

Electronic Supplementary information

For

The Nature of Metal-Metal Bonding in Re-, Ru- and Os-Corrole Dimer

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Further explanation and redox potentials obtained from DFT:

The oxidized forms of $[M_2\text{-Model}]^{1+}$ (M=Re, Ru or Os): One electron removal from the $[Re_2\text{-Model}]^0$ system occurs either from the metal-based orbitals or the ligand-based orbitals giving a $[Re_2\text{-Model}]^{1+}$ molecule. Our DFT using OLYP and B3LYP calculations show that the single electron removal is removed from ligand-based orbitals. Furthermore, the δ^* metal-based orbital is populated as shown in Scheme 1, one of the δ manifold electrons is coupled antiferromagnetically to the electron on the ligands giving a 2A ground state. The Mulliken spin density of 0.98 (OLYP) on each ruthenium centre. The Re-Re bond length of 2.21 Å is slightly longer than that of the neutral molecule $[Re_2\text{-Model}]^0$ (2.20 Å) suggesting that the populated weakly bonding δ orbital has a small impact on the total bond strength. This behaviour is also observed using B3LYP, the Mulliken spin density of 1.0 on each metal centre. The Re-Re bond length of 2.24 Å is also slightly longer than in the $[Re_2\text{-Model}]^0$ molecule (2.20 Å). Removing an electron from the neutral molecule leads to populating the δ^* orbitals which are consistent with the finding of Ghosh and co-workers.¹

For the $[Ru_2\text{-Model}]^{1+}$ molecule, Mulliken spin density of 0.002 and 0.001 on each Ru centre calculated using OLYP and B3LYP functionals, respectively. This suggested that the unpaired electron is removed almost entirely from ligand-based orbitals. Supportive evidence to this is that the predicted Ru-Ru bond length was calculated to be exactly similar to that in the $[Ru_2\text{-Model}]^0$ (2.14 Å). For the $[Os_2\text{-Model}]^{1+}$ molecule, Mulliken spin density of 0.05 and 0.01 on each Os centre calculated using OLYP and B3LYP, respectively. Those results suggested that the unpaired electron is mainly removed from ligand-based orbitals. However, the Os-Os bond length of 2.21 Å (OLYP) is slightly shorter than in the $[Os_2\text{-Model}]^0$ (2.22 Å). The spin-density profiles of the $[Os_2\text{-Model}]^{1+}$, shown in Fig. ESI4, indicates that the δ^* (HOMO-2) orbital is fully occupied since if the electron is removed from this orbital, it would then be empty.

The first oxidation potentials of the three molecules were found experimentally to be nearly identical (0.51 V for Re, 0.52 V for Ru, and 0.55 V for Os).^{1,2} Our oxidation potential calculations (see the computational details in main text) are in a good agreement with the experimental values as shown in Table ESI1. The difference between the calculated oxidation potential between the Re-complex and the Ru- and Os-complex are just 0.06 V and 0.08 V, respectively. These results are suggested that the removal of the unpaired electron occurs from the same type of orbital in all molecules. The unpaired electron is removed from ligand-based orbitals of all three complexes with a slightly different degree as shown by Mulliken spin densities. Furthermore, the computed metal-metal bond distances in all systems are slightly changed upon first oxidation compared to neutral molecules confirming the removal is indeed from the ligand-based orbital.

Table ESI1. Comparison of the computed and experimental first oxidation ($E^{1/2}_{ox1}$) and first reduction ($E^{1/2}_{red1}$) of the $\{M[\text{TpMePC}]\}_2$ (M=Re or Ru or Os) complexes. $E^{1/2}$ values in V calculated against SCE.

	Computed		Experimental	
	$E^{1/2}_{ox1}$	$E^{1/2}_{red1}$	$E^{1/2}_{ox1}$	$E^{1/2}_{red1}$
$\{Re[\text{TpMePC}]\}_2$	0.23	-1.30	0.51	-0.55
$\{Ru[\text{TpMePC}]\}_2$	0.14	-1.85	0.52	-0.85

{Os[TPMePC]} ₂	0.18	-2.25	0.55	-1.31
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The reduced forms of [M₂-Model]¹⁻ (M=Re, Ru or Os): Adding one electron to the [Re₂-Model]⁰ system produces [Re₂-Model]¹⁻. DFT calculations show that the single electron is added to a metal-based orbital giving Mulliken spin density of 0.52 and 0.50 on each Re centre with OLYP and B3LYP, respectively. The Re-Re bond distance of 2.22 Å (OLYP) in the [Re₂-Model]¹⁻ is slightly longer than that in the neutral molecule (2.20 Å) as expected since adding one electron to the weakly overlap δ^* orbital results in decreasing the formal bond order from 4.0 in [Re₂-Model]⁰ to 3.5 in [Re₂-Model]¹⁻. The unpaired electron occupied metal-based orbitals in the [Ru₂-Model]¹⁻ as suggested by Mulliken spin density. However, the Mulliken spin density on each Ru centre is 0.31 and 0.41 using OLYP and B3LYP, respectively, less than those of the [Re₂-Model]¹⁻. The Ru-Ru bond distance is longer than that in the neutral form (2.19 vs. 2.14 (OLYP)). In contrast to the [Re₂-Model]¹⁻, the electron is added to the ligand-based orbitals in the [Os₂-Model]¹⁻ molecule as suggested by Mulliken spin density. The Mulliken density on each osmium centre is equal to 0.005 and 0.009 with OLYP and B3LYP, respectively. The Os-Os bond distance predicts to be the same as that in the neutral molecule, [Os₂-Model]⁰, (2.22 Å (OLYP)).

Computed first reduction potentials of the [Re₂-Model]¹⁻, [Ru₂-Model]¹⁻ and [Os₂-Model]¹⁻ molecules show very different behaviour compared to that of the first oxidation potentials as shown in Table ESI1 (see the computational details in main text). The computed difference between the reduction potential between the Re-complex and the Ru- and Os-complex are 0.54 V and 0.95 V, respectively. That results are in agreement with the experimental trend as the experimental reduction potentials proved to be very different for the Re and Os metals (-0.55 V for Re and -1.31 V for Os) and for the Ru-analogue is located in between them (-0.85 V).^{1,2} These results suggesting the electron addition were occupied different types of orbitals. This adding an electron to metal-based orbital in the [Re₂-Model]¹⁻ complex while this electron occupied ligand-based orbital in the [Os₂-Model]¹⁻. In the case [Ru₂-Model]¹⁻ in between those of Re and Os-corrole as suggested by Mulliken spin density.

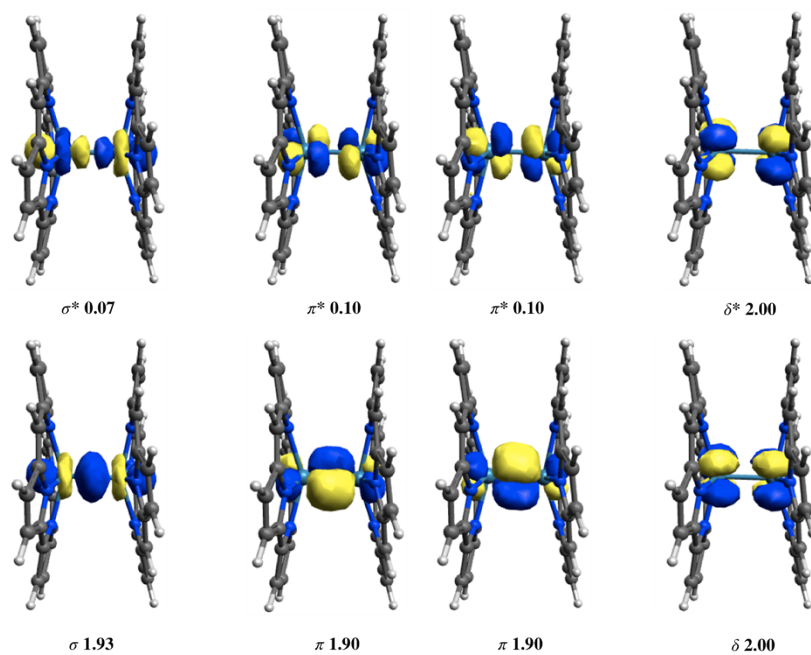


Fig. ESI1. Active space natural orbitals with occupations of the $[\text{Os}_2\text{-Model}]^0$ complex (CAS(10,8)).

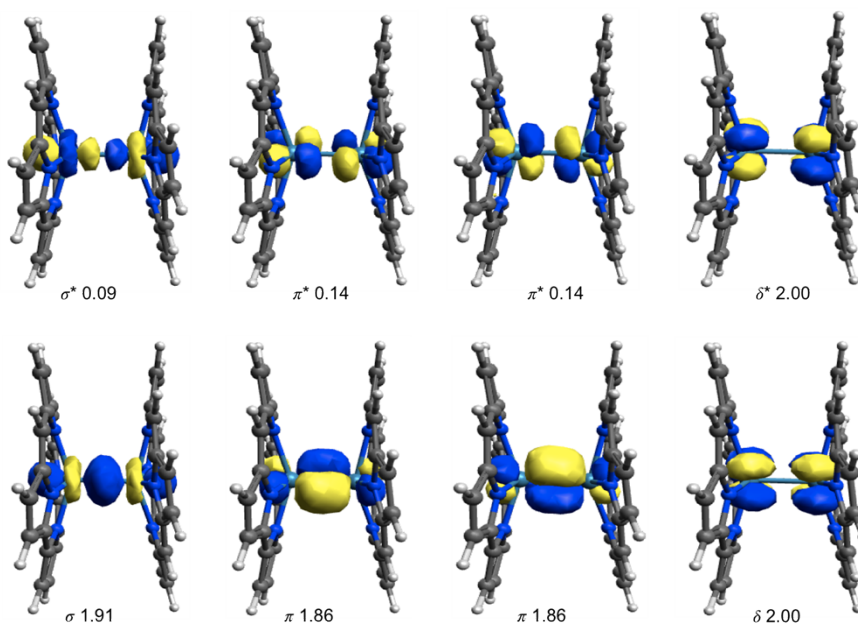


Fig. ESI2. Active space natural orbitals with occupations of the $[\text{Ru}_2\text{-Model}]^0$ complex (CAS(10,8)).

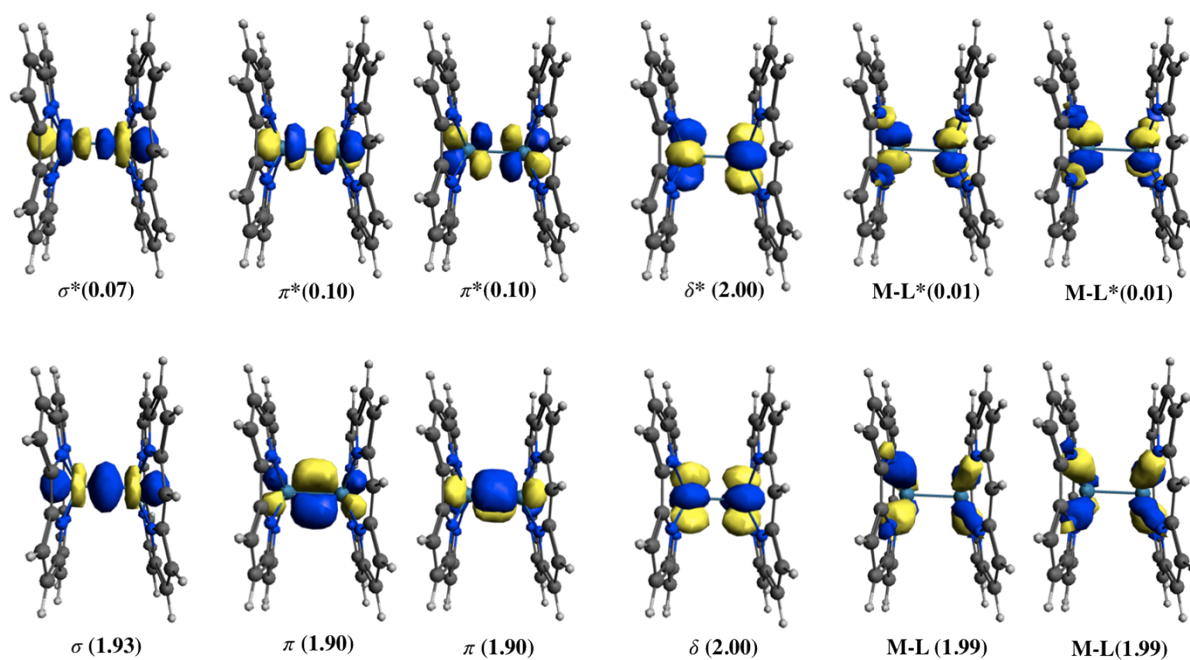


Fig. ESI3. Active space natural orbitals with occupations of the $[\text{Os}_2\text{-Model}]^0$ complex (CAS(14,12)).

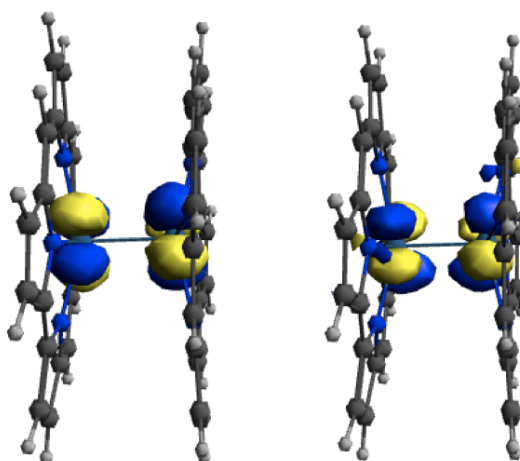


Fig. ESI4. DFT spin-density profile of the $[\text{OS}_2\text{-Model}]^{1+}$ complex.

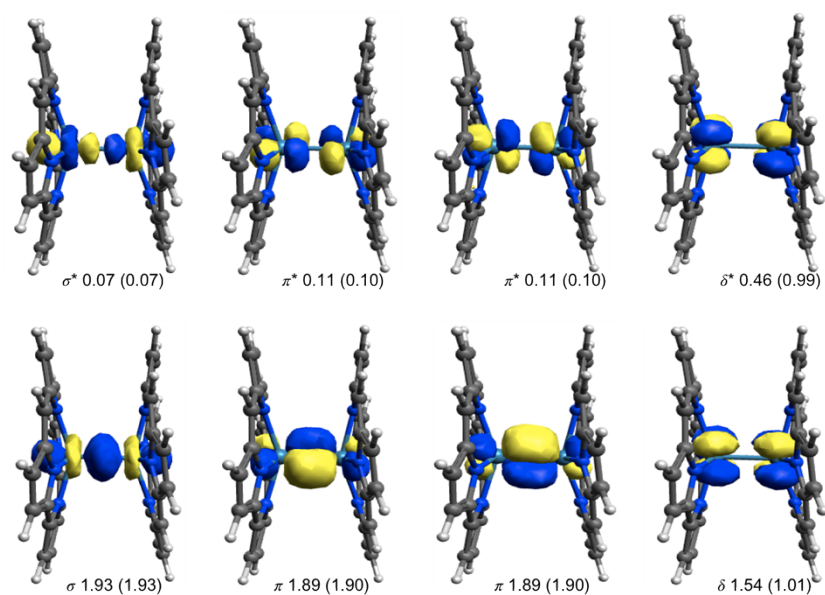


Fig. ESI5. Active space natural orbitals with occupations of the $[\text{Re}_2\text{-Model}]^{1+}$ complex (CAS(8,8)). The occupations of triplet state in the parentheses.

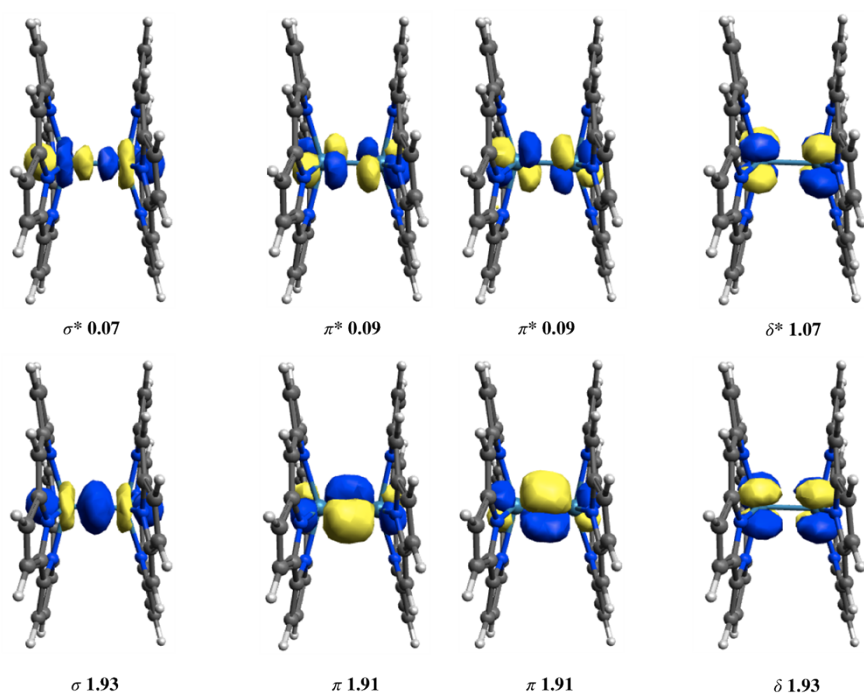


Fig. ESI6. Active space natural orbitals with occupations of the $[\text{Re}_2\text{-Model}]^{1-}$ complex (CAS(9,8)).

Cartesian Coordinates

Optimized geometry of {Re[TpMePC]}₂⁰

Re	8.07598549150596	10.72683012659914	10.11858761069554
Re	6.88328484253585	9.84902306531949	11.73795149745493
N	6.79184492361732	12.08486839500468	9.31112903035535
N	8.16650389356428	8.49044582272336	12.54540730767051
N	7.72047719586345	9.58611024185481	8.48288072325285
N	7.23980191649149	10.98971203263960	13.37311662555476
N	9.96676169871490	10.05591385952112	10.34158719221023
N	4.99302952128506	10.52034306977993	11.51565166230284
N	8.69821053468717	12.50754312379644	10.86150460068502
N	6.25988449006191	8.06840492850365	10.99579665071910
C	6.82970929520124	13.40162692674748	9.76164141994981
C	8.12834664280266	7.17373953121716	12.09491850517175
C	5.81207100752522	14.10847444061455	9.05918667484833
C	9.14644160239759	6.46676892318234	12.79650834118495
H	5.59180661744741	15.17313355029338	9.15329549763083
H	9.36653416862246	5.40209275858843	12.70214443169096
C	5.18554554517681	13.20160303798699	8.19399321843848
C	9.77417417578623	7.37375465674373	13.66069603356458
H	4.38515092889256	13.42267271454222	7.48815142898742
H	10.57536884488667	7.15282477657350	14.36568394733371
C	5.82418500169958	11.92241516764111	8.33861951092121
C	9.13510981363358	8.65280305750426	13.51694104377849
C	5.67830257982294	10.71880821572648	7.59068364334558
C	9.28160186489535	9.85617468255322	14.26496774236829
C	6.59024684813986	9.63084025608481	7.65454450849365
C	8.36979737012394	10.94427219330774	14.20167358717567
C	6.57307812723919	8.39082944501151	6.92759626217060
C	8.38698712230242	12.18365285732878	14.92967352530370
H	5.82444868646313	8.10168237796890	6.19439246016949
H	9.13539129509460	12.47191576447888	15.66342693105248
C	7.66861909122003	7.63626866886988	7.31178558869208
C	7.29205701677929	12.93896048627585	14.54529491059763
H	7.92972760515534	6.64025531535294	6.95896544952811
H	7.03114696924797	13.93488314476923	14.89849602404190
C	8.42067428310546	8.38845527465609	8.27577250688048
C	6.54023159976352	12.18763035716406	13.58050967555155
C	9.64302125361584	8.03213061741917	8.90772654800115
C	5.31833739953349	12.54473034361000	12.94823485450098
C	10.37986688539983	8.81813051594368	9.83548414515238
C	4.58124645408176	11.75913810358174	12.02045015403673
C	11.69203403517801	8.57418038989801	10.36532025276340
C	3.26952965306590	12.00421650700149	11.49022590689514
H	12.29371384059288	7.69157056933911	10.15433715641041
H	2.66883573924315	12.88767768123324	11.70050611114104
C	12.05143743445515	9.65708219847616	11.15137464484914
C	2.90924484704815	10.92138400398054	10.70453486487733
H	12.99389233578046	9.78122391162943	11.67944795700149
H	1.96686772477720	10.79811930141449	10.17611878848478
C	10.97765924239602	10.61414971792504	11.13621693741776
C	3.98197743733768	9.96323291877273	10.72046930280831
C	10.91203136116504	11.89253765565781	11.75555664733495
C	4.04643011464470	8.68459730064368	10.10166881453014
C	9.84043800020286	12.81374488747893	11.58114086484757
C	5.11719816964699	7.76256680579071	10.27681506018639
C	9.73496492795250	14.20805029001665	11.91371551212691
C	5.22062324775136	6.36759601401795	9.94647263371627
H	10.47823049225362	14.77076415488638	12.47817515037425
H	4.47624919507376	5.80487843577078	9.38351691083298
C	8.55750804518188	14.71269836527700	11.34534744593362
C	6.39810780881871	5.86251327870905	10.51434508369261

H	8.20579929617024	15.74536284707883	11.38573914057237
H	6.74869703353504	4.82942378699021	10.47503345491378
C	7.91473924331066	13.64134991865293	10.66353971477085
C	7.04273116776780	6.93419161885773	11.19374516212928
C	4.50155547838362	10.60835942085870	6.70096774629913
C	10.45941905990932	9.96674189945830	15.15331800632674
C	3.22190922999467	10.89604912622887	7.20946167125485
C	11.73848649829836	9.67998820833649	14.64291543663754
H	3.13487137389060	11.21228549190594	8.24873059762013
H	11.82423506483053	9.36409610026026	13.60341613148213
C	2.07914653354231	10.72463512444291	6.42889330893721
C	12.88227746114845	9.85261352055664	15.42172303212686
H	1.09366074702400	10.91506340387624	6.86811526428771
H	13.86727319009176	9.66324810222975	14.98095981407070
C	2.16788607309172	10.26628437257641	5.10551710967221
C	12.79508980239914	10.31037204910119	16.74539502055305
C	3.45001792025305	10.01998595638563	4.58155450893752
C	11.51347822609758	10.55486701741728	17.27151509855835
H	3.54943211125167	9.68800707687361	3.54078214070021
H	11.41535979671429	10.88696986994255	18.31236753731540
C	4.59647300366795	10.18880029866160	5.35979382814130
C	10.36603819170159	10.38565375561533	16.49479361893169
H	5.58180527735084	10.00740276033207	4.92107909413216
H	9.38117589265604	10.56597591421177	16.93497072162532
C	0.94066949867166	10.00720993551196	4.27874466177611
C	14.02337776403934	10.57299594788617	17.56947349651885
H	1.04376431792811	10.42975240264164	3.26132013287998
H	13.92373307454192	10.15021418625965	18.58713862905109
H	0.03856048404422	10.43282018214434	4.75209380710184
H	14.92569550952548	10.15000774735388	17.09416519019483
H	0.77655994870475	8.91812164264836	4.16443152012289
H	14.18453819121020	11.66258693541501	17.68340809911026
C	10.24147993968076	6.72538850184569	8.53000425678018
C	4.72218638264534	13.85321146289803	13.32359538831105
C	10.54623998794900	6.41117579352297	7.19217713662862
C	4.41829634189642	14.17054856969728	14.66086998584938
H	10.34751756784285	7.15091514381643	6.41039953612205
H	4.61603413580820	13.43204853818450	15.44405987400086
C	11.10666264233886	5.17644545004152	6.85669937210401
C	3.86138431703170	15.40744615344987	14.99420679609467
H	11.33793282957191	4.95628408950315	5.80727880381531
H	3.63143252484371	15.63037745276041	16.04332855506304
C	11.38623228176526	4.21017305390752	7.84072123813071
C	3.58258605472156	16.37197139971896	14.00825689887783
C	11.08492941315606	4.52947592518839	9.17583287598786
C	3.88117839738177	16.04875941921104	12.67348466320552
H	11.28695817220161	3.79360325176299	9.96373393337802
H	3.68026973781148	16.78349180327154	11.88423304842996
C	10.52587360086413	5.76471678270144	9.51580538955372
C	4.43825850066016	14.81197944599212	12.33584164446646
H	10.29045239046037	5.99708148219931	10.55663362988154
H	4.67131622945356	14.57638608509604	11.29519588450941
C	12.01332825792004	2.89452122713416	7.47043986834897
C	2.96111491861738	17.69084945454168	14.37652905349488
H	11.54975458490659	2.47295136539682	6.55873816080508
H	3.42868006124429	18.11339547111953	15.28574429809172
H	11.91895804593463	2.15861593718617	8.2885523798465
H	3.05575885681902	18.42409308666816	13.55575750710791
H	13.09352243827360	3.02186699227361	7.25400464035079
H	1.88110611599519	17.56787537612784	14.59633900397124
C	12.03660520521790	12.31388762181327	12.62250569293745
C	2.92167258849117	8.26387062539821	9.23474313755121
C	13.37968748385964	12.25505543569243	12.20407057034514

C	1.57824892089927	8.32796610910350	9.65141501122778
H	13.61134762341462	11.94952250007957	11.17966156772989
H	1.34634725081617	8.63672877634623	10.67479254052433
C	14.41504372528780	12.60070481103250	13.07495040878452
C	0.54294453926095	7.98153755246531	8.78083780000694
C	14.15285398816518	13.02269518584472	14.39099212761180
C	0.80531535999553	7.55534058329580	7.46617548662306
C	12.81098721100643	13.11758787574032	14.79204905372268
C	2.14727756059445	7.45703644782234	7.06632537179649
H	12.57467779429228	13.43538689223548	15.81329359460529
H	2.38381341450727	7.13481877160124	6.04652213099020
C	11.77422869513130	12.77481387304744	13.92445271355505
C	3.18408761921732	7.79924632527166	7.93410484758671
H	10.73952398377788	12.82128169041274	14.26046643839120
H	4.21888211447333	7.75081911019098	7.59861213618328
H	15.45350641259266	12.54609107281479	12.72574910446616
H	-0.49578830865532	8.04105484448999	9.12843971826411
C	15.27970199663614	13.32829669690892	15.33714752936121
C	-0.32150982693945	7.24512975343080	6.52149259186011
H	15.74904511089750	12.39107066891853	15.69530877427186
H	14.92248483862965	13.88100639954073	16.22382556151001
H	16.07158388100802	13.92095987430476	14.84165775799605
H	-0.79534791236451	8.18035450203219	6.16411105959339
H	0.03676899517753	6.69378437978382	5.63442072245076
H	-1.11027371189252	6.64916706903901	7.01809565425210

Optimized geometry of {Os[TpMePC]}₂⁰

Os	8.03424314770732	10.77110156212573	10.09553736004800
Os	6.92736560944241	9.80640904899963	11.75952039488678
N	6.75063590500415	12.04599861916295	9.31231033858660
N	8.21127310395872	8.53192784071260	12.54341538922120
N	7.68916421061947	9.56703466673867	8.53634509920519
N	7.27257801247286	11.01139015284526	13.31820392399899
N	9.88483488099980	10.05435660473593	10.31428554732895
N	5.07678156407677	10.52312054576500	11.54014285516478
N	8.66674505945910	12.47857018501955	10.84741246116686
N	6.29482881884214	8.09833821385013	11.00867201474313
C	6.78608346789808	13.36233753448751	9.76897112950763
C	8.17517322198216	7.21501125757643	12.08831178182137
C	5.76096438339930	14.06862428727309	9.08152260539352
C	9.20004838825732	6.50913018615281	12.77656654328341
H	5.53682782945636	15.13175655720078	9.18252429619920
H	9.42368170235652	5.44577138322446	12.67698280227171
C	5.12950109322484	13.16363459210449	8.21636051810751
C	9.83248504345109	7.41506753177744	13.64007161149781
H	4.31448085470899	13.38319488026653	7.52741062156902
H	10.64773664487329	7.19601776832073	14.32894534098498
C	5.77671491014886	11.89130541695708	8.34892905592770
C	9.18560334043909	8.68749376958794	13.50632587877300
C	5.64171477702409	10.69130373613798	7.60749571986614
C	9.32128681886618	9.88848056738033	14.24627781593688
C	6.56079155774135	9.61704116117647	7.70102064030271
C	8.40192271134583	10.96264261300839	14.15244318341463
C	6.54027006849716	8.38602330853934	6.95905142468636
C	8.42286835123235	12.19466835473303	14.89281036156174
H	5.78878608728396	8.10768375682774	6.22520399959191
H	9.17539594786133	12.47460946903161	15.62496743225039
C	7.63504983576226	7.62953803401032	7.33138902125267
C	7.32708370671384	12.95005617788773	14.52121784583363
H	7.90047735122593	6.63869533250904	6.96831908062953
H	7.06168095323081	13.94116195879083	14.88352390546288
C	8.37837978397988	8.37818344544747	8.30301994047333
C	6.58308365098092	12.20020755964365	13.55105764849500

C	9.59593021297077	8.01520584077917	8.91664791771999
C	5.36524178505315	12.56251151464986	12.93757563896534
C	10.31067885080107	8.81868981293586	9.83239089493532
C	4.65074274536666	11.75877519186079	12.02185821694763
C	11.61018730123106	8.56328865380838	10.38276668796773
C	3.35130321215810	12.01389308679244	11.47123848357014
H	12.20739267872300	7.67451222926065	10.18672807331829
H	2.75394178664238	12.90261238449668	11.66705755746988
C	11.95538212188843	9.64223194785268	11.17579833935987
C	3.00642943608236	10.93485057386482	10.67822495204124
H	12.88393982292079	9.76327131802290	11.72763069324479
H	2.07801594151185	10.81363993948765	10.12627997811057
C	10.88524853258506	10.60174649619009	11.13380943540075
C	4.07651571341157	9.97534221366906	10.72075587239717
C	10.84962113666585	11.87430630503942	11.75951488226611
C	4.11207794550293	8.70233773594905	10.09601841760551
C	9.78634744520473	12.79509715348824	11.58803450471873
C	5.17513276365274	7.78144700840456	10.26827512211771
C	9.65846082172074	14.17965645772492	11.94225392188025
C	5.30266868154255	6.39644113597284	9.91556588477905
H	10.37860131926513	14.74358274767342	12.53412847541014
H	4.58208397897118	5.83190603511025	9.32478677605547
C	8.47907436367664	14.67367633759640	11.36703149683592
C	6.48213298786852	5.90277228431790	10.49099648447990
H	8.10334089161757	15.69670906756288	11.42787320232803
H	6.85753490807267	4.87955975731119	10.43116929392306
C	7.86593206376884	13.60349032617632	10.66028583411619
C	7.09527034548919	6.97333737117811	11.19714898795594
C	4.48768507889234	10.57779302429600	6.68758271652394
C	10.47627626741557	10.00259721416253	15.16493627426195
C	3.19463808752378	10.85765778590355	7.16468171234464
C	11.76833778890375	9.71891494624100	14.68732427940631
H	3.08038499094714	11.16954217315238	8.20199366600896
H	11.88104865584411	9.40478325057013	13.65046073576658
C	2.07215754269708	10.68412271300473	6.35592419366795
C	12.89187680503115	9.89106594638129	15.49491665410692
H	1.07548193470215	10.86793248840422	6.77197161809025
H	13.88776515252943	9.70390893960501	15.07848326721682
C	2.19549491909162	10.23158912547458	5.03314085066531
C	12.77068722188305	10.34651507193566	16.81685703109181
C	3.49162659546351	9.99892285839391	4.53865441313230
C	11.47550066200326	10.58338781058817	17.31188860622025
H	3.61905704748237	9.67514243055362	3.49836534837583
H	11.34969186462461	10.90925300687438	18.35172216594620
C	4.61789166885922	10.17073280742923	5.34585864986391
C	10.34813228629400	10.41237613122458	16.50608425800549
H	5.61460978553023	9.99941317098072	4.92944995914518
H	9.35213019770134	10.58580720849979	16.92333386933455
C	0.98862572257561	9.96150738593706	4.18009263337624
C	13.97878044335415	10.61369250225424	17.66904700104131
H	1.13559445995776	10.32491601744716	3.14570142060937
H	13.83312197094539	10.24707648295331	18.70252477509949
H	0.08358791805698	10.43467112348902	4.60020525174920
H	14.88297432428059	10.14132713043603	17.24628098240361
H	0.79694603202485	8.87213464168590	4.11987443049795
H	14.17096616461104	11.70277927780197	17.73237230842369
C	10.20254366264426	6.71465240935220	8.53056301022448
C	4.75735011012529	13.86212669614454	13.32478437534188
C	10.51723161703949	6.42173031954335	7.19019819152013
C	4.44227151036904	14.15329669257980	14.66542933397566
H	10.31930035876126	7.17204664166405	6.41834269267746
H	4.64130072956374	13.40249582182316	15.43653344382044
C	11.08404871456027	5.19424741368136	6.83905850395427

C	3.87289054948395	15.37927372241190	15.01767524200701
H	11.32196912888868	4.99103943611861	5.78767714597934
H	3.63423067739857	15.58089768961349	16.06919467197015
C	11.36168316698487	4.21425834551182	7.80986448492845
C	3.59359087289657	16.35971425086422	14.04780795575388
C	11.05180917728531	4.51273224778170	9.14760719168435
C	3.90485222972874	16.06340291913545	12.70990189308716
H	11.25209567600868	3.76624908482410	9.92592118166674
H	3.70327697315687	16.81027472253135	11.93229520565419
C	10.48532469192836	5.74048544950664	9.50251876772939
C	4.47345133613023	14.83695790191434	12.35382141521107
H	10.24503359496983	5.95638489127517	10.54504707783014
H	4.71453520896821	14.62266944367272	11.31114595246455
C	11.99354237335682	2.90548111232814	7.42329795614129
C	2.95791958959062	17.66634772743986	14.43535996541517
H	11.53434004522251	2.49545142902162	6.50412464880467
H	3.41436035840273	18.07589341450666	15.35611277352472
H	11.89804902819668	2.15767775427259	8.23076943554690
C	3.05320433815768	18.41573424126561	13.62933214357179
H	13.07419060563561	3.03840331647316	7.21268672890485
H	1.87716589395543	17.53053070034163	14.64360338161825
C	11.99133612774695	12.28999013136774	12.60709402442655
C	2.97051107918305	8.28667478631585	9.24829528545060
C	13.32809322070080	12.21047475164780	12.17155246384183
C	1.63365905982441	8.36862126585652	9.68296455445404
H	13.54265844391923	11.89245729892648	11.14730969780518
H	1.41903151190711	8.68756820766968	10.70688147242269
C	14.37990164687566	12.54887999543991	13.02561824204406
C	0.58177463633000	8.03168935421459	8.82842119052080
C	14.14161359755465	12.98616394323228	14.34109960820987
C	0.82008903540240	7.59360472765306	7.51324252039524
C	12.80655036586053	13.10983334946717	14.75624681962053
C	2.15520862997226	7.46738067082341	7.09895854886609
H	12.58736779422813	13.44333365348603	15.77633607468373
H	2.37438805418885	7.13290924876517	6.07917908104607
C	11.75427416313072	12.77331961753123	13.90550331835102
C	3.20753309964832	7.80240882255276	7.95022579415394
H	10.72572594658186	12.84013396929837	14.25426466965146
H	4.23617412930156	7.73445198586042	7.60194336629854
H	15.41264728780368	12.47438967424313	12.66341231654595
H	-0.45107839796306	8.10845897974844	9.18984975440609
C	15.28354590768686	13.27280635057953	15.27480997462516
C	-0.32173129255534	7.30905338674948	6.57875266030152
H	15.70665278806050	12.32725888721224	15.66775895369994
H	14.95496370327958	13.87353619084252	16.14129854442266
H	16.10259378529428	13.80760050694257	14.75849438916296
H	-0.73903861183460	8.25524484112099	6.18116013729917
H	0.00523059287561	6.70319799881148	5.71520510234613
H	-1.14448070254250	6.78070793515993	7.09577197617993

Optimized geometry of [Re₂-Model]⁰ (DFT-OLYP)

Re	8.01419189080941	10.63910224538826	10.03021631647108
Re	6.93410384128856	9.91070858434557	11.80298345187591
N	6.80167791159309	12.00885852144264	9.16223174508296
N	8.14569116727147	8.54465778613857	12.67783724060970
N	7.64671156402216	9.41272439076163	8.47122956196566
N	7.35812591460833	11.17092143714130	13.31739641516338
N	9.88470231634826	9.93545315258871	10.30213727010657
N	5.06577600139113	10.63571365262061	11.56509538958614
N	8.70164379159188	12.43314526628517	10.69644584211782
N	6.20466486947091	8.10840590915953	11.19785405068057
C	6.87383479851617	13.34213152862984	9.55275370149126
C	8.04462407567280	7.20240163339626	12.32745080396321

C	5.88310334544091	14.04739214590781	8.81030691405672
C	9.04884962341873	6.50492147787601	13.05950594990575
H	5.67810305733841	15.11651091886228	8.87691515690878
H	9.23806950758919	5.43162543586805	13.01744865910231
C	5.25586504343441	13.12778924756612	7.96017298916296
C	9.71486938765330	7.43977065793562	13.86237616787520
H	4.45979528411711	13.33855812547994	7.24464840622079
H	10.53026042121612	7.23845465358358	14.55851309113048
C	5.86615196498271	11.84201810378592	8.15698553195479
C	9.11526258610331	8.72737893640415	13.64789142945075
C	5.73245145386064	10.62393334876149	7.45861556482379
C	9.28764745093414	9.96362667895739	14.30424274397841
C	6.57741045124166	9.50539972541863	7.57591700670375
C	8.45776497299025	11.09166039529834	14.17709363852251
C	6.63201800584804	8.33420817252081	6.74145415915503
C	8.46497047999584	12.30304877623994	14.95280484658555
H	5.92860006966428	8.11894496448240	5.93586318828604
H	9.20515176763530	12.53898825057960	15.71852548115867
C	7.74227209872926	7.59111210110236	7.10662995073289
C	7.36633667928394	13.06204212416424	14.58590195906588
H	8.09908787420419	6.66544054841288	6.65321967062321
H	7.05685509555205	14.02300992283946	14.99844378395231
C	8.40759212827665	8.27907391497198	8.18176825842336
C	6.64397681473139	12.34271140039813	13.57022402469736
C	9.63148752500186	7.97075953763236	8.80364642228329
C	5.41135407178580	12.65644666434870	12.96894920764331
C	10.34209524283619	8.73860669833267	9.74625838099399
C	4.65377092038153	11.86600353293440	12.08327294627691
C	11.64344366706026	8.48917174984408	10.30824823910055
C	3.33786806424549	12.11945017958755	11.55824754611349
H	12.25655131738549	7.61791699221825	10.07436941723792
H	2.75186456177747	13.01332143872819	11.77556435632951
C	11.95658647578397	9.53708366406619	11.15765973867786
C	2.97051530574171	11.04140794845805	10.77081035159669
H	12.87800209697957	9.67586590808591	11.72470469793544
H	2.02543617215204	10.89766242735244	10.24536643805204
C	10.86369916487242	10.47121153434234	11.14373130745275
C	4.04566545962748	10.08616588510296	10.78379772672428
C	10.79560065385295	11.74805482031197	11.72739373049599
C	4.06896778886881	8.78726603003625	10.24672083731252
C	9.79520020215917	12.71343346423024	11.49000550713941
C	5.06636579058249	7.81571222463295	10.47397092379902
C	9.71519131686028	14.11284283355995	11.80788563094054
C	5.10168647656001	6.40142274356791	10.21855283249390
H	10.43387996343109	14.65748866970129	12.42126098793238
H	4.34021950446300	5.84460305997915	9.67069590637767
C	8.59779125407155	14.64584049380314	11.15519296202158
C	6.23881029341762	5.87368003952107	10.84136430846023
H	8.27311139746043	15.68695927064557	11.16544051733190
H	6.53802008000274	4.82521054401491	10.86962956381579
C	7.96223115526071	13.58234146451325	10.44796099152110
C	6.92698664194664	6.95337453846136	11.47065825916393
H	4.96323463959756	10.57330970646153	6.68424652413828
H	10.08688342412407	10.02872041500409	15.04662910144605
H	10.11753814588481	7.04857539992738	8.47568142829357
H	4.96019531111952	13.60631954259475	13.26577418600258
H	11.64245639973340	12.04520228401748	12.35016454879520
H	3.18806580814518	8.47921415866547	9.67806411450771

Optimized geometry of [Re₂-Model]⁰ (DFT-B3LYP)

Re	8.02230915708155	10.63615532848865	10.02351534657593
Re	6.93524712812229	9.92771994457497	11.81917728808357
N	6.82558740569696	12.00811925667558	9.13588171904013

N	8.12600994780040	8.54988890757213	12.70598503100099
N	7.65328539363464	9.41010823040923	8.46189123617634
N	7.33744897291089	11.16370526009607	13.36405152855752
N	9.90767159850967	9.95577245613962	10.26960063883022
N	5.05406466278380	10.62891936200903	11.59445848015341
N	8.73365812769334	12.44354084170330	10.65534503762016
N	6.19461981926494	8.12244246482659	11.21245220832820
C	6.88982331537030	13.33278697593883	9.52924906948627
C	8.04048862482296	7.22200593527015	12.32772924182711
C	5.88411846841127	14.03362191128237	8.80546602273006
C	9.04739614912637	6.51666403762639	13.04556677808321
H	5.67085668755286	15.09919102508677	8.87857139489123
H	9.24683196002098	5.44784350073153	12.98112841240983
C	5.25471166594880	13.11388264435308	7.96332560175530
C	9.69981509932060	7.43769859690433	13.86863761886714
H	4.44808807711805	13.32190248961290	7.26085277551989
H	10.51359209106616	7.22737596136744	14.56209535762146
C	5.87889847205139	11.83468964220823	8.14613770076573
C	9.08763127977566	8.72193629964601	13.68153175562259
C	5.73919329479709	10.61361179943995	7.45216802042633
C	9.25153250957817	9.94870409188746	14.35993493653703
C	6.58345874168480	9.49760728424182	7.57178054591464
C	8.42098333194430	11.07432040028031	14.23755544481024
C	6.62886950319413	8.31436142984354	6.75239989027700
C	8.41300582531188	12.27568968524138	15.03086206140997
H	5.92232313432147	8.08886142846606	5.95395315087039
H	9.13825495731955	12.50478085650817	15.81128168115544
C	7.73103191416722	7.57236509300085	7.12327690989540
C	7.32152468741361	13.03315405687789	14.65991092800942
H	8.07610998846416	6.63715050793247	6.68354540074994
H	7.00467653103283	13.98620435231158	15.08213153324755
C	8.40381649971763	8.27311724140576	8.18675738308886
C	6.61675073844758	12.32307853960556	13.62391028355652
C	9.62651711555885	7.96562605491468	8.81036463794733
C	5.39023471726778	12.64032406857094	13.01290271268911
C	10.34400819418691	8.74490730349055	9.73801850706742
C	4.64517224101945	11.85546565708447	12.11205314796313
C	11.64336612409427	8.48606158523956	10.30192352926919
C	3.33947590767014	12.12381878816703	11.56742962527837
H	12.24290509173011	7.60206437238136	10.08715165415708
H	2.75701113455743	13.02026245279209	11.77750444489639
C	11.97643767704043	9.54417200375368	11.12160591270026
C	2.97604696731737	11.05674384584094	10.77287578530978
H	12.90259371138863	9.67810941208532	11.67981986592769
H	2.03812014404689	10.92616258969251	10.23383507397377
C	10.89590013596174	10.49304118729751	11.09422605645386
C	4.04356882665852	10.09287456688632	10.79672813938065
C	10.84147525887785	11.77524683068370	11.66296850646773
C	4.06930710704594	8.80139922588776	10.24739219858350
C	9.83471686026441	12.73536935606955	11.42709737233560
C	5.06889558874633	7.83193504594969	10.47641048478929
C	9.75091179666094	14.13551579947604	11.73824528291581
C	5.12150826953400	6.42392072417211	10.19472857024999
H	10.47485035460513	14.69041817084087	12.33408519015939
H	4.37252915674917	5.86806938341435	9.63145054748700
C	8.62210664583843	14.65400828116357	11.10331844119078
C	6.25771777887778	5.90039150623086	10.81235767468773
H	8.29050319070454	15.69146198929446	11.11057048338814
H	6.57067642110040	4.85716495139010	10.82204264287262
C	7.98725277861827	13.57962583249300	10.41311893932818
C	6.92647291502005	6.97862388868352	11.46357946359501
H	4.96037758897945	10.55823713194068	6.68883632897248
H	10.04350434614413	10.00417127293115	15.10956287594609

H	10.10565219489562	7.03581619807232	8.49716207745644
H	4.93267580091246	13.58487211311157	13.31392624348850
H	11.69403896215681	12.07755633951413	12.27426847907625
H	3.19877323429039	8.50007423091606	9.66134069009878

Optimized geometry of [Os₂-Model]⁰ (DFT-OLYP)

Os	8.04836493602547	10.72855064324709	10.08143314493882
Os	6.91334962843710	9.84892683926877	11.77343152866172
N	6.81530373257514	12.02011204397832	9.24527874475791
N	8.14759910474280	8.56069654114521	12.61305696785453
N	7.65576988877867	9.45589542842630	8.59907738397869
N	7.30161309069056	11.12427935259603	13.25447820538074
N	9.86572649840964	9.95356402642624	10.34059616023804
N	5.09486109442657	10.62015399591396	11.51081609409088
N	8.73068317368880	12.45158331268505	10.75410163013788
N	6.23518980285199	8.12370922584170	11.10203327451319
C	6.86343792623335	13.34465535495780	9.66971226390639
C	8.10253609292743	7.23552119868007	12.19026591545781
C	5.80444665748807	14.02963392113126	9.00935567550068
C	9.16143449118570	6.55321943439330	12.85354446657344
H	5.56122091604614	15.08680736124262	9.12217199374545
H	9.40652153886319	5.49626160905496	12.74278122269916
C	5.15199577849522	13.10624518451549	8.18070282056600
C	9.81113525501526	7.47895108209975	13.68174363721425
H	4.30200763297993	13.30419401869016	7.52667831647214
H	10.66037847358674	7.28337002961210	14.33746517647653
C	5.81611567534385	11.84222958299494	8.31133597301728
C	9.14505590149167	8.74164763843999	13.54825594723441
C	5.67309911404218	10.61691877793920	7.63905212044489
C	9.28495448548534	9.96814886082154	14.21900228035899
C	6.54144139253342	9.52078888111341	7.75775588647893
C	8.41482763661934	11.06254669956671	14.09751790585303
C	6.50012741348503	8.28947679446127	7.01594687532930
C	8.45299849567625	12.29501659064688	14.83754610007401
H	5.73741089869953	8.04325207799288	6.27607803015037
H	9.21434239629368	12.54372887783035	15.57798585382540
C	7.58103195129839	7.51600695746048	7.40060165561261
C	7.37091136591148	13.06574314655069	14.45072707109738
H	7.85472364515323	6.52555278950779	7.03569487881906
H	7.09483273214358	14.05612681436018	14.81400647033680
C	8.32115153107818	8.25475274502928	8.38728498167667
C	6.63360551866661	12.32439615183476	13.46388753059471
C	9.51641622990684	7.89830556864443	9.02717687001278
C	5.43862638897722	12.67787331504161	12.82179277526306
C	10.25897181198509	8.69128925229738	9.91320645025314
C	4.69882012654397	11.88241661033215	11.93568144072097
C	11.53437203782588	8.40725101462690	10.51280116894222
C	3.42404508778012	12.16351633128736	11.33340519599202
H	12.09255271927662	7.48144675704722	10.37006266994352
H	2.86424513756204	13.08871421895828	11.47359901006918
C	11.90046075680796	9.50653826645921	11.26929461110582
C	3.06098724741258	11.06247017730089	10.57803735256466
H	12.81450573215218	9.63807433948724	11.84980652548273
H	2.14822695860400	10.92865492256043	9.99602412625901
C	10.86045147091048	10.49373282361020	11.16068758056842
C	4.10229171959409	10.07704401135203	10.69003073685986
C	10.84705475908406	11.78234255609555	11.71654213434178
C	4.11877760933274	8.78770289608109	10.13599919349005
C	9.85484638964701	12.75191862415334	11.49467461200755
C	5.11252241404818	7.82028034604500	10.36041367977901
C	9.76717033231173	14.14565351436104	11.81952935823250
C	5.20331114213798	6.42633783713674	10.03735412067749
H	10.49694037553981	14.69968573785624	12.41103426840030

H	4.47532682758995	5.87015680831625	9.44566555656641
C	8.60926864873501	14.66128922868734	11.22089541812480
C	6.36131493812348	5.91362286482129	10.63833172702374
H	8.26595604369746	15.69592401743157	11.25496059768536
H	6.70649124342708	4.87953241481320	10.60627326210612
C	7.96384717309176	13.59260161627572	10.53681930161993
C	7.00394256893246	6.98444066819233	11.32173366318663
H	4.85274223868536	10.51832833438563	6.92453243670457
H	10.10400479973345	10.06913176864649	14.93469595840759
H	9.93082525861443	6.91802789570847	8.78115000551856
H	5.02221012347740	13.65779986288537	13.06579302875412
H	11.70839911101743	12.06262973322401	12.32710678666921
H	3.25885871006400	8.50509167542057	9.52450419259779

Optimized geometry of [Os₂-Model]⁰ (DFT-B3LYP)

Os	8.05331981784954	10.72350538930830	10.07606066216230
Os	6.90858608979637	9.85390798784700	11.77857761762366
N	6.84062719218080	12.03380157063019	9.20638396562293
N	8.12367293462470	8.54972920401496	12.65411564811483
N	7.68204721135423	9.46693561657871	8.55599231699273
N	7.27261675378605	11.11565442664220	13.29613221523346
N	9.89702618800097	9.96315961599628	10.29857374907405
N	5.06278962234552	10.60753206208357	11.55066196221373
N	8.76143025320314	12.46417440795508	10.71775967442959
N	6.20754723425136	8.10924232694902	11.13973622141063
C	6.89837037365780	13.35183002931820	9.62396832060605
C	8.07117215073049	7.23047062274107	12.23978861748253
C	5.85117899753195	14.04633518285721	8.95483123966598
C	9.11938255146062	6.54119406474777	12.91272556347033
H	5.61987057169577	15.10556103804338	9.05923374502047
H	9.35454766581260	5.48252856568400	12.81138701203353
C	5.19963343345702	13.12989465130666	8.12549044813056
C	9.76583340505536	7.46184546815779	13.74143187342192
H	4.36169135089126	13.33674985221363	7.46069843734144
H	10.60278728070304	7.25936769334465	14.40883526072998
C	5.85111235871718	11.86074297185738	8.26580917158543
C	9.11051290839850	8.72851264654939	13.59644656098824
C	5.70994758700183	10.63584304901647	7.58925808840542
C	9.24615443147232	9.95550495186404	14.27028552331127
C	6.57625213633350	9.53822481541602	7.70895715815775
C	8.37657478714715	11.05000820660244	14.14591261176834
C	6.54575939209534	8.31500522737969	6.95130510463956
C	8.40160786321403	12.27534023170488	14.90035555419788
H	5.79398794430064	8.07430689633097	6.20010628560147
H	9.15089906744252	12.52034891605711	15.65263912523294
C	7.62502907084500	7.54658033542489	7.32970095598863
C	7.32079964655323	13.03939618240374	14.51744598605741
H	7.90837835616107	6.56661256380564	6.94754938029512
H	7.03343052479807	14.01941751091212	14.89645309727117
C	8.35531366880301	8.27735084853877	8.33103456988873
C	6.59503500452890	12.30366889776749	13.51648497619457
C	9.55507045287582	7.92206174045808	8.96464394846668
C	5.39537732630743	12.65335729191576	12.87959305140207
C	10.29543898229204	8.71224618405629	9.85605525270278
C	4.65929264220975	11.85826858119686	11.98904163565801
C	11.58100890555671	8.43365443195107	10.43869817474900
C	3.37394843221869	12.13101754489239	11.40314618185612
H	12.14906146518749	7.51808324272301	10.27837319499893
H	2.80263421021111	13.04519500592965	11.55974224660515
C	11.94558830194914	9.52567491337620	11.19584289658684
C	3.01446760339280	11.03573719009526	10.64835513259261
H	12.86809238493571	9.66031098097001	11.75997727571408
H	2.09351044856830	10.89652974331437	10.08278996302930

C	10.89616657493852	10.50631246479390	11.10599971759515
C	4.06707452874689	10.05892792074815	10.74260774178450
C	10.88598144703352	11.79586872398871	11.65981571717185
C	4.08264439268934	8.76805656320231	10.19200824135318
C	9.89104417809944	12.76609112199923	11.44352806863759
C	5.08035030396282	7.80163589973862	10.41265472787521
C	9.81170657063612	14.16345703383128	11.75310705370414
C	5.16474568987508	6.40371849500484	10.10709260077871
H	10.54916690889000	14.72362786184809	12.32689752415351
H	4.43019442556775	5.83960437840565	9.53343751207559
C	8.65471154859804	14.67460474316395	11.15961291835421
C	6.32233767156698	5.89793860451767	10.70407219127598
H	8.31809638469705	15.71025268492701	11.18069240785800
H	6.66228818389412	4.86331143935694	10.68653326702617
C	8.00259361788980	13.59934514163520	10.49249303381533
C	6.96967936169097	6.97713260891295	11.36947770105246
H	4.89931707663753	10.54396964571890	6.86378448345705
H	10.05489519221349	10.05183172807087	14.99727653370204
H	9.97905563298948	6.95096082803547	8.70204188445693
H	4.96785699970424	13.62387937693151	13.13853669476739
H	11.75556364682073	12.08062102371279	12.25531505379664
H	3.21510268095153	8.47892083252542	9.59564727058114

Optimized geometry of [Re₂-Model]¹⁺ (DFT-OLYP)

Re	8.07557344306438	10.68797473430092	10.08041680191033
Re	6.92481825814924	9.86813251988523	11.78189678163115
N	6.80179879270120	12.05650397437205	9.28975719458257
N	8.14902420787081	8.51273235793572	12.67448022434598
N	7.61367197118881	9.43957850786541	8.56040552790100
N	7.31602716974133	11.15832621223494	13.28598745341022
N	9.93966155523066	9.94171492805397	10.30948381243235
N	5.07928467670264	10.61887980852110	11.44425827298163
N	8.74933446946437	12.47667867072964	10.76851969424383
N	6.26720864244539	8.06621044022567	11.11549516314314
C	6.85684940441727	13.37723207355973	9.70980803365066
C	8.08133530995573	7.17557102617704	12.31184648772476
C	5.78386287608184	14.06060863894932	9.06642786770565
C	9.07575599342158	6.48979153104976	13.06914830512362
H	5.54450000667375	15.11822040533528	9.17899137231779
H	9.28395524885029	5.42044598194411	13.02563279256519
C	5.11258315114381	13.13369376664966	8.25822117281829
C	9.70469100844180	7.43065253945751	13.89592624918582
H	4.25417878344815	13.33191330757242	7.61566326116350
H	10.49533164363193	7.23471851006713	14.62125968798042
C	5.77914084288896	11.86346764725348	8.37533289329158
C	9.09191698576078	8.71223185599496	13.66997139865152
C	5.61653795054385	10.63884559278562	7.69741039251900
C	9.22336258222665	9.95408824957441	14.32695792516977
C	6.48458116759190	9.51704815562198	7.74925168816006
C	8.38703502638017	11.08846010319301	14.17587371846180
C	6.45215236020190	8.30869750720992	6.97241354161021
C	8.39340255641439	12.32414013131102	14.90857289067141
H	5.68571102148227	8.06917891503894	6.23468253542151
H	9.11221123498051	12.57548729596762	15.68914658854478
C	7.56078348634487	7.54361064069945	7.30896104641528
C	7.32751162638162	13.09831410461608	14.46832609751150
H	7.84843503520866	6.57785412564411	6.89236635042249
H	7.03335337812988	14.08406985444288	14.82963798280563
C	8.31628086935736	8.26029473940786	8.30157169870180
C	6.62548047261075	12.35919770938056	13.45526842129861
C	9.55254846606661	7.93335291949013	8.90331617360692
C	5.43429121658211	12.68731491253425	12.76379110100759
C	10.33536249183253	8.70572769994246	9.79569965238116

C	4.68593074209896	11.89002265910024	11.86840858891224
C	11.65266946546691	8.44880818167293	10.31192521340831
C	3.41453253265309	12.15378462772492	11.25032171752516
H	12.23952708574969	7.55650616624901	10.09137116685831
H	2.84064810084077	13.07089700968191	11.38500530528547
C	12.03121514712424	9.53382843075072	11.09197476969513
C	3.06074666975000	11.04242662568617	10.49665922025561
H	12.98049571131583	9.67455352161390	11.61002761859535
H	2.15006038617734	10.90343347235619	9.91338541240068
C	10.95929924169470	10.49115345978980	11.08458945955772
C	4.10461519805176	10.06348248986024	10.61834834598465
C	10.91388687677999	11.78762603369052	11.65827931932157
C	4.16964537488561	8.75330281113433	10.07844993359860
C	9.90269810962324	12.75505897607080	11.48328312874660
C	5.15436044994330	7.77944021592378	10.34205023445953
C	9.83172727952895	14.15374609939992	11.81471699789320
C	5.22280758153541	6.37047173159320	10.06055407641089
H	10.58659945105139	14.70127981752143	12.38020934809807
H	4.49359068852014	5.81470442698522	9.47005377341282
C	8.66669404510075	14.68338463220933	11.24414668872168
C	6.34198531624773	5.84354967184271	10.71941654273290
H	8.33717837042114	15.72178574318849	11.28478982413180
H	6.65609688878073	4.79962263586874	10.73383317068332
C	7.99306165519478	13.62237084030742	10.57139873347241
C	6.99228402189082	6.91758433362605	11.39493510179956
H	4.77883593158625	10.56349240935199	7.00004266105320
H	10.00206455058995	10.03137766546296	15.09006119522224
H	9.99003330241604	6.98005065035149	8.59600962844497
H	5.00679100629994	13.66539972172572	12.99776216441890
H	11.79491260681256	12.08873201122874	12.23069266749653
H	3.32445082825605	8.44965083303395	9.45613973793005

Optimized geometry of [Re₂-Model]¹⁺ (DFT-B3LYP)

Re	8.06397201860708	10.72921801296404	10.06608929313459
Re	6.90152237678081	9.84984482147116	11.79100711740774
N	6.82215746389212	12.09986463632452	9.23283454445064
N	8.15700275616412	8.51180567395921	12.65680401489300
N	7.62621496955209	9.47558692154428	8.53893491856625
N	7.29220766925881	11.12830488208683	13.30978390265387
N	9.91731557225052	9.95879830261654	10.32135222511962
N	5.03697120681403	10.58067140812998	11.50063922238171
N	8.76084716645484	12.51019944948746	10.74296420124428
N	6.24713635902951	8.04889553785748	11.12537000704824
C	6.89860028187210	13.41751061670166	9.63516378744614
C	8.10995873385940	7.18810712308009	12.26890530436394
C	5.85686888925566	14.11881896511944	8.96333165644818
C	9.15134347767372	6.51306019649805	12.96612281227412
H	5.63837598877202	15.18116281428977	9.05780793208190
H	9.38951850822100	5.45359416497929	12.88833660951915
C	5.18809741338558	13.20168909609945	8.14774929691614
C	9.78986886602296	7.45137610844421	13.78309956115786
H	4.35445209026323	13.41669658282899	7.48052531683362
H	10.61538408815967	7.25855054548074	14.46701893149775
C	5.82455164054296	11.92078916567752	8.29322018929428
C	9.13459704755426	8.71831352645374	13.61101977791850
C	5.66985815149801	10.69625599703817	7.61265723690951
C	9.25624430310262	9.95465076062254	14.27985701691788
C	6.52288898551165	9.56478921771353	7.69888849699280
C	8.38561213946623	11.06859056603595	14.16718195458913
C	6.48091687670606	8.34303079483782	6.94397763167707
C	8.39308318965535	12.29926826941144	14.90859057588606
H	5.73119653163769	8.10646077429236	6.19008411596206
H	9.12655551145392	12.55842709567417	15.67101813862182

C	7.55420376362411	7.55831004510888	7.32688922453055
C	7.30994378893424	13.05848856570844	14.50212974724954
H	7.82536643950477	6.57852246706052	6.93641033876082
H	7.01416937377097	14.03692928178683	14.87787585145298
C	8.29757087274881	8.27616299948350	8.32720948030535
C	6.59603747665884	12.31593978138183	13.49913275526425
C	9.50312233712109	7.92238402095683	8.97667060048446
C	5.39211116236781	12.63970655599504	12.82765447223879
C	10.28247691836616	8.69615191457967	9.87059465694372
C	4.64180374275816	11.84226680232300	11.93256851201320
C	11.56808189418832	8.40741352742030	10.44594749776186
C	3.35895126673709	12.09967006390500	11.33532788615857
H	12.13034875894485	7.48968237065041	10.27974008792826
H	2.77688064467129	13.00813999970955	11.48314325989589
C	11.95597369038674	9.50061716487981	11.20046953881027
C	3.00250446973438	10.99063099015203	10.58889042579748
H	12.88748323957606	9.61959357694997	11.75228393678003
H	2.08150850532368	10.84775046256803	10.02521078438564
C	10.92186906776893	10.49483948398729	11.11973017855773
C	4.05451979807720	10.01778164325630	10.69503143626676
C	10.89550888405863	11.80071446786728	11.67280835524394
C	4.11448919113273	8.70651729806825	10.15464568701933
C	9.90678148117500	12.78535960106748	11.46415822173504
C	5.11859541304749	7.74523325168642	10.38757620064018
C	9.85419749829335	14.18927588832601	11.76505717809487
C	5.20502162426151	6.33943142583522	10.09899483295646
H	10.60798142169475	14.74016321455305	12.32605968643289
H	4.47175349160428	5.76896871231958	9.53044763714999
C	8.70611690171730	14.72227500729949	11.17063517562061
C	6.35263087640166	5.83468784496438	10.71676574231557
H	8.39285052727585	15.76479815895404	11.18646276514275
H	6.68720900931263	4.79869287124100	10.71470078408167
C	8.02846690792982	13.65704469620563	10.51298929863309
C	6.99841660685279	6.91908179403858	11.37662961045007
H	4.85408692770781	10.62752021087451	6.89035919944610
H	10.05864561103338	10.04601641674865	15.01459058547757
H	9.91527442906399	6.94663301364098	8.71184101264970
H	4.95756990723370	13.61001311328678	13.07622979717662
H	11.76929764732699	12.08959091098700	12.26025870921980
H	3.25584815819356	8.39515835645022	9.55656305871786

Optimized geometry of [Os₂-Model]¹⁺ (DFT-OLYP)

Os	8.03437874464217	10.72670239064336	10.08124628743069
Os	6.90519133434518	9.84470474702063	11.76122068932548
N	6.72820910614745	11.85853980164194	9.14211014450999
N	8.08750234900405	8.42829705293187	12.43792490017794
N	7.80072447107731	9.32612276697812	8.69214224469920
N	7.50381907978552	11.02824864030048	13.24453131672279
N	9.87050934091325	10.09660269368995	10.51937426645429
N	5.17198575146615	10.80035522907591	11.59287875940348
N	8.51932644401400	12.52101536120696	10.71925712137546
N	6.07370192061446	8.22805628342747	11.01009348069792
C	6.63082659227160	13.19476321039496	9.51384084419355
C	7.93792740164727	7.14866842149850	11.92576381298075
C	5.54232942793637	13.74778480299188	8.78853895449370
C	9.01012170316672	6.36455888231728	12.44593074021001
H	5.19169121500601	14.77806913973005	8.84884660708339
H	9.19095805629677	5.31098447808999	12.23289023421761
C	5.01520950370729	12.73127913297891	7.97329892631161
C	9.77642839690936	7.19187371881061	13.27413540051116
H	4.17511900123859	12.82056480584244	7.28418398121922
H	10.66650513870459	6.90681673641562	13.83506551084075
C	5.78900216132964	11.54594602306681	8.18580821860355

C	9.16844907142241	8.49675207001220	13.29315115974988
C	5.77306021168466	10.26695102597953	7.59275165490373
C	9.44108867223527	9.66473985296169	14.01201058255405
C	6.71849109008522	9.25005230339420	7.81027825721670
C	8.64583907211640	10.83598200144065	14.01170553732867
C	6.79376411340914	7.96899655802453	7.16440210788569
C	8.84267223217602	12.02685517990319	14.79110648411063
H	6.08286195421404	7.61171851862812	6.41905965070409
H	9.66639010097024	12.17702572484898	15.48923408653108
C	7.91355149498183	7.30787090809236	7.64542415189075
C	7.82468555062217	12.91532955590194	14.48403341606594
H	8.26736525501478	6.31405771373669	7.37108726976679
H	7.66717302447634	13.91315045222164	14.89285249301677
C	8.55183704314212	8.16789697377232	8.60080321977742
C	6.96470177304243	12.28055636675944	13.52105865153827
C	9.72919375601246	7.93778825997680	9.34366924961258
C	5.78442559950502	12.76561060776044	12.94671522106317
C	10.36656122414241	8.83480476352223	10.20719218387978
C	4.91827286665388	12.07213600422566	12.07543767594754
C	11.61362948997538	8.67810358746229	10.90822407863462
C	3.66259150064050	12.50297670462671	11.53047725432802
H	12.23890910296976	7.78650861824758	10.86809338514108
H	3.20406828971389	13.47355405163855	11.72006915161317
C	11.85926814888725	9.85260645153597	11.60031403950504
C	3.17137524185079	11.47579049402261	10.73875717609105
H	12.71788881111276	10.08397818576136	12.23097375788423
H	2.23576749655065	11.45981278324700	10.17939461550322
C	10.76290390648360	10.75023072004904	11.35982128659835
C	4.11183272111938	10.39095740471156	10.77946333154739
C	10.60046664231221	12.06481184762471	11.85906506206260
C	3.99944369663145	9.13326326958197	10.16004290091564
C	9.55317961600692	12.93248019481970	11.53510107562533
C	4.90672259936821	8.06400679504256	10.29840488964756
C	9.29926527340018	14.31830080832249	11.83415245792838
C	4.87887339034430	6.69687495899056	9.87423915810388
H	9.92339050639287	14.94627772438608	12.46998095677696
H	4.09163140567592	6.23933010616330	9.27462531623800
C	8.14649769610845	14.71004750689400	11.14603548935142
C	6.02398337587868	6.05938380532856	10.38226920785570
H	7.69550196462695	15.70235889829786	11.14466291293442
H	6.29333894477020	5.01092206154713	10.25495053820672
C	7.66025862089485	13.57217292588386	10.43505451483128
C	6.76714389613766	7.02776190134963	11.10800747173636
H	4.99123814411458	10.05745568718625	6.85924753064106
H	10.31636115347655	9.67047789869075	14.66433755928226
H	10.21668149440734	6.97222716206966	9.19500740506687
H	5.47773576587092	13.77258265590177	13.23676208298076
H	11.38672259607787	12.43615117930603	12.51899796432716
H	3.10046726206859	8.96285445109299	9.56343193363408

Optimized geometry of [Os₂-Model]¹⁺ (DFT-B3LYP)

Os	8.05532704036933	10.71850792311529	10.07551713109106
Os	6.90573423981851	9.85886908871629	11.77913108480639
N	6.82433032280042	12.01268310135673	9.22773361518614
N	8.13554764060710	8.56207013663216	12.62471497805062
N	7.67790436656840	9.44724067476110	8.58004582360441
N	7.28633276285661	11.12821289528703	13.27550828371326
N	9.88386599102052	9.95040098787750	10.32300166405246
N	5.07811240190362	10.62976110499713	11.53410493516792
N	8.73996810598076	12.44970413462515	10.74104651153437
N	6.21812322141556	8.12932040320394	11.11248282276000
C	6.86824830371292	13.33496016711041	9.66409413016566
C	8.08949531784753	7.24027462859349	12.18704629598135

C	5.79997175623817	14.01979063542904	8.99983135719561
C	9.15747044794407	6.55346733438143	12.84952233461899
H	5.55096125475307	15.07315438226215	9.11683278657164
H	9.40499962278266	5.49988392909517	12.73132667202300
C	5.16812799434146	13.10571372930873	8.16577872423108
C	9.79149152160809	7.46603029374747	13.68379023952807
H	4.32237589027944	13.30182732321569	7.50848116780498
H	10.63768378783604	7.26814388154703	14.33998312461328
C	5.84207276263921	11.83640975402183	8.29522178190055
C	9.11914429619968	8.73617662909995	13.55620925861682
C	5.69570943553954	10.60289465416211	7.62212003138026
C	9.26810796001034	9.96920462350273	14.23000387976382
C	6.55861208525820	9.50869982188611	7.74693273202298
C	8.40670801164912	11.06462151422400	14.10716985399577
C	6.51799425243187	8.26587013686609	7.00682900279550
C	8.45004400437453	12.30697915753630	14.84785651255032
H	5.75574207239154	8.01417383386302	6.27059603691123
H	9.21365192300941	12.55724386074329	15.58317284132113
C	7.60117961864950	7.50931578650106	7.37835588001176
C	7.36733807853387	13.06523000608694	14.47828166900094
H	7.88009944822713	6.52344603044927	7.00951298003465
H	7.09030377647043	14.05126413049519	14.84808370073736
C	8.34672163347953	8.25747989314450	8.36539659974427
C	6.61962774812071	12.31875829586815	13.49168689225650
C	9.54677881624752	7.90406548529881	9.00027030534930
C	5.41927685421781	12.67445089265781	12.85823327984497
C	10.28113887047599	8.69892218303348	9.89313668024250
C	4.68299951610141	11.88151684976873	11.96553270953188
C	11.55957228377321	8.41265043813359	10.50422213378410
C	3.40436164744259	12.17004848551378	11.35583287612564
H	12.12200700052358	7.49175531340212	10.35791828446225
H	2.84335562973796	13.09157854535670	11.50353339287353
C	11.91300850050865	9.49682782721667	11.26801622872009
C	3.04872131451767	11.08705870805468	10.59142858443216
H	12.82299938632940	9.62670181962619	11.85238794161018
H	2.13801418934545	10.95893550705239	10.00779661147958
C	10.86893138215655	10.49203005998736	11.15198140797803
C	4.09158438352893	10.09033517347606	10.70559051225685
C	10.85536037503471	11.77997910487298	11.69817930229812
C	4.10274229622133	8.80273323285004	10.15813538032791
C	9.85677342301686	12.75237159413192	11.46682968199770
C	5.10016575742214	7.82892573647633	10.38749718072558
C	9.76349980837754	14.15410269041688	11.79595703355785
C	5.19124005236182	6.42720693934848	10.05697432933756
H	10.49336077765537	14.70953050160214	12.38295306386496
H	4.46003357081828	5.87336220807333	9.47014940327242
C	8.60637365178273	14.66003006402325	11.21669818133856
C	6.34810138563171	5.91917534910166	10.63464367882319
H	8.25754081870919	15.69064734906201	11.25436558245011
H	6.69548236807380	4.88811560748913	10.59575807667395
C	7.96014929173609	13.58409243856704	10.52673179935264
C	6.99649728572209	6.99364406349615	11.32507870517925
H	4.87607023082057	10.50650315851926	6.90843796895604
H	10.08891212254816	10.06391708005590	14.94256823924483
H	9.96833964319114	6.92983763646301	8.74805806126364
H	4.99949797333892	13.64913805593141	13.11164286151004
H	11.71287010532157	12.06619205438524	12.30906986853484
H	3.24410018963964	8.51832296284085	9.54800731685429

Optimized geometry of [Re₂-Model]¹⁻ (DFT-OLYP)

Re	8.06134731102773	10.73344833577053	10.09668900473163
Re	6.93111058413595	9.86822863139438	11.79298528814414
N	6.81526241998564	12.08652732261743	9.25107457349819

N	8.16525343089033	8.52776866837393	12.68089149424394
N	7.62515341010405	9.46218422226691	8.57498465919175
N	7.25260981298551	11.12212392068284	13.35991293083408
N	9.93191411503074	9.96249265508034	10.28014293661237
N	5.05705860214836	10.60036698976570	11.51821591702746
N	8.79317280671781	12.51796338202705	10.72067300019118
N	6.27777399641544	8.08241718251776	11.10310952724211
C	6.93828281302826	13.42424372274053	9.59929619892995
C	8.09192954338990	7.19501039379505	12.29931486332065
C	5.93211547076626	14.13588863933287	8.87802246458902
C	9.06057891001313	6.48665544112445	13.07287133069071
H	5.75523692182236	15.21213106800076	8.91966436207164
H	9.26026824654993	5.41479821751908	13.02218208488908
C	5.24053938014584	13.20707851480978	8.08623952848191
C	9.67387854865776	7.40928748179258	13.93329261856220
H	4.42651045913654	13.42189763783184	7.39162816722732
H	10.43867618798048	7.19316380510690	14.68156039137701
C	5.83454688745694	11.91443645209288	8.29948113734253
C	9.07032184798837	8.69539683031729	13.70570056160810
C	5.67344334176776	10.68014734083013	7.63036552940869
C	9.15715866690646	9.91602114372611	14.41421953208694
C	6.51753502514531	9.55788408864778	7.73327826288669
C	8.29785184005149	11.02422376049105	14.27798027002867
C	6.48129187965661	8.34740452647453	6.95003938651014
C	8.24273309467706	12.20631995188672	15.10376689707570
H	5.72533293565067	8.12082888774322	6.19602310498255
H	8.93192119672436	12.42268148232112	15.92220589755391
C	7.56835624958584	7.56822364070622	7.30869465530899
C	7.15928423187178	12.96696205849836	14.69649283390121
H	7.85053913398183	6.59590679693736	6.90163606933369
H	6.81505222739306	13.91157781046988	15.12123111683390
C	8.30758985860195	8.28204041958693	8.32159547485447
C	6.51458807123696	12.26974113481969	13.60963602304119
C	9.53657724349416	7.93845177535727	8.91965316588640
C	5.31399124604569	12.59738863732225	12.94752601238942
C	10.31828736105749	8.72335616301008	9.79119288534579
C	4.60953018435482	11.81781687909784	12.00753915982428
C	11.65449145037217	8.46908044238546	10.27367017173335
C	3.30618875220878	12.05663096485642	11.43596649281468
H	12.23211999464851	7.56799664529226	10.06040590176221
H	2.69467917459832	12.93994824035465	11.62784120107919
C	12.05731498519098	9.57341682663676	11.00604123352006
C	2.98503435814053	10.96652216922987	10.64424790001529
H	13.02320018604052	9.72923973191512	11.49020320831284
H	2.06320726242595	10.80650709184944	10.08205211493557
C	10.98021574115850	10.53361016865395	11.00076109633148
C	4.07896544312034	10.02860001622131	10.70530663790763
C	10.98797439193475	11.84252984749387	11.52184906840639
C	4.14138236386859	8.73624274070806	10.14869931266525
C	9.98210778139858	12.82087242592896	11.34709175000103
C	5.15175397353808	7.77426472962541	10.37279918461649
C	9.98240341213268	14.24385591347332	11.55958514794911
C	5.21250739345049	6.36193402040804	10.10643547659982
H	10.78335266476646	14.81197322556626	12.03631642919049
H	4.47118492266975	5.79261281348243	9.54307995731574
C	8.81204989154041	14.76527495274132	10.98839144041319
C	6.35242410996289	5.85080053831669	10.74383135748246
H	8.52731978648264	15.81782082863369	10.93924834624680
H	6.66927584832025	4.80662197937173	10.76717630628704
C	8.07508710892148	13.67212675528990	10.43976712523947
C	7.01362619679248	6.94089617811206	11.38696379927068
H	4.86392712204627	10.61012861199763	6.89864463031633
H	9.90480399336294	9.98009277961706	15.20996448694562

H	9.96548183736245	6.97791473856260	8.62150454543830
H	4.83904963787309	13.53552565122591	13.24761453591759
H	11.90407190003379	12.15331741349997	12.03226317789504
H	3.27918282105544	8.42564554566060	9.55228864532910

Optimized geometry of [Re₂-Model]¹⁻ (DFT-B3LYP)

Re	8.05531767003900	10.71537549212013	10.07525017926188
Re	6.90529787470760	9.86289859226308	11.77912780666564
N	6.82802844453073	12.06954741538292	9.18651153121845
N	8.13496142460784	8.51076872525648	12.66741850247713
N	7.68858788593875	9.46334191330039	8.50790802538240
N	7.27082119223007	11.11554759049583	13.34625980026909
N	9.94332833188251	9.97406693006227	10.28447343731254
N	5.01596232213388	10.60145433915780	11.57043101068573
N	8.76605704340989	12.50822939720434	10.71531065457941
N	6.19690753926645	8.06896303934911	11.13960366949752
C	6.92644039977024	13.39330747669726	9.55810303951391
C	8.03838724597214	7.18682619071318	12.29605137187316
C	5.93347478936817	14.10806820146712	8.82291542480380
C	9.03317174765484	6.47382829781714	13.03051338012406
H	5.74300610978740	15.17985574118853	8.87795876902918
H	9.22542232726711	5.40235592289518	12.97539807669501
C	5.28121861645868	13.18911834087121	7.99442198857932
C	9.68580128059396	7.39420780954192	13.85703499571627
H	4.48821569810903	13.40865557105277	7.27917341834794
H	10.48059709670024	7.17626118222436	14.57077652351136
C	5.88410760318578	11.90085346981672	8.20477994057736
C	9.07999781221729	8.68128971164198	13.64777558154564
C	5.75994997687617	10.67220694079727	7.51320504001178
C	9.20273575334511	9.91023924588332	14.33901984632800
C	6.61342506819070	9.55999990672005	7.63143284091974
C	8.34696429019558	11.02081582680160	14.22175219089117
C	6.62455025330444	8.36311404113279	6.82318763885382
C	8.33390675986655	12.21726058105894	15.03058499497001
H	5.90404182184364	8.13900920018519	6.03605761690445
H	9.05449282397683	12.44249077540480	15.81731771671996
C	7.70808531013306	7.59943972012577	7.20221246175212
C	7.24876403371470	12.97907966139318	14.65239112398857
H	8.02256217741560	6.64401299432525	6.78202759773595
H	6.93278178706244	13.93379890791900	15.07304483958965
C	8.39978544108376	8.30790363399562	8.25479417657893
C	6.55736882684870	12.26934489929159	13.60047818394564
C	9.61450050031080	7.96991957118290	8.88538308303258
C	5.34131354531691	12.60501930673247	12.97121848051625
C	10.35553557299435	8.75097086832944	9.79537447892124
C	4.60136998122058	11.82311293691716	12.06104923428138
C	11.67532320570252	8.49822659990399	10.32702640088516
C	3.28049859878242	12.07319343871303	11.53080168329662
H	12.26879106771089	7.60628436230599	10.12574729521333
H	2.68490410569588	12.96333453993991	11.73386735369509
C	12.03812521702372	9.58947658855869	11.08738337266895
C	2.91985067515871	10.98219409411353	10.76892079820656
H	12.98205187652621	9.74241302803135	11.61138760068627
H	1.97592522076612	10.82765090627734	10.24540729188982
C	10.95399892823871	10.54301646549567	11.05155379509224
C	4.00600738819467	10.03092056108261	10.80352957834380
C	10.93130134187564	11.84307017885979	11.58876697015761
C	4.03082774297565	8.73102021581562	10.26593400161163
C	9.92210821781641	12.81501785036995	11.38806188324768
C	5.04136270300377	7.76051790606296	10.46670509048662
C	9.88966200715673	14.23241046116613	11.62726156962298
C	5.07573913343349	6.34308448919149	10.22784488415940
H	10.65986859724536	14.80586051975454	12.14355756515459

H	4.30623364269941	5.76843650524061	9.71182554159372
C	8.73280423883037	14.74184096334036	11.02842458935175
C	6.23365579650336	5.83548736224286	10.82615332468638
H	8.42864689177814	15.78789130654877	10.99253238602002
H	6.53948441610758	4.78991418139327	10.86184852314411
C	8.03844515528253	13.64505857567729	10.43500415282041
C	6.92634004464281	6.93326717705768	11.41973621206248
H	4.97986170519732	10.60405244895081	6.75087229051881
H	9.98348800907897	9.97986561108804	15.10054110391812
H	10.06623147189917	7.02154757414557	8.58471267250901
H	4.88775722272120	13.55218252717913	13.27291944791365
H	11.82131330731909	12.15316181940964	12.14201180427788
H	3.14113769110084	8.41953137336599	9.71295214315575

Optimized geometry of [Os₂-Model]¹⁻ (DFT-OLYP)

Os	8.05594899642740	10.70534180971547	10.07732792239914
Os	6.90203520405349	9.87176535770171	11.77642265401296
N	6.75951891880426	11.86084903814550	9.15214009315892
N	8.07750632190245	8.46446383202615	12.50584706353535
N	7.78621936016652	9.31877379445162	8.66498146859922
N	7.42335191305124	11.05236881490398	13.29660812391199
N	9.90985484574607	10.06221180882057	10.43353244071733
N	5.14247334697628	10.79803302798640	11.58683555134094
N	8.59184774251634	12.50020049132307	10.69847460028328
N	6.09177058527157	8.23886523328085	11.03513208822602
C	6.67962262642632	13.20055468537308	9.54155961982836
C	7.95143318710376	7.17683556886783	11.99125222238041
C	5.56496226495559	13.75508236839676	8.86505039117802
C	9.0152888625723	6.41211675224240	12.53960177946483
H	5.21478166893988	14.78492684097704	8.94899725951807
H	9.21363046511597	5.35772216485692	12.34131348278184
C	4.99635501018724	12.74128294130416	8.06767806345164
C	9.75096748750353	7.25654111364537	13.39625245883274
H	4.12448135678070	12.83708012142487	7.41919808641844
H	10.63162957139195	6.98277283158038	13.97912491636981
C	5.77257788240873	11.55091557065444	8.23928418394441
C	9.13697188934082	8.54610590497871	13.38468277706950
C	5.71062261369976	10.26822459664450	7.65877348569667
C	9.37767262630421	9.73789599626123	14.10549495555219
C	6.66963537003269	9.24573067927292	7.82896228128023
C	8.56662983818772	10.88024867763968	14.08363330452556
C	6.71136628868931	7.96676201206594	7.18476645116690
C	8.71938404664878	12.07829824029363	14.86900241562918
H	5.96194798654095	7.60843222661502	6.47767274531202
H	9.52992082511274	12.24728758356537	15.57988672896444
C	7.85205068434370	7.29550146428025	7.62033965519092
C	7.67984851600395	12.93678443986691	14.55988748472783
H	8.18754873263682	6.29901737734063	7.32979477875127
H	7.49361587567875	13.93000135503058	14.97053075684992
C	8.53100358573909	8.14530574058776	8.54564273186753
C	6.85065205057372	12.29249759283820	13.57673463023145
C	9.73916646784367	7.91598352044665	9.23244703997719
C	5.67545224842495	12.76312338131763	12.98616319852306
C	10.39689403772097	8.80198423416083	10.08895259916544
C	4.85648869651599	12.07504689952959	12.06980369172091
C	11.65887057590823	8.63095185690455	10.75816848265721
C	3.62244703288167	12.49162078884024	11.48383697797909
H	12.27776494460674	7.73526678773399	10.69119495116684
H	3.14369900927091	13.45543712957700	11.66216221786838
C	11.92067270505874	9.78462052594851	11.47475036979458
C	3.17297704902691	11.46065822254259	10.66149672690801
H	12.79377983631566	9.99659110398430	12.09413226668800
H	2.26490082291828	11.44391710332761	10.05728962117074

C	10.82760482658874	10.70128932693051	11.27343022077351
C	4.11799183748830	10.38600599966014	10.73147187428795
C	10.69770904247489	11.99837528000691	11.78700907740557
C	4.04837544411090	9.13080805150486	10.08836458167600
C	9.64963558012673	12.89840628411914	11.48837358419589
C	4.95534314447730	8.06767483762600	10.27172960975197
C	9.43337844770915	14.27877192530042	11.78526107218867
C	4.96528653196669	6.70384007377700	9.83718465506037
H	10.08146098074928	14.89921616084080	12.40598789999040
H	4.20998432588418	6.23934224144443	9.20182768264612
C	8.25490483101666	14.68964096769017	11.12930594012012
C	6.10327126471764	6.07697288932026	10.38430730481912
H	7.82361827287464	15.69177226635645	11.13829326263200
H	6.39381213874489	5.03378565053216	10.25146761650276
C	7.73579008298569	13.56568099501374	10.43309458877131
C	6.80710232182317	7.04347557839859	11.14463025034744
H	4.89098595303250	10.06035816679004	6.96739476626557
H	10.24353501487045	9.76353847021903	14.77127224847801
H	10.22042599194165	6.94936605493158	9.06473782352637
H	5.34828049934422	13.76419472301296	13.27757283998423
H	11.50114623617296	12.35120763822890	12.43787206118144
H	3.18110523288639	8.95676680902146	9.44761324260521

Optimized geometry of [Os₂-Model]¹⁻ (DFT-B3LYP)

Os	8.06295970310305	10.69757395274376	10.07304923294344
Os	6.89878587847709	9.88042162420240	11.78167782643552
N	6.84944162083575	12.01002086847606	9.20763179219282
N	8.12093124572323	8.58463517222882	12.65966709890836
N	7.68445921767437	9.43392283975522	8.55495559139985
N	7.25945546038387	11.15671591156071	13.29370122158959
N	9.90400853873261	9.91983260429559	10.29883259710675
N	5.05143444477749	10.63912161812219	11.54425421858511
N	8.77797680719516	12.43229175444155	10.72363099705638
N	6.20278528476096	8.13517164649303	11.13835817900273
C	6.88761046548107	13.32185862099901	9.65612584658157
C	8.09688417059971	7.26970161728150	12.21879862153049
C	5.81351886110847	13.99992774921640	9.03271397636287
C	9.17415757252022	6.60525979617837	12.85101159755683
H	5.55700223576383	15.05087840936846	9.16387336497576
H	9.44059746243953	5.55586924659854	12.72742258429165
C	5.15381935947033	13.07563957626764	8.19786866158948
C	9.82221137062948	7.54065483465968	13.68266531007398
H	4.28913373164588	13.27622885437247	7.56550062163394
H	10.68599972920064	7.35176850309472	14.31984122711567
C	5.83024857078423	11.82497730717037	8.30137967963286
C	9.13478392510055	8.78453678451650	13.56875513444651
C	5.67509529166263	10.58110015884365	7.64004851517088
C	9.27648258334421	10.03394356209096	14.22240402223692
C	6.55909548754162	9.49494507050508	7.73382536951247
C	8.38233524907290	11.11147393207946	14.11905798990978
C	6.51439185498037	8.26199778906033	6.99101680490451
C	8.41284942275311	12.34920340823509	14.85387914953886
H	5.74366277018096	8.00874503413395	6.26294508235279
H	9.17874212846827	12.61445827279316	15.58276466198650
C	7.60608802544871	7.49801747504204	7.35323991038317
C	7.31453008414002	13.10040219947986	14.48345524344330
H	7.87819208506932	6.51209977834391	6.97680409345409
H	7.03162099492821	14.08593677434444	14.85286751482989
C	8.35340085068226	8.23291935162486	8.33181731998966
C	6.57823375507280	12.35260019261281	13.50705252670348
C	9.55540780948475	7.87798564213865	8.95867745513757
C	5.37449074743649	12.69180504753451	12.87358646244465
C	10.29613691826436	8.65841412192039	9.85742485845401

C	4.64520884443559	11.89900718834964	11.97724084853561
C	11.56308667160525	8.36483972497419	10.46017664444282
C	3.37722283730467	12.17663126368115	11.36793060492942
H	12.12366523132451	7.44261900652187	10.30840739458814
H	2.80706875018245	13.09414460791780	11.51230146429169
C	11.92376558627366	9.44721703986512	11.23897529674213
C	3.03009783536752	11.08666020671732	10.59438250593083
H	12.83297036110135	9.56193055640218	11.82925331465300
H	2.12419967770989	10.95959404385857	10.00155262600502
C	10.88936342791525	10.44319270596772	11.13505599664624
C	4.07401996516914	10.10122437121954	10.70778233316852
C	10.86977457763531	11.71930731613943	11.72055124888390
C	4.10763460164846	8.82236141817470	10.13028007597701
C	9.88751915419460	12.71390816167352	11.48775300688505
C	5.09891089399349	7.83862084842802	10.37172324095637
C	9.79327392842575	14.09265227791189	11.83883513520998
C	5.20764478905954	6.45904049811962	10.02877729932124
H	10.51178443234185	14.64045730135383	12.44825768952428
H	4.49666491516166	5.90091812519374	9.41986370277440
C	8.62940660728002	14.61713000347367	11.24162424627911
C	6.37384998793018	5.94891627971426	10.63381261194367
H	8.28128536311465	15.64811700311775	11.29940067136652
H	6.73157935842834	4.92080277715620	10.58384369928149
C	8.00237843979651	13.56616051844564	10.53163567204486
C	6.98818614404547	7.00999466898992	11.34001683522331
H	4.83914418691948	10.47500436514522	6.94563647604296
H	10.10868172390978	10.15190834942239	14.91939830526807
H	9.97109076374705	6.90103078706125	8.70165548290361
H	4.94814809374524	13.66607435210384	13.12320174784299
H	11.72168482288133	11.98327995267789	12.35050679409798
H	3.26071631241274	8.54668717739502	9.49860466677383

¹ B. Alemayehu, L. J. McCormick-McPherson, J. Conradie and A. Ghosh, *Inorg. Chem.*, 2021, 60, 8315-8321.

² A. B. Alemayehu, L. J. McCormick, H. Vazquez-Lima and A. Ghosh, *Inorg. Chem.*, 2019, 58, 2798-2806.