Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information to:

N-Heterocyclic Olefins as Initiators for the Polymerization of (Meth)Acrylic Monomers: A Combined Experimental and Theoretical Approach

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Contents

Experimental

Materials and Synthesis

N,*N*-Dimethylacrylamide (DMAA), methyl acrylate (MA), *tert*-butyl methacrylate (tBuMA), C_6H_6 and C_6D_6 were dried over CaH_2, distilled under nitrogen atmosphere, degassed and then stored under protective conditions (glove box, LabMaster, *MBraun*, Germany). Methyl methacrylate (MMA) was purified according to a procedure by McGrath.[i] All acrylic monomers were kept in brown bottles at -36°C. The THF and toluene used for polymerizations was taken from a solvent purification system (*MBraun*, Germany) and stored inside the glove box over molecular sieve. Sodium was employed to dry DME, which was distilled under nitrogen atmosphere, degassed and stored over molecular sieve in the glove box. Likewise, dry LiCl was stored under exclusion of humidity.

All NHOs were prepared according to published procedures [ii,iii] and their identity confirmed by ^{1}H and ^{13}C NMR (Scheme S1). Characterization of compounds **1**,[iv] **2**,[v] **3**,[vi] **4**,[vii] **5**[viii] and **6**[viii] is available from the cited sources. The NHOs were stored under nitrogen at -36°C.

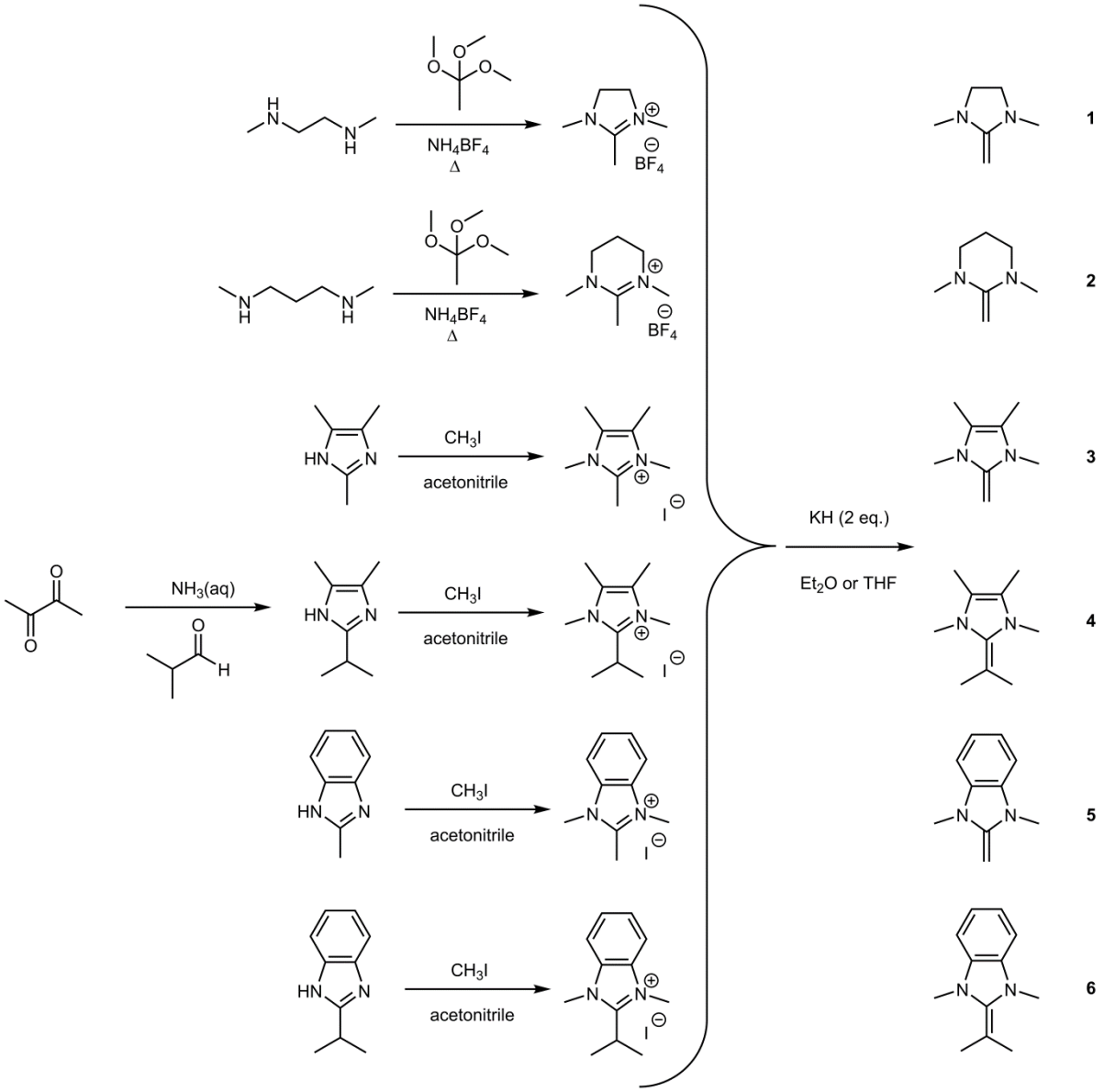

Figure S1. Schematic preparation of NHOs **1**-**6**.

General procedure for the organopolymerization of acrylic monomers via NHO-initiation

For a typical polymerization reaction, monomer (250-500 mg; 2.5-5.0 mmol) was dissolved in THF or toluene (2-7 mL) in a small vial inside the glove box. Likewise, the catalyst (0.025 mmol) was dissolved in the same solvent (0.5 mL), to generate a ratio of monomer to NHO of 1:200 and an initial monomer concentration of 0.25-3.33 mol/L. Both solutions were then pre-cooled in the box freezer (-36°C) for at least 1.5 h. The catalyst solution was then quickly added to the vigorously stirred monomer solution using a pipette. During polymerization, typically a pale yellow discolouration appeared. The

reaction was placed back in the freezer on top of a suitable flat-top stirrer. After the desired reaction time, the mixture was removed from the box and quenched by application of a small amount of MeOH (0.1 mL), upon which the discoloration disappeared. The polymer was then precipitated from diethyl ether and washed one to three times with the same solvent before it was subjected to pump evacuation until a constant weight was achieved. Molecular weights were determined by GPC (chloroform) and tacticity by ^{13}C NMR (MeOD for PDMAA, $CDCl_3$ for all others), while conversion was checked by ^{1}H NMR analysis of aliquots removed before precipitation ($CDCl_3$).

General procedure for the polymerization of acrylic monomers by NHO/LiCl

These polymerizations were assembled by addition of LiCl (0.125 mmol) to monomer/THF (2.5 mmol DMAA monomer in 2 mL solvent). This suspension was stirred for 30 minutes at room temperature to generate a clear solution, which was then pre-cooled alongside a separate, catalyst-containing solution (0.025 mmol in 0.5 mL THF). Addition of the catalyst solution to the monomer/LiCl solution (ratio NHO/LiCl/DMAA = 1:5:100) quickly (< two minutes) resulted in solidification of the whole mixture, which was then removed from the glove box and re-dissolved in MeOH. After precipitation from diethyl ether and vacuum drying, molecular weight was determined by GPC (chloroform). Tacticity and conversion were calculated from ^{13}C- and ^{1}H NMR experiments.

Characterization and analysis

For NMR spectra, a *Bruker* Avance III 400 spectrometer was employed. All chemical shifts are given in reference to deuterated solvent peaks (CD_3OD: δ = 4.87/49.00 ppm; C_6D_6: δ = 7.16/128.06 ppm, $CDCl_3$: δ = 7.26/77.16 ppm for $^{1}H/^{13}C$). IR measurements were recorded on a *Bruker* Alpha FT-IR-spectrometer (4000 – 400 cm^{-1}). GPC (chloroform, 35°C) was used to determine molecular weights (polystyrene calibration, 800 g/mol – $2*10^6$ g/mol). A chromatographic assembly consisting of a *PSS* SDV 5 µm 8*50mm precolumn, three *PSS* SDV 100 000 Å 5 µm 8*50mm columns in combination with an *Agilent* 1200 Series G1362A RI- detector, was employed. A flow rate of 1 ml/min and a sample concentration of 3 mg/mL were used for GPC analysis (injection volume: 100µL).

Computational details

DFT calculations were performed by using the Gaussian 09 package.[ix] Geometries were optimized at the generalized gradient approximation (GGA) level using the BP86[x]functional and the SVP basis set.[xi] The reported free energies were built through single point energy calculations on the BP86/SVP geometries using the hybrid meta GGA (HMGGA) M06[xii] functional and the triple-ζ TZVP basis set.[xiii] Solvent effects were included with the PCM model using toluene as solvent.[xiv] To these M06/TZVP electronic energies in solvent, zero point energy and thermal corrections were included from the gas-phase frequency calculations at the BP86/SVP level with a temperature of 298 K and a pressure of 1354 atm.[xv]

%V_{Bur} Calculations

The $\%V_{Bur}$ values have been calculated with the SambVca 2.0 package.[xvi] The radius of the sphere around the center atom was set to 3.5 Å, while for the atoms we adopted the Bondi radii scaled by 1.17, and a mesh of 0.1 Å was used to scan the sphere for buried voxels.

Parr electrophilicity index Calculation

$$\omega = \frac{\mu^2}{2\eta}$$

where μ is the chemical potential calculated as $\frac{(\varepsilon_{LUMO} + \varepsilon_{HOMO})}{2}$ and η is the molecular hardness given by $\frac{(\varepsilon_{LUMO} - \varepsilon_{HOMO})}{2}$.[xvii-xviii]

Data analysis

A multiple linear regression approach has been used to model the relationship between the dependent variable, $\Delta G_{\mathbf{A\text{-}B}}$ for each monomer considered with NHO **3**, and two independent variables, $\%V_{Bur}$ and ω of the monomer. The DFT calculated $\Delta G_{\mathbf{A\text{-}B}}$ is plotted versus the fitted $\Delta G_{\mathbf{A\text{-}B}}$ ($\%V_{Bur}$, ω) in Figure S9 for the four experimentally tested monomers and in Figure 5 in the manuscript for the complete set of monomers considered.

Results

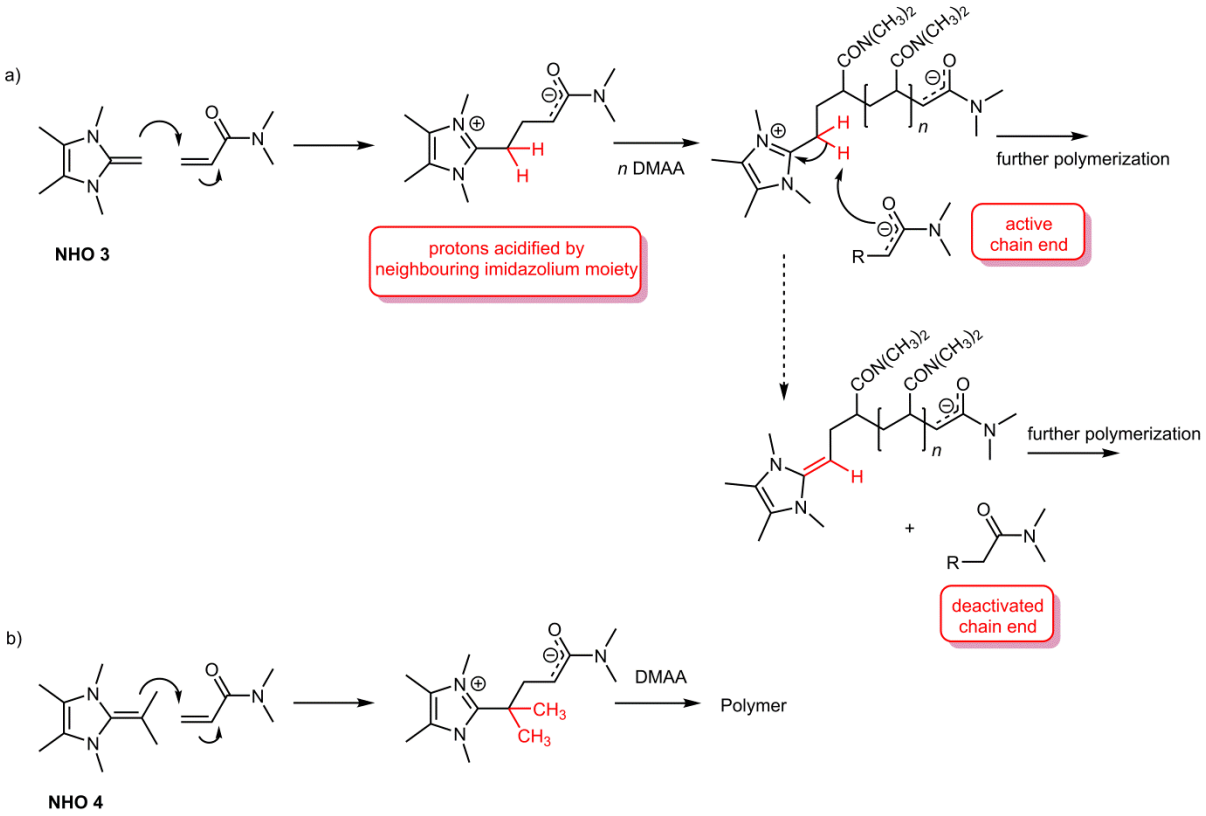

Figure S2. Addition of NHO **3** to the Michael acceptor system will result in the formation of a zwitterionic species; the enolate will enable the anionic propagation of the polymerization. However, the protons introduced by the NHO, now directly adjacent to an aromatic, positively charged imidazolium moiety, will be relatively acidic. Deprotonation could occur either inter- or intramolecularly by the strongly basic enolate chain ends, resulting in deactivation (intermolecular reaction shown here). Such a proposed side reaction is additionally favoured by the fact that both termini of the polymer form the counter ion pair in this polymerization. Application of NHO **4** eliminates this side reaction pathway.

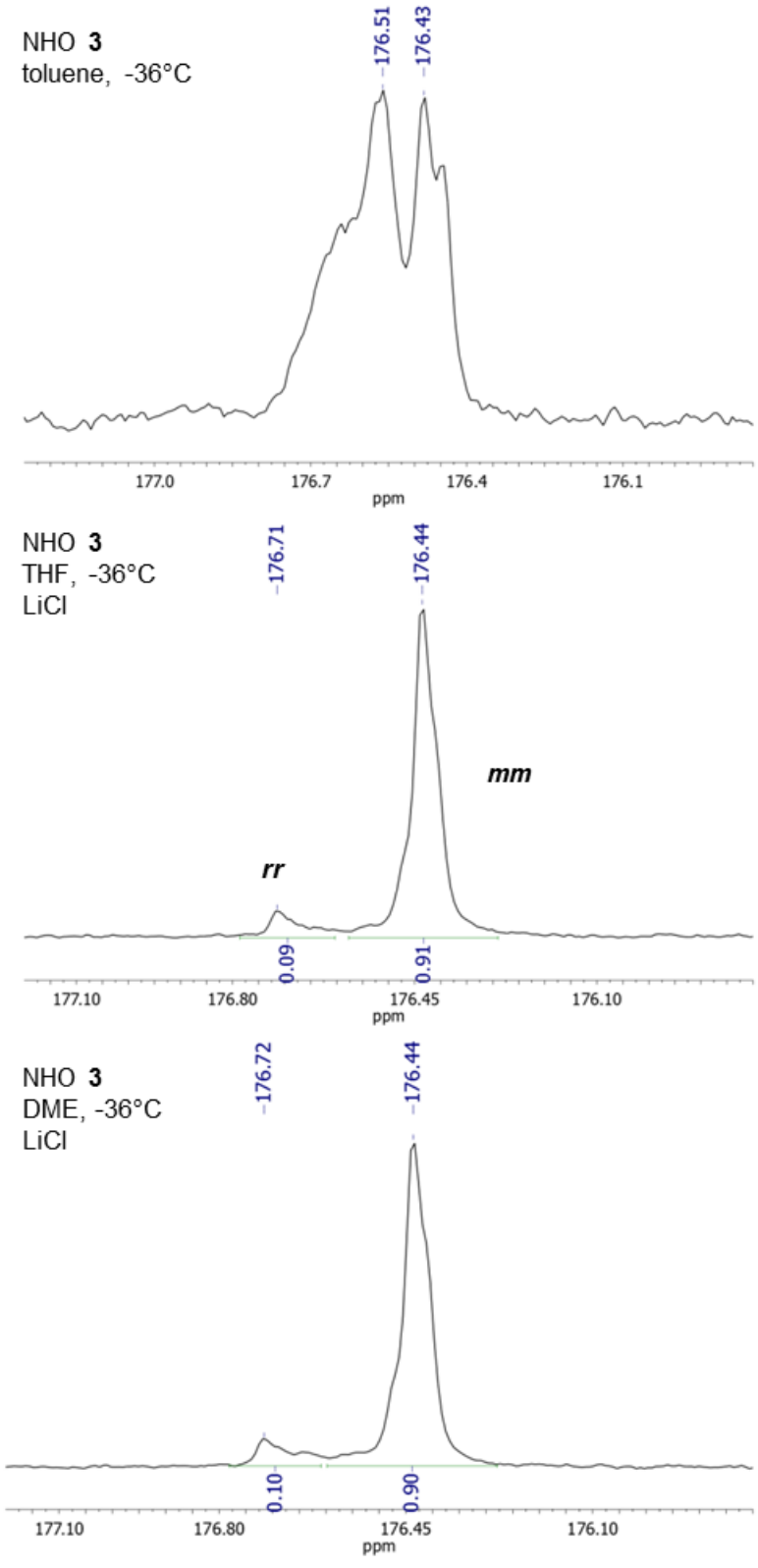

Figure S3. ^{13}C NMR analysis (100 MHz, 300K, CD_3OD) of the carbonyl area of PDMAA prepared by NHO **3** in the absence (top) and presence of LiCl. For more detailed reaction conditions and polymer properties, see Table 1, entry 4, and Table 2, entries 2 and 11.

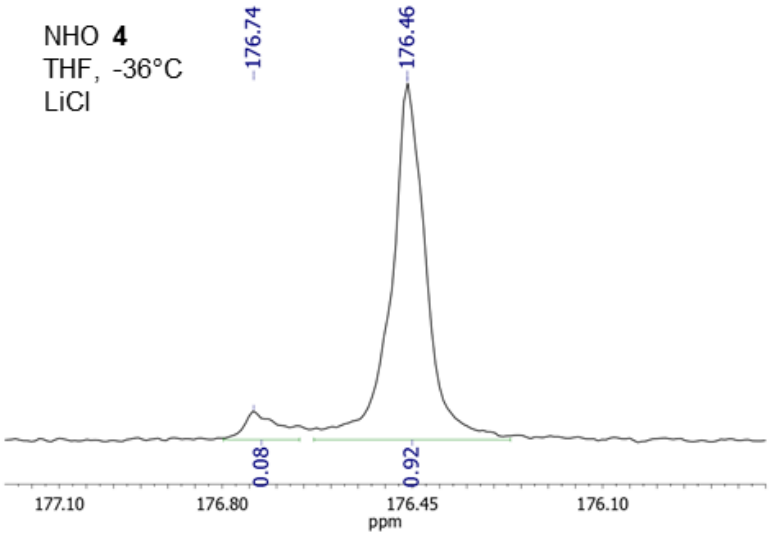

Figure S4. ^{13}C NMR analysis (100 MHz, 300K, CD_3OD) of the carbonyl area of PDMAA prepared by NHO **4** in the presence of LiCl. For more detailed reaction conditions and polymer properties, see Table 2, entry 6. The high degree of isotacticity is very similar to the results obtained from NHO **3** (Figure S3).

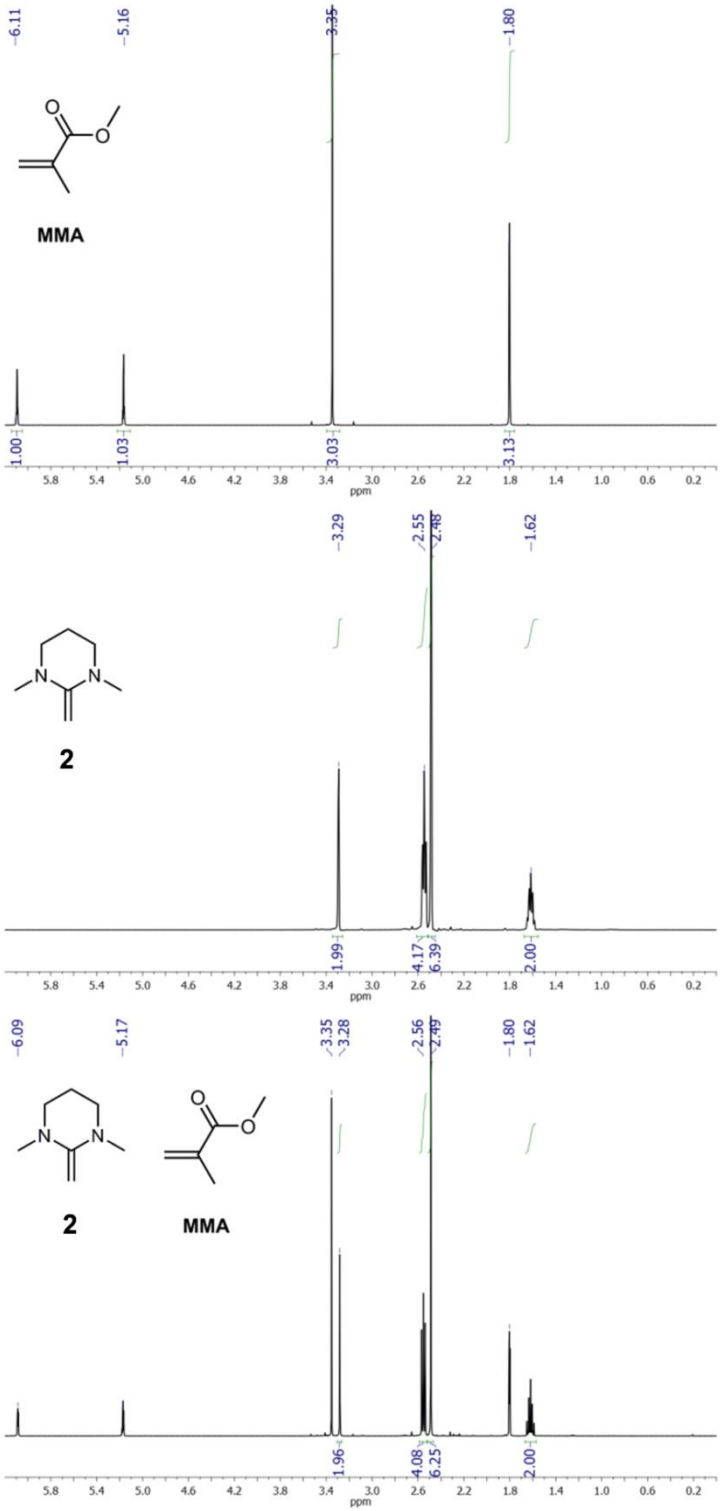

Figure S5. ^{1}H NMR analysis (400 MHz, 300K, C_6D_6) of MMA (top), NHO **2** (middle) and an equimolar mixture of both (bottom). Chemical shifts and integrals of the NHO, including the olefinic signals, remain virtually unchanged upon addition of MMA.

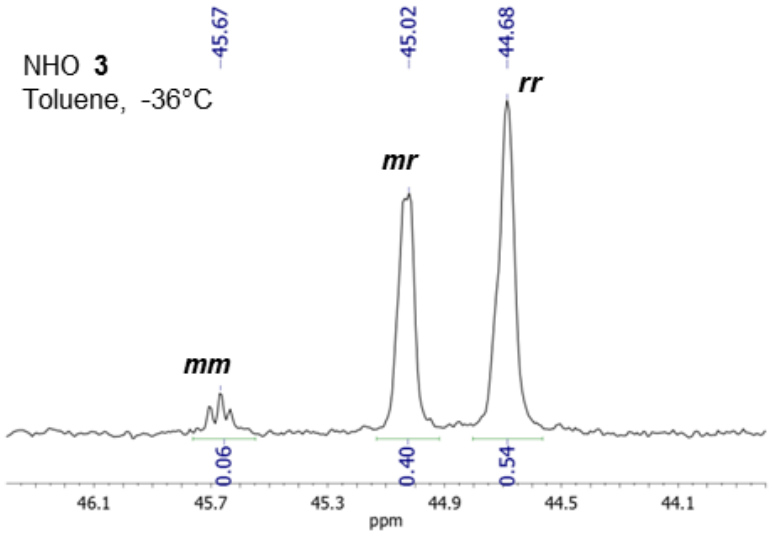

Figure S6. ^{13}C NMR analysis (100 MHz, 300K, $CDCl_3$) of the quaternary carbon area of PMMA prepared by NHO **3** in toluene without further additives. See Table 3, entry 4, for more details on reaction conditions.

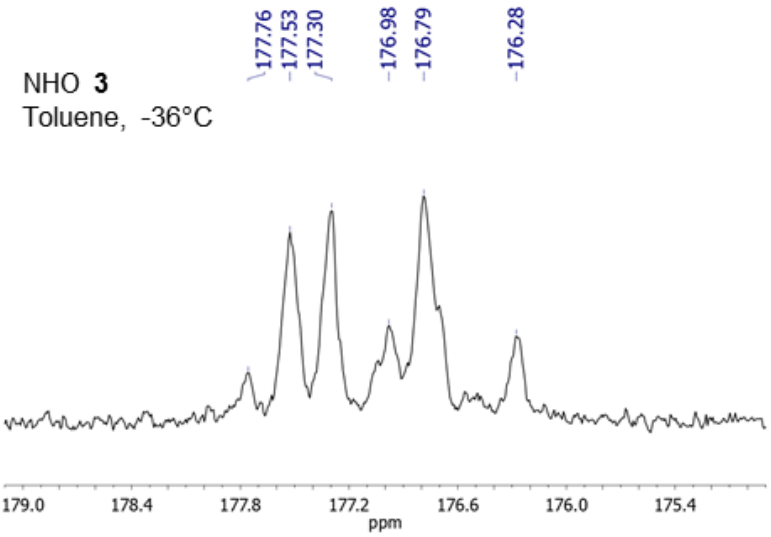

Figure S7. ^{13}C NMR analysis (100 MHz, 300K, $CDCl_3$) of the carbonyl carbon area of PtBuMA prepared by NHO **3** in toluene without further additives. See Table 3, entry 6, for more details on reaction conditions. The polymer is found to be largely atactic.[xix]

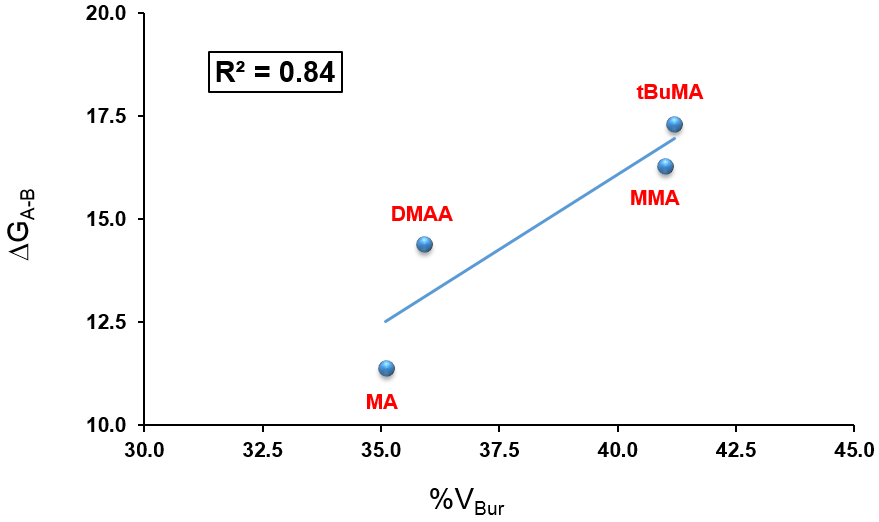

Figure S8. Fitting of ΔG_{A-B} using the $\%V_{Bur}$ of the four monomers experimentally tested.

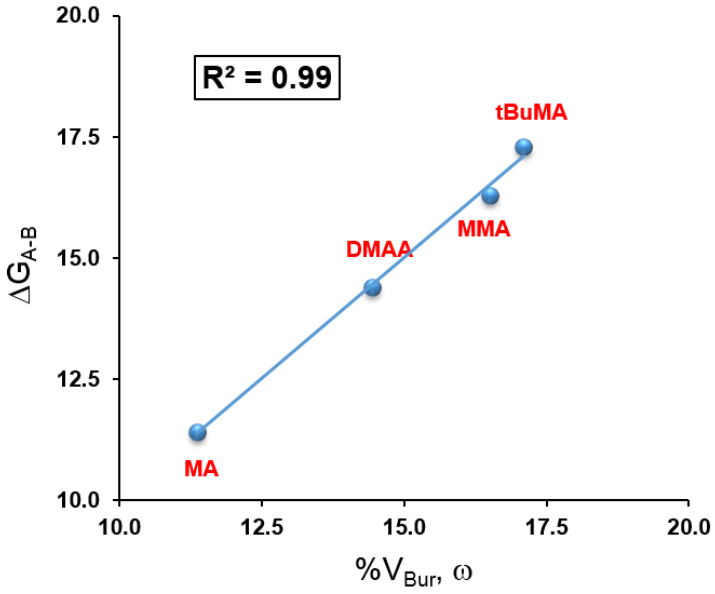

Figure S9. Fitting of ΔG_{A-B} using the $\%V_{Bur}$ and the Parr electrophilicity index, ω, of the four monomers experimentally tested.

Table S1. Percent of buried volume, $\%V_{Bur,}$ and Parr electrophilicity index for the eight monomers considered in this work.

Monomer	$\%V_{Bur}$	ω
MMA	41.0	4.33
MA	35.1	4.71
tBuMA	41.2	4.18
DMAA	35.9	3.88
DMMAA	44.4	2.91
MAM	40.8	3.56
EA	35.1	4.67
MBL	39.5	4.86

Cartesian coordinates

MMA

C	0.742932	-0.916640	0.000000
C	0.000000	0.388980	0.000000
C	2.244496	-0.783305	0.000000
O	0.548039	1.481413	0.000000
O	-1.353443	0.239467	0.000000
C	-2.103467	1.462025	0.000000
H	-3.168997	1.167515	0.000000
H	-1.871448	2.070900	0.898316
H	-1.871448	2.070900	-0.898316
H	2.736660	-1.775160	0.000000
H	2.589586	-0.209831	-0.885892
H	2.589586	-0.209831	0.885892
C	0.085477	-2.099096	0.000000
H	0.636389	-3.054119	0.000000
H	-1.013723	-2.139191	0.000000

1

C	-0.000232	0.688454	-0.000530
N	1.110365	-0.149916	-0.207852
C	0.752370	-1.517729	0.150214
C	-0.751362	-1.518287	-0.150956
N	-1.109983	-0.150640	0.206827
C	-2.456101	0.324962	-0.010011
C	2.455913	0.325960	0.012267
H	-1.316371	-2.259040	0.454155
H	-0.937287	-1.740353	-1.234852
H	1.317938	-2.258321	-0.454570
H	0.938410	-1.739268	1.234216
H	-3.177896	-0.450218	0.319155
H	-2.643027	1.233485	0.599138
H	-2.672174	0.577826	-1.079340
H	3.178752	-0.447088	-0.319709
H	2.642573	1.237232	-0.592738
H	2.670820	0.574177	1.082934
C	-0.000922	2.053135	-0.000893
H	0.933851	2.618715	-0.096676
H	-0.936259	2.617776	0.094926

(1)A-B(MMA)

C	1.476582	1.105165	-0.623236
C	1.604858	-0.331389	-0.586565
C	0.434366	1.631859	-1.425229
C	2.383977	1.984782	0.207440
H	2.254473	1.850289	1.307938
H	3.457573	1.772833	0.010034
H	2.209741	3.058500	-0.017699
O	2.679495	-0.750832	0.192345
O	0.885366	-1.169896	-1.165801
C	2.910609	-2.154515	0.210647
H	3.859451	-2.307751	0.761404
H	2.092437	-2.704439	0.727271

H	2.994425	-2.572038	-0.815504
H	0.511368	2.696778	-1.709546
H	0.090366	0.980124	-2.244181
C	-1.360931	1.825791	-0.563770
H	-2.006823	2.052634	-1.426046
H	-1.197655	2.699187	0.085667
C	-1.466048	-1.092347	1.689754
C	-1.846389	-1.690274	0.329650
H	-2.330145	-1.066681	2.400117
H	-0.630040	-1.631927	2.180647
H	-2.662851	-2.438866	0.388969
H	-0.947982	-2.133204	-0.166435
N	-2.264525	-0.499173	-0.422320
N	-1.065309	0.265302	1.312403
C	-1.623332	0.605510	0.103937
C	-0.627491	1.199670	2.325882
H	-0.168352	2.088568	1.856784
H	-1.461934	1.529488	2.992054
H	0.151111	0.719181	2.952268
C	-2.502030	-0.661544	-1.846420
H	-2.887103	0.280278	-2.283208
H	-1.569518	-0.962547	-2.376567
H	-3.273635	-1.443719	-1.999441

(1)B(MMA)

C	-1.428664	0.658189	0.291552
N	-2.297739	-0.150015	-0.384697
C	-2.112456	-1.531757	0.095621
C	-1.490165	-1.328185	1.486412
N	-0.939923	0.028790	1.381145
C	-2.576426	0.017429	-1.804686
C	-0.116597	0.566251	2.444802
C	-0.965331	1.981360	-0.149239
C	0.408782	1.886571	-1.028441
C	1.521683	1.102651	-0.443913
C	2.626755	1.778924	0.326200
C	1.436333	-0.292231	-0.633485
O	0.522239	-0.913114	-1.252667
O	2.482039	-1.032381	-0.045163
C	2.515724	-2.407246	-0.385678
H	2.330944	2.145377	1.347420
H	3.473881	1.082610	0.482900
H	3.025256	2.675939	-0.204400
H	3.435225	-2.822847	0.074516
H	1.631944	-2.966119	-0.000272
H	2.546372	-2.568513	-1.486449
H	0.691591	2.949682	-1.188582
H	0.090273	1.463786	-2.004234
H	-1.746800	2.478986	-0.757315
H	-0.768129	2.627002	0.728654
H	-2.236036	-1.372344	2.315575
H	-0.683254	-2.057962	1.702590
H	-3.071581	-2.087296	0.111935
H	-1.372430	-2.022644	-0.577852
H	0.217940	1.588569	2.199029
H	-0.679299	0.584958	3.407893
H	0.792392	-0.058150	2.568141
H	-2.761255	1.083477	-2.038637
H	-1.714453	-0.350872	-2.404443
H	-3.490999	-0.552829	-2.063836

(1)B-Bspiro$_O$(MMA)

C	1.818465	-1.043569	-0.167217
C	1.416105	0.220743	-0.582762
C	0.779074	-2.100393	-0.382721
C	3.112458	-1.349937	0.539300
H	3.768572	-0.457453	0.546893
H	2.980516	-1.664210	1.607402
H	3.682358	-2.178183	0.053388
O	2.288166	1.291162	-0.290265
O	0.282710	0.480092	-1.122819
C	2.111560	2.456713	-1.077681
H	2.714208	3.260186	-0.607587
H	2.470432	2.309583	-2.124741
H	1.045097	2.765870	-1.128792
H	0.431985	-2.126960	-1.440757
H	1.174423	-3.111802	-0.144764
C	-0.520327	-1.922525	0.505419
H	-0.249741	-2.101252	1.565341
H	-1.263129	-2.703370	0.234001
C	-2.612227	1.070730	-0.322017
C	-1.957723	1.510881	1.004894
H	-3.710636	1.227729	-0.343279
H	-2.146641	1.595851	-1.184613
H	-2.695152	1.693157	1.819239
H	-1.344086	2.428272	0.879784
N	-1.100466	0.370338	1.348292
N	-2.283917	-0.361423	-0.400023
C	-1.214164	-0.603854	0.415712
C	-2.421094	-1.011455	-1.693931
H	-1.667882	-0.612813	-2.409140
H	-2.272691	-2.104393	-1.592484
H	-3.445896	-0.840073	-2.080434
C	-0.030888	0.543509	2.313892
H	0.485178	-0.417079	2.490743
H	0.729490	1.262487	1.935581

H	-0.450166	0.916970	3.273690

(1)Bspiro$_O$(MMA)

C	0.871914	-0.500104	-0.182537
N	2.059122	-0.116507	-0.893322
C	3.024480	0.508309	0.014845
C	2.379997	0.337535	1.400305
N	1.349977	-0.676304	1.167858
C	1.971307	0.436862	-2.228642
C	0.414716	-0.836219	2.266245
C	0.180088	-1.722199	-0.810010
C	-1.264642	-1.987463	-0.356034
C	-2.073750	-0.721005	-0.222355
C	-3.570884	-0.837638	-0.105868
C	-1.434118	0.482316	-0.220104
O	-0.088094	0.685057	-0.265666
O	-2.137638	1.654108	-0.233659
C	-1.567533	2.778958	0.433404
H	-4.043078	0.147107	0.072305
H	-4.026880	-1.269718	-1.027485
H	-3.860348	-1.517129	0.729638
H	-2.299177	3.602529	0.322536
H	-1.411013	2.579306	1.518530
H	-0.599640	3.084165	-0.015215
H	-1.285151	-2.572003	0.596848
H	-1.746295	-2.664139	-1.100310
H	0.171403	-1.546961	-1.905386
H	0.840122	-2.593082	-0.626713
H	3.095001	-0.007978	2.177679
H	1.936385	1.302801	1.756158
H	4.017130	0.005836	-0.057665
H	3.184206	1.586919	-0.222347
H	-0.170697	0.091883	2.489114
H	-0.298284	-1.656857	2.067194
H	0.982735	-1.104370	3.182286
H	1.259051	-0.144031	-2.847800
H	1.643399	1.506042	-2.248210
H	2.963857	0.369932	-2.723793

(1)Bspiro$_C$(MMA)

N	-0.476169	-1.217384	0.609192
C	-0.825295	0.181742	0.260115
N	-1.684478	0.054866	-0.910041
C	-1.756335	-1.356041	-1.311980
C	-1.451076	-2.102574	-0.015019
C	0.496982	1.124058	0.088461
C	0.389968	2.062134	-1.117651
C	-1.259797	1.128490	1.438883
C	0.142853	1.790758	1.448029
C	-2.905909	0.828244	-1.033212
C	-0.137839	-1.558703	1.979202
C	1.788441	0.323795	0.083946
O	2.479714	0.072422	1.060237
O	2.097189	-0.123401	-1.164557
C	3.258053	-0.961701	-1.247399
H	3.113987	-1.891453	-0.658917
H	3.387422	-1.202723	-2.318815
H	4.155987	-0.440251	-0.856759
H	-2.713044	1.909119	-0.879208
H	-3.295669	0.729366	-2.068021
H	-3.730778	0.529744	-0.332853
H	0.660091	-0.897117	2.366912
H	-1.012096	-1.531259	2.683311
H	0.264987	-2.593504	2.001749
H	1.237878	2.779845	-1.133262
H	0.389376	1.491403	-2.065114
H	-0.547067	2.653958	-1.073738
H	0.803710	1.436507	2.262722
H	0.155586	2.899940	1.442144
H	-1.583105	0.618122	2.368136
H	-2.063500	1.831696	1.148805
H	-1.019673	-3.115146	-0.175327
H	-2.383572	-2.227786	0.603159
H	-2.756455	-1.601414	-1.723996
H	-0.995043	-1.594798	-2.090675

(1)B-C(MMA)

C	2.267451	1.234895	-0.097741
C	1.502341	2.318991	0.363276
C	1.884611	3.103175	1.602841
C	0.320339	2.699463	-0.384542
O	-0.253143	3.869133	0.112970
C	-1.374814	4.353717	-0.611384
O	-0.190898	2.140233	-1.374367
C	1.735195	-0.717933	0.767462
C	2.263809	-1.529084	-0.302452
O	3.605613	-1.837355	-0.159473
C	4.185786	-2.556806	-1.244946
O	1.646707	-1.898607	-1.327502
C	2.416148	-0.738637	2.122156
H	2.158597	0.169161	2.709792
H	3.517986	-0.774464	2.014683
H	2.126371	-1.622875	2.741838
C	0.237090	-0.533719	0.748852
H	5.249532	-2.711655	-0.979400
H	4.112235	-1.991301	-2.198421
H	3.687955	-3.538685	-1.398589

H	2.065207	0.881992	-1.121820
H	3.309190	1.133507	0.249004
H	1.972034	4.191741	1.393002
H	2.859813	2.753006	2.000715
H	1.138376	3.013225	2.425496
H	-2.228125	3.638960	-0.582946
H	-1.673020	5.304491	-0.127194
H	-1.131327	4.533926	-1.680845
H	-0.044000	0.140205	-0.083236
H	-0.091068	-0.015478	1.674853
C	-1.974777	-1.515379	0.137726
N	-3.066523	-1.413301	0.944219
C	-4.247574	-1.027138	0.158372
C	-3.616138	-0.511536	-1.150185
N	-2.264158	-1.089236	-1.107005
H	-3.535869	0.599187	-1.178283
H	-4.843476	-0.256443	0.689425
C	-3.206768	-1.944860	2.285160
H	-3.697379	-2.945827	2.289164
H	-2.215003	-2.033315	2.765109
H	-3.822265	-1.252916	2.896283
C	-1.306707	-0.790133	-2.173223
H	-0.348962	-1.323239	-1.998443
H	-1.743276	-1.105456	-3.143015
H	-1.080892	0.301771	-2.181504
H	-4.160012	-0.841462	-2.058445
H	-4.903587	-1.914283	-0.008083
C	-0.604788	-1.860534	0.572388
H	-0.614497	-2.475329	1.493000
H	-0.103216	-2.434802	-0.238223

(1)C(MMA)

C	-3.712617	-1.372106	0.634328
C	-3.538576	-1.362522	-0.895852
N	-2.127359	-1.745731	-1.065765
C	-1.458143	-1.465320	0.083129
N	-2.325573	-1.365521	1.112443
C	-1.546960	-1.629065	-2.397750
C	0.027912	-1.604265	0.221080
C	0.740076	-0.592210	1.157418
C	1.968394	0.138612	0.556684
C	2.611211	0.988211	1.677141
C	-2.041429	-1.296608	2.530947
C	2.992070	-0.879627	0.057040
O	2.844370	-2.095171	0.004166
O	4.135951	-0.276116	-0.374625
C	5.145205	-1.153464	-0.891885
C	1.520251	1.078923	-0.645933
C	0.550033	2.179059	-0.305211
C	-0.814256	1.899312	-0.379988
O	-1.378459	0.793035	-0.709366
C	1.071174	3.567988	-0.008334
O	-1.660631	2.986955	-0.062633
C	-3.032494	2.805192	-0.324761
H	1.857129	1.695862	2.076431
H	3.468803	1.572478	1.291148
H	2.973053	0.352314	2.513792
H	5.983525	-0.504574	-1.206046
H	4.763266	-1.734852	-1.756499
H	5.484082	-1.871856	-0.116736
H	1.086660	0.419578	-1.432942
H	2.455372	1.507384	-1.069460
H	0.274226	4.324816	-0.148607
H	1.914976	3.835168	-0.688552
H	1.465467	3.712516	1.028318
H	-3.478371	1.972788	0.270325
H	-3.536462	3.752372	-0.041432
H	-3.245780	2.593266	-1.399297
H	1.061384	-1.107126	2.088424
H	0.040453	0.218594	1.443382
H	-2.729004	-1.979264	3.075854
H	-1.005092	-1.614160	2.738519
H	-2.183391	-0.266785	2.926598
H	-0.597681	-2.194284	-2.458636
H	-2.251950	-2.076417	-3.126360
H	-1.363026	-0.559545	-2.635048
H	0.247647	-2.649002	0.537469
H	0.451436	-1.524760	-0.794467
H	-4.263134	-0.482172	1.005120
H	-4.234755	-2.283278	1.009128
H	-3.677627	-0.339791	-1.307202
H	-4.211649	-2.072794	-1.418623

(1)C-Cspiro$_C$(MMA)

C	-0.816723	-1.189068	0.706705
N	-1.897120	-1.143472	1.579888
C	-3.133538	-1.225364	0.790794
C	-2.671547	-1.977509	-0.469969
N	-1.221751	-1.772693	-0.452982
C	-1.908731	-0.320772	2.771745
C	-0.407869	-2.295429	-1.532703
C	0.592357	-1.364981	1.235019
C	1.427532	-0.123433	1.587710
C	2.003478	0.715734	0.405796
C	2.688685	1.968705	0.994283
C	0.875334	1.113581	-0.614768

C	-0.517860	1.356216	-0.060311
C	-0.692122	2.500283	0.927896
C	3.019963	-0.170539	-0.337093
O	2.746057	-1.192296	-0.956553
C	-1.563191	1.144508	-1.024943
O	-1.518045	0.447567	-2.055320
O	-2.775311	1.795023	-0.694056
C	-3.828292	1.644708	-1.634404
O	4.299263	0.272620	-0.235857
C	5.289934	-0.523689	-0.907402
H	6.254775	-0.009139	-0.745698
H	5.065895	-0.598877	-1.990959
H	5.323318	-1.550203	-0.488099
H	0.789312	0.331749	-1.393563
H	1.248876	2.025181	-1.151146
H	-4.374318	0.678835	-1.499832
H	-4.539819	2.476024	-1.456331
H	-3.450866	1.670444	-2.677563
H	0.827400	0.566457	2.213500
H	2.276530	-0.457597	2.225089
H	-0.962586	-0.442050	3.334639
H	-2.045515	0.758996	2.534878
H	-2.737088	-0.651379	3.431645
H	0.646325	-1.982548	-1.414845
H	-0.458239	-3.409924	-1.559606
H	-0.774614	-1.881545	-2.492619
H	0.484576	-1.986860	2.153153
H	1.161039	-1.984472	0.516041
H	3.168822	2.568892	0.196413
H	1.940772	2.610096	1.498203
H	3.472574	1.700693	1.731471
H	-1.760699	2.677901	1.153908
H	-0.168505	2.342412	1.896278
H	-0.287821	3.462571	0.519474
H	-3.924789	-1.761479	1.355285
H	-3.497512	-0.201660	0.544453
H	-2.894918	-3.070925	-0.416250
H	-3.110994	-1.569447	-1.402117

(1)Cspiro$_C$(MMA)

C	-0.598406	-0.602608	-0.700870
C	-0.853236	0.784625	0.106301
C	0.505278	1.532418	0.313778
C	1.562006	1.272530	-0.765290
C	2.026479	-0.221899	-0.769937
C	0.826584	-1.163633	-0.440883
N	-1.874819	1.608473	-0.570256
C	-3.055793	1.788569	0.275244
C	-2.544156	1.457551	1.675940
N	-1.528569	0.453667	1.400351
C	-0.755472	0.043567	2.557652
C	-1.512785	2.721990	-1.418224
C	3.056184	-0.333913	0.377432
O	4.309167	0.006285	-0.028337
C	5.315576	0.001512	0.997557
C	-1.594438	-1.631519	-0.119822
O	-2.856241	-1.449710	-0.602130
C	-3.840421	-2.354882	-0.084886
O	2.806944	-0.627802	1.535528
O	-1.309201	-2.549221	0.631545
C	2.683237	-0.567381	-2.123964
C	-0.874475	-0.456808	-2.215601
H	6.261629	0.280214	0.498272
H	5.402569	-1.002557	1.460496
H	5.070116	0.731240	1.796415
H	0.893507	-1.465764	0.620013
H	0.938356	-2.108635	-1.013778
H	-3.969169	-2.213624	1.008536
H	-4.782602	-2.120642	-0.614517
H	-3.546206	-3.409281	-0.264336
H	1.175308	1.521740	-1.776128
H	2.441458	1.934830	-0.614336
H	-0.676436	2.455545	-2.093606
H	-2.370723	2.984029	-2.074705
H	-1.217244	3.660647	-0.874744
H	0.026582	-0.688523	2.285258
H	-0.261183	0.896111	3.095097
H	-1.431014	-0.455650	3.284746
H	0.315424	2.620023	0.422092
H	0.936107	1.202675	1.280819
H	3.108988	-1.592182	-2.114047
H	1.928669	-0.524227	-2.934691
H	3.501179	0.137545	-2.370817
H	-0.756038	-1.439532	-2.719540
H	-1.901660	-0.091909	-2.391446
H	-0.169450	0.245727	-2.701298
H	-3.883324	1.101758	-0.020165
H	-3.437474	2.830382	0.207847
H	-3.330401	1.045727	2.346842
H	-2.125578	2.372207	2.181645

(1)C-D(MMA)

N	-1.970540	-2.224429	-0.556681
C	-3.366828	-2.606409	-0.769070
C	-4.136248	-1.326416	-0.385758
N	-3.138562	-0.567394	0.369110

C	-1.881727	-1.092248	0.211598
C	-3.490940	0.648171	1.084837
C	-0.694747	-0.421102	0.692230
C	0.483906	-1.162904	1.358242
C	1.854311	-0.446569	1.166136
C	1.695120	1.120866	1.003208
C	0.965306	1.647588	-0.220698
C	1.735835	1.733132	-1.522903
C	-0.896833	-3.084530	-1.011546
C	2.749006	-0.719322	2.399297
C	2.545987	-1.006767	-0.081336
O	3.829565	-0.577134	-0.185823
C	4.544884	-1.006143	-1.353610
O	2.046827	-1.755894	-0.913313
C	-0.138790	2.529584	0.025319
O	-0.497080	3.311886	-1.076149
C	-1.637358	4.139214	-0.899414
O	-0.826966	2.593633	1.073672
H	3.756622	-0.279584	2.267707
H	2.288129	-0.266510	3.301772
H	2.868083	-1.808277	2.585660
H	5.584152	-0.652943	-1.221986
H	4.517067	-2.110134	-1.454365
H	4.103588	-0.557946	-2.268098
H	1.168510	1.479685	1.913747
H	2.728472	1.541832	1.042763
H	1.144369	2.258336	-2.296014
H	2.701419	2.285204	-1.406015
H	1.993506	0.732386	-1.936227
H	-2.586595	3.554611	-0.907140
H	-1.647330	4.846543	-1.752725
H	-1.597622	4.697069	0.060136
H	0.281131	-1.220570	2.449278
H	0.579093	-2.208538	1.007704
H	-1.100947	-3.396379	-2.058834
H	-0.812722	-4.009798	-0.393834
H	0.074138	-2.551263	-0.995054
H	-3.751586	0.443720	2.148349
H	-4.378448	1.101102	0.596809
H	-2.663378	1.394301	1.057656
H	-1.013870	0.412616	1.348593
H	-0.187491	0.275903	-0.149394
H	-4.475372	-0.751483	-1.280978
H	-5.032883	-1.539113	0.234255
H	-3.644431	-3.474763	-0.122903
H	-3.535964	-2.910040	-1.824151

(1)D(MMA)

C	5.190317	-1.069250	0.300790
N	4.112226	-1.166684	-0.675124
C	3.179983	-0.131599	-0.436700
N	3.823438	0.804034	0.401247
C	5.234889	0.439833	0.530943
C	3.688877	-2.473702	-1.123032
C	1.906745	-0.136438	-0.954465
C	0.792754	0.869042	-0.839520
C	-0.317646	0.539798	0.250675
C	0.294586	0.609372	1.660733
C	3.515065	2.221210	0.399571
C	-0.910806	-0.865996	-0.032742
C	-2.167858	-1.251774	0.791910
C	-2.081537	-2.700912	1.325948
C	-1.362746	1.653978	0.112436
O	-1.422479	2.665442	0.791684
C	-3.442387	-1.150842	-0.045439
O	-3.595574	-1.616280	-1.160112
O	-4.445104	-0.538056	0.648428
C	-5.717491	-0.501032	-0.016718
O	-2.205770	1.428447	-0.937069
C	-3.169711	2.461737	-1.190274
H	-2.289783	-0.570661	1.660121
H	-3.733386	2.139110	-2.084825
H	-2.668499	3.433543	-1.377176
H	-3.851989	2.583174	-0.324189
H	-0.099060	-1.594412	0.176132
H	-1.150919	-0.973037	-1.111086
H	-6.084691	-1.526568	-0.228640
H	-6.408554	0.020059	0.671235
H	-5.646991	0.044446	-0.980090
H	0.262946	0.929712	-1.815531
H	1.160613	1.892921	-0.628658
H	4.190876	2.729016	1.117155
H	3.650453	2.701009	-0.601562
H	2.479182	2.412574	0.740375
H	3.179204	-2.405270	-2.106267
H	4.582685	-3.115495	-1.257748
H	2.991663	-2.982585	-0.409653
H	1.662255	-1.028259	-1.550270
H	-0.423609	0.274070	2.437703
H	1.196261	-0.033769	1.711372
H	0.576018	1.650523	1.914255
H	-2.985563	-2.977025	1.907676
H	-1.980944	-3.417062	0.484108
H	-1.198849	-2.814710	1.988293
H	5.632161	0.719763	1.529650

H	5.867789	0.938950	-0.248072
H	6.141725	-1.478215	-0.100024
H	4.952589	-1.610222	1.254722

3

C	-0.686895	0.968122	0.000008
N	-1.108467	-0.379769	-0.000479
C	-0.000002	-1.232679	-0.000302
N	1.108465	-0.379776	-0.000314
C	0.686901	0.968120	0.000069
C	-2.457502	-0.885303	0.000312
C	-0.000008	-2.606918	0.000037
C	2.457498	-0.885316	0.000206
C	-1.652413	2.107763	-0.000039
C	1.652425	2.107754	0.000145
H	-3.177530	-0.046247	-0.000591
H	-2.651040	-1.517420	-0.897241
H	-2.650930	-1.515532	0.899249
H	3.177529	-0.046262	-0.000517
H	2.650997	-1.515773	0.898964
H	2.650958	-1.517206	-0.897527
H	0.941634	-3.168473	0.000194
H	-0.941654	-3.168465	0.000060
H	-1.107068	3.071206	0.000338
H	-2.314541	2.105319	-0.895571
H	-2.315094	2.104953	0.895077
H	1.107084	3.071200	0.000425
H	2.314972	2.104947	0.895361
H	2.314686	2.105303	-0.895288

(3)A-B(MMA)

C	-1.133599	-0.929069	0.873517
N	-1.380252	0.386923	1.205582
C	-2.012828	1.040417	0.137364
C	-2.170280	0.116458	-0.873340
N	-1.617007	-1.090861	-0.410861
C	-0.799042	1.044746	2.366858
C	-1.520818	-2.333585	-1.152155
C	-0.354287	-1.866934	1.598188
C	1.674666	-1.578312	1.313897
C	2.109425	-1.002318	0.100439
C	2.352186	-1.832847	-1.137746
C	2.212753	0.437143	0.057623
O	1.983058	1.244622	0.979193
O	2.638469	0.906563	-1.182502
C	2.834847	2.313102	-1.261443
H	1.521334	-1.776074	-1.886797
H	3.260881	-1.503732	-1.683848
H	2.481260	-2.905541	-0.878009
H	3.191866	2.521375	-2.289298
H	1.893681	2.874009	-1.069813
H	3.586118	2.667199	-0.522369
H	1.901023	-2.646135	1.480361
H	1.795883	-0.945114	2.207329
H	-0.375646	-1.750088	2.693090
H	-0.486640	-2.913110	1.280934
C	-2.792187	0.258080	-2.224021
C	-2.389161	2.485090	0.193631
H	-0.470306	-2.544088	-1.451517
H	-1.889603	-3.181257	-0.537575
H	-2.142183	-2.270255	-2.063761
H	-0.848930	0.368571	3.242809
H	0.266689	1.299928	2.147004
H	-1.377110	1.957102	2.604478
H	-1.499406	3.138250	0.324262
H	-2.890278	2.788459	-0.745248
H	-3.089250	2.704719	1.029380
H	-3.664609	-0.418099	-2.364860
H	-3.155655	1.293486	-2.366750
H	-2.070572	0.046659	-3.043245

(3)B(MMA)

C	1.690116	0.830563	0.856611
N	0.632566	0.031952	1.307994
C	0.632008	-1.148022	0.630179
N	1.711674	-1.131742	-0.203699
C	2.361734	0.099589	-0.102699
C	-0.386274	0.503838	2.242544
C	-0.388156	-2.217368	0.739279
C	-1.641052	-2.022470	-0.235737
C	-2.271468	-0.670321	-0.169406
C	-3.512188	-0.438390	0.652516
C	1.846258	-2.034022	-1.340125
C	-1.566188	0.337396	-0.842537
O	-0.509416	0.197881	-1.527382
O	-2.086238	1.651063	-0.646301
C	-1.625234	2.629260	-1.561319
H	-3.356334	-0.484610	1.766924
H	-3.934366	0.564238	0.442697
H	-4.311472	-1.188478	0.439721
H	-1.807305	3.624538	-1.104560
H	-0.544254	2.497162	-1.782962
H	-2.176449	2.583208	-2.531889
H	-2.357865	-2.826935	0.041507
H	-1.271704	-2.245793	-1.261341
H	0.098069	-3.199636	0.550799
H	-0.758475	-2.250258	1.784607

C	1.927757	2.208388	1.380043
C	3.531502	0.467601	-0.954720
H	-1.079999	-0.318447	2.484510
H	0.096205	0.870327	3.172784
H	-0.980257	1.311503	1.768579
H	1.561842	-3.061357	-1.043505
H	1.167799	-1.677823	-2.143749
H	2.895277	-2.046372	-1.688296
H	3.928192	1.455150	-0.652199
H	4.363250	-0.264253	-0.869449
H	3.246889	0.537728	-2.026667
H	2.805177	2.662113	0.881818
H	1.056115	2.869590	1.187971
H	2.122322	2.219129	2.474314

(3)B-Bspiro$_O$(MMA)

C	0.396847	-0.256419	-0.685633
N	1.505963	0.543317	-1.063796
C	2.570302	0.334139	-0.144438
C	2.236909	-0.736415	0.634370
N	0.962371	-1.203323	0.206464
C	1.332179	1.798857	-1.772370
C	0.148840	-2.056159	1.058124
C	-0.495455	-0.742070	-1.832554
C	-1.884013	-1.281656	-1.449573
C	-2.593498	-0.432519	-0.425507
C	-4.064390	-0.672397	-0.205586
C	-1.891322	0.518607	0.264691
O	-0.575201	0.772063	0.186107
O	-2.556993	1.351783	1.133635
C	-1.782868	2.077316	2.082171
H	-4.457171	-0.050661	0.621332
H	-4.668839	-0.443426	-1.115838
H	-4.274816	-1.740699	0.040688
H	-2.510320	2.646909	2.693189
H	-1.195413	1.405850	2.748183
H	-1.076510	2.784259	1.597750
H	-1.811183	-2.349070	-1.115789
H	-2.493381	-1.339572	-2.383137
H	-0.641116	0.127912	-2.504734
H	0.085472	-1.495929	-2.404047
C	3.018438	-1.449051	1.688889
C	3.828208	1.136898	-0.201632
H	-0.204408	-1.528955	1.973907
H	-0.739491	-2.407388	0.506177
H	0.732445	-2.946911	1.366105
H	0.605653	1.674630	-2.598150
H	0.963223	2.615737	-1.112326
H	2.294043	2.107522	-2.227102
H	2.494666	-1.465716	2.670341
H	3.228216	-2.508161	1.415211
H	3.994352	-0.950468	1.846374
H	4.336049	1.053601	-1.189561
H	3.652737	2.220074	-0.017159
H	4.543945	0.784950	0.566246

(3)Bspiro$_O$(MMA)

N	-1.489079	-0.672845	-0.996618
C	-0.370214	0.160994	-0.678138
N	-0.962918	1.215707	0.092554
C	-2.249676	0.790934	0.538530
C	-2.569038	-0.357209	-0.124819
C	0.487568	0.556272	-1.890594
C	1.871430	1.145449	-1.576624
C	2.592618	0.391213	-0.487202
C	1.892458	-0.483189	0.293668
O	0.559806	-0.717305	0.256143
C	4.070191	0.626230	-0.312527
O	2.544652	-1.269304	1.207290
C	1.809096	-1.720510	2.342233
C	-0.147999	2.090624	0.921038
C	-1.289936	-2.017089	-1.509281
H	4.465053	0.086454	0.569072
H	4.654793	0.292835	-1.202500
H	4.298069	1.710565	-0.182933
H	2.519562	-2.318120	2.945814
H	1.435275	-0.872204	2.960346
H	0.943489	-2.353144	2.056555
H	1.790280	2.234454	-1.331064
H	2.476910	1.126136	-2.513414
H	0.632311	-0.367231	-2.488605
H	-0.120786	1.247863	-2.507924
C	-3.064679	1.624670	1.472212
C	-3.835568	-1.148892	-0.134914
H	0.207989	1.593477	1.853792
H	0.739243	2.435992	0.361620
H	-0.734858	2.987249	1.203745
H	-0.506427	-2.013470	-2.291634
H	-0.981274	-2.744070	-0.723304
H	-2.223482	-2.379143	-1.984591
H	-4.055976	1.160063	1.637901
H	-2.586908	1.745002	2.470057
H	-3.241504	2.649334	1.072147
H	-3.680002	-2.208664	0.166715
H	-4.569338	-0.712043	0.569797
H	-4.311611	-1.165479	-1.142109

(3)Bspiro$_C$(MMA)

C	-1.174788	-1.092009	-0.205080
C	0.312601	-0.736879	0.462046
C	0.038628	-1.883942	1.494225
C	-1.419478	-2.049202	0.995204
N	1.451908	-0.846440	-0.447756
C	2.139219	0.404686	-0.481797
C	1.529892	1.271980	0.376438
N	0.422096	0.630504	0.987733
C	3.242920	0.645535	-1.462376
C	1.799759	2.724233	0.613477
C	0.016498	0.965126	2.343168
C	2.221725	-2.074588	-0.558695
C	-2.073010	0.126042	-0.205518
O	-2.005206	0.809674	-1.381767
C	-2.772043	2.020275	-1.435801
O	-2.751170	0.512791	0.736697
C	-1.067369	-1.762118	-1.575263
H	-2.443445	2.733324	-0.652049
H	-2.600523	2.447595	-2.441151
H	-3.851932	1.814605	-1.283643
H	1.556735	-2.945935	-0.719361
H	2.880273	-2.012974	-1.448453
H	2.871431	-2.291222	0.327664
H	-0.995223	0.565122	2.547181
H	0.721544	0.605684	3.135690
H	-0.058660	2.066805	2.437993
H	3.563700	1.705083	-1.436124
H	4.147347	0.029115	-1.258500
H	2.923047	0.414871	-2.504604
H	2.629671	3.077264	-0.028605
H	0.906399	3.351145	0.390437
H	2.088752	2.937876	1.666613
H	-2.070646	-2.039843	-1.962212
H	-0.583237	-1.088232	-2.307734
H	-0.467043	-2.692741	-1.516271
H	-2.178875	-1.646560	1.693223
H	-1.710842	-3.079898	0.707567
H	0.166627	-1.599009	2.556903
H	0.670555	-2.775088	1.315988

(3)B-C(MMA)

C	-3.286877	-0.362646	-0.919649
N	-1.951391	-0.776529	-0.931624
C	-1.650173	-1.402663	0.236860
N	-2.786686	-1.391993	0.995697
C	-3.821303	-0.757353	0.293193
C	-0.994676	-0.476566	-2.007601
C	-0.286349	-1.842202	0.618478
C	0.650997	-0.612298	0.906574
C	2.135616	-0.873354	0.760165
C	2.531222	-1.638561	-0.392712
O	3.859054	-2.036060	-0.370310
C	4.316678	-2.700853	-1.544462
C	-2.925536	-1.943053	2.337330
C	2.947251	-0.976667	2.037478
O	1.826607	-1.902598	-1.397035
C	2.739737	1.104291	-0.076345
C	2.040075	2.200775	0.450257
C	2.470772	2.886469	1.731763
C	0.880216	2.694651	-0.264960
O	0.361697	3.848698	0.322814
C	-0.733129	4.440903	-0.361107
O	0.351488	2.246223	-1.301234
H	2.777127	-0.092091	2.688811
H	4.031627	-1.033872	1.818624
H	2.694976	-1.881564	2.643633
H	5.385079	-2.934740	-1.370342
H	4.212178	-2.061383	-2.447105
H	3.751182	-3.639319	-1.732646
H	2.494173	0.804970	-1.107874
H	3.779533	0.927931	0.244338
H	2.589489	3.983326	1.594458
H	3.440848	2.478556	2.084489
H	1.737574	2.763094	2.561930
H	-1.626829	3.776434	-0.368572
H	-0.973499	5.375537	0.183212
H	-0.484529	4.672225	-1.419446
H	0.349019	0.206889	0.220990
H	0.438160	-0.225794	1.926412
C	-3.896601	0.379220	-2.062793
H	-3.684709	-2.751132	2.352850
H	-1.957041	-2.359735	2.664494
H	-3.227667	-1.151373	3.052029
H	-0.080051	-1.094288	-1.884932
H	-1.470910	-0.694493	-2.982654
H	-0.680255	0.591289	-1.940262
C	-5.195321	-0.600724	0.858106
H	-0.321566	-2.547558	1.472326
H	0.161561	-2.377996	-0.249170
H	-5.843818	-0.065627	0.139188
H	-5.675581	-1.579930	1.073199
H	-5.195328	-0.016180	1.803469
H	-4.940959	0.660938	-1.830701
H	-3.330120	1.308231	-2.284063

H	-3.909475	-0.229000	-2.992531

(3)C(MMA)

C	-2.409536	-1.607957	-0.115346
N	-1.029936	-1.702404	0.089924
C	-0.656604	-0.887729	1.114687
N	-1.807019	-0.345959	1.623203
C	-2.900276	-0.746560	0.844100
C	-0.138073	-2.475246	-0.770460
C	0.662280	-0.925160	1.827385
C	1.595542	0.308366	1.788817
C	2.378537	0.661558	0.497229
C	1.430553	0.963137	-0.747688
C	0.093451	1.603551	-0.480465
C	0.064663	3.012118	0.081826
C	-1.825277	0.751999	2.573624
C	3.266145	-0.502857	0.056791
O	3.086468	-1.696182	0.293778
C	3.248973	1.904054	0.813855
O	4.287426	-0.089479	-0.740108
C	5.105199	-1.126852	-1.301742
C	-0.973353	1.132595	-1.294132
O	-0.994106	0.134576	-2.059478
O	-2.151615	1.923241	-1.191542
C	-3.169373	1.617257	-2.126019
H	5.884562	-0.612879	-1.893877
H	4.505990	-1.794902	-1.954244
H	5.568225	-1.743579	-0.504453
H	1.230309	0.019124	-1.295926
H	2.060020	1.578682	-1.441647
H	-3.749610	0.705239	-1.845017
H	-3.863325	2.483391	-2.139545
H	-2.762066	1.442507	-3.144956
H	1.019833	1.213784	2.067441
H	2.342061	0.150932	2.598839
H	-1.063008	0.590716	3.359730
H	-1.603084	1.702183	2.041902
H	-2.817562	0.813307	3.056534
H	0.904458	-2.373091	-0.418520
H	-0.425037	-3.546384	-0.755547
H	-0.208801	-2.055464	-1.792945
H	0.430996	-1.132243	2.897817
H	1.235808	-1.799797	1.468821
H	3.834371	2.209734	-0.073439
H	2.607901	2.756025	1.112543
H	3.961586	1.702429	1.642360
H	-0.956021	3.437676	0.028364
H	0.398050	3.094558	1.144509
H	0.738551	3.703869	-0.488808
C	-4.281868	-0.227423	1.067100
C	-3.077297	-2.262923	-1.275683
H	-4.989222	-0.723429	0.376037
H	-4.643238	-0.413594	2.101889
H	-4.337061	0.865907	0.874967
H	-4.173351	-2.120143	-1.226580
H	-2.701537	-1.790446	-2.209337
H	-2.878617	-3.354382	-1.323266

3-C-CspiroC(MMA)

N	-1.664505	-0.144797	1.677003
C	-2.845675	-0.637850	1.091867
C	-2.469196	-1.512835	0.099311
N	-1.066688	-1.533971	0.068243
C	-0.559293	-0.533128	0.902066
C	-4.201277	-0.208265	1.547625
C	-3.282075	-2.301350	-0.872231
C	-0.297203	-2.429756	-0.784267
C	0.793163	-0.759386	1.572716
C	1.821285	0.380047	1.545374
C	2.409328	0.750605	0.144572
C	1.286757	0.867498	-0.945484
C	-0.110595	1.250832	-0.471379
C	-1.135578	0.944218	-1.459406
O	-2.263961	1.762416	-1.353047
C	-3.349659	1.428516	-2.206737
C	-1.629809	0.814882	2.759019
C	3.341892	-0.413226	-0.240596
O	4.658357	-0.114575	-0.091667
C	5.576807	-1.179954	-0.387977
O	2.972540	-1.523557	-0.600794
O	-1.097402	0.045999	-2.314367
C	3.194160	2.073587	0.278605
C	-0.253550	2.604504	0.216087
H	6.588219	-0.762696	-0.230312
H	5.457299	-1.522965	-1.435842
H	5.406693	-2.047299	0.282447
H	1.198940	-0.090749	-1.492019
H	1.654226	1.602118	-1.706414
H	-3.916692	0.553243	-1.812312
H	-4.019465	2.310967	-2.231746
H	-3.001538	1.176012	-3.229852
H	1.379480	1.301356	1.975183
H	2.661150	0.108980	2.223057
H	-0.610191	0.860897	3.186678
H	-1.909908	1.839867	2.433608
H	-2.319578	0.503806	3.570829

H	0.776357	-2.169192	-0.742455
H	-0.418306	-3.486683	-0.456361
H	-0.618368	-2.320767	-1.837143
H	0.592858	-1.038861	2.631953
H	1.254298	-1.658088	1.118551
H	-4.984701	-0.732198	0.967117
H	-4.381449	-0.435032	2.622031
H	-4.357886	0.884680	1.410580
H	-4.364062	-2.155113	-0.689512
H	-3.056146	-1.975994	-1.911756
H	-3.075779	-3.392108	-0.810074
H	3.719661	2.321955	-0.665271
H	2.497566	2.904043	0.506914
H	3.954588	2.022719	1.083647
H	-1.312188	2.827880	0.445446
H	0.323380	2.688023	1.160303
H	0.106729	3.436678	-0.439983

(3)Cspiro$_C$(MMA)

C	0.129249	0.806125	-0.788435
C	0.591713	-0.573649	-0.071712
C	-0.649536	-1.488499	0.179831
C	-1.800439	-1.302191	-0.813465
C	-2.430215	0.127383	-0.698592
C	-1.320902	1.178515	-0.384739
N	1.667105	-1.251913	-0.850119
C	2.818862	-1.401570	-0.023792
C	2.597365	-0.812035	1.183765
N	1.298344	-0.239919	1.205926
C	4.078075	-1.991014	-0.575366
C	3.544790	-0.587976	2.319733
C	0.588846	-0.116051	2.470111
C	1.342746	-2.321241	-1.778073
C	-3.380313	0.053593	0.517353
O	-4.636345	-0.327446	0.164545
C	-5.562120	-0.496450	1.251268
C	1.047458	1.911469	-0.212649
O	2.296644	1.853448	-0.746034
C	3.225505	2.817268	-0.233241
O	-3.062715	0.244103	1.681181
O	0.709077	2.776037	0.578333
C	-3.209948	0.468734	-1.985877
C	0.315203	0.781275	-2.323223
H	-6.526287	-0.777342	0.789364
H	-5.667630	0.444124	1.829155
H	-5.218324	-1.292406	1.943437
H	-1.326834	1.391888	0.700153
H	-1.584828	2.143344	-0.867256
H	3.369366	2.681363	0.858684
H	4.176484	2.642988	-0.769557
H	2.865135	3.852027	-0.408185
H	-1.458830	-1.451530	-1.859190
H	-2.585096	-2.071759	-0.647387
H	0.525958	-2.014721	-2.459402
H	2.224649	-2.530421	-2.416668
H	1.043190	-3.288788	-1.297065
H	-0.382287	0.394036	2.328114
H	0.392576	-1.091840	2.983857
H	1.180728	0.517022	3.162134
H	-0.318017	-2.546210	0.214541
H	-1.048257	-1.264916	1.188108
H	4.900093	-1.917030	0.162927
H	3.975767	-3.067464	-0.840086
H	4.404921	-1.461074	-1.499930
H	4.537126	-1.023274	2.092591
H	3.690245	0.496892	2.530115
H	3.192627	-1.051425	3.267926
H	-3.747115	1.434455	-1.886043
H	-2.511170	0.558170	-2.841575
H	-3.958255	-0.311654	-2.226584
H	0.095511	1.783679	-2.747369
H	1.355843	0.510965	-2.578642
H	-0.366765	0.062470	-2.818391

(3)C-D(MMA)

C	-3.373085	-1.644699	-0.471337
C	-3.842539	-0.455398	0.041280
N	-2.749479	0.194627	0.635610
C	-1.606350	-0.577413	0.506777
N	-1.995389	-1.703736	-0.193934
C	-5.219754	0.123957	0.026226
C	-2.796710	1.455954	1.363702
C	-0.302016	-0.125567	0.901489
C	0.783868	-1.018144	1.528921
C	2.239087	-0.578175	1.166061
C	3.176650	-0.862608	2.365280
C	-1.118197	-2.781045	-0.630364
C	-4.086947	-2.731621	-1.207536
C	2.731290	-1.394712	-0.036300
O	2.066118	-2.172293	-0.711015
O	4.047023	-1.175312	-0.291904
C	4.591584	-1.866029	-1.425753
C	2.327755	0.960507	0.820720
C	1.525989	1.449351	-0.383008
C	0.711658	2.623066	-0.157152
O	0.176950	2.952702	0.923517

C	2.126046	1.217068	-1.759291
O	0.435853	3.349158	-1.313381
C	-0.475205	4.430030	-1.159096
H	4.228110	-0.616809	2.120011
H	2.868798	-0.243720	3.233624
H	3.132874	-1.929327	2.673413
H	5.671176	-1.628375	-1.438069
H	4.434324	-2.960428	-1.338471
H	4.113410	-1.516624	-2.364348
H	1.979709	1.508981	1.722191
H	3.409764	1.200872	0.694699
H	1.515138	1.703141	-2.543096
H	3.163178	1.624195	-1.844780
H	2.183947	0.137085	-2.016035
H	-1.522927	4.075569	-1.024209
H	-0.414956	5.025810	-2.091374
H	-0.218847	5.060703	-0.282013
H	0.684544	-0.969430	2.635396
H	0.664195	-2.085229	1.259550
H	-1.431647	-3.128589	-1.634087
H	-1.156255	-3.647285	0.066115
H	-0.070402	-2.427996	-0.697763
H	-2.768243	1.284503	2.462132
H	-3.734818	1.984359	1.114502
H	-1.931781	2.105120	1.096825
H	-0.422943	0.787651	1.514303
H	0.332162	0.487459	-0.039079
H	-5.169937	-2.510239	-1.262288
H	-3.973046	-3.718939	-0.709477
H	-3.722169	-2.847742	-2.252160
H	-5.920902	-0.572681	-0.471535
H	-5.264902	1.087656	-0.527450
H	-5.609780	0.312904	1.050285

(3)D(MMA)

N	3.603552	-1.189451	-0.572584
C	2.689602	-0.124659	-0.511458
N	3.419838	0.931168	0.054837
C	4.749334	0.518018	0.314044
C	4.858851	-0.793968	-0.070596
C	1.383200	-0.205735	-0.966798
C	0.258655	0.787468	-0.895395
C	-0.850274	0.503224	0.220782
C	-1.465167	-0.899436	-0.020896
C	-2.709525	-1.255997	0.835929
C	-4.000261	-1.152677	0.024345
O	-4.977383	-0.506946	0.725222
C	-6.262478	-0.461733	0.086149
C	2.952661	2.297106	0.150082
C	5.768377	1.426406	0.920642
C	6.023652	-1.726021	0.002970
C	3.243490	-2.491785	-1.073649
C	-1.871742	1.631465	0.061489
O	-2.749494	1.380897	-0.954835
C	-3.689602	2.428790	-1.232921
O	-1.884536	2.677947	0.689975
O	-4.186188	-1.641346	-1.075346
C	-0.219188	0.600879	1.619490
H	-2.805440	-0.559100	1.694780
H	-4.290310	2.078448	-2.092364
H	-3.166673	3.374032	-1.485628
H	-4.340887	2.616725	-0.354818
H	-0.657728	-1.633294	0.186934
H	-1.727896	-1.025059	-1.091965
H	-6.649028	-1.484901	-0.101479
H	-6.931334	0.080962	0.779386
H	-6.204420	0.067178	-0.887303
H	-0.285764	0.802876	-1.866128
H	0.613209	1.823250	-0.728585
H	3.745604	2.923384	0.598453
H	2.704347	2.719204	-0.849773
H	2.051900	2.380000	0.794009
H	2.958493	-2.453052	-2.150436
H	4.097245	-3.185429	-0.964214
H	2.374675	-2.908791	-0.514038
H	1.128026	-1.169305	-1.431665
C	-2.629889	-2.697056	1.392248
H	6.720388	0.881908	1.070668
H	5.995588	2.309273	0.281116
H	5.453072	1.815284	1.915062
H	6.903199	-1.206214	0.428701
H	5.822101	-2.611355	0.647669
H	6.322122	-2.111450	-0.997818
H	-0.937990	0.321135	2.417577
H	0.657405	-0.075978	1.680419
H	0.104668	1.639708	1.830737
H	-3.524179	-2.951793	1.998392
H	-2.557227	-3.428465	0.560685
H	-1.734261	-2.811347	2.036977

tbuMA

C	-3.068038	-1.326257	0.000000
C	-2.131966	-0.144384	0.000000
C	-2.541606	1.144752	0.000000
C	-0.667807	-0.506679	0.000000
O	0.140090	0.580732	0.000000

C	1.615917	0.455369	0.000000
O	-0.283613	-1.670079	0.000000
C	2.079284	1.918515	0.000000
C	2.079284	-0.265515	1.275960
C	2.079284	-0.265515	-1.275960
H	-4.126634	-1.001320	0.000000
H	-2.888792	-1.971556	-0.885532
H	-2.888792	-1.971556	0.885532
H	-3.614511	1.399128	0.000000
H	-1.815607	1.970741	0.000000
H	3.187033	1.970269	0.000000
H	1.704090	2.449075	-0.898555
H	1.704090	2.449075	0.898555
H	3.187846	-0.260966	-1.324832
H	1.728308	-1.314103	-1.290497
H	1.694447	0.254673	-2.177161
H	3.187846	-0.260966	1.324832
H	1.694447	0.254673	2.177161
H	1.728308	-1.314103	1.290497

(3)A-B(tbuMA)

C	-2.246979	0.670203	-0.550353
N	-1.938731	-0.490960	-1.226986
C	-2.050822	-1.593191	-0.365539
C	-2.435434	-1.110553	0.867527
N	-2.546511	0.285270	0.742661
C	-1.340991	-0.507384	-2.553947
C	-2.877273	1.221199	1.799975
C	-2.080797	2.000325	-1.014080
C	-0.117420	2.644753	-0.895480
C	0.743665	2.029461	0.039692
C	0.806839	2.481170	1.480220
C	1.499047	0.883846	-0.414357
O	1.478521	0.389741	-1.562679
O	2.301850	0.363222	0.593690
C	3.263072	-0.704180	0.336455
C	3.950865	-0.892755	1.698722
C	2.537049	-1.998959	-0.077311
C	4.288054	-0.265331	-0.726087
H	-0.422976	3.686507	-0.694637
H	0.108093	2.434582	-1.953144
H	-2.220616	2.138633	-2.097526
H	-2.607225	2.760922	-0.416806
C	-2.716956	-1.833545	2.144247
C	-1.773739	-2.992293	-0.810759
H	-1.985029	1.807384	2.111744
H	-3.663529	1.927204	1.460209
H	-3.262715	0.669349	2.676299
H	-1.878991	0.199299	-3.216974
H	-0.265264	-0.210258	-2.478481
H	-1.430599	-1.520764	-2.986490
H	-3.763202	-1.688185	2.494034
H	-2.567422	-2.921167	2.005582
H	-2.042204	-1.511772	2.967408
H	-0.720269	-3.122463	-1.139785
H	-1.950045	-3.700428	0.021126
H	-2.428948	-3.302132	-1.654282
H	4.715452	-1.694964	1.642858
H	4.448292	0.046054	2.016851
H	3.207777	-1.167687	2.475262
H	3.260668	-2.837401	-0.158866
H	1.777836	-2.270469	0.685835
H	2.032093	-1.856486	-1.050857
H	5.071574	-1.042623	-0.848885
H	3.787030	-0.097441	-1.697710
H	4.783182	0.677542	-0.414120
H	1.852022	2.545525	1.849450
H	0.342179	3.483198	1.602312
H	0.287469	1.787585	2.188226

(3)B(tbuMA)

C	-2.488650	-1.193824	-0.202883
C	-1.838308	-1.188946	1.015010
N	-1.470872	0.137301	1.273026
C	-1.853409	0.925383	0.232121
N	-2.516381	0.127718	-0.652746
C	-1.524084	-2.303427	1.957350
C	-0.643315	0.535365	2.409262
C	-1.595233	2.379696	0.087330
C	-0.227997	2.736176	-0.643413
C	0.975274	2.068069	-0.056479
C	1.117799	0.717401	-0.397746
O	2.169365	0.047229	0.288304
C	2.856238	-1.063984	-0.344809
C	-2.770560	0.518308	-2.033438
C	-3.058893	-2.327763	-0.989928
C	1.869337	2.816608	0.897042
O	0.356748	0.061035	-1.180914
H	1.393090	3.061135	1.886478
H	2.774757	2.221926	1.127137
H	2.207299	3.798933	0.486621
C	4.124489	-1.247195	0.506145
C	1.984314	-2.335687	-0.286924
C	3.233165	-0.721206	-1.799051
H	-0.145229	3.844761	-0.597749
H	-0.360108	2.456526	-1.712101

H	-2.452331	2.839249	-0.452802
H	-1.584902	2.839002	1.097243
H	-0.568795	1.635117	2.448141
H	-1.094358	0.161152	3.351437
H	0.382663	0.133201	2.283164
H	-3.135721	1.562253	-2.070998
H	-1.817080	0.438642	-2.596746
H	-3.542027	-0.139617	-2.473325
H	-2.972635	-3.270344	-0.417183
H	-4.134871	-2.179510	-1.225327
H	-2.517079	-2.472348	-1.949200
H	-1.890932	-3.264079	1.549313
H	-0.429233	-2.404677	2.112543
H	-1.995417	-2.161766	2.953980
H	4.718924	-2.114821	0.150154
H	4.761569	-0.340346	0.459001
H	3.854319	-1.420717	1.568578
H	3.851816	-1.529819	-2.242452
H	2.317920	-0.587991	-2.407324
H	3.816488	0.222300	-1.830618
H	2.510166	-3.201998	-0.743299
H	1.756532	-2.593997	0.769787
H	1.036038	-2.143266	-0.823057

(3)Bspiro$_C$(tbuMA)

N	1.057009	0.347135	1.154478
C	1.348822	-0.749093	0.219797
N	2.106548	-0.095199	-0.847338
C	2.210380	1.298944	-0.554754
C	1.596225	1.551982	0.636345
C	0.003447	-1.607645	-0.263237
C	-0.011094	-1.877069	-1.769052
C	1.882994	-2.087247	0.836745
C	0.517635	-2.784155	0.614186
C	3.228007	-0.756435	-1.494840
C	2.792826	2.250257	-1.551401
C	1.352360	2.859487	1.321402
C	0.960366	0.122789	2.586988
C	-1.282058	-0.976972	0.245840
O	-1.739622	-1.154723	1.369438
O	-1.829326	-0.154611	-0.683227
C	-3.068405	0.609993	-0.420774
C	-2.854463	1.580366	0.751510
C	-3.277316	1.378808	-1.732935
C	-4.233782	-0.359100	-0.163307
H	2.942712	-1.766238	-1.849540
H	3.521605	-0.178289	-2.393989
H	4.136671	-0.857903	-0.847611
H	0.294998	-0.737895	2.790829
H	1.945301	-0.045156	3.093137
H	0.485634	1.004410	3.062033
H	2.656524	3.296916	-1.216337
H	3.884910	2.101105	-1.709336
H	2.305834	2.148846	-2.548519
H	1.746774	3.697378	0.714578
H	0.266694	3.042881	1.490028
H	1.846075	2.916887	2.316969
H	-0.894374	-2.485898	-2.055562
H	-0.038651	-0.929298	-2.339909
H	0.892106	-2.440170	-2.081753
H	-0.082635	-2.892538	1.538423
H	0.556326	-3.765254	0.098062
H	2.246794	-2.018686	1.880924
H	2.698799	-2.527183	0.232003
H	-4.194666	1.999255	-1.672825
H	-2.414901	2.044982	-1.937357
H	-3.383069	0.677514	-2.585367
H	-5.181899	0.210777	-0.073988
H	-4.340556	-1.071034	-1.007600
H	-4.073638	-0.931394	0.769457
H	-3.746296	2.231313	0.864236
H	-2.691247	1.029004	1.695771
H	-1.974792	2.227326	0.558486

(3)B-C(tbuMA)

C	-2.874661	-3.347698	0.140835
C	-2.542690	-2.710316	-1.040526
N	-1.239784	-2.225040	-0.890080
C	-0.769010	-2.536786	0.346961
N	-1.764745	-3.217807	0.988455
C	-3.331164	-2.501622	-2.291210
C	-0.530153	-1.409040	-1.886781
C	0.532935	-2.074363	0.883963
C	0.539893	-0.521648	1.134489
C	1.911606	0.121913	1.166040
C	2.448004	0.532451	2.522838
C	-1.705915	-3.740643	2.347211
C	-4.119238	-4.064023	0.552784
C	2.818005	-0.268611	0.119252
O	2.499395	-0.898234	-0.924342
O	4.110229	0.182587	0.322702
C	5.162551	0.001454	-0.675828
C	1.348661	2.084399	0.212799
C	0.133397	2.627350	0.649540
C	-1.070307	2.354212	-0.118170
O	-1.187726	1.612002	-1.115895

C	0.052210	3.516575	1.874979
O	-2.149819	3.074680	0.381417
C	-3.454405	3.068783	-0.267861
H	1.708265	1.158566	3.067701
H	3.383044	1.117286	2.423682
H	2.684458	-0.339385	3.181897
C	6.379696	0.676101	-0.021969
C	4.795436	0.716317	-1.989212
C	5.440298	-1.496871	-0.901532
H	1.373180	1.637183	-0.793635
H	2.292102	2.526340	0.572254
H	-0.403447	4.503512	1.641305
H	1.064505	3.697713	2.292104
H	-0.571692	3.080882	2.688064
C	-4.067616	1.655041	-0.236126
C	-4.284962	4.025489	0.603934
C	-3.349164	3.610868	-1.705826
H	-0.078322	-0.052473	0.342062
H	0.004523	-0.305359	2.083980
H	-1.741852	-4.849348	2.346516
H	-0.765421	-3.415084	2.824823
H	-2.555329	-3.353308	2.944054
H	0.552179	-1.366849	-1.640405
H	-0.674481	-1.858822	-2.887534
H	-0.914809	-0.364451	-1.856027
H	0.811399	-2.644213	1.792416
H	1.312085	-2.261971	0.109596
H	-4.852550	-4.059912	-0.275492
H	-3.923022	-5.125391	0.817933
H	-4.608038	-3.587284	1.429962
H	-4.346464	-2.927493	-2.183680
H	-3.437592	-1.421466	-2.524890
H	-2.852711	-2.985497	-3.169507
H	-5.100617	1.674177	-0.643458
H	-3.448853	0.961141	-0.835143
H	-4.114621	1.281648	0.808298
H	-5.322491	4.105137	0.218354
H	-4.323785	3.662484	1.651391
H	-3.831938	5.037607	0.608955
H	-4.359529	3.699485	-2.158082
H	-2.884474	4.618402	-1.699736
H	-2.726724	2.940604	-2.327343
H	6.317912	-1.627233	-1.569371
H	5.666374	-1.994242	0.064774
H	4.560439	-1.987207	-1.357619
H	5.647573	0.671400	-2.700020
H	3.910097	0.243803	-2.453537
H	4.564662	1.783703	-1.793016
H	7.268165	0.601121	-0.682268
H	6.173817	1.748718	0.170591
H	6.618632	0.191733	0.946856

(3)C(tbuMA)

C	-2.853194	-2.076852	0.011923
C	-2.196245	-2.042819	-1.200905
N	-0.828286	-2.021643	-0.920374
C	-0.630243	-2.016890	0.423074
N	-1.864501	-2.094330	1.002805
C	-2.715805	-1.916212	-2.591217
C	0.201042	-1.883730	-1.947113
C	0.673780	-2.242448	1.124932
C	1.301903	-1.111148	1.975738
C	1.964731	0.124263	1.310481
C	2.545065	0.992385	2.455728
C	-2.109604	-1.884419	2.420163
C	-4.308813	-1.991377	0.325207
C	0.955922	0.985413	0.430700
C	-0.479311	1.103421	0.880587
C	-1.444076	1.044549	-0.153586
O	-2.786156	1.281646	0.296452
C	-3.601904	2.237153	-0.436397
C	3.084452	-0.294555	0.346571
O	3.960260	0.716670	0.145905
C	5.073213	0.628966	-0.829147
C	-0.778209	1.764817	2.210377
O	3.156089	-1.378374	-0.235578
O	-1.257158	0.784312	-1.376052
C	5.738114	2.006822	-0.704699
C	4.518264	0.417864	-2.246320
C	6.043918	-0.486996	-0.411525
H	0.930338	0.580726	-0.602666
H	1.443693	1.990133	0.341598
C	-4.160633	1.611222	-1.730960
C	-4.750820	2.570801	0.530690
C	-2.791283	3.507257	-0.760447
H	0.540175	-0.718454	2.679026
H	2.077226	-1.604577	2.602774
H	-1.322867	-2.377874	3.021810
H	-2.105010	-0.794079	2.632366
H	-3.087584	-2.317338	2.698329
H	1.199258	-1.855868	-1.474058
H	0.150933	-2.734084	-2.656802
H	0.026398	-0.920156	-2.464966
H	0.512564	-3.110754	1.804346
H	1.424554	-2.573831	0.384267

H	3.020561	1.905291	2.051915
H	1.740370	1.302259	3.150123
H	3.309582	0.437675	3.041423
H	-1.863217	1.962305	2.308461
H	-0.474599	1.171015	3.107508
H	-0.246715	2.745939	2.320958
H	-4.901361	-2.077689	-0.604895
H	-4.649278	-2.794128	1.013723
H	-4.545582	-1.006145	0.782242
H	-3.817430	-2.013716	-2.606068
H	-2.450258	-0.909325	-2.978863
H	-2.296161	-2.684579	-3.274154
H	6.609041	2.075718	-1.387881
H	5.021957	2.812024	-0.965277
H	6.091080	2.179117	0.332213
H	5.343474	0.496534	-2.984215
H	4.048629	-0.578064	-2.345967
H	3.765573	1.195761	-2.488336
H	6.931097	-0.479487	-1.078238
H	6.396097	-0.325860	0.628187
H	5.558570	-1.478642	-0.475256
H	-5.466218	3.281682	0.066511
H	-5.309275	1.651335	0.805201
H	-4.359243	3.025842	1.463441
H	-4.847632	2.316630	-2.246487
H	-3.322568	1.349057	-2.403198
H	-4.730498	0.686997	-1.498171
H	-3.434258	4.263710	-1.257486
H	-2.379313	3.954833	0.167253
H	-1.948464	3.262935	-1.436658

(3)C-Cspiro$_C$(tbuMA)

C	-0.603205	-1.540801	0.305829
N	-1.664742	-2.080450	1.042513
C	-2.784379	-2.250596	0.210030
C	-2.368735	-2.003959	-1.078581
N	-1.011918	-1.658194	-1.021567
C	-1.694680	-2.197054	2.484484
C	-4.126544	-2.634748	0.740116
C	-3.112330	-2.057954	-2.370755
C	-0.195132	-1.425659	-2.205752
C	0.833775	-1.898288	0.667212
C	1.626434	-0.952620	1.579194
C	2.010402	0.436804	0.976364
C	2.551312	1.328995	2.114192
C	0.789914	1.113000	0.260003
C	-0.607795	0.792060	0.780002
C	-0.893765	1.144034	2.235167
C	3.099331	0.158751	-0.086951
O	2.875031	-0.380809	-1.166501
C	-1.640454	1.166762	-0.177126
O	-1.514502	1.179928	-1.414934
O	-2.845858	1.520099	0.435389
C	-3.914984	2.186065	-0.300979
O	4.330870	0.534204	0.322124
C	5.539220	0.344495	-0.520616
C	6.656171	0.923944	0.357887
C	5.396191	1.147189	-1.823038
C	5.766517	-1.152693	-0.779669
H	0.807522	0.859462	-0.816603
H	0.972418	2.218219	0.299544
C	-4.523606	1.257579	-1.366920
C	-4.953252	2.495325	0.790879
C	-3.395212	3.493671	-0.928378
H	1.060816	-0.765681	2.514212
H	2.558352	-1.473674	1.892768
H	-2.124561	-1.296742	2.973294
H	-2.292650	-3.081848	2.781711
H	-0.667857	-2.339945	2.873057
H	0.809340	-1.069544	-1.911954
H	-0.083125	-2.363474	-2.794258
H	-0.653925	-0.636194	-2.829585
H	0.807732	-2.909455	1.134460
H	1.400023	-2.028678	-0.275422
H	-4.855986	-2.714466	-0.088475
H	-4.114252	-3.617823	1.261671
H	-4.520348	-1.883751	1.459831
H	-4.166966	-2.348004	-2.202698
H	-3.106985	-1.068663	-2.876906
H	-2.670693	-2.794077	-3.077505
H	2.931038	2.291509	1.717180
H	1.741784	1.555945	2.835198
H	3.382204	0.841093	2.662399
H	-1.954157	0.963962	2.493672
H	-0.269047	0.580453	2.959815
H	-0.702914	2.228123	2.444567
H	6.735070	-1.296748	-1.301591
H	5.808783	-1.710432	0.178579
H	4.959137	-1.575410	-1.405768
H	7.630384	0.855245	-0.167413
H	6.458375	1.989642	0.591125
H	6.734029	0.368390	1.314383
H	6.344510	1.095517	-2.396885
H	4.578588	0.747929	-2.451239
H	5.188568	2.213950	-1.600686

H	-4.228798	4.047468	-1.409105
H	-2.953116	4.144867	-0.145972
H	-2.621454	3.275192	-1.688184
H	-5.828924	3.022836	0.359498
H	-5.309344	1.558951	1.268006
H	-4.509556	3.136347	1.579714
H	-5.415456	1.732497	-1.827983
H	-3.775367	1.044289	-2.151872
H	-4.842049	0.300046	-0.905378

(3)Cspiro$_C$(tbuMA)

N	-1.321963	0.992596	1.152985
C	-0.710361	0.982103	-0.213244
N	-1.722568	1.743013	-1.004985
C	-2.691177	2.292943	-0.113523
C	-2.446873	1.857665	1.153660
C	0.696942	1.663410	-0.208661
C	1.683984	1.125527	-1.248317
C	2.052860	-0.370743	-0.969653
C	0.813634	-1.129746	-0.399210
C	-0.585931	-0.545450	-0.734532
C	-1.617959	-1.387291	0.071261
O	-1.316709	-2.160653	0.968736
C	-0.918382	-0.694899	-2.236684
C	3.137596	-0.322938	0.139422
O	2.890415	-0.239579	1.335448
C	2.598403	-1.030065	-2.253325
C	-1.303469	2.559189	-2.132280
C	-3.840108	3.094071	-0.638069
C	-3.233643	2.085613	2.405539
C	-0.512591	0.864038	2.354338
O	4.384462	-0.316857	-0.382510
C	5.596230	-0.208651	0.470889
O	-2.872526	-1.212521	-0.404226
C	-4.013867	-2.010181	0.099099
C	6.736288	-0.250588	-0.555290
C	5.670840	-1.412494	1.422714
C	5.585437	1.129325	1.225495
H	0.903971	-1.181479	0.701281
H	0.844406	-2.186228	-0.740717
C	-4.238805	-1.748035	1.595667
C	-5.192177	-1.479701	-0.729108
C	-3.768714	-3.499641	-0.194090
H	1.269064	1.198810	-2.275339
H	2.608136	1.743482	-1.260980
H	-0.654234	1.980731	-2.816435
H	-2.195388	2.856611	-2.720117
H	-0.758777	3.499479	-1.855927
H	0.287218	0.114340	2.208488
H	-0.030788	1.818108	2.689511
H	-1.145937	0.495833	3.186932
H	0.564642	2.760152	-0.308899
H	1.156572	1.505169	0.785786
H	-4.546744	3.343063	0.177372
H	-3.525225	4.056720	-1.100440
H	-4.408142	2.534788	-1.417533
H	-4.127092	2.706112	2.198521
H	-3.582471	1.130340	2.860026
H	-2.642219	2.611119	3.188090
H	2.960593	-2.059544	-2.053403
H	1.799559	-1.096039	-3.018839
H	3.442001	-0.452251	-2.678882
H	-0.929212	-1.769174	-2.517365
H	-1.912198	-0.264573	-2.455663
H	-0.167749	-0.199037	-2.882393
H	-4.667796	-4.088555	0.082256
H	-3.576595	-3.656063	-1.275725
H	-2.904851	-3.880132	0.382305
H	-5.156234	-2.275197	1.931064
H	-3.380596	-2.105688	2.193811
H	-4.377812	-0.663909	1.778508
H	-6.125044	-2.012593	-0.453244
H	-5.338972	-0.395919	-0.548654
H	-5.009446	-1.630175	-1.812467
H	7.716145	-0.179651	-0.040879
H	6.711624	-1.197521	-1.131568
H	6.654989	0.593333	-1.270083
H	6.541087	1.253025	1.775690
H	5.489072	1.977137	0.516206
H	4.751627	1.169577	1.950716
H	6.631028	-1.387742	1.978270
H	4.838689	-1.396721	2.150653
H	5.630726	-2.362907	0.851889

(3)C-D(tbuMA)

N	-1.381100	-2.880015	-0.362829
C	-2.629345	-3.413050	-0.730628
C	-3.597151	-2.650247	-0.114225
N	-2.928684	-1.666834	0.631553
C	-1.558965	-1.811096	0.494095
C	-2.756713	-4.592674	-1.638763
C	-5.086653	-2.760310	-0.158040
C	-3.553957	-0.669931	1.489628
C	-0.605227	-0.879343	1.034435
C	0.739967	-1.291573	1.661083
C	1.865591	-0.218720	1.501218

C	1.283554	1.236881	1.302168
C	0.391115	1.495024	0.092639
C	1.077158	1.706418	-1.243632
C	-0.104605	-3.365287	-0.869336
C	2.738759	-0.210438	2.781171
C	2.766487	-0.598625	0.307176
O	3.882367	0.163438	0.274791
C	4.982337	-0.061185	-0.695691
O	2.528883	-1.494246	-0.499520
C	-0.851701	2.183014	0.370142
O	-1.337914	2.888345	-0.727967
C	-2.531799	3.719641	-0.650917
O	-1.504279	2.102608	1.436765
H	3.570907	0.514125	2.694306
H	2.116621	0.077154	3.654094
H	3.171920	-1.213149	2.986189
C	5.998701	1.020475	-0.305075
C	5.570042	-1.465957	-0.487644
C	4.488147	0.150913	-2.134301
H	0.701105	1.470447	2.219271
H	2.159558	1.928836	1.294019
H	0.340257	1.929582	-2.037810
H	1.805126	2.555631	-1.220587
H	1.645641	0.809135	-1.565692
C	-3.789725	2.871116	-0.382551
C	-2.609434	4.346040	-2.053966
C	-2.356502	4.816305	0.416509
H	0.582773	-1.454908	2.749451
H	1.114705	-2.253300	1.260907
H	-0.201177	-3.610579	-1.945461
H	0.225466	-4.280314	-0.330802
H	0.679511	-2.590738	-0.759143
H	-3.485331	-0.962042	2.560245
H	-4.620239	-0.571745	1.216917
H	-3.057839	0.318982	1.369335
H	-1.138189	-0.206126	1.732175
H	-0.287458	0.043150	0.228733
H	-3.819946	-4.879415	-1.748391
H	-2.209892	-5.479421	-1.250832
H	-2.364009	-4.386851	-2.659020
H	-5.387271	-3.624819	-0.780079
H	-5.562160	-1.856684	-0.598887
H	-5.528583	-2.906993	0.851699
H	-3.479191	5.030977	-2.129778
H	-1.686774	4.921219	-2.271980
H	-2.713598	3.558046	-2.828032
H	-3.231229	5.500296	0.413318
H	-2.254509	4.361713	1.419917
H	-1.447808	5.416513	0.203104
H	-4.703669	3.490460	-0.505495
H	-3.844598	2.029271	-1.104305
H	-3.767379	2.463194	0.644592
H	6.890537	0.963799	-0.961857
H	5.551807	2.030048	-0.405788
H	6.328162	0.889804	0.745591
H	5.349442	0.093659	-2.831918
H	3.748540	-0.620062	-2.418988
H	4.022311	1.150607	-2.243083
H	6.464530	-1.594216	-1.131722
H	5.884734	-1.604466	0.567204
H	4.832737	-2.248367	-0.748010

(3)D(tbuMA)

C	5.865355	-1.244396	-0.293098
N	4.570011	-1.406790	-0.821699
C	3.765906	-0.297453	-0.508821
N	4.606461	0.543442	0.237236
C	5.892186	-0.037468	0.358142
C	4.076558	-2.534769	-1.570359
C	2.451227	-0.160640	-0.923133
C	1.429556	0.897818	-0.616004
C	0.301692	0.496162	0.438850
C	0.942979	0.201909	1.804046
C	4.273841	1.890994	0.643908
C	7.006305	0.625560	1.100160
C	6.934138	-2.274841	-0.456273
C	-0.493450	-0.717723	-0.106964
C	-1.702272	-1.168938	0.751411
C	-1.421722	-2.454561	1.566507
C	-0.593839	1.740072	0.579351
O	-0.527953	2.536738	1.506226
C	-2.951256	-1.402918	-0.111260
O	-2.950979	-1.578405	-1.319048
O	-4.059264	-1.425006	0.676352
C	-5.396801	-1.762555	0.135976
O	-1.419750	1.874743	-0.490920
C	-2.335392	3.028334	-0.637440
H	-1.981304	-0.371959	1.476173
C	-3.029496	2.741713	-1.975955
C	-1.530514	4.335825	-0.706115
C	-3.350580	3.033308	0.517152
H	0.222113	-1.561570	-0.211122
H	-0.850025	-0.489142	-1.130495
C	-5.380553	-3.186429	-0.442848
C	-6.293871	-1.687573	1.379036

C	-5.824491	-0.720712	-0.909973
H	0.888750	1.173496	-1.548608
H	1.889287	1.834128	-0.243740
H	5.133591	2.332538	1.180572
H	4.043040	2.541322	-0.229679
H	3.400488	1.910452	1.329988
H	3.781273	-2.244043	-2.605136
H	4.859304	-3.312535	-1.637469
H	3.178783	-2.978205	-1.081073
H	2.095995	-0.979925	-1.565511
H	7.906491	-0.018570	1.087435
H	7.299359	1.603152	0.654554
H	6.753816	0.815573	2.167854
H	7.867025	-1.940084	0.036462
H	6.656447	-3.253182	-0.002524
H	7.177921	-2.468006	-1.525235
H	0.185001	-0.076595	2.564462
H	1.675277	-0.624909	1.704557
H	1.463516	1.099547	2.194620
H	-2.284583	-2.722476	2.208452
H	-1.212969	-3.308655	0.887866
H	-0.533925	-2.315657	2.215263
H	-4.115799	3.817797	0.341570
H	-3.869080	2.054169	0.577960
H	-2.851324	3.232225	1.483831
H	-6.407177	-3.478282	-0.746551
H	-4.719925	-3.249622	-1.327911
H	-5.030063	-3.912534	0.319343
H	-2.212978	5.182865	-0.926585
H	-1.013846	4.534084	0.251245
H	-0.775959	4.284573	-1.517961
H	-7.343114	-1.925981	1.110481
H	-5.956487	-2.408954	2.150608
H	-6.266965	-0.670950	1.820973
H	-6.873061	-0.911310	-1.219709
H	-5.776155	0.301873	-0.482489
H	-5.175235	-0.766685	-1.803850
H	-3.769456	3.536088	-2.203131
H	-2.289090	2.704765	-2.800494
H	-3.553735	1.765742	-1.942390

MA

C	2.365149	0.837496	0.000000
C	1.462801	-0.162356	0.000000
H	1.760098	-1.223644	0.000000
C	0.000000	0.128940	0.000000
O	-0.715601	-1.032453	0.000000
C	-2.141687	-0.872460	0.000000
O	-0.512963	1.236257	0.000000
H	-2.565251	-1.893464	0.000000
H	-2.477763	-0.314306	0.898302
H	-2.477763	-0.314306	-0.898302
H	2.023236	1.886025	0.000000
H	3.448375	0.639543	0.000000

(3)A-B(MA)

C	1.183234	1.146131	0.320176
N	1.199729	0.133910	1.255425
C	1.468327	-1.092840	0.628434
C	1.641319	-0.837203	-0.713876
N	1.435381	0.543055	-0.892995
C	0.676489	0.276420	2.604909
C	1.556219	1.283451	-2.136964
C	0.750551	2.481416	0.491617
C	-1.340905	2.438229	0.137731
C	-1.817089	1.387297	-0.663226
H	-1.909379	1.486415	-1.756305
C	-2.145407	0.114071	-0.078294
O	-2.059433	-0.220652	1.116798
O	-2.613448	-0.791107	-1.026256
C	-3.029879	-2.048066	-0.507235
H	-3.413974	-2.629974	-1.368234
H	-2.190681	-2.599718	-0.028572
H	-3.829177	-1.935908	0.257377
H	-1.358302	3.461228	-0.272829
H	-1.571200	2.375759	1.214080
H	0.791764	2.883551	1.515046
H	1.092081	3.195207	-0.272915
C	1.947014	-1.762480	-1.845353
C	1.498974	-2.382081	1.382177
H	0.656707	1.908211	-2.298682
H	2.455756	1.938816	-2.129640
H	1.641383	0.575238	-2.980436
H	0.944983	1.272848	3.005624
H	-0.431426	0.162677	2.572865
H	1.124491	-0.491273	3.263484
H	2.890660	-1.498740	-2.371921
H	2.060400	-2.796890	-1.468807
H	1.131923	-1.774904	-2.602165
H	0.514529	-2.602875	1.848397
H	1.741345	-3.219767	0.700779
H	2.262302	-2.380649	2.190930

(3)B(MA)

C	-2.057722	-0.358692	-0.293843
C	-1.406700	-1.024331	0.725101
N	-0.538208	-0.102899	1.320777

C	-0.632560	1.093146	0.679356
N	-1.585650	0.954280	-0.285564
C	-1.497087	-2.443542	1.179133
C	0.413721	-0.466779	2.367732
C	0.204975	2.291508	0.925993
C	1.561312	2.308243	0.076862
C	2.339689	1.042331	0.136970
C	1.881129	-0.040815	-0.618323
O	2.597963	-1.248456	-0.371655
C	2.420547	-2.273673	-1.332357
C	-1.720076	1.871897	-1.410024
C	-3.039576	-0.857581	-1.301715
H	3.223234	0.938839	0.783398
O	0.894767	-0.062722	-1.410329
H	2.607699	-3.247560	-0.831832
H	1.393460	-2.250046	-1.756784
H	3.142930	-2.175517	-2.179609
H	2.139266	3.176241	0.461822
H	1.262807	2.554335	-0.968582
H	-0.398058	3.203149	0.717567
H	0.464726	2.327716	2.003466
H	0.959515	0.431688	2.699754
H	-0.124309	-0.925888	3.223951
H	1.163467	-1.170428	1.953945
H	-1.597747	2.915298	-1.063438
H	-0.924922	1.628413	-2.146211
H	-2.722489	1.766255	-1.864043
H	-3.324807	-1.901615	-1.072092
H	-3.972286	-0.254170	-1.319447
H	-2.605891	-0.848422	-2.324879
H	-2.234228	-2.996025	0.566489
H	-0.520406	-2.962398	1.075361
H	-1.812702	-2.530376	2.241228

(3)Bspiro$_C$(MA)

N	-0.758612	0.492496	1.167831
C	-0.396159	1.082402	-0.086605
N	-1.415039	0.579390	-0.965864
C	-1.976644	-0.593042	-0.380752
C	-1.582248	-0.631318	0.930311
C	1.263147	0.862717	-0.606713
H	1.236015	0.848666	-1.712242
C	-0.028247	2.589154	-0.062058
C	1.490541	2.278649	-0.046532
C	-1.305032	0.736037	-2.399180
C	-2.917678	-1.474463	-1.133966
C	-1.977147	-1.573969	2.019938
C	-0.095122	0.802421	2.420596
C	2.049141	-0.291088	-0.110352
O	2.541609	-0.425118	1.007455
O	2.132202	-1.280959	-1.061367
C	2.796827	-2.476833	-0.642258
H	2.275604	-2.947777	0.218019
H	2.784365	-3.158557	-1.513498
H	3.842849	-2.269079	-0.333628
H	-1.037091	1.782438	-2.649778
H	-0.540845	0.063916	-2.863096
H	-2.282004	0.528245	-2.879166
H	0.969748	0.483418	2.435252
H	-0.141375	1.893577	2.627480
H	-0.629177	0.296868	3.247596
H	-3.274645	-2.299816	-0.487772
H	-3.818618	-0.921460	-1.487554
H	-2.451195	-1.938587	-2.032066
H	-2.626908	-2.375146	1.618027
H	-1.097826	-2.063227	2.494540
H	-2.546046	-1.067568	2.833077
H	1.906036	2.233938	0.980060
H	2.136700	2.945723	-0.653448
H	-0.467565	3.175488	0.772292
H	-0.341232	3.070361	-1.011147

(3)B-C(MA)

N	1.865394	-1.705482	-0.809123
C	2.870649	-1.292444	0.075324
C	2.231128	-0.901536	1.236605
N	0.863739	-1.106220	1.035270
C	0.644225	-1.582441	-0.213503
C	4.318473	-1.304724	-0.291481
C	2.758852	-0.279466	2.484648
C	-0.162019	-0.763176	2.026014
C	-0.674195	-1.825883	-0.855275
C	-1.201443	-0.588502	-1.667869
C	-2.525293	-0.023612	-1.228908
C	-3.319787	-0.500950	-0.146787
O	-4.603115	0.034811	-0.172816
C	-5.436110	-0.320111	0.925238
C	2.105016	-2.132753	-2.181319
H	-3.096914	0.487602	-2.017772
O	-2.997659	-1.259239	0.805580
C	-1.907258	2.080743	-0.254376
C	-0.717295	2.543371	-0.801958
H	-0.711184	3.066302	-1.771750
C	0.559346	2.444179	-0.131487
O	1.562417	3.063328	-0.870047
C	2.839222	3.115337	-0.250911

O	0.821810	1.935212	0.972605
H	-6.402045	0.195945	0.758798
H	-5.003057	0.000528	1.897827
H	-5.602944	-1.418085	0.981350
H	-1.911850	1.701935	0.779892
H	-2.874069	2.436533	-0.635094
H	3.274453	2.100474	-0.104730
H	3.491602	3.700664	-0.928350
H	2.797631	3.606213	0.745807
H	-1.254053	-0.881372	-2.741652
H	-0.429925	0.235147	-1.641163
H	2.803892	-2.992713	-2.204226
H	1.149633	-2.435878	-2.643958
H	2.534628	-1.301265	-2.775861
H	-1.174842	-0.986908	1.625352
H	0.012944	-1.346842	2.951760
H	-0.081502	0.325086	2.217331
H	-0.598334	-2.721456	-1.505691
H	-1.424653	-2.058783	-0.066497
H	4.926050	-0.930902	0.553943
H	4.682516	-2.326299	-0.535761
H	4.534019	-0.655741	-1.167616
H	3.864850	-0.252710	2.470834
H	2.378946	0.762611	2.552790
H	2.441587	-0.829256	3.395100

(3)C(MA)

C	2.718989	-1.112531	0.084186
C	2.221812	-0.711100	1.306045
N	0.831345	-0.860744	1.251830
C	0.459718	-1.271726	0.004044
N	1.619753	-1.515333	-0.688315
C	2.898894	-0.093515	2.481941
C	-0.065400	-0.471917	2.336675
C	-0.874430	-1.866144	-0.356850
C	-1.716355	-1.166254	-1.444861
C	-2.431840	0.144305	-1.054231
H	-2.938432	0.511076	-1.971328
C	1.646683	-1.742384	-2.120586
C	4.117055	-1.127599	-0.438033
C	-1.473630	1.284492	-0.546644
C	-0.100013	1.276694	-1.152834
C	0.983362	1.783335	-0.392627
O	2.140869	1.993359	-1.184585
C	3.231093	2.588668	-0.504585
C	-3.511505	-0.079852	-0.012720
O	-4.651707	0.595767	-0.315710
C	-5.699571	0.525225	0.665512
H	-0.005796	1.363266	-2.249547
O	-3.396829	-0.734731	1.019678
O	1.030353	2.031343	0.835360
H	-6.531730	1.134240	0.267375
H	-5.357297	0.929329	1.640351
H	-6.027935	-0.523109	0.820323
H	-1.359096	1.211794	0.555088
H	-2.028122	2.242474	-0.713145
H	3.748567	1.873795	0.179702
H	3.950455	2.919335	-1.281977
H	2.914724	3.457166	0.112531
H	-1.072728	-0.937967	-2.317875
H	-2.481488	-1.896163	-1.790837
H	0.921730	-2.531574	-2.401635
H	1.378019	-0.796086	-2.643673
H	2.655436	-2.070595	-2.429494
H	-1.114250	-0.661175	2.042999
H	0.166459	-1.052487	3.253044
H	0.060056	0.614444	2.513663
H	-0.676833	-2.912123	-0.687325
H	-1.488912	-1.951204	0.560112
H	4.823104	-0.823568	0.357629
H	4.426368	-2.136619	-0.788805
H	4.240631	-0.418221	-1.284729
H	3.998460	-0.133619	2.365170
H	2.589476	0.972992	2.545781
H	2.640784	-0.596950	3.437466

(3)C-Cspiro$_C$(MA)

C	2.694906	-1.186304	0.082902
C	2.249737	-0.705045	1.294638
N	0.850179	-0.764215	1.274111
C	0.422273	-1.159814	0.030137
N	1.556270	-1.549877	-0.654801
C	2.990579	-0.095264	2.436104
C	0.009047	-0.296712	2.371620
C	-0.938332	-1.759103	-0.236762
C	-1.798443	-1.118244	-1.341626
C	-2.443384	0.246137	-0.991853
H	-2.937604	0.609383	-1.916428
C	1.546545	-1.856161	-2.070412
C	4.079661	-1.321835	-0.457616
C	-3.534504	0.060917	0.050940
O	-3.366183	-0.348835	1.194316
O	-4.761506	0.405141	-0.421367
C	-5.847695	0.273872	0.511825
C	-1.413963	1.318062	-0.507852
C	-0.038993	1.172383	-1.104813

C	1.064931	1.769967	-0.432651
O	1.137839	2.137090	0.759375
H	0.041618	1.150867	-2.206562
O	2.191269	1.902039	-1.275239
C	3.330527	2.487450	-0.668221
H	-6.753028	0.613225	-0.023883
H	-5.672788	0.898368	1.411639
H	-5.964080	-0.780104	0.838132
H	-1.324375	1.273093	0.596580
H	-1.873890	2.317911	-0.713241
H	3.858952	1.774233	0.009295
H	4.018800	2.775319	-1.488981
H	3.064512	3.379591	-0.062174
H	-1.185170	-0.970470	-2.252886
H	-2.602440	-1.837300	-1.614378
H	0.758732	-2.600842	-2.301301
H	1.350311	-0.929986	-2.657149
H	2.520966	-2.283990	-2.368552
H	-1.057977	-0.430935	2.114245
H	0.231960	-0.868939	3.296139
H	0.194144	0.784371	2.525779
H	-0.776589	-2.833887	-0.484087
H	-1.517166	-1.755435	0.707330
H	4.818560	-1.023689	0.310170
H	4.316830	-2.366718	-0.756838
H	4.237437	-0.670537	-1.344721
H	4.083043	-0.195779	2.291459
H	2.741274	0.987651	2.489583
H	2.734129	-0.562073	3.410819

(3)Cspiro$_C$(MA)

C	-2.645239	-1.109491	0.455451
C	-2.194836	-1.324886	-0.818149
N	-0.775681	-1.304341	-0.803090
C	-0.349863	-0.665556	0.445922
N	-1.508949	-0.959803	1.301408
C	-2.954621	-1.655831	-2.060477
C	-0.002938	-1.209298	-2.031250
C	0.967599	-1.293670	0.998576
C	1.936689	-0.300240	1.650783
C	2.427052	0.779504	0.639898
H	2.873450	1.608930	1.225791
C	-1.607232	-0.402913	2.631903
C	-4.028703	-1.194569	1.011071
C	3.554350	0.183485	-0.198889
O	3.427057	-0.422629	-1.251020
O	4.758446	0.362574	0.407165
C	5.885171	-0.230808	-0.260892
C	1.265217	1.294729	-0.253415
C	-0.125480	0.947279	0.317120
C	-1.227597	1.625280	-0.464090
O	-1.267443	1.770082	-1.678437
H	-0.190548	1.335851	1.353475
O	-2.183764	2.141054	0.371976
C	-3.307146	2.743427	-0.283508
H	6.770251	0.020456	0.351652
H	5.995417	0.177067	-1.286368
H	5.766903	-1.331408	-0.335508
H	1.369444	0.872998	-1.270447
H	1.349421	2.395305	-0.372414
H	-3.896334	1.976077	-0.829356
H	-3.922846	3.198910	0.514263
H	-2.980129	3.513726	-1.011369
H	1.447307	0.216496	2.503272
H	2.808341	-0.834700	2.084081
H	-0.678470	-0.613855	3.202757
H	-1.794596	0.700156	2.664447
H	-2.433189	-0.898008	3.181502
H	1.078418	-1.314235	-1.812231
H	-0.279184	-2.043976	-2.708593
H	-0.151402	-0.248252	-2.575908
H	0.674850	-2.093417	1.709150
H	1.482860	-1.805554	0.159809
H	-4.761545	-1.371908	0.200071
H	-4.136053	-2.032140	1.739508
H	-4.337222	-0.265807	1.541519
H	-4.043293	-1.677833	-1.859017
H	-2.775829	-0.910407	-2.866742
H	-2.672510	-2.652769	-2.469361

(3)C-Cspiro$_C$(MA)

C	2.694906	-1.186304	0.082902
C	2.249737	-0.705045	1.294638
N	0.850179	-0.764215	1.274111
C	0.422273	-1.159814	0.030137
N	1.556270	-1.549877	-0.654801
C	2.990579	-0.095264	2.436104
C	0.009047	-0.296712	2.371620
C	-0.938332	-1.759103	-0.236762
C	-1.798443	-1.118244	-1.341626
C	-2.443384	0.246137	-0.991853
H	-2.937604	0.609383	-1.916428
C	1.546545	-1.856161	-2.070412
C	4.079661	-1.321835	-0.457616
C	-3.534504	0.060917	0.050940
O	-3.366183	-0.348835	1.194316

O	-4.761506	0.405141	-0.421367
C	-5.847695	0.273872	0.511825
C	-1.413963	1.318062	-0.507852
C	-0.038993	1.172383	-1.104813
C	1.064931	1.769967	-0.432651
O	1.137839	2.137090	0.759375
H	0.041618	1.150867	-2.206562
O	2.191269	1.902039	-1.275239
C	3.330527	2.487450	-0.668221
H	-6.753028	0.613225	-0.023883
H	-5.672788	0.898368	1.411639
H	-5.964080	-0.780104	0.838132
H	-1.324375	1.273093	0.596580
H	-1.873890	2.317911	-0.713241
H	3.858952	1.774233	0.009295
H	4.018800	2.775319	-1.488981
H	3.064512	3.379591	-0.062174
H	-1.185170	-0.970470	-2.252886
H	-2.602440	-1.837300	-1.614378
H	0.758732	-2.600842	-2.301301
H	1.350311	-0.929986	-2.657149
H	2.520966	-2.283990	-2.368552
H	-1.057977	-0.430935	2.114245
H	0.231960	-0.868939	3.296139
H	0.194144	0.784371	2.525779
H	-0.776589	-2.833887	-0.484087
H	-1.517166	-1.755435	0.707330
H	4.818560	-1.023689	0.310170
H	4.316830	-2.366718	-0.756838
H	4.237437	-0.670537	-1.344721
H	4.083043	-0.195779	2.291459
H	2.741274	0.987651	2.489583
H	2.734129	-0.562073	3.410819

(3)Cspiro$_C$(MA)

C	-2.645239	-1.109491	0.455451
C	-2.194836	-1.324886	-0.818149
N	-0.775681	-1.304341	-0.803090
C	-0.349863	-0.665556	0.445922
N	-1.508949	-0.959803	1.301408
C	-2.954621	-1.655831	-2.060477
C	-0.002938	-1.209298	-2.031250
C	0.967599	-1.293670	0.998576
C	1.936689	-0.300240	1.650783
C	2.427052	0.779504	0.639898
H	2.873450	1.608930	1.225791
C	-1.607232	-0.402913	2.631903
C	-4.028703	-1.194569	1.011071
C	3.554350	0.183485	-0.198889
O	3.427057	-0.422629	-1.251020
O	4.758446	0.362574	0.407165
C	5.885171	-0.230808	-0.260892
C	1.265217	1.294729	-0.253415
C	-0.125480	0.947279	0.317120
C	-1.227597	1.625280	-0.464090
O	-1.267443	1.770082	-1.678437
H	-0.190548	1.335851	1.353475
O	-2.183764	2.141054	0.371976
C	-3.307146	2.743427	-0.283508
H	6.770251	0.020456	0.351652
H	5.995417	0.177067	-1.286368
H	5.766903	-1.331408	-0.335508
H	1.369444	0.872998	-1.270447
H	1.349421	2.395305	-0.372414
H	-3.896334	1.976077	-0.829356
H	-3.922846	3.198910	0.514263
H	-2.980129	3.513726	-1.011369
H	1.447307	0.216496	2.503272
H	2.808341	-0.834700	2.084081
H	-0.678470	-0.613855	3.202757
H	-1.794596	0.700156	2.664447
H	-2.433189	-0.898008	3.181502
H	1.078418	-1.314235	-1.812231
H	-0.279184	-2.043976	-2.708593
H	-0.151402	-0.248252	-2.575908
H	0.674850	-2.093417	1.709150
H	1.482860	-1.805554	0.159809
H	-4.761545	-1.371908	0.200071
H	-4.136053	-2.032140	1.739508
H	-4.337222	-0.265807	1.541519
H	-4.043293	-1.677833	-1.859017
H	-2.775829	-0.910407	-2.866742
H	-2.672510	-2.652769	-2.469361

(3)C-D(MA)

N	-1.736604	-1.678214	-0.129176
C	-3.103889	-1.623251	-0.453058
C	-3.588166	-0.424464	0.024567
N	-2.514548	0.232716	0.645040
C	-1.372712	-0.542655	0.566089
C	-3.795749	-2.721667	-1.193329
C	-4.963499	0.155416	-0.044565
C	-2.565032	1.530129	1.308538
C	-0.074345	-0.086311	0.985723
C	0.992555	-0.974242	1.658483
C	2.435173	-0.527651	1.297337

C	2.553054	1.011518	0.984489
C	1.816331	1.438904	-0.268839
H	2.292368	1.215619	-1.239689
C	-0.833960	-2.746080	-0.539500
H	3.109448	-0.738049	2.155168
C	2.989275	-1.320855	0.125579
O	4.338890	-1.187758	0.032800
C	4.957836	-1.849306	-1.081105
O	2.345069	-1.994479	-0.668896
C	0.968700	2.593787	-0.248920
O	0.782959	3.145023	-1.516303
C	-0.172241	4.194028	-1.596364
O	0.338153	3.042133	0.733472
H	6.040445	-1.642090	-0.996691
H	4.770361	-2.942491	-1.047897
H	4.565282	-1.458216	-2.042218
H	2.142563	1.569461	1.854026
H	3.638304	1.255151	0.935930
H	-1.218629	3.811789	-1.543456
H	-0.021803	4.684048	-2.578984
H	-0.043718	4.931485	-0.775975
H	0.874601	-0.908065	2.761893
H	0.871907	-2.044428	1.400987
H	-1.145700	-3.129022	-1.530323
H	-0.846082	-3.592751	0.181227
H	0.203053	-2.364099	-0.626388
H	-2.521054	1.413187	2.413073
H	-3.512436	2.034350	1.046062
H	-1.708348	2.171601	0.994634
H	-0.206680	0.843705	1.570523
H	0.572228	0.457633	0.048324
H	-4.876522	-2.501144	-1.283387
H	-3.697022	-3.701184	-0.677126
H	-3.400609	-2.852827	-2.224982
H	-5.649761	-0.550887	-0.549328
H	-4.990717	1.107455	-0.618950
H	-5.383967	0.365090	0.963171

(3)D(MA)

C	-3.949028	0.044092	-0.851315
C	-4.085066	-1.158165	-0.205134
N	-3.050217	-1.242104	0.746921
C	-2.254951	-0.088237	0.708514
N	-2.815257	0.701169	-0.310280
C	-5.072791	-2.259252	-0.413435
C	-2.777072	-2.340539	1.639495
C	-1.171929	0.142627	1.540673
C	-0.143548	1.231681	1.410716
C	0.918106	0.991015	0.261245
C	1.584690	2.317770	-0.060038
O	2.821654	2.449639	0.499672
C	3.458442	3.721834	0.300331
C	-2.558838	2.122156	-0.475835
C	-4.760324	0.630100	-1.960701
C	1.861237	-0.173621	0.591684
C	2.760010	-0.602874	-0.571875
C	3.577389	-1.848069	-0.269784
O	4.590267	-1.993294	-1.171259
C	5.401300	-3.165969	-1.001800
O	1.051601	3.219112	-0.692367
O	3.372552	-2.639746	0.632819
H	0.332857	0.744121	-0.651954
H	3.456308	0.204859	-0.880185
H	2.150017	-0.831198	-1.476657
H	4.432659	3.661606	0.819491
H	2.844260	4.542824	0.724080
H	3.608517	3.925216	-0.779979
H	1.241216	-1.039097	0.906974
H	2.490171	0.095616	1.466781
H	4.790501	-4.088878	-1.084365
H	6.158935	-3.134089	-1.806380
H	5.895048	-3.167392	-0.008021
H	0.418262	1.324459	2.365474
H	-0.594783	2.229263	1.232505
H	-3.146344	2.495980	-1.334548
H	-2.860691	2.701233	0.427338
H	-1.491614	2.339070	-0.685357
H	-2.891744	-2.041141	2.706891
H	-3.474387	-3.173729	1.435275
H	-1.734043	-2.709220	1.506869
H	-0.972912	-0.641405	2.284643
H	-5.550553	-0.080467	-2.270964
H	-5.269129	1.577496	-1.672391
H	-4.143818	0.851357	-2.860823
H	-5.787927	-1.985622	-1.212646
H	-4.588674	-3.214628	-0.718430
H	-5.668162	-2.472680	0.502532

DMAA

C	-1.448817	0.657806	0.040914
C	-0.327208	-0.345183	0.002461
O	-0.568821	-1.557677	-0.013802
C	-2.724751	0.228488	-0.015354
H	-3.572588	0.930272	0.021373
H	-2.928792	-0.851988	-0.097052
H	-1.243859	1.735462	0.132932

N	0.980935	0.131219	-0.004979
C	1.404332	1.521106	-0.028472
H	0.556102	2.207804	-0.187254
H	1.913912	1.810265	0.920304
H	2.127932	1.688660	-0.858092
C	2.063559	-0.842783	0.021758
H	2.706836	-0.694674	0.918478
H	1.615203	-1.852576	0.048875
H	2.706592	-0.746943	-0.882133

(3)A-B(DMAA)

C	-1.487147	1.111998	0.159850
N	-1.869693	0.259709	-0.853919
C	-1.894399	-1.060416	-0.382774
C	-1.564908	-1.025910	0.954047
N	-1.289910	0.317986	1.269285
C	-1.849418	0.641403	-2.256558
C	-0.978225	0.849242	2.584671
C	-1.143775	2.481698	0.064938
C	0.912426	2.569971	-0.352269
C	1.717611	1.534399	0.154661
C	1.852810	0.294746	-0.592551
O	1.164002	0.029153	-1.612844
C	2.848216	-1.951381	-0.781520
H	3.862001	-2.177487	-1.188161
H	2.582951	-2.772167	-0.070541
H	2.119701	-1.939637	-1.614277
H	1.022769	3.574903	0.088928
H	0.745532	2.566812	-1.441589
H	-1.562079	3.028941	-0.793622
H	-1.198344	3.048119	1.007054
C	-1.457105	-2.129256	1.954345
C	-2.207028	-2.219499	-1.271135
H	-0.120644	1.545269	2.520309
H	-1.849906	1.386983	3.022480
H	-0.698918	0.020245	3.259767
H	-2.287968	1.651704	-2.376274
H	-0.794551	0.633863	-2.608445
H	-2.458043	-0.069219	-2.846199
H	-1.447942	-2.329533	-2.075400
H	-2.214043	-3.160162	-0.688075
H	-3.202747	-2.122557	-1.756698
H	-2.152271	-1.999715	2.813235
H	-1.701522	-3.097685	1.477712
H	-0.428232	-2.218489	2.368548
H	2.171066	1.640934	1.152205
N	2.805845	-0.647259	-0.152928
C	3.719406	-0.414023	0.945390
H	3.318642	-0.732849	1.941336
H	4.660584	-0.981286	0.775272
H	3.987469	0.658902	1.011554

(3)B(DMAA)

N	-1.943416	0.833032	-0.282942
C	-2.385651	-0.492612	-0.334571
C	-1.703908	-1.180418	0.647143
N	-0.848159	-0.261711	1.269824
C	-0.952841	0.945725	0.648948
C	-3.395741	-0.970020	-1.325523
C	-1.762145	-2.615772	1.053744
C	0.167637	-0.649402	2.241826
C	-0.255844	2.205729	1.033347
C	1.075334	2.529615	0.242138
C	2.074749	1.420689	0.246346
C	1.744132	0.287647	-0.512758
O	0.652762	0.207794	-1.189816
C	-2.107924	1.798711	-1.360850
N	2.584805	-0.880779	-0.495874
C	2.475536	-1.768228	-1.640913
H	3.012924	1.534493	0.805506
H	2.679688	-2.823244	-1.348576
H	1.444041	-1.680390	-2.031997
H	3.185391	-1.505944	-2.469799
H	1.486397	3.452745	0.705783
H	0.761985	2.798849	-0.794585
H	-0.982636	3.041763	0.917542
H	-0.016629	2.152694	2.115057
H	0.708452	0.248905	2.586854
H	-0.303010	-1.173210	3.099659
H	0.915496	-1.306310	1.750261
H	-2.098613	2.828361	-0.953402
H	-1.259635	1.675916	-2.066778
H	-3.074453	1.631579	-1.870327
H	-3.633243	-2.035474	-1.144542
H	-4.349329	-0.402371	-1.263401
H	-3.019209	-0.886880	-2.367976
H	-2.498177	-3.161430	0.433376
H	-0.778620	-3.115525	0.921209
H	-2.061692	-2.744256	2.116544
C	3.907277	-0.793263	0.088219
H	4.356619	-1.807918	0.148933
H	4.613714	-0.141439	-0.490329
H	3.852172	-0.387461	1.119886

(3)B-Bspiro$_O$(DMAA)

C	0.526256	0.504327	0.576568
N	1.325772	-0.539655	1.126171

C	2.407151	-0.808406	0.240485
C	2.443402	0.194200	-0.686951
N	1.384846	1.094999	-0.388454
C	0.717013	-1.585808	1.928483
C	0.900171	2.111121	-1.301971
C	-0.154194	1.430536	1.592216
C	-1.416267	2.165184	1.103119
C	-2.407332	1.203158	0.505189
C	-1.968405	0.040697	-0.075525
O	-0.658685	-0.255869	-0.252556
C	-2.397035	-1.759255	-1.696896
H	-2.842536	-2.776763	-1.659826
H	-2.715821	-1.283368	-2.660747
H	-1.296598	-1.853197	-1.704709
H	-1.133334	2.979579	0.392142
H	-1.861746	2.693993	1.974876
H	-0.440885	0.805324	2.462971
H	0.622373	2.139691	1.948387
C	3.430150	0.461915	-1.775350
C	3.335545	-1.957783	0.459977
H	-0.023561	1.786340	-1.831819
H	0.681582	3.061670	-0.770563
H	1.680458	2.327220	-2.055213
H	0.050568	-1.140668	2.693367
H	0.109485	-2.293058	1.319630
H	1.503402	-2.150409	2.466914
H	2.964137	0.463712	-2.786488
H	3.942540	1.443167	-1.650745
H	4.214444	-0.319590	-1.779958
H	3.822876	-1.920065	1.461103
H	2.822876	-2.943063	0.386344
H	4.141866	-1.951748	-0.298944
H	-3.478840	1.432649	0.558780
N	-2.807152	-0.993722	-0.527090
C	-4.236875	-0.831507	-0.365287
H	-4.680277	-0.051639	-1.038033
H	-4.741177	-1.795071	-0.586902
H	-4.474091	-0.549374	0.681144

(3)Bspiro$_O$(DMAA)

N	-1.503112	-0.415961	-1.133493
C	-0.475117	0.445845	-0.604463
N	-1.132674	1.068623	0.524668
C	-2.287733	0.299046	0.858547
C	-2.510475	-0.598179	-0.143681
C	0.122668	1.391662	-1.662020
C	1.416303	2.108962	-1.246510
C	2.359194	1.165690	-0.549433
C	1.942068	-0.052956	-0.084851
O	0.644406	-0.483460	-0.118753
C	2.296920	-1.872131	1.538749
C	-0.344524	1.686054	1.580914
C	-1.150042	-1.478652	-2.059057
H	2.793715	-2.865748	1.511251
H	2.500160	-1.417755	2.542825
H	1.207410	-2.020279	1.437700
H	1.174990	2.998778	-0.613047
H	1.888598	2.541035	-2.158605
H	0.337309	0.770806	-2.557161
H	-0.674040	2.107991	-1.944904
C	-3.113143	0.622225	2.061132
C	-3.649919	-1.538816	-0.362853
H	0.159418	0.941638	2.242869
H	0.437963	2.334979	1.148937
H	-0.999158	2.323643	2.208429
H	-0.461817	-1.091043	-2.835727
H	-0.650900	-2.346043	-1.567888
H	-2.059867	-1.837951	-2.580660
H	-4.006829	-0.030299	2.102922
H	-2.558188	0.480507	3.015427
H	-3.471638	1.677290	2.050189
H	-3.319875	-2.597867	-0.452682
H	-4.362256	-1.488620	0.483293
H	-4.217825	-1.298018	-1.290974
H	3.404216	1.470513	-0.407204
N	2.780816	-1.044475	0.440758
C	4.209479	-0.808327	0.428820
H	4.737314	-1.757877	0.655914
H	4.531935	-0.462753	-0.574569
H	4.544846	-0.045095	1.178393

(3)Bspiro$_C$(DMAA)

C	0.610757	0.845420	0.530183
N	0.994659	-0.406560	1.151550
C	2.016621	-1.021047	0.382898
C	2.475107	-0.111229	-0.522540
N	1.749798	1.106965	-0.334916
C	0.118218	-1.102545	2.058653
C	2.479821	-2.410962	0.664108
C	3.608813	-0.201545	-1.489260
C	1.645208	2.084280	-1.392638
C	0.155453	1.967415	1.522204
H	0.524664	2.958292	1.187618
C	-0.911851	0.944904	-0.109579
C	-1.561776	-0.334726	-0.617661
N	-2.947065	-0.470277	-0.546989

C	-3.539195	-1.744702	-0.926244
C	-1.334219	1.736639	1.162665
H	0.472262	1.821080	2.575473
H	-0.832025	1.638791	-0.973456
O	-0.855092	-1.237752	-1.080951
H	-1.942535	2.651719	1.008311
H	-1.859732	1.098795	1.902643
H	1.232178	3.036991	-0.998806
H	2.652121	2.317260	-1.793712
H	1.004780	1.762709	-2.255169
H	-0.144995	-0.461391	2.929058
H	-0.834463	-1.456355	1.592438
H	0.636888	-1.992592	2.463945
H	3.323961	-2.678092	-0.000632
H	2.832523	-2.540430	1.713654
H	1.673182	-3.158898	0.492615
H	4.084808	-1.199795	-1.432447
H	3.290541	-0.051582	-2.546093
H	4.401689	0.554691	-1.280492
H	-4.159559	-1.645240	-1.846745
H	-2.717713	-2.457531	-1.125923
H	-4.192472	-2.135262	-0.113482
C	-3.885652	0.603806	-0.278415
H	-4.641977	0.664855	-1.094593
H	-4.440272	0.451154	0.676945
H	-3.368708	1.577707	-0.227282

(3)B-C(DMAA)

C	1.067539	2.781775	-0.262530
C	-0.064569	2.889597	-1.050784
N	-1.123767	2.346136	-0.314608
C	-0.669709	1.914688	0.892380
N	0.658401	2.199250	0.937942
C	-0.231578	3.432946	-2.432098
C	-2.512657	2.271166	-0.775789
C	-1.453880	1.230497	1.961296
C	-1.138315	-0.285221	2.168612
C	-1.475984	-1.229561	1.037392
C	1.571428	1.860509	2.028136
C	2.500871	3.076762	-0.552609
C	-2.765663	-1.189381	0.418114
O	-3.571491	-0.202554	0.518121
C	-4.530910	-2.298298	-0.894143
C	0.182514	-1.014758	-0.907773
C	1.307294	-1.810277	-0.803750
C	2.572270	-1.301047	-0.276867
O	2.743470	-0.095653	0.056652
C	4.963637	-1.682762	0.158931
H	-4.580069	-2.599395	-1.965444
H	-4.954927	-1.284656	-0.769364
H	-5.164098	-3.015855	-0.313291
H	0.272667	0.061092	-0.708198
H	-0.698186	-1.346201	-1.474013
H	5.393283	-2.203190	1.045467
H	5.677858	-1.810908	-0.689128
H	4.861968	-0.605295	0.383760
H	-1.694597	-0.549634	3.105622
H	-0.063301	-0.409890	2.425986
H	2.199174	2.741225	2.267138
H	0.987906	1.585423	2.923303
H	2.207301	1.012139	1.691648
H	-3.014423	1.381969	-0.314035
H	-3.053455	3.206083	-0.519427
H	-2.514880	2.146410	-1.874162
H	-1.283367	1.773354	2.918804
H	-2.530198	1.294326	1.710618
H	2.605937	3.536484	-1.553333
H	2.947839	3.773625	0.188153
H	3.072958	2.123023	-0.535080
H	0.726617	3.854825	-2.789755
H	-0.538304	2.646491	-3.154918
H	-0.991857	4.241654	-2.474277
H	1.241917	-2.858760	-1.130636
H	-0.973665	-2.201095	1.127002
N	3.644801	-2.195755	-0.165356
N	-3.158536	-2.265510	-0.423155
H	2.598556	-4.043523	-0.172274
C	-2.465425	-3.539313	-0.425396
H	-2.708537	-4.177911	0.462626
H	-2.748783	-4.111932	-1.334382
H	-1.367769	-3.399282	-0.452663

(3)C(DMAA)

C	-0.618518	-1.456354	0.459321
N	-1.784290	-1.388695	1.178379
C	-2.870652	-1.272478	0.298804
C	-2.357719	-1.367743	-0.978708
N	-0.975081	-1.528711	-0.854089
C	-1.828187	-1.104376	2.598766
C	-4.277097	-1.095163	0.769486
C	-3.011954	-1.224562	-2.310206
C	-0.067845	-1.604133	-1.996654
C	0.706910	-1.854140	1.036843
C	1.537102	-0.773949	1.766483
C	2.277442	0.267932	0.900428
C	3.416446	-0.368629	0.093673

N	4.549936	0.384825	-0.167654
C	4.800807	1.749115	0.269043
C	1.361681	1.075331	-0.078390
C	-0.001199	1.438335	0.448317
C	-1.035870	1.687699	-0.507945
N	-2.170019	2.459546	-0.104632
C	-2.343550	2.949972	1.240048
O	-1.014597	1.269985	-1.709736
O	3.309572	-1.519914	-0.367737
C	5.602372	-0.199106	-0.989743
C	-3.324288	2.488716	-0.974028
H	6.567781	-0.223186	-0.435967
H	5.753970	0.394037	-1.919646
H	5.300335	-1.228566	-1.254666
H	1.229307	0.501907	-1.017919
H	1.955799	1.974383	-0.393142
H	-2.977819	2.257922	-1.999490
H	-4.114426	1.738308	-0.699084
H	-3.804558	3.493077	-0.962642
H	0.879825	-0.213593	2.461508
H	2.288455	-1.307120	2.389162
H	-1.095243	-1.732589	3.141446
H	-1.579121	-0.030602	2.769692
H	-2.836518	-1.323215	2.994853
H	0.967300	-1.762149	-1.642632
H	-0.359897	-2.446229	-2.656427
H	-0.124246	-0.631849	-2.527754
H	0.507542	-2.684620	1.753209
H	1.346058	-2.283111	0.242452
H	-4.961534	-1.050041	-0.098554
H	-4.614593	-1.936272	1.415167
H	-4.411094	-0.153594	1.343807
H	-4.108107	-1.124237	-2.198892
H	-2.618224	-0.301383	-2.789001
H	-2.813384	-2.088530	-2.979249
H	2.700448	0.985257	1.636922
H	-0.019030	1.981361	1.408888
H	-3.131723	3.732948	1.253140
H	-2.647026	2.165255	1.985873
H	-1.409645	3.414545	1.621247
H	5.706445	1.800130	0.917216
H	4.978691	2.412490	-0.607314
H	3.945336	2.161132	0.830323

(3)C-Cspiro$_C$(DMAA)

N	-1.800611	-1.328852	1.156788
C	-2.904366	-1.226801	0.293119
C	-2.414209	-1.316709	-0.991827
N	-1.024700	-1.456062	-0.896776
C	-0.633614	-1.313470	0.414162
C	-4.307158	-1.085692	0.787011
C	-3.099666	-1.201307	-2.310914
C	-0.145337	-1.549074	-2.057254
C	0.674240	-1.835026	0.955761
C	1.568037	-0.858773	1.743512
C	2.304830	0.214495	0.911595
C	1.374365	0.987963	-0.075589
C	-0.022450	1.226238	0.445423
C	-1.023721	1.643127	-0.503479
C	-3.270186	2.570183	-0.921371
C	-1.825998	-1.068609	2.578737
C	3.471815	-0.398768	0.122728
C	5.646489	-0.165663	-0.970889
O	3.416723	-1.570526	-0.287052
O	-0.977887	1.357257	-1.735702
H	6.609629	-0.137820	-0.413131
H	5.779487	0.407841	-1.915789
H	5.386439	-1.213276	-1.208334
H	1.312634	0.435861	-1.035610
H	1.896961	1.941135	-0.348724
H	-2.925665	2.358550	-1.951584
H	-4.116646	1.873841	-0.682603
H	-3.668358	3.608853	-0.870179
H	0.960234	-0.334785	2.508874
H	2.321658	-1.461858	2.293870
H	-1.097750	-1.716770	3.106207
H	-1.562810	-0.003683	2.780742
H	-2.832632	-1.281559	2.982944
H	0.890148	-1.746949	-1.725218
H	-0.470965	-2.382681	-2.712838
H	-0.169946	-0.580828	-2.596654
H	0.430267	-2.705765	1.607911
H	1.284147	-2.244690	0.128915
H	-5.008132	-1.058045	-0.068746
H	-4.612669	-1.936328	1.436718
H	-4.458571	-0.150110	1.367857
H	-4.192759	-1.094166	-2.176349
H	-2.719807	-0.297250	-2.835157
H	-2.922803	-2.083192	-2.963316
H	2.700098	0.940324	1.655439
H	-0.071991	1.641820	1.466903
N	4.567669	0.398263	-0.169596
N	-2.134290	2.405977	-0.040505
C	-2.301097	2.827856	1.329424
H	-2.977103	3.709758	1.369636

H	-2.744621	2.047970	2.004918
H	-1.331155	3.135134	1.771748
C	4.757345	1.783859	0.227821
H	5.662725	1.894366	0.868893
H	4.900397	2.431893	-0.666438
H	3.886491	2.170310	0.783931

(3)Cspiro$_C$(DMAA)

C	0.188183	0.851210	-0.424911
C	0.724257	-0.549080	0.080307
C	-0.491282	-1.462277	0.462539
C	-1.720441	-1.330935	-0.449853
C	-2.284612	0.131831	-0.457500
C	-1.246345	1.141465	0.071259
N	1.621068	-1.174076	-0.942268
C	2.698756	-1.814723	-0.244256
C	2.724163	-1.347172	1.036638
N	1.669291	-0.418100	1.219759
C	3.696580	-2.655695	-0.972752
C	3.747333	-1.571780	2.103773
C	1.182904	-0.079392	2.546971
C	1.039071	-1.846504	-2.087912
C	-3.560242	0.201136	0.408833
C	-5.977294	-0.099512	0.633784
C	1.098154	2.029618	0.006660
C	2.882497	3.620873	-0.469958
O	-3.499371	0.515604	1.601222
O	0.842510	2.646887	1.048868
H	-6.431122	-1.111798	0.732599
H	-6.736489	0.574444	0.177319
H	-5.700673	0.275993	1.635903
H	-1.276753	1.141396	1.177280
H	-1.540713	2.168954	-0.225325
H	2.446496	4.041520	0.454647
H	3.955881	3.382713	-0.295371
H	2.826003	4.375527	-1.286768
H	-1.477031	-1.636715	-1.486600
H	-2.500442	-2.044496	-0.106221
H	0.353867	-1.161928	-2.631106
H	1.844219	-2.119668	-2.799583
H	0.473396	-2.783929	-1.848548
H	0.548351	0.825532	2.486708
H	0.618904	-0.898507	3.060597
H	2.044687	0.188079	3.190209
H	-0.137903	-2.514443	0.514253
H	-0.811209	-1.193279	1.489244
H	4.502295	-2.981682	-0.286633
H	3.254474	-3.576736	-1.415656
H	4.180751	-2.099060	-1.810086
H	4.525564	-2.278172	1.756225
H	4.257259	-0.623631	2.390579
H	3.307523	-1.993304	3.034508
H	0.161803	0.792011	-1.535021
H	-2.531371	0.408448	-1.503718
N	2.132424	2.422516	-0.821990
N	-4.770163	-0.143581	-0.181464
C	-4.965085	-0.601528	-1.546293
H	-5.447875	-1.605813	-1.558592
H	-5.627688	0.092082	-2.114455
H	-4.007650	-0.683816	-2.088571
C	2.532944	1.752525	-2.050012
H	2.113015	2.245637	-2.959283
H	3.640458	1.783134	-2.137024
H	2.241270	0.683899	-2.014400

(3)C-D(DMAA)

C	-3.548146	-1.881222	0.636116
C	-3.910490	-1.035982	-0.391725
N	-2.730874	-0.471753	-0.897910
C	-1.638865	-0.957525	-0.209650
N	-2.147567	-1.813189	0.747786
C	-5.261870	-0.717228	-0.944229
C	-2.633052	0.477226	-2.003343
C	-0.288672	-0.475711	-0.386689
C	0.950849	-1.392916	-0.381479
C	2.219943	-0.618086	0.053705
C	-1.358207	-2.464189	1.780812
C	-4.387896	-2.742646	1.522464
C	3.467083	-1.301887	-0.534856
O	3.402888	-1.978775	-1.567799
C	5.880885	-1.697728	-0.470301
C	2.172179	0.899612	-0.356199
C	1.180639	1.709604	0.455062
C	0.261940	2.604011	-0.201278
O	-0.142403	2.420376	-1.391506
C	-1.438448	4.381433	-0.005512
H	6.613792	-0.911909	-0.764056
H	5.578428	-2.270470	-1.366121
H	6.380740	-2.376939	0.257208
H	1.914033	0.975410	-1.434509
H	3.204263	1.315181	-0.268346
H	-1.522200	4.110409	-1.075171
H	-2.396072	4.112057	0.510244
H	-1.313702	5.485171	0.083973
H	1.136096	-1.795091	-1.399188
H	0.825920	-2.278925	0.274562

H	-1.997266	-2.663870	2.661489
H	-0.923770	-3.426374	1.434750
H	-0.533513	-1.795857	2.094990
H	-2.300216	-0.032117	-2.933052
H	-3.626498	0.926853	-2.181410
H	-1.896113	1.283100	-1.763428
H	-0.270787	0.159816	-1.294632
H	0.002581	0.423089	0.378508
H	-5.448504	-2.687478	1.211689
H	-4.084604	-3.811386	1.479436
H	-4.344587	-2.428449	2.589068
H	-6.038361	-1.306280	-0.420115
H	-5.522777	0.356555	-0.820131
H	-5.338225	-0.953160	-2.027742
H	2.279190	-0.642960	1.164904
H	1.474455	1.909282	1.499664
N	4.684019	-1.105839	0.110404
N	-0.290155	3.682961	0.533013
C	4.908805	-0.312848	1.306267
H	5.369994	-0.931641	2.111290
H	5.603988	0.533811	1.100076
H	3.967982	0.112043	1.695271
C	0.080890	3.987348	1.896407
H	-0.136726	5.056089	2.112197
H	-0.462652	3.377118	2.663805
H	1.167862	3.831270	2.052724

(3)D(DMAA)

C	4.714258	-0.580512	-0.025714
N	3.866620	-0.122527	-1.053959
C	2.729404	0.496552	-0.513236
N	2.892507	0.389249	0.877970
C	4.119981	-0.256168	1.167230
C	4.069544	-0.260853	-2.473441
C	1.722311	1.071323	-1.270867
C	0.387266	1.591488	-0.796698
C	-0.643542	0.464899	-0.419157
H	-0.066403	-0.263738	0.187364
C	2.118967	1.132829	1.856904
C	4.578869	-0.518256	2.564728
C	5.989873	-1.306163	-0.302942
C	-1.156563	-0.322966	-1.643857
C	-1.942102	-1.600953	-1.291129
H	-2.047314	-2.217898	-2.210896
C	-1.693524	0.930537	0.609021
O	-1.623240	0.482730	1.770899
C	-3.381147	-1.307906	-0.844780
O	-4.107244	-0.596428	-1.555071
N	-3.837755	-1.883367	0.323996
C	-5.203453	-1.598354	0.747152
N	-2.645086	1.873409	0.274600
C	-3.630740	2.251584	1.279712
H	-1.370821	-2.208460	-0.563206
H	-3.667882	3.357517	1.392088
H	-3.339022	1.786427	2.238988
H	-4.646098	1.899632	0.988162
H	-0.254993	-0.606605	-2.229914
H	-1.788782	0.298425	-2.310434
H	-5.711983	-1.067805	-0.078562
H	-5.747168	-2.540826	0.976092
H	-5.220240	-0.955874	1.656276
H	-0.037702	2.228058	-1.602769
H	0.479771	2.267391	0.080078
H	2.480899	0.876924	2.869736
H	2.233609	2.232035	1.720487
H	1.038957	0.880542	1.821767
H	4.172021	0.730498	-2.972903
H	4.988338	-0.844247	-2.667517
H	3.208476	-0.784788	-2.949823
H	1.880274	1.038432	-2.357862
H	5.530529	-1.083743	2.551708
H	4.762043	0.415718	3.142539
H	3.844620	-1.121877	3.144185
H	6.494943	-1.568375	0.646485
H	5.828440	-2.255780	-0.862183
H	6.705498	-0.694972	-0.897661
C	-2.979234	-2.580482	1.284708
H	-3.622751	-3.035977	2.062460
H	-2.410406	-3.405756	0.809675
H	-2.271023	-1.880654	1.780571
C	-2.903469	2.394647	-1.062166
H	-3.178768	3.468859	-0.989184
H	-2.005932	2.324461	-1.699325
H	-3.731464	1.837217	-1.554126

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C	-1.566828	0.683261	-0.000435
C	-1.566646	-0.683540	-0.000707
N	-0.220413	-1.113416	-0.000410
C	0.662196	0.000163	-0.000055
N	-0.220718	1.113522	0.000000
C	-2.722103	-1.631240	-0.001465
C	0.148762	-2.516189	0.005104
C	2.051480	0.000180	-0.000094
C	0.147950	2.516442	0.001442
C	-2.722543	1.630645	-0.001081

H	-0.775071	-3.122979	0.003314
H	0.734149	-2.803598	-0.891246
H	0.727153	-2.798212	0.907874
H	-0.776127	3.122864	0.000262
H	0.728269	2.800909	0.902139
H	0.731165	2.801886	-0.897002
C	2.879780	1.284578	0.001624
C	2.879591	-1.284328	-0.004653
H	-3.673460	-1.065228	-0.002225
H	-2.737062	-2.293546	-0.896838
H	-2.738481	-2.293417	0.893969
H	-3.673746	1.064375	-0.001755
H	-2.738970	2.292769	0.894390
H	-2.737810	2.292995	-0.896417
H	3.955999	-1.018986	-0.003325
H	2.738599	-1.935523	0.886734
H	2.739052	-1.928341	-0.901458
H	3.956142	1.019049	0.002362
H	2.739965	1.932951	-0.892100
H	2.738320	1.931459	0.896109

(4)A-B(MMA)

C	1.352320	0.411714	0.120081
N	0.952087	1.339937	-0.834309
C	0.084323	2.279649	-0.261051
C	-0.055007	1.958676	1.065295
N	0.721794	0.805319	1.292083
C	0.949686	1.158968	-2.286695
C	0.853046	0.214954	2.619801
C	2.085538	-0.805248	-0.140372
C	0.622159	-2.028018	-0.916669
C	-0.617643	-2.109329	-0.237233
C	-0.836904	-3.043770	0.931962
C	-1.666167	-1.207512	-0.649974
O	-1.644171	-0.370735	-1.574323
O	-2.824480	-1.353953	0.114303
C	-3.928387	-0.562370	-0.306319
H	-0.823904	-2.533037	1.929322
H	-1.825195	-3.547548	0.878112
H	-0.053798	-3.831289	0.964379
H	-4.758371	-0.787113	0.392476
H	-3.693247	0.523988	-0.277152
H	-4.238630	-0.804332	-1.346544
H	1.282934	-2.914044	-0.868294
H	0.589649	-1.558666	-1.914299
C	-0.855790	2.631785	2.132171
C	-0.562109	3.362114	-1.062424
H	0.294289	-0.740337	2.700748
H	1.912330	0.042089	2.878388
H	0.434518	0.920384	3.359325
H	1.767491	0.494504	-2.599253
H	-0.025997	0.706806	-2.570911
H	1.092825	2.139543	-2.780303
H	-1.245532	2.940965	-1.830343
H	-1.161329	4.019906	-0.404642
H	0.181887	4.002015	-1.584238
H	-0.228985	3.021921	2.964773
H	-1.396094	3.496516	1.702080
H	-1.618656	1.955049	2.574303
C	3.174526	-0.726344	-1.223717
H	4.080668	-1.273533	-0.889905
H	2.868384	-1.200606	-2.185908
H	3.506011	0.309139	-1.447809
C	2.562891	-1.670292	1.028423
H	3.381379	-1.201823	1.622942
H	1.754557	-1.977609	1.715270
H	2.979959	-2.612038	0.613548

(4)B(MMA)

C	-2.497440	-0.268968	-0.168210
C	-1.964952	-0.698840	1.025970
N	-0.789826	0.032564	1.231947
C	-0.592254	0.902952	0.196637
N	-1.646302	0.724179	-0.660104
C	-2.449332	-1.746809	1.974367
C	0.158415	-0.317258	2.298231
C	0.501991	1.968499	0.095758
C	1.776264	1.390614	-0.666668
C	2.296322	0.057291	-0.212210
C	1.581456	-1.040265	-0.717021
O	2.092259	-2.309696	-0.357617
C	1.491657	-3.411940	-1.009914
C	-1.649828	1.105050	-2.075957
C	-3.717873	-0.736201	-0.892534
C	3.629249	-0.054108	0.492057
O	0.517825	-0.990877	-1.410451
H	3.651310	0.380794	1.525689
H	3.921543	-1.118178	0.591077
H	4.455998	0.462305	-0.058492
H	1.828447	-4.324949	-0.476158
H	0.381320	-3.349031	-0.996631
H	1.800990	-3.492283	-2.079772
H	2.555994	2.180431	-0.562117
H	1.497594	1.360339	-1.748103
C	-0.011918	3.226470	-0.653843
C	0.935613	2.457178	1.505186

H	1.180678	-0.203921	1.885464
H	-0.007920	0.289914	3.210597
H	0.019604	-1.385535	2.540810
H	-1.927766	2.164249	-2.225230
H	-0.647551	0.870721	-2.485346
H	-2.384661	0.470702	-2.600610
H	-4.307383	-1.410620	-0.242731
H	-4.379901	0.104517	-1.188808
H	-3.462681	-1.308996	-1.810720
H	-3.450463	-2.102613	1.665132
H	-1.778428	-2.633181	1.993160
H	-2.534866	-1.368369	3.014787
H	1.527934	3.385919	1.381219
H	0.071602	2.699181	2.160467
H	1.589068	1.733609	2.022002
H	0.738814	4.032835	-0.531739
H	-0.115029	3.062883	-1.741908
H	-0.976251	3.604664	-0.251489

(4)B-Bspiro$_O$(MMA)

C	0.417372	-0.364461	-0.115198
N	1.508632	-0.202004	-1.017001
C	2.621770	0.366838	-0.337367
C	2.308981	0.438611	0.987869
N	0.999482	-0.082464	1.149457
C	1.331395	-0.012761	-2.452937
C	0.241569	0.081136	2.381365
C	-0.445046	-1.672702	-0.224403
C	-1.741447	-1.561404	0.629295
C	-2.536596	-0.298365	0.401088
C	-3.992028	-0.288955	0.791536
C	-1.921206	0.777940	-0.177303
O	-0.623834	0.870310	-0.511532
O	-2.655472	1.889291	-0.515179
C	-1.965135	3.133215	-0.596718
H	-4.439354	0.714838	0.659945
H	-4.593627	-1.007695	0.185439
H	-4.134629	-0.590871	1.856092
H	-2.731125	3.889890	-0.856214
H	-1.494265	3.412766	0.373586
H	-1.175106	3.125017	-1.376305
H	-1.505831	-1.706307	1.711207
H	-2.371796	-2.445461	0.372065
C	3.136574	0.878658	2.151055
C	3.891127	0.707239	-1.047253
H	0.703601	0.877761	2.995848
H	-0.797619	0.394011	2.159696
H	0.212805	-0.845384	2.997884
H	0.284801	0.266309	-2.668858
H	1.968339	0.824132	-2.801167
H	1.600739	-0.913431	-3.046604
H	2.734993	1.790337	2.648733
H	3.217332	0.091210	2.933677
H	4.163855	1.121744	1.817116
H	4.282126	-0.149981	-1.639838
H	3.783325	1.564005	-1.750580
H	4.672941	0.990483	-0.315960
C	-0.873507	-1.973869	-1.680418
H	-0.012384	-2.204807	-2.335826
H	-1.527310	-2.870834	-1.675970
H	-1.455312	-1.143509	-2.125317
C	0.420827	-2.847179	0.280792
H	0.715972	-2.713194	1.340838
H	-0.142313	-3.800491	0.197580
H	1.349603	-2.939730	-0.318981

(4)Bspiro$_O$(MMA)

N	-1.471360	0.243712	-1.047639
C	-0.339591	0.276303	-0.116015
N	-0.936218	-0.147234	1.160986
C	-2.292164	-0.522332	0.930450
C	-2.608663	-0.288862	-0.372426
C	0.354234	1.693847	-0.032811
C	1.633135	1.582027	0.834672
C	2.519640	0.425813	0.435824
C	1.966871	-0.601774	-0.262627
O	0.641723	-0.718831	-0.595278
C	3.977775	0.451996	0.812712
O	2.713191	-1.620166	-0.774156
C	2.160289	-2.937705	-0.721212
C	-0.155788	-0.938451	2.105857
C	-1.255654	-0.157800	-2.436779
H	4.488276	-0.487934	0.528787
H	4.515054	1.293469	0.317207
H	4.110186	0.602445	1.909028
H	2.911914	-3.604299	-1.185740
H	1.986891	-3.265006	0.329606
H	1.205648	-3.010407	-1.281274
H	1.353615	1.519327	1.915468
H	2.199180	2.537597	0.745145
C	-3.164960	-0.955460	2.065087
C	-3.925428	-0.392213	-1.073377
H	-0.053085	-2.009165	1.802461
H	0.861298	-0.522512	2.216381
H	-0.641653	-0.907452	3.102067
H	-0.319688	0.278704	-2.824227

H	-1.192296	-1.264246	-2.568322
H	-2.088770	0.221576	-3.063810
H	-4.209677	-1.089306	1.723625
H	-2.840884	-1.921920	2.511199
H	-3.172053	-0.205654	2.889056
H	-3.911297	-1.130369	-1.905948
H	-4.718114	-0.710802	-0.369085
H	-4.235087	0.583533	-1.512677
C	0.743733	2.208900	-1.436912
H	-0.150066	2.351306	-2.076329
H	1.239164	3.197699	-1.338709
H	1.454544	1.533294	-1.954118
C	-0.634221	2.690859	0.598803
H	-0.927939	2.367702	1.616902
H	-0.172559	3.698618	0.663972
H	-1.554122	2.769539	-0.016112

(4)Bspiro$_C$(MMA)

C	-1.030213	0.644390	0.845772
C	0.412501	0.424191	-0.170429
C	0.027065	1.841697	-0.807945
C	-0.978335	2.117197	0.354691
N	1.632314	0.365239	0.612753
C	2.341529	-0.834389	0.363575
C	1.689490	-1.512640	-0.621503
N	0.569908	-0.735422	-1.030484
C	3.600570	-1.171087	1.095405
C	2.025341	-2.813207	-1.275113
C	-0.543777	-1.419805	-1.666432
C	2.150240	1.349658	1.540087
C	-2.271188	-0.058863	0.372852
O	-2.491088	-1.233990	1.052512
C	-3.647386	-1.971258	0.645101
O	-3.042089	0.317427	-0.507992
C	-0.777631	0.359240	2.331023
H	-3.520188	-2.375108	-0.383028
H	-3.751754	-2.804167	1.365668
H	-4.554976	-1.333592	0.651750
H	1.404806	2.139272	1.733605
H	2.397917	0.888143	2.521551
H	3.073831	1.849111	1.162837
H	-1.299721	-0.705183	-2.025037
H	-0.180043	-1.987921	-2.546198
H	-1.049989	-2.135569	-0.976952
H	4.013474	-2.128880	0.724228
H	4.392226	-0.399019	0.967327
H	3.438690	-1.286381	2.190895
H	2.966464	-3.220919	-0.857649
H	1.239436	-3.588552	-1.132070
H	2.171978	-2.702779	-2.373930
H	-1.699367	0.513112	2.931611
H	-0.460059	-0.691095	2.483863
H	-0.000462	1.020437	2.754023
C	-0.692085	1.722424	-2.169268
H	-1.662276	1.198325	-2.089838
H	-0.909100	2.742557	-2.550708
H	-0.048079	1.213547	-2.916703
C	1.186541	2.837061	-1.004687
H	0.805200	3.767051	-1.476864
H	1.691344	3.135816	-0.068733
H	1.954463	2.412326	-1.685904
H	-1.957769	2.523552	0.032151
H	-0.562160	2.792032	1.133297

(4)B-C(MMA)

C	2.383805	-2.191173	-0.556657
C	3.420291	-1.289979	-0.476784
N	3.008206	-0.271863	0.391283
C	1.718923	-0.501107	0.804762
N	1.357767	-1.703866	0.261406
C	4.748743	-1.307118	-1.162205
C	3.762366	0.976103	0.503252
C	0.866732	0.280499	1.814910
C	-0.569065	0.604151	1.225157
C	-0.759729	1.824328	0.335930
C	-1.424365	3.034552	0.971860
C	0.078983	-2.415968	0.359028
C	2.266209	-3.455508	-1.344218
C	0.221128	2.030636	-0.691320
O	1.082985	1.206794	-1.080408
O	0.096885	3.250837	-1.342892
C	0.948282	3.442779	-2.467169
C	-2.326286	1.162808	-1.032323
C	-3.367053	0.416082	-0.450918
C	-3.317681	-1.023478	-0.560605
O	-2.433629	-1.732968	-1.086371
C	-4.540595	1.075075	0.245778
O	-4.452123	-1.632213	-0.028283
C	-4.510807	-3.044830	-0.171452
H	-2.369712	2.744816	1.477920
H	-1.669840	3.802886	0.212571
H	-0.783678	3.534107	1.738209
H	0.597395	4.365607	-2.969049
H	0.902818	2.584510	-3.169954
H	2.011780	3.576042	-2.164601
H	-1.642918	0.609314	-1.697301

H	-2.518316	2.211133	-1.315435
H	-5.512030	0.679401	-0.121620
H	-4.530474	2.171898	0.075125
H	-4.545149	0.912303	1.348484
H	-4.435420	-3.357179	-1.235580
H	-3.689193	-3.552741	0.381717
H	-5.487277	-3.360347	0.246068
H	-1.229104	0.728017	2.110338
H	-0.965592	-0.291565	0.708982
H	0.271926	-3.492146	0.199729
H	-0.358936	-2.298884	1.362533
H	-0.671645	-2.059112	-0.389169
H	3.191036	1.776992	-0.003531
H	3.963305	1.242433	1.554427
H	4.730457	0.843676	-0.008839
H	3.178902	-3.610057	-1.950048
H	2.143370	-4.350970	-0.697096
H	1.401918	-3.425062	-2.040662
H	4.857951	-2.245116	-1.738659
H	4.862505	-0.466515	-1.880128
H	5.597153	-1.261835	-0.446256
C	0.716185	-0.606265	3.091191
H	0.132200	-1.531582	2.927562
H	1.707758	-0.897044	3.498000
H	0.185234	-0.025986	3.873344
C	1.496638	1.603371	2.307325
H	1.678347	2.325021	1.492343
H	0.772653	2.076284	3.000282
H	2.431597	1.442473	2.881845

(4)C(MMA)

C	2.695887	-1.221248	0.780618
N	1.308201	-1.349291	0.923592
C	0.687007	-1.140479	-0.285713
N	1.707814	-0.937300	-1.200368
C	2.943685	-0.945688	-0.543407
C	0.699319	-1.506521	2.245567
C	-0.724924	-1.614972	-0.698852
C	-1.582866	-0.528348	-1.432127
C	-2.289368	0.608329	-0.640783
C	-1.330579	1.428942	0.281231
C	0.015566	1.841223	-0.279067
C	0.037619	2.883372	-1.386901
C	1.532047	-0.275478	-2.484302
C	-3.500628	0.025557	0.119607
O	-4.290179	-0.782221	-0.347900
C	-2.972346	1.530614	-1.698083
O	-3.660416	0.555796	1.361606
C	-4.827533	0.119653	2.075911
C	1.112294	1.775328	0.629910
O	1.157344	1.259312	1.772157
O	2.293595	2.384601	0.117989
C	3.373560	2.487135	1.025274
H	-4.814017	0.660171	3.040182
H	-4.801792	-0.976491	2.246548
H	-5.750738	0.358618	1.509195
H	-1.141339	0.858656	1.213186
H	-1.913943	2.327896	0.609289
H	3.983646	1.551272	1.062552
H	4.025222	3.311278	0.667062
H	3.025761	2.695157	2.059336
H	-0.963712	-0.039252	-2.205697
H	-2.381870	-1.083467	-1.968941
H	0.803466	-0.804565	-3.124790
H	1.167919	0.756828	-2.275973
H	2.499104	-0.245177	-3.015746
H	-0.157720	-0.823258	2.344984
H	0.404444	-2.557145	2.440675
H	1.436377	-1.186630	2.998927
C	-0.515330	-2.802306	-1.693861
C	-1.543276	-2.213954	0.469801
H	-3.495956	2.371166	-1.197451
H	-2.220748	1.962502	-2.384496
H	-3.714883	0.963068	-2.295425
H	1.048911	3.319061	-1.496748
H	-0.266559	2.512955	-2.395066
H	-0.665944	3.726876	-1.164027
C	4.231803	-0.635414	-1.232607
C	3.638347	-1.303496	1.935092
H	5.080699	-0.806781	-0.544142
H	4.395907	-1.271418	-2.129014
H	4.273275	0.428300	-1.552677
H	4.683117	-1.230964	1.578235
H	3.461138	-0.460554	2.637759
H	3.542897	-2.255378	2.499723
H	-1.499811	-3.245794	-1.948110
H	-0.037087	-2.495109	-2.644184
H	0.112681	-3.595859	-1.238332
H	-2.510893	-2.565625	0.064135
H	-1.033698	-3.085302	0.926043
H	-1.770423	-1.482277	1.265747

(4)C-Cspiro$_C$(MMA)

N	-1.627062	-1.206060	1.012804
C	-2.883672	-1.216752	0.388166
C	-2.672621	-1.048335	-0.956087

N	-1.284799	-0.919578	-1.153589
C	-0.618356	-0.865776	0.085938
C	-4.153140	-1.383290	1.157511
C	-3.653743	-0.985142	-2.080446
C	-0.747954	-0.653533	-2.487912
C	0.814762	-1.502650	0.257360
C	1.764135	-0.647499	1.146028
C	2.295643	0.706282	0.590777
C	1.171151	1.580160	-0.044639
C	-0.221758	1.428520	0.549636
C	-1.287545	1.903329	-0.316684
O	-2.432748	2.293018	0.388175
C	-3.554298	2.654555	-0.404512
C	-1.512999	-1.208733	2.460408
C	3.413533	0.496718	-0.455245
O	4.388466	-0.342174	0.008829
C	5.509099	-0.530041	-0.868794
O	3.492744	1.036829	-1.544555
O	-1.279468	1.952727	-1.555381
C	2.999202	1.460035	1.759740
C	-0.368110	1.807848	2.018437
H	6.210406	-1.195836	-0.332604
H	5.996467	0.438591	-1.102480
H	5.191010	-0.995423	-1.824777
H	1.118966	1.376645	-1.131184
H	1.509613	2.645854	0.013098
H	-4.106674	1.751109	-0.754615
H	-4.224571	3.255904	0.241596
H	-3.249529	3.236889	-1.298617
H	1.264263	-0.432901	2.111910
H	2.640219	-1.281054	1.399485
H	-0.471545	-1.022439	2.764592
H	-2.137157	-0.410978	2.912800
H	-1.831546	-2.185966	2.884292
H	0.105013	0.038605	-2.433917
H	-0.453233	-1.588782	-3.011248
H	-1.515631	-0.130888	-3.082058
H	-5.017187	-1.423208	0.467268
H	-4.164921	-2.318227	1.759655
H	-4.329794	-0.538019	1.858636
H	-4.680530	-1.147942	-1.700165
H	-3.634351	0.007064	-2.582534
H	-3.459768	-1.755508	-2.858725
H	3.478493	2.390320	1.389928
H	2.264320	1.749273	2.535347
H	3.781446	0.829941	2.228727
H	-1.418827	1.739680	2.353491
H	0.248651	1.190223	2.703113
H	-0.049231	2.866694	2.192443
C	0.651244	-2.900217	0.928067
H	1.623413	-3.434604	0.900828
H	0.341644	-2.848222	1.988810
H	-0.092843	-3.516360	0.383002
C	1.534764	-1.801294	-1.082449
H	1.725029	-0.908486	-1.701485
H	2.518577	-2.254195	-0.845116
H	0.974852	-2.536593	-1.692357

(4)Cspiro$_C$(MMA)

C	-0.189104	1.013182	0.664104
C	-0.651546	-0.458224	0.080155
C	0.658147	-1.422321	-0.101269
C	1.766481	-1.044033	0.912009
C	2.362633	0.380211	0.719224
C	1.262609	1.383352	0.264777
N	-1.697897	-1.059760	0.938604
C	-2.890968	-1.312369	0.210982
C	-2.721811	-0.871504	-1.064949
N	-1.412621	-0.336655	-1.189995
C	-4.085868	-1.926334	0.865196
C	-3.680787	-0.866178	-2.211079
C	-1.004120	0.360259	-2.395170
C	-1.518089	-1.621154	2.258895
C	3.493191	0.387652	-0.337168
O	4.405928	-0.596542	-0.101626
C	5.535782	-0.617553	-0.988525
C	-1.125288	2.078308	0.048688
O	-2.385839	1.995437	0.550164
C	-3.323183	2.948896	0.030891
O	3.624926	1.195175	-1.240203
O	-0.798535	2.935372	-0.756065
C	3.059313	0.836185	2.033639
C	-0.370963	1.159372	2.198775
H	6.176011	-1.452113	-0.648248
H	6.091890	0.341133	-0.943674
H	5.212112	-0.781915	-2.036775
H	1.327213	1.517836	-0.831081
H	1.491572	2.393872	0.664240
H	-3.460149	2.816009	-1.061982
H	-4.275389	2.759277	0.559278
H	-2.977123	3.987272	0.212373
H	1.367836	-1.115252	1.945912
H	2.584454	-1.792963	0.861286
H	-0.478501	-1.495359	2.604614
H	-2.170363	-1.133109	3.021506

H	-1.735598	-2.715178	2.293208
H	-0.096067	0.959860	-2.220074
H	-0.794943	-0.324496	-3.251691
H	-1.781310	1.082468	-2.727171
H	-4.914630	-2.022237	0.137054
H	-3.888919	-2.944251	1.271845
H	-4.462562	-1.312370	1.715278
H	-4.621512	-1.376335	-1.926058
H	-3.954922	0.160491	-2.546218
H	-3.276903	-1.392136	-3.105411
H	3.556608	1.819419	1.897596
H	2.321553	0.943205	2.852760
H	3.826157	0.100360	2.349159
H	-0.101753	2.194589	2.498589
H	-1.419494	0.985773	2.495610
H	0.279917	0.477130	2.775467
C	1.252990	-1.364461	-1.530986
H	1.533941	-0.351777	-1.869833
H	2.171699	-1.987781	-1.559950
H	0.546440	-1.787836	-2.270588
C	0.248372	-2.900756	0.102116
H	1.062004	-3.566140	-0.256944
H	0.061826	-3.165794	1.159411
H	-0.666030	-3.137449	-0.479768

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