

SUPPLEMENTARY MATERIAL

Kinetic and Computational Studies of Rhenium Catalysis for Oxygen Atom Transfer Reactions

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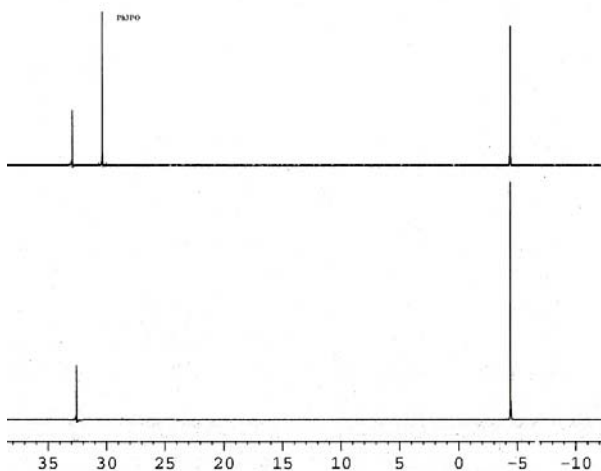


Figure S-1: ^{31}P -NMR in CDCl_3 spectrum before and after completion (3.0 h) of a reaction between 60 mM pyridine oxide, 140 mM PPh_3 , and 11 mM Re catalyst

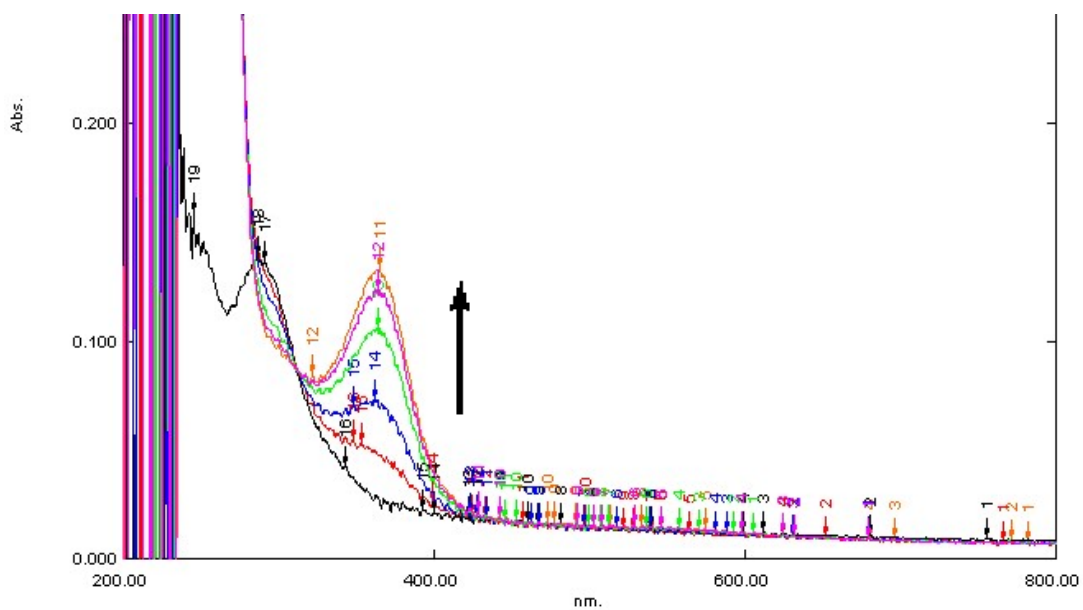


Figure S-2: UV repeated scan experiment of the monomerization reaction of Pyridine with $\{\text{MeReO}(\text{edt})\}_2$ every 3 min at the following concentration; 1.5 mM pyridine and 0.01 mM Re catalyst.

Table S3 : Initial rate M/s and rate constant (k) L mol⁻¹ s⁻¹ of picoline oxide

Ph ₃ As/10 ⁻³ M	PicO/10 ⁻³ M	1/10 ⁻³ M	Ri x10 ⁻⁵ M/s	k ^a / L mol ⁻¹ s ⁻¹
20	0.6	0.04	0.648	270.0
20	1.0	0.04	1.011	252.6
20	1.5	0.04	1.589	264.8
20	2.0	0.04	1.981	247.6
50	0.6	0.04	0.648	270.1
50	1.3	0.04	1.259	251.8
50	0.4	0.04	0.424	282.9
50	0.7	0.04	0.788	271.7
30	0.6	0.08	1.196	249.2
30	0.8	0.08	1.745	272.6
30	0.4	0.08	0.819	272.9
30	0.6	0.08	1.342	268.5
20	0.8	0.08	1.770	276.6
20	0.8	0.016	0.320	250.0
20	0.8	0.04	0.819	255.9
20	0.8	0.10	1.981	247.6
30	1.0	0.04	1.106	267.4
50	1.0	0.04	1.180	294.9
60	1.0	0.04	1.195	298.7
80	1.0	0.04	1.150	287.4

$$k = 268.1 \pm 3.5$$

$$^a k = Ri / [1][PicO]$$

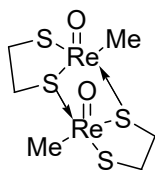
Table S-4 : Initial rate M/s and rate constant (k) L mol⁻¹ s⁻¹ of Pyridine oxide

Ph ₃ As/10 ⁻³ M	PyNO/10 ⁻³ M	1/10 ⁻³ M	Ri x10 ⁻⁵ M/s	k ^a / L mol ⁻¹ s ⁻¹
20	1.5	0.07	1.73	159.1
20	1.5	0.07	1.73	159.1
20	1.5	0.07	1.73	159.1
20	2.0	0.29	9.3	160.1
20	2.0	0.07	2.15	149.3
20	2.0	0.07	2.15	148.3
12	1.0	0.07	1.06	146.6
7.5	1.0	0.15	2.50	172.7
20	2.0	0.29	9.33	160.9
20	2.0	0.07	2.15	149.3
20	2.0	0.07	2.15	148.3
16	1.0	0.07	1.06	146.6
12	1.0	0.07	1.02	141.2
20	1.0	0.07	1.18	162.8
20	1.0	0.10	1.66	166

$$k = 155.3 \pm 2.3$$

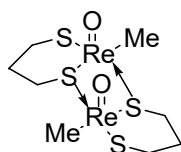
$$^a k = Ri / [1][PyNO]$$

Table S-5: Coordinate and absolute energy of the computational study



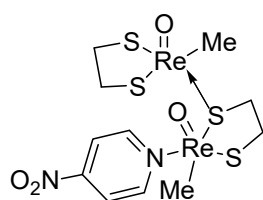
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RE	75.0	0.2836208720	1.7454054704	-0.9644159830
C	6.0	0.7797803270	-2.6998113430	0.6661058501
C	6.0	-0.3937966666	2.7571343870	0.7871777054
S	16.0	-1.9856635703	-1.9165551913	1.3114993881
S	16.0	-1.7179654671	0.3632347675	-0.8895062029
H	1.0	0.3673215298	-3.4861170014	1.3075561894
H	1.0	1.2062105585	-1.9305069166	1.3244635038
H	1.0	1.5950250034	-3.1202549161	0.0658389249
C	6.0	-3.4194316072	-0.7659293256	0.9802222352
C	6.0	-2.9423625982	0.6029797045	0.5094917917
H	1.0	-3.9706569074	-0.6712662953	1.9223943445
H	1.0	-4.0763846136	-1.2352129401	0.2411520424
H	1.0	-2.4489169734	1.1503980358	1.3138869862
H	1.0	-3.7623926228	1.2078197959	0.1092322039
S	16.0	2.3461701353	1.9550741027	0.0139704836
S	16.0	1.0428193082	-0.4441845977	-1.6102314080
O	8.0	0.1384629474	2.8460226272	-2.2113425174
C	6.0	2.8083490258	-0.6250238632	-1.0085363146
H	1.0	3.3224877173	-1.2650669790	-1.7325363500
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H	1.0	-1.4103346665	3.1447023701	0.6517130198
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S	16.0	-0.5748767586	-1.3399202297	0.6092031736
H	1.0	-3.0878322986	2.5177752826	-1.2322725096
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S	16.0	0.5361776392	1.3779971092	0.6840433522
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H	1.0	1.4405195493	-2.9977204483	-1.3052018923
H	1.0	2.6272957689	-1.9669533301	-2.1505743218
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H	1.0	-0.9947399064	-2.8347249811	-1.2819030068
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H	1.0	-4.6269681582	-2.0852141706	-1.0075035863
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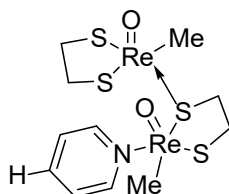
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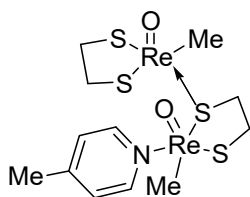
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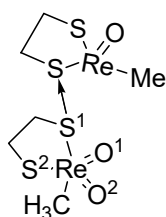
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C	6.0	-1.2922415995	-1.1361318914	2.1262103187
C	6.0	3.4714627126	1.3767893793	1.1950351152
S	16.0	-3.8920531756	-0.4749933185	0.7840168357
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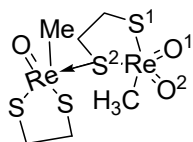
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RE	75.0	-2.3753979073	-0.5193025787	-0.1035217599
C	6.0	-4.5024474994	-0.8093239182	0.0258761995
C	6.0	0.9914475318	-2.0385511330	-0.7722510114
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S	16.0	2.6503266641	1.6724286190	-0.6082898658
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C	6.0	4.9665699982	0.2198564019	-0.0035162166
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S	16.0	-3.2909634408	1.6342775826	0.3434334813
S	16.0	-0.3524572681	0.8461385193	-0.4226234063
O	8.0	-2.2486438976	-1.2346216887	-1.6393381446
C	6.0	-0.5993115520	2.3245768917	0.6538028592
H	1.0	0.2291721711	3.0037870052	0.4293033029

H	1.0	-0.5396275171	2.0107524009	1.6986116404
C	6.0	-1.9486676382	2.9178622921	0.2967449143
H	1.0	-1.9315903514	3.3669201289	-0.7003594406
H	1.0	-2.2415040708	3.6841634341	1.0218288487
H	1.0	-4.5913167533	-1.9007618469	-0.0371739729
H	1.0	-5.0127258034	-0.3391732967	-0.8152981638
H	1.0	-4.9104073816	-0.4568214390	0.9733206743
O	8.0	-1.9977643441	-1.4800735629	1.2380153736

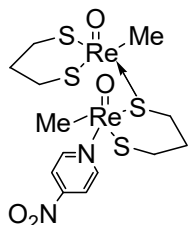
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O	8.0	1.8065853749	-0.3756467100	-2.3303975972
RE	75.0	1.9197590060	0.3400242843	-0.8133443624
RE	75.0	-2.3383311586	-0.7777923824	-0.0428460216
C	6.0	-1.0528959950	-1.7449996443	-1.4580954096
C	6.0	2.1694710469	2.4665158211	-0.9706370506
S	16.0	4.1328209392	0.3697364086	-0.2637451929
S	16.0	1.6049927780	-0.9673397648	1.0625556764
H	1.0	2.1706603614	2.8995909229	0.0407720973
H	1.0	1.3676868364	2.9483529433	-1.5450294887
H	1.0	3.1309765187	2.7352582595	-1.4217796011
C	6.0	4.3759029214	-1.2090029155	0.7015848157
C	6.0	3.2983104646	-1.3505193214	1.7685890890
H	1.0	5.3736883558	-1.1565588327	1.1519811598
H	1.0	4.3511324239	-2.0499087619	0.0007148834
H	1.0	3.4750425663	-0.6594146732	2.5993728651
H	1.0	3.2507136686	-2.3706886879	2.1643875900
S	16.0	-0.5682714506	0.9161738537	-0.5787548528
S	16.0	-2.7526454226	0.7609521113	1.6956775488
O	8.0	-2.4390578918	-2.1393648838	0.9552500708
C	6.0	-2.0652504680	2.3948800253	1.1976640001
H	1.0	-2.1147226190	3.0332188684	2.0863191662
H	1.0	-2.6899511470	2.8323705208	0.4140150826
C	6.0	-0.6295321096	2.2109109811	0.7431999086
H	1.0	0.0090022145	1.8845598977	1.5683223226
H	1.0	-0.2211211041	3.1267296077	0.3077784801
H	1.0	-1.6857712613	-2.5882271556	-1.7603969375
H	1.0	-0.1518272483	-2.0994578562	-0.9558042677

H	1.0	-0.7928716221	-1.1408358230	-2.3262035065
O	8.0	-3.6499259787	-0.5904270931	-1.0905904678

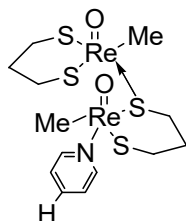
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O	8.0	3.0947281539	1.9842521227	-1.2592036564
RE	75.0	2.4445228613	1.1297600939	0.0276973957
RE	75.0	-1.1031962435	-1.7770476950	0.1020350045
C	6.0	2.7442562055	2.2693358521	1.8147633629
C	6.0	-0.5005189032	-1.4233631717	2.1159667027
S	16.0	4.1470320149	-0.0484357519	1.0059398901
S	16.0	1.2597141666	-0.7853413174	-0.6900802026
S	16.0	-3.1791347134	-2.2032683348	0.9681369746
S	16.0	-1.9528525619	-0.2094356255	-1.3727917236
O	8.0	-0.5983628668	-3.2904216980	-0.4338160322
H	1.0	3.7851000349	2.3057634668	2.1483099128
H	1.0	2.1657881341	1.8050075422	2.6268676980
H	1.0	2.3679669374	3.2910270839	1.6771765584
H	1.0	-0.4347160584	-2.4109730868	2.5936036044
H	1.0	-1.2481042328	-0.8595663212	2.6884875577
H	1.0	0.4797041153	-0.9403734092	2.2266840400
C	6.0	2.2620239110	-2.3503958073	-0.6954371022
H	1.0	2.1059251279	-2.8706483034	0.2545535903
H	1.0	1.7989673618	-2.9520757505	-1.4821339835
C	6.0	3.7513403737	-2.1291354876	-0.9673827106
H	1.0	4.1762134208	-3.0736444867	-1.3375706704
H	1.0	3.8889358813	-1.3865259841	-1.7640601150
C	6.0	4.5316819785	-1.7149698478	0.2805294856
H	1.0	5.6047496640	-1.6756205220	0.0602899407
H	1.0	4.3838437052	-2.4513888825	1.0797092064
C	6.0	-4.3247488951	-2.3061649568	-0.4965823328
H	1.0	-3.8210356389	-2.9413145587	-1.2304659399
H	1.0	-5.2120230656	-2.8465675139	-0.1485369267
C	6.0	-4.7386139748	-0.9608639014	-1.1385482505
H	1.0	-4.9296979098	-1.1362234211	-2.2056336733
H	1.0	-5.6869507143	-0.6189323728	-0.7005833292
C	6.0	-3.7317733518	0.1869429072	-0.9754655828
H	1.0	-4.0006847724	1.0118361311	-1.6455321793
H	1.0	-3.7557310960	0.5599340430	0.0522837469

C	6.0	-0.3124206979	1.9590740105	1.2362024694
C	6.0	0.0905666832	2.8155261995	-0.8892734358
C	6.0	-1.5185622347	2.6392287661	1.3291572026
H	1.0	0.0219140534	1.3238014666	2.0455749720
C	6.0	-1.0919825318	3.5374545054	-0.8697908304
H	1.0	0.7501686334	2.8407104183	-1.7468418517
C	6.0	-1.8959693952	3.4398421079	0.2601534789
H	1.0	-2.1469119219	2.5493673360	2.2065238136
H	1.0	-1.3861473944	4.1500669804	-1.7125477946
N	7.0	0.4960348087	2.0467373032	0.1540417105
N	7.0	-3.1712403931	4.1784684158	0.3220815590
O	8.0	-3.8534845482	4.0315378600	1.3330246154
O	8.0	-3.4583941111	4.8853635951	-0.6408161698

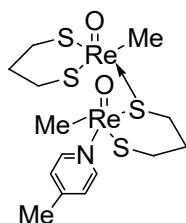
E= -2669.179638 Hartree



O	8.0	3.2305312427	1.0966548084	-1.4750970262
RE	75.0	2.5599758627	0.4689007539	-0.0721267808
RE	75.0	-1.8896127178	-0.9042605546	0.2245193117
C	6.0	3.4683647682	1.3909347383	1.6267204247
C	6.0	-1.3424325385	-0.6806417964	2.2709838872
S	16.0	3.9279329672	-1.2319133168	0.6340552966
S	16.0	0.7101585130	-0.9277976781	-0.4399070175
S	16.0	-4.0180634674	-0.4238095859	0.9189670712
S	16.0	-1.9399637187	0.7803109753	-1.3672794746
O	8.0	-1.9791693692	-2.5320383800	-0.1953409351
H	1.0	4.5002521242	1.0773172063	1.8108325312
H	1.0	2.8850533318	1.1045604348	2.5153628875
H	1.0	3.4279348692	2.4840216305	1.5396654813
H	1.0	-1.8297875106	-1.4854991058	2.8375796569
H	1.0	-1.7275974018	0.2594114051	2.6884552223
H	1.0	-0.2624162126	-0.7366269216	2.4610488399
C	6.0	1.0830611339	-2.7464239334	-0.4211032135
H	1.0	1.0044753425	-3.1111596460	0.6080314581
H	1.0	0.2665333214	-3.1871784263	-0.9979909852
C	6.0	2.4439159429	-3.0858438191	-1.0347316608
H	1.0	2.4178330053	-4.1352255957	-1.3653965432
H	1.0	2.6124221468	-2.4795641855	-1.9345878420
C	6.0	3.6095471278	-2.9278263606	-0.0585442613

H	1.0	4.5487699336	-3.2143290220	-0.5456479492
H	1.0	3.4705280607	-3.5907498030	0.8048221709
C	6.0	-4.9994363244	-0.1272272010	-0.6344184958
H	1.0	-4.7312670073	-0.9338191082	-1.3221547382
H	1.0	-6.0525789878	-0.2620841273	-0.3634549578
C	6.0	-4.7965161299	1.2489236512	-1.3098896876
H	1.0	-4.9934979628	1.1330618982	-2.3842559539
H	1.0	-5.5419412343	1.9610660549	-0.9274876868
C	6.0	-3.4152832329	1.8874839108	-1.1011746587
H	1.0	-3.2833891952	2.7210557038	-1.8008196680
H	1.0	-3.3352203870	2.2819089261	-0.0848186626
C	6.0	0.4153594468	2.1817608204	1.4439512296
C	6.0	0.8974537651	2.9566477732	-0.6895095341
C	6.0	-0.4413296566	3.2508049508	1.6807674395
H	1.0	0.5699017337	1.4201988543	2.1978953627
C	6.0	0.0701488132	4.0564766095	-0.5138093972
H	1.0	1.4357762816	2.7952943603	-1.6146509797
C	6.0	-0.6154187835	4.2145303885	0.6906804414
H	1.0	-0.9552911887	3.3144748210	2.6341273186
H	1.0	-0.0348079149	4.7710781183	-1.3236861752
H	1.0	-1.2713830083	5.0648837579	0.8513163703
N	7.0	1.0838942155	2.0290560156	0.2811218832

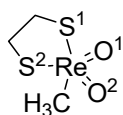
E= -2464.771938 Hartree



O	8.0	3.1546203721	1.0285170284	-1.6452850988
RE	75.0	2.5151711428	0.4621977113	-0.2032221286
RE	75.0	-1.7794566858	-1.2115010347	0.2023868744
C	6.0	3.3677981913	1.5906813515	1.4003276413
C	6.0	-1.1770623727	-0.9149688950	2.2282483269
S	16.0	3.9727666608	-1.0835741888	0.6577001602
S	16.0	0.7701652269	-1.0825990989	-0.5317775499
S	16.0	-3.8996455312	-0.7797085641	0.9735357573
S	16.0	-1.9901590977	0.3808473594	-1.4742684654
O	8.0	-1.8372896549	-2.8542908649	-0.1548800771
H	1.0	4.4132480359	1.3471821066	1.6118641161
H	1.0	2.7981412870	1.3767756101	2.3172514184
H	1.0	3.2755355197	2.6652105030	1.1958798863
H	1.0	-1.6281251993	-1.7175341012	2.8271368187

H	1.0	-1.5757687210	0.0243071143	2.6342507348
H	1.0	-0.0912111508	-0.9373614594	2.3902511339
C	6.0	1.2512012561	-2.8711989674	-0.4030709840
H	1.0	1.1233339273	-3.1982409750	0.6340048407
H	1.0	0.5032138980	-3.3872307574	-1.0105632044
C	6.0	2.6690787215	-3.1491950752	-0.9087742915
H	1.0	2.7358090658	-4.2140165576	-1.1781823120
H	1.0	2.8571251757	-2.5785698540	-1.8275384580
C	6.0	3.7524672707	-2.8520207480	0.1280046065
H	1.0	4.7343144425	-3.1475714212	-0.2605938303
H	1.0	3.5708591432	-3.4325827196	1.0408455740
C	6.0	-4.9573631875	-0.6357334742	-0.5516806186
H	1.0	-4.6629959844	-1.4639309000	-1.2018438661
H	1.0	-5.9886441799	-0.8185855687	-0.2296671552
C	6.0	-4.8658167600	0.7041150205	-1.3160115431
H	1.0	-5.1036434764	0.5124671701	-2.3712892814
H	1.0	-5.6326830124	1.3973951194	-0.9406194089
C	6.0	-3.5128783481	1.4222719986	-1.2082527661
H	1.0	-3.4535852677	2.2197799767	-1.9579924812
H	1.0	-3.4136816444	1.8764308343	-0.2184703106
C	6.0	0.2523300871	2.0820274409	1.2504849037
C	6.0	0.6527318655	2.7648152664	-0.9233514479
C	6.0	-0.6845634296	3.0885957712	1.4321070551
H	1.0	0.4701056909	1.3812434011	2.0466830419
C	6.0	-0.2598095617	3.8010890657	-0.7974316510
H	1.0	1.1885891630	2.5972561274	-1.8489135240
C	6.0	-0.9613077904	3.9912810441	0.3980424263
H	1.0	-1.1958282611	3.1595769443	2.3877413565
H	1.0	-0.4280066741	4.4530999075	-1.6494782504
N	7.0	0.9266652793	1.9120959181	0.0920483058
C	6.0	-1.9676103839	5.1015946202	0.5670468772
H	1.0	-2.9443028062	4.7036748046	0.8675242467
H	1.0	-1.6517765705	5.8047319994	1.3479731130
H	1.0	-2.1023956712	5.6661240101	-0.3600705112

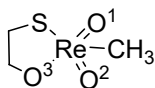
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S	16.0	-0.4307603268	-0.9511474812	-1.8405607211
RE	75.0	-0.5868172723	-1.1998753285	0.5022835706
C	6.0	-0.1154531781	-0.6848573002	2.5538184965
H	1.0	0.9581317285	-0.7307536805	2.7336798890

H	1.0	-0.6317234136	-1.4826863227	3.0989870227
H	1.0	-0.5191770680	0.2860507768	2.8388133526
O	8.0	-2.2578323010	-1.1724687478	0.7914035720
S	16.0	0.6157399472	0.8813005681	0.4580771887
C	6.0	0.9639518053	1.3384986586	-1.3022031606
H	1.0	1.0379686604	2.4315698181	-1.3334387613
H	1.0	1.9293395839	0.9118075830	-1.5894049593
C	6.0	-0.1458653052	0.8320403172	-2.2071101894
H	1.0	0.1317109477	0.8909793108	-3.2655734885
H	1.0	-1.0769130727	1.3842616063	-2.0520833744
O	8.0	0.1276992659	-2.7347198307	0.6133115098

E= -1144.245153 Hartree



O	8.0	1.5560287059	0.0229521048	-2.0461415962
RE	75.0	1.1794677409	-0.1043835446	-0.3929549116
S	16.0	-0.9675790790	-0.7689874448	0.4430985469
O	8.0	2.5292934204	-0.1625482741	0.6331644248
O	8.0	0.3923065155	1.5708699230	-0.0196517647
C	6.0	1.1028226562	-2.2548268070	-0.5966418337
H	1.0	2.0813186136	-2.4758435898	-1.0353938438
H	1.0	0.3115295125	-2.5718548461	-1.2759811289
H	1.0	1.0065943694	-2.7394338002	0.3742778913
C	6.0	-0.9834153806	1.9169384893	0.1517087586
C	6.0	-1.6346644994	0.8536361613	1.0135882544
H	1.0	-1.3910629835	0.9913920291	2.0714329900
H	1.0	-2.7224789884	0.8403037264	0.8974280042
H	1.0	-1.0037086287	2.9078405175	0.6186800058
H	1.0	-1.4564518678	1.9739454051	-0.8366137972

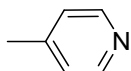
E = -821.338848 Hartree



C	6.0	1.1239828688	0.7147190158	0.0000589775
C	6.0	1.1876810492	-0.6702616191	0.0000479453
C	6.0	-0.0000634081	-1.3800324803	-0.0000048238
C	6.0	-1.1876986083	-0.6700418726	-0.0001225990
C	6.0	-1.1239264059	0.7148387898	-0.0000890676
H	1.0	2.0495686702	1.3078822687	0.0001526173
H	1.0	2.1562936762	-1.1807571158	0.0001578454
H	1.0	-2.1563178121	-1.1804792127	-0.0001669341
H	1.0	-2.0495323494	1.3080493377	-0.0001008527

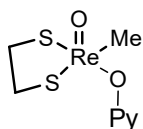
N 7.0 0.0000675289 1.4111173147 0.0000206493
 H 1.0 -0.0001652793 -2.4761643762 0.0000462325

E(M11-L) = -248.310827 Hartree



C 6.0 1.2141727733 1.1203826410 0.0067326441
 C 6.0 -0.1689528842 1.1809309546 -0.0085982836
 C 6.0 -0.9009526353 -0.0001593656 -0.0154637302
 C 6.0 -0.1687929272 -1.1811065420 -0.0104522975
 C 6.0 1.2143464752 -1.1204354113 0.0051502989
 H 1.0 1.8018045311 2.0495888014 0.0098965457
 H 1.0 -0.6778977289 2.1523065276 -0.0184649331
 H 1.0 -0.6776151708 -2.1525258749 -0.0216227315
 H 1.0 1.8020107175 -2.0496131248 0.0070709326
 N 7.0 1.9167144275 0.0000033221 0.0139465982
 C 6.0 -2.3893067093 0.0000792971 -0.0025981339
 H 1.0 -2.7744642700 0.0044110741 1.0316083509
 H 1.0 -2.8027019756 0.8898128912 -0.5022952374
 H 1.0 -2.8029546236 -0.8937051915 -0.4948700233

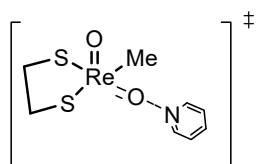
E(M11-L) = -287.6360917 Hartree



O 8.0 0.5968954348 -1.1073979525 1.7938453394
 RE 75.0 0.6735977031 -0.6155692017 0.2003099788
 S 16.0 2.7637458990 0.1302530750 -0.1484551676
 O 8.0 -1.1829206019 -1.2466679436 -0.4656189158
 S 16.0 -0.0284239174 1.4984016250 -0.3024708109
 C 6.0 1.1259207939 -2.1523612867 -1.1302310826
 C 6.0 2.6336235664 1.9201350524 0.1554413011
 C 6.0 1.4756122795 2.4870049652 -0.6058811284
 H 1.0 0.9991161519 -1.7257446317 -2.1456006409
 H 1.0 0.4081159629 -2.9896274284 -1.0552990350
 H 1.0 2.1557060380 -2.5451111478 -1.0853437032
 H 1.0 2.5104972715 2.0960816046 1.2405472823
 H 1.0 3.5822044951 2.3913356942 -0.1601536534
 H 1.0 1.2555749313 3.5264640647 -0.3023732802
 H 1.0 1.6842860041 2.4857846701 -1.6919929637
 C 6.0 -2.9348855066 -0.0196767867 -1.2209331747

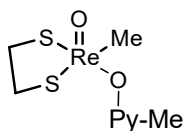
C	6.0	-2.5342149930	-0.2312626820	1.0741565947
C	6.0	-4.0510844874	0.7487744688	-0.9809161219
H	1.0	-2.5456044642	-0.2944169639	-2.2022889738
C	6.0	-3.6455684120	0.5285201330	1.3581878389
H	1.0	-1.8389491442	-0.6535955098	1.8069466818
C	6.0	-4.4183698482	1.0294814700	0.3237064519
H	1.0	-4.6165879022	1.1350271661	-1.8322217578
H	1.0	-3.8893965976	0.7282642510	2.4043060830
N	7.0	-2.2213533059	-0.4933981199	-0.1986692856
H	1.0	-5.3004673510	1.6413414145	0.5336221436

E(M11-L) = -1393.0159371 Hartree



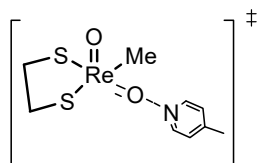
O	8.0	0.7974022593	-1.0604233922	1.7617120134
RE	75.0	0.7035601677	-0.5519703508	0.1782506824
S	16.0	2.7740813969	0.2300829335	-0.4471674071
O	8.0	-0.9258040328	-1.1492563067	-0.4706101639
S	16.0	-0.0107353788	1.6329277861	-0.1305979128
C	6.0	1.3096850010	-2.1405700572	-1.0703919459
C	6.0	2.6928196126	1.9613855921	0.0724258730
C	6.0	1.4718742524	2.6081836201	-0.5074528811
H	1.0	1.0571806864	-1.8777646652	-2.1132778512
H	1.0	0.7428185404	-3.0565210119	-0.8304746875
H	1.0	2.3897906715	-2.3625881961	-1.0380002792
H	1.0	2.6760463464	2.0193827729	1.1768954069
H	1.0	3.6102549463	2.4705067292	-0.2774658955
H	1.0	1.3179322662	3.6244985586	-0.1001049499
H	1.0	1.5634856714	2.6943961139	-1.6062470291
C	6.0	-3.1018226754	-0.2378829162	-1.3091094325
C	6.0	-2.5820530323	0.0912402900	0.9297253881
C	6.0	-4.3642614715	0.2922415715	-1.1327114545
H	1.0	-2.7086476948	-0.6197182798	-2.2566839623
C	6.0	-3.8333316797	0.6207634538	1.1818048387
H	1.0	-1.7808634194	-0.0241684657	1.6752448293
C	6.0	-4.7321178293	0.7247952268	0.1331774259
H	1.0	-5.0464094707	0.3687937107	-1.9840282531
H	1.0	-4.0918838553	0.9459899609	2.1933091827
N	7.0	-2.2787353966	-0.2953859619	-0.2872153031
H	1.0	-5.7304058818	1.1407412835	0.3031037682

E(M11-L) = -1392.9952714 Hartree



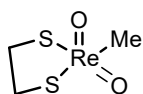
O	8.0	0.8385723327	-0.9543602075	1.8439213363
RE	75.0	0.9327298324	-0.5372129010	0.2295751521
S	16.0	2.9166858359	0.4752829295	-0.0711577549
O	8.0	-0.7743949454	-1.4431814471	-0.4966772350
S	16.0	-0.0250927195	1.4310636057	-0.4276633520
C	6.0	1.6657794599	-2.0616881902	-0.9859104288
C	6.0	2.5298518346	2.2448203923	0.1054388759
C	6.0	1.3441872847	2.5961659747	-0.7385663460
H	1.0	1.5458844933	-1.7060757436	-2.0290037817
H	1.0	1.0633793610	-2.9846510496	-0.9024381559
H	1.0	2.7343170881	-2.3062765237	-0.8620567832
H	1.0	2.3311195906	2.4702130035	1.1699812599
H	1.0	3.4198681867	2.8220662039	-0.2046296614
H	1.0	0.9716419865	3.6129669953	-0.5181107433
H	1.0	1.6042905091	2.5543554449	-1.8128886066
C	6.0	-2.6848608314	-0.5635872066	-1.3599468059
C	6.0	-2.3081833979	-0.5312581097	0.9406743081
C	6.0	-3.9057164232	0.0407714359	-1.1922112056
H	1.0	-2.2439825290	-0.8519448185	-2.3154017426
C	6.0	-3.5265025980	0.0714546394	1.1479150955
H	1.0	-1.5799894371	-0.7835423663	1.7186449853
C	6.0	-4.3614249362	0.3792149511	0.0798430460
H	1.0	-4.5020311664	0.2656051287	-2.0816197665
H	1.0	-3.8166640081	0.3129169078	2.1747462280
N	7.0	-1.9243783786	-0.8405554153	-0.2997208498
C	6.0	-5.6779085995	1.0391417136	0.2764890713
H	1.0	-5.7512394039	1.9658336811	-0.3151495006
H	1.0	-6.5037852506	0.3867916482	-0.0522873591
H	1.0	-5.8532585008	1.2965524935	1.3307172607

E(M11-L) = -1432.34301130 Hartree



O	8.0	1.1599781481	-1.0306091900	1.7756714427
RE	75.0	1.0028177929	-0.5611454058	0.1854584875
S	16.0	2.9831869487	0.4181672321	-0.4578787956
O	8.0	-0.5578154950	-1.3381488029	-0.4359955960
S	16.0	0.0692624737	1.5345955390	-0.1570346674
C	6.0	1.7595448811	-2.0972318270	-1.0464168204
C	6.0	2.7261532177	2.1329099187	0.0594880584
C	6.0	1.4490098160	2.6534631931	-0.5267206089
H	1.0	1.4808689527	-1.8709125301	-2.0913319035
H	1.0	1.2850588142	-3.0616096801	-0.7962704030
H	1.0	2.8563083224	-2.2121069154	-1.0151393607
H	1.0	2.6976604559	2.1894464417	1.1638980675
H	1.0	3.5894343652	2.7321339140	-0.2858221333
H	1.0	1.1921131691	3.6497025246	-0.1214513845
H	1.0	1.5374625316	2.7474728926	-1.6251470630
C	6.0	-2.7752518451	-0.5611333342	-1.3380482005
C	6.0	-2.3609112161	-0.2205839847	0.9136245159
C	6.0	-4.0556179855	-0.0678502393	-1.2131469651
H	1.0	-2.3370809067	-0.9290051195	-2.2714846251
C	6.0	-3.6374068774	0.2650397244	1.1109792508
H	1.0	-1.5907137252	-0.3018735676	1.6948100647
C	6.0	-4.5133241383	0.3583215586	0.0335204815
H	1.0	-4.7008016991	-0.0109086608	-2.0963126086
H	1.0	-3.9468676775	0.5761991452	2.1142133391
N	7.0	-1.9918143129	-0.6027918881	-0.2852471012
C	6.0	-5.8828417739	0.9128248929	0.1971314694
H	1.0	-5.9062663106	1.9762162350	-0.0954560262
H	1.0	-6.6134867271	0.3897205531	-0.4382418757
H	1.0	-6.2268491989	0.8540373808	1.2400909614

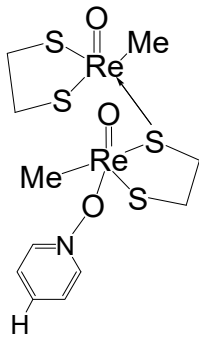
E(M11-L) = -1432.3217325 Hartree



S	16.0	-0.4287096496	-0.9444106275	-1.8429930948
RE	75.0	-0.5836917410	-1.2000494909	0.5003963998
C	6.0	-0.1180606526	-0.6819578618	2.5514289910
H	1.0	0.9554932934	-0.7226134141	2.7327092943
H	1.0	-0.6316327960	-1.4808403663	3.0976313415
H	1.0	-0.5261138796	0.2878342458	2.8341937300
O	8.0	-2.2552644005	-1.1801328859	0.7863476869
S	16.0	0.6135786510	0.8860201735	0.4535748834
C	6.0	0.9642773285	1.3311411290	-1.3012909540

H	1.0	1.0475628646	2.4235117885	-1.3365091630
H	1.0	1.9252578810	0.8958532563	-1.5902387195
C	6.0	-0.1476056058	0.8340562963	-2.1992911097
H	1.0	0.1247904322	0.8967631466	-3.2589355012
H	1.0	-1.0775631103	1.3863331495	-2.0371902531
O	8.0	0.1376813859	-2.7315085917	0.6101664156

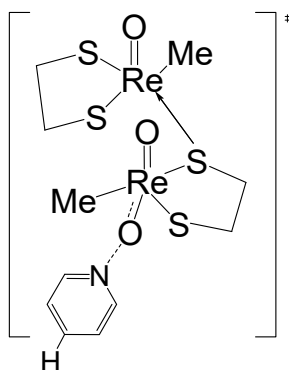
E(M11-L) = -1144.733725 Hartree



O	8.0	-3.2516234333	-1.1384393403	0.6760638860
RE	75.0	-1.9799667814	-0.0541058028	0.5405048703
RE	75.0	2.0643692051	-0.8066928675	-0.1954482870
S	16.0	-2.6783263882	1.9652004723	1.4041419192
S	16.0	-1.8833079535	1.0034352059	-1.5210341615
C	6.0	-0.8243663898	-0.1689273056	2.3550551470
H	1.0	-0.6577679445	0.7833071012	2.8735769947
H	1.0	0.1387136242	-0.6919635865	2.2847861346
H	1.0	-1.4650135725	-0.7652500308	3.0223442231
C	6.0	-3.4754164908	2.8141073007	-0.0573361019
C	6.0	-2.5883314849	2.7265063741	-1.2891569956
H	1.0	-3.6547024901	3.8560531862	0.2339789217
H	1.0	-4.4416972358	2.3304304451	-0.2341812279
H	1.0	-1.7453038975	3.4237827546	-1.2133235598
H	1.0	-3.1475795279	2.9613417713	-2.2018790784
S	16.0	2.4200565624	-2.8009554560	0.8610184922
C	6.0	3.3106816260	-0.0604701346	1.3690016990
S	16.0	-0.1977443120	-1.5305083394	-0.4858985752
O	8.0	2.9212033014	-0.8327625639	-1.6354464858
C	6.0	-0.3188058274	-3.1458125491	0.4443278149
H	1.0	-1.1459395929	-3.6993331950	-0.0121911576
H	1.0	-0.5707623563	-2.9219572045	1.4844667769
C	6.0	1.0007155418	-3.8966944215	0.3430466181
H	1.0	1.1815031831	-4.2529026973	-0.6764897707
H	1.0	1.0037569926	-4.7587880963	1.0189154385
H	1.0	3.7738908504	0.9009759792	1.1177442746
H	1.0	4.0965156630	-0.7542881872	1.6832228023
H	1.0	2.6549788113	0.1041398074	2.2365579945
C	6.0	2.7430447552	2.6258259525	-0.5687269475
C	6.0	1.0385583194	3.0285631114	1.0429789856
C	6.0	3.2457981563	3.9081351527	-0.3848841045
H	1.0	3.1466140818	1.8981570740	-1.2603842040
C	6.0	1.5175496677	4.3177445360	1.2470975805
H	1.0	0.1545049743	2.6132517344	1.5125946799
C	6.0	2.6359391806	4.7689731959	0.5357409522
H	1.0	4.1041439963	4.2214880276	-0.9659616182

H	1.0	1.0063677592	4.9551119929	1.9577786361
H	1.0	3.0177037436	5.7715364255	0.6876839793
N	7.0	1.6695410224	2.2150283449	0.1565300273
O	8.0	1.1097451710	1.0150456331	-0.0869768323

E(M11-L) = -2461.981092 Hartree

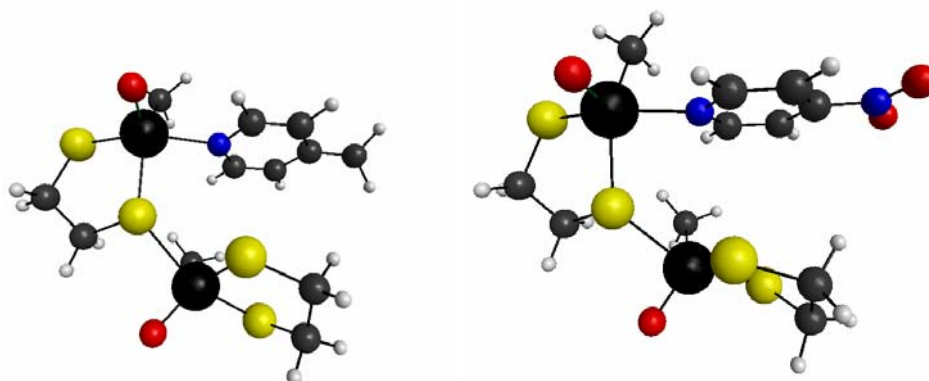


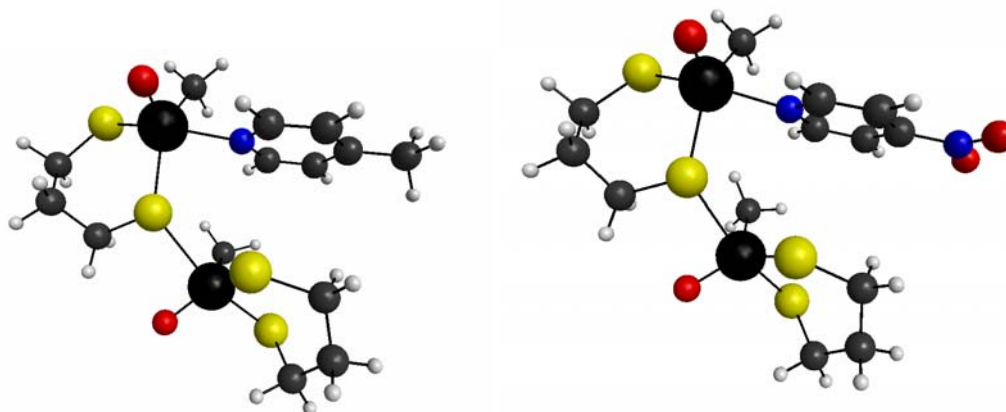
O	8.0	2.8545502271	-2.2259736565	-0.3232370655
RE	75.0	1.9516258349	-0.8153403683	-0.2260809785
RE	75.0	-2.1492397579	-0.3013698119	0.3130061222
S	16.0	3.2354036980	0.8916116465	-1.0853814983
S	16.0	2.1020649333	0.2692752080	1.8145680282
C	6.0	0.8448434002	-0.6047310916	-2.0615814761
H	1.0	1.0001107548	0.3365620268	-2.6022342093
H	1.0	-0.2336563423	-0.8012987935	-2.0114528841
H	1.0	1.2785401644	-1.3910391586	-2.6982556554
C	6.0	4.1989421716	1.5054638038	0.3924450412
C	6.0	3.2850898387	1.7069262512	1.5910691008
H	1.0	4.6827280621	2.4434549224	0.0946360136
H	1.0	4.9762756962	0.7667371458	0.6130239248
H	1.0	2.6852718477	2.6179590834	1.4781498997
H	1.0	3.8592826726	1.7867419530	2.5210366981
S	16.0	-2.9377911078	-2.1312887340	-0.8880131761
C	6.0	-3.0860810629	0.7618818247	-1.2743664244
S	16.0	-0.2083424299	-1.7065040450	0.7675670237
O	8.0	-3.1080321799	-0.1428473196	1.6797575220
C	6.0	-0.5011680141	-3.2838822360	-0.1771330853
H	1.0	0.0599725030	-4.0634876654	0.3495006472
H	1.0	-0.0811713396	-3.1602533355	-1.1781333155
C	6.0	-1.9877166151	-3.5944836527	-0.2400693941
H	1.0	-2.3846312742	-3.8614850237	0.7445040049
H	1.0	-2.1769167048	-4.4262546119	-0.9274524511

H	1.0	-3.3878694183	1.7593338523	-0.9356846206
H	1.0	-3.9583131158	0.2545629405	-1.6959274606
H	1.0	-2.3463388579	0.8876927655	-2.0757327141
C	6.0	-1.8116101099	3.3629156704	0.5400005881
C	6.0	0.0191563008	3.0293191482	-0.9137959014
C	6.0	-1.7586513619	4.7424623120	0.3460640788
H	1.0	-2.5213992298	2.8697150305	1.1947501473
C	6.0	0.1148303416	4.4036506641	-1.1463744730
H	1.0	0.7102500098	2.3032283023	-1.3290508318
C	6.0	-0.7848669484	5.2692122800	-0.5139026498
H	1.0	-2.4614685290	5.3844844973	0.8631297877
H	1.0	0.8890318926	4.7765440868	-1.8058887751
H	1.0	-0.7225671162	6.3391267054	-0.6779380698
N	7.0	-0.9488345219	2.5683826988	-0.1099576531
O	8.0	-0.8035643117	1.0099146846	0.4068561348

E(M11-L) = -2461.962642 Hartree

Figure S-6: MacMolplt structure of the open-half optimized structures





Derivation of rate law S-7: Steady state approximation

During the experiment, none of the proposed intermediates have been detected and the rhenium dimer is the only observed complex. the steady state approximation is valid. Equation 1 shows the derived steady state rate law. ([I₁] is the steady state concentration)

$$R = k_2[I_1] \dots\dots\dots 1$$

$$[I_1] = \frac{k_1}{k_2+k_{-1}} [1][PyNO] \dots\dots\dots 2$$

The assumption of $k_{-1} \gg k_2$ rate constant. Then equation 2 can be simplified to equation 3 in which $K_{eq} = k_1/k_{-1}$.

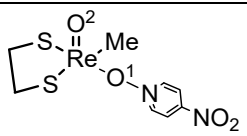
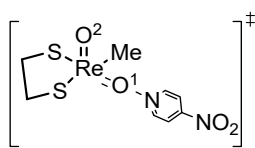
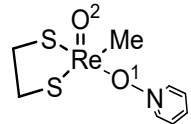
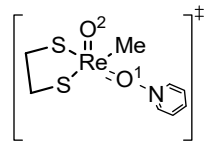
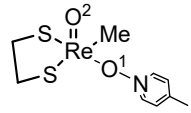
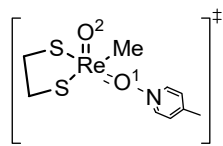
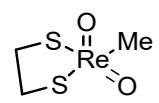
$$[I_1] = K_{eq} [1][PyNO] \dots\dots\dots 3$$

substituting eq 3 into eq 2 leads to eq 4.

$$R = K_{eq} k_2 [1][PyNO] \dots\dots\dots 4$$

$$R = k [1][PyNO], k = K_{eq} k_2 \dots\dots\dots 5$$

Table S-8: Selected bond lengths (Å) and Mulliken charges on Re, O, and N

	Re-O ¹	O ¹ -N	Charge, Re	Charge, O ¹	Charge, N
	2.12	1.32	0.42	-0.52	-0.04
	1.90	1.59	0.54	-0.53	-0.19
	2.10	1.34	0.41	-0.53	-0.06
	1.90	1.62	0.54	-0.53	-0.20
	2.09	1.35	0.42	-0.54	-0.06
	1.89	1.62	0.54	-0.53	-0.21
	1.69		0.64	-0.45	