

Supporting Information of:

Alternating Ring-Opening Metathesis Polymerization promoted by Ruthenium Catalysts bearing Unsymmetrical NHC ligands

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NMR Spectra

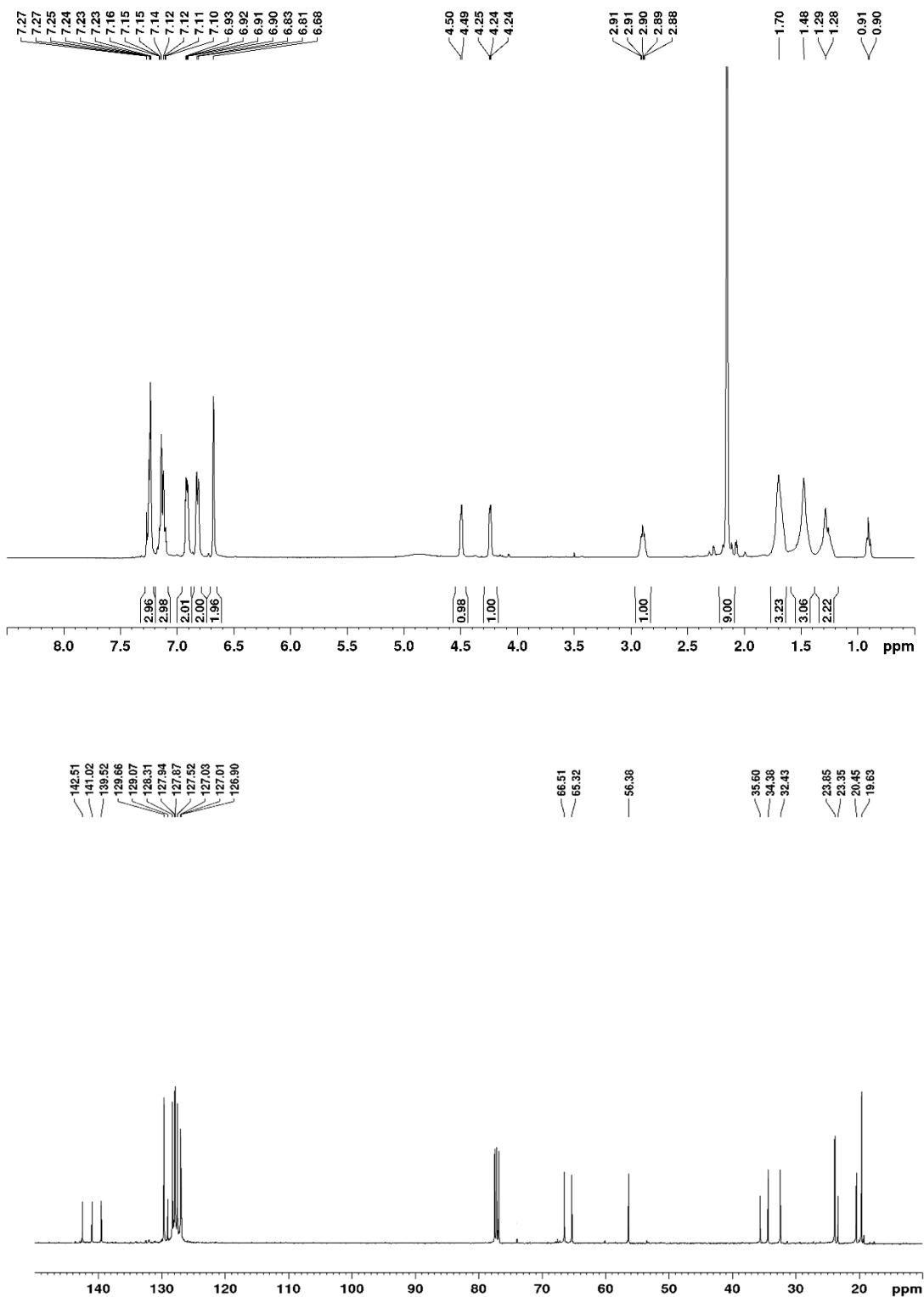


Figure S1: ^1H (top) and $^{13}\text{C}\{^1\text{H}\}$ (bottom) NMR spectra of $\text{N}^1\text{-cyclopentyl-N}^2\text{-(2-mesityl)-1,2-diphenylethane-1,2-diamine (B)}$.

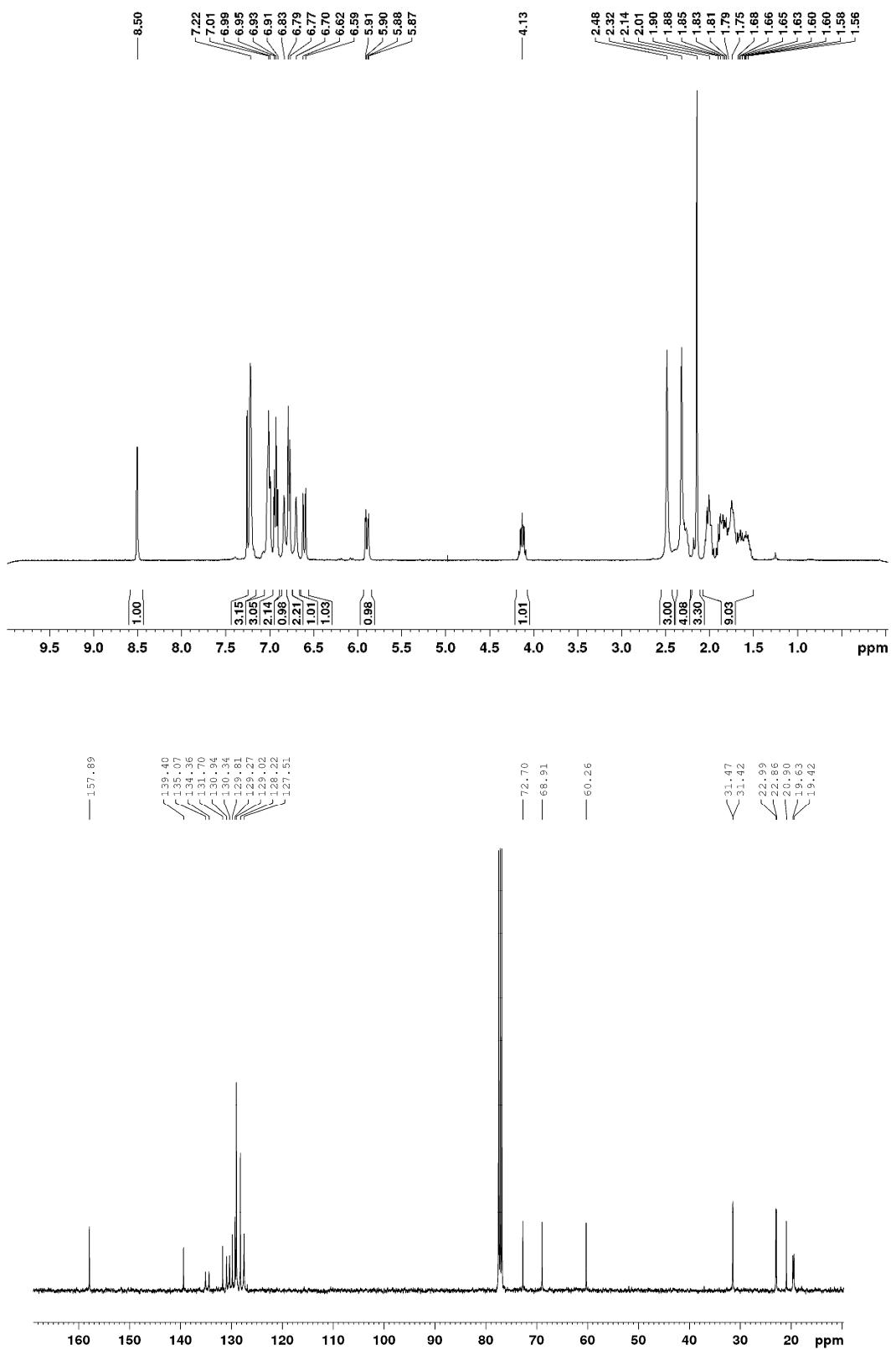


Figure S2: ^1H (top) and $^{13}\text{C}\{\text{H}\}$ (bottom) NMR spectra of 1-cyclopentyl-3-mesityl-4,5-diphenyl-4,5-dihydro-1H-imidazol-3-ium tetrafluoroborate (**C**).

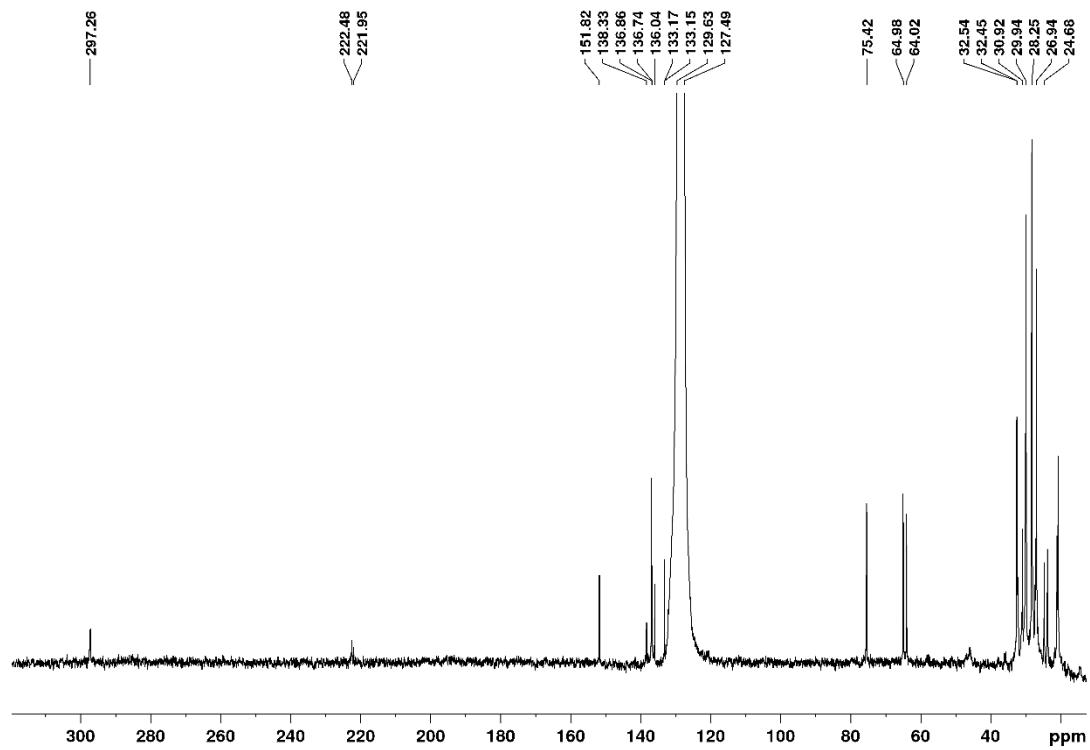
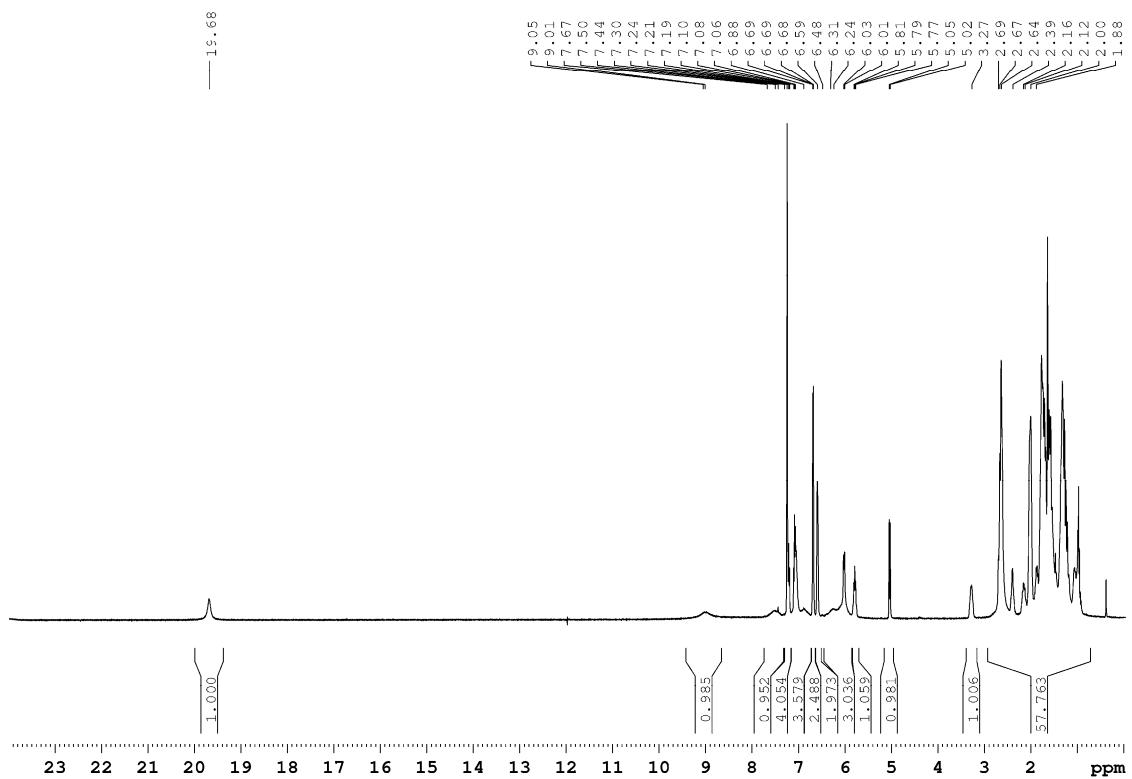


Figure S3: ^1H (top) and $^{13}\text{C}\{\text{H}\}$ (bottom) NMR spectra [1-cyclopentyl-3-mesityl-4,5-diphenyl-2-imidazolidinylidene](dichloro)(benzilydene)(tricyclohexylphosphine)ruthenium (**2**).

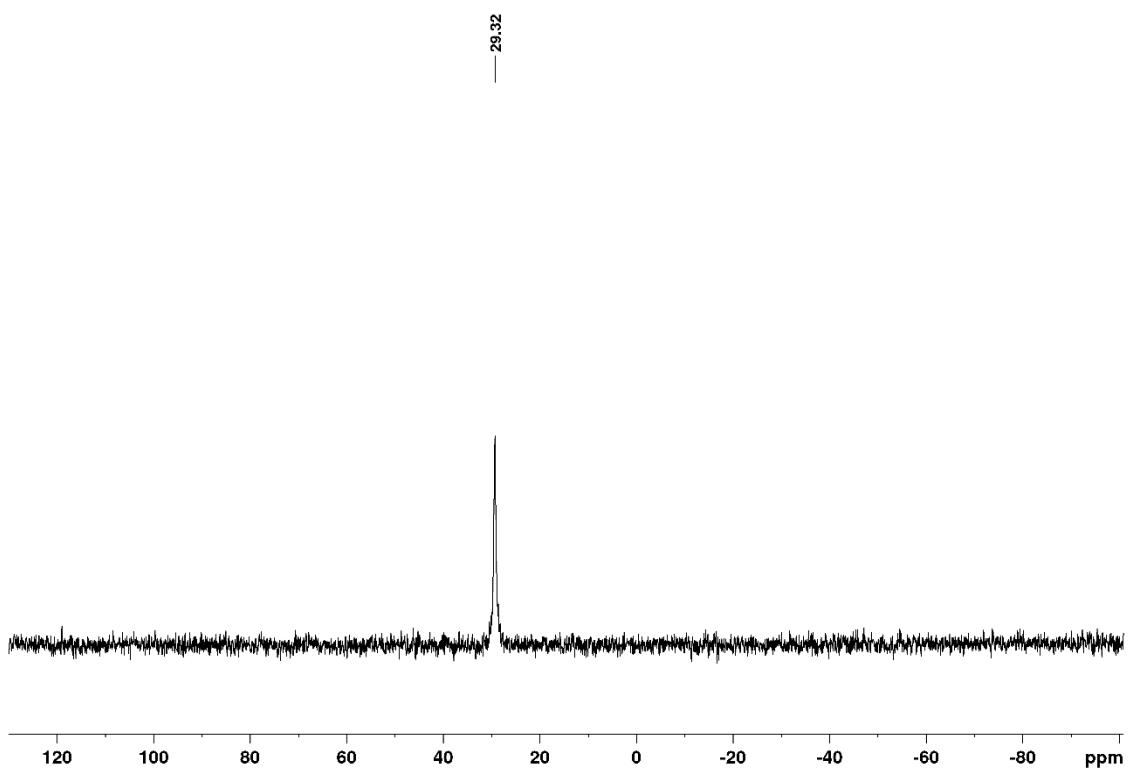


Figure S4: $^{31}\text{P}\{\text{H}\}$ NMR spectrum of [1-cyclopentyl-3-mesyl-4,5-diphenyl-2-imidazolidinylidene] (dichloro)(benzilydene)(tricyclohexylphosphine)ruthenium (**2**).

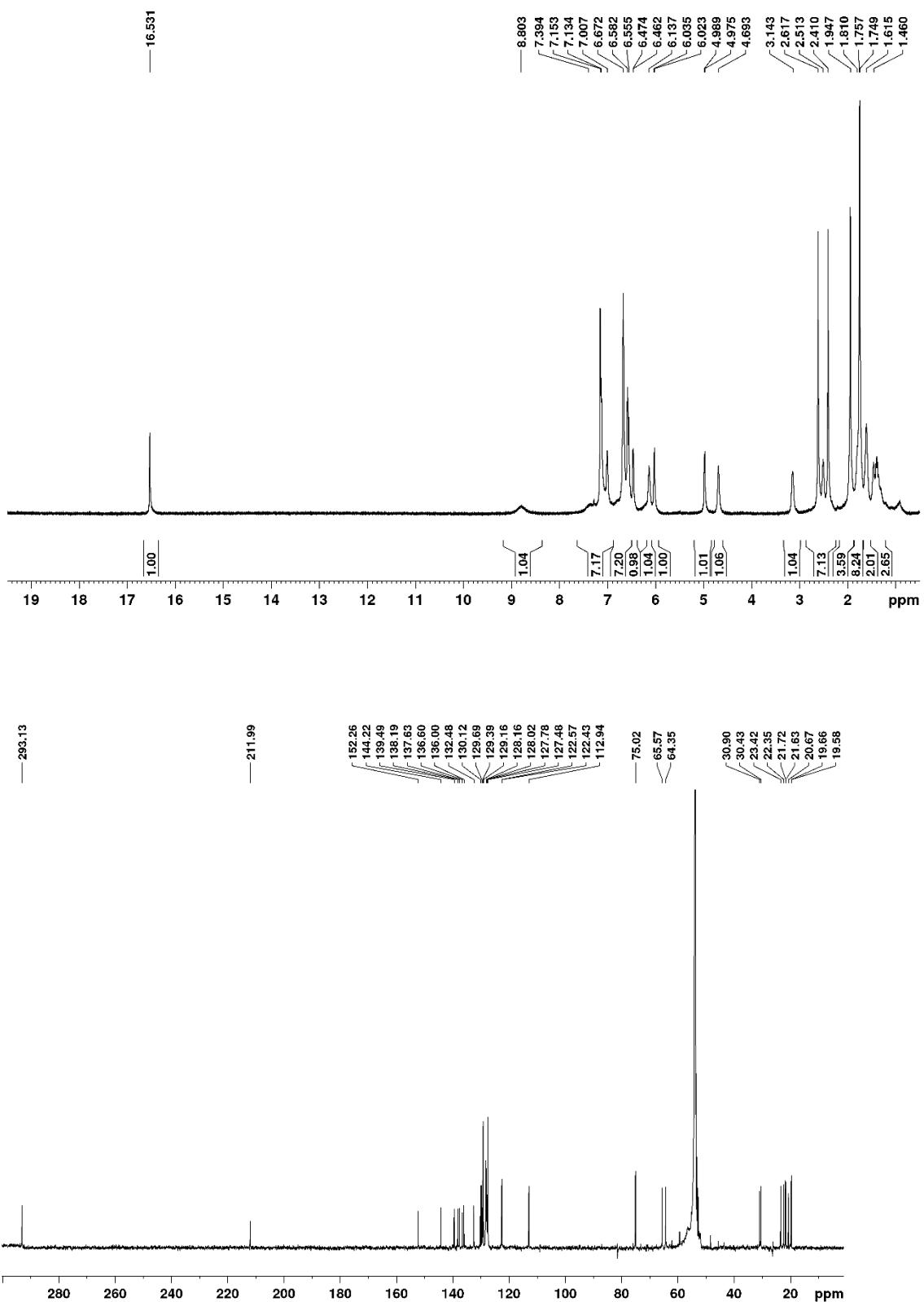


Figure S5: ^1H (top) and $^{13}\text{C}\{\text{H}\}$ (bottom) NMR spectra of [1-cyclopentyl-3-mesityl-4,5-diphenyl-2-imidazolidinylidene](dichloro)(benzilydene)(2-isopropoxyphenylmethylene)ruthenium (**4**).

ESI-FT-ICR

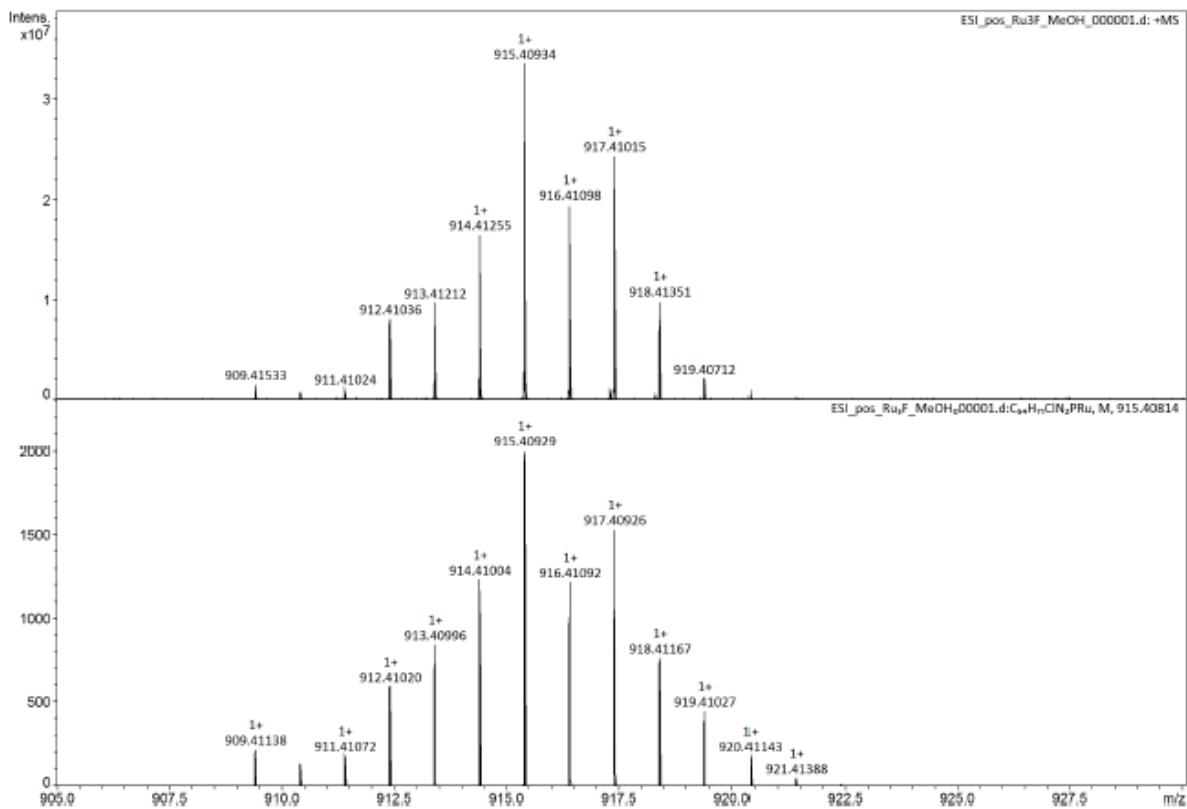


Figure S6: experimental (top) and calculated (bottom) ESI-FT-ICR analysis of 1-cyclopentyl-3-cyclohexyl-4,5-diphenyl-2-imidazolidinylidene](dichloro)(benzilydene)(tricyclohexylphosphine) ruthenium (**2**).

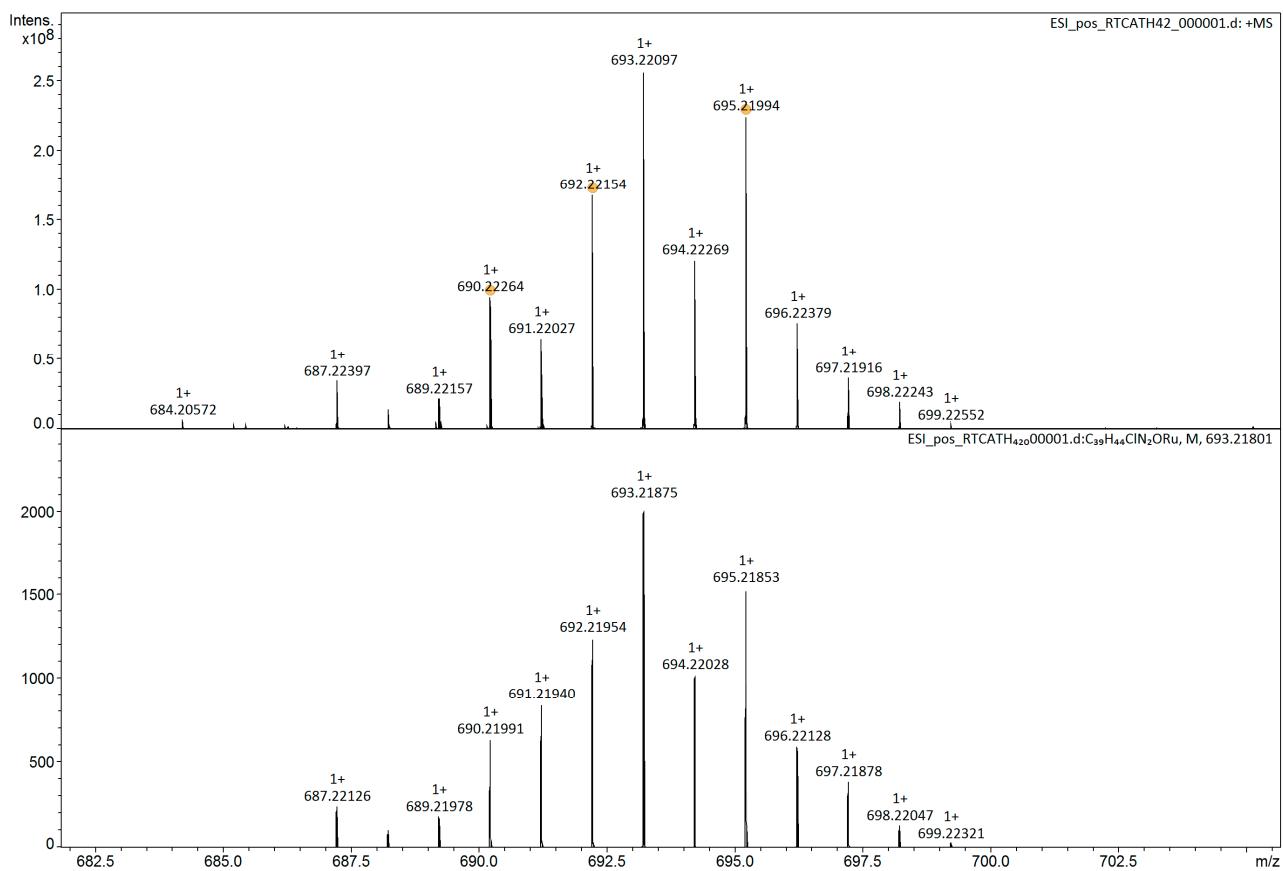


Figure S7: experimental (top) and calculated (bottom) ESI-FT-ICR analysis of [1-cyclopentyl-3-mesityl-4,5-diphenyl-2-imidazolidinylidene](dichloro)(benzilydene)(2-isopropoxyphenylmethylenec) ruthenium (**4**)

NMR Spectra of copolymers

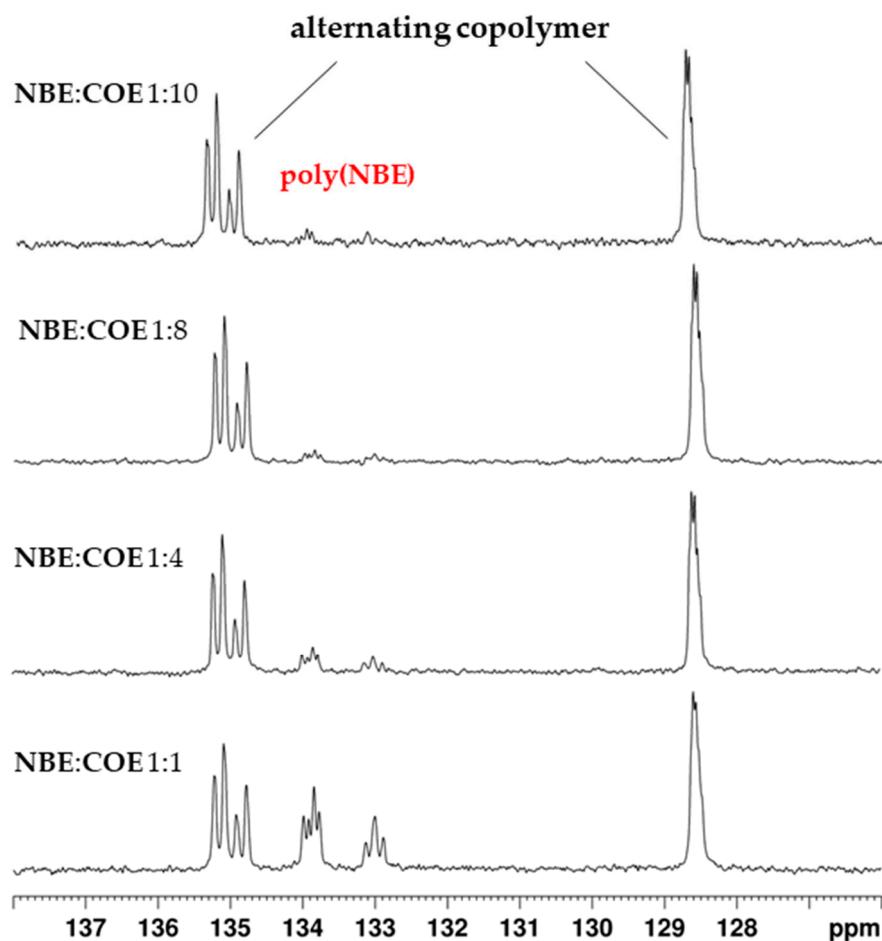


Figure S8: ^{13}C NMR (150 MHz) spectra of the olefinic region of the alternating NBE-COE copolymers obtained by catalyst **2** (Table 1, entries 5-8).

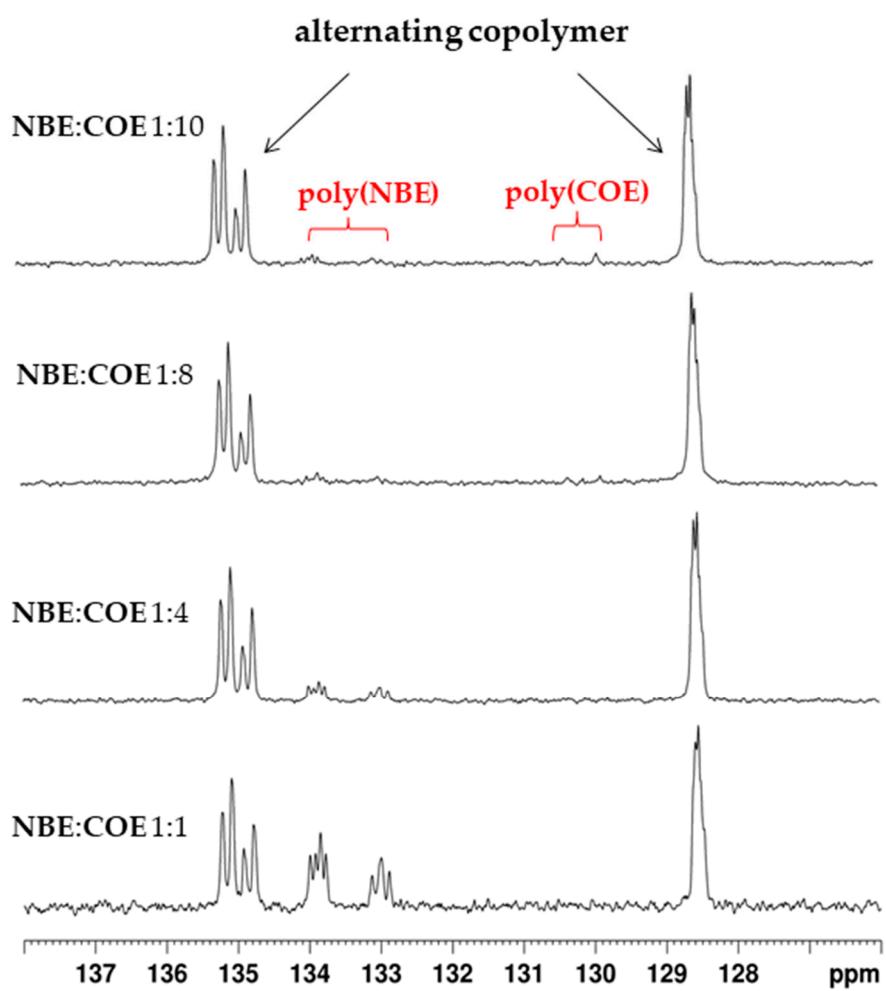


Figure S9: ^{13}C NMR (150 MHz) spectra of the olefinic region of the alternating NBE-CPE copolymers obtained by catalyst **2** (Table 2, entries 5-8).

DSC thermograms of alternating copolymers

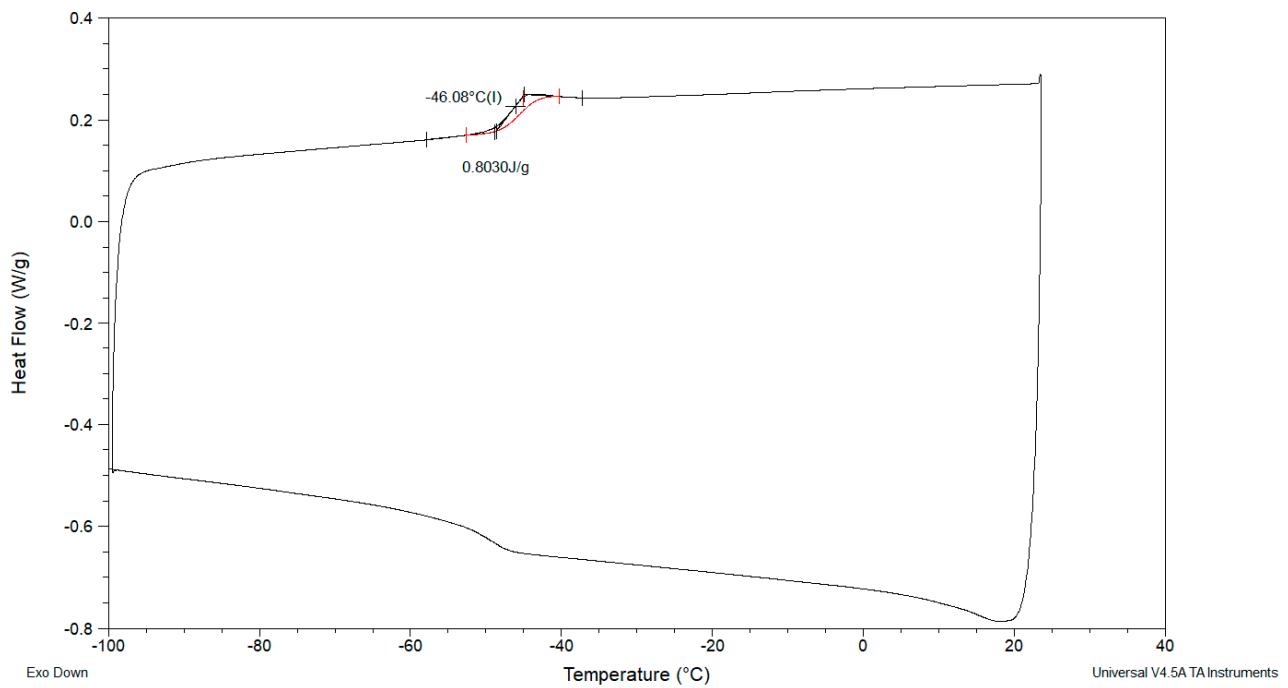


Figure S10: Thermogram of the alternating NBE-COE copolymer produced by **1** (Table 1, entry 4).

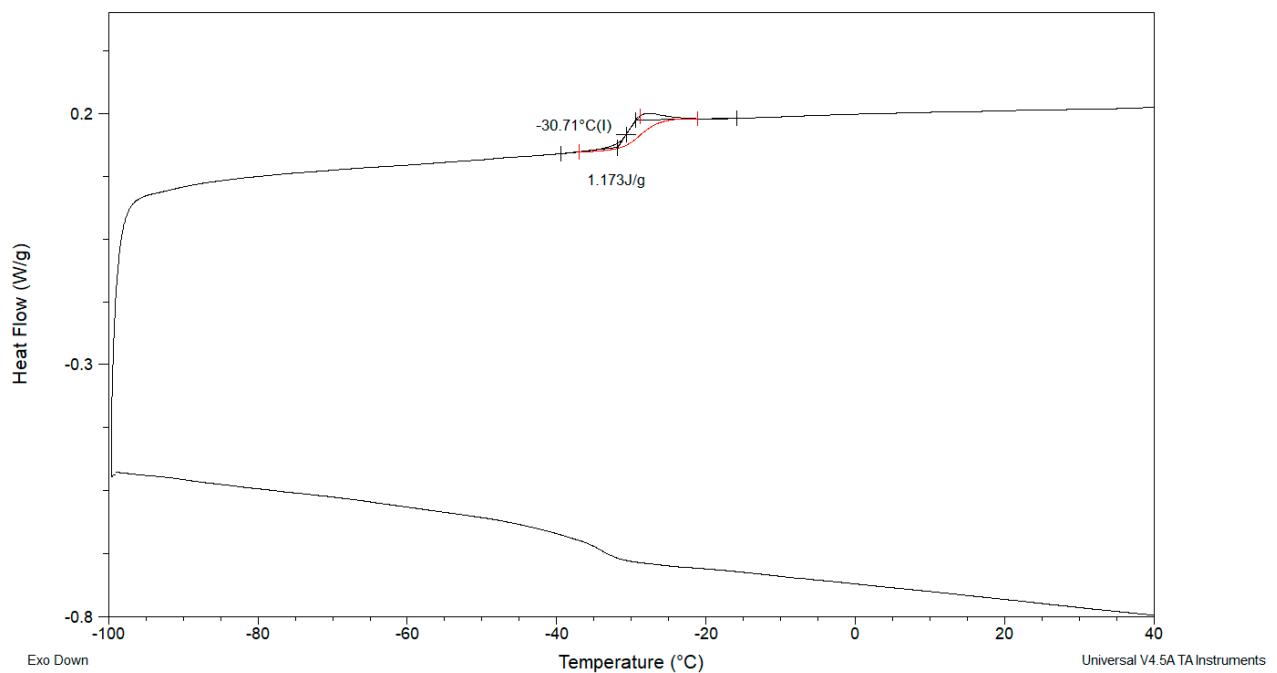


Figure S11: Thermogram of the alternating NBE-CPE copolymer produced by **1** (Table 2, entry 4).

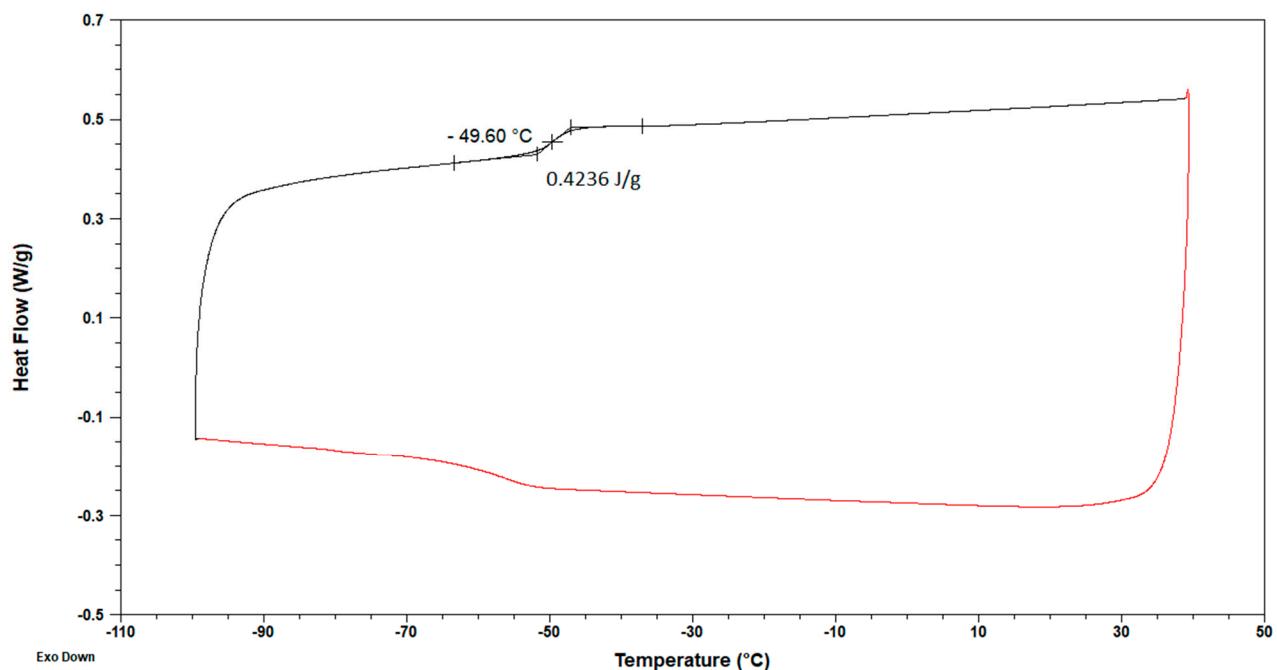


Figure S12: Thermogram of the alternating NBE-COE copolymer produced by **2** (Table 1, entry 8).

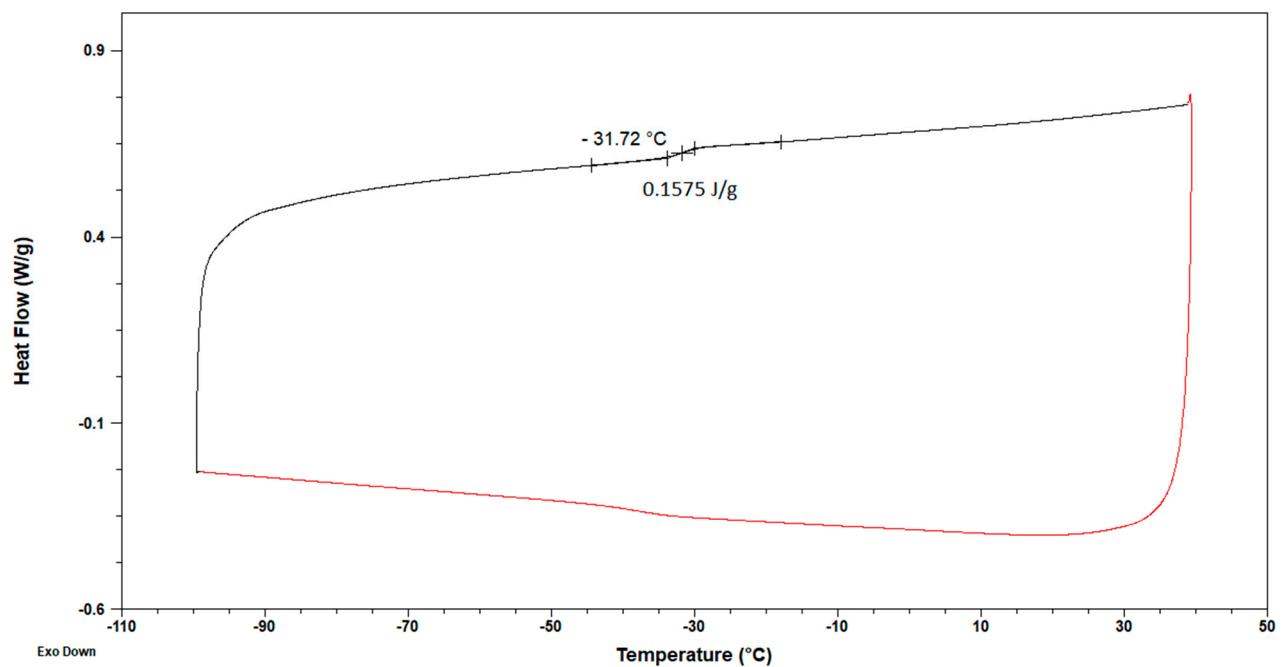


Figure S13: Thermogram of the alternating NBE-CPE copolymer produced by **2** (Table 2, entry 8).

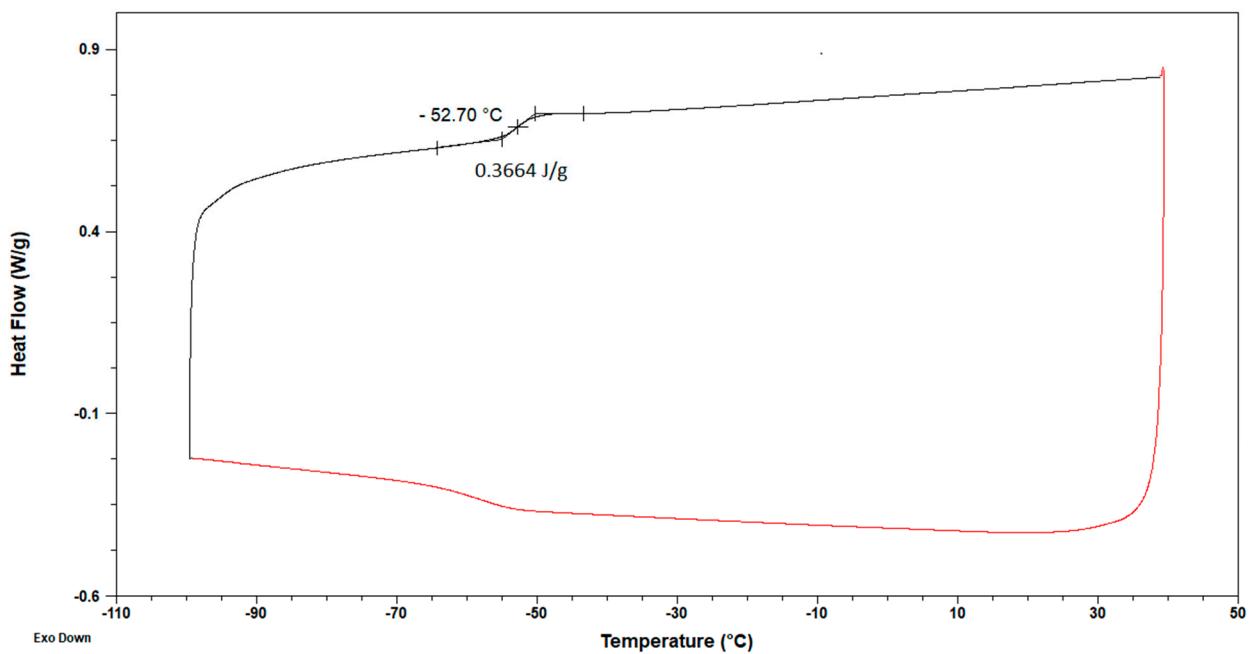


Figure S14: Thermogram of the alternating NBE-COE copolymer produced by **3** (Table 1, entry 12).

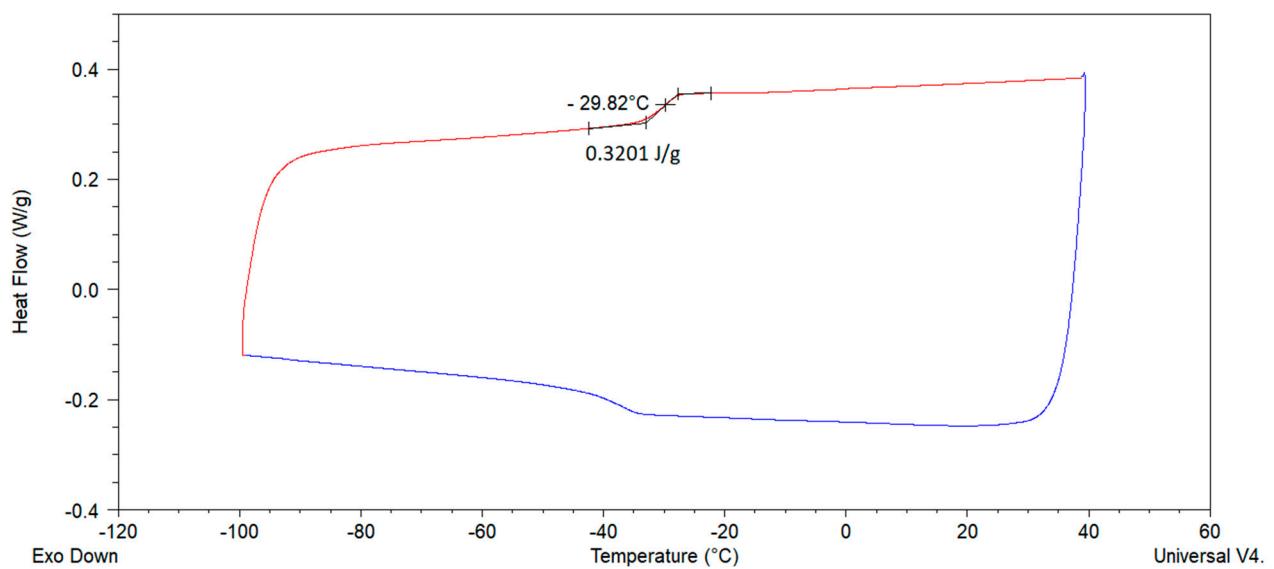


Figure S15: Thermogram of the alternating NBE-CPE copolymer produced by **3** (Table 2, entry 12).

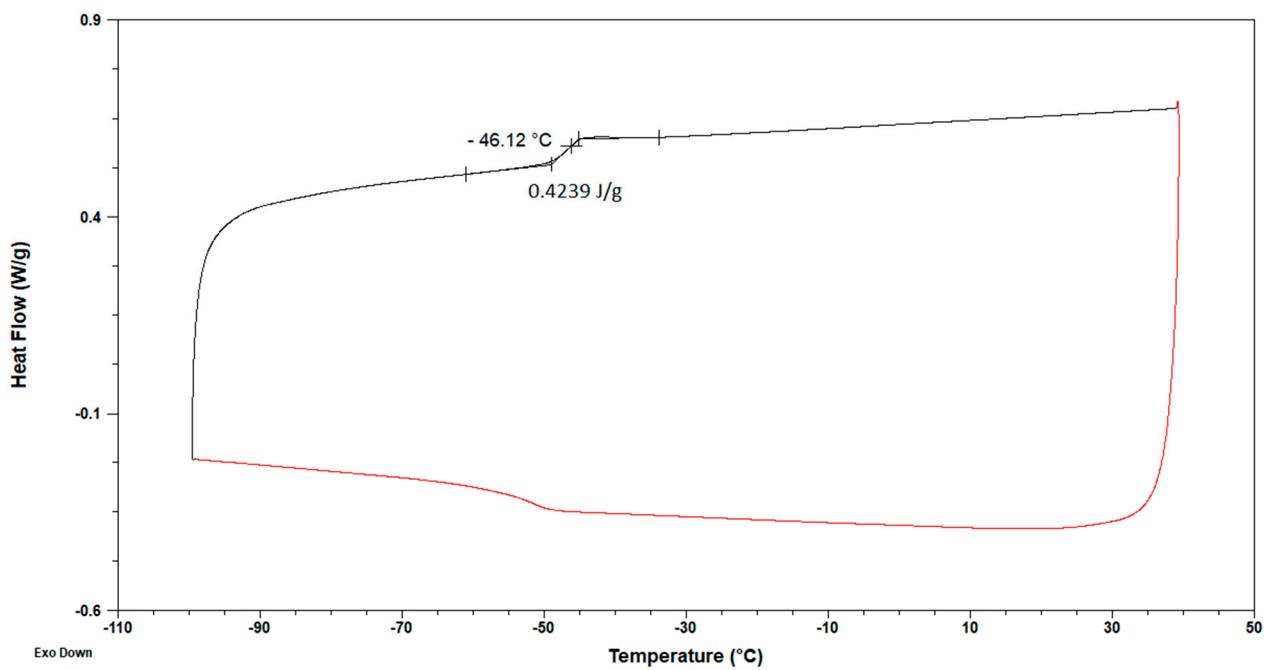


Figure S16: Thermogram of the alternating NBE-COE copolymer produced by **4** (Table 1, entry 16).

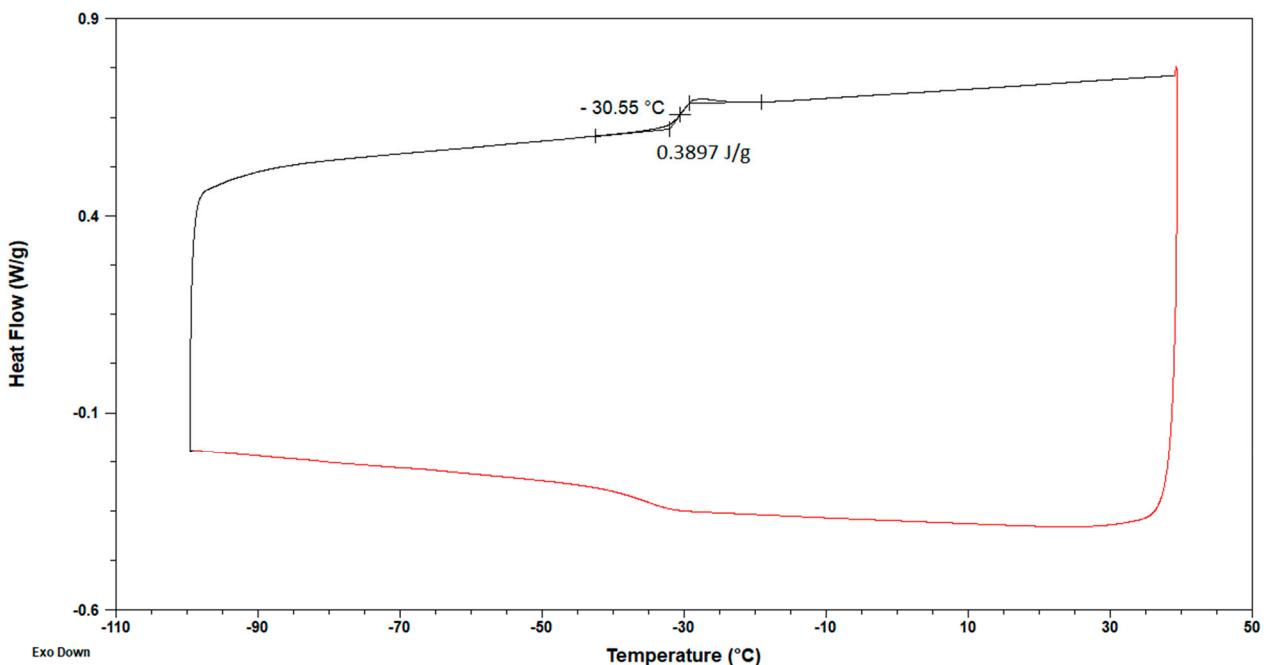


Figure S17: Thermogram of the alternating NBE-CPE copolymer produced by **4** (Table 2, entry 16).

Computational details

Computational details relative to calculations on Hoveyda-Grubbs-type catalysts

The DFT calculations were performed with the Gaussian09 set of programs,[58] using the BP86 functional of Becke and Perdew.[59,60] The electronic configuration of the molecular systems was described with the standard split-valence basis set with a polarization function of Ahlrichs and co-workers for H, C, N, O, and Cl (SVP keyword in Gaussian).[61] For Ru we used the small-core, quasi-relativistic Stuttgart/Dresden effective core potential, with an associated (8s7p6d)/[6s5p3d] valence basis set contracted according to a (311111/221111/411) scheme (standard SDD keywords in gaussian09).[62-64] The geometry optimizations were performed without symmetry constraints, and the characterization of the located stationary points was performed by analytical frequency calculations.

Improved electronic energies were obtained by single-point calculations, on the gas phase optimized structures, using diffuse function basis set (6-311++G(d,p))[65] and solvent effects including contributions of non electrostatic terms, based on the polarizable continuous solvation model PCM using CH₂Cl₂ as a solvent.[66,67] Free energies reported herein were obtained by adding these energies to the free energy thermal corrections of the SVP optimization level.

%V_{Bur} calculation. %V_{Bur} was calculated with the software developed by Cavallo and coworkers [54], starting from DFT optimized structures by choosing the metal as center of the sphere, selecting atomic bondi radii scaled by 1.17 and radius sphere of 3.5.

Cartesian coordinates and energies

“SD” are improved energies obtained considering solvent and diffuse functions as reported in computational details.

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3 E(gas) = -2750.77592503 G(SD) = -2752.090988			
Ru	1.619678	-0.341465	-0.079089
Cl	1.979793	-0.615245	-2.399978
C1	1.433907	-1.231041	2.103458
N	-0.978435	-1.501640	-0.490475
N	-1.263340	0.693465	-0.389083
C	-0.317095	-0.310314	-0.307298
C	-2.441390	-1.337798	-0.572668
H	-2.851715	-1.962750	-1.392457
C	-2.506941	0.159026	-1.026435
H	-2.336758	0.144842	-2.127635
C	2.023389	1.448423	0.131991
H	1.266753	2.255545	0.135284
C	3.404541	1.879591	0.256205
C	3.772881	3.246754	0.336289
H	2.973372	4.004864	0.317898
C	5.118699	3.626467	0.430243
H	5.392581	4.691029	0.490208
C	6.118360	2.636209	0.447407
H	7.178834	2.925465	0.521000
C	5.789515	1.268335	0.374072
H	6.591108	0.517390	0.391849
C	4.438125	0.895539	0.276531
O	3.968376	-0.388238	0.176649
C	4.879207	-1.530212	0.335960

H	5.793913	-1.281721	-0.246589
C	4.209330	-2.740853	-0.302676
H	3.322499	-3.053072	0.285827
H	4.926739	-3.586625	-0.320550
H	3.891587	-2.513235	-1.339065
C	5.210877	-1.729531	1.814952
H	5.689786	-0.832886	2.256538
H	5.909457	-2.583876	1.931597
H	4.281371	-1.941755	2.380837
C	-0.310005	-2.794670	-0.718271
H	0.778653	-2.595665	-0.571965
C	-0.709335	-3.887532	0.293149
H	-1.804258	-4.075449	0.221687
H	-0.509970	-3.524032	1.321331
C	0.053899	-5.197890	0.026625
H	1.137989	-5.034994	0.226964
H	-0.278033	-5.975589	0.747584
C	-0.125164	-5.686514	-1.420381
H	0.466146	-6.611597	-1.594222
H	-1.192499	-5.963117	-1.585326
C	0.277587	-4.594496	-2.425114
H	0.104145	-4.936051	-3.468338
H	1.371156	-4.399492	-2.342800
C	-0.480980	-3.279073	-2.176271
H	-0.119067	-2.483490	-2.860153
H	-1.564659	-3.438242	-2.383227
C	-1.046890	2.105632	-0.246352
C	-0.979486	2.676021	1.055180
C	-0.819570	4.072149	1.165081
H	-0.767444	4.515893	2.173693
C	-0.720423	4.910954	0.037564
C	-0.756378	4.308765	-1.235102
H	-0.644769	4.938837	-2.133807
C	-0.913327	2.918594	-1.404627
C	-0.993501	1.825084	2.300948
H	-1.139361	2.447507	3.205509
H	-0.038589	1.266840	2.414424
H	-1.786868	1.051873	2.273977
C	-0.883876	2.323303	-2.793610
H	-1.905640	2.083732	-3.161536
H	-0.280945	1.391679	-2.825741
H	-0.441987	3.039192	-3.514491
C	-0.598940	6.411191	0.188398
H	-0.031806	6.863540	-0.650564
H	-0.095428	6.689575	1.136472
H	-1.602106	6.892512	0.199061
C	-3.188999	-1.685194	0.713416
C	-2.575935	-1.626626	1.982737
H	-1.504974	-1.379217	2.065481
C	-3.315604	-1.920053	3.142718
H	-2.820603	-1.875467	4.126055
C	-4.672306	-2.276732	3.051226
H	-5.247510	-2.509908	3.961534
C	-5.287684	-2.346492	1.788841
H	-6.347799	-2.634295	1.704181
C	-4.549346	-2.053653	0.630741

H	-5.038591	-2.109856	-0.356013
C	-3.793652	0.918260	-0.787428
C	-4.213929	1.353273	0.488276
H	-3.580408	1.165798	1.365962
C	-5.438646	2.021021	0.648302
H	-5.746780	2.355781	1.651470
C	-6.270126	2.260287	-0.460075
H	-7.230010	2.785149	-0.330056
C	-5.866551	1.829070	-1.734895
H	-6.506861	2.012998	-2.612248
C	-4.636050	1.169579	-1.893489
H	-4.319655	0.841455	-2.898129

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4 E(gas) = -2711.48384812 G(SD) = -2712.789211

Ru	1.618802	-0.460976	-0.135063
Cl	1.986523	-0.664501	-2.461027
Cl	1.411187	-1.419359	2.016731
N	-0.989585	-1.567744	-0.599901
N	-1.252776	0.622003	-0.404210
C	-0.316270	-0.391643	-0.367030
C	-2.449960	-1.392363	-0.656288
H	-2.875359	-1.980577	-1.496467
C	-2.509862	0.123071	-1.045642
H	-2.355376	0.153849	-2.148790
C	2.053490	1.312966	0.140639
H	1.311858	2.133502	0.173664
C	3.442627	1.712235	0.284527
C	3.837953	3.068039	0.413932
H	3.053864	3.842275	0.420421
C	5.190744	3.417506	0.524399
H	5.485251	4.473656	0.622820
C	6.170788	2.407814	0.508198
H	7.236543	2.673288	0.593916
C	5.815118	1.050161	0.386044
H	6.601347	0.283004	0.378848
C	4.456943	0.707763	0.273450
O	3.962755	-0.562468	0.129897
C	4.848806	-1.728532	0.246022
H	5.764190	-1.483022	-0.336962
C	4.142494	-2.902004	-0.422212
H	3.253123	-3.205623	0.167133
H	4.836345	-3.765897	-0.472121
H	3.820633	-2.634882	-1.447936
C	5.188304	-1.983375	1.714818
H	5.688242	-1.112040	2.182872
H	5.871052	-2.854476	1.796149
H	4.259800	-2.197837	2.281444
C	-0.336376	-2.853221	-0.846256
C	-1.017603	2.026042	-0.216812
C	-0.935691	2.552559	1.102041
C	-0.758105	3.942564	1.255617
H	-0.695914	4.353481	2.277493
C	-0.654201	4.815691	0.155099
C	-0.704472	4.255428	-1.136267
H	-0.589423	4.913017	-2.014638
C	-0.880365	2.873669	-1.349476

C	-0.951209	1.662735	2.320533
H	-1.114655	2.254637	3.242442
H	0.010434	1.114730	2.427160
H	-1.731901	0.878792	2.261635
C	-0.867988	2.322537	-2.756952
H	-1.895463	2.109005	-3.125026
H	-0.278585	1.384050	-2.823347
H	-0.421002	3.054959	-3.457793
C	-0.512714	6.308743	0.352872
H	0.071283	6.777499	-0.465327
H	-0.016808	6.550934	1.314723
H	-1.508723	6.804664	0.365779
C	-3.177619	-1.792518	0.625956
C	-2.532374	-1.817206	1.880436
H	-1.454309	-1.595980	1.950703
C	-3.249760	-2.162974	3.040135
H	-2.730088	-2.183882	4.011442
C	-4.615003	-2.488893	2.962947
H	-5.172620	-2.762984	3.872803
C	-5.262022	-2.475814	1.714414
H	-6.329216	-2.739426	1.640434
C	-4.546289	-2.131766	0.556276
H	-5.059912	-2.125174	-0.419635
C	-3.784495	0.884896	-0.755180
C	-4.184822	1.257844	0.546381
H	-3.545607	1.013067	1.405713
C	-5.395823	1.936809	0.754983
H	-5.688441	2.222705	1.777723
C	-6.233481	2.249254	-0.330409
H	-7.182515	2.783056	-0.162620
C	-5.850208	1.879520	-1.630569
H	-6.495805	2.120945	-2.489935
C	-4.633244	1.208307	-1.837305
H	-4.332499	0.928711	-2.861230
C	-0.465453	-3.380843	-2.306658
C	-0.372361	-4.930699	-2.199015
C	-0.124985	-5.232682	-0.696859
C	-0.764366	-4.043690	0.038422
H	-1.440663	-3.069029	-2.737047
H	0.320359	-2.925679	-2.941684
H	0.423922	-5.353145	-2.845139
H	-1.324655	-5.398218	-2.527558
H	0.966812	-5.253262	-0.484780
H	-0.532509	-6.213492	-0.377177
H	-0.432975	-3.925732	1.089104
H	-1.872041	-4.141872	0.042690
H	0.747269	-2.680655	-0.647780

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Buchmeiser complex E(gas)=-2363.96183964 G(SD) = -2365.072286

Ru	0.145625	-0.762781	0.169473
Cl	-0.697734	-1.029885	-2.020814
Cl	0.169652	-1.254221	2.480459
N	-2.179513	0.905683	0.690584
N	-0.417893	2.224629	0.546996
C	-0.823174	0.912565	0.461964
C	-2.693776	2.208681	1.131408

H	-3.651258	2.449404	0.625744
C	-1.549846	3.154099	0.743086
H	-1.760724	3.709845	-0.199583
C	1.861587	-0.165692	-0.157413
H	2.165862	0.897881	-0.144596
C	2.910257	-1.116833	-0.483268
C	4.226881	-0.714384	-0.823395
H	4.460147	0.362604	-0.823218
C	5.205934	-1.659618	-1.158613
H	6.224089	-1.334952	-1.422843
C	4.877555	-3.027930	-1.156186
H	5.640273	-3.777753	-1.420113
C	3.581831	-3.465023	-0.817648
H	3.353772	-4.539488	-0.821447
C	2.605453	-2.511613	-0.483419
O	1.304790	-2.784322	-0.150307
C	0.847221	-4.169227	0.029938
H	1.268942	-4.748792	-0.821358
C	-0.672145	-4.157217	-0.085459
H	-1.118265	-3.592557	0.758991
H	-1.051273	-5.198626	-0.045127
H	-0.992806	-3.690271	-1.036964
C	1.347803	-4.721389	1.365217
H	2.453082	-4.691175	1.440583
H	1.026682	-5.777957	1.475250
H	0.926351	-4.127588	2.200971
C	-3.044458	-0.285476	0.751387
H	-2.451779	-1.101066	0.274816
C	-3.360461	-0.697587	2.197592
H	-3.951808	0.074283	2.732394
H	-2.414398	-0.866708	2.748664
H	-3.946164	-1.639002	2.211847
C	0.870138	2.787045	0.260075
C	1.758426	3.044283	1.335344
C	2.999111	3.646328	1.043567
H	3.700994	3.839853	1.872289
C	3.367314	4.000105	-0.270528
C	2.459176	3.723855	-1.313795
H	2.734153	3.979522	-2.351191
C	1.207014	3.122361	-1.077503
C	1.401296	2.639674	2.746628
H	2.221540	2.884360	3.449529
H	1.195399	1.549615	2.812311
H	0.485727	3.157267	3.105968
C	0.276952	2.794508	-2.222221
H	-0.705811	3.302885	-2.118780
H	0.066876	1.703909	-2.272971
H	0.713766	3.109224	-3.190018
C	4.687349	4.683533	-0.552702
H	5.091391	4.400477	-1.546061
H	5.449456	4.437136	0.213982
H	4.570569	5.790056	-0.553605
H	-2.874773	2.207242	2.231079
H	-1.314441	3.900535	1.529068
C	-4.281293	-0.072521	-0.140048
C	-4.096599	0.193326	-1.517018

C	-5.198495	0.399713	-2.361636
C	-6.507805	0.347279	-1.847876
C	-6.702934	0.080645	-0.483509
C	-5.597852	-0.128942	0.363042
H	-3.072086	0.216543	-1.923996
H	-5.033260	0.596683	-3.433226
H	-7.372546	0.509893	-2.511049
H	-7.722819	0.033711	-0.068805
H	-5.776155	-0.339707	1.428014

13

cpe E(gas) = -195.178261062 G(SD) = -195.2865533

C	-0.674600	1.077978	-0.050112
C	0.674782	1.077865	-0.050118
H	-1.306347	1.979175	-0.108563
H	1.306661	1.978973	-0.108577
C	1.237611	-0.320440	0.108509
C	-1.237662	-0.320247	0.108510
C	-0.000103	-1.227554	-0.142981
H	-1.652460	-0.454464	1.136560
H	-2.078411	-0.536411	-0.586648
H	-0.000149	-1.555436	-1.204363
H	-0.000176	-2.145954	0.478828
H	1.652391	-0.454726	1.136558
H	2.078325	-0.536776	-0.586637

17

nbe E(gas) = -272.525533005 G(SD) = -272.672461

C	-1.280783	0.676987	-0.509321
C	-1.280681	-0.677065	-0.509442
H	-1.928348	1.343220	-1.100086
H	-1.928096	-1.343275	-1.100401
C	-0.087802	-1.131716	0.326360
C	-0.088004	1.131662	0.326602
C	-0.042441	-0.000180	1.385593
C	1.192862	0.781734	-0.519459
H	-0.117498	2.174801	0.697772
H	-0.927382	-0.000240	2.054667
H	0.886435	-0.000154	1.996429
C	1.193000	-0.781459	-0.519496
H	-0.117208	-2.174936	0.697320
H	2.102381	-1.186556	-0.027560
H	1.145576	-1.217551	-1.537716
H	2.102271	1.187071	-0.027792
H	1.144969	1.217848	-1.537651

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3-CPE E(gas) = -2945.92932680 G(SD) = -2947.329784

Ru	1.066606	-1.187846	0.215898
Cl	1.396653	-1.250582	-2.167549
Cl	0.128435	-1.847309	2.352510
N	-1.745116	-1.256107	-0.528472
N	-1.238393	0.881676	-0.277692
C	-0.746038	-0.395910	-0.172278
C	-3.026912	-0.567008	-0.787904
H	-3.500473	-0.975603	-1.703520
C	-2.479705	0.858915	-1.123080
H	-2.139486	0.801152	-2.182121
C	1.833718	0.359964	0.921256

H	1.162417	0.827796	1.670442
C	3.145371	1.011960	0.980398
C	-1.558346	-2.702017	-0.747816
C	-0.559106	2.108106	0.041776
C	-0.560445	2.576193	1.386781
C	0.053586	3.813018	1.662458
H	0.053928	4.177879	2.703636
C	0.658947	4.595339	0.658617
C	0.647946	4.098843	-0.657134
H	1.125739	4.686134	-1.459501
C	0.054242	2.864309	-0.991048
C	-1.156083	1.769200	2.516367
H	-1.088555	2.323576	3.472947
H	-0.646166	0.788202	2.648109
H	-2.222421	1.520561	2.340668
C	0.093670	2.370064	-2.417432
H	-0.890937	2.491682	-2.919733
H	0.377489	1.297174	-2.470870
H	0.827116	2.951553	-3.009968
C	1.328010	5.908407	0.998507
H	1.493247	6.530344	0.095985
H	2.320378	5.738956	1.471207
H	0.724406	6.499619	1.718208
C	-4.032760	-0.661656	0.356888
C	-3.632787	-0.846469	1.697420
H	-2.566539	-0.988996	1.939172
C	-4.593286	-0.888787	2.724004
H	-4.265990	-1.040644	3.765061
C	-5.960546	-0.750050	2.427324
H	-6.710050	-0.788372	3.233988
C	-6.366946	-0.574793	1.092574
H	-7.436360	-0.474620	0.847314
C	-5.408255	-0.532182	0.066923
H	-5.733533	-0.393980	-0.977765
C	-3.427107	2.034616	-1.030407
C	-3.925869	2.544390	0.188070
H	-3.609842	2.095408	1.139206
C	-4.829988	3.618593	0.198925
H	-5.202585	4.003824	1.161246
C	-5.262525	4.197881	-1.006915
H	-5.972102	5.040543	-0.994330
C	-4.781788	3.695840	-2.227863
H	-5.111391	4.141003	-3.180096
C	-3.869312	2.627685	-2.234783
H	-3.489330	2.242895	-3.196262
C	3.391859	-2.119853	0.208547
C	2.440825	-3.122269	0.316126
C	4.264376	-2.087851	1.448516
C	3.485427	-2.944324	2.477273
H	5.241385	-2.558864	1.180090
H	4.507200	-1.068554	1.812947
C	2.596485	-3.881587	1.622939
H	4.148042	-3.490905	3.178668
H	2.823366	-2.287827	3.079137
H	3.110014	-4.847218	1.398394
H	1.633013	-4.122290	2.116288

H	3.660601	-1.625922	-0.734945
H	1.932709	-3.558588	-0.561668
C	3.471552	1.557148	2.256899
C	4.715858	2.128387	2.544326
C	5.676732	2.203397	1.521552
C	5.382099	1.732354	0.232834
C	4.122221	1.158717	-0.067065
H	2.707324	1.487518	3.048084
H	4.933384	2.511924	3.552860
H	6.667102	2.644792	1.718216
H	6.147381	1.821781	-0.549587
O	3.755914	0.772343	-1.310106
C	4.643593	0.949709	-2.446090
C	3.751973	1.111968	-3.674444
H	5.220461	1.890611	-2.295807
C	5.604360	-0.237730	-2.559738
H	4.377018	1.220946	-4.584381
H	3.091393	0.229051	-3.785055
H	3.112323	2.011252	-3.578876
H	6.317887	-0.075976	-3.394219
H	6.192589	-0.382205	-1.630928
H	5.037877	-1.169189	-2.764043
C	-1.728386	-3.080961	-2.234906
H	-0.492368	-2.901549	-0.480728
C	-1.448994	-4.576206	-2.469339
H	-2.771986	-2.852838	-2.552669
H	-1.043343	-2.452775	-2.841273
C	-2.308037	-5.468467	-1.558239
H	-1.618053	-4.826059	-3.538909
H	-0.370487	-4.776378	-2.274322
C	-2.128040	-5.084335	-0.080302
H	-3.381099	-5.356331	-1.839171
H	-2.056172	-6.539805	-1.714608
C	-2.417550	-3.592695	0.170971
H	-2.782696	-5.704559	0.568826
H	-1.082583	-5.308832	0.233511
H	-3.495104	-3.385443	-0.015263
H	-2.210252	-3.329346	1.227608

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4-CPE E(gas)=-2906.63733518 G(SD) = -2908.028567

Ru	1.092996	-1.238244	0.139702
Cl	1.427263	-1.193240	-2.241090
Cl	0.184896	-2.036665	2.241151
N	-1.701482	-1.401910	-0.628780
N	-1.302803	0.744170	-0.283344
C	-0.748679	-0.509967	-0.224605
C	-3.013666	-0.770087	-0.867568
H	-3.462263	-1.163852	-1.803172
C	-2.537358	0.695210	-1.137927
H	-2.189257	0.700113	-2.195979
C	1.790677	0.312781	0.907165
H	1.093134	0.731341	1.661572
C	3.077254	1.008999	1.003370
C	-1.448735	-2.823914	-0.865685
C	-0.689822	1.986598	0.100359
C	-0.724041	2.387235	1.466470

C	-0.175795	3.638665	1.807281
H	-0.201380	3.952081	2.864774
C	0.396525	4.498077	0.847985
C	0.420186	4.066377	-0.490359
H	0.873621	4.715240	-1.258708
C	-0.108155	2.821457	-0.889031
C	-1.283084	1.494845	2.549447
H	-1.277430	2.013357	3.528230
H	-0.704551	0.549281	2.655379
H	-2.322898	1.173349	2.337313
C	-0.034196	2.398021	-2.336675
H	-1.019631	2.496734	-2.842478
H	0.299889	1.343228	-2.437259
H	0.675653	3.040437	-2.893986
C	0.996071	5.824907	1.257147
H	1.137701	6.496840	0.387049
H	1.991619	5.682365	1.732040
H	0.357571	6.350250	1.997538
C	-4.015530	-0.967154	0.267967
C	-3.606765	-1.225947	1.593535
H	-2.535741	-1.349341	1.826121
C	-4.563887	-1.366455	2.614736
H	-4.229925	-1.574976	3.643786
C	-5.935337	-1.253470	2.327156
H	-6.681817	-1.368477	3.129321
C	-6.349765	-1.005685	1.006304
H	-7.422354	-0.925024	0.767815
C	-5.395090	-0.865168	-0.014176
H	-5.726585	-0.670861	-1.047888
C	-3.542971	1.816772	-1.000819
C	-4.065546	2.252560	0.236204
H	-3.725518	1.784050	1.169493
C	-5.022870	3.278418	0.288052
H	-5.413521	3.606536	1.264276
C	-5.485183	3.881771	-0.894709
H	-6.236488	4.686302	-0.849956
C	-4.980444	3.453182	-2.133875
H	-5.332722	3.918366	-3.068249
C	-4.015022	2.433724	-2.181632
H	-3.616250	2.107091	-3.156918
C	-1.541620	-3.266486	-2.353463
C	-1.886510	-4.783882	-2.311867
C	-1.972609	-5.156421	-0.805939
C	-2.329133	-3.836340	-0.102903
H	-2.342248	-2.692176	-2.866237
H	-0.596530	-3.028624	-2.880915
H	-1.136823	-5.400898	-2.847959
H	-2.860974	-4.972714	-2.809585
H	-0.983932	-5.511715	-0.440909
H	-2.699662	-5.968267	-0.600096
H	-2.123911	-3.830345	0.985697
H	-3.404997	-3.595995	-0.248527
H	-0.402813	-2.998182	-0.517643
C	3.458460	-2.070168	0.107388
C	2.553819	-3.118890	0.146636
C	4.315959	-2.067088	1.358154

C	3.570243	-3.018094	2.327146
H	5.318050	-2.472958	1.076302
H	4.503544	-1.059400	1.782655
C	2.730214	-3.942451	1.411066
H	4.253104	-3.575312	3.000207
H	2.875251	-2.429884	2.961480
H	3.286333	-4.871503	1.138650
H	1.773569	-4.251857	1.878639
H	3.713078	-1.512510	-0.803951
H	2.073408	-3.525999	-0.760239
C	3.379542	1.507562	2.304322
C	4.600892	2.111907	2.621347
C	5.559765	2.270192	1.606190
C	5.285412	1.847635	0.296263
C	4.049034	1.240178	-0.033061
H	2.617073	1.373241	3.088862
H	4.802110	2.457195	3.646951
H	6.532063	2.739901	1.826030
H	6.047499	2.002670	-0.479035
O	3.698007	0.897677	-1.293584
C	4.578661	1.160518	-2.418213
C	3.681531	1.339334	-3.640258
H	5.116293	2.116869	-2.225438
C	5.587276	0.019439	-2.581554
H	4.301633	1.514081	-4.543285
H	3.058667	0.435168	-3.790873
H	3.004712	2.206002	-3.506734
H	6.294010	0.246490	-3.406556
H	6.180502	-0.141517	-1.658655
H	5.059299	-0.924467	-2.827553

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B-CPE E(gas) = -2559.11819666 G(SD) = -2560.309748

Ru	0.257656	-0.807243	-0.677578
Cl	0.933210	-1.454297	1.540000
Cl	0.513597	-0.275244	-3.045218
N	2.625269	0.970468	-0.493453
N	0.825147	2.223272	-0.290432
C	1.262743	0.935439	-0.434177
C	3.158286	2.340550	-0.571326
H	4.027826	2.464674	0.105490
C	1.944281	3.184104	-0.161488
H	2.011169	3.549113	0.888629
C	-1.442859	-0.047049	-0.764325
H	-1.496997	0.748812	-1.537690
C	-2.794452	-0.354304	-0.289848
C	3.524260	-0.179006	-0.710820
C	-0.505488	2.708547	-0.053253
C	-1.206427	3.329240	-1.120718
C	-2.476601	3.875746	-0.851431
H	-3.032870	4.351861	-1.676568
C	-3.053140	3.831727	0.434105
C	-2.316683	3.228277	1.472743
H	-2.742246	3.199718	2.490144
C	-1.042531	2.666283	1.259528
C	-0.619158	3.380504	-2.512167
H	-1.352789	3.785165	-3.236952

H	-0.296692	2.372824	-2.857325
H	0.280699	4.033034	-2.557199
C	-0.270902	2.040815	2.395665
H	0.741946	2.484988	2.500835
H	-0.121485	0.951445	2.236073
H	-0.800124	2.185802	3.357725
C	-4.435231	4.391403	0.687676
H	-4.524531	4.815290	1.708891
H	-5.206754	3.595127	0.597518
H	-4.697124	5.185512	-0.040487
H	3.492129	2.565449	-1.609635
H	1.783964	4.064989	-0.815486
C	-0.855469	-3.039821	-0.547039
C	0.297192	-3.053537	-1.320798
C	-2.056305	-3.404045	-1.397208
C	-1.542147	-3.254205	-2.849597
H	-2.316162	-4.465617	-1.163901
H	-2.970552	-2.812801	-1.184219
C	-0.012552	-3.467874	-2.748483
H	-2.036355	-3.945567	-3.561789
H	-1.729727	-2.217391	-3.200251
H	0.259571	-4.544635	-2.861116
H	0.553760	-2.892948	-3.508073
H	-0.864803	-3.051600	0.551144
H	1.310195	-3.154607	-0.887547
C	-3.827925	-0.015112	-1.212505
C	-5.172916	-0.336136	-1.001922
C	-5.530066	-0.998011	0.185216
C	-4.557370	-1.307462	1.148278
C	-3.195129	-0.972220	0.949058
H	-3.527605	0.496609	-2.141226
H	-5.932893	-0.075750	-1.754310
H	-6.580094	-1.272503	0.376395
H	-4.872264	-1.813238	2.070562
O	-2.237587	-1.163622	1.883275
C	-2.556315	-1.751020	3.175085
C	-1.555398	-1.188655	4.181272
H	-3.577206	-1.417352	3.468594
C	-2.513057	-3.278618	3.083071
H	-1.739759	-1.632599	5.181034
H	-0.519602	-1.421510	3.863692
H	-1.655864	-0.088883	4.265772
H	-2.815695	-3.730663	4.050360
H	-3.195634	-3.662720	2.298124
H	-1.482373	-3.615384	2.849778
H	2.904665	-1.074916	-0.477351
C	3.991280	-0.276304	-2.170849
C	4.656261	-0.150891	0.330038
H	4.590002	-1.197211	-2.321854
H	3.106708	-0.314237	-2.837519
H	4.621817	0.587671	-2.466821
C	6.019202	-0.112162	-0.031084
C	7.025221	-0.082932	0.953211
C	6.683336	-0.094164	2.314774
C	5.326677	-0.139508	2.686134
C	4.323396	-0.167187	1.704885

H	6.312645	-0.105884	-1.091479
H	8.083750	-0.051859	0.648428
H	7.470814	-0.072698	3.085120
H	5.046413	-0.161451	3.751707
H	3.261246	-0.224836	1.995717

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3-NBE E(gas)=-3023.27822299 G(SD) = -3024.71668

Ru	-1.073320	-0.952404	-0.132117
Cl	-1.272286	-0.903861	2.270568
Cl	-0.232212	-1.796390	-2.252283
N	1.750833	-1.383767	0.559355
N	1.517388	0.793647	0.261347
C	0.865257	-0.411206	0.201651
C	3.118395	-0.860202	0.770058
H	3.557398	-1.303485	1.686534
C	2.769753	0.632736	1.075936
H	2.453371	0.647942	2.143627
C	-1.639987	0.652931	-0.894084
H	-0.946669	0.975744	-1.698670
C	-2.840100	1.494133	-0.923254
C	1.387729	-2.788012	0.825587
C	0.994465	2.087414	-0.087214
C	1.013155	2.504163	-1.448641
C	0.553301	3.799710	-1.754911
H	0.566336	4.124894	-2.809021
C	0.086154	4.688255	-0.766368
C	0.079948	4.242196	0.567620
H	-0.289084	4.915194	1.360029
C	0.521691	2.954332	0.932756
C	1.471768	1.592709	-2.562463
H	1.439399	2.117954	-3.537168
H	0.846934	0.674743	-2.642678
H	2.507078	1.226214	-2.407646
C	0.475169	2.523945	2.379378
H	1.486485	2.536916	2.841483
H	0.059291	1.499527	2.488795
H	-0.153657	3.218044	2.970920
C	-0.425898	6.062014	-1.137464
H	-0.416941	6.751556	-0.269456
H	-1.473779	6.008808	-1.506725
H	0.179748	6.518925	-1.947192
C	4.074184	-1.115495	-0.392692
C	3.620321	-1.284281	-1.718052
H	2.538824	-1.294660	-1.932907
C	4.541678	-1.478938	-2.762828
H	4.171730	-1.616372	-3.791532
C	5.922389	-1.509407	-2.499606
H	6.640421	-1.666585	-3.320374
C	6.381163	-1.350585	-1.179860
H	7.460377	-1.382226	-0.960487
C	5.461787	-1.156404	-0.135965
H	5.828115	-1.032335	0.896834
C	3.858819	1.671464	0.925295
C	4.378498	2.086000	-0.320145
H	3.973596	1.663812	-1.249600
C	5.415614	3.030278	-0.385361

H	5.802819	3.343216	-1.367919
C	5.961682	3.571044	0.791966
H	6.775451	4.311627	0.736780
C	5.460707	3.161906	2.039192
H	5.878478	3.578395	2.969545
C	4.415951	2.224713	2.100611
H	4.021567	1.913051	3.082567
C	-3.435821	-1.516902	0.077877
C	-2.642889	-2.611589	-0.278609
C	-4.476819	-1.367257	-1.026770
C	-3.708445	-1.864719	-2.271728
C	-5.446266	-2.585407	-0.788173
H	-4.988346	-0.389024	-1.099282
C	-3.202188	-3.157920	-1.591484
H	-4.373373	-2.064306	-3.138106
H	-2.882325	-1.199445	-2.585384
C	-4.566390	-3.818009	-1.180137
H	-2.522287	-3.801485	-2.179388
H	-3.581798	-1.149387	1.102228
H	-2.147048	-3.270116	0.458741
C	-3.141670	2.038130	-2.205755
C	-4.293102	2.789729	-2.462686
C	-5.175707	3.054996	-1.401960
C	-4.894725	2.587340	-0.108930
C	-3.729513	1.826981	0.159381
H	-2.438193	1.821962	-3.026325
H	-4.498240	3.166591	-3.476316
H	-6.091690	3.643509	-1.572390
H	-5.595927	2.826414	0.701443
O	-3.373074	1.425143	1.400284
C	-4.176408	1.773090	2.559269
C	-3.228250	1.809312	3.754782
H	-4.592444	2.794431	2.402297
C	-5.318978	0.768443	2.737380
H	-3.795136	2.039846	4.680001
H	-2.719704	0.831271	3.868656
H	-2.451717	2.586881	3.616872
H	-5.968469	1.072399	3.584378
H	-5.951876	0.698084	1.829728
H	-4.912048	-0.239331	2.958830
C	1.568901	-3.153030	2.315062
H	0.295519	-2.849773	0.606287
C	1.099161	-4.590841	2.599592
H	2.646344	-3.063941	2.585702
H	1.002083	-2.424909	2.931460
C	1.792976	-5.610906	1.681737
H	1.275579	-4.838509	3.668497
H	-0.003425	-4.645941	2.449497
C	1.609538	-5.237450	0.201339
H	2.881449	-5.640245	1.921191
H	1.404653	-6.634363	1.875249
C	2.086415	-3.804237	-0.099094
H	2.149814	-5.954216	-0.453642
H	0.532220	-5.325588	-0.069828
H	3.188198	-3.740145	0.044789
H	1.875389	-3.537901	-1.154222

H	-4.998249	-4.368285	-2.042392
H	-4.447151	-4.547164	-0.352236
H	-5.815023	-2.627552	0.257271
H	-6.334920	-2.491961	-1.447614

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4-NBE E(gas) = -2983.98618840 G(SD) = -2985.415543

Ru	-1.083430	-1.011983	-0.065640
Cl	-1.288427	-0.865831	2.329855
Cl	-0.264594	-1.980767	-2.140123
N	1.716067	-1.499206	0.661858
N	1.560652	0.668782	0.270230
C	0.866972	-0.513022	0.253820
C	3.099301	-1.018718	0.856833
H	3.519728	-1.440176	1.793240
C	2.803453	0.497818	1.097944
H	2.483767	0.569464	2.162355
C	-1.603097	0.579647	-0.887262
H	-0.892236	0.864737	-1.690860
C	-2.787906	1.440272	-0.956703
C	1.308489	-2.875814	0.947321
C	1.089011	1.962099	-0.144999
C	1.127795	2.308311	-1.525725
C	0.716769	3.602535	-1.898802
H	0.7444895	3.873688	-2.967829
C	0.278936	4.556080	-0.958079
C	0.250913	4.178132	0.396381
H	-0.097530	4.902697	1.151737
C	0.643485	2.894613	0.827647
C	1.554750	1.323876	-2.588869
H	1.554613	1.801307	-3.588362
H	0.890032	0.431658	-2.630871
H	2.570594	0.918227	-2.404813
C	0.572418	2.535547	2.292586
H	1.580571	2.533136	2.761788
H	0.119249	1.532860	2.445797
H	-0.034557	3.278702	2.846103
C	-0.178137	5.927820	-1.401505
H	-0.204670	6.644586	-0.556391
H	-1.202322	5.885340	-1.833029
H	0.486010	6.345400	-2.186559
C	4.045095	-1.359348	-0.292552
C	3.579113	-1.605549	-1.601422
H	2.495880	-1.611814	-1.809297
C	4.490493	-1.882772	-2.636457
H	4.111391	-2.079892	-3.652029
C	5.872107	-1.919604	-2.379520
H	6.582051	-2.141150	-3.192436
C	6.342296	-1.684667	-1.075079
H	7.422277	-1.720665	-0.860204
C	5.433460	-1.408294	-0.040653
H	5.808628	-1.225234	0.980104
C	3.928557	1.490498	0.908226
C	4.462151	1.836495	-0.352148
H	4.042235	1.392202	-1.264494
C	5.531044	2.741331	-0.453637
H	5.928643	3.001462	-1.447372

C	6.095328	3.309651	0.701913
H	6.934018	4.019105	0.618278
C	5.580463	2.968446	1.963866
H	6.012148	3.407507	2.877328
C	4.503983	2.071054	2.061333
H	4.098571	1.813226	3.054349
C	1.392890	-3.285765	2.444661
C	1.546715	-4.834870	2.438838
C	1.554707	-5.253510	0.942249
C	2.046443	-4.003058	0.194713
H	2.274463	-2.802836	2.917452
H	0.501374	-2.918746	2.990641
H	0.737125	-5.339824	3.004276
H	2.499864	-5.130900	2.925415
H	0.523400	-5.499943	0.606707
H	2.177306	-6.149986	0.745329
H	1.816747	-4.000878	-0.888962
H	3.146300	-3.887790	0.311241
H	0.240880	-2.935045	0.632033
C	-3.466950	-1.498017	0.155768
C	-2.704590	-2.632985	-0.133362
C	-4.495302	-1.377678	-0.963981
C	-3.732386	-1.962924	-2.173474
C	-5.501788	-2.552868	-0.669407
H	-4.977211	-0.390247	-1.092626
C	-3.269517	-3.231982	-1.420647
H	-4.396123	-2.189449	-3.034155
H	-2.884596	-1.339503	-2.514160
C	-4.655604	-3.829532	-0.987177
H	-2.604438	-3.925745	-1.966975
H	-3.607850	-1.069896	1.156962
H	-2.234164	-3.264198	0.643354
C	-3.083251	1.928025	-2.262669
C	-4.222771	2.686536	-2.551540
C	-5.097129	3.016891	-1.502334
C	-4.819611	2.606744	-0.189078
C	-3.666470	1.840356	0.111466
H	-2.386476	1.660791	-3.073899
H	-4.424983	3.018623	-3.581298
H	-6.003474	3.612334	-1.698246
H	-5.513274	2.896500	0.611248
O	-3.309606	1.493533	1.369033
C	-4.101371	1.908383	2.513608
C	-3.145397	1.986397	3.700937
H	-4.503059	2.927332	2.310310
C	-5.257619	0.930695	2.745347
H	-3.702586	2.269142	4.617516
H	-2.651941	1.006569	3.857986
H	-2.357808	2.744267	3.521995
H	-5.897826	1.284533	3.579958
H	-5.896524	0.826571	1.845175
H	-4.863910	-0.071167	3.012742
H	-5.096817	-4.412415	-1.822870
H	-4.563987	-4.516548	-0.120618
H	-5.879423	-2.528272	0.373432
H	-6.382330	-2.469162	-1.340912

B-NBE E(gas) = -2636.46675370 G(SD) = -2637.698798

Ru	0.224263	-0.734817	-0.510159
Cl	0.935336	-1.073891	1.765607
Cl	0.494300	-0.589618	-2.928959
N	2.764889	0.826561	-0.636179
N	1.095752	2.261518	-0.617044
C	1.408306	0.932334	-0.555455
C	3.415188	2.108111	-0.959712
H	4.326289	2.255412	-0.345686
C	2.303799	3.118150	-0.652299
H	2.441059	3.618829	0.333196
C	-1.402690	0.162121	-0.666495
H	-1.400680	0.862159	-1.529521
C	-2.765363	0.035341	-0.142308
C	3.553202	-0.420673	-0.647580
C	-0.180198	2.900392	-0.453376
C	-0.841315	3.406451	-1.603612
C	-2.056308	4.095062	-1.420961
H	-2.582659	4.482909	-2.309545
C	-2.617003	4.297960	-0.143235
C	-1.917477	3.803884	0.975440
H	-2.329892	3.967649	1.985389
C	-0.697106	3.110648	0.850763
C	-0.271652	3.189723	-2.986508
H	-0.987610	3.517799	-3.765605
H	-0.021288	2.119834	-3.161878
H	0.667148	3.766480	-3.141103
C	0.039796	2.610976	2.069364
H	1.078184	3.004191	2.111683
H	0.120963	1.503002	2.072895
H	-0.473848	2.928948	2.997571
C	-3.947571	4.998014	0.019691
H	-4.012380	5.536467	0.987115
H	-4.783523	4.264367	-0.002100
H	-4.131188	5.727245	-0.795345
H	3.710903	2.127428	-2.033191
H	2.204489	3.908562	-1.423078
C	-1.053945	-2.747951	0.033783
C	0.011481	-2.979095	-0.841167
C	-2.310368	-3.221056	-0.687507
C	-1.960812	-2.950809	-2.168414
C	-2.182057	-4.791339	-0.649433
H	-3.276305	-2.834696	-0.310319
C	-0.574646	-3.630705	-2.092547
H	-2.652439	-3.455858	-2.874746
H	-1.890789	-1.877004	-2.423023
C	-0.987091	-5.070418	-1.619206
H	0.054537	-3.590615	-3.000439
H	-0.970467	-2.676009	1.126508
H	1.045247	-3.188492	-0.503943
C	-3.788251	0.308882	-1.096462
C	-5.149011	0.131739	-0.824210
C	-5.529341	-0.303064	0.456767
C	-4.562022	-0.532464	1.447675
C	-3.182976	-0.344755	1.182249

H	-3.471437	0.645392	-2.097019
H	-5.903389	0.329969	-1.600850
H	-6.593082	-0.456911	0.700208
H	-4.894312	-0.854323	2.443408
O	-2.219533	-0.458209	2.123556
C	-2.550071	-0.800218	3.496702
C	-1.469180	-0.181889	4.379860
H	-3.526822	-0.328284	3.748876
C	-2.650055	-2.320184	3.654725
H	-1.660551	-0.436684	5.442443
H	-0.470069	-0.562132	4.087206
H	-1.464152	0.921371	4.281624
H	-2.964045	-2.579365	4.687087
H	-3.387704	-2.759501	2.952956
H	-1.662671	-2.788092	3.464485
H	2.864007	-1.196741	-0.243548
C	3.971624	-0.825275	-2.068743
C	4.710140	-0.303096	0.359364
H	4.484518	-1.808215	-2.053283
H	3.070219	-0.904733	-2.708587
H	4.665653	-0.090125	-2.526681
C	6.062204	-0.443204	-0.017287
C	7.091685	-0.319926	0.934973
C	6.784075	-0.056615	2.279222
C	5.437808	0.077848	2.667066
C	4.411379	-0.043862	1.717539
H	6.327378	-0.652386	-1.064333
H	8.141502	-0.431613	0.619160
H	7.589904	0.039062	3.024586
H	5.183819	0.272016	3.721715
H	3.355139	0.040041	2.022888
H	-1.305201	-5.679663	-2.491131
H	-0.148448	-5.608618	-1.131272
H	-2.007818	-5.171579	0.378008
H	-3.122856	-5.253010	-1.016682