STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 76 (2020)

Supporting information for article:

Intra- and intermolecular interactions in a series of chlorido- tricarbonyl-diazabutadiene rhenium(I) complexes: structural, theoretical, non-covalent interaction index and natural bond orbital studies

Reza Kia and Azadeh Kalaghchi

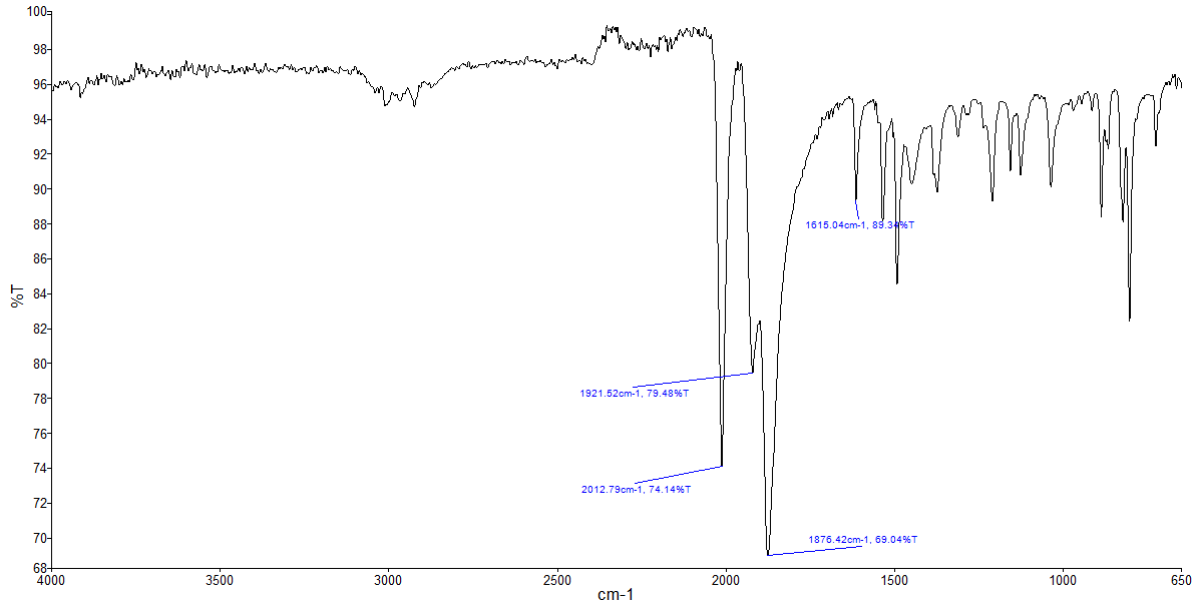


Fig. S1. The FTIR spectrum of **1** in KBr pellet.

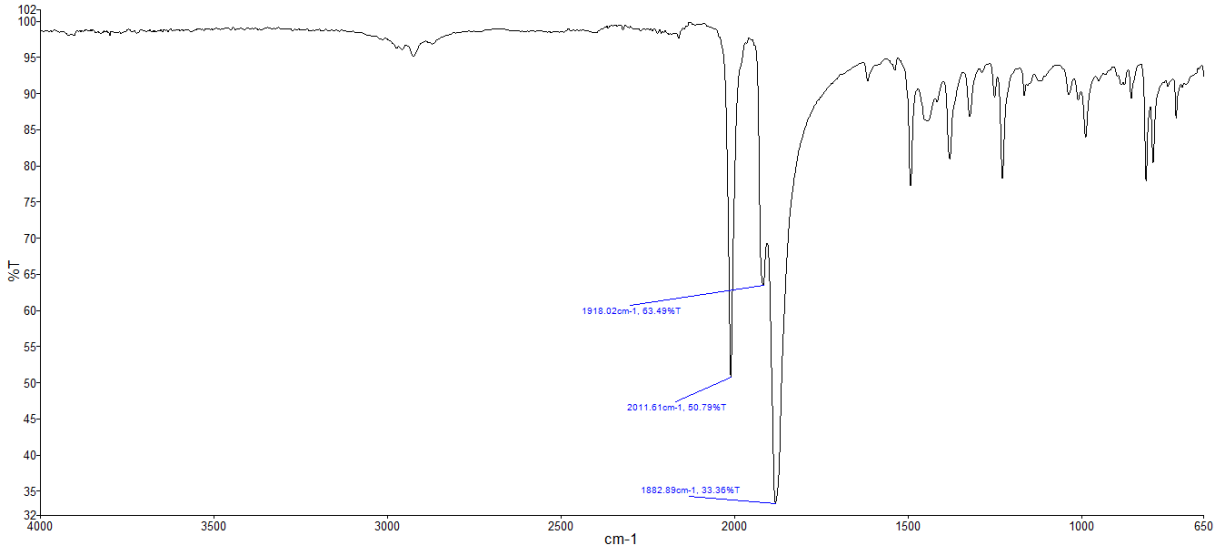


Fig. S2. The FTIR spectrum of **2** in KBr pellet.

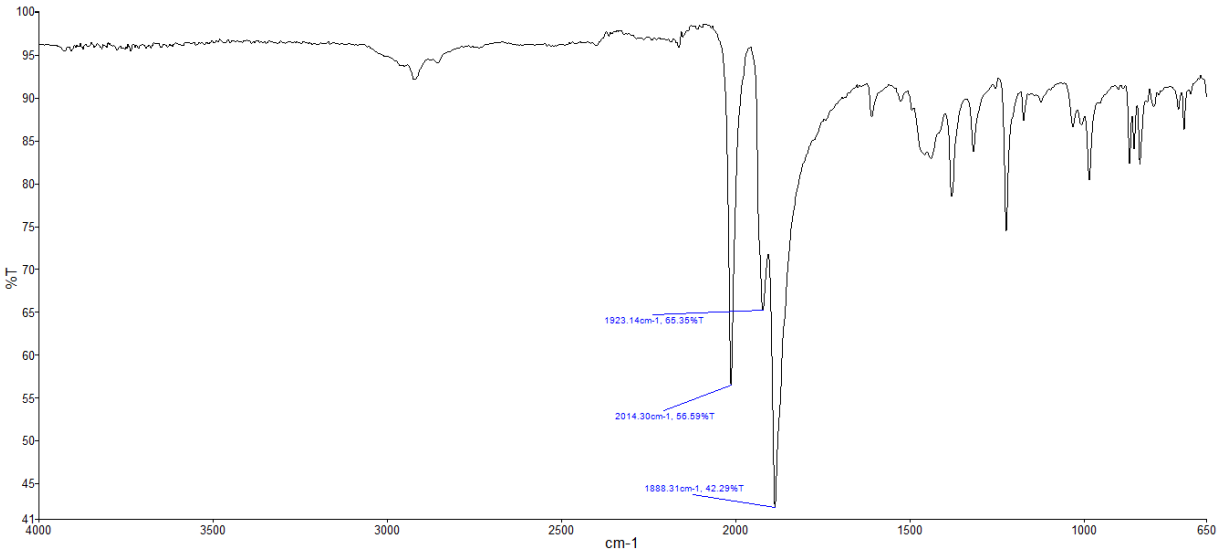


Fig. S3. The FTIR spectrum of **3** in KBr pellet.

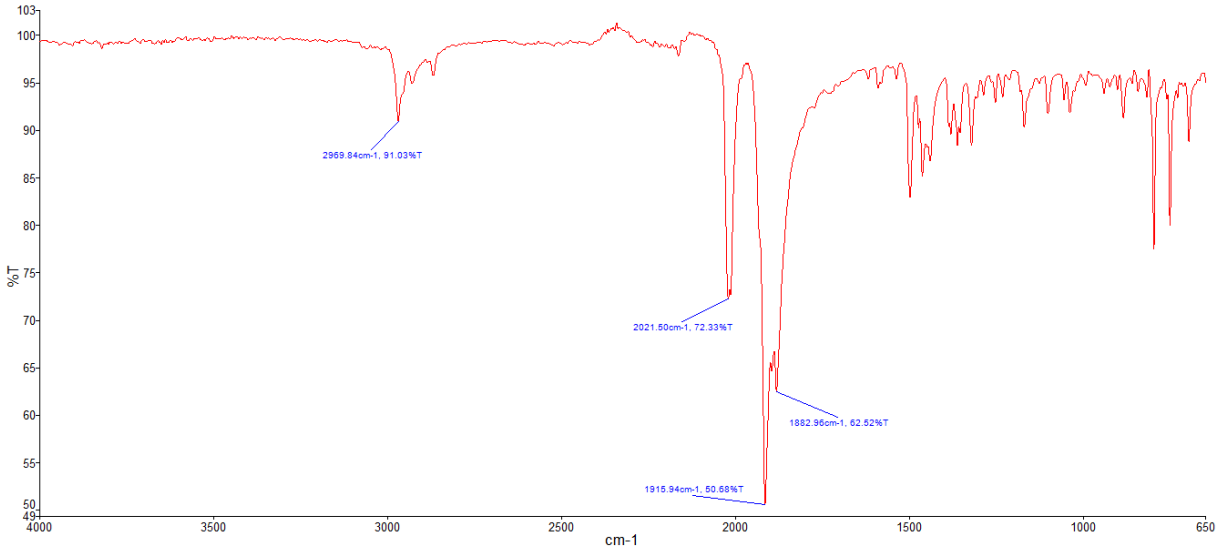
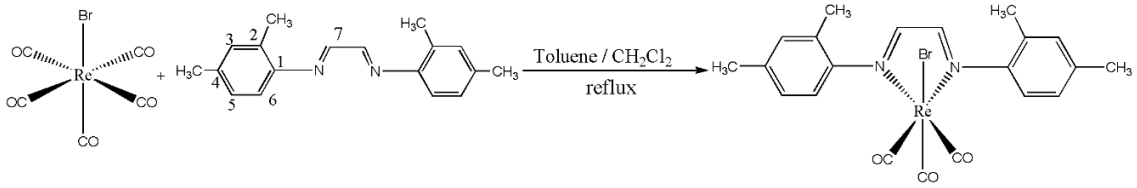


Fig. S4. The FTIR spectrum of **4** in KBr pellet.



[Re(CO)$_3$($^{2,4\text{-Me}_2}$DAB)Br]

^{1}H-NMR (δ_{ppm} $CDCl_3$): 2.40 (s, 6H, 2-CH_3), 2.41 (s, 6H, 4-CH_3), 7.10-7.46 (m, 6H, aromatic hydrogens), 8.61 (s, 2H, iminic hydrogens).

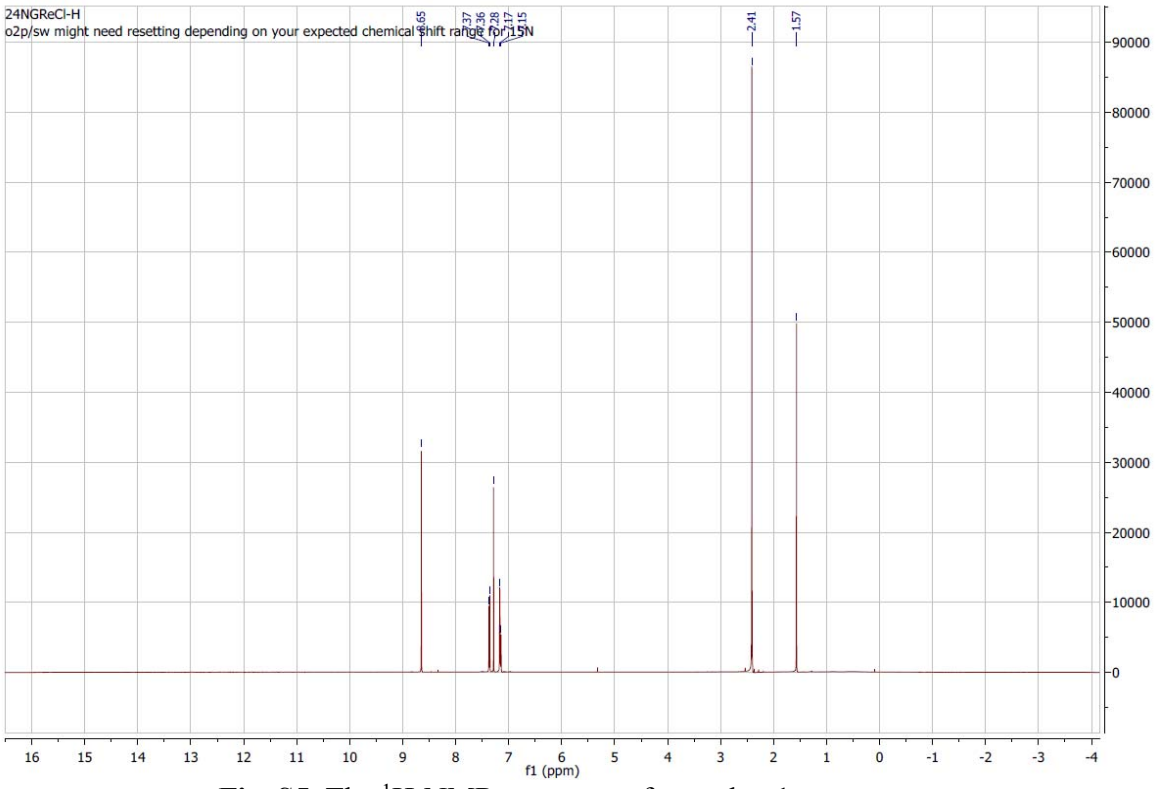


Fig. S5. The ^{1}H-NMR spectrum of complex **1**.

^{13}C{^{1}H}-NMR (500 MHz, $CDCl_3$): 18.06 (2-CH_3), 21.05 (4-CH_3), 123.14 (C6), 127.12 (C2), 127.55 (C5), 132.14 (C3), 138.64 (C4), 148.85 (C1), 165.02 (iminic carbon), 182.94 (CO_{ax}), 194.79 (CO_{eq}).

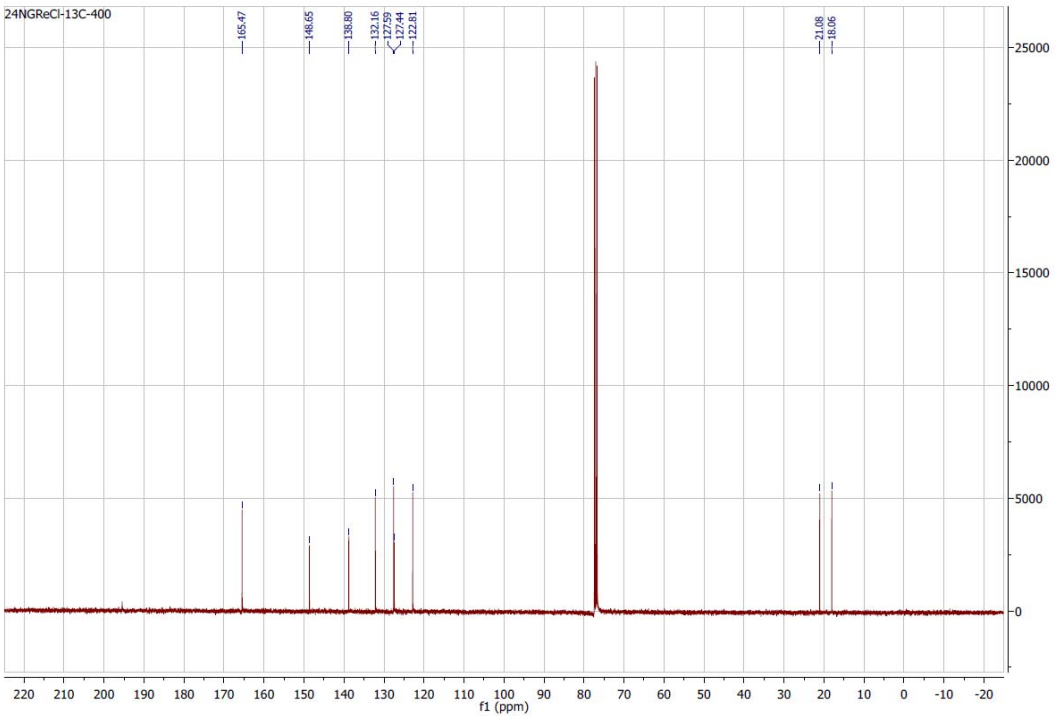
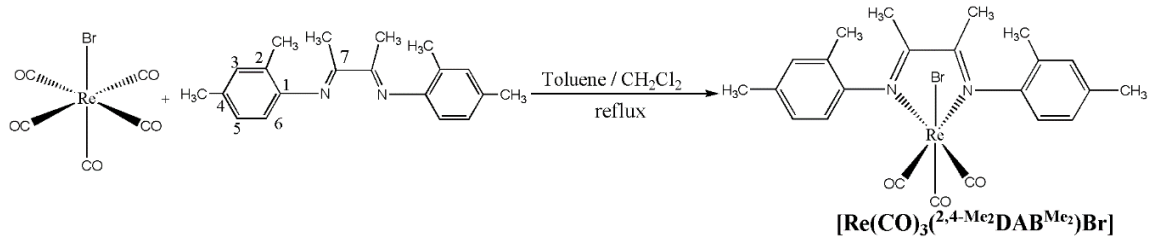


Fig. S6. The $^{13}C\{^{1}H\}$-NMR spectrum of complex **1**.



^{1}H-NMR (δ_{ppm} $CDCl_3$): 2.10 (s, 6H, 2-CH_3), 2.20 (m, 6H, 4-(CH_3)), 2.35 (s, 6H, 7-CH_3), 7.0-7.5 (m, 6H, aromatic hydrogens).

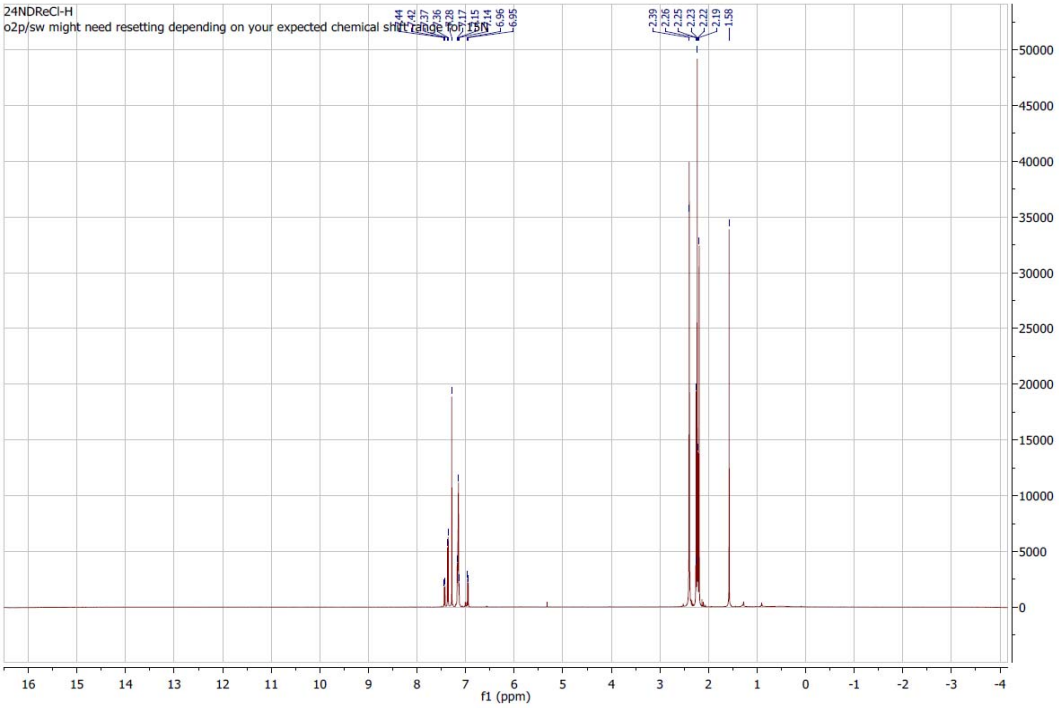


Fig. S7. The ^{1}H-NMR spectrum of complex **2**.

$^{13}C\{^{1}H\}$-NMR (500 MHz, $CDCl_3$): 17.02 (2-CH_3), 20.41 (4-CH_3), 20.97 (7-CH_3), 121.37 (C6), 126.09 (C2), 128.36 (C5), 132.16 (C3), 137.31 (C4), 146.39 (C1), 174.97 (iminic carbon) ,185.01 (CO_{ax}), 195.28 (CO_{eq}).

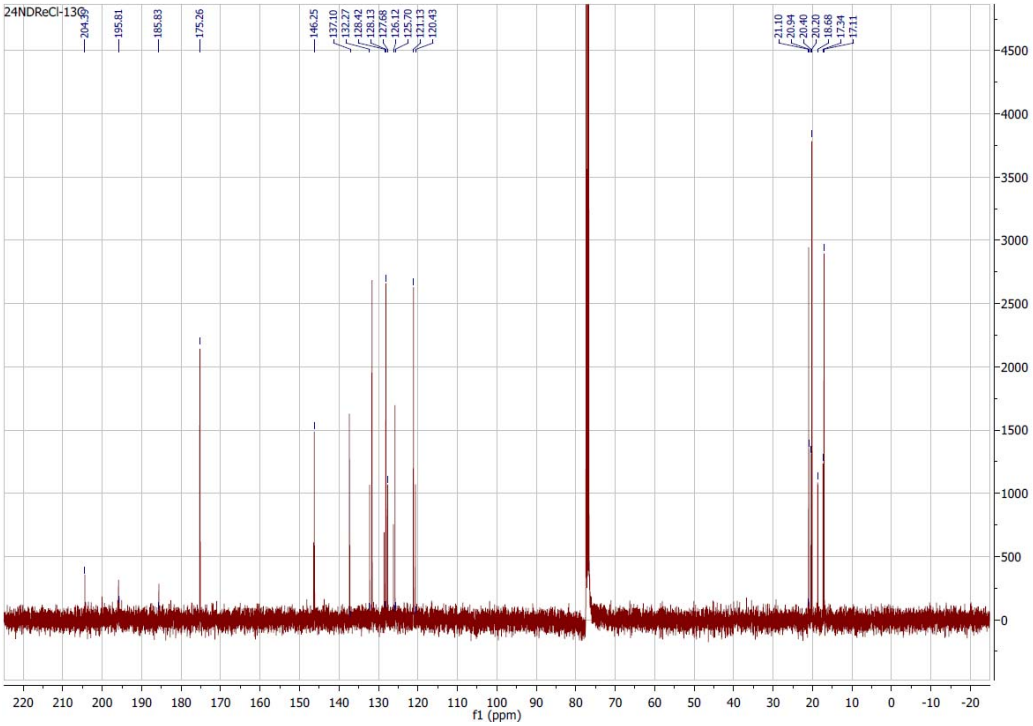
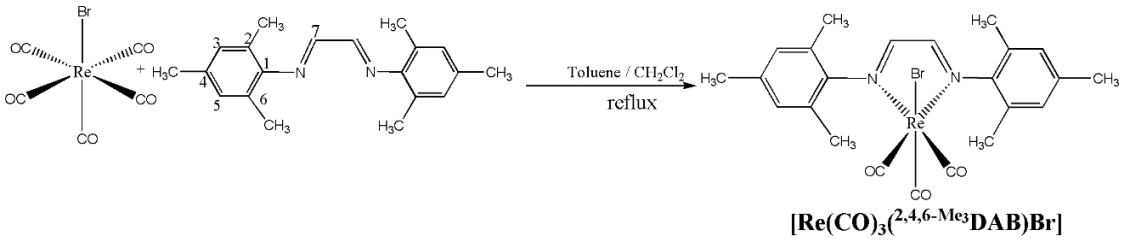


Fig. S8. The $^{13}C\{^{1}H\}$-NMR spectrum of complex **2**.



^{1}H-NMR (δ_{ppm} $CDCl_3$): 2.28 (s, 6H, 6-CH_3), 2.37 (s, 6H, 2-CH_3), 2.60 (s, 6H, 4-CH_3), 7.0-7.28 (m, 4H, aromatic hydrogens), 8.69 (s, 2H, iminic hydrogens).

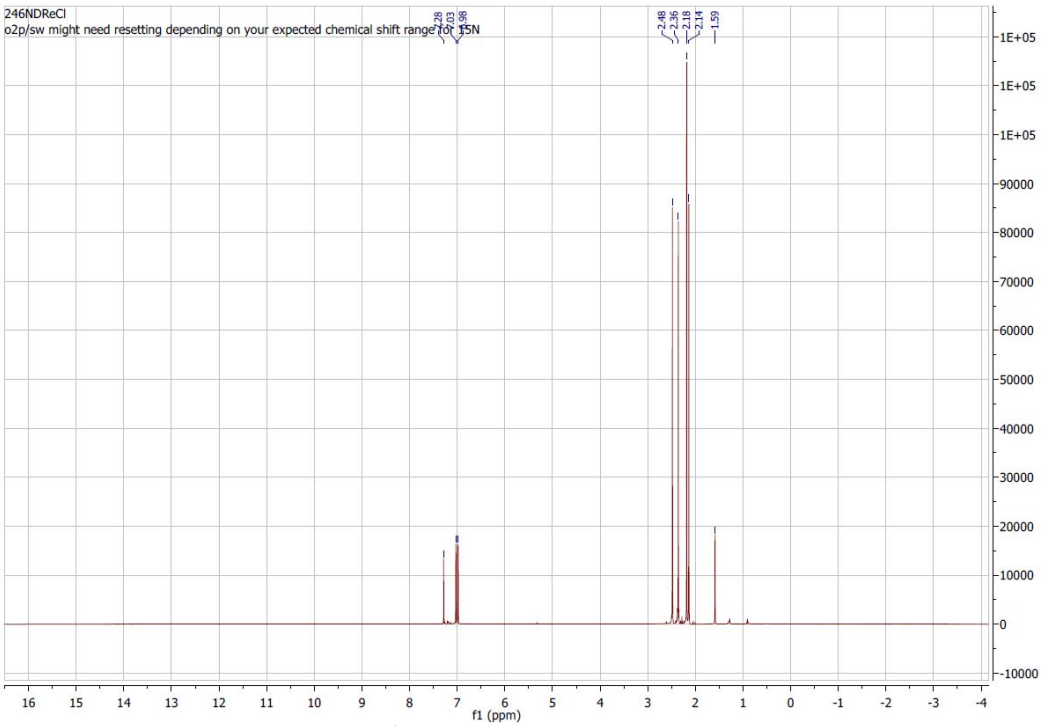


Fig. S9. The ^{1}H-NMR spectrum of complex **3**.

$^{13}C\{^{1}H\}$-NMR (500 MHz, $CDCl_3$): 19.03 (6-CH_3), 20.77 (2-CH_3), 20.89 (4-CH_3), 128.29 (C6), 129.64 (C5), 129.94 (C2), 130.25 (C3), 137.97 (C4), 148.44 (C1), 165.88 (iminic carbon) ,183.89 (CO_{ax}), 194.17 (CO_{eq}).

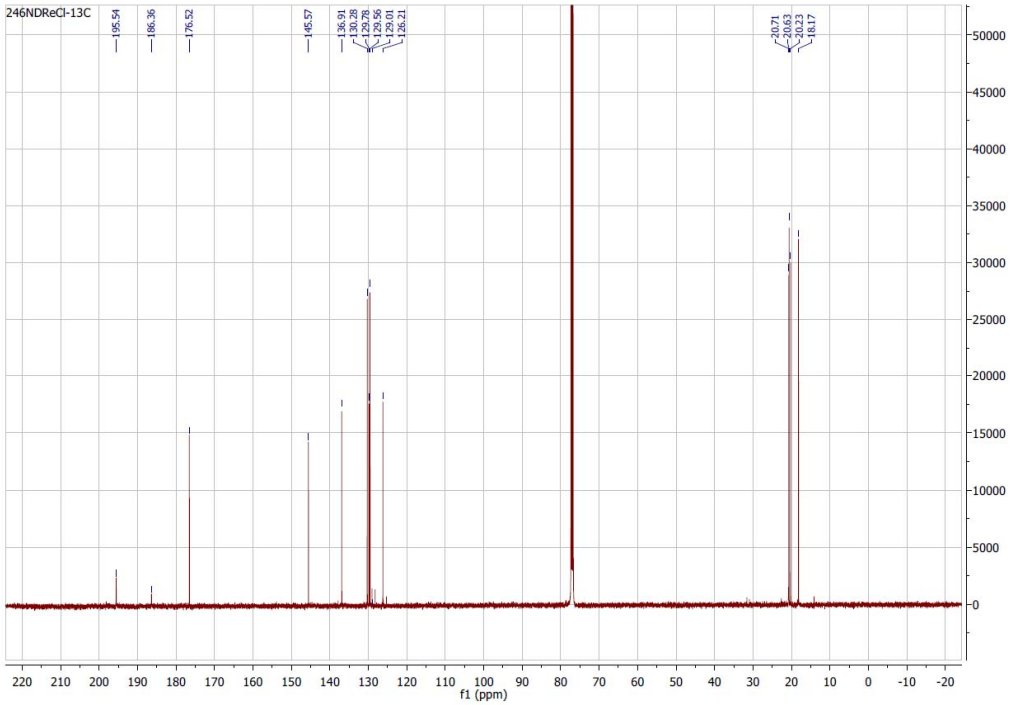
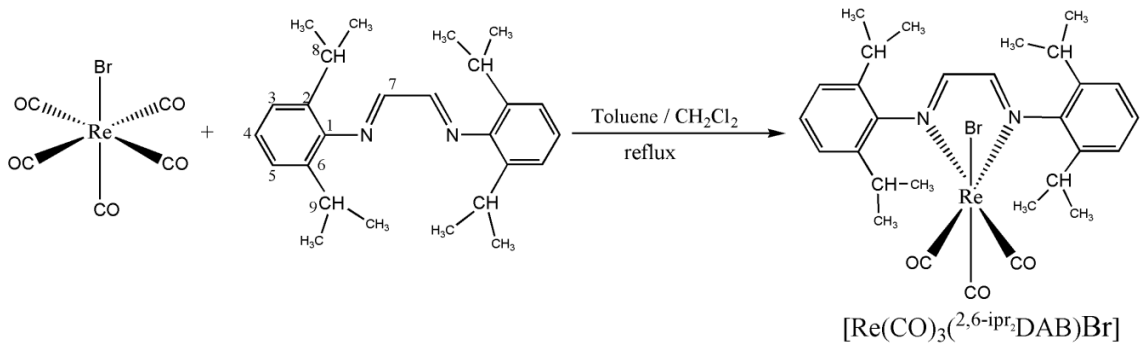


Fig. S10. The $^{13}C\{^{1}H\}$-NMR spectrum of complex **3**.



^{1}H-NMR (δ_{ppm} $CDCl_3$): 1.1(m, 12H, 8-$(CH_3)_2$), 1.35 (m, 12H, 9-$(CH_3)_2$), 2.75 (m, 2H, isopropyl hydrogens (8-CH)), 4 (m, 2H, isopropyl hydrogens (9-CH)), 7.1-7.4 (m, 6H, aromatic hydrogens), 8.7 (s, 2H, iminic hydrogens).

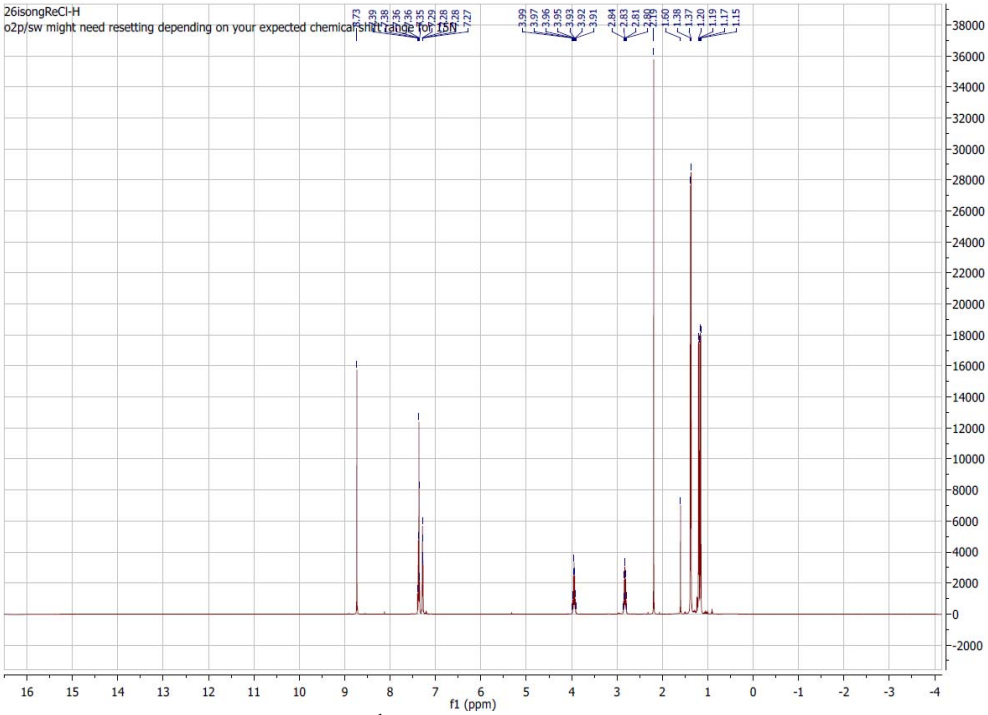


Fig. S11. The ^{1}H-NMR spectrum of complex **4**.

$^{13}C\{^{1}H\}$-NMR (500 MHz, $CDCl_3$) : 23.18 and 26.44 and 27.08 and 28.38 (methyls carbon), 28.55 (isopropyl carbon), 124.19 (C5), 124.91 (C3), 129.09 (C4), 139.54 (C6), 141.01 (C2), 148.14 (C1), 166.22 (iminic carbon), 182.58(CO_{ax}), 194.19(CO_{eq}).

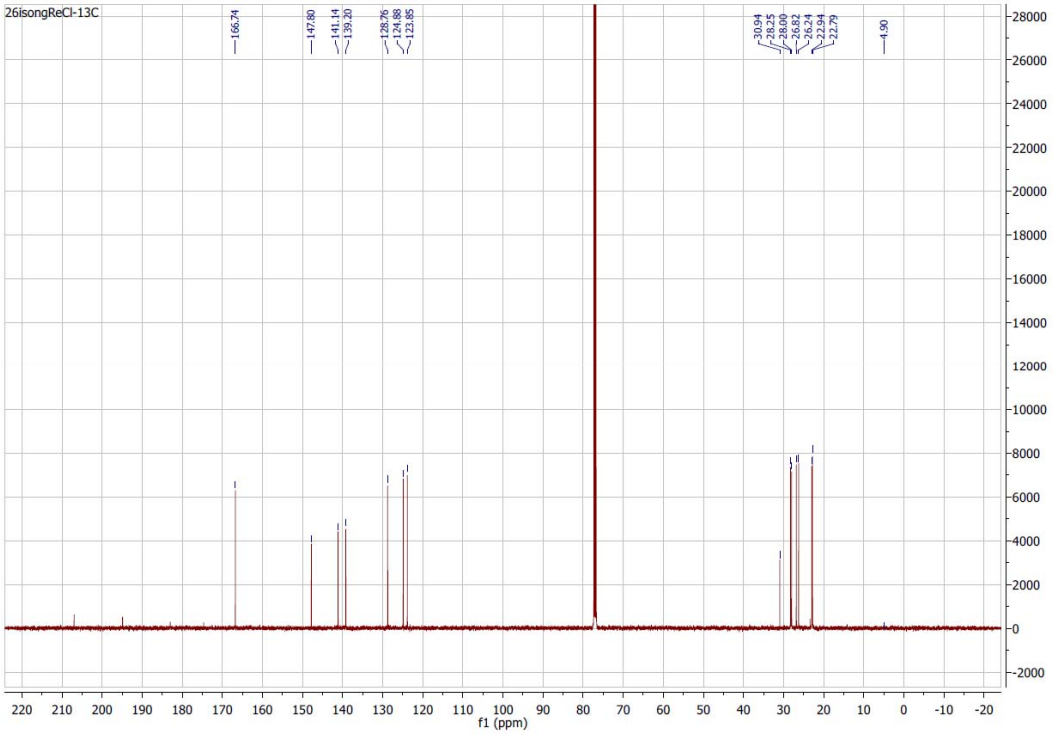


Fig. S12. The $^{13}C\{^{1}H\}$-NMR spectrum of complex **4**.

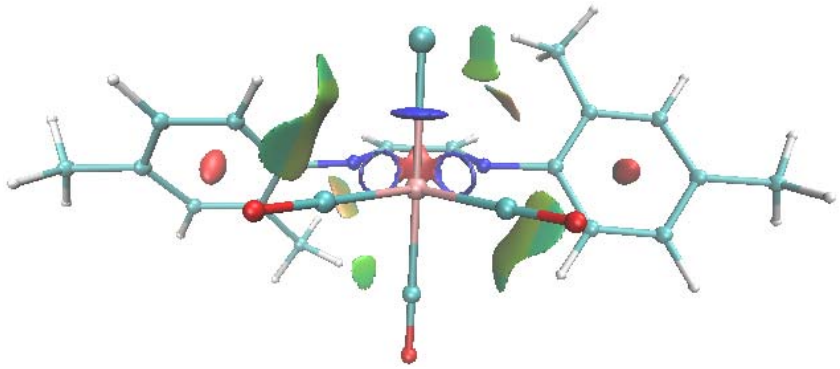


Fig. S13. The NCI plot of complex **1** derived from the optimized structure.

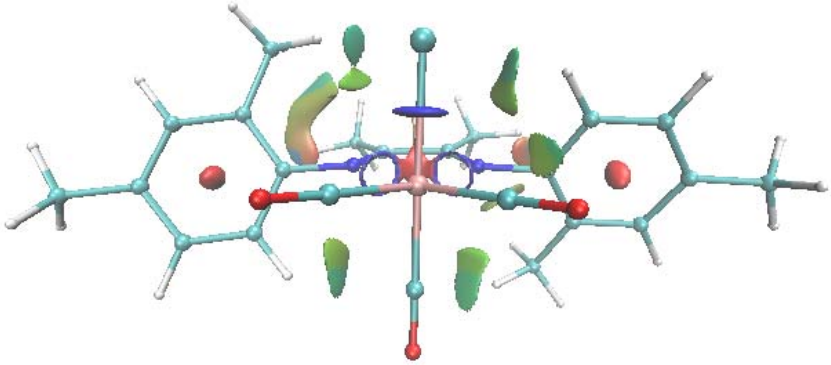


Fig. S14. The NCI plot of complex **2** derived from the optimized structure.

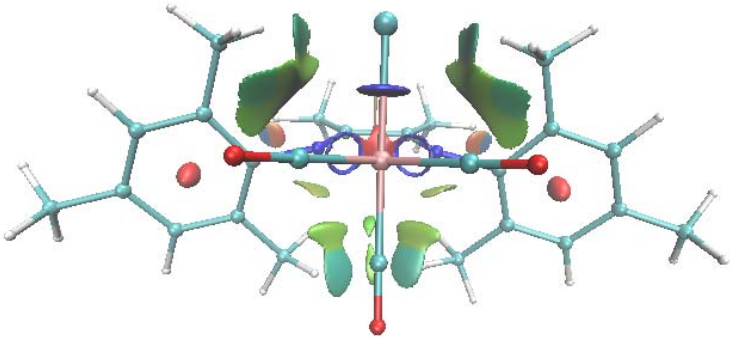


Fig. S15. The NCI plot of complex **3** derived from the optimized structure.

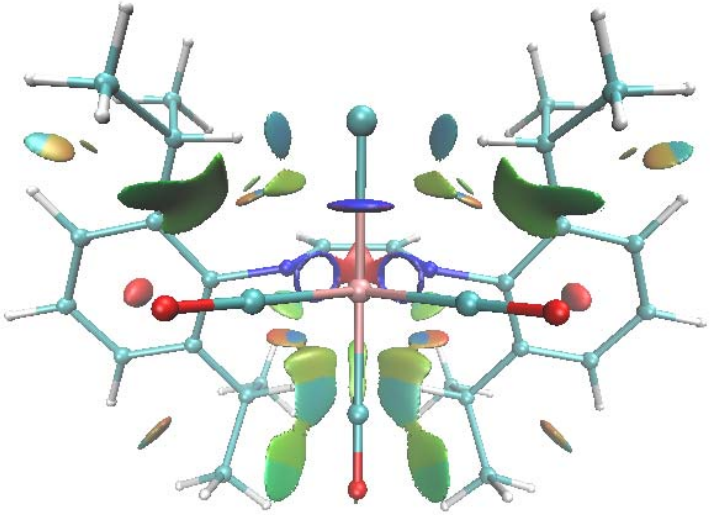


Fig. S16. The NCI plot of complex **3** derived from the optimized structure.

Cartesian coordinates of the optimized structure of complex **1**

Re	-0.01109100	0.79868900	0.03012100
Cl	0.17268300	0.56537500	-2.46986400
O	-0.26160400	1.03466400	3.08807100
C	-0.16652700	0.93941000	1.93408900
O	-2.17138000	2.98168000	-0.31782400
C	-1.35843700	2.17020600	-0.18242600
O	2.21859800	2.94036700	-0.00552100
C	1.37365900	2.15119000	0.01922700
C	0.72122400	-2.08972400	-0.07299600
H	1.27674300	-3.02340800	-0.11155000
N	1.30851900	-0.94597500	0.07272300
C	3.29685300	-0.21217000	1.21528500
H	2.64331700	0.23647900	1.95763900
C	-2.74030000	-0.89977800	-0.07686700
N	-1.31559800	-0.94084800	-0.07973900

C	3.54421400	-1.47913200	-0.85264300
C	3.00911200	-2.16883600	-2.07883000
H	3.72458700	-2.07230800	-2.90068500
H	2.05721300	-1.74052300	-2.40744500
H	2.85795300	-3.24237700	-1.91155300
C	-2.86345200	-2.23846600	2.10016900
H	-2.65802600	-3.29001600	1.86604800
H	-3.54138700	-2.22752500	2.95827600
H	-1.91865300	-1.78106900	2.41112800
C	-0.72170100	-2.08844400	-0.13226000
H	-1.27606100	-3.02086500	-0.21312000
C	4.92900500	-1.35929700	-0.68769200
H	5.57206000	-1.78894600	-1.45320100
C	-3.36748100	-0.19751500	-1.11069000
H	-2.75356600	0.26539100	-1.87846300
C	-3.48926800	-1.51485700	0.93825000
C	4.67174500	-0.14048000	1.35834400
H	5.09498400	0.37442800	2.21701800
C	-4.75013400	-0.13056600	-1.16707100
H	-5.22728300	0.40062000	-1.98684300
C	5.51634900	-0.71481200	0.39967300
C	-5.53377100	-0.73118700	-0.17358600
C	7.00901600	-0.62037700	0.53706400
H	7.52019600	-1.13273200	-0.28281100
H	7.34637600	-1.06653500	1.47991200
H	7.33866000	0.42525100	0.54148400
C	2.72887000	-0.89503300	0.13293800
C	-4.88203900	-1.40042700	0.86150300
H	-5.47708900	-1.85483700	1.65125400
C	-7.03285100	-0.64223200	-0.22111200
H	-7.36705500	0.40161200	-0.19653900
H	-7.49229700	-1.16434000	0.62298200
H	-7.42431100	-1.08216700	-1.14585800

Cartesian coordinates of the optimized structure of complex **2**

Re	-0.00761900	-0.87986800	-0.01819000
Cl	0.00478500	-0.58222200	-2.52644300
C	-0.03629100	-1.08981100	1.88075500
O	-0.05088600	-1.23395100	3.03531500
C	1.37904600	-2.22048700	-0.16124000
O	2.23552400	-2.99217200	-0.26385600
C	-1.36748100	-2.24351400	-0.19454300

O	-2.19959400	-3.03977500	-0.30891700
C	2.71144200	0.72991600	0.16885600
C	3.58177400	0.99748300	-0.89740500
C	4.94738700	0.76879700	-0.68374100
H	5.63134600	0.96365900	-1.50767300
C	5.46260100	0.30752500	0.52563500
C	4.56226100	0.05447900	1.56790300
H	4.92786100	-0.30642700	2.52612200
C	3.20210900	0.24940700	1.38712200
H	2.50464700	0.04010800	2.19287300
C	0.73677100	2.03856300	-0.03675300
C	-0.74550900	2.03226800	-0.11645100
C	-2.72729600	0.72995900	-0.03191600
C	-3.35238400	0.25911400	-1.18811400
H	-2.74533400	0.04077700	-2.06215200
C	-4.72807100	0.07715000	-1.20764900
H	-5.20584000	-0.27915200	-2.11715700
C	-5.50082800	0.33884900	-0.07075200
C	-4.84727900	0.79230600	1.07507000
H	-5.43160400	0.99503700	1.97064500
C	-3.46503900	1.00278300	1.12833800
C	6.93642800	0.07832100	0.71032200
H	7.49782100	0.33931500	-0.19138100
H	7.32901200	0.67845400	1.53957900
H	7.14642700	-0.97143300	0.94694200
C	1.46020000	3.34111600	0.00815100
H	1.00787500	3.99840300	0.75809000
H	2.51441500	3.20268400	0.25023300
H	1.38583300	3.85576400	-0.95714900
C	-1.47888600	3.32113800	-0.27064900
H	-1.07592400	3.87920400	-1.12289500
H	-2.54474000	3.15478900	-0.42995300
H	-1.34972500	3.95240000	0.61623200
C	-6.98915000	0.12852700	-0.08696300
H	-7.44286700	0.40679000	0.86867200
H	-7.46454900	0.72535300	-0.87410400
H	-7.23813100	-0.92059600	-0.28562700
C	-2.81903800	1.50226500	2.38998000
H	-1.90394200	0.95046900	2.62812000
H	-2.54903000	2.56327100	2.31541900
H	-3.50439600	1.40141900	3.23599000
N	1.29175000	0.87175400	0.04605100
N	-1.30154300	0.86621500	-0.03771300
C	3.11023000	1.50964400	-2.22931800
H	3.78686000	1.18020800	-3.02355600
H	2.10371600	1.15670800	-2.47055800

H	3.10057700	2.60728300	-2.25142800

Cartesian coordinates of the optimized structure of complex **3**

Re	0.00552000	-0.90390600	-0.36565900
Cl	-0.01146700	-2.09622500	1.85754800
C	0.03378700	-0.08693100	-2.09266700
O	0.05603800	0.34588600	-3.17356800
C	-1.37445400	-2.10581800	-0.99784200
O	-2.22125700	-2.80906200	-1.35372700
C	1.38573400	-2.11941600	-0.97047800
O	2.23032500	-2.83234700	-1.31198800
C	-2.71160400	0.67144600	0.31698000
C	-3.66339300	-0.15964300	0.92760000
C	-4.99958000	-0.01664000	0.54603900
H	-5.74128700	-0.65313600	1.02470400
C	-5.41074500	0.91041900	-0.40977700
C	-4.43984500	1.74114300	-0.96830300
H	-4.73593100	2.49625000	-1.69383400
C	-3.09211200	1.65028700	-0.61888400
C	-0.75083000	1.31408300	1.48871400
C	0.73509500	1.31647500	1.49632600
C	2.70536700	0.67715400	0.33762400
C	3.65946200	-0.16846800	0.92482800
C	4.99240500	-0.02107800	0.53566100
H	5.73693700	-0.66733300	0.99656600
C	5.39740700	0.92109900	-0.40893800
C	4.42462600	1.76396900	-0.94480500
H	4.71608400	2.52907300	-1.66171300
C	3.08019200	1.67289500	-0.58177600
C	-3.29914200	-1.16048100	1.98443400
H	-2.75151500	-2.01074500	1.56626600
H	-4.20135100	-1.54009200	2.47246000
H	-2.64744300	-0.73015300	2.75188900
C	-6.85101600	1.00881900	-0.82814000
H	-7.10611200	2.02398700	-1.14837800
H	-7.52437900	0.72559800	-0.01297800
H	-7.06034500	0.33849600	-1.67150000
C	-2.10276600	2.60800400	-1.22214300
H	-2.60464000	3.27621500	-1.92709800
H	-1.30668300	2.08951400	-1.76399100
H	-1.62079100	3.23436700	-0.46191400
C	-1.48770600	2.25375000	2.38218500
H	-2.56661200	2.13966300	2.27231900
H	-1.21981000	3.29458800	2.16599500
H	-1.21530800	2.06312200	3.42641400
C	1.46060400	2.26478300	2.38982500
H	2.54083300	2.14994800	2.29330000

H	1.17647700	2.08342200	3.43256100
H	1.19470600	3.30345000	2.16118100
C	3.29843400	-1.18456100	1.96818100
H	4.20265500	-1.58240100	2.43758800
H	2.73559100	-2.02154000	1.54358100
H	2.66190700	-0.75956000	2.75132400
C	6.83408700	1.01995800	-0.83949000
H	7.08267500	2.03189300	-1.17445500
H	7.04003500	0.33921900	-1.67530700
H	7.51468200	0.74980500	-0.02578400
C	2.09098900	2.65766600	-1.14044300
H	1.16815200	2.17728700	-1.47496400
H	2.52297600	3.19175200	-1.99114300
H	1.80981600	3.41002700	-0.39222600
N	-1.30757900	0.53997900	0.61060600
N	1.30312200	0.53670500	0.63100700

Cartesian coordinates of the optimized structure of complex **4**

Re	-0.00007500	-0.39007300	0.96391800
Cl	0.00039300	-2.78960500	0.21343500
O	-0.00093000	2.37802200	2.30374700
C	-0.00054600	1.36204800	1.74048700
O	2.25166800	-1.16262600	2.94029600
C	1.39729600	-0.87169100	2.21951400
O	-2.25159000	-1.16351000	2.94020100
C	-1.39732500	-0.87227400	2.21941200
N	1.31752400	0.03386100	-0.72589400
C	2.74404400	0.27271800	-0.69182600
C	3.64492000	-0.79603600	-0.84125200
C	5.01106800	-0.50726000	-0.76742200
H	5.72577600	-1.31750600	-0.88439800
C	5.46988700	0.78572500	-0.56193300
H	6.53642600	0.98558100	-0.50790300
C	4.55829800	1.82695700	-0.44430600
H	4.92111400	2.84209100	-0.31132500
C	3.18165200	1.60076700	-0.50917800
C	0.72476200	0.08954900	-1.87393700
H	1.27824600	0.23353100	-2.79995500
C	3.20525500	-2.21775700	-1.12947600
H	2.11591600	-2.26369200	-1.05985400
C	2.23011200	2.78271300	-0.45939400
H	1.22030500	2.40197900	-0.27719400
C	3.75710000	-3.20908600	-0.10209600
H	4.85189500	-3.26012600	-0.13135800
H	3.37248800	-4.21407300	-0.30952900
H	3.45627900	-2.93554100	0.91459000

C	3.60130400	-2.62867900	-2.55232300
H	3.17586100	-1.95041500	-3.30074900
H	3.24041500	-3.64116100	-2.76706000
H	4.69047800	-2.62647600	-2.68016800
C	2.55694800	3.76179900	0.67044100
H	2.61860100	3.25357400	1.63783800
H	1.77501300	4.52626800	0.73722900
H	3.50637000	4.28043700	0.49659900
C	2.20917200	3.50919700	-1.81023900
H	3.19877500	3.91801900	-2.04630700
H	1.49530900	4.34072000	-1.78540000
H	1.92204700	2.83895800	-2.62810000
N	-1.31753600	0.03367000	-0.72600100
C	-2.74402100	0.27277000	-0.69201300
C	-3.64504400	-0.79597200	-0.84061400
C	-5.01114600	-0.50697600	-0.76689800
H	-5.72597300	-1.31720000	-0.88328800
C	-5.46977300	0.78621500	-0.56225200
H	-6.53628100	0.98625000	-0.50828000
C	-4.55804200	1.82740700	-0.44537800
H	-4.92072500	2.84266600	-0.31299800
C	-3.18142500	1.60100500	-0.51021700
C	-0.72467800	0.08950800	-1.87399100
H	-1.27809000	0.23356000	-2.80004100
C	-3.20548700	-2.21787700	-1.12807600
H	-2.11618000	-2.26392000	-1.05801300
C	-2.22972900	2.78286000	-0.46114200
H	-1.21997100	2.40212600	-0.27862500
C	-3.75786900	-3.20880500	-0.10060200
H	-4.85265100	-3.25982200	-0.13034600
H	-3.37321600	-4.21388200	-0.30752300
H	-3.45751900	-2.93493800	0.91613700
C	-3.60101100	-2.62923200	-2.55094800
H	-3.17514500	-1.95129800	-3.29943300
H	-3.24020900	-3.64185000	-2.76519300
H	-4.69013500	-2.62687200	-2.67922300
C	-2.55649300	3.76273500	0.66803700
H	-2.61837600	3.25515500	1.63575400
H	-1.77439200	4.52707100	0.73441500
H	-3.50577200	4.28148300	0.49373800
C	-2.20863300	3.50852800	-1.81242600
H	-3.19818400	3.91730700	-2.04878700
H	-1.49469000	4.33999500	-1.78804300
H	-1.92153900	2.83779400	-2.62988900