorhenium. The search is set up with rhenium bound to three oxygen atoms by "double bond" and to a methyl group by "single bound". In blue, hits displaying a contact between the rhenium atom and a nucleophile (nucleophile=N, P, O, S, Se, F, Cl, Br, I) shorter than the sum of the respective van der Waals radii. According to Batsanov,[1] the crystallographic vdW radius of rhenium was set to 205 pm.

APAZOH	BUCQEW	KUHPUA01	TAHWAC	VUFQET
APAZUN	BUCQIA	NEXSAL	TAHWEG	VUFQIX
APIZIJ	ECIYIY	NEXSEP	TAHWIK	VUKFUE
BOTBIW	KATREC	NEXSIT	TAHWOQ	XANKIG
BOTBOC	KAZNII	NEXSOZ	TAHWUW	XODMIN
BOTBUI	KELZAC	NEXSUF	TAHXAD	YIDKAZ
BOTCAP	KELZEG	NEZWOE	TAHXEH	YIFSEL
BOWHEB	KEXSOV	NIFZIL	TULKIV	YOXVAI01
BUCQAS	KUHPUA	PELFAP	VOKHIO	YOXVAI02

S.4. Computational Data

The energetic features of the adducts analyzed in this work were calculated at the PBE0[2]-D3[3]/def2-TZVP[4] level of theory using either the crystallographic coordinates or fully optimized geometries. This level of theory has been used before[5,6,7] to analyze similar interactions and it has been proved to provide results similar to high level ab initio methods.[8] The GAUSSIAN-16 program has been used for the energetic calculations and NBO analysis.[9] The basis set superposition error for the calculation of interaction energies has been corrected using the counterpoise method.[10] Molecular electrostatic potential (MEP) surfaces have been computed at the same level of theory and represented using several isovalues of electron density to map the electrostatic potential. The QTAIM analysis[11] has been performed using the AIMAll program at the same level of theory.[12]

In order to assess the nature of interactions in terms of being attractive or repulsive and revealed them in real space,[13] we have used NCIPLOT index, which is a method for plotting non-covalent interaction regions,[14] based on the NCI (Non-Covalent Interaction) visualization index derived from the electronic density.[15] The reduced density gradient (RDG), coming from the density and its first derivative, is plotted as a function of the density (mapped as isosurfaces) over the assembly of interest. The sign of the second Hessian eigenvalue times the electron density [i.e. sign(λ_2)ρ in atomic units] enables the identification of attractive/stabilizing (blue-green coloured isosurfaces) or repulsive (yellow-red coloured isosurfaces) interactions using 3D-Plots. For the plots shown in Figures 3 and 4 of the main text the NCIplot index parameters are: RGD = 0.45; ρ cut off = 0.04 a.u.; color range: –0.03 a.u. ≤ sign(λ_2)ρ ≤ 0.03 a.u.

S.4.1. Cartesian Coordinates

1·Acetonitrile adduct (Figure 3a)

Re	0.00000000	0.00000000	0.61273592
O	0.00000000	1.67026612	0.28869327
O	1.44649289	-0.83513306	0.28869327
O	-1.44649289	-0.83513306	0.28869327
C	0.00000000	0.00000000	2.68853924
H	0.00000000	-1.03100517	3.04697827
H	0.89287667	0.51550258	3.04697827
H	-0.89287667	0.51550258	3.04697827
C	0.00000000	0.00000000	-3.27455787
C	0.00000000	0.00000000	-4.72146674
H	-0.88852699	-0.51299129	-5.09244566
H	0.00000000	1.02598259	-5.09244566
H	0.88852699	-0.51299129	-5.09244566
N	0.00000000	0.00000000	-2.12893113

2· Pyridine adduct (Figure 3b)

Re	-0.07915156	0.98747801	0.00000000
O	1.62714530	0.86504020	0.00000000
O	-0.91751984	0.67119458	1.45079402
O	-0.91751984	0.67119458	-1.45079402
C	-0.21525857	3.07231888	0.00000000
H	-1.26577981	3.36997329	0.00000000
H	0.27575003	3.46888571	0.89108449

H	0.27575003	3.46888571	-0.89108449
C	1.32432911	-2.07347167	0.00000000
C	1.46424615	-3.45119304	0.00000000
C	0.32155825	-4.23398955	0.00000000
C	-0.91751984	-3.61217999	0.00000000
C	-0.96369677	-2.22978967	0.00000000
N	0.13547443	-1.48072195	0.00000000
H	0.39444840	-5.31558610	0.00000000
H	2.17955100	-1.40559956	0.00000000
H	2.45214172	-3.89426291	0.00000000
H	-1.83643713	-4.18468659	0.00000000
H	-1.90617283	-1.69301140	0.00000000

3a (Figure 4)

N	4.72860840	2.42503659	7.39687853
C	6.03903502	3.91147204	9.37805544
C	6.79183118	4.72171552	10.40526298
H	6.99033348	5.59244369	10.02622083
H	7.63738134	4.28215515	10.58590682
C	6.56231133	3.79035974	8.09463111
H	7.36445470	4.20822076	7.87869047
C	5.89388882	3.05417298	7.14434495
H	6.26140599	2.98715042	6.29302400
C	4.22927562	2.53417404	8.62697809
H	3.42666325	2.10552573	8.81830909
C	4.84520473	3.25229578	9.63275721
H	4.46094153	3.29415176	10.47859060
N	8.12639083	7.21897384	14.72482560
C	6.81596421	5.73253839	12.74364869
C	6.06316929	4.92225611	11.71653331
H	5.86466575	4.05156674	12.09548330
H	5.21761789	5.36185529	11.53579730
C	6.29268790	5.85365069	14.02707302
H	5.49055305	5.43569788	14.24297489
C	6.96111041	6.58983745	14.97735918
H	6.59359324	6.65686001	15.82868012
C	8.62572485	7.10979760	13.49481819
H	9.42823635	7.53847637	13.30339287
C	8.00969610	6.39166752	12.48903690
H	8.39405770	6.34985868	11.64311353
Re	3.51895528	1.22067299	5.64139720
O	5.11089647	0.80862779	5.17611570
O	2.82787000	0.43371654	6.98726656
O	2.94614017	2.76810201	5.22840666
C	2.50889164	0.14453875	4.16096723
H	1.57160880	0.34775745	4.20096243
H	2.63922699	-0.79566061	4.30364473
H	2.85250115	0.38799059	3.29799257
Re	9.33604394	8.42333744	16.48030693
O	7.74400313	8.83537431	16.94558625
O	10.02702960	9.21028556	15.13443540
O	9.90885906	6.87590843	16.89329747
C	10.34610759	9.49947168	17.96073690
H	11.28339166	9.29621418	17.92083386
H	10.21577348	10.43963224	17.81815155
H	10.00249808	9.25601984	18.82371155

3b (Figure 4)

N	0.59732511	1.48317217	15.03442904
N	0.89333128	3.71850074	16.26854120
C	0.49796584	3.94392922	14.86972602
H	1.18240733	4.45706904	14.41261051
H	-0.33025413	4.44817667	14.83934071
C	-0.15415760	2.88269635	16.92193213
H	-1.00060313	3.35574554	16.90954370
H	0.08850857	2.72158403	17.84654009
C	-0.30398762	1.56085214	16.20124498
H	-0.10155244	0.83628012	16.81293500
H	-1.22194902	1.45747049	15.90612099
C	0.30498222	2.57721805	14.15788042
H	-0.61098940	2.50328146	13.84642857

H	0.88813702	2.53291896	13.38351423
C	2.00990775	1.62983912	15.51260959
H	2.61563156	1.61783078	14.75524624
H	2.23773417	0.88843130	16.09522246
C	2.16052932	2.95342908	16.27505349
H	2.42141656	2.76976065	17.19142767
H	2.85999971	3.48465160	15.86464771
Re	1.13817987	5.89686691	17.38161103
O	-0.54123737	5.95183498	17.11009144
O	1.68390490	4.95959928	18.69482273
O	2.19388143	6.14134293	16.07651992
C	1.32600842	7.80088147	18.24482551
H	2.25560134	7.98012989	18.42213472
H	0.98724255	8.46261613	17.63728622
H	0.83320000	7.83243174	19.06445415
Re	0.30826575	-0.60529073	13.84284056
O	-1.24938989	0.01878126	13.52198607
O	1.62792464	-0.01303107	12.92780859
O	0.63035750	-1.27613554	15.34306897
C	0.05455404	-2.41518763	12.84083805
H	-0.68467724	-2.89225624	13.22387038
H	0.85313942	-2.94105451	12.92294649
H	-0.12173845	-2.24436639	11.91200042

3c (Figure 4)

Re	6.46772074	6.19366638	1.50827852
C	7.36328400	6.50708406	7.14501190
C	5.62548654	6.34374887	5.50086358
H	4.77053715	6.06697389	5.26146437
C	6.10184668	6.09537687	6.76143117
H	5.56585939	5.64039188	7.37035729
C	8.13231904	7.16290309	6.19150294
H	8.99278176	7.44450845	6.40453625
C	7.63113541	7.39329225	4.94551692
H	8.15070581	7.83887830	4.31634714
N	6.39587793	6.98558768	4.61746065
O	5.88364947	7.30954328	3.41470729
O	6.03136832	7.71622828	0.90340002
O	7.95521598	6.04727741	2.33624776
O	6.63455169	5.18999766	0.13620157
C	4.90085489	5.01896136	2.24303744
H	4.79850340	4.23917015	1.69204397
H	4.08601616	5.52715883	2.23168476
H	5.09661136	4.74993066	3.14390672
C	7.84820026	6.30322008	8.53193450
C	9.09488849	7.06045065	10.43505964
H	9.66254611	7.68489314	10.82603850
C	8.70018556	7.21004914	9.13142312
H	9.01241909	7.93584532	8.64056444
C	7.42838268	5.22498356	9.30125369
H	6.86519571	4.58379001	8.93142654
C	7.84005744	5.10286537	10.59444989
H	7.54842664	4.38156094	11.10339619
N	8.66014357	6.01276603	11.14148236
O	8.97559746	5.92683122	12.44802165
Re	10.53591560	4.44867378	13.22337116
O	9.54310400	4.65500130	14.58209351
O	9.94431262	3.51153713	11.92292807
O	11.90458482	3.59513973	13.78562221
C	11.71358095	6.09416024	12.69389047
H	12.64144338	5.87540385	12.80948001
H	11.48990569	6.84231737	13.25304423
H	11.55148420	6.32263179	11.77531958

3d (Figure 4)

Re	1.03760762	5.83701893	1.28398541
O	2.62826773	5.26988704	1.56344433
O	1.10159523	6.64399853	-0.22874707
O	-0.21093146	4.66863641	1.13361949
C	-0.31263726	4.76735187	4.06788071
H	-1.07364115	4.80893606	3.53453698
C	1.93113662	5.08834651	4.35027454
H	2.76006721	5.33534138	4.00960372
C	1.85425423	4.69300972	5.65766163
H	2.61379131	4.69012061	6.19399183

C	-0.44204488	4.33259783	5.35840481
H	-1.27070004	4.06040785	5.68113487
N	0.65064643	4.30191352	6.16511871
N	0.86545807	5.13760835	3.53751447
O	0.55397310	3.88854049	7.37686573
C	0.50680798	7.59963107	2.32336841
H	1.21610480	7.84384355	2.92209358
H	-0.29679966	7.44446377	2.82604289
H	0.35894413	8.30954650	1.69490495

S.5. References

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