

Probing Heterocycle Conformation with Residual Dipolar Couplings

Chakicherla Gayathri,^a M. Carmen de la Fuente,^b Burkhard Luy,^c Roberto R. Gil^{*a} and Armando Navarro-Vázquez^{*d}

^a Department of Chemistry, Carnegie Mellon University, 4400 Fifth Avenue, Pittsburgh, Pennsylvania 15213, USA. Fax: +1 412 2681061; Tel: +1 412 2684313; E-mail: rgil@andrew.cmu.edu

^b Departamento de Química Orgánica, Facultade de Química, Universidade de Santiago de Compostela, 15782 Santiago de Compostela, Spain.

^c Department Chemie, Lehrstuhl für Organische Chemie II, Technische Universität München 85747 Garching, Germany;

^d Departamento de Química Orgánica, Universidade de Vigo, 36310, Vigo, Spain. Fax: +34 986 812262; Tel: +34 986812226; E-mail: armando.navarro@uvigo.es

Computational methodology:

The conformational space of **1** was first explored by means of a simulated annealing methodology using the MM3 force field¹ as implemented in the TINKER² program and in-house python scripts. The so-obtained geometries were then refined at the DFT level using both the hybrid GGA B3LYP³ and the meta-GGA-hybrid M052X⁴ functionals, as we wanted to evaluate whether the better handling of medium-size correlation and dispersion effects in M052X would be important in the computation of relative conformational energies.⁵ The 6-31+G** basis set and the was employed with both functionals, and the gaussian integration FineGrid (pruned(75,302)). Analytical frequencies were computed in all cases to verify the character of the stationary points and to compute-zero point vibrational corrections. These computations were performed with the Gaussian03 program.⁶ Solvation effects were taken into account by single point computations on gas phase geometries, using the IEFPCM model⁷ with CHCl₃ parameters as implemented in Gaussian09,⁸ using the 6-31+G** basis sets and the gaussian UltraFine integration grid (pruned (99,590)).

Benzazepine 1 DFT optimized cartesian coordinates (Å)

B3LYP geometries

```
45
1A
C      -3.566304   -0.071308   -0.037419
C      -2.932805    1.194357   -0.032235
C      -1.557349    1.265101   -0.248277
C      -0.784996    0.110888   -0.472225
C      -1.410993   -1.137636   -0.474770
C      -2.797241   -1.213954   -0.255506
C       0.698679    0.231394   -0.732591
C       1.659278   -0.402536    0.317230
N       1.758337   -1.874277    0.202916
C       0.496508   -2.607687    0.391731
C      -0.590101   -2.389067   -0.675077
C       3.027721    0.247355    0.132563
C       3.815610   -0.040254   -0.992963
C       5.036695    0.606255   -1.192335
C       5.491331    1.555720   -0.270824
C       4.715234    1.849109    0.852384
C       3.493192    1.197564    1.049741
C       2.741639   -2.415848    1.148443
O      -4.914556   -0.065778    0.179921
C      -5.601347   -1.308171    0.172395
O      -3.746502    2.269046    0.189032
C      -3.162766    3.563067    0.193883
H      -1.062853    2.230242   -0.253339
H      -3.271353   -2.189267   -0.256913
H       0.953514   -0.200367   -1.709883
H       0.952911    1.293722   -0.792760
H       1.286172   -0.124873    1.322978
H       0.767023   -3.669129    0.377717
H       0.062365   -2.404322    1.391215
H      -1.255479   -3.259647   -0.650939
H      -0.109505   -2.391277   -1.663202
H       3.473215   -0.788508   -1.701751
H       5.635589    0.368363   -2.067309
H       6.441926    2.057950   -0.426159
H       5.060148    2.580262    1.578373
H       2.896711    1.426928    1.929836
H       2.449583   -2.254026    2.204257
H       2.840138   -3.493414    0.986351
H       3.719457   -1.959125    0.993634
H      -5.236895   -1.974794    0.964996
H      -6.649500   -1.068073    0.356473
```

H	-5.508803	-1.812979	-0.798105
H	-2.410242	3.662260	0.987107
H	-2.703313	3.800818	-0.774458
H	-3.982621	4.256961	0.384947

45

1B

C	-3.553195	-0.081988	0.155207
C	-2.974025	1.175032	-0.142124
C	-1.609269	1.240100	-0.400595
C	-0.778244	0.098678	-0.385659
C	-1.353256	-1.144956	-0.093609
C	-2.737387	-1.208034	0.171962
C	0.696751	0.318165	-0.696943
C	1.711484	-0.496568	0.142238
N	1.894967	-1.858807	-0.383264
C	0.687940	-2.490333	-0.929845
C	-0.571316	-2.447861	-0.041852
C	3.046201	0.244885	0.195285
C	3.961054	0.165184	-0.864186
C	5.149799	0.898130	-0.835072
C	5.444688	1.721857	0.255958
C	4.542255	1.803474	1.319500
C	3.353540	1.068358	1.286424
C	2.589740	-2.713268	0.576394
O	-4.895854	-0.080645	0.402448
C	-5.522963	-1.316777	0.708853
O	-3.826166	2.241965	-0.145667
C	-3.295578	3.524307	-0.445631
H	-1.156108	2.199895	-0.622672
H	-3.171735	-2.177259	0.392139
H	0.911238	0.144873	-1.760560
H	0.914727	1.376300	-0.526098
H	1.318824	-0.530417	1.177259
H	0.453553	-2.041525	-1.901504
H	0.949131	-3.534146	-1.132853
H	-0.291864	-2.681866	0.995983
H	-1.239948	-3.259874	-0.354270
H	3.738478	-0.491052	-1.700108
H	5.849111	0.823422	-1.663584
H	6.371068	2.288780	0.279437
H	4.764853	2.432572	2.177040
H	2.658309	1.131146	2.120977
H	2.813630	-3.679996	0.114880
H	3.537043	-2.249638	0.863772
H	2.012696	-2.897173	1.503059
H	-6.576051	-1.082522	0.870842
H	-5.432755	-2.030246	-0.120754
H	-5.105339	-1.764682	1.620097
H	-2.856789	3.552877	-1.451556
H	-4.140909	4.212377	-0.400080
H	-2.539068	3.828928	0.289322

1C

C	2.951908	-0.277313	0.289236
C	2.529173	0.791114	-0.536483
C	1.312006	0.686826	-1.207358
C	0.493299	-0.450304	-1.087511
C	0.912213	-1.508378	-0.273423
C	2.138857	-1.404115	0.407185
C	-0.812968	-0.521054	-1.847276
C	-2.131633	-0.636634	-1.039192
N	-2.329024	-1.990041	-0.472725
C	-1.344457	-2.517146	0.476312
C	0.059185	-2.747326	-0.112391
C	-2.391194	0.541608	-0.089718
C	-1.575982	0.858282	1.012047
C	-1.883481	1.936195	1.847252
C	-3.008587	2.727431	1.601855
C	-3.826807	2.430483	0.509919
C	-3.517897	1.348685	-0.318493
C	-3.690717	-2.184220	0.019240
O	4.152599	-0.109240	0.917842
C	4.627322	-1.155703	1.751501

O	3.371314	1.863814	-0.604620
C	2.987498	2.969569	-1.409190
H	0.975106	1.503222	-1.836086
H	2.454164	-2.228832	1.036858
H	-0.901951	0.373794	-2.472815
H	-0.798891	-1.382713	-2.529144
H	-2.916817	-0.566886	-1.803031
H	-1.269045	-1.909698	1.396915
H	-1.730466	-3.494647	0.788173
H	-0.063916	-3.256975	-1.078483
H	0.581952	-3.449397	0.547380
H	-0.684822	0.277908	1.215117
H	-1.234840	2.159860	2.689868
H	-3.242780	3.565261	2.252469
H	-4.704993	3.036141	0.303182
H	-4.166566	1.126030	-1.163128
H	-3.913433	-1.632901	0.950064
H	-4.407295	-1.858985	-0.742159
H	-3.858679	-3.250109	0.206053
H	3.943275	-1.345090	2.589158
H	4.775109	-2.085046	1.186047
H	5.587274	-0.812423	2.139811
H	2.882018	2.682736	-2.463639
H	2.048067	3.415485	-1.057938
H	3.792964	3.698954	-1.312448

45

1D

C	-3.560467	-0.070684	0.117645
C	-2.952234	1.194050	-0.051930
C	-1.593243	1.253241	-0.355105
C	-0.805348	0.095258	-0.500669
C	-1.408529	-1.158403	-0.330120
C	-2.780691	-1.217509	-0.021784
C	0.665913	0.257827	-0.840119
C	1.641137	-0.347959	0.209123
N	1.792793	-1.815319	0.150082
C	0.588895	-2.567616	0.496657
C	-0.625752	-2.450337	-0.457815
C	3.025471	0.305969	0.220168
C	3.828691	0.132944	1.358662
C	5.103872	0.692870	1.435501
C	5.608392	1.437947	0.364013
C	4.824447	1.613091	-0.776877
C	3.543595	1.052015	-0.846234
C	2.491906	-2.335315	-1.019628
O	-4.893370	-0.060843	0.414878
C	-5.551527	-1.305853	0.593948
O	-3.768134	2.278547	0.101595
C	-3.204829	3.571633	-0.060967
H	-1.118678	2.219274	-0.486449
H	-3.237630	-2.192302	0.108009
H	0.876711	-0.176121	-1.827465
H	0.870421	1.328866	-0.930473
H	1.198256	-0.148072	1.194680
H	0.882759	-3.623399	0.556260
H	0.275578	-2.263503	1.504174
H	-1.298132	-3.291791	-0.252022
H	-0.283051	-2.587979	-1.493256
H	3.444980	-0.457688	2.186212
H	5.703606	0.549938	2.330213
H	6.600768	1.876192	0.419929
H	5.205761	2.185606	-1.617989
H	2.956206	1.199405	-1.747129
H	2.662244	-3.407947	-0.877592
H	1.959415	-2.208110	-1.979122
H	3.466745	-1.850755	-1.113685
H	-5.509217	-1.918224	-0.316285
H	-5.123103	-1.870712	1.432232
H	-6.591131	-1.061630	0.816963
H	-2.801982	3.710887	-1.072724
H	-4.023867	4.273700	0.101505
H	-2.412369	3.760955	0.674836

45
1E

C	2.958578	-0.072693	0.229803
C	2.342527	0.995269	-0.465023
C	1.105439	0.779725	-1.064182
C	0.450645	-0.466374	-1.004344
C	1.054521	-1.521586	-0.313774
C	2.304503	-1.299630	0.298022
C	-0.883187	-0.626659	-1.700507
C	-2.104012	-0.889559	-0.773962
N	-1.866591	-2.003890	0.159768
C	-1.061846	-3.091680	-0.402052
C	0.455478	-2.914191	-0.176583
C	-2.512803	0.378877	-0.031175
C	-1.888230	0.758892	1.165306
C	-2.238695	1.951698	1.802615
C	-3.217304	2.785966	1.253447
C	-3.847799	2.414976	0.062857
C	-3.497334	1.218746	-0.569788
C	-3.120727	-2.477241	0.740970
O	4.170503	0.201680	0.796991
C	4.825344	-0.832295	1.515714
O	3.028520	2.176290	-0.483052
C	2.434798	3.284539	-1.143291
H	0.616521	1.590923	-1.591223
H	2.764554	-2.118735	0.840383
H	-1.106535	0.278684	-2.273218
H	-0.824926	-1.435439	-2.437711
H	-2.938473	-1.150318	-1.457396
H	-1.353607	-4.018067	0.102625
H	-1.286999	-3.258833	-1.469434
H	0.979867	-3.608781	-0.850788
H	0.679643	-3.260145	0.840074
H	-1.134704	0.106403	1.593194
H	-1.745226	2.230553	2.729811
H	-3.490262	3.712056	1.751581
H	-4.617280	3.049489	-0.368483
H	-3.999790	0.930724	-1.491123
H	-2.913034	-3.220706	1.516215
H	-3.651777	-1.643498	1.207420
H	-3.796754	-2.933482	-0.009026
H	4.227361	-1.167107	2.373498
H	5.048340	-1.692543	0.870940
H	5.759683	-0.397887	1.874243
H	3.136718	4.111112	-1.023529
H	2.288750	3.084446	-2.212952
H	1.472508	3.553949	-0.689300

45
1F

C	2.898044	-0.348235	0.460845
C	2.597713	0.631732	-0.512822
C	1.384994	0.555162	-1.193963
C	0.447362	-0.465837	-0.947390
C	0.753664	-1.446149	0.005591
C	1.975675	-1.364853	0.699320
C	-0.831733	-0.503065	-1.765242
C	-2.195059	-0.497789	-1.008960
N	-2.526214	-1.760638	-0.333648
C	-1.611998	-2.198923	0.721615
C	-0.180818	-2.603569	0.297772
C	-2.432079	0.708418	-0.088478
C	-1.809623	1.945966	-0.308374
C	-2.111058	3.058107	0.483250
C	-3.045298	2.956766	1.515537
C	-3.678411	1.731889	1.742046
C	-3.376953	0.624394	0.946564
C	-2.949513	-2.825953	-1.231022
O	4.097765	-0.212715	1.098834
C	4.446458	-1.171703	2.085880
O	3.546637	1.595161	-0.706544
C	3.298781	2.597023	-1.680588
H	1.150965	1.301903	-1.944611
H	2.200883	-2.125751	1.437975
H	-0.824462	0.335101	-2.470832

H	-0.832337	-1.403683	-2.395084
H	-2.949288	-0.408916	-1.805115
H	-1.546800	-1.404103	1.473374
H	-2.086588	-3.060488	1.209026
H	-0.237088	-3.271304	-0.574329
H	0.249628	-3.207215	1.105734
H	-1.078573	2.056801	-1.100498
H	-1.610302	4.003309	0.291876
H	-3.277033	3.819440	2.133730
H	-4.411308	1.636781	2.538876
H	-3.873918	-0.324773	1.117431
H	-2.162172	-3.223372	-1.897194
H	-3.329980	-3.664704	-0.637394
H	-3.767317	-2.465755	-1.864820
H	5.427587	-0.871391	2.456520
H	3.728844	-1.173228	2.916761
H	4.512243	-2.181730	1.660544
H	4.177394	3.243676	-1.670700
H	3.177889	2.163815	-2.682291
H	2.409129	3.190214	-1.431253

45
1G

C	-3.477750	-0.369250	-0.149770
C	-3.126796	1.000531	-0.112843
C	-1.792170	1.367078	-0.293026
C	-0.793974	0.405243	-0.509403
C	-1.141067	-0.950368	-0.543977
C	-2.481329	-1.323172	-0.363863
C	0.650554	0.792897	-0.714760
C	1.595758	0.391840	0.455837
N	1.156751	-0.831470	1.154105
C	0.957764	-2.072187	0.408689
C	-0.051578	-1.973608	-0.764770
C	3.066338	0.408120	0.026173
C	3.988569	1.202396	0.723545
C	5.342196	1.222919	0.375622
C	5.803399	0.437580	-0.682989
C	4.899109	-0.361341	-1.388829
C	3.546777	-0.373007	-1.039257
C	1.871764	-1.059762	2.401973
O	-4.803182	-0.651646	0.029417
C	-5.209688	-2.010811	-0.000614
O	-4.155474	1.875693	0.098440
C	-3.857187	3.262191	0.147987
H	-1.512257	2.414650	-0.269687
H	-2.739850	-2.376082	-0.392146
H	1.014407	0.348413	-1.648261
H	0.742824	1.875820	-0.849704
H	1.488608	1.174588	1.218110
H	1.905314	-2.508451	0.038365
H	0.559373	-2.786894	1.138675
H	-0.486281	-2.967248	-0.918985
H	0.484344	-1.735808	-1.692910
H	3.639995	1.816393	1.551135
H	6.033219	1.851465	0.930657
H	6.854247	0.448873	-0.957621
H	5.245951	-0.973876	-2.216618
H	2.863257	-0.992626	-1.611618
H	2.916273	-1.395575	2.268168
H	1.889793	-0.136496	2.991128
H	1.343516	-1.821027	2.986383
H	-4.727782	-2.593377	0.795616
H	-6.288512	-2.001111	0.161902
H	-4.993122	-2.475033	-0.971829
H	-4.809763	3.764099	0.324118
H	-3.166068	3.496600	0.968323
H	-3.429643	3.616873	-0.799140

45
1H

C	2.833545	-0.170522	0.705137
C	2.780379	0.152467	-0.672034
C	1.597499	-0.072144	-1.367900
C	0.448465	-0.612557	-0.752685

C	0.503843	-0.939459	0.606862
C	1.703665	-0.708838	1.311484
C	-0.774937	-0.827116	-1.630803
C	-2.175228	-0.620860	-0.996932
N	-2.632648	-1.764015	-0.180229
C	-1.602607	-2.447921	0.608089
C	-0.666481	-1.516347	1.386296
C	-2.371744	0.726115	-0.282018
C	-3.345309	0.858802	0.719404
C	-3.605214	2.096455	1.313144
C	-2.896130	3.232778	0.915173
C	-1.927555	3.115606	-0.084075
C	-1.670749	1.875920	-0.676665
C	-3.416416	-2.730642	-0.939534
O	4.020706	0.075555	1.333095
C	4.122342	-0.223485	2.717204
O	3.922860	0.671507	-1.211428
C	3.921088	1.009575	-2.589836
H	1.546397	0.176507	-2.422447
H	1.735805	-0.966281	2.364482
H	-0.688956	-0.165925	-2.500251
H	-0.762301	-1.844003	-2.048986
H	-2.866558	-0.589450	-1.849610
H	-2.131719	-3.089494	1.323635
H	-0.990679	-3.125508	-0.020146
H	-0.257964	-2.092003	2.224895
H	-1.260346	-0.709378	1.834184
H	-3.888629	-0.026613	1.032094
H	-4.363299	2.171248	2.088399
H	-3.094340	4.195570	1.377663
H	-1.364087	3.988495	-0.402363
H	-0.906345	1.814196	-1.443788
H	-3.815471	-3.490458	-0.258788
H	-4.264434	-2.234452	-1.421446
H	-2.833700	-3.258721	-1.720674
H	3.402822	0.357931	3.308301
H	3.970209	-1.293596	2.909776
H	5.136793	0.054691	3.006455
H	3.176622	1.785035	-2.813561
H	4.919108	1.396001	-2.801483
H	3.730353	0.130850	-3.219933

45

1I

C	-3.541989	-0.149614	0.309110
C	-3.047816	1.105157	-0.121109
C	-1.701663	1.217904	-0.451081
C	-0.809269	0.126876	-0.381684
C	-1.300063	-1.117108	0.037935
C	-2.665508	-1.227137	0.376494
C	0.642139	0.392193	-0.761790
C	1.671153	-0.450749	0.035174
N	1.909704	-1.804558	-0.530762
C	0.674699	-2.518438	-0.876120
C	-0.451527	-2.377213	0.152157
C	2.997049	0.255567	0.303336
C	3.511286	1.266251	-0.520215
C	4.738351	1.873015	-0.233069
C	5.474526	1.476835	0.885329
C	4.974689	0.467345	1.713769
C	3.749448	-0.134330	1.421878
C	2.835355	-1.857344	-1.658228
O	-4.869829	-0.195658	0.624105
C	-5.411980	-1.429692	1.069541
O	-3.956871	2.122748	-0.171708
C	-3.511608	3.400150	-0.602323
H	-1.311421	2.177834	-0.770818
H	-3.036198	-2.194889	0.696195
H	0.789475	0.235027	-1.840019
H	0.835850	1.454806	-0.586089
H	1.229871	-0.622170	1.023389
H	0.286732	-2.202332	-1.864501
H	0.938220	-3.579060	-0.972820
H	-0.029311	-2.479254	1.162173

H	-1.117634	-3.238319	0.025816
H	2.959948	1.587028	-1.399129
H	5.116908	2.654980	-0.885603
H	6.425782	1.950260	1.110987
H	5.536440	0.151808	2.588611
H	3.367689	-0.923636	2.064248
H	3.809834	-1.453387	-1.379248
H	2.972654	-2.905311	-1.944707
H	2.476279	-1.314367	-2.554442
H	-6.466952	-1.235177	1.267866
H	-5.324554	-2.208905	0.301003
H	-4.925478	-1.773037	1.991898
H	-4.390728	4.045448	-0.573160
H	-2.741462	3.804864	0.067277
H	-3.119909	3.364956	-1.627383

45
1J

C	3.517356	-0.159765	-0.089971
C	2.967885	1.136094	0.055103
C	1.598386	1.309841	-0.119959
C	0.734413	0.244391	-0.448707
C	1.280967	-1.036921	-0.592143
C	2.667012	-1.215293	-0.404801
C	-0.735794	0.604721	-0.640126
C	-1.808321	-0.510700	-0.441802
N	-1.481795	-1.496360	0.587297
C	-0.633292	-2.599508	0.125547
C	0.431967	-2.241310	-0.937718
C	-3.218590	0.071566	-0.239376
C	-4.202275	-0.691851	0.408965
C	-5.508087	-0.217873	0.549809
C	-5.863995	1.033776	0.039621
C	-4.898383	1.801761	-0.613157
C	-3.590425	1.325164	-0.750154
C	-1.174987	-0.961181	1.910306
O	4.865380	-0.265376	0.099407
C	5.464460	-1.545170	-0.037129
O	3.850187	2.129500	0.369726
C	3.349339	3.448540	0.528802
H	1.170680	2.299352	-0.000591
H	3.074039	-2.214023	-0.517047
H	-0.961532	1.423573	0.053311
H	-0.864669	1.029618	-1.646025
H	-1.870596	-1.078282	-1.378619
H	-0.134196	-3.022582	1.003701
H	-1.267190	-3.397582	-0.293497
H	-0.062327	-2.082859	-1.904913
H	1.073611	-3.119418	-1.079127
H	-3.921771	-1.661222	0.807826
H	-6.248312	-0.828040	1.060591
H	-6.879029	1.404802	0.149679
H	-5.158325	2.776191	-1.017799
H	-2.865325	1.945228	-1.266531
H	-1.953136	-0.247722	2.200021
H	-1.192202	-1.776526	2.641538
H	-0.198610	-0.455907	1.984858
H	5.062359	-2.258128	0.694553
H	5.327811	-1.947453	-1.049477
H	6.528486	-1.395620	0.151525
H	2.621652	3.506583	1.348780
H	4.215287	4.066651	0.769889
H	2.885521	3.817194	-0.395446

45
1K

C	3.140470	0.477038	-0.557271
C	3.115140	-0.711813	0.209818
C	1.904972	-1.137117	0.744551
C	0.693474	-0.438949	0.545227
C	0.717431	0.731909	-0.223210
C	1.950762	1.167557	-0.756446
C	-0.516732	-1.036304	1.257522
C	-1.874720	-0.297686	1.262259
N	-1.657257	1.111806	1.633409

C	-1.368556	2.073198	0.575201
C	-0.521873	1.527448	-0.583442
C	-2.793933	-0.562295	0.056621
C	-2.401601	-1.321799	-1.056361
C	-3.284442	-1.568219	-2.112525
C	-4.583593	-1.058130	-2.080041
C	-4.991845	-0.301766	-0.977890
C	-4.107787	-0.063003	0.076101
C	-2.522658	1.675519	2.655033
O	4.359598	0.850825	-1.047681
C	4.436607	2.041823	-1.815809
O	4.312488	-1.350249	0.368064
C	4.339870	-2.545523	1.132634
H	1.880686	-2.037606	1.349370
H	1.956620	2.074714	-1.349947
H	-0.669208	-2.069737	0.917186
H	-0.234565	-1.117688	2.314460
H	-2.413472	-0.731042	2.113686
H	-2.299724	2.486232	0.137573
H	-0.844014	2.917100	1.044999
H	-0.222614	2.392008	-1.186520
H	-1.160323	0.924483	-1.235427
H	-1.393203	-1.718679	-1.114560
H	-2.951880	-2.159373	-2.961403
H	-5.270343	-1.250276	-2.899305
H	-6.001685	0.096944	-0.933932
H	-4.448930	0.513215	0.930564
H	-2.039077	2.558844	3.090567
H	-3.514251	2.000058	2.283621
H	-2.678747	0.951775	3.460860
H	5.486413	2.148211	-2.093047
H	3.825622	1.974716	-2.725649
H	4.123745	2.917851	-1.232598
H	5.378017	-2.880769	1.121517
H	4.026724	-2.367716	2.169897
H	3.702398	-3.321847	0.689314

M052X geomet

45

1A

C	-3.538974	-0.069676	-0.043149
C	-2.906488	1.190235	-0.037430
C	-1.538368	1.264675	-0.262657
C	-0.775671	0.110738	-0.494158
C	-1.398910	-1.130197	-0.495274
C	-2.779391	-1.210648	-0.267724
C	0.704398	0.220001	-0.752989
C	1.633085	-0.397663	0.319113
N	1.742715	-1.858405	0.215447
C	0.479211	-2.573546	0.408131
C	-0.572509	-2.373699	-0.688547
C	2.997419	0.243344	0.139045
C	3.798204	-0.103237	-0.953453
C	5.017833	0.532396	-1.163431
C	5.452812	1.526152	-0.286054
C	4.660599	1.875404	0.803737
C	3.439307	1.234633	1.013631
C	2.687308	-2.361955	1.212278
O	-4.879600	-0.060389	0.180430
C	-5.546173	-1.309059	0.173656
O	-3.715833	2.258218	0.192408
C	-3.111262	3.538033	0.201195
H	-1.041028	2.225610	-0.268541
H	-3.250344	-2.184697	-0.269560
H	0.965259	-0.240922	-1.712042
H	0.965605	1.276992	-0.831042
H	1.243797	-0.114413	1.314501
H	0.739352	-3.633864	0.435765
H	0.029545	-2.321426	1.385542
H	-1.233704	-3.243380	-0.684013
H	-0.062295	-2.361718	-1.657183
H	3.462793	-0.888956	-1.620539
H	5.631732	0.251877	-2.010884
H	6.402850	2.019568	-0.449920

H	4.992859	2.641332	1.494043
H	2.826015	1.504392	1.866941
H	2.347281	-2.154315	2.241312
H	2.789147	-3.441476	1.094391
H	3.666041	-1.907827	1.075495
H	-5.161754	-1.963771	0.960980
H	-6.592954	-1.087267	0.363449
H	-5.445670	-1.802148	-0.797350
H	-2.355246	3.609332	0.988457
H	-2.656261	3.763980	-0.767390
H	-3.913131	4.243730	0.401245

45

1B

C	-3.526926	-0.093681	0.179514
C	-2.971614	1.157685	-0.158781
C	-1.615823	1.239505	-0.428647
C	-0.773260	0.112194	-0.387392
C	-1.324279	-1.124139	-0.058975
C	-2.700732	-1.204244	0.220659
C	0.695434	0.343844	-0.696099
C	1.692574	-0.501025	0.115679
N	1.894128	-1.819279	-0.482730
C	0.665900	-2.445174	-0.969235
C	-0.522514	-2.408871	0.001897
C	3.015239	0.241027	0.206020
C	3.929908	0.194159	-0.848307
C	5.112298	0.927131	-0.787719
C	5.394935	1.715110	0.327308
C	4.488094	1.763532	1.383250
C	3.305276	1.028690	1.320285
C	2.620773	-2.690257	0.431011
O	-4.860520	-0.101966	0.439031
C	-5.445619	-1.343968	0.783214
O	-3.838123	2.204074	-0.185748
C	-3.309823	3.475063	-0.516937
H	-1.176197	2.195911	-0.679175
H	-3.114022	-2.172734	0.470358
H	0.913581	0.197521	-1.760096
H	0.913208	1.392164	-0.484854
H	1.292746	-0.592064	1.141908
H	0.367304	-1.974933	-1.909086
H	0.916586	-3.481572	-1.203808
H	-0.167826	-2.589574	1.023254
H	-1.194885	-3.237417	-0.235426
H	3.708610	-0.437813	-1.700141
H	5.816555	0.880262	-1.609721
H	6.317216	2.280992	0.375005
H	4.703154	2.366269	2.257404
H	2.602091	1.062604	2.146208
H	2.845652	-3.634444	-0.066785
H	3.562623	-2.217409	0.710257
H	2.061824	-2.905023	1.356853
H	-6.499313	-1.138858	0.952311
H	-5.338402	-2.067097	-0.030348
H	-4.999054	-1.748313	1.696091
H	-2.875340	3.470186	-1.520670
H	-4.150779	4.162739	-0.486748
H	-2.554130	3.787210	0.209577

45

1C

C	2.847969	-0.316680	0.280493
C	2.444097	0.730627	-0.572619
C	1.255017	0.609097	-1.278531
C	0.447493	-0.530304	-1.157966
C	0.847017	-1.566034	-0.320442
C	2.047519	-1.446331	0.394761
C	-0.864757	-0.605285	-1.894841
C	-2.141245	-0.626953	-1.032356
N	-2.385752	-1.943160	-0.421697
C	-1.390674	-2.472948	0.506196
C	-0.032009	-2.776908	-0.135095
C	-2.275061	0.571210	-0.094326
C	-1.366441	0.869923	0.931083

C	-1.569572	1.968431	1.764357
C	-2.678739	2.793287	1.594150
C	-3.589329	2.510407	0.579932
C	-3.384474	1.409593	-0.248541
C	-3.706795	-1.989526	0.191054
O	4.021172	-0.125261	0.938816
C	4.458881	-1.160893	1.799243
O	3.276428	1.803026	-0.629162
C	2.882433	2.885923	-1.453020
H	0.921933	1.413060	-1.921048
H	2.345461	-2.256492	1.047156
H	-0.941419	0.258344	-2.559366
H	-0.898459	-1.504167	-2.519237
H	-2.959757	-0.524355	-1.752410
H	-1.254273	-1.828983	1.390103
H	-1.804114	-3.417669	0.868775
H	-0.217213	-3.272242	-1.093825
H	0.489627	-3.493510	0.503877
H	-0.484721	0.261784	1.076286
H	-0.850698	2.180668	2.546675
H	-2.830325	3.646715	2.243762
H	-4.457557	3.141734	0.433526
H	-4.102743	1.194266	-1.033355
H	-3.779421	-1.381964	1.105863
H	-4.451155	-1.623647	-0.519146
H	-3.950397	-3.024307	0.438494
H	3.738065	-1.334797	2.603314
H	4.622231	-2.089137	1.244333
H	5.399686	-0.817841	2.221359
H	2.805857	2.575528	-2.498983
H	1.927334	3.302637	-1.121345
H	3.663524	3.634561	-1.351349

45
1D

C	-3.541009	-0.078054	0.102934
C	-2.937646	1.185958	-0.046092
C	-1.585578	1.257879	-0.352366
C	-0.803836	0.103964	-0.517717
C	-1.399759	-1.145549	-0.364756
C	-2.766371	-1.219282	-0.055434
C	0.663547	0.257989	-0.851993
C	1.608067	-0.313909	0.228943
N	1.769082	-1.771737	0.218155
C	0.556681	-2.516260	0.524701
C	-0.597476	-2.418737	-0.493105
C	2.991965	0.322356	0.221422
C	3.797849	0.138520	1.349017
C	5.082973	0.665777	1.404408
C	5.590479	1.382929	0.320478
C	4.801877	1.562982	-0.810731
C	3.509809	1.036101	-0.858938
C	2.493343	-2.299523	-0.927329
O	-4.866746	-0.071696	0.401716
C	-5.507183	-1.326192	0.543765
O	-3.753893	2.258800	0.128118
C	-3.171847	3.543360	0.003217
H	-1.112270	2.223460	-0.471734
H	-3.216340	-2.196352	0.060958
H	0.882296	-0.207940	-1.819293
H	0.869456	1.324052	-0.964304
H	1.154340	-0.076249	1.198620
H	0.850703	-3.565229	0.625459
H	0.191264	-2.181495	1.500869
H	-1.264156	-3.271533	-0.341368
H	-0.196203	-2.517370	-1.507588
H	3.405306	-0.437821	2.179315
H	5.689219	0.518008	2.290053
H	6.591383	1.794863	0.359370
H	5.188796	2.111232	-1.661232
H	2.917134	1.179155	-1.754219
H	2.615804	-3.375843	-0.790748
H	2.002144	-2.137405	-1.898128
H	3.484470	-1.848003	-0.971852
H	-5.445632	-1.904793	-0.382267

H	-5.070108	-1.899556	1.366296
H	-6.547285	-1.104228	0.767120
H	-2.769111	3.696069	-1.002074
H	-3.975362	4.251958	0.185391
H	-2.379637	3.688503	0.743047

45
1E

C	2.798993	0.053768	0.146216
C	2.055692	1.080207	-0.470006
C	0.857588	0.766559	-1.098062
C	0.380194	-0.548604	-1.122422
C	1.106281	-1.562572	-0.509182
C	2.316491	-1.250036	0.122258
C	-0.962587	-0.880556	-1.708859
C	-2.017181	-1.099856	-0.597412
N	-1.530704	-2.015283	0.434651
C	-0.872515	-3.198511	-0.108932
C	0.603878	-2.986764	-0.554424
C	-2.392480	0.241472	0.004496
C	-1.638867	0.798295	1.040891
C	-1.946069	2.066142	1.529125
C	-3.005987	2.792394	0.987515
C	-3.763277	2.240863	-0.043688
C	-3.456183	0.970794	-0.528507
C	-2.630181	-2.404372	1.308649
O	3.962041	0.439108	0.737061
C	4.727451	-0.563187	1.378739
O	2.583729	2.330958	-0.386600
C	1.810704	3.391327	-0.919662
H	0.258725	1.543020	-1.555404
H	2.875547	-2.043292	0.600582
H	-1.317096	-0.074164	-2.353549
H	-0.896593	-1.781104	-2.326782
H	-2.916332	-1.523481	-1.084141
H	-0.881319	-3.948145	0.683160
H	-1.460429	-3.623023	-0.940958
H	0.721718	-3.369372	-1.573866
H	1.251966	-3.597552	0.076546
H	-0.817722	0.224007	1.452490
H	-1.355394	2.487949	2.333701
H	-3.244283	3.777077	1.370976
H	-4.594860	2.793219	-0.464547
H	-4.049521	0.539147	-1.328630
H	-2.244721	-2.993141	2.142017
H	-3.112739	-1.513939	1.710922
H	-3.392251	-3.000614	0.777373
H	4.162044	-1.029752	2.190602
H	5.048113	-1.329182	0.666625
H	5.598729	-0.056560	1.785579
H	2.371689	4.299408	-0.714752
H	1.680399	3.278064	-1.999804
H	0.831430	3.443707	-0.434791

45
1F

C	2.824643	-0.398706	0.461439
C	2.556333	0.555268	-0.539648
C	1.356747	0.486822	-1.232801
C	0.400419	-0.505141	-0.963586
C	0.677269	-1.461662	0.009470
C	1.887913	-1.390070	0.716131
C	-0.874955	-0.541409	-1.777811
C	-2.214368	-0.458907	-1.004678
N	-2.591314	-1.680247	-0.297465
C	-1.681821	-2.117772	0.753746
C	-0.285326	-2.586843	0.309366
C	-2.351113	0.758631	-0.093085
C	-1.642063	1.939416	-0.324191
C	-1.845885	3.066187	0.470399
C	-2.766540	3.033356	1.513089
C	-3.485297	1.863292	1.748810
C	-3.280690	0.740580	0.951804
C	-3.027099	-2.752401	-1.172772
O	4.013723	-0.265709	1.105465

C	4.316189	-1.214676	2.111419
O	3.523991	1.487462	-0.747132
C	3.279125	2.468217	-1.737477
H	1.146831	1.211267	-2.009051
H	2.087468	-2.136371	1.473338
H	-0.847579	0.266404	-2.513541
H	-0.903786	-1.467981	-2.361818
H	-2.982854	-0.339383	-1.778521
H	-1.566430	-1.300250	1.470372
H	-2.180919	-2.941460	1.273424
H	-0.380275	-3.239870	-0.565677
H	0.136179	-3.204353	1.106635
H	-0.918192	1.992539	-1.124891
H	-1.279764	3.968666	0.273361
H	-2.922535	3.907500	2.133377
H	-4.208848	1.823539	2.554387
H	-3.838992	-0.169817	1.128868
H	-2.246164	-3.165923	-1.828581
H	-3.414187	-3.570796	-0.561692
H	-3.839116	-2.390095	-1.806838
H	5.293022	-0.936035	2.497756
H	3.578920	-1.179585	2.918631
H	4.360484	-2.225643	1.696344
H	4.156171	3.109870	-1.743118
H	3.154497	2.009843	-2.722715
H	2.392674	3.060540	-1.492193

45

1G

C	-3.443115	-0.402263	-0.141030
C	-3.124551	0.969971	-0.134123
C	-1.807515	1.366043	-0.337617
C	-0.796688	0.422226	-0.547467
C	-1.111103	-0.933633	-0.550793
C	-2.434729	-1.336860	-0.347901
C	0.636671	0.829548	-0.761620
C	1.561470	0.470709	0.426173
N	1.115551	-0.716242	1.163837
C	0.972161	-1.978860	0.452879
C	0.001341	-1.931018	-0.745235
C	3.026467	0.434726	0.008894
C	3.966123	1.200743	0.703025
C	5.319887	1.153820	0.376405
C	5.758525	0.327333	-0.654585
C	4.833768	-0.444271	-1.355479
C	3.481269	-0.387722	-1.028588
C	1.881716	-0.907471	2.383455
O	-4.753836	-0.706957	0.060132
C	-5.105634	-2.077168	0.070375
O	-4.167351	1.818361	0.075199
C	-3.877537	3.202849	0.116124
H	-1.548306	2.416756	-0.336304
H	-2.664846	-2.394259	-0.351366
H	1.011706	0.366841	-1.677291
H	0.709521	1.907793	-0.918681
H	1.460907	1.282714	1.153787
H	1.942233	-2.392078	0.129378
H	0.564690	-2.677911	1.188078
H	-0.409964	-2.932239	-0.889521
H	0.545975	-1.689790	-1.662358
H	3.630753	1.841618	1.511988
H	6.028975	1.760423	0.926592
H	6.809755	0.285547	-0.911807
H	5.164869	-1.088132	-2.161294
H	2.778404	-0.987887	-1.593938
H	2.916070	-1.238558	2.199822
H	1.918556	0.030168	2.942267
H	1.383368	-1.654728	3.004207
H	-4.586886	-2.610095	0.872346
H	-6.177579	-2.107114	0.247488
H	-4.880053	-2.548591	-0.890584
H	-4.825870	3.699237	0.304271
H	-3.176065	3.433086	0.923289
H	-3.466721	3.547438	-0.837231

45
1H

C	2.752171	-0.079501	0.736590
C	2.734424	-0.057715	-0.673562
C	1.567551	-0.402252	-1.334803
C	0.400356	-0.780006	-0.644743
C	0.421858	-0.814107	0.745822
C	1.606856	-0.458838	1.415762
C	-0.818227	-1.118810	-1.481016
C	-2.192427	-0.731812	-0.899887
N	-2.704782	-1.689824	0.087526
C	-1.694396	-2.249557	0.980715
C	-0.767621	-1.205253	1.598116
C	-2.284553	0.711561	-0.406176
C	-3.278132	1.070028	0.509260
C	-3.439462	2.395072	0.905434
C	-2.609329	3.388669	0.390069
C	-1.619705	3.042503	-0.525397
C	-1.460175	1.715460	-0.921068
C	-3.455282	-2.768669	-0.534158
O	3.925583	0.278126	1.320662
C	3.966903	0.290252	2.735817
O	3.894530	0.314522	-1.275809
C	3.906628	0.355075	-2.690380
H	1.538181	-0.378684	-2.416714
H	1.608808	-0.486806	2.497547
H	-0.704740	-0.634724	-2.454188
H	-0.845815	-2.194326	-1.691376
H	-2.891923	-0.788574	-1.740919
H	-2.233998	-2.762485	1.781054
H	-1.081322	-3.012893	0.468931
H	-0.380858	-1.618137	2.532869
H	-1.353775	-0.320578	1.863853
H	-3.909997	0.289807	0.914068
H	-4.214430	2.651021	1.618278
H	-2.731020	4.419272	0.700185
H	-0.962801	3.803122	-0.929790
H	-0.672966	1.469293	-1.622054
H	-3.856855	-3.419859	0.244634
H	-4.293016	-2.361791	-1.102334
H	-2.840484	-3.390453	-1.207893
H	3.236241	0.994885	3.142571
H	3.781656	-0.707992	3.142489
H	4.970958	0.610882	3.000481
H	3.179711	1.079838	-3.068220
H	4.909815	0.665641	-2.969935
H	3.696564	-0.631489	-3.113416

45
1I

C	-3.528573	-0.160763	0.305915
C	-3.042079	1.095675	-0.111004
C	-1.702664	1.220852	-0.439196
C	-0.811145	0.133378	-0.379476
C	-1.293353	-1.109272	0.026264
C	-2.653849	-1.232699	0.363775
C	0.636879	0.407161	-0.746005
C	1.644656	-0.436209	0.057826
N	1.903193	-1.771296	-0.516804
C	0.676285	-2.453341	-0.919664
C	-0.441505	-2.362656	0.115154
C	2.966973	0.261733	0.322817
C	3.466008	1.283914	-0.485304
C	4.706980	1.860780	-0.217268
C	5.466381	1.419585	0.862512
C	4.978966	0.394450	1.672315
C	3.740508	-0.178060	1.400060
C	2.833012	-1.767419	-1.637678
O	-4.849764	-0.211978	0.618820
C	-5.368938	-1.460341	1.038112
O	-3.954205	2.101983	-0.150342
C	-3.494208	3.379322	-0.552165
H	-1.314223	2.182134	-0.748880
H	-3.016030	-2.204234	0.673410
H	0.795798	0.257587	-1.820470

H	0.823757	1.464377	-0.549563
H	1.195203	-0.609753	1.039541
H	0.296202	-2.067488	-1.881892
H	0.935356	-3.503409	-1.078382
H	-0.010695	-2.479862	1.115489
H	-1.102776	-3.219411	-0.033393
H	2.895326	1.630246	-1.338967
H	5.079361	2.652902	-0.855478
H	6.428832	1.869893	1.072010
H	5.562338	0.043794	2.515048
H	3.363620	-0.985429	2.018206
H	3.813567	-1.415987	-1.322026
H	2.934893	-2.792307	-1.998898
H	2.490941	-1.145857	-2.482805
H	-6.423574	-1.290856	1.237914
H	-5.260521	-2.214170	0.253190
H	-4.873213	-1.804702	1.950217
H	-4.363067	4.031228	-0.518877
H	-2.727991	3.753270	0.132794
H	-3.095713	3.350535	-1.570344

45

1J

C	3.462523	-0.133568	-0.058520
C	2.894898	1.153072	0.039791
C	1.539298	1.312802	-0.203919
C	0.711361	0.233287	-0.559439
C	1.276856	-1.034341	-0.662782
C	2.647868	-1.200552	-0.404190
C	-0.755987	0.551268	-0.797187
C	-1.795549	-0.566839	-0.499556
N	-1.409011	-1.493361	0.548914
C	-0.574116	-2.597850	0.087804
C	0.445214	-2.242809	-1.009893
C	-3.182357	0.024006	-0.234456
C	-4.084683	-0.649697	0.593621
C	-5.369897	-0.155681	0.802223
C	-5.781522	1.020693	0.180072
C	-4.894229	1.696171	-0.653021
C	-3.606534	1.202647	-0.856256
C	-1.021334	-0.882663	1.812639
O	4.793029	-0.219307	0.202909
C	5.384262	-1.503766	0.135528
O	3.748335	2.152532	0.384138
C	3.209474	3.456882	0.499643
H	1.092222	2.294337	-0.115112
H	3.066454	-2.195205	-0.483371
H	-1.001962	1.414223	-0.171811
H	-0.884235	0.881299	-1.834248
H	-1.910896	-1.173521	-1.402722
H	-0.039659	-2.990052	0.956277
H	-1.216839	-3.402766	-0.290464
H	-0.076071	-2.074256	-1.956355
H	1.094307	-3.107666	-1.170591
H	-3.756411	-1.563534	1.072531
H	-6.050231	-0.691720	1.453270
H	-6.780518	1.406378	0.342404
H	-5.200597	2.610822	-1.146314
H	-2.937813	1.746336	-1.511654
H	-1.759089	-0.121159	2.075423
H	-1.040829	-1.644550	2.595279
H	-0.027744	-0.417863	1.803758
H	4.925926	-2.184492	0.858570
H	5.298488	-1.923484	-0.870783
H	6.432892	-1.360986	0.382334
H	2.441476	3.496474	1.277457
H	4.042171	4.097805	0.776578
H	2.787850	3.792921	-0.451847

45

1K

C	3.075923	0.521940	-0.536448
C	3.076430	-0.690717	0.182312
C	1.885848	-1.149689	0.717073
C	0.668130	-0.458865	0.560798

C	0.664767	0.734068	-0.159786
C	1.881898	1.204008	-0.693446
C	-0.512304	-1.098452	1.274100
C	-1.868501	-0.383463	1.279595
N	-1.667864	1.001412	1.713321
C	-1.431895	2.004569	0.689877
C	-0.581786	1.526145	-0.488200
C	-2.726278	-0.590191	0.031482
C	-2.282725	-1.310071	-1.081568
C	-3.107214	-1.492590	-2.190251
C	-4.392407	-0.957350	-2.206792
C	-4.847913	-0.240122	-1.102570
C	-4.022377	-0.064423	0.004660
C	-2.561254	1.504131	2.738093
O	4.278033	0.924263	-1.027722
C	4.308843	2.146194	-1.741132
O	4.278234	-1.315671	0.296546
C	4.309139	-2.531641	1.019935
H	1.875379	-2.070264	1.287098
H	1.866944	2.130559	-1.251404
H	-0.639768	-2.127890	0.922470
H	-0.224091	-1.169667	2.326879
H	-2.432905	-0.860860	2.086634
H	-2.382410	2.387802	0.277391
H	-0.932397	2.846136	1.181145
H	-0.287103	2.418702	-1.044911
H	-1.205877	0.944019	-1.166009
H	-1.275793	-1.709031	-1.101557
H	-2.740142	-2.049943	-3.043617
H	-5.032863	-1.099314	-3.068553
H	-5.847556	0.177306	-1.099922
H	-4.392374	0.482066	0.863782
H	-2.106700	2.383530	3.201737
H	-3.550447	1.809155	2.358277
H	-2.702382	0.751128	3.514566
H	5.345207	2.293609	-2.033404
H	3.679541	2.095198	-2.634324
H	3.983231	2.977441	-1.109214
H	5.342902	-2.866112	0.994303
H	3.998300	-2.379220	2.057570
H	3.668258	-3.283854	0.550828

2. DFT computed absolute energies and zero point vibrational energies

Conformer	B3LYP			M052X		
	E (-a.u) ^a	E (-a.u) ^b	ZPVE (a.u) ^a	E (-a.u) ^a	E (-a.u) ^b	ZPVE (a.u) ^a
A	943.10022	943.10744	0.38424	942.99195	943.00039	0.39172
B	943.09655	943.10373	0.38428	942.98888	942.99737	0.39137
C	943.09666	943.10400	0.38473	942.98979	942.99844	0.39240
D	943.09606	943.10350	0.38444	942.98795	942.99677	0.39163
E	943.09531	943.10243	0.38458	942.98919	942.99752	0.39161
F	943.09429	943.10176	0.38472	942.98708	942.99610	0.39186
G	943.09356	943.10156	0.38459	942.98517	942.99481	0.39210
H	943.09130	943.09862	0.38442	942.98497	942.99374	0.39156
I	943.09105	943.09871	0.38447	942.98401	942.99302	0.39192
J	943.08846	943.09558	0.38417	942.98157	942.98962	0.39133
K	943.08511	943.09255	0.38454	942.97695	942.98583	0.39187

a) Gas phase, normal grid. b) IEFCM, ultrafine grid single point computation

Table 1 Experimental and back-computed $^1D_{CH}$ RDCs for **1**

$^1D_{CH}$	Experimental	Computed $\langle ^1D_{CH} \rangle^a$	
		B3LYP	M052X
C-H1a	3.20	4.32 [0.29]	4.18 [0.31]
C-H1b	7.70	6.86 [0.27]	7.03 [0.28]
C-H2a	5.60	5.66 [0.21]	5.85 [0.25]
C-H4a	4.20	4.82 [0.24]	4.78 [0.27]
C-H4b	2.20	1.73 [0.50]	1.59 [0.45]
C-H5a	0.10	-0.59 [0.25]	-0.50 [0.25]
C-H5b	5.20	4.65 [0.40]	4.58 [0.41]
C-H6	2.80	2.50 [0.26]	2.50 [0.27]
C-H9	2.20	2.23 [0.26]	2.15 [0.27]
C-H2'	3.00	3.49 [0.28]	3.28 [0.27]
C-H3'	2.80	3.48 [0.28]	3.33 [0.27]
C-H4'	-9.20	-9.09 [0.48]	-9.07 [0.46]
C-H10	0.00	0.38 [0.16]	0.15 [0.17]

^a In brackets computed standard deviations

3. Alignment tensor computations for conformer **1A**

B3LYP geometry

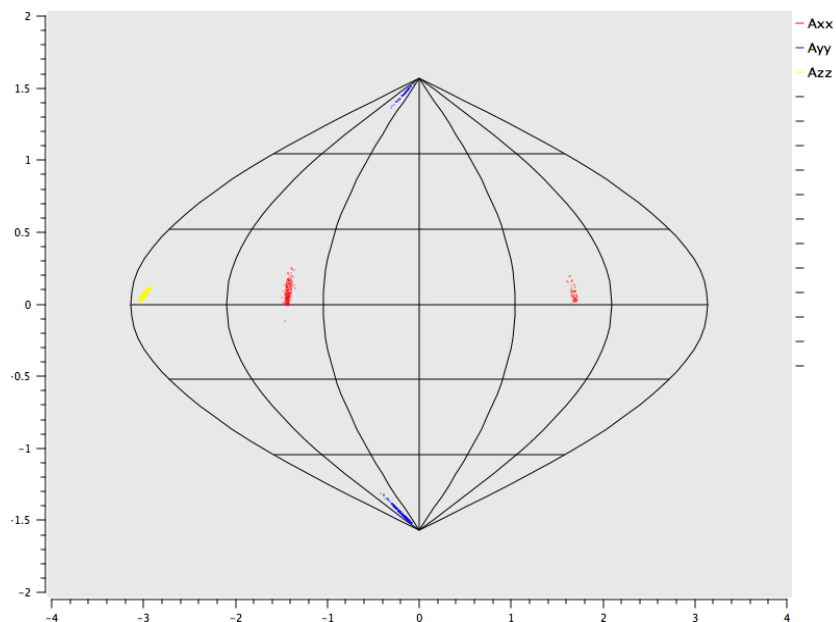
Single point computation:

Alignment tensor
 Axx=-6.36596e-05
 Ayy=-0.000162893
 Azz=0.000226553
 Saupe tensor
 Sxx=-9.54894e-05
 Syy=-0.00024434
 Szz=0.00033983
 (0.1325,0.989231,0.0621703,)
 (-0.0583528,0.0703997,-0.995811,)
 (-0.989464,0.128317,0.0670524,)

SVD condition number is 5.38996
 Axial component Aa=0.00033983
 rhombic component Ar=9.92339e-05
 rhombicity R=0.292011
 Asimmetry parameter etha=0.438016
 GD0=0.000410792
 Euler Angles
 Set 1
 (62.4106,81.6754,-23.7686)
 Set 2
 (-117.589,98.3246,156.231)

Montecarlo bootstrapping computation
 Gaussian distribution size=256
 RDC Error=1.5 Hz
 Alignment tensor
 <Axx>=-6.24381e-05 stdved=4.54166e-06
 <Ayy>=-0.000164461 stdved=1.26407e-05
 <Azz>=0.000226899 stdved=1.28149e-05
 Quality factors statistic
 <Q>=0.145593
 StdDev(Q)=0.0113819
 Highest Q=0.185862

Lowest $Q=0.127067$



Sason-Flamsteed projection of alignment tensor eigenvectors distribution (1A, B3LYP)

M052X geometry

Conformer 1

Alignment tensor

Axx=-6.21809e-05

Ayy=-0.000166047

Azz=0.000228228

Saupe tensor

Sxx=-9.32714e-05

Syy=-0.00024907

Szz=0.000342341

(0.140543, 0.988163, 0.0614917,)

(-0.039264, 0.0676221, -0.996938,)

(-0.989296, 0.137698, 0.048303,)

SVD condition number is 5.41546

Axial component Aa=0.000342341

rhombic component Ar=0.000103866

rhombicity R=0.303398

Asimmetry parameter etha=0.455097

GDO=0.000415266

Euler Angles

Set 1

(70.6697, 81.6092, -15.609)

Set 2

(-109.33, 98.3908, 164.391)

Montecarlo bootstrapping distribution:

Gaussian distribution size=256

RDC Error=1.5 Hz

Alignment tensor

<Axx>=-6.11177e-05 stdved=4.46158e-06

<Ayy>=-0.00016745 stdved=1.24848e-05

<Azz>=0.000228568 stdved=1.25575e-05

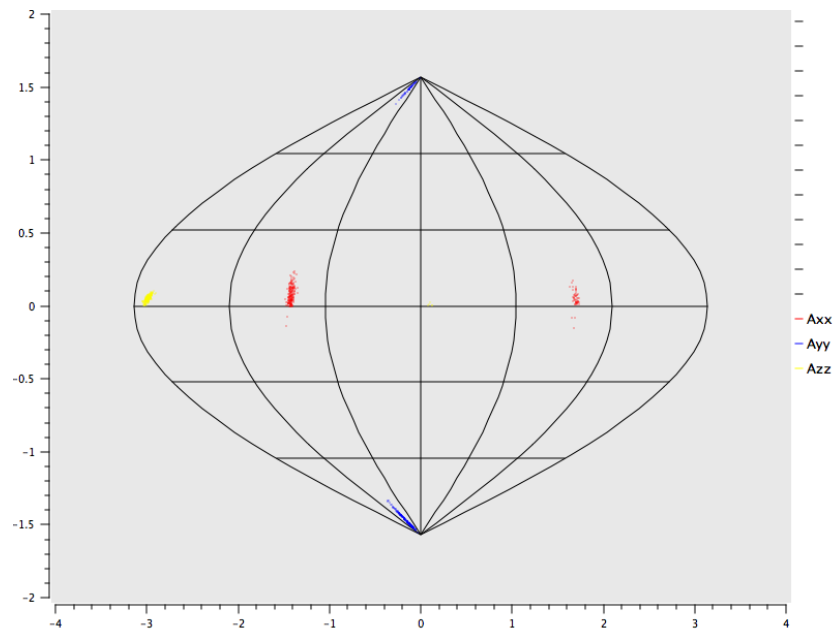
Quality factors statistic

<Q>=0.132545

StdDev(Q)=0.0115594

Highest $Q=0.171022$

Lowest $Q=0.113639$



Sason-Flamsteed projection of alignment tensor eigenvectors distribution (1A, M052X)

- 1 (a) N. L. Allinger, Y. H. Yuh, and J. H. Lii *J. Am. Chem. Soc.* 1989, **111**, 8551; (b) J. H. Lii, and N. L. Allinger, *J. Am. Chem. Soc.* 1989, **111**, 8566; (c) J. H. Lii, and N. L. Allinger, *J. Am. Chem. Soc.* 1989, **111**, 8576
- 2 J. W. Ponder Tinker Software Tools for Molecular Design. Version 4.2 2004 (<http://dasher.wustl.edu/tinker>).
- 3 (a) A. D. Becke, *Phys. Rev. A* 1988, **38**, 3098; (b) C. Lee, W. Yang, and R. G. Parr, *Phys. Rev. B* 1988, **37**, 785
- 4 Y. Zhao, N. E. Shultz, D. G. Truhlar, *J. Chem. Theory. Comput.* 2006, **2**, 364.
- 5 Y. Zhao, D. G. Truhlar, *Acc. Chem. Res.* 2008, **41**, 157
- 6 Gaussian 03, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.
- 7 J. Tomasi, B. Mennucci, R. Cammi *Chem. Rev.* 2005, **105**, 2999
- 8 Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.