

Supporting information

New indenylidene-type metathesis catalysts bearing unsymmetrical N-heterocyclic ligands with mesityl and nitrobenzyl substituents

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Stanisław Witkowski, Jacek W. Morzycki

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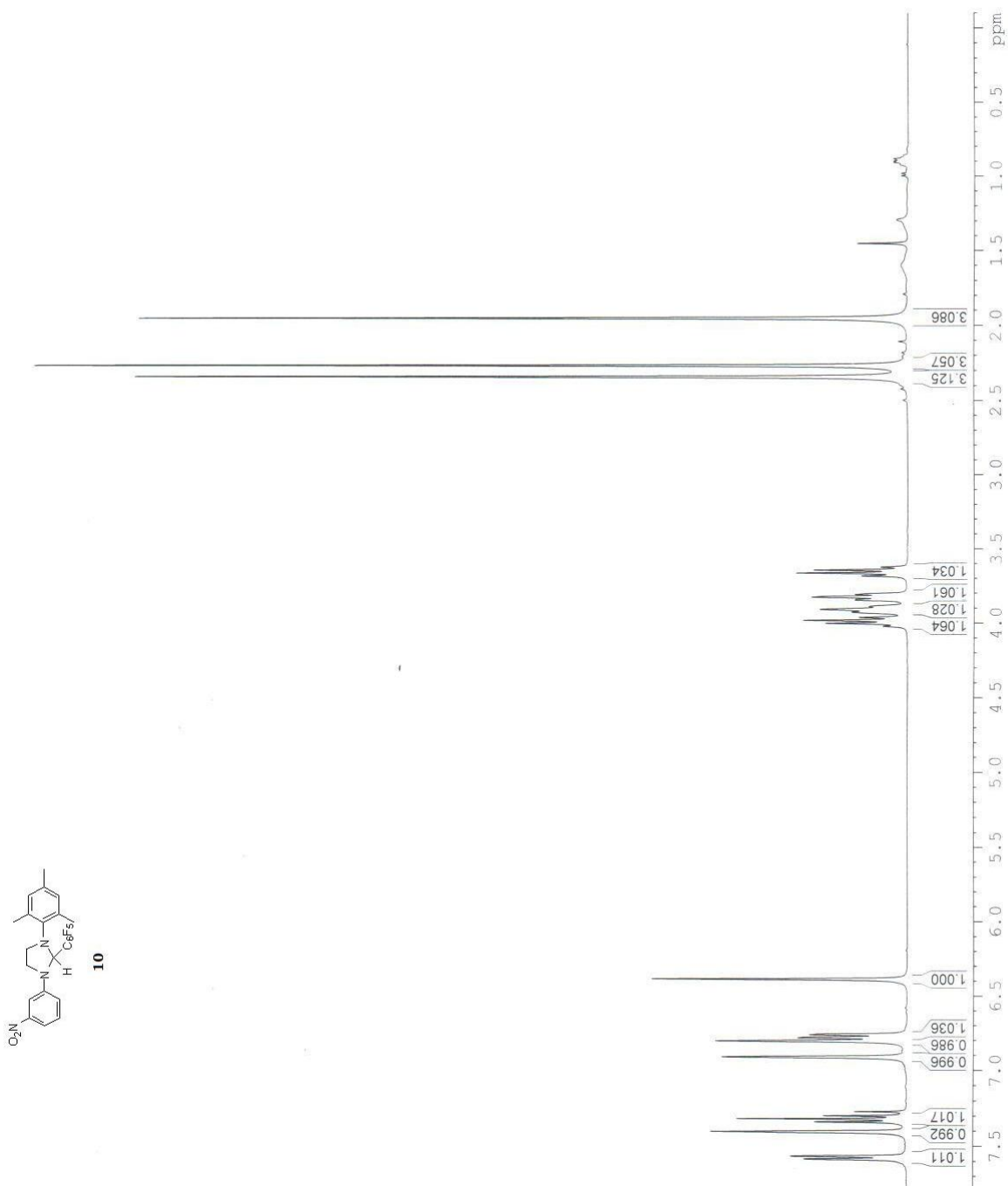
* e-mail: marta.terpilowska@gmail.com

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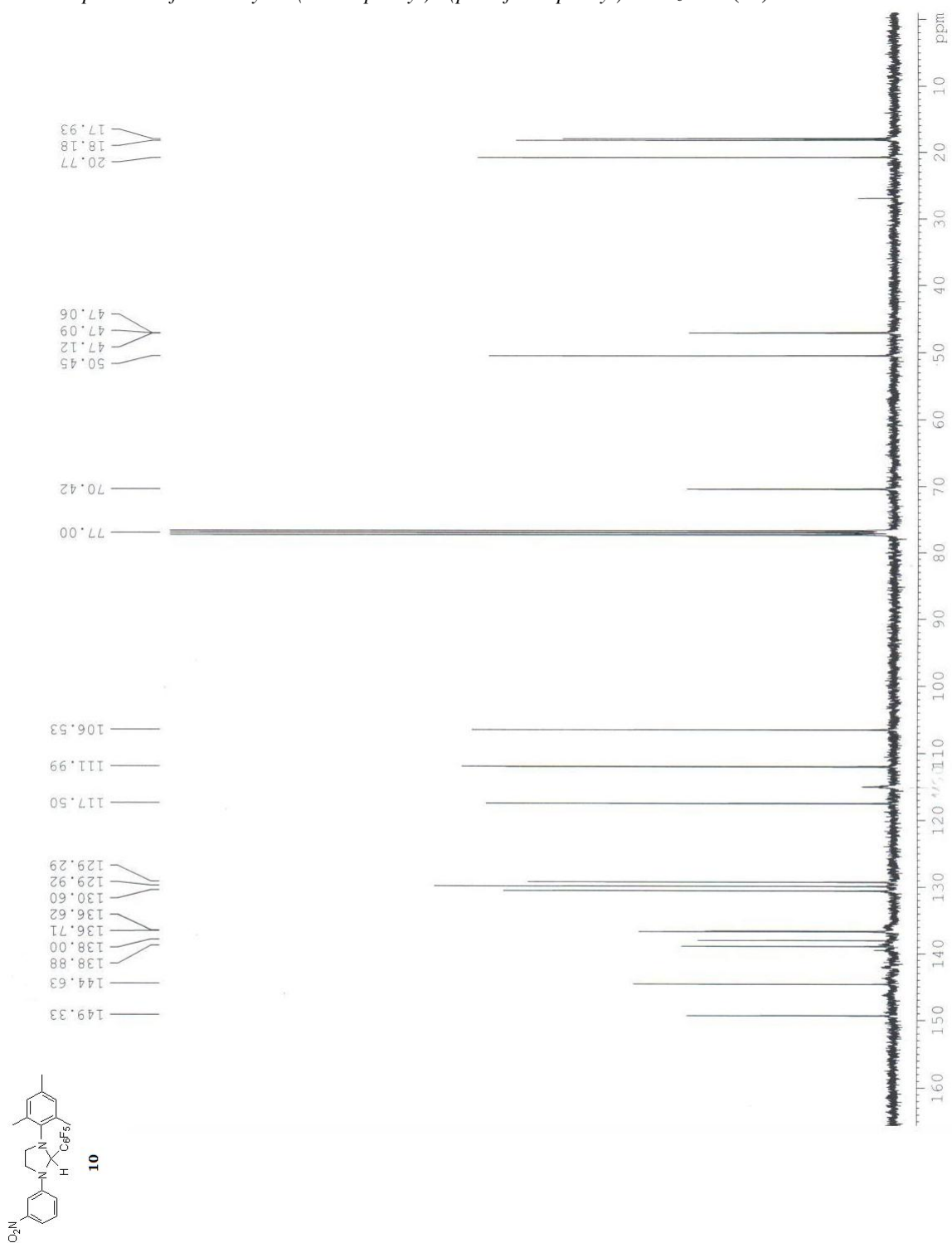
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1. Copies of NMR spectra of new compounds

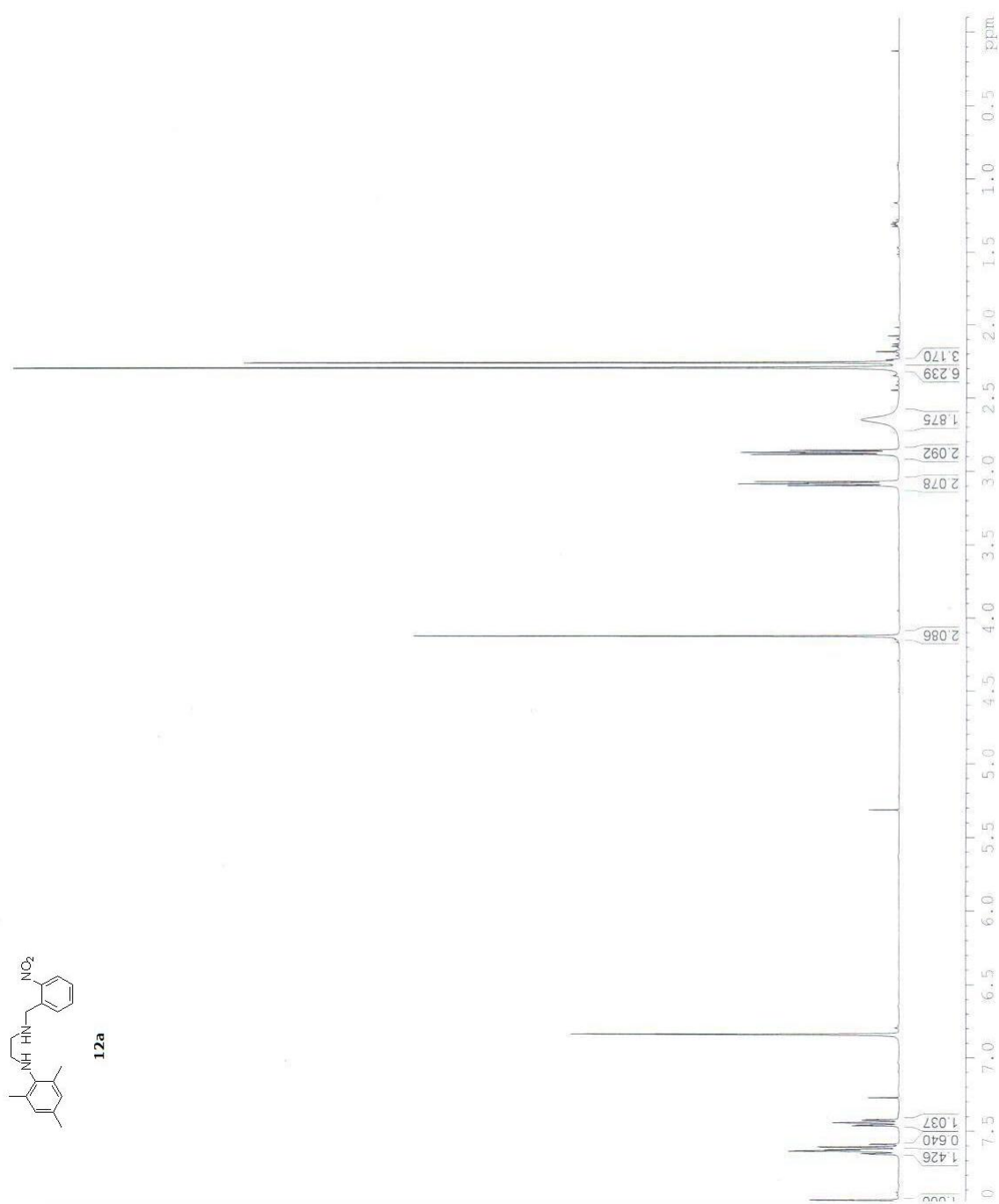
1.1. ^1H NMR spectrum of *N*-mesityl-*N*-(3-nitrophenyl)-2-(pentafluorophenyl)imidazoline (**10**)



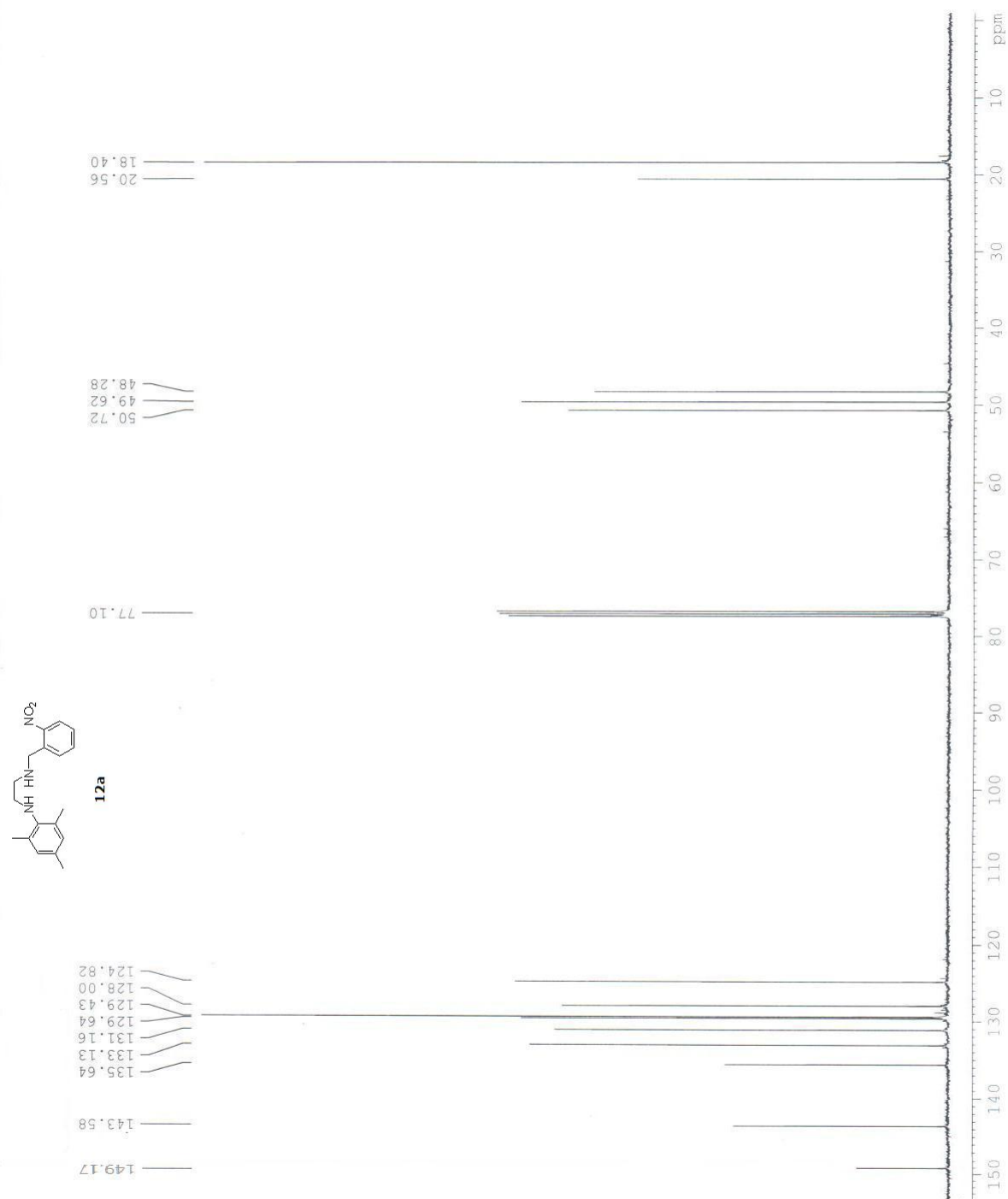
1.2. ^{13}C NMR spectrum of *N*-mesityl-*N*-(3-nitrophenyl)-2-(pentafluorophenyl)imidazoline (**10**)



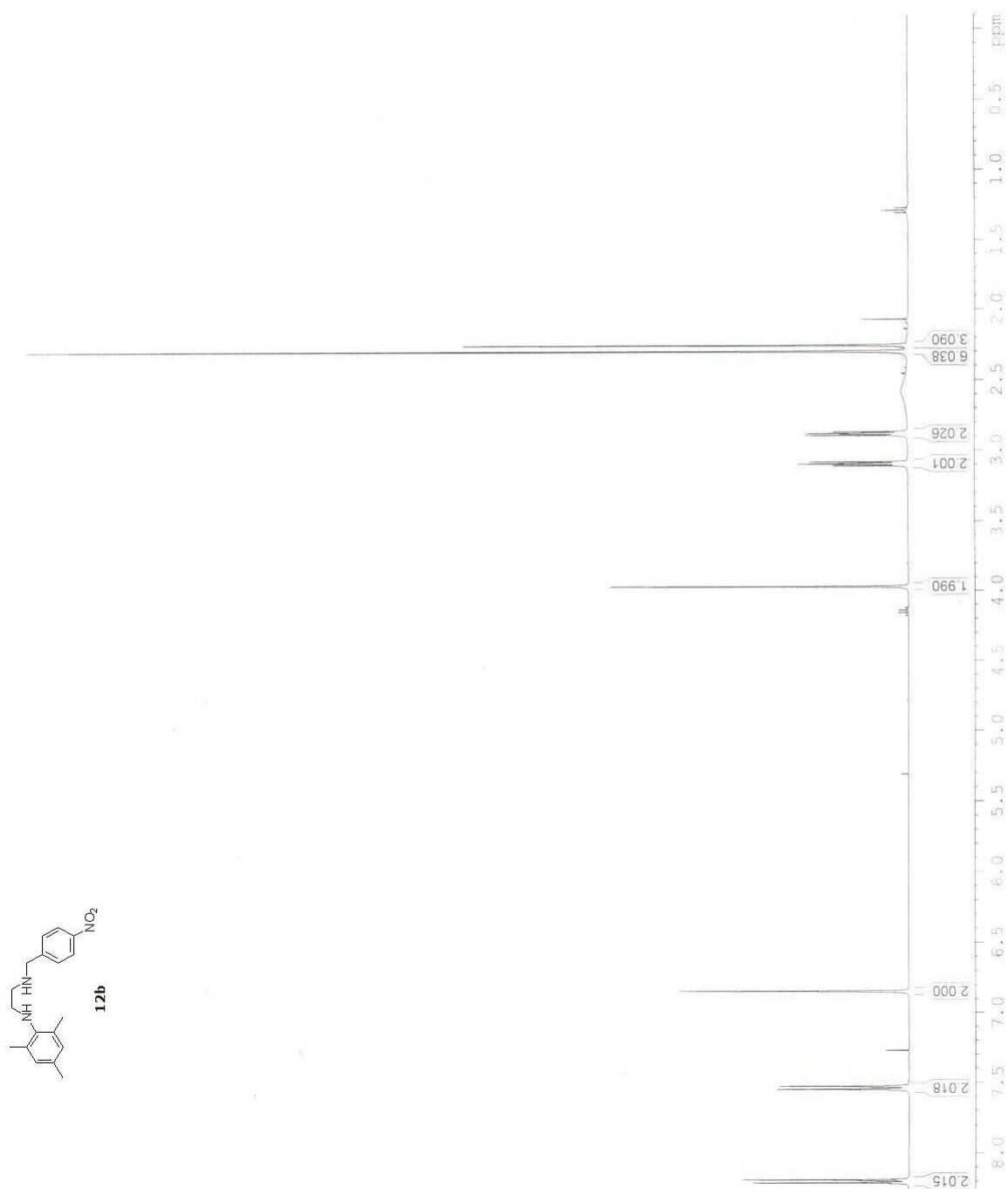
1.3. ^1H NMR spectrum of *N*-(2-nitrobenzyl)-*N*-mesitylethylenediamine (**12a**)



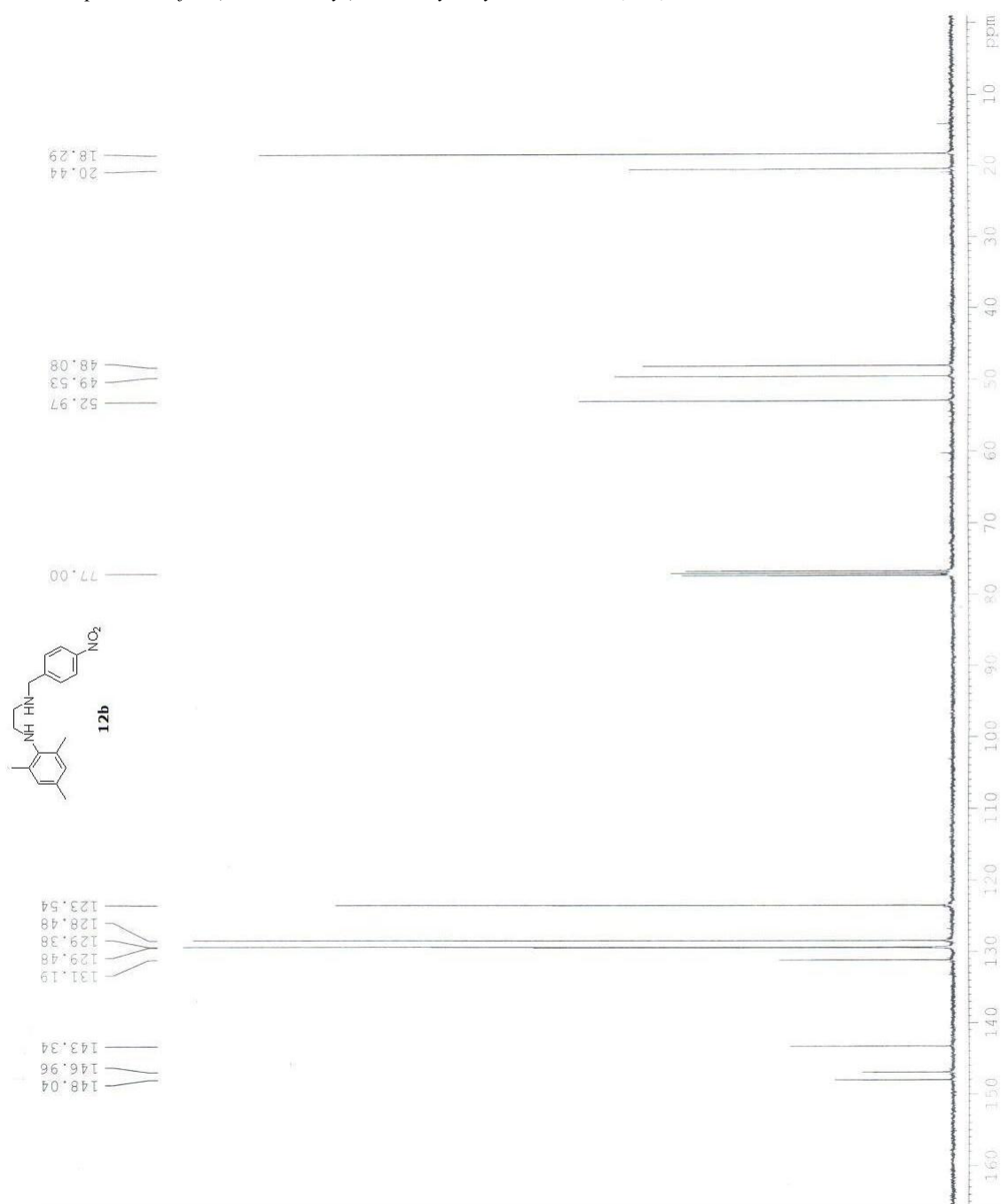
1.4. ^{13}C NMR spectrum of *N*-(2-nitrobenzyl)-*N*-mesitylethylenediamine (**12a**)



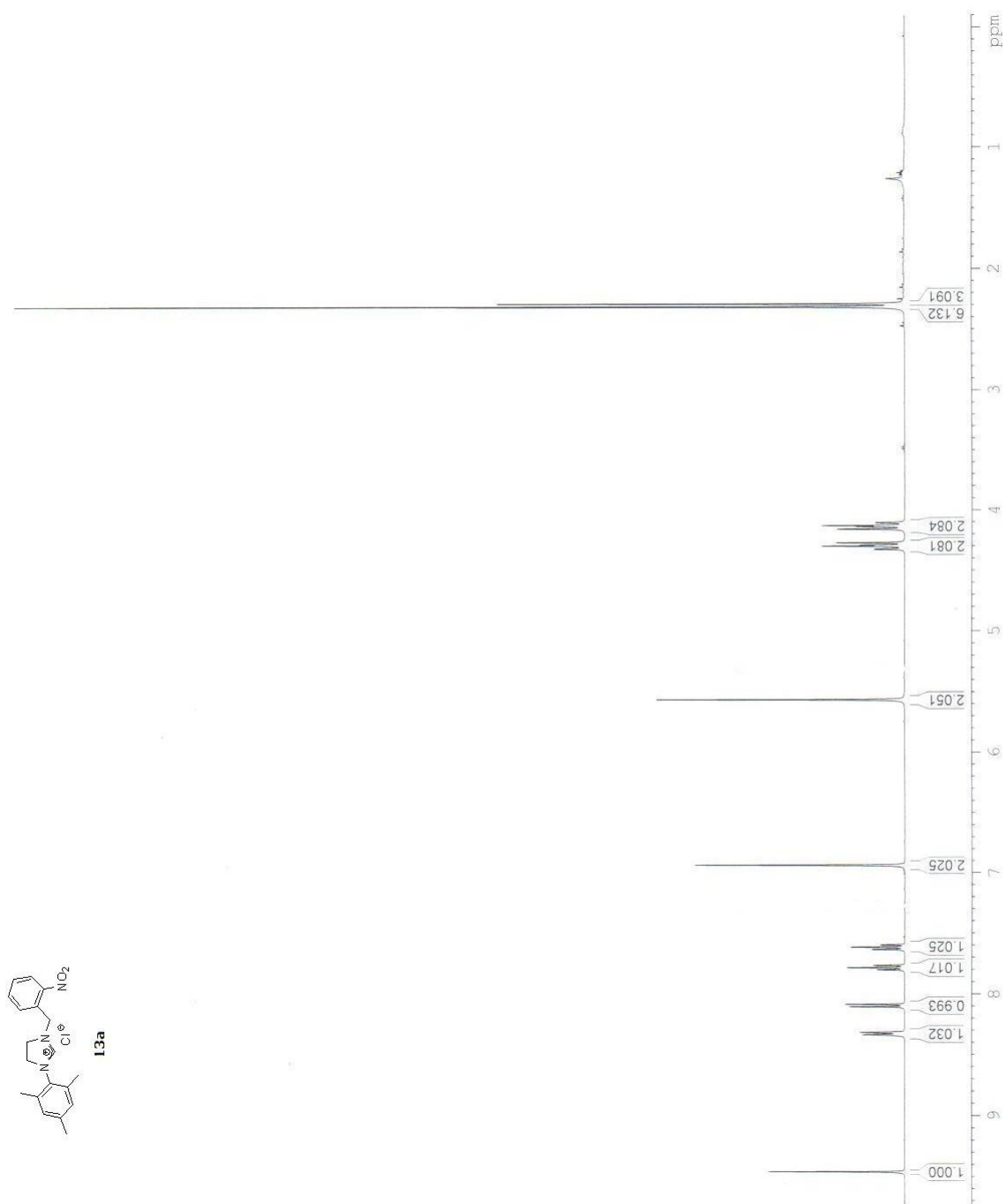
1.5. ^1H NMR spectrum of *N*-(4-nitrobenzyl)-*N*-mesitylethylenediamine (**12b**)



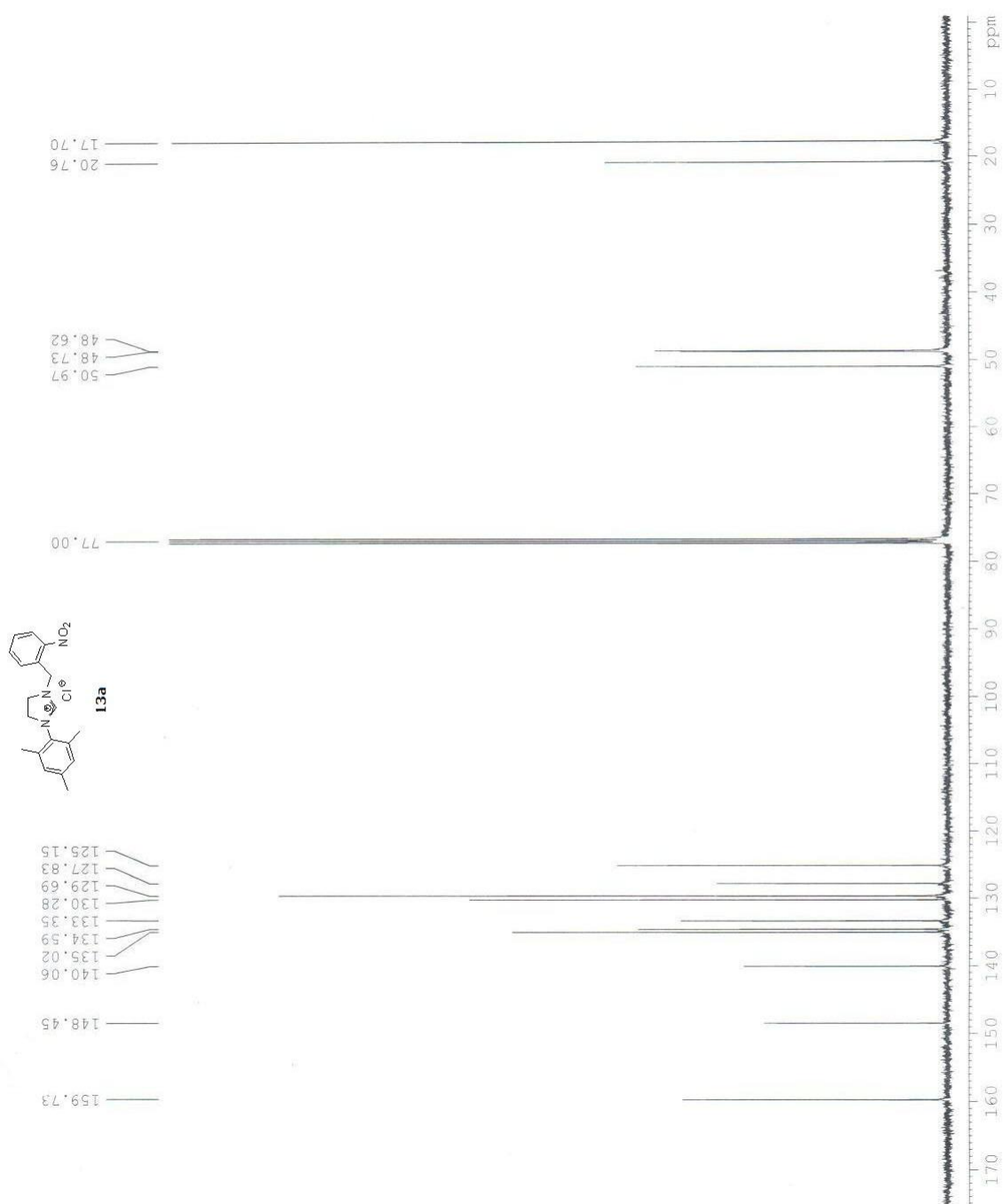
1.6. ^{13}C NMR spectrum of *N*-(4-nitrobenzyl)-*N*-mesitylethylenediamine (**12b**)



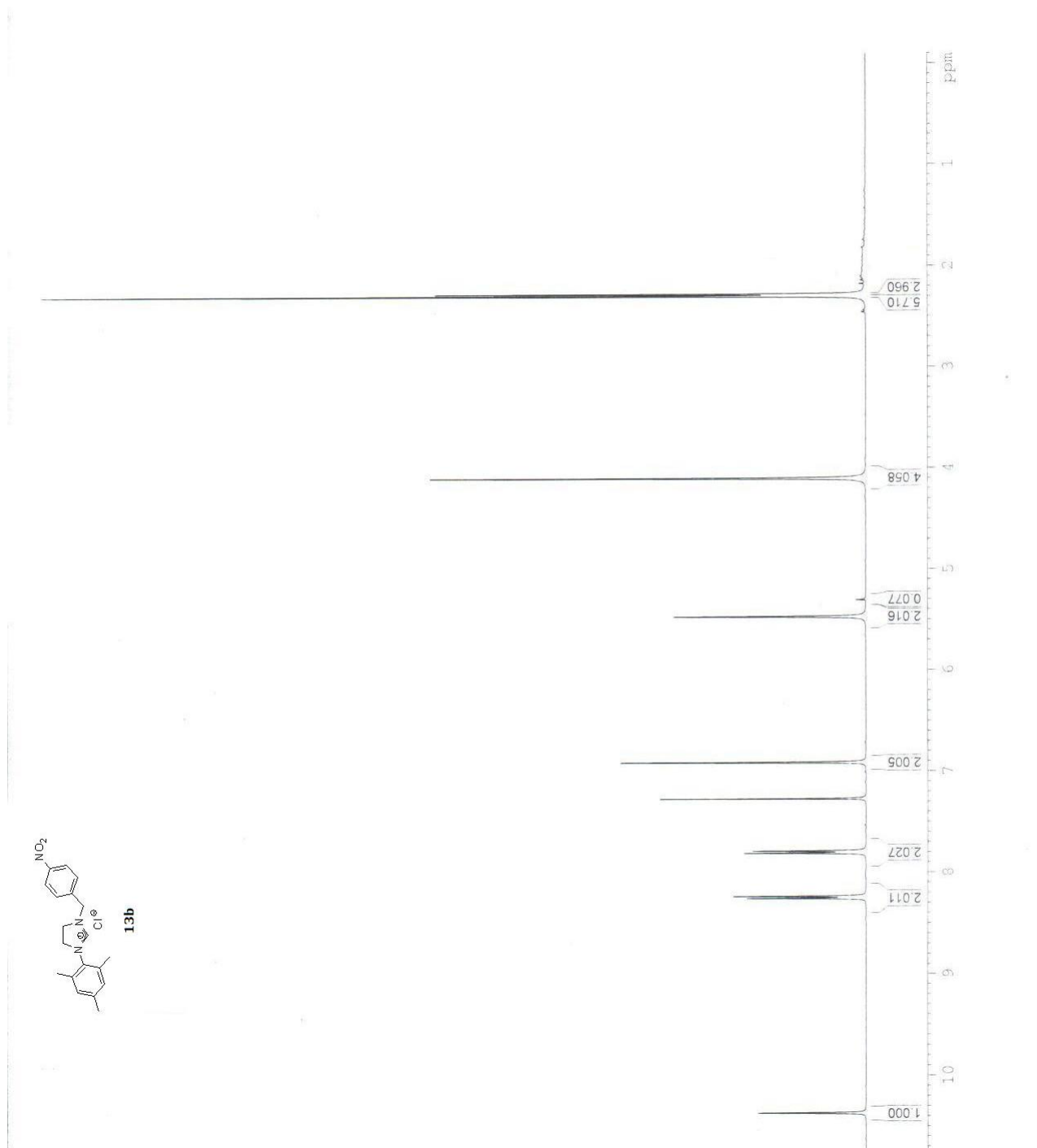
1.7. ^1H NMR spectrum of 1-Mesityl-3-(2-nitrobenzyl)imidazolium chloride (**13a**)



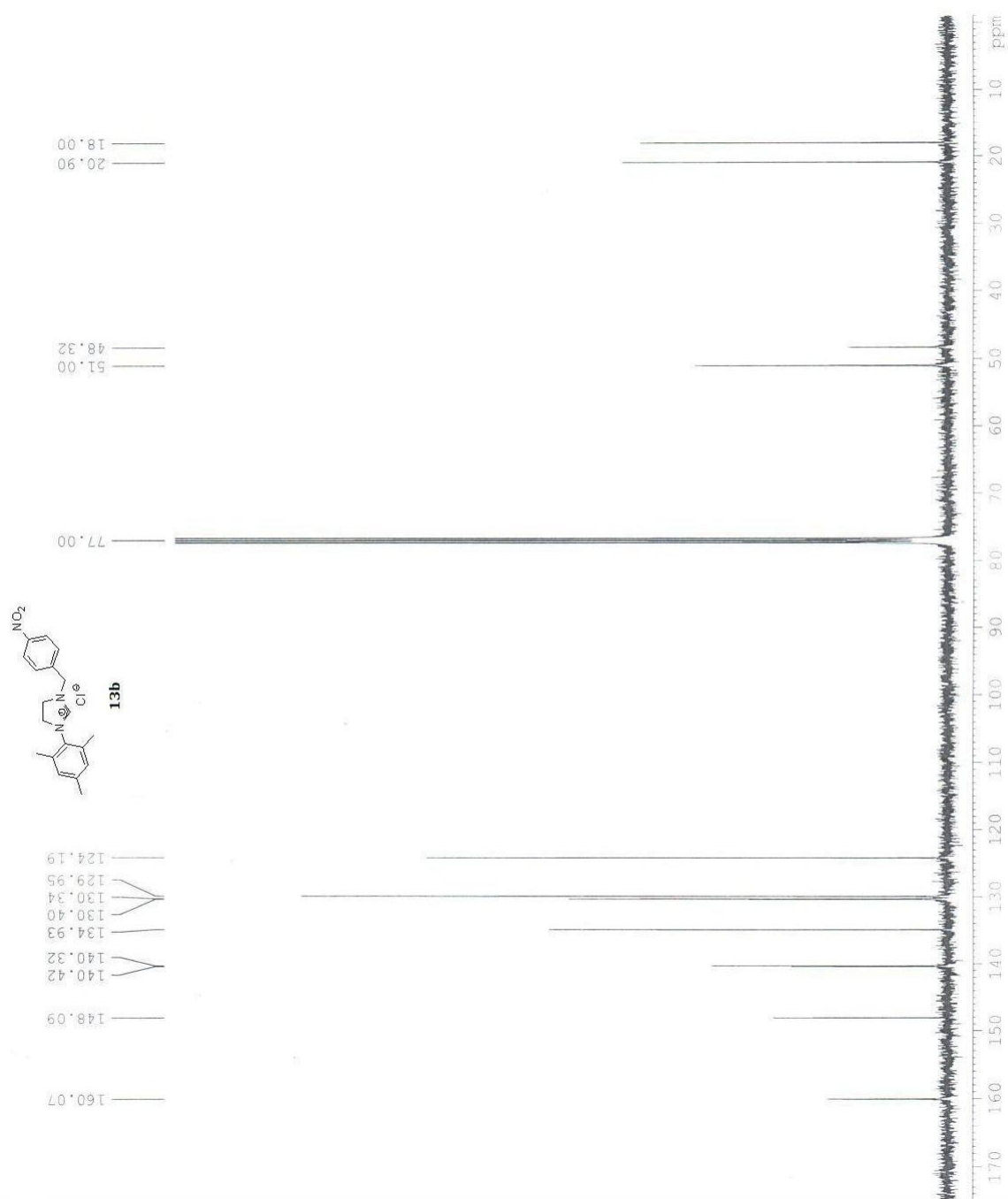
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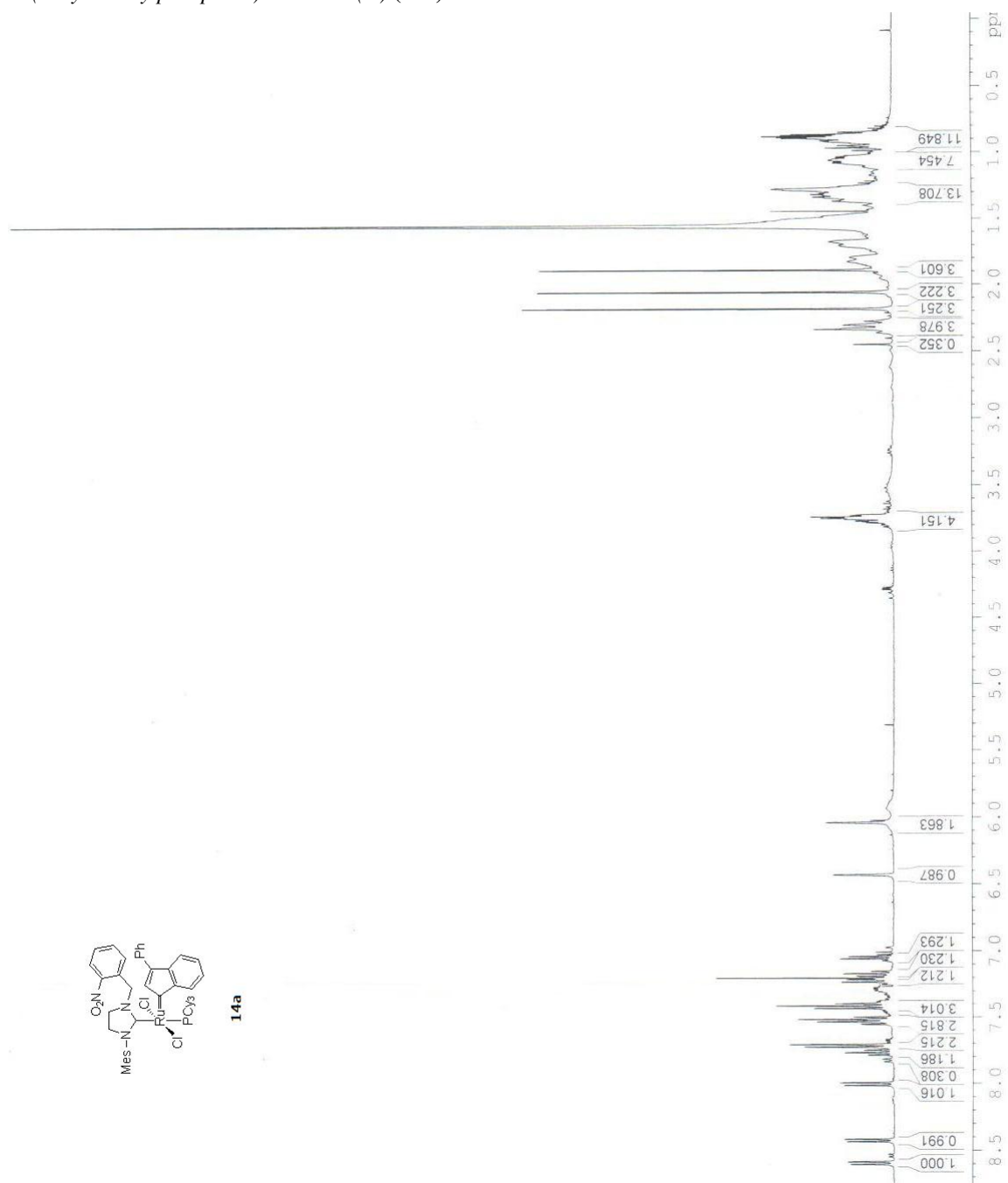
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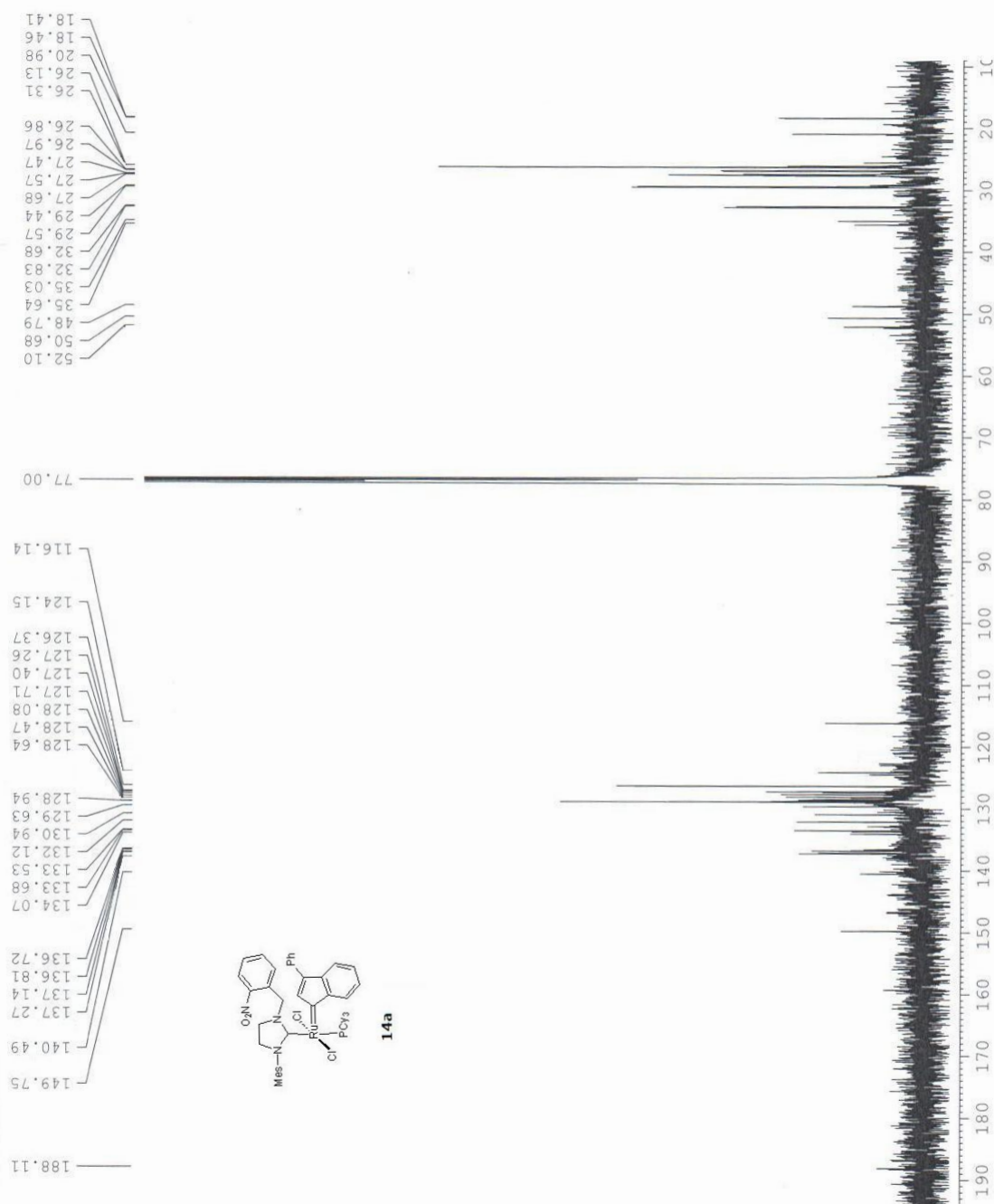
1.10. ^{13}C NMR spectrum of 1-Mesityl-3-(4-nitrobenzyl)imidazolium chloride (**13b**)



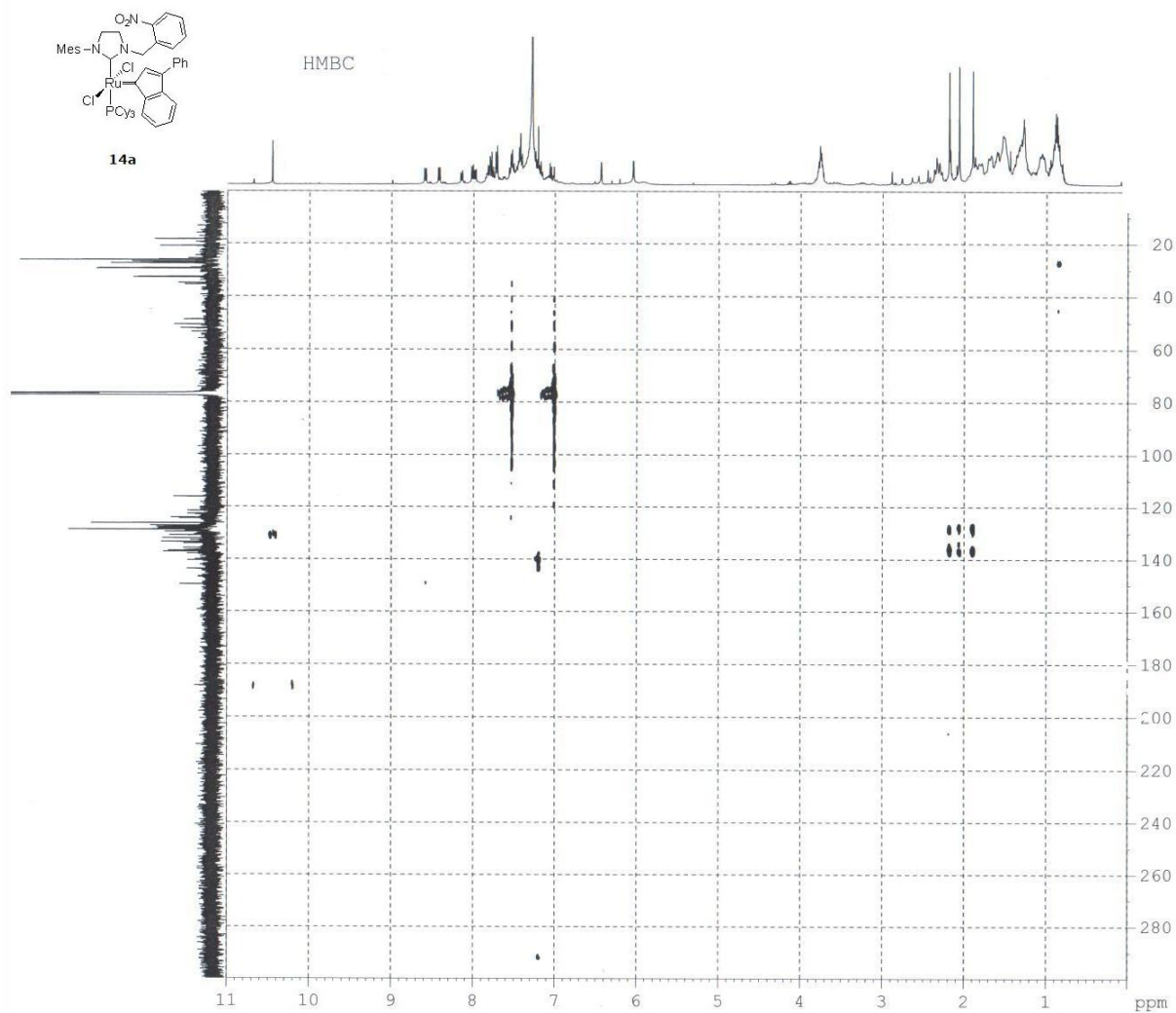
1.11. ^1H NMR spectrum of [1-Mesityl-3-(2-nitrobenzyl)-2-imidazolidinylidene]dichloro-(3-phenyl-1H-inden-1-ylidene) (tricyclohexylphosphine)ruthenium(II) (**14a**)



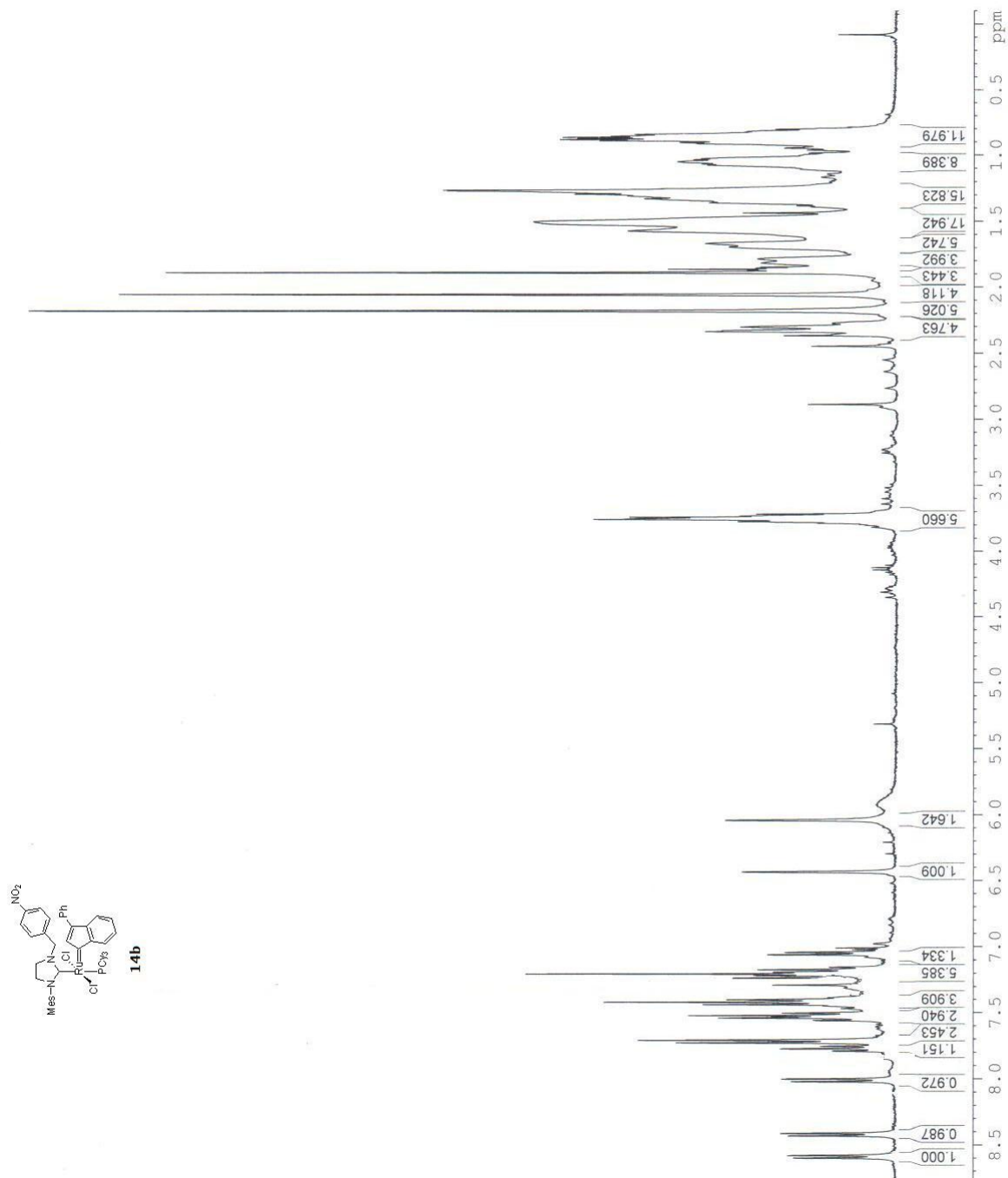
1.12. ^{13}C NMR spectrum of [1-Mesityl-3-(2-nitrobenzyl)-2-imidazolidinylidene]dichloro-(3-phenyl-1H-inden-1-ylidene) (tricyclohexylphosphine)ruthenium(II) (**14a**)



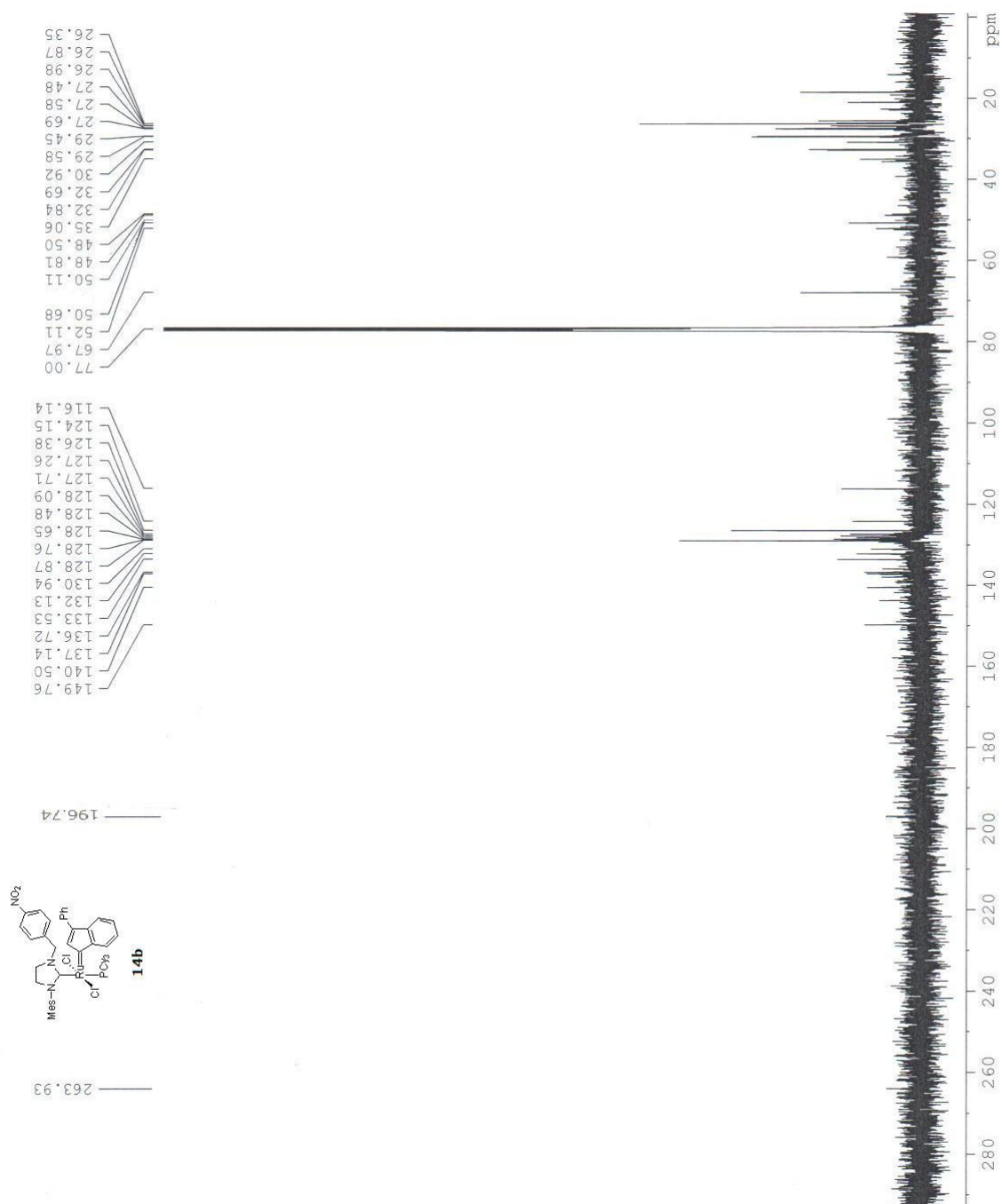
1.13. HMBC correlations between ^{13}C and ^1H NMR spectrum of [1-Mesityl-3-(2-nitrobenzyl)-2-imidazolidinylidene]dichloro-(3-phenyl-1H-inden-1-ylidene)(tricyclohexylphosphine)ruthenium(II) (**14a**)



1.14. ^1H NMR spectrum of [1-Mesityl-3-(2-nitrobenzyl)-2-imidazolidinylidene]dichloro-(3-phenyl-1H-inden-1-ylidene) (tricyclohexylphosphine)ruthenium(II) (**14b**)



1.15. ^{13}C NMR spectrum of [1-Mesityl-3-(2-nitrobenzyl)-2-imidazolidinylidene]dichloro-(3-phenyl-1H-inden-1-ylidene) (tricyclohexylphosphine)ruthenium(II) (**14b**)



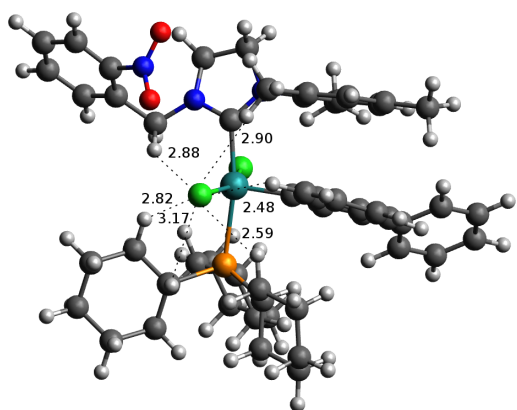
2. DFT calculations

To estimate the most stable structures of new indenylidene-type metathesis catalysts we performed geometry optimization of 13 conformers of each complex. Our main goal was to appoint additional intramolecular interactions which impact the stability of the examined ruthenium complexes. Therefore, we modified the structures of catalysts changing the possibility for hydrogen bonds formation, π - π stacking interactions and specific $\text{NO}_2 \cdots \text{Ru}$ interactions. The used computational setup for all performed calculations is included in the manuscript.

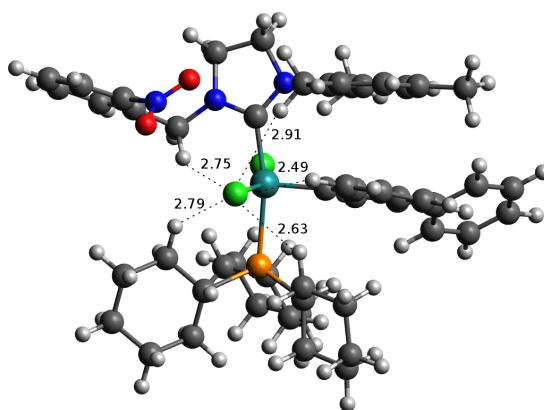
Due to the fact that some of the calculated conformers converged to the same local minima or had very similar values of absolute energy we have chosen only 6 conformers for further analysis. Fig. 1 and Fig. 2 contain the selected local minima after the geometry optimization of **14a,b**. The corresponding relative energy value for all local minima are also given in the figures. The relative energy value is the difference between the values of absolute energy for the particular local minimum and the global minimum, respectively. The higher is the value of relative energy the less stable is the structure of the complex. The most stable structure – the global minimum – is marked with the relative energy equal to 0.0. kJ/mol.

Two synthesized ruthenium complexes differs with the position of the nitro group in the phenyl ring bonded to the *N*-heterocyclic carbene ligand. The comparative analysis of their global minima indicated that complex **14b**, with the nitro group in *para*- position, is more stable than the complex **14a**, with the nitro group linked in *ortho*- position. The value of their absolute energy difference is 51.4 kJ/mol, which is caused with stronger C-H $\cdots\pi$ interactions and C-H \cdots Cl hydrogen bonds in the case of **14b** catalyst. The detailed structural parameters of all C-H \cdots Cl H-bonds formed in the examined structures are listed in Table 1 and Table 2. Even if C-H \cdots Cl H-bonds belong to the weak H-bonds, their amount in the case of synthesized catalysts is enough to influence the structural stability of **14a,b**. The structure **14a(1)** has additional weak C-H \cdots O H-bonds formed between the H atom from the mesityl group as the proton donor and the O atom from the nitro group as the proton acceptor. The structural parameters of the mentioned C-H \cdots O H-bonds in **14a(1)** equal to 3.01 Å, 3.08 Å and 140.56°, 119.98° for the H \cdots O distance and \angle CHO, respectively. Such H-bonds are too weak to stabilize efficiently the structure. Therefore, their absence does not influence the stability of the structure **14b(1)**, which is more stable than **14a(1)**.

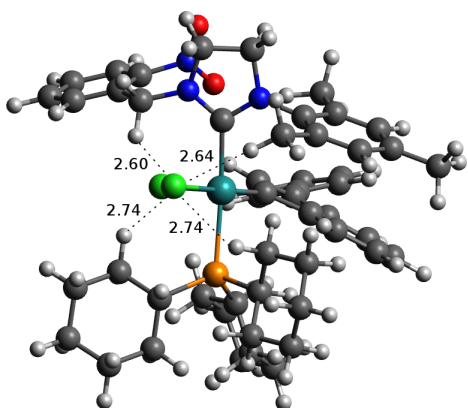
Among other specific intramolecular interactions in the synthesized ruthenium catalysts are C-H $\cdots\pi$ H-bonds and π - π stacking interactions. In the case of complex **14b** the nitro group is located far from mesityl group allowing it to locate in the preferable position for π - π stacking interactions and C-H $\cdots\pi$ H-bonds formation with the indenylidene ligand. As the result, the energy gain of such interactions is higher in the case of **14b** than **14a**. Moreover, the preferable position of the indenylidene ligand is on the side of mesityl group (like in **14b(1)**), but not on the side of nitrobenzyl one (**14b(2)**), see Fig 2. Similar behavior can be also seen from the structures **14a(1)** and **14a(4)** in Fig 1. Such specific arrangement of indenylidene ligand causes better *Z*-selectivity of the synthesized complexes comparing with the commercial one (**5**). In all examined complexes no interactions between nitro group and the ruthenium atom were identified.



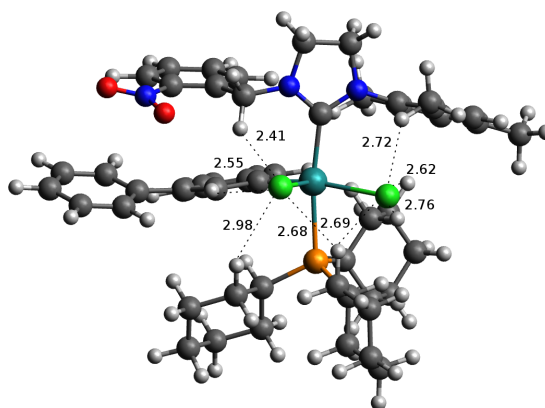
14a(1): $E_{rel} = 0.0$ kJ / mol



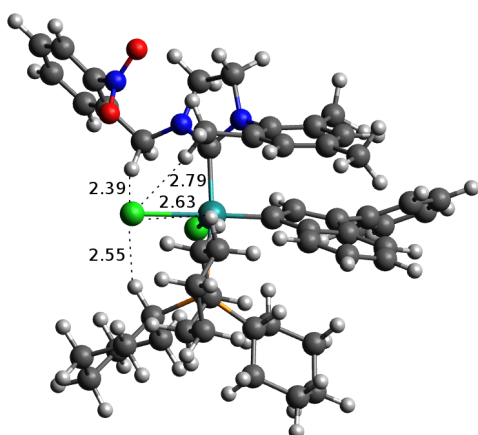
14a(2): $E_{rel} = 6.0$ kJ / mol



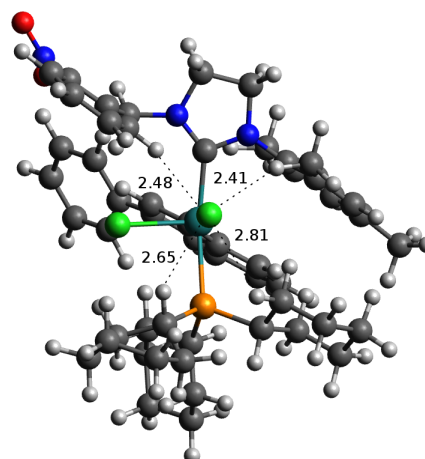
14a(3): $E_{rel} = 40.6$ kJ / mol



14a(4): $E_{rel} = 58.3$ kJ / mol

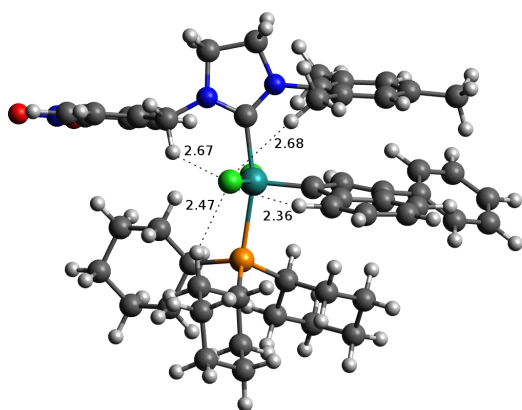


14a(5): $E_{rel} = 69.9$ kJ / mol

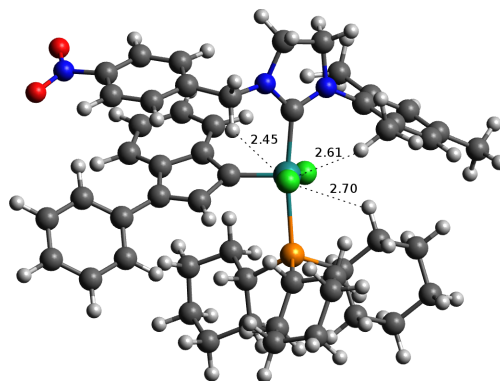


14a(6): $E_{rel} = 82.1$ kJ / mol

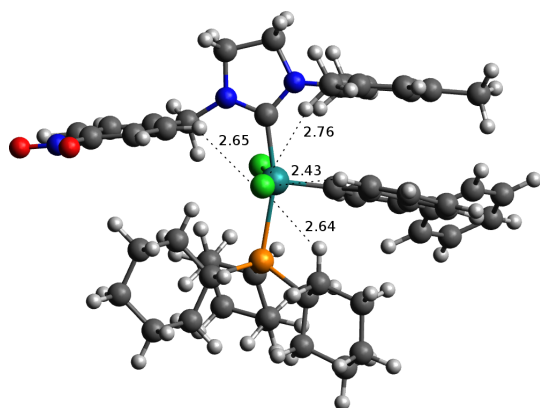
Figure 1: Selected structures of the optimized local minima of **14a** complex with the corresponding relative energy value.



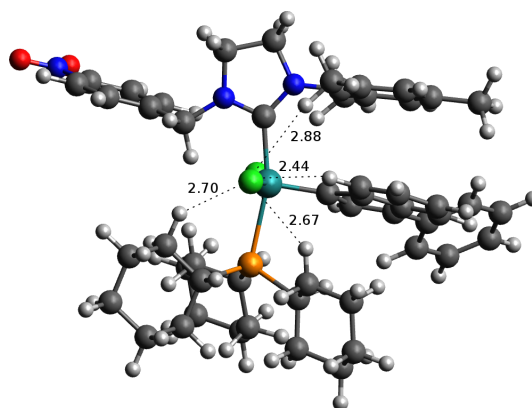
14b(1): $E_{rel} = 0.0$ kJ / mol



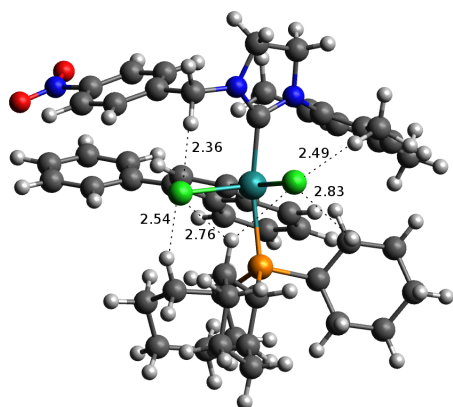
14b(2): $E_{rel} = 17.7$ kJ / mol



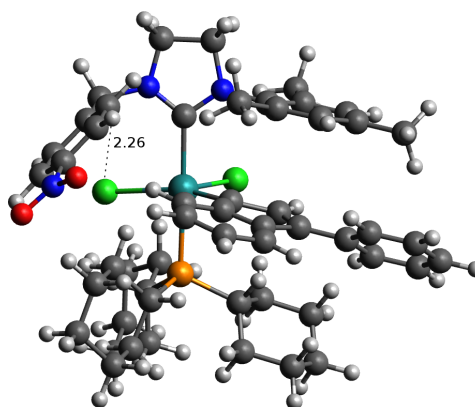
14b(3): $E_{rel} = 22.3$ kJ / mol



14b(4): $E_{rel} = 28.1$ kJ / mol



14b(5): $E_{rel} = 78.4$ kJ / mol



14b(6): $E_{rel} = 106.2$ kJ / mol

Figure 2: Selected structures of optimized local minima of **14b** complex with the corresponding relative energy value.

Table 1: The structural parameters of C-H...Cl H-bonds in **14a** complexes

Label	E_{rel} [kJ/mol]	H...Cl [Å]	\angle CHCl [°]
14a(1)	0.0	2.90	170.90
		2.48	137.43
		2.59	138.49
		2.82	134.79
		2.88	145.54
		2.97	113.70
		2.70	118.16
		2.62	122.37
		2.67	117.28
		2.62	171.60
14a(2)	6.0	2.91	167.84
		2.49	139.25
		2.63	137.90
		2.79	138.90
		2.75	143.34
		3.04	111.32
		2.70	117.55
		2.66	117.57
		2.58	174.39
14a(3)	40.6	2.64	176.30
		2.74	120.11
		2.74	134.62
		2.60	128.99
		2.62	111.68
		2.76	116.91
		2.59	154.41
14a(4)	58.3	2.41	141.51
		2.55	116.21
		2.63	137.90
		2.98	151.95
		2.68	135.05
		2.72	113.27
		2.62	123.11
		2.76	112.02
2.69	123.83		
14a(5)	69.9	2.79	174.78
		2.63	121.68
		2.55	133.59
		2.39	152.54
		2.98	132.86
14a(6)	82.1	2.41	148.06
		2.81	110.24
		2.65	138.09
		2.48	163.45
		2.37	139.55
		2.56	140.21

Table 2: The structural parameters of C-H...Cl H-bonds in **14b** complexes

Label	E_{rel} [kJ/mol]	H...Cl [Å]	\angle CHCl [°]
14b(1)	0.0	2.68	175.59
		2.36	142.76
		2.47	151.49
		2.67	127.67
		2.59	144.34
		2.70	165.01
		2.53	119.83
		2.74	134.16
		2.89	115.67
14b(2)	17.7	2.93	126.40
		2.61	165.47
		2.70	120.17
		2.45	136.77
		2.57	121.09
		2.82	114.76
14b(3)	22.3	2.95	110.14
		2.76	161.96
		2.43	139.78
		2.64	136.68
		2.65	134.65
		2.72	121.88
14b(4)	28.1	2.57	118.76
		2.55	117.05
		2.88	165.83
		2.44	141.55
		2.67	143.34
		2.70	138.71
		2.64	145.70
14b(5)	78.4	2.72	117.04
		2.58	123.43
		2.58	118.32
		2.51	176.58
		2.76	111.18
		2.54	152.55
14b(6)	106.2	2.36	128.56
		2.49	169.76
		2.83	119.86
		2.68	140.50
		2.26	139.23
		2.86	114.33
14b(6)	106.2	2.61	123.12
		2.89	123.91
		2.60	147.65

3. The final xyz coordinates of the examined indenylidene-type metathesis catalysts

14a(1) – global minimum

125

Coordinates from ORCA-job

C 0.66424970393847 2.26817380788507 3.23953003980830
N 1.89370261645935 2.73004739868184 2.97801344384945
C 2.27588711459624 3.83649388579400 3.88210870385391
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C 2.88887543892701 2.08043895196817 2.18401525849845
H 2.74420453485200 4.64241252643709 3.31773869206353
H 2.97315476464641 3.47411225013635 4.64326441285647
H 0.45165207213573 5.04499382017445 3.92668678540974
H 0.99108148209031 4.48447580556700 5.53627932074401
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Ru -0.58912922882720 1.12719407472610 2.07270289653130
Cl -0.61238835868456 -0.78490849380331 3.64685890707175
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H -6.98757110303472 -1.03541101767780 4.41178343985819
C -4.05463465551828 0.42489473496398 3.22099664271767
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H -3.07467475992011 0.59466626595796 3.66882689545903
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Coordinates from ORCA-job

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C 4.04093809706793 0.38548214970178 0.71700087931281
C 4.01349831749434 -0.93879106644552 1.14284594201919
C 3.25260845759492 -1.26353224458469 2.27012826839563
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C 3.39154155106348 2.81131982453159 0.89143283968771
H 4.61185786788940 0.64794032237508 -0.16766704228537
C 4.77815042026801 -2.00838528836110 0.40602164179733
H 3.23055534602372 -2.29017239175811 2.62206908665558

C 1.79113083663490 -0.65091572522827 4.23478372773158
H 3.48205496043827 2.83970995647952 -0.19597185289605
H 2.51219943457080 3.39051595214741 1.16632440354285
H 4.26785675230008 3.31960410504098 1.30985461119239
H 4.10601234306735 -2.79026325815079 0.03965574370385
H 5.3080600001408 -1.59525727532713 -0.45373908875126
H 5.51211841237880 -2.49066558854174 1.05915143013855
H 2.26958326565746 -0.18416604070571 5.10283814119737
H 0.75237138032912 -0.31408719805747 4.22874301650486
H 1.80165614516677 -1.73031950063243 4.39403462434358
C -1.25499230474386 5.30036504241667 3.86099063927761
C -2.51416120919273 5.80255271330783 4.21169126844008
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Coordinates from ORCA-job

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Coordinates from ORCA-job

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H -9.70798306853624 -1.57282507928446 4.51886238785734
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14a(6)

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Coordinates from ORCA-job

C 0.62743031027453 3.67355334681425 2.08877505925612
N 1.77925123714653 3.13149151025180 2.54448607468933
C 2.60693279680982 4.07975500886338 3.30944978328147
C 1.64410682217835 5.26159292649047 3.47550055144634
N 0.55471409040389 4.92863956261962 2.53908881025648
C 2.30845046175664 1.90259377098690 2.03233664883855
H 3.50283762588270 4.34288838826616 2.73856746156035
H 2.91485918972805 3.64584876557804 4.26067711602718
H 1.24248804911144 5.33353403868879 4.49009005453627
H 2.08932123175882 6.22281964705041 3.20899119295084
C -0.46091482884475 5.93153424620279 2.26942513284015
Ru -0.61428037292653 2.35297932142944 1.03295827624332
Cl -1.39511491736932 1.66252471170421 3.39863195300345
Cl -2.54971861719888 3.81597944503692 0.90754675195967
P -2.06207468173276 0.43866590191539 0.25319305690089
C -3.79276344964927 0.47778218728913 1.08325077920064
C -4.41058461877472 -0.86658393655828 1.48975344852792
H -3.54983762879411 1.02752937292257 1.99449259921603
C -5.50604153292804 -0.61380345983162 2.55541764025668
H -4.84153897556179 -1.35217237975540 0.60672387753915
H -3.67979707106145 -1.56012673062559 1.90074119831412
C -6.18961733258719 0.75816447104101 2.38151967980566
H -6.25207464353411 -1.41385854640894 2.49749333414191

H -5.05738334871850 -0.67134738644138 3.55160573205065
C -6.25495198754449 1.13527215359811 0.90029615908075
H -7.19067168331884 0.73807068440780 2.82217102172661
H -5.62759234535684 1.52574861823085 2.92262144521403
C -4.83847518980603 1.28225822231840 0.28598900801271
H -6.81424679313506 0.35725423580615 0.36650926890690
H -6.81237076147043 2.06546516860762 0.76143182728274
H -4.87756007480577 0.93062547535886 -0.74572186292891
H -4.53479375839263 2.32714378873805 0.26329621126665
C -1.40780850054086 -1.30747679051427 0.70361948896081
C -2.24932921004982 0.30536624185780 -1.63648567810616
C -2.63725452124487 1.62288583386008 -2.32131817720516
H -1.21757875003257 0.10730534898601 -1.93845646656995
C -2.45834287363907 1.48979054919321 -3.83809887712357
H -3.67571915171327 1.87871746878499 -2.10182178260314
H -2.03922254873527 2.44639841233399 -1.93342911965106
C -3.29351051481242 0.32654790566153 -4.38850816359360
H -2.74074217795601 2.42632899152409 -4.32967482195634
H -1.39762333461962 1.32224109861752 -4.06272988717853
C -2.96647807067646 -0.98953154854945 -3.67120347138372
H -4.35843762823582 0.55527353337180 -4.24887077345051
H -3.13505814518802 0.21597137840902 -5.46629372685331
C -3.10461819203865 -0.86250953572869 -2.14534753160086
H -3.61193950614468 -1.79397687893828 -4.03853338676639
H -1.93489547043173 -1.27944614853173 -3.90843305526633
H -4.15532683233364 -0.69987912077770 -1.88457172046338
H -2.80727236344608 -1.80185525855046 -1.67076680735777
C -1.06481743207251 -1.44245531256977 2.19335017400243
H -2.24889136155859 -1.96897415445637 0.47709657714748
C -0.76081623463087 -2.90476342287880 2.54176024973244
H -0.19490099430779 -0.81794015374429 2.41221427867676
H -1.85723229479007 -1.05078734311568 2.82862784296770
C 0.37245337917083 -3.46909235036139 1.67752594068681
H -0.50472962210770 -2.98621855878253 3.60314706409141
H -1.66628655661863 -3.50722657526092 2.39147777188716
C 0.09476278634661 -3.26130467379940 0.18499414721828
H 0.52771704087277 -4.53142093479214 1.89089820614105
H 1.30467787986536 -2.95460290549841 1.93623565961014
C -0.21320854251391 -1.78965925930241 -0.12825263172713
H -0.76045930282844 -3.87797202974913 -0.11967973067520
H 0.95005070421038 -3.59755125741354 -0.41160271243829
H 0.66466659290556 -1.18888726794749 0.12834616791392
H -0.38881141869795 -1.67211411988027 -1.19934439239333
C -0.03123055716134 2.95865240043429 -0.67873754029608
C -0.23227828204321 4.30077165803139 -1.22978814806400
C 0.26355722073992 4.40764720388242 -2.49733439729464
C 0.87559728535578 3.10450644962835 -2.86220677368102
C 0.69524360360420 2.23344275822987 -1.75986498405684
C 1.56571013120942 2.68415754399745 -3.98600457591445
C 0.17297291490659 5.58646745920408 -3.35777425788684
H -0.78939499545457 5.06927177998918 -0.72056397672834
C -0.05064892001417 5.46551963405775 -4.73910657520629

C -0.18582716082476 6.59614499564663 -5.53704763359906
C -0.08982077872858 7.86752137077896 -4.97499039746180
C 0.13238015380590 8.00198762226090 -3.60485192811819
C 0.25956970523773 6.87461949468463 -2.80397356481109
H -0.16123990745851 4.48193054502604 -5.17800372002038
H -0.37552516179746 6.48462430344250 -6.59868656375295
H -0.19204454095636 8.74812766527039 -5.59856424762523
H 0.20638582851395 8.98786932132940 -3.16009939474596
H 0.44216444362026 6.98205358037114 -1.74115065278369
C 2.05430260703218 1.36531640137093 -4.02567581462531
H 1.74198501378159 3.35200636653787 -4.81991549600488
H 2.59009861635707 1.02280365452093 -4.90380496203558
C 1.86018819248589 0.50273899680520 -2.95451958994256
C 1.18100844808168 0.94357396028291 -1.80730004059283
H 2.24160185590513 -0.51095509913299 -2.99746386288894
H 1.04895287090387 0.28607827838703 -0.96462949308685
C 2.96937642640086 1.91078983433120 0.78923969307276
C 3.49137063454776 0.71001006413501 0.30976971784442
C 3.38353136440815 -0.47831188144405 1.03269171891611
C 2.79052892525174 -0.43620933160815 2.29442056390438
C 2.27072549149207 0.74328992466027 2.82904879764771
C 3.18761596619035 3.18361287856969 0.01381882027342
H 3.98436093541270 0.70613262951695 -0.65606476221451
C 3.88247819388946 -1.77742608279644 0.45450485404631
H 2.74358219582581 -1.34031453663357 2.89164216583025
C 1.76204437175319 0.77924106450591 4.24246670966351
H 3.39773928265980 2.96263865073567 -1.03233817814035
H 2.32575665675475 3.84795717580577 0.04977832199873
H 4.04789521659249 3.72927966180665 0.41834616937319
H 3.10987420299162 -2.24349848056264 -0.16741641178638
H 4.76082219849933 -1.62152622538032 -0.17604095057853
H 4.14244062613196 -2.49076552279551 1.23899320293598
H 2.48658777153472 1.28430983156766 4.89171514303467
H 0.80916666090419 1.30314100321965 4.30791528238254
H 1.62544691365722 -0.23271398389019 4.62632534824657
C -1.36838506877048 6.17449724660575 3.46081522945935
C -1.76271266254504 5.07532724695733 4.22958394256403
C -2.59359978572617 5.22517026549561 5.33302812932886
C -3.04235473619888 6.48848845138036 5.71656129637793
C -2.66599674235194 7.59758298271653 4.97570259554218
C -1.85375240543570 7.42888473704970 3.85436913181844
H -1.44085739084248 4.08115851767583 3.94467041825482
H -2.89440596133008 4.34334614958461 5.88623813855875
H -2.98989598353470 8.59508518626896 5.23663440729936
H 0.04603930072432 6.84387665822164 1.96211750490913
H -1.07496908083382 5.58662418630041 1.44029028996829
N -1.54894995357889 8.65068866014773 3.08877728191037
H -3.68747839944900 6.60911904701316 6.57857886674998
O -1.54169031999411 9.71562024064691 3.69287611942874
O -1.33423846507890 8.53935371310183 1.88408108652554

14b(1) – global minimum

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Coordinates from ORCA-job

C -2.12019530777102 2.84581625868012 -0.92230748248688
N -1.25188365545675 2.91316998365970 0.10394749805338
C -1.00185480745445 4.30143310342485 0.54697651521300
C -1.63212469003175 5.12236188250268 -0.57946167570802
N -2.41238973166227 4.10660131007018 -1.29727636341409
C -0.78292211059093 1.84547859813809 0.93057223976483
H 0.06733509016488 4.47902745443996 0.66196148504364
H -1.48709390239516 4.47134709800391 1.51282163112377
H -0.88545312051274 5.56388817191719 -1.24760278480951
H -2.28611120358644 5.91837637538891 -0.21600134463425
C -3.31427511741901 4.51267315399558 -2.35174464474492
Ru -2.88707269823547 1.19294724649225 -1.90619284184301
Cl -5.09404839171870 1.91133214463077 -0.96546119547733
Cl -0.79489455963636 1.13938553514609 -3.31070176256079
P -3.81659714106504 -0.35455335033591 -3.65478457963921
C -5.60396088926920 -0.97310851767335 -3.45891291681611
C -6.04550729089410 -2.13697676287389 -4.36148033321125
H -5.59801751637618 -1.32785213233101 -2.42110989844503
C -7.43440773496476 -2.63527692597629 -3.93433160626217
H -6.08818642694050 -1.80175380417833 -5.40091288377942
H -5.33501805357363 -2.96296582262323 -4.32837980096954
C -8.47209983350968 -1.50699147448798 -3.95957110576160
H -7.74980327818486 -3.45805320789548 -4.58435609599155
H -7.36764633460626 -3.04380126030298 -2.91821880011496
C -8.01146422329218 -0.30649754682651 -3.12523376070176
H -8.62592725646084 -1.18543375077155 -4.99793184542311
H -9.43885234508260 -1.87407271388300 -3.60048226489035
C -6.61918832544038 0.17793746969137 -3.54924312598477
H -8.73007875342359 0.51501403948386 -3.20886726387329
H -7.97742388670606 -0.58556530538220 -2.06462586200979
H -6.66682841125716 0.53897150041416 -4.58208045761102
H -6.30599233662960 1.00727233537509 -2.91841680863350
C -2.67673796015997 -1.87991581128712 -3.78247456029675
C -3.62581774857920 0.57257395408953 -5.30769553498585
C -3.87398062364131 2.07372459746548 -5.10323191711822
H -2.55531887398510 0.45437304284652 -5.50411594535461
C -3.54483503288736 2.86619005608105 -6.37334604467822
H -4.91364502334305 2.24995031692753 -4.80728717531351
H -3.23507617433714 2.42851448642157 -4.29198726635701
C -4.31362796771010 2.33319505119510 -7.58655041089790
H -3.76157602841285 3.92631174790343 -6.21772227301271
H -2.46744991057326 2.79037659904530 -6.56199507463644
C -4.07178935013665 0.83198249349901 -7.77761301261987
H -5.38807367755196 2.50615215429914 -7.44026389864255
H -4.02617777071024 2.88379596668989 -8.48764492002642
C -4.42358470788344 0.04469567088205 -6.50681717264291
H -4.65966667037640 0.45438360869629 -8.62037610058736
H -3.01706150942488 0.66282397509798 -8.02718290616643
H -5.49481796149679 0.15663166895000 -6.31193476834738

H -4.24125465266398 -1.01905262676452 -6.66209420627571
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C -1.42368104795518 -3.60313002697568 -5.11971658674089
H -3.44971954813599 -2.95619249056581 -5.50705145813649
H -2.22182970368782 -1.75709452869661 -5.90459917162533
C -1.72440247235406 -4.66020881781678 -4.05119250320317
H -1.32491909829301 -4.07134803225099 -6.10443124847675
H -0.45903637591417 -3.13054283793180 -4.89692684248187
C -1.92859113789471 -4.01315013681411 -2.67717322057449
H -2.63359542038656 -5.20930554555506 -4.33201428227898
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H -3.16126135696493 -2.48889810033652 -1.75122506434414
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C -1.00316760844440 -1.90385871862354 0.05590347022640
C -2.29907557147956 -1.97575885592806 0.77968642467985
C -3.15278180707213 -0.97405662609587 0.24601781120318
C -2.72027554361818 -2.76524036722287 1.83521785326556
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C -0.04704227902760 -4.15264992738483 0.60640681684456
C 1.03775408037951 -5.01771229338563 0.70834985444341
C 2.32151568782683 -4.57339394799167 0.40355576022206
C 2.50935523247562 -3.25845080691491 -0.02379077640737
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H -1.04246184961201 -4.52376239457081 0.80587166217525
H 0.87747823901775 -6.04329472896979 1.02085365500309
H 3.16761077997928 -5.24532659174789 0.49007604041127
H 3.50368101299753 -2.90608355034515 -0.27433278574339
H 1.58210598112196 -1.37501302405120 -0.45197416003470
C -4.02193619590928 -2.59493228255407 2.33610581866878
H -2.06106659596467 -3.48807509162065 2.29740007211810
H -4.35830219510172 -3.20925365244559 3.16414135759826
C -4.87491524146854 -1.65367438836196 1.77909017920499
C -4.44220134430672 -0.83041491448594 0.72683051650668
H -5.88161933870786 -1.53933478301525 2.16418654653009
H -5.09351186597246 -0.07626895641895 0.31032672959506
C 0.53576268264495 1.39972132134676 0.76281436920348
C 1.00908525416103 0.41641946177686 1.62733723341274
C 0.19560350551846 -0.14920163124557 2.61141939231197
C -1.10299847935965 0.33472176387380 2.76031081343910
C -1.60886883191420 1.34858927792440 1.94706860457238
C 1.39372596875775 1.93443486198031 -0.35293804343729
H 2.02571207665587 0.05752070527944 1.51069007002414
C 0.69569098789279 -1.29092531917106 3.45638311003147
H -1.74767079795798 -0.09436512999290 3.51992066772703
C -2.99471538038775 1.89244134521918 2.16859366185872

H 2.36885450603120 1.44431627990465 -0.35550793078022
H 0.91511432808247 1.77110899030145 -1.32243789691997
H 1.56651165303156 3.01087747419833 -0.25607915954827
H 0.53245793721927 -2.24298394691899 2.93976817301431
H 1.76785432342889 -1.20705101215565 3.64785965819154
H 0.17545158784311 -1.33627425430969 4.41480345711967
H -3.57218723349527 1.94684816834502 1.24543840650066
H -3.54076507804272 1.26315027605751 2.87177147899606
H -2.95268450895729 2.90393187370481 2.58969828045764
C -2.61933237955544 5.07552369767859 -3.57305365428874
C -3.22314342489880 6.10649060379089 -4.29850971279658
C -2.64105436367831 6.59272610333740 -5.46203139276986
C -1.43995301555821 6.03506351996173 -5.88509964279454
C -0.81210062908245 5.01632459697639 -5.17824028099777
C -1.40591486367745 4.54131240302665 -4.01634415118979
H -4.16039302214374 6.52867912475674 -3.95318119677839
H -3.09258999870909 7.38563742531037 -6.04122558303494
N -0.82038538755203 6.53513674835979 -7.12847801439700
H 0.11434963692462 4.60142308693454 -5.54800049516423
H -3.93594438724950 3.65573967195387 -2.61626803012844
H -4.00904985315993 5.25635797871114 -1.94626554301996
H -0.94397434291695 3.72021092995734 -3.48226438652231
O 0.22938739801847 6.01761658702953 -7.48666551606336
O -1.39537278241456 7.43484761554340 -7.72786834170926

14b(2)

125

Coordinates from ORCA-job

C -0.18928918966509 0.82195927381262 0.97672544955149
N -0.68281612168032 0.56839086955170 2.20270024512392
C 0.15545115304408 1.10153646007358 3.29215229711810
C 1.13959071476907 1.98825271631188 2.52850677000057
N 0.93613612388922 1.56484703934645 1.13173856030619
C -1.90786269843803 -0.10934997772397 2.50419210054048
H 0.65152594241154 0.28075811976481 3.81761995832744
H -0.45774121870862 1.65065899315213 4.00800476879296
H 2.17639660472924 1.84415900174937 2.83766121533994
H 0.89843756426991 3.05400654685821 2.62249151518511
C 1.59083267788680 2.33459093964143 0.09034385634679
Ru -1.13658334206715 0.26740848356821 -0.79127811349538
Cl -1.39265801761473 -2.09800333596618 -0.13557879631843
Cl -1.44014748911257 2.69770695626911 -1.24085956809178
P -2.60425895585835 -0.35384990170227 -2.77012839498963
C -4.10715186768885 -1.36859516732962 -2.18757806926514
C -5.26908700905958 -1.52485157651090 -3.17978916762245
H -3.65207537465588 -2.34956437369442 -2.01142298116819
C -6.33085421788979 -2.48216972043636 -2.61775797778999
H -5.73258165042784 -0.55002130944145 -3.36069793905520
H -4.92040011380129 -1.88776289900025 -4.14448549165921
C -6.84374362093957 -2.01030668714863 -1.25324176961914
H -7.16037164728657 -2.57563572733883 -3.32625698606792

H -5.89035529618266 -3.48188309561478 -2.51332367600425
C -5.68947252052424 -1.80557014780259 -0.26642926469907
H -7.37994005646900 -1.06064914885432 -1.38192394976666
H -7.56764745356974 -2.72689490435335 -0.85067785083457
C -4.62018738642070 -0.86189155218232 -0.82846884811759
H -6.06479945948350 -1.41240050912376 0.68126239747849
H -5.22029432546820 -2.77106752222419 -0.04050296112625
H -5.04276675847787 0.14139425717224 -0.93704271824159
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C -5.58717916644131 -2.11099344981632 3.46846261310289
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O 7.19869942792796 -0.50983382311808 -1.19647085707015
O 6.95779612576508 0.75408389833950 -2.94354210194190

14b(3)

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Coordinates from ORCA-job

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H 6.09325126053306 -4.50632824952635 -1.47899954808383
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C -3.33083247161396 -2.01376917143832 2.65683538308089
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Coordinates from ORCA-job

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H -4.20859126110380 -1.46228004470176 -1.97192229286219
C -6.71668100805660 -0.81928070623566 -2.90250808481932
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H -5.09438326623068 -1.13790797930840 -4.29869461370123
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C 4.35045870772577 -1.65515272972107 -0.16068082501682
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C 2.40832409104891 -1.27328868453864 1.25421849642597
C 3.06729078746497 1.87177619262237 -0.83185734466129
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C 5.44516790154896 -2.57203449450162 -0.64147203267193
H 3.54817546192319 -3.08250397857498 1.23081986922963
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H 3.75161016899198 1.99847741856271 -1.67223669286035
H 2.05813554884937 2.09528940501971 -1.17766023436448
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H 0.38937942159395 -1.63196056818216 1.92892762726612
H 1.57613773307230 -2.82507577854257 2.48164015038375
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O -2.51229512963855 8.58461940259242 0.82369713506627
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14b(5)

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Coordinates from ORCA-job

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C 0.12551954324139 -1.77420420525665 1.24130459363225
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H 0.01055103354682 1.97765500023149 3.50723653461976
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H -7.48840579845733 -1.72557802221288 -3.74256089721225
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H -7.34092870836334 1.26539509655375 -4.37044388555520
H -8.71196727635360 0.42819205078077 -3.65060520143231
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O 3.40019980039617 5.38638141062544 -1.35912397701006
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Coordinates from ORCA-job

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H -5.20648896709246 -1.18470796098213 -4.10234827909462
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H -7.42143706153248 -0.08404005518021 -4.06821178794668

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H -0.55737077097102 2.58600202187039 -4.60236832935157
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H 2.76217498231493 3.24621318666734 -5.94510269772841
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