

Supporting Information

Asymmetric Aromatic Finkelstein Reaction: A Peptide Catalysis Platform for Diarylmethine Desymmetrization

Tobias Morack^a, Tyler E. Myers^a, Lucas J. Karas^b, Melissa A. Hardy^b, Brandon Q. Mercado^a,
Matthew S. Sigman^{b*}, Scott J. Miller^{a*}

^aDepartment of Chemistry, Yale University, New Haven, Connecticut 06520 – 8170, United States

^bDepartment of Chemistry, University of Utah, 315 South 1400 East, Salt Lake City, Utah 84112, United States

1. Optimized Cartesian coordinates for all structures

3-conf01

- Electronic Energy (Eh): -6818.72907025

- Cartesian Coordinates:

Br	3.420116	-0.613522	2.251994
C	2.875182	0.228927	0.639925
C	1.702247	0.974529	0.653464
C	1.242617	1.622669	-0.498225
C	-0.036330	2.445498	-0.561738
C	-0.074594	3.718043	0.363886
C	1.206368	4.528180	0.120340
C	-1.285166	4.571572	-0.044689
C	-0.195099	3.403072	1.860546
C	-1.296945	1.592556	-0.502903
C	-1.538510	0.647968	0.498619
C	-2.716881	-0.088511	0.521599
Br	-2.962870	-1.346980	1.922064
C	-3.708052	0.081180	-0.459899
N	-4.880561	-0.685987	-0.395764
C	-5.942656	-0.652626	-1.239689
C	-7.067811	-1.649460	-0.858955
F	-6.781669	-2.343910	0.253402
F	-8.198605	-0.992199	-0.650270
F	-7.252910	-2.515439	-1.844304
O	-6.093210	0.041789	-2.214019
C	-3.465124	1.019125	-1.470488
C	-2.282762	1.749813	-1.481683
C	2.017417	1.483664	-1.653930
C	3.192145	0.741114	-1.680769
C	3.647296	0.093971	-0.525979
N	4.823068	-0.669732	-0.490048
C	5.697564	-0.896873	-1.502704
C	6.900638	-1.785851	-1.094052
F	8.028593	-1.103536	-1.229396
F	6.953533	-2.856527	-1.871034
F	6.820093	-2.201691	0.179615
O	5.639161	-0.490968	-2.636613
H	1.158454	1.043417	1.593297
H	-0.035827	2.872406	-1.576483
H	1.177791	5.469526	0.690335
H	1.320284	4.784214	-0.945307
H	2.104449	3.973616	0.430247
H	-2.235905	4.057322	0.159810
H	-1.258392	4.821495	-1.117467
H	-1.288733	5.517825	0.517468
H	-0.327723	4.340447	2.422440
H	0.707348	2.921202	2.261740
H	-1.065948	2.767107	2.079032
H	-0.804630	0.459276	1.279961
H	-4.933339	-1.339875	0.379881
H	-4.214628	1.163200	-2.245179
H	-2.127766	2.471637	-2.286930
H	1.694944	1.973535	-2.575766
H	3.772400	0.652933	-2.596319
H	5.037902	-1.099913	0.404803

3-conf02

- Electronic Energy (Eh): -6818.72892987

- Cartesian Coordinates:

Br	4.699145	1.414238	-2.090259
C	3.385492	0.905266	-0.818076
C	2.227388	1.667049	-0.721015
C	1.220210	1.349891	0.195641
C	-0.010552	2.245033	0.265064
C	0.019109	3.296778	1.435420

C	-1.208543	4.207332	1.292163
C	0.021914	2.675542	2.837738
C	1.288808	4.148295	1.283092
C	-1.316559	1.479874	0.105720
C	-1.831401	0.599702	1.063735
C	-3.029860	-0.071862	0.852721
Br	-3.650883	-1.245601	2.209902
C	-3.773022	0.102733	-0.326862
N	-4.976630	-0.597599	-0.494144
C	-5.823356	-0.552956	-1.553705
C	-7.062159	-1.472143	-1.395431
F	-7.074277	-2.379124	-2.361021
F	-7.071887	-2.119757	-0.219861
F	-8.170091	-0.750732	-1.473474
O	-5.713674	0.098278	-2.562634
C	-3.261828	0.982015	-1.288507
C	-2.062113	1.647515	-1.065250
C	1.423494	0.224653	1.000177
C	2.577223	-0.546202	0.912024
C	3.587450	-0.219164	-0.000764
N	4.769569	-0.962895	-0.130536
C	5.142927	-2.060858	0.574100
C	6.526909	-2.622736	0.157416
F	7.348426	-2.609241	1.196581
F	7.094009	-1.908236	-0.827136
F	6.395934	-3.870550	-0.267124
O	4.534924	-2.619359	1.453048
H	2.112674	2.532013	-1.376988
H	0.047670	2.873436	-0.636961
H	-1.182800	5.006077	2.049231
H	-2.147040	3.648529	1.423440
H	-1.237798	4.686044	0.300082
H	0.852522	1.967030	2.973056
H	-0.923308	2.165371	3.070179
H	0.145976	3.469795	3.589961
H	1.292309	4.960444	2.025957
H	1.347001	4.610379	0.284387
H	2.201069	3.552310	1.434426
H	-1.310669	0.422727	2.002398
H	-5.238338	-1.207911	0.274658
H	-3.818137	1.134600	-2.210372
H	-1.696024	2.325744	-1.839714
H	0.668367	-0.084976	1.721288
H	2.709632	-1.416388	1.550645
H	5.418970	-0.631204	-0.837818

3-conf03

- Electronic Energy (Eh): -6818.7289882

- Cartesian Coordinates:

Br	-4.245726	1.119522	2.496613
C	-3.199036	0.865101	0.933974
C	-2.035836	1.611329	0.786721
C	-1.216984	1.476513	-0.338872
C	0.044164	2.326505	-0.415117
C	0.112197	3.336043	-1.620843
C	0.332545	2.670741	-2.985274
C	-1.198290	4.134877	-1.653722
C	1.276609	4.306273	-1.367743
C	1.318273	1.519486	-0.203857
C	1.622500	0.364249	-0.929315
C	2.810871	-0.324100	-0.716650
Br	3.144615	-1.881978	-1.749490
C	3.749494	0.108086	0.235854
N	4.935003	-0.619951	0.415019
C	5.954335	-0.351128	1.269308

C	7.117705	-1.373024	1.185981
F	8.228766	-0.757613	0.807644
F	7.318432	-1.924418	2.372969
F	6.871870	-2.357815	0.307954
O	6.045826	0.564391	2.048901
C	3.443257	1.259071	0.971597
C	2.251324	1.938715	0.749000
C	-1.623058	0.554227	-1.310191
C	-2.784345	-0.198087	-1.174760
C	-3.600033	-0.058080	-0.045405
N	-4.780599	-0.792311	0.139674
C	-5.325421	-1.714175	-0.693882
C	-6.643377	-2.331156	-0.158206
F	-6.497582	-3.639120	-0.006605
F	-7.625939	-2.107827	-1.017784
F	-7.005132	-1.815396	1.026883
O	-4.906139	-2.087318	-1.761218
H	-1.763984	2.316941	1.574167
H	-0.014675	2.988448	0.462588
H	0.467470	3.447384	-3.753827
H	-0.527261	2.062621	-3.298312
H	1.235418	2.042163	-2.995815
H	-1.385970	4.634000	-0.689343
H	-2.062756	3.490899	-1.872921
H	-1.152103	4.913404	-2.430628
H	1.297694	5.084233	-2.146041
H	2.248605	3.791336	-1.383280
H	1.175656	4.811905	-0.393939
H	0.929928	-0.028095	-1.671783
H	5.033773	-1.445079	-0.169354
H	4.151100	1.609039	1.719335
H	2.045942	2.832261	1.343106
H	-1.035557	0.404421	-2.214713
H	-3.075923	-0.906295	-1.946840
H	-5.281885	-0.603460	1.002860

3-conf04

- Electronic Energy (Eh): -6818.72878518

- Cartesian Coordinates:

Br	-4.598256	-1.589695	-1.776400
C	-3.373731	-0.881343	-0.510616
C	-2.197609	-1.579433	-0.264620
C	-1.253428	-1.115905	0.656601
C	0.000714	-1.946564	0.895172
C	-0.047536	-2.835425	2.192871
C	-0.140371	-2.035263	3.497624
C	-1.276765	-3.752275	2.100056
C	1.217809	-3.704194	2.225748
C	1.288507	-1.159863	0.691941
C	2.090165	-1.479284	-0.408420
C	3.280462	-0.807727	-0.660817
Br	4.301152	-1.314567	-2.178645
C	3.726975	0.223116	0.181864
N	4.934022	0.876378	-0.106756
C	5.527420	1.874914	0.595022
C	6.865940	2.355416	-0.023144
F	6.786344	3.643259	-0.321757
F	7.850684	2.178274	0.845136
F	7.179500	1.689111	-1.145288
O	5.137108	2.402474	1.606640
C	2.927597	0.548978	1.284397
C	1.738871	-0.130297	1.525987
C	-1.538122	0.087384	1.309201
C	-2.710619	0.795593	1.071107
C	-3.657948	0.322656	0.154599
N	-4.856303	0.996956	-0.122217
C	-5.308414	2.150454	0.431547
C	-6.691403	2.596840	-0.109597
F	-6.600693	3.810738	-0.630435

F	-7.573047	2.621118	0.879503
F	-7.159702	1.772478	-1.059683
O	-4.770129	2.830849	1.268978
H	-2.018484	-2.511083	-0.804649
H	0.001893	-2.691000	0.084148
H	-0.247090	-2.728912	4.345905
H	-1.015379	-1.368803	3.510389
H	0.763633	-1.439513	3.685775
H	-1.265977	-4.348631	1.173415
H	-2.215866	-3.179706	2.123682
H	-1.291325	-4.454484	2.947484
H	1.180977	-4.401151	3.077015
H	2.127509	-3.094239	2.328870
H	1.315925	-4.303278	1.305980
H	1.783733	-2.274507	-1.090747
H	5.415692	0.555414	-0.941709
H	3.253697	1.343915	1.951041
H	1.164648	0.166328	2.402145
H	-0.834425	0.508005	2.025991
H	-2.907566	1.728898	1.593426
H	-5.451716	0.560530	-0.820141

3-conf05

- Electronic Energy (Eh): -6818.72907057

- Cartesian Coordinates:

Br	2.962245	-1.346916	1.922114
C	2.716564	-0.088520	0.521532
C	1.538258	0.648051	0.498312
C	1.296907	1.592581	-0.503322
C	0.036402	2.445665	-0.562407
C	0.074803	3.718450	0.362894
C	-1.205962	4.528764	0.118903
C	0.194967	3.403891	1.859670
C	1.285623	4.571614	-0.045714
C	-1.242591	1.622930	-0.498672
C	-1.702339	0.975301	0.653263
C	-2.875231	0.229643	0.639932
Br	-3.420340	-0.612084	2.252313
C	-3.647199	0.094120	-0.526020
N	-4.822954	-0.669603	-0.489861
C	-5.696615	-0.898387	-1.502878
C	-6.900140	-1.786561	-1.093694
F	-8.027723	-1.103513	-1.228883
F	-6.953988	-2.857342	-1.870405
F	-6.819585	-2.202141	0.180048
O	-5.637397	-0.494155	-2.637331
C	-3.191954	0.740772	-1.681047
C	-2.017250	1.483377	-1.654395
C	2.282856	1.749614	-1.482007
C	3.465152	1.018824	-1.470591
C	3.707875	0.080979	-0.459860
N	4.880293	-0.686327	-0.395518
C	5.942642	-0.652899	-1.239123
C	7.067562	-1.649988	-0.858286
F	6.780831	-2.345014	0.253554
F	8.198284	-0.992878	-0.648657
F	7.253162	-2.515452	-1.843986
O	6.093625	0.041776	-2.213192
H	0.804218	0.459418	1.279524
H	0.035954	2.872315	-1.577259
H	-1.177343	5.470233	0.688700
H	-2.104192	3.974409	0.428759
H	-1.319609	4.784583	-0.946824
H	1.065401	2.767451	2.078442
H	-0.707836	2.922732	2.260917
H	0.328153	4.341376	2.421247
H	1.289081	5.518178	0.515922
H	1.259284	4.820951	-1.118640
H	2.236223	4.057358	0.159408

H	-1.158613	1.044622	1.593104
H	-5.038151	-1.098918	0.405316
H	-3.772056	0.652112	-2.596643
H	-1.694669	1.972827	-2.576419
H	2.128032	2.471362	-2.287358
H	4.214797	1.162778	-2.245169
H	4.932675	-1.340522	0.379891

3-conf06

- Electronic Energy (Eh): -6818.72893001

- Cartesian Coordinates:

Br	3.651107	-1.244675	2.210333
C	3.029900	-0.071455	0.852788
C	1.831489	0.600225	1.063732
C	1.316517	1.480021	0.105456
C	0.010521	2.245249	0.264654
C	-0.019197	3.297187	1.434827
C	-0.022520	2.676200	2.837258
C	1.208661	4.207478	1.291720
C	-1.288689	4.148944	1.282046
C	-1.220205	1.350049	0.195367
C	-2.227439	1.667018	-0.721283
C	-3.385498	0.905142	-0.818183
Br	-4.699224	1.413805	-2.090416
C	-3.587345	-0.219193	-0.000721
N	-4.769415	-0.963021	-0.130320
C	-5.142750	-2.060819	0.574596
C	-6.526639	-2.622938	0.157931
F	-7.094538	-1.907695	-0.825633
F	-6.395212	-3.870245	-0.268031
F	-7.347687	-2.610996	1.197445
O	-4.534670	-2.619185	1.453567
C	-2.577024	-0.546068	0.912033
C	-1.423352	0.224879	1.000036
C	2.061879	1.647168	-1.065712
C	3.261531	0.981535	-1.288905
C	3.772867	0.102631	-0.326987
N	4.976433	-0.597803	-0.494166
C	5.822828	-0.553906	-1.554022
C	7.061971	-1.472546	-1.395249
F	7.075445	-2.378913	-2.361348
F	7.071088	-2.120828	-0.220042
F	8.169593	-0.750443	-1.471895
O	5.712818	0.096571	-2.563402
H	1.310897	0.423626	2.002544
H	-0.047675	2.873492	-0.637487
H	-0.146662	3.470609	3.589304
H	0.922538	2.165908	3.070101
H	-0.853286	1.967847	2.972453
H	1.238279	4.685972	0.299543
H	2.147027	3.648540	1.423369
H	1.182846	5.006384	2.048618
H	-1.292215	4.961199	2.024796
H	-2.201117	3.553177	1.433242
H	-1.346521	4.610896	0.283258
H	-2.112804	2.531889	-1.377395
H	-5.418932	-0.631438	-0.837546
H	-2.709294	-1.416209	1.550743
H	-0.668145	-0.084596	1.721135
H	1.695676	2.325091	-1.840391
H	3.817668	1.133714	-2.210941
H	5.238249	-1.207761	0.274880

3-conf07

- Electronic Energy (Eh): -6818.72898831

- Cartesian Coordinates:

Br	3.144651	-1.881744	1.749668
C	2.810890	-0.323941	0.716724

C	1.622519	0.364416	0.929349
C	1.318282	1.519598	0.203805
C	0.044149	2.326587	0.415022
C	0.112144	3.336179	1.620714
C	1.276414	4.306545	1.367492
C	-1.198424	4.134871	1.653695
C	0.332710	2.670927	2.985133
C	-1.216994	1.476580	0.338801
C	-2.035907	1.611425	-0.786732
C	-3.199125	0.865196	-0.933926
Br	-4.245924	1.119676	-2.496476
C	-3.600038	-0.058022	0.045443
N	-4.780618	-0.792263	-0.139570
C	-5.325245	-1.714308	0.693907
C	-6.643072	-2.331515	0.158185
F	-7.005126	-1.815473	-1.026673
F	-6.496865	-3.639392	0.006107
F	-7.625596	-2.108815	1.017963
O	-4.905866	-2.087475	1.761199
C	-2.784280	-0.198061	1.174748
C	-1.623000	0.554264	1.310130
C	2.251318	1.938770	-0.749083
C	3.443261	1.259122	-0.971633
C	3.749508	0.108188	-0.235815
N	4.935010	-0.619869	-0.414926
C	5.954308	-0.351188	-1.269302
C	7.117542	-1.373243	-1.186084
F	8.228930	-0.757860	-0.808738
F	7.317469	-1.925319	-2.372908
F	6.872016	-2.357527	-0.307401
O	6.045811	0.564264	-2.048976
H	0.929960	-0.027856	1.671865
H	-0.014704	2.988479	-0.462720
H	1.297572	5.084440	2.145849
H	1.175222	4.812251	0.393751
H	2.248461	3.791700	1.382811
H	-2.062781	3.490838	1.873152
H	-1.386338	4.633813	0.689270
H	-1.152182	4.913533	2.430460
H	0.467397	3.447595	3.753701
H	1.235772	2.042622	2.995638
H	-0.526894	2.062529	3.298177
H	-1.764113	2.317063	-1.574173
H	-5.281920	-0.603467	-1.002758
H	-3.075800	-0.906310	1.946810
H	-1.035454	0.404455	2.214621
H	2.045920	2.832273	-1.343249
H	4.151089	1.609044	-1.719404
H	5.033820	-1.444889	0.169592

3-conf08

- Electronic Energy (Eh): -6818.72896148

- Cartesian Coordinates:

Br	4.630075	1.430984	-2.136276
C	3.362776	0.918939	-0.819199
C	2.198234	1.666812	-0.694354
C	1.223066	1.347073	0.255530
C	-0.016219	2.227998	0.347918
C	-0.005318	3.243744	1.549656
C	-0.045779	2.581011	2.931833
C	1.274552	4.087436	1.452317
C	-1.222657	4.168038	1.404937
C	-1.317727	1.461619	0.159050
C	-1.803407	0.508955	1.061121
C	-3.003224	-0.153582	0.830362
Br	-3.584901	-1.427989	2.112034
C	-3.776651	0.102634	-0.314419
N	-4.980607	-0.591668	-0.503092
C	-5.859852	-0.466444	-1.529168

C	-7.098412	-1.390350	-1.398909
F	-8.196737	-0.655581	-1.295803
F	-7.199876	-2.161443	-2.470156
F	-7.031602	-2.185996	-0.320106
O	-5.782611	0.263344	-2.486005
C	-3.294005	1.053761	-1.220812
C	-2.092580	1.709372	-0.978212
C	1.467094	0.234290	1.066586
C	2.627579	-0.522640	0.950969
C	3.604511	-0.193580	0.003350
N	4.791788	-0.923453	-0.154524
C	5.200202	-2.009361	0.549345
C	6.577567	-2.558998	0.096048
F	7.107937	-1.845165	-0.909187
F	6.447834	-3.811027	-0.316529
F	7.428685	-2.529811	1.110682
O	4.626043	-2.566208	1.451795
H	2.052602	2.523237	-1.355416
H	0.042163	2.884828	-0.533496
H	0.033351	3.354650	3.711160
H	0.792489	1.884631	3.080731
H	-0.989864	2.046654	3.109103
H	1.358980	4.579037	0.469684
H	2.177618	3.477647	1.604087
H	1.269211	4.876193	2.219994
H	-1.208760	4.943631	2.185959
H	-2.167972	3.612953	1.498020
H	-1.225420	4.676622	0.427393
H	-1.258313	0.265279	1.970456
H	-5.214022	-1.267182	0.218940
H	-3.873664	1.269980	-2.115137
H	-1.749384	2.445461	-1.709080
H	0.742376	-0.075310	1.817890
H	2.791845	-1.383002	1.595529
H	5.415286	-0.590523	-0.884135

3-conf09

- Electronic Energy (Eh): -6818.72878622

- Cartesian Coordinates:

Br	-4.301142	1.314754	2.178639
C	-3.280426	0.807536	0.660951
C	-2.090141	1.479046	0.408387
C	-1.288469	1.159353	-0.691888
C	-0.000728	1.946056	-0.895344
C	0.047392	2.834619	-2.193274
C	1.276811	3.751279	-2.100989
C	0.139726	2.034158	-3.497883
C	-1.217795	3.703620	-2.226021
C	1.253478	1.115537	-0.656674
C	2.197684	1.579353	0.264383
C	3.373898	0.881440	0.510427
Br	4.598478	1.590213	1.775926
C	3.658179	-0.322675	-0.154542
N	4.856661	-0.996767	0.122279
C	5.308788	-2.150390	-0.431241
C	6.691845	-2.596581	0.109900
F	7.573267	-2.621734	-0.879368
F	7.160505	-1.771621	1.059293
F	6.601054	-3.810101	0.631647
O	4.770383	-2.831109	-1.268322
C	2.710839	-0.795907	-1.070865
C	1.538239	-0.087877	-1.309016
C	-1.738793	0.129545	-1.525654
C	-2.927497	-0.549706	-1.283879
C	-3.726905	-0.223546	-0.181455
N	-4.933920	-0.876797	0.107358
C	-5.527973	-1.874583	-0.594925
C	-6.866560	-2.354855	0.023262
F	-6.787378	-3.642841	0.321365

F	-7.851379	-2.177029	-0.844805
F	-7.179722	-1.688875	1.145710
O	-5.138171	-2.401682	-1.606981
H	-1.783725	2.274448	1.090513
H	-0.001897	2.690696	-0.084513
H	1.291147	4.453414	-2.948484
H	2.215819	3.178574	-2.124931
H	1.266489	4.347714	-1.174395
H	1.014445	1.367324	-3.510637
H	0.246654	2.727606	-4.346301
H	-0.764559	1.438773	-3.685822
H	-1.181139	4.400234	-3.077575
H	-1.315443	4.303077	-1.306449
H	-2.127659	3.093814	-2.328569
H	2.018509	2.511088	0.804244
H	5.452243	-0.559968	0.819806
H	2.907809	-1.729302	-1.593014
H	0.834504	-0.508759	-2.025616
H	-1.164538	-0.167300	-2.401716
H	-3.253594	-1.344791	-1.950343
H	-5.415380	-0.555937	0.942468

3-conf10

- Electronic Energy (Eh): -6818.72906228

- Cartesian Coordinates:

Br	2.941515	-1.325007	1.937444
C	2.706155	-0.081672	0.521744
C	1.530743	0.658867	0.485217
C	1.297384	1.592490	-0.528383
C	0.039397	2.448124	-0.602120
C	0.082277	3.736853	0.300542
C	1.287338	4.585658	-0.133879
C	-1.202379	4.540054	0.053697
C	0.218076	3.449286	1.801504
C	-1.240139	1.627448	-0.524140
C	-1.709733	1.014239	0.642583
C	-2.881236	0.266231	0.640679
Br	-3.440813	-0.527324	2.272395
C	-3.641440	0.093467	-0.528048
N	-4.816299	-0.670961	-0.480022
C	-5.672769	-0.943354	-1.496940
C	-6.868098	-1.836995	-1.075920
F	-8.008217	-1.220846	-1.346900
F	-6.830840	-2.980381	-1.744683
F	-6.854115	-2.124871	0.235063
O	-5.598789	-0.581568	-2.644767
C	-3.175973	0.705250	-1.697891
C	-2.003094	1.450965	-1.682543
C	2.287666	1.734666	-1.504878
C	3.467141	0.999628	-1.480172
C	3.702001	0.072591	-0.457689
N	4.870540	-0.699325	-0.379819
C	5.936595	-0.680586	-1.219170
C	7.053765	-1.680592	-0.823474
F	8.188211	-1.028833	-0.617489
F	7.236686	-2.558347	-1.798795
F	6.758779	-2.361172	0.295116
O	6.095642	0.003064	-2.199740
H	0.791905	0.482279	1.264897
H	0.039198	2.856719	-1.624368
H	1.293916	5.541553	0.411697
H	1.250267	4.816888	-1.210538
H	2.241057	4.077148	0.071096
H	-2.096546	3.990070	0.382459
H	-1.326662	4.775359	-1.015557
H	-1.170179	5.492184	0.605315
H	0.358118	4.396600	2.344602
H	1.090119	2.815681	2.022055
H	-0.680509	2.976634	2.221691

H	-1.174731	1.113147	1.584865
H	-5.047402	-1.061786	0.428799
H	-3.746818	0.587072	-2.615959
H	-1.672356	1.912633	-2.615938
H	2.138506	2.447352	-2.319313
H	4.220327	1.131609	-2.253391
H	4.916146	-1.345185	0.403073

3-conf11

- Electronic Energy (Eh): -6818.72898858

- Cartesian Coordinates:

Br	3.146079	-1.880638	1.751049
C	2.811468	-0.323614	0.717206
C	1.623109	0.364692	0.930013
C	1.318272	1.519325	0.203823
C	0.044084	2.326188	0.415103
C	0.112006	3.335776	1.620801
C	1.276260	4.306160	1.367589
C	-1.198594	4.134408	1.653727
C	0.332498	2.670541	2.985235
C	-1.217030	1.476135	0.338871
C	-2.036115	1.611266	-0.786522
C	-3.199358	0.865116	-0.933725
Br	-4.246403	1.120028	-2.496041
C	-3.600175	-0.058345	0.045463
N	-4.780796	-0.792451	-0.139574
C	-5.325561	-1.714554	0.693760
C	-6.643386	-2.331606	0.157867
F	-7.625648	-2.110204	1.018242
F	-7.006040	-1.814376	-1.026311
F	-6.496784	-3.639262	0.004264
O	-4.906162	-2.088029	1.760943
C	-2.784246	-0.198693	1.174602
C	-1.622907	0.553579	1.309997
C	2.250735	1.938020	-0.749820
C	3.442673	1.258406	-0.972560
C	3.749493	0.108018	-0.236149
N	4.935009	-0.619971	-0.415416
C	5.953817	-0.351640	-1.270492
C	7.117538	-1.373106	-1.186842
F	8.228272	-0.757236	-0.808259
F	7.318779	-1.924490	-2.373734
F	6.871863	-2.357923	-0.308799
O	6.044680	0.563284	-2.050863
H	0.931073	-0.027124	1.673247
H	-0.014830	2.988096	-0.462625
H	1.297546	5.083953	2.146050
H	1.174963	4.811994	0.393925
H	2.248299	3.791286	1.382702
H	-2.062931	3.490349	1.873191
H	-1.386509	4.633328	0.689287
H	-1.152380	4.913088	2.430477
H	0.466595	3.447225	3.753896
H	1.235865	2.042681	2.995990
H	-0.526916	2.061713	3.297969
H	-1.764429	2.317099	-1.573826
H	-5.282309	-0.603172	-1.002542
H	-3.075680	-0.907104	1.946551
H	-1.035249	0.403487	2.214372
H	2.044889	2.831100	-1.344469
H	4.150051	1.607940	-1.720941
H	5.034211	-1.444678	0.169475

3-conf12

- Electronic Energy (Eh): -6818.72892945

- Cartesian Coordinates:

Br	4.699325	1.413516	-2.090466
C	3.385487	0.904996	-0.818292

C	2.227442	1.666907	-0.721545
C	1.220139	1.350060	0.195079
C	-0.010518	2.245366	0.264263
C	0.019394	3.297486	1.434281
C	0.022381	2.676715	2.836814
C	1.289131	4.148872	1.281512
C	-1.208196	4.208101	1.290893
C	-1.316573	1.480232	0.105240
C	-1.831609	0.600683	1.063736
C	-3.030021	-0.071018	0.852920
Br	-3.651307	-1.243875	2.210755
C	-3.772954	0.102798	-0.326920
N	-4.976471	-0.597716	-0.494008
C	-5.823050	-0.553732	-1.553718
C	-7.061585	-1.473259	-1.395311
F	-7.071689	-2.119858	-0.219183
F	-8.169779	-0.752436	-1.474626
F	-7.072728	-2.381118	-2.360115
O	-5.713402	0.097154	-2.562888
C	-3.261607	0.981514	-1.289005
C	-2.061931	1.647153	-1.065953
C	1.423186	0.224946	0.999837
C	2.576850	-0.546040	0.911997
C	3.587245	-0.219279	-0.000711
N	4.769316	-0.963142	-0.130174
C	5.142601	-2.060843	0.574920
C	6.526388	-2.623195	0.158212
F	7.347857	-2.610265	1.197381
F	7.093825	-1.908776	-0.826202
F	6.394895	-3.870901	-0.266586
O	4.534624	-2.618875	1.454190
H	2.112877	2.531719	-1.377746
H	0.047706	2.873464	-0.637976
H	0.146924	3.471180	3.588735
H	0.852788	1.967962	2.972134
H	-0.922943	2.166952	3.069723
H	1.347290	4.610539	0.282611
H	2.201382	3.552925	1.433063
H	1.292693	4.961336	2.024033
H	-1.182306	5.007052	2.047741
H	-2.146734	3.649423	1.422407
H	-1.237492	4.686541	0.298681
H	-1.311053	0.424364	2.002622
H	-5.238207	-1.207656	0.275080
H	-3.817789	1.133538	-2.211042
H	-1.695722	2.324911	-1.840774
H	0.667892	-0.084498	1.720862
H	2.709097	-1.416088	1.550836
H	5.418644	-0.631941	-0.837753

3-conf13

- Electronic Energy (Eh): -6818.728776270001

- Cartesian Coordinates:

Br	-4.281118	1.281783	2.207652
C	-3.272920	0.800720	0.673188
C	-2.082951	1.474163	0.424323
C	-1.290121	1.173121	-0.687551
C	-0.000681	1.958777	-0.884089
C	0.054191	2.854270	-2.177057
C	0.160710	2.061023	-3.485116
C	-1.213335	3.719582	-2.215092
C	1.279798	3.774681	-2.070732
C	1.250332	1.122772	-0.647607
C	2.203920	1.586809	0.263570
C	3.377575	0.883171	0.505409
Br	4.615802	1.592369	1.757346
C	3.649456	-0.326980	-0.153836
N	4.845833	-1.006549	0.118561
C	5.287419	-2.165992	-0.431270

C	6.672208	-2.616417	0.101924
F	7.150699	-1.790708	1.045761
F	6.579984	-3.828036	0.627639
F	7.546871	-2.647922	-0.893228
O	4.739144	-2.848566	-1.260403
C	2.692266	-0.800583	-1.059728
C	1.522283	-0.086851	-1.293697
C	-1.749308	0.160327	-1.537230
C	-2.937908	-0.520520	-1.299412
C	-3.728166	-0.213375	-0.185003
N	-4.934580	-0.869098	0.100657
C	-5.534806	-1.854320	-0.614004
C	-6.868725	-2.344673	0.006407
F	-6.783818	-3.635346	0.291598
F	-7.858604	-2.161680	-0.854593
F	-7.177996	-1.690772	1.137008
O	-5.152794	-2.364756	-1.637507
H	-1.769472	2.255882	1.118948
H	-0.002011	2.698768	-0.068975
H	0.280402	2.759024	-4.328076
H	-0.742650	1.469523	-3.688644
H	1.033471	1.391455	-3.490395
H	-1.319968	4.313558	-1.292968
H	-2.120530	3.107684	-2.328040
H	-1.172124	4.421013	-3.062488
H	1.297858	4.481238	-2.914461
H	2.221040	3.205520	-2.090960
H	1.260511	4.366394	-1.141266
H	2.034308	2.523041	0.798702
H	5.448654	-0.569136	0.809460
H	2.879535	-1.738833	-1.576743
H	0.809296	-0.508186	-2.000968
H	-1.182415	-0.120942	-2.423192
H	-3.271079	-1.302102	-1.978256
H	-5.409970	-0.561190	0.944079

8-conf01

- Electronic Energy (Eh): -7051.02245105

- Cartesian Coordinates:

Br	2.909749	-1.649341	2.277826
C	2.643064	-0.729842	0.638333
C	1.512316	0.063514	0.502251
C	1.267643	0.763508	-0.682088
C	0.045607	1.657070	-0.826311
C	-1.229513	0.837636	-0.700947
C	-1.850639	0.601038	0.527870
C	-2.986777	-0.195110	0.611336
Br	-3.774399	-0.463656	2.317976
C	-3.551887	-0.787171	-0.531124
N	-4.700034	-1.582212	-0.397717
C	-5.388318	-2.220353	-1.377662
C	-6.617931	-3.009056	-0.857423
F	-7.723677	-2.532233	-1.410199
F	-6.499031	-4.288896	-1.176115
F	-6.753280	-2.925293	0.475409
O	-5.153124	-2.233961	-2.560303
C	-2.931945	-0.545544	-1.763771
C	-1.795844	0.251831	-1.834956
C	2.189892	0.629959	-1.719517
C	3.326058	-0.163972	-1.595041
C	3.575874	-0.860761	-0.407436
N	4.703118	-1.675819	-0.224115
C	5.708360	-1.914178	-1.103464
C	6.794940	-2.875248	-0.555663
F	6.532173	-3.284927	0.695240
F	7.971041	-2.265708	-0.546679
F	6.876285	-3.948399	-1.327933
O	5.837271	-1.474328	-2.218996
H	0.811851	0.126186	1.336576

H	0.064137	2.032091	-1.859311
H	-1.462862	1.049278	1.443662
H	-5.051316	-1.687179	0.549683
H	-3.356324	-0.990984	-2.660548
H	-1.334551	0.417739	-2.811676
H	2.025853	1.163273	-2.659011
H	4.034426	-0.253798	-2.415301
H	4.766741	-2.137530	0.678581
C	0.106950	2.872810	0.125387
H	0.085033	2.482717	1.159182
C	-1.089752	3.837728	-0.039341
C	1.413454	3.687928	-0.009414
H	-2.033112	3.275939	0.038004
C	-1.029725	4.547137	-1.401977
C	-1.037910	4.891331	1.078114
C	2.278239	3.014696	0.094871
C	1.474253	4.398824	-1.370859
C	1.459439	4.742086	1.107930
H	-1.896540	5.220959	-1.501314
H	-1.109090	3.821643	-2.228117
C	0.275774	5.349152	-1.513861
H	-1.104549	4.400437	2.063679
H	-1.908060	5.563597	0.996810
C	0.264884	5.697073	0.974716
H	1.486016	3.669865	-2.197448
H	2.417307	4.964651	-1.446925
H	1.443861	4.247699	2.093693
H	2.405035	5.306007	1.048466
H	0.317744	5.853443	-2.492485
C	0.323467	6.397943	-0.391496
H	0.300144	6.449466	1.778755
H	1.247341	6.994868	-0.470958
H	-0.521303	7.099456	-0.493728

8-conf02

- Electronic Energy (Eh): -7051.02238132

- Cartesian Coordinates:

Br	-3.795870	-1.172900	2.804956
C	-3.009626	-0.438924	1.241217
C	-1.868666	0.342389	1.377230
C	-1.246642	0.910691	0.263473
C	0.031539	1.711937	0.458957
C	1.246396	0.799983	0.388649
C	1.543826	0.084797	-0.774377
C	2.669612	-0.724237	-0.842565
Br	3.010913	-1.663605	-2.456594
C	3.543941	-0.856244	0.252421
N	4.668852	-1.686700	0.136040
C	5.622252	-1.930938	1.069698
C	6.727628	-2.904801	0.585757
F	7.905323	-2.298453	0.617093
F	6.772125	-3.964466	1.379033
F	6.517864	-3.335115	-0.668108
O	5.695734	-1.485704	2.188179
C	3.240882	-0.144646	1.418595
C	2.110348	0.665006	1.474960
C	-1.816740	0.669740	-0.989150
C	-2.957838	-0.110638	-1.137452
C	-3.578483	-0.684052	-0.020518
N	-4.731501	-1.477906	-0.112807
C	-5.422739	-1.813892	-1.230850
C	-6.656757	-2.709863	-0.949838
F	-7.758131	-2.098626	-1.360368
F	-6.800593	-2.988157	0.355238
F	-6.537196	-3.856918	-1.601214
O	-5.186268	-1.499573	-2.370945
H	-1.454895	0.505949	2.374490
H	-0.000935	2.094790	1.488859
H	0.888977	0.148214	-1.644896

H	4.774022	-2.156646	-0.758532
H	3.903670	-0.235381	2.276015
H	1.904374	1.210575	2.399080
H	-1.376234	1.107768	-1.886840
H	-3.387285	-0.283743	-2.121447
H	-5.084226	-1.839427	0.768697
C	0.164488	2.920309	-0.494936
H	0.193708	2.523179	-1.525616
C	1.473889	3.716065	-0.290486
C	-1.024184	3.904377	-0.403188
H	2.332617	3.029107	-0.341682
C	1.468771	4.434956	1.068175
C	1.599954	4.762097	-1.409148
H	-1.970105	3.356455	-0.531221
C	-1.030253	4.621601	0.956602
C	-0.892520	4.949948	-1.521704
H	2.414766	4.986807	1.194201
H	1.422600	3.711621	1.898515
C	0.279114	5.404529	1.137686
H	1.632691	4.261686	-2.391408
H	2.549381	5.311836	-1.299047
C	0.414842	5.736128	-1.349404
H	-1.166915	3.902673	1.781078
H	-1.890906	5.308926	1.003274
H	-0.911278	4.453781	-2.506639
H	-1.755175	5.636090	-1.493551
H	0.273592	5.914581	2.114237
C	0.406852	6.445016	0.013890
H	0.507315	6.482612	-2.154403
H	-0.431267	7.160071	0.063944
H	1.333967	7.028217	0.142500

8-conf03

- Electronic Energy (Eh): -7051.02217156
- Cartesian Coordinates:

Br	-3.798073	-1.147875	2.662009
C	-3.061172	-0.457575	1.054802
C	-1.899419	0.301115	1.130878
C	-1.311526	0.837265	-0.016669
C	-0.012405	1.618017	0.112623
C	1.182562	0.687508	-0.023143
C	2.075605	0.531245	1.036552
C	3.186438	-0.298407	0.918910
Br	4.357137	-0.455945	2.404730
C	3.444694	-1.005374	-0.266468
N	4.576652	-1.830869	-0.342784
C	4.996382	-2.573027	-1.398326
C	6.299646	-3.365360	-1.118059
F	6.767740	-3.158252	0.122823
F	6.075610	-4.663337	-1.258178
F	7.240975	-2.999660	-1.975373
O	4.482156	-2.675134	-2.484278
C	2.542850	-0.850673	-1.329377
C	1.436877	-0.020970	-1.200457
C	-1.937186	0.588055	-1.240854
C	-3.099453	-0.169543	-1.329142
C	-3.686058	-0.711088	-0.178239
N	-4.857932	-1.481667	-0.210366
C	-5.602856	-1.818054	-1.293385
C	-6.839923	-2.686857	-0.947863
F	-6.936422	-2.939569	0.366831
F	-6.765711	-3.847232	-1.582206
F	-7.946206	-2.063716	-1.325747
O	-5.409625	-1.523050	-2.446627
H	-1.442942	0.472834	2.107932
H	0.012366	2.000694	1.142729
H	1.912765	1.067191	1.973787
H	5.146828	-1.868872	0.497141
H	2.725553	-1.393836	-2.253696

H	0.753822	0.066180	-2.047826
H	-1.524146	1.000773	-2.163146
H	-3.572164	-0.349474	-2.291869
H	-5.180926	-1.823563	0.690158
C	0.087365	2.825923	-0.845713
H	0.055938	2.430747	-1.876815
C	1.416673	3.603052	-0.709658
C	-1.081333	3.825421	-0.688143
H	2.261729	2.904516	-0.809512
C	1.494268	4.317253	0.649313
C	1.496509	4.651318	-1.830640
H	-2.039803	3.290086	-0.767067
C	-1.004943	4.538235	0.671973
C	-0.995664	4.873157	-1.809034
H	2.452921	4.856224	0.725932
H	1.482990	3.591887	1.479271
C	0.323149	5.302280	0.785322
H	1.469500	4.153796	-2.814472
H	2.457892	5.187864	-1.770447
C	0.329751	5.640960	-1.704510
H	-1.108297	3.818929	1.500984
H	-1.851864	5.237666	0.765908
H	-1.073665	4.380887	-2.792954
H	-1.846093	5.570778	-1.732738
H	0.376779	5.808840	1.762266
C	0.404723	6.345009	-0.340734
H	0.389312	6.389034	-2.511125
H	-0.419583	7.071174	-0.243587
H	1.345353	6.915116	-0.260549

8-conf04

- Electronic Energy (Eh): -7051.02245124
- Cartesian Coordinates:

Br	2.911253	-1.648384	2.277999
C	2.644008	-0.729142	0.638453
C	1.512908	0.063772	0.502475
C	1.267801	0.763580	-0.681850
C	0.045459	1.656734	-0.826024
C	-1.229469	0.837055	-0.700607
C	-1.850196	0.599833	0.528288
C	-2.986351	-0.196306	0.611715
Br	-3.773334	-0.465707	2.318524
C	-3.551893	-0.787749	-0.530856
N	-4.699943	-1.582885	-0.397539
C	-5.389785	-2.218720	-1.377922
C	-6.618365	-3.008982	-0.857596
F	-6.496115	-4.289306	-1.173587
F	-6.755405	-2.922981	0.474911
F	-7.724429	-2.535867	-1.412626
O	-5.156084	-2.230011	-2.560880
C	-2.932260	-0.545601	-1.763555
C	-1.796157	0.251763	-1.834705
C	2.190019	0.630360	-1.719391
C	3.326513	-0.163072	-1.595008
C	3.576744	-0.859736	-0.407383
N	4.704428	-1.674183	-0.224094
C	5.708459	-1.914099	-1.104416
C	6.795665	-2.874404	-0.556488
F	7.971616	-2.264536	-0.548889
F	6.876774	-3.948242	-1.327818
F	6.533865	-3.282987	0.694972
O	5.836017	-1.475889	-2.220745
H	0.812560	0.126166	1.336917
H	0.063822	2.031743	-1.859028
H	-1.462174	1.047584	1.444215
H	-5.050684	-1.688728	0.549963
H	-3.356959	-0.990493	-2.660459
H	-1.335181	0.418118	-2.811499
H	2.025625	1.163584	-2.658873

H	4.034758	-0.252801	-2.415387
H	4.768852	-2.135012	0.678998
C	0.106478	2.872569	0.125631
H	0.085069	2.482486	1.159442
C	-1.090730	3.836899	-0.038775
C	1.412555	3.688340	-0.009609
H	-2.033811	3.274688	0.038887
C	-1.031453	4.546235	-1.401467
C	-1.039066	4.890563	1.078622
H	2.277710	3.015553	0.094437
C	1.472601	4.399248	-1.371084
C	1.458359	4.742555	1.107689
H	-1.898650	5.219586	-1.500642
H	-1.110639	3.820608	-2.227507
C	0.273588	5.348944	-1.513774
H	-1.105171	4.399664	2.064218
H	-1.909570	5.562400	0.997556
C	0.263293	5.696948	0.974804
H	1.484522	3.670301	-2.197680
H	2.415344	4.965560	-1.447415
H	1.443322	4.248189	2.093468
H	2.403658	5.306940	1.047922
H	0.315006	5.853223	-2.492426
C	0.321083	6.397797	-0.391457
H	0.298427	6.449395	1.778798
H	1.244619	6.995198	-0.471244
H	-0.524087	7.098862	-0.493443

8-conf05

- Electronic Energy (Eh): -7051.02233886
- Cartesian Coordinates:

Br	3.992789	-0.520816	2.459846
C	3.127247	-0.242107	0.793152
C	1.971684	0.529570	0.771532
C	1.294016	0.772359	-0.425795
C	-0.000197	1.569026	-0.483336
C	-1.197039	0.654115	-0.275521
C	-2.149176	0.501336	-1.282992
C	-3.261631	-0.313570	-1.097369
Br	-4.514622	-0.468078	-2.514613
C	-3.462408	-1.008540	0.106127
N	-4.598678	-1.818750	0.251338
C	-4.967987	-2.548511	1.333906
C	-6.295866	-3.324072	1.134009
F	-6.083714	-4.623497	1.278442
F	-7.183894	-2.933675	2.036317
F	-6.827456	-3.124458	-0.082155
O	-4.394772	-2.650551	2.390015
C	-2.501434	-0.857521	1.116300
C	-1.394479	-0.042600	0.919609
C	1.823984	0.218091	-1.592589
C	2.978917	-0.555166	-1.583325
C	3.655742	-0.802907	-0.382360
N	4.825375	-1.574354	-0.311457
C	5.487291	-2.176549	-1.331385
C	6.754071	-2.946988	-0.877362
F	6.647865	-4.223968	-1.211942
F	6.944670	-2.881281	0.449633
F	7.825027	-2.438270	-1.468786
O	5.204588	-2.172088	-2.503713
H	1.613114	0.953596	1.710349
H	-0.075883	1.946142	-1.512932
H	-2.031658	1.028206	-2.232057
H	-5.214605	-1.854875	-0.555838
H	-2.639261	-1.391524	2.053606
H	-0.665169	0.042079	1.727814
H	1.318760	0.390467	-2.546226
H	3.374333	-0.975977	-2.504884
H	5.217804	-1.689814	0.618485

C	-0.033221	2.782230	0.472793
H	0.044686	2.391036	1.503250
C	-1.356645	3.577933	0.401632
C	1.139694	3.764738	0.251882
H	-2.205167	2.891736	0.547232
C	-1.493393	4.288504	-0.954527
C	-1.364515	4.630826	1.521074
H	2.093702	3.216684	0.283575
C	1.003979	4.473498	-1.105561
C	1.126034	4.817085	1.371636
H	-2.447055	4.840746	-0.984347
H	-1.534516	3.560208	-1.780940
C	-0.317004	5.256285	-1.153917
H	-1.294428	4.136225	2.504279
H	-2.320046	5.180816	1.507724
C	-0.191915	5.603463	1.331783
H	1.054355	3.749418	-1.935269
H	1.854937	5.160124	-1.245886
H	1.247070	4.326783	2.352242
H	1.981265	5.502185	1.249396
H	-0.413256	5.760352	-2.128845
C	-0.326327	6.303814	-0.029279
H	-0.199721	6.354964	2.137361
H	0.502126	7.017755	-0.171265
H	-1.261645	6.887062	-0.063820

8-conf06

- Electronic Energy (Eh): -7051.02217173
- Cartesian Coordinates:

Br	-3.798239	-1.147853	2.662073
C	-3.061266	-0.457686	1.054837
C	-1.899486	0.300984	1.130904
C	-1.311527	0.837005	-0.016655
C	-0.012437	1.617806	0.112595
C	1.182590	0.687378	-0.023209
C	2.075699	0.531261	1.036473
C	3.186587	-0.298293	0.918847
Br	4.357409	-0.455635	2.404588
C	3.444845	-1.005338	-0.266502
N	4.576899	-1.830699	-0.342780
C	4.996669	-2.572980	-1.398234
C	6.300131	-3.364976	-1.117955
F	6.076176	-4.663098	-1.257107
F	7.241073	-2.999782	-1.975849
F	6.768667	-3.157023	0.122629
O	4.482333	-2.675422	-2.484102
C	2.542936	-0.850798	-1.329370
C	1.436902	-0.021154	-1.200470
C	-1.937124	0.587676	-1.240861
C	-3.099417	-0.169860	-1.329131
C	-3.686124	-0.711263	-0.178194
N	-4.858046	-1.481731	-0.210328
C	-5.602999	-1.818042	-1.293362
C	-6.840161	-2.686735	-0.947874
F	-7.946366	-2.063654	-1.325970
F	-6.936835	-2.939293	0.366849
F	-6.765892	-3.847215	-1.582051
O	-5.409705	-1.523047	-2.446592
H	-1.443059	0.472766	2.107969
H	0.012349	2.000497	1.142695
H	1.912822	1.067272	1.973663
H	5.147206	-1.868441	0.497064
H	2.725619	-1.394069	-2.253628
H	0.753826	0.065879	-2.047833
H	-1.523994	1.000256	-2.163174
H	-3.572107	-0.349865	-2.291856
H	-5.181150	-1.823528	0.690195
C	0.087222	2.825701	-0.845759
H	0.055781	2.430516	-1.876858

C	1.416489	3.602901	-0.709726
C	-1.081530	3.825133	-0.688165
H	2.261583	2.904412	-0.809593
C	1.494069	4.317097	0.649252
C	1.496254	4.651187	-1.830695
H	-2.039968	3.289743	-0.767081
C	-1.005153	4.537922	0.671963
C	-0.995931	4.872875	-1.809050
H	2.452692	4.856122	0.725845
H	1.482856	3.591728	1.479207
C	0.322894	5.302050	0.785296
H	1.469261	4.153679	-2.814535
H	2.457604	5.187793	-1.770511
C	0.329439	5.640757	-1.704538
H	-1.108434	3.818579	1.500950
H	-1.852114	5.237299	0.765942
H	-1.073922	4.380605	-2.792970
H	-1.846397	5.570452	-1.732743
H	0.376510	5.808608	1.762241
C	0.404382	6.344795	-0.340754
H	0.388946	6.388843	-2.511146
H	-0.419971	7.070903	-0.243589
H	1.344976	6.914962	-0.260572

8-conf07

- Electronic Energy (Eh): -7051.02233881

- Cartesian Coordinates:

Br	-4.514072	-0.468687	2.514898
C	-3.261398	-0.313645	1.097429
C	-2.148982	0.501309	1.283053
C	-1.197058	0.654451	0.275430
C	-0.000202	1.569323	0.483292
C	1.293934	0.772516	0.425762
C	1.971523	0.529600	-0.771597
C	3.126971	-0.242228	-0.793245
Br	3.992399	-0.521121	-2.459966
C	3.655445	-0.803066	0.382274
N	4.824941	-1.574714	0.311339
C	5.486959	-2.176737	1.331296
C	6.753685	-2.947282	0.877293
F	6.647473	-4.224210	1.212080
F	6.944204	-2.881794	-0.449725
F	7.824698	-2.438508	1.468555
O	5.204349	-2.172106	2.503649
C	2.978698	-0.555206	1.583250
C	1.823865	0.218213	1.592540
C	-1.394711	-0.041894	-0.919874
C	-2.501653	-0.856828	-1.116581
C	-3.462390	-1.008258	-0.106241
N	-4.598611	-1.818540	-0.251432
C	-4.968144	-2.547931	-1.334168
C	-6.295660	-3.324064	-1.134043
F	-6.827925	-3.123473	0.081656
F	-6.082613	-4.623547	-1.276929
F	-7.183491	-2.935252	-2.037184
O	-4.395236	-2.649475	-2.390493
H	-2.031315	1.027933	2.232238
H	-0.075879	1.946408	1.512901
H	1.612934	0.953640	-1.710401
H	5.217292	-1.690299	-0.618623
H	3.374098	-0.976045	2.504804
H	1.318713	0.390682	2.546200
H	-0.665606	0.043104	-1.728235
H	-2.639663	-1.390553	-2.054022
H	-5.214506	-1.854707	0.555765
C	-0.033121	2.782561	-0.472774
H	0.044775	2.391440	-1.503260
C	1.139864	3.764966	-0.251791
C	-1.356496	3.578348	-0.401571

H	2.093829	3.216838	-0.283519
C	1.004188	4.473631	1.105703
C	1.126275	4.817394	-1.371473
H	-2.205057	2.892207	-0.547215
C	-1.493205	4.288831	0.954638
C	-1.364291	4.631314	-1.520937
H	1.855192	5.160188	1.246085
H	1.054510	3.749487	1.935360
C	-0.316744	5.256504	1.154108
H	1.247278	4.327155	-2.352115
H	1.981549	5.502432	-1.249186
C	-0.191621	5.603857	-1.331567
H	-1.534406	3.560468	1.780989
H	-2.446824	4.841149	0.984490
H	-1.294233	4.136777	-2.504177
H	-2.319781	5.181377	-1.507557
H	-0.412965	5.760509	2.129072
C	-0.325991	6.304116	0.029546
H	-0.199372	6.355419	-2.137089
H	-1.261269	6.887428	0.064125
H	0.502512	7.017988	0.171595

8-conf08

- Electronic Energy (Eh): -7051.02245126

- Cartesian Coordinates:

Br	2.910422	-1.648652	2.278059
C	2.643387	-0.729553	0.638400
C	1.512561	0.063705	0.502351
C	1.267637	0.763418	-0.682095
C	0.045528	1.656881	-0.826318
C	-1.229522	0.837345	-0.700875
C	-1.850660	0.600839	0.527934
C	-2.986755	-0.195391	0.611461
Br	-3.774361	-0.463783	2.318126
C	-3.551783	-0.787629	-0.530933
N	-4.699808	-1.582822	-0.397502
C	-5.389234	-2.219398	-1.377682
C	-6.618197	-3.009047	-0.857294
F	-7.724193	-2.534180	-1.411082
F	-6.497504	-4.289104	-1.174724
F	-6.754302	-2.924273	0.475403
O	-5.155212	-2.231363	-2.560566
C	-2.931784	-0.546127	-1.763588
C	-1.795750	0.251316	-1.834839
C	2.189700	0.629671	-1.719670
C	3.325929	-0.164166	-1.595225
C	3.576028	-0.860651	-0.407493
N	4.703420	-1.675492	-0.224128
C	5.708037	-1.914799	-1.103953
C	6.795107	-2.875135	-0.555792
F	6.877445	-3.948279	-1.327910
F	6.532318	-3.284847	0.695081
F	7.970812	-2.264747	-0.546565
O	5.836150	-1.476095	-2.220022
H	0.812239	0.126490	1.336788
H	0.064003	2.031856	-1.859337
H	-1.462954	1.049181	1.443704
H	-5.050659	-1.688413	0.549987
H	-3.356116	-0.991647	-2.660352
H	-1.334425	0.417132	-2.811558
H	2.025432	1.162752	-2.659256
H	4.034092	-0.254238	-2.415634
H	4.767387	-2.136701	0.678801
C	0.106751	2.872695	0.125306
H	0.084635	2.482678	1.159121
C	-1.089912	3.837619	-0.039706
C	1.413288	3.687787	-0.009289
H	-2.033298	3.275850	0.037453
C	-1.029595	4.546998	-1.402346

C	-1.038284	4.891250	1.077735
H	2.278045	3.014555	0.095185
C	1.474359	4.398635	-1.370745
C	1.459068	4.741972	1.108045
H	-1.896382	5.220825	-1.501867
H	-1.108797	3.821484	-2.228482
C	0.275932	5.348997	-1.513991
H	-1.105140	4.400376	2.063293
H	-1.908396	5.563540	0.996231
C	0.264546	5.696963	0.974587
H	1.486225	3.669636	-2.197299
H	2.417451	4.964417	-1.446662
H	1.443307	4.247597	2.093809
H	2.404672	5.305893	1.048739
H	0.318099	5.853273	-2.492612
C	0.323418	6.397807	-0.391634
H	0.299659	6.449374	1.778614
H	1.247320	6.994707	-0.470924
H	-0.521324	7.099325	-0.494053

8-conf09

- Electronic Energy (Eh): -7051.02217191
- Cartesian Coordinates:

Br	-3.798147	-1.147650	2.662158
C	-3.061197	-0.457571	1.054872
C	-1.899462	0.301169	1.130903
C	-1.311496	0.837118	-0.016687
C	-0.012420	1.617953	0.112541
C	1.182613	0.687529	-0.023227
C	2.075734	0.531442	1.036434
C	3.186629	-0.298124	0.918808
Br	4.357385	-0.455467	2.404610
C	3.444883	-1.005182	-0.266527
N	4.576882	-1.830625	-0.342792
C	4.996721	-2.572732	-1.398326
C	6.299664	-3.365493	-1.117793
F	6.074826	-4.663490	-1.256768
F	7.240935	-3.001048	-1.975652
F	6.768183	-3.157639	0.122802
O	4.482742	-2.674605	-2.484421
C	2.542983	-0.850618	-1.329410
C	1.436939	-0.021010	-1.200500
C	-1.937063	0.587680	-1.240886
C	-3.099286	-0.169966	-1.329131
C	-3.685983	-0.711309	-0.178165
N	-4.857834	-1.481897	-0.210289
C	-5.602485	-1.818687	-1.293375
C	-6.839884	-2.687007	-0.947809
F	-7.945952	-2.063134	-1.325181
F	-6.936165	-2.940094	0.366830
F	-6.766468	-3.847186	-1.582558
O	-5.408879	-1.524188	-2.446683
H	-1.443061	0.473048	2.107962
H	0.012348	2.000674	1.142627
H	1.912900	1.067470	1.973622
H	5.146982	-1.868641	0.497179
H	2.725746	-1.393786	-2.253712
H	0.753828	0.065996	-2.047835
H	-1.523947	1.000228	-2.163219
H	-3.571912	-0.350117	-2.291860
H	-5.180998	-1.823542	0.690269
C	0.087234	2.825834	-0.845836
H	0.055876	2.430626	-1.876924
C	1.416457	3.603112	-0.709757
C	-1.081577	3.825200	-0.688317
H	2.261597	2.904673	-0.809579
C	1.493935	4.317343	0.649204
C	1.496207	4.651367	-1.830757
H	-2.039989	3.289765	-0.767258

C	-1.005299	4.538039	0.671795
C	-0.995992	4.872923	-1.809227
H	2.452525	4.856415	0.725849
H	1.482707	3.591991	1.479171
C	0.322701	5.302244	0.785169
H	1.469286	4.153824	-2.814578
H	2.457525	5.188022	-1.770549
C	0.329334	5.640883	-1.704682
H	-1.108577	3.818725	1.500804
H	-1.852305	5.237364	0.765715
H	-1.073913	4.380626	-2.793135
H	-1.846501	5.570446	-1.732969
H	0.376250	5.808833	1.762102
C	0.404185	6.344962	-0.340911
H	0.388834	6.388950	-2.511308
H	-0.420202	7.071033	-0.243798
H	1.344744	6.915177	-0.260705

8-conf10

- Electronic Energy (Eh): -7051.0223387
- Cartesian Coordinates:

Br	3.992437	-0.521153	2.459981
C	3.127067	-0.242150	0.793253
C	1.971557	0.529589	0.771627
C	1.293999	0.772550	-0.425737
C	-0.000206	1.569248	-0.483285
C	-1.196994	0.654267	-0.275518
C	-2.149017	0.501274	-1.283060
C	-3.261403	-0.313726	-1.097438
Br	-4.514178	-0.468605	-2.514835
C	-3.462245	-1.008542	0.106141
N	-4.598414	-1.818913	0.251275
C	-4.968082	-2.548042	1.334143
C	-6.295542	-3.324249	1.133930
F	-7.183959	-2.934448	2.036053
F	-6.826919	-3.124819	-0.082342
F	-6.082692	-4.623615	1.278278
O	-4.395326	-2.649240	2.390579
C	-2.501378	-0.857284	1.116386
C	-1.394481	-0.042301	0.919692
C	1.824025	0.218401	-1.592548
C	2.978933	-0.554910	-1.583279
C	3.655636	-0.802827	-0.382299
N	4.825178	-1.574419	-0.311378
C	5.487645	-2.175759	-1.331452
C	6.753858	-2.947063	-0.877317
F	6.945472	-2.879857	0.449457
F	7.824980	-2.440541	-1.470188
F	6.645789	-4.224422	-1.210084
O	5.205599	-2.170293	-2.503935
H	1.612888	0.953529	1.710446
H	-0.075861	1.946378	-1.512881
H	-2.031456	1.028052	-2.232172
H	-5.214031	-1.855433	-0.556111
H	-2.639346	-1.391164	2.053748
H	-0.665252	0.042545	1.727955
H	1.318903	0.390922	-2.546211
H	3.374434	-0.975564	-2.504873
H	5.217509	-1.690044	0.618584
C	-0.033294	2.782440	0.472834
H	0.044639	2.391276	1.503299
C	-1.356767	3.578069	0.401657
C	1.139570	3.765001	0.251896
H	-2.205244	2.891816	0.547267
C	-1.493554	4.288587	-0.954530
C	-1.364692	4.630984	1.521065
H	2.093603	3.216984	0.283598
C	1.003814	4.473714	-1.105568
C	1.125850	4.817380	1.371620

H	-2.447243	4.840783	-0.984370
H	-1.534654	3.560242	-1.780902
C	-0.317218	5.256415	-1.153951
H	-1.294581	4.136414	2.504284
H	-2.320249	5.180932	1.507703
C	-0.192144	5.603680	1.331741
H	1.054249	3.749621	-1.935262
H	1.854730	5.160390	-1.245900
H	1.246912	4.327117	2.352243
H	1.981041	5.502526	1.249360
H	-0.413494	5.760455	-2.128890
C	-0.326600	6.303979	-0.029342
H	-0.199992	6.355208	2.137294
H	0.501813	7.017962	-0.171363
H	-1.261953	6.887172	-0.063901

8-conf11

- Electronic Energy (Eh): -7051.022338919999

- Cartesian Coordinates:

Br	-4.513849	-0.469078	2.514938
C	-3.261187	-0.313873	1.097475
C	-2.148869	0.501213	1.283119
C	-1.196960	0.654471	0.275505
C	-0.000204	1.569484	0.483348
C	1.294000	0.772787	0.425815
C	1.971593	0.529925	-0.771554
C	3.127053	-0.241876	-0.793222
Br	3.992501	-0.520719	-2.459942
C	3.655542	-0.802740	0.382280
N	4.825023	-1.574397	0.311328
C	5.487060	-2.176394	1.331290
C	6.753369	-2.947558	0.877203
F	6.944565	-2.881031	-0.449663
F	7.824509	-2.440281	1.469451
F	6.645877	-4.224736	1.210747
O	5.204657	-2.171461	2.503692
C	2.978829	-0.554876	1.583268
C	1.823967	0.218512	1.592584
C	-1.394512	-0.041895	-0.919805
C	-2.501352	-0.856965	-1.116524
C	-3.462086	-1.008504	-0.106199
N	-4.598231	-1.818889	-0.251419
C	-4.967719	-2.548243	-1.334189
C	-6.295315	-3.324257	-1.134198
F	-7.183423	-2.934441	-2.036661
F	-6.827054	-3.124571	0.081876
F	-6.082658	-4.623652	-1.278293
O	-4.394802	-2.649697	-2.390522
H	-2.031270	1.027841	2.232310
H	-0.075911	1.946567	1.512957
H	1.612980	0.953987	-1.710340
H	5.217333	-1.690059	-0.618639
H	3.374246	-0.975664	2.504837
H	1.318847	0.390969	2.546261
H	-0.665399	0.043183	-1.728150
H	-2.639276	-1.390708	-2.053966
H	-5.214000	-1.855343	0.555863
C	-0.033269	2.782695	-0.472727
H	0.044718	2.391577	-1.503208
C	1.139573	3.765263	-0.251695
C	-1.356763	3.578278	-0.401573
H	2.093610	3.217262	-0.283404
C	1.003745	4.473893	1.105798
C	1.125869	4.817702	-1.371367
H	-2.205211	2.892007	-0.547253
C	-1.493622	4.288724	0.954641
C	-1.364665	4.631254	-1.520927
H	1.854636	5.160585	1.246211
H	1.054152	3.749754	1.935452

C	-0.317309	5.256566	1.154166
H	1.246980	4.327489	-2.352009
H	1.981035	5.502867	-1.249040
C	-0.192146	5.603968	-1.331501
H	-1.534746	3.560342	1.780978
H	-2.447318	4.840910	0.984467
H	-1.294494	4.136741	-2.504170
H	-2.320234	5.181181	-1.507577
H	-0.413639	5.760541	2.129131
C	-0.326669	6.304190	0.029616
H	-0.199978	6.355536	-2.137013
H	-1.262036	6.887360	0.064170
H	0.501726	7.018181	0.171701

9-conf10

- Electronic Energy (Eh): -6896.16284408

- Cartesian Coordinates:

Br	3.779976	0.304701	2.189987
C	2.969377	0.336921	0.473322
C	1.849857	1.139963	0.288003
C	1.212959	1.206594	-0.953336
C	-0.052221	2.021419	-1.177204
C	-0.102746	3.355571	-0.400328
C	-1.413489	4.111053	-0.658091
C	-1.462561	5.446554	0.084365
C	-0.260606	6.327416	-0.252369
C	1.049986	5.585369	0.004098
C	1.095797	4.251618	-0.741283
C	-1.277666	1.156038	-0.923643
C	-1.501924	0.580395	0.329694
C	-2.632321	-0.189690	0.565990
Br	-2.870329	-0.938725	2.294184
C	-3.584510	-0.421260	-0.444183
N	-4.709628	-1.209535	-0.159123
C	-5.733049	-1.529269	-0.990504
C	-6.815233	-2.419504	-0.326449
F	-6.513293	-2.731003	0.943681
F	-7.978794	-1.785357	-0.324917
F	-6.946187	-3.549639	-1.004086
O	-5.882286	-1.202488	-2.141775
C	-3.355766	0.152389	-1.700061
C	-2.220270	0.924995	-1.924940
C	1.744471	0.443087	-1.994953
C	2.863275	-0.362630	-1.821500
C	3.500130	-0.432799	-0.575537
N	4.632029	-1.227744	-0.341311
C	5.283620	-2.027812	-1.222595
C	6.499848	-2.765841	-0.605427
F	6.318608	-4.075675	-0.685899
F	7.602478	-2.446006	-1.265832
F	6.686185	-2.453166	0.686605
O	5.023573	-2.216414	-2.384874
H	1.486932	1.727172	1.132757
H	-0.070620	2.284723	-2.247958
H	-0.068515	3.132637	0.683425
H	-2.275249	3.490535	-0.369444
H	-1.509761	4.291205	-1.745236
H	-2.402611	5.970170	-0.149478
H	-1.477173	5.252663	1.171833
H	-0.310136	6.617455	-1.317149
H	-0.294046	7.262654	0.328195
H	1.910123	6.207802	-0.288001
H	1.155772	5.397458	1.087642
H	2.041593	3.732174	-0.525831
H	1.088785	4.441056	-1.830645
H	-0.785183	0.723423	1.140039
H	-4.754648	-1.580929	0.785377
H	-4.080298	-0.015821	-2.493499
H	-2.073424	1.363320	-2.914944

H	1.268421	0.471609	-2.978168
H	3.260698	-0.948267	-2.647267
H	5.001887	-1.193882	0.604229

9-conf02

- Electronic Energy (Eh): -6896.16280295

- Cartesian Coordinates:

Br	-2.959823	-1.010175	-2.471640
C	-2.653046	-0.173620	-0.795317
C	-1.527404	0.625834	-0.651966
C	-1.254647	1.265997	0.559784
C	-0.036816	2.165220	0.710729
C	-0.157167	3.463475	-0.117594
C	1.036075	4.397756	0.124922
C	0.922417	5.697738	-0.671079
C	-0.390450	6.422500	-0.378995
C	-1.587118	5.503309	-0.618123
C	-1.470458	4.201625	0.175068
C	1.232824	1.368167	0.449508
C	1.822918	0.664479	1.501863
C	2.948343	-0.123611	1.295681
Br	3.691431	-1.046519	2.778341
C	3.532874	-0.240822	0.022474
N	4.669456	-1.046748	-0.141371
C	5.366781	-1.278993	-1.281797
C	6.573140	-2.233410	-1.086133
F	7.692957	-1.620604	-1.439473
F	6.705925	-2.635963	0.187287
F	6.419927	-3.311320	-1.840931
O	5.152506	-0.839316	-2.384211
C	2.943553	0.466997	-1.032261
C	1.817252	1.252903	-0.814067
C	-2.143035	1.067850	1.616164
C	-3.272971	0.266143	1.484643
C	-3.551113	-0.371339	0.270236
N	-4.674090	-1.190385	0.078562
C	-5.647287	-1.489863	0.975041
C	-6.745201	-2.426005	0.407043
F	-7.918018	-1.809566	0.433178
F	-6.499646	-2.792483	-0.860519
F	-6.824313	-3.524680	1.142010
O	-5.743812	-1.114901	2.117275
H	-0.852108	0.740948	-1.501423
H	-0.005910	2.475022	1.768780
H	-0.170991	3.194468	-1.190997
H	1.981093	3.888931	-0.117503
H	1.079198	4.632969	1.204591
H	1.781555	6.349740	-0.448835
H	0.978310	5.466736	-1.749959
H	-0.393636	6.755805	0.674236
H	-0.474183	7.331665	-0.994834
H	-2.526231	6.016516	-0.358745
H	-1.651144	5.263493	-1.694567
H	-2.331011	3.551601	-0.043949
H	-1.516923	4.425474	1.257423
H	1.395285	0.725059	2.504772
H	5.003271	-1.507900	0.700154
H	3.384483	0.393189	-2.023633
H	1.399632	1.795616	-1.664351
H	-1.957450	1.556774	2.575552
H	-3.954810	0.124469	2.319941
H	-4.760080	-1.605044	-0.844934

9-conf03

- Electronic Energy (Eh): -6896.16257292

- Cartesian Coordinates:

Br	-4.405146	-0.018741	2.396835
----	-----------	-----------	----------

C	-3.204209	0.173013	0.939376
C	-2.098197	1.002466	1.097521
C	-1.183985	1.181513	0.059856
C	0.009251	2.108968	0.234869
C	-0.087423	3.366385	-0.657055
C	1.079389	4.329854	-0.399983
C	0.984683	5.592521	-1.256365
C	-0.351009	6.307170	-1.058317
C	-1.521384	5.359155	-1.314390
C	-1.424193	4.094488	-0.461064
C	1.302034	1.321806	0.077348
C	1.849369	0.683586	1.192522
C	2.996175	-0.093094	1.083489
Br	3.676790	-0.926595	2.647072
C	3.646328	-0.263351	-0.151203
N	4.802321	-1.055513	-0.216895
C	5.565291	-1.324740	-1.306158
C	6.771849	-2.250652	-1.003299
F	6.852894	-2.577078	0.296066
F	6.662535	-3.372658	-1.699498
F	7.899669	-1.645559	-1.343371
O	5.405262	-0.937540	-2.437017
C	3.099707	0.379222	-1.268967
C	1.951033	1.153565	-1.148089
C	-1.412170	0.497618	-1.137185
C	-2.514123	-0.330140	-1.306828
C	-3.436815	-0.509076	-0.265881
N	-4.565064	-1.334994	-0.382190
C	-4.964032	-2.052581	-1.462561
C	-6.268315	-2.856901	-1.223927
F	-6.768323	-2.668008	0.007310
F	-7.190709	-2.488155	-2.099990
F	-6.031028	-4.151724	-1.373404
O	-4.430359	-2.127044	-2.541337
H	-1.956737	1.521457	2.047620
H	-0.017772	2.467781	1.277539
H	-0.044757	3.049569	-1.716350
H	2.041996	3.826730	-0.576024
H	1.068394	4.611876	0.669286
H	1.822653	6.267646	-1.022622
H	1.095347	5.316458	-2.320292
H	-0.409693	6.684549	-0.021683
H	-0.418100	7.188027	-1.715908
H	-2.479280	5.867286	-1.122463
H	-1.529870	5.072821	-2.381243
H	-2.263090	3.421312	-0.693816
H	-1.527102	4.363658	0.607074
H	1.371260	0.787262	2.168776
H	5.097674	-1.471247	0.661749
H	3.591748	0.263712	-2.231902
H	1.567312	1.643866	-2.044772
H	-0.710432	0.603498	-1.967130
H	-2.677076	-0.853213	-2.246283
H	-5.150881	-1.392178	0.445846

9-conf04

- Electronic Energy (Eh): -6896.161022760001

- Cartesian Coordinates:

Br	2.521230	-1.121039	2.291380
C	2.433013	-0.216007	0.625012
C	1.306345	0.545158	0.346235
C	1.188280	1.234274	-0.864822
C	-0.019270	2.110258	-1.155197
C	0.136716	3.532898	-0.562502
C	1.264881	4.318244	-1.244705
C	1.330166	5.760485	-0.740099
C	1.474700	5.818013	0.780754
C	0.372848	5.016488	1.473719
C	0.327528	3.577011	0.959442

C	-1.330383	1.406536	-0.808404
C	-1.491295	0.065629	-1.180653
C	-2.674474	-0.614474	-0.932783
Br	-2.803199	-2.431496	-1.467610
C	-3.760115	0.015752	-0.297233
N	-4.934671	-0.712593	-0.057222
C	-6.071021	-0.281441	0.545630
C	-7.168420	-1.371925	0.649916
F	-6.788525	-2.534553	0.097421
F	-7.454774	-1.599887	1.923403
F	-8.266955	-0.965706	0.031670
O	-6.302981	0.814586	0.992212
C	-3.605573	1.356407	0.067591
C	-2.413942	2.030692	-0.188464
C	2.232937	1.118347	-1.782334
C	3.367137	0.357903	-1.513578
C	3.490126	-0.324159	-0.297644
N	4.608186	-1.105990	0.028666
C	5.720635	-1.319146	-0.718425
C	6.767180	-2.228765	-0.024256
F	6.335050	-2.696373	1.157177
F	7.046102	-3.266231	-0.797624
F	7.882014	-1.544793	0.191570
O	5.970840	-0.885101	-1.815391
H	0.501911	0.592389	1.082042
H	-0.042204	2.250371	-2.250301
H	-0.797602	4.072317	-0.801053
H	1.124268	4.305803	-2.338471
H	2.229730	3.819433	-1.046075
H	2.163801	6.291842	-1.225208
H	0.407473	6.290032	-1.037573
H	2.456636	5.400705	1.066623
H	1.466557	6.863329	1.127206
H	0.522317	5.022034	2.564646
H	-0.603084	5.500980	1.290159
H	-0.466670	3.012886	1.473521
H	1.277649	3.077393	1.215097
H	-0.672774	-0.464384	-1.671155
H	-4.922943	-1.677703	-0.374534
H	-4.432229	1.865239	0.557844
H	-2.353572	3.075958	0.114437
H	2.166473	1.636729	-2.741778
H	4.170055	0.279955	-2.242846
H	4.571452	-1.563545	0.935052

9-conf05

- Electronic Energy (Eh): -6896.16089681

- Cartesian Coordinates:

Br	2.715460	-1.347114	2.127325
C	2.601053	-0.397617	0.487496
C	1.433148	0.298387	0.207793
C	1.294600	1.016779	-0.983725
C	0.040336	1.825366	-1.271901
C	0.099675	3.238065	-0.639196
C	1.181443	4.112602	-1.287402
C	1.148154	5.542031	-0.744750
C	1.273887	5.568301	0.778599
C	0.220320	4.678426	1.438048
C	0.274123	3.253463	0.885533
C	-1.228238	1.030408	-0.968792
C	-2.342649	1.577660	-0.331498
C	-3.490910	0.819851	-0.117095
Br	-4.954530	1.641481	0.771477
C	-3.577982	-0.515786	-0.536903
N	-4.754033	-1.241004	-0.294910
C	-5.015744	-2.533563	-0.614924
C	-6.424227	-3.007159	-0.171391
F	-7.143486	-2.020899	0.386867
F	-7.096841	-3.461952	-1.216984

F	-6.309384	-3.981807	0.719533
O	-4.293941	-3.318931	-1.177154
C	-2.463635	-1.064186	-1.187870
C	-1.322441	-0.301511	-1.391999
C	2.361851	0.996742	-1.882125
C	3.537097	0.301880	-1.612585
C	3.680401	-0.408959	-0.415449
N	4.840162	-1.127974	-0.089991
C	5.978495	-1.243754	-0.819292
C	7.065326	-2.114337	-0.137088
F	8.147735	-1.384079	0.089418
F	6.654673	-2.618862	1.036779
F	7.391095	-3.126931	-0.925669
O	6.222017	-0.756143	-1.895086
H	0.613187	0.270603	0.927240
H	0.025767	1.993135	-2.363183
H	-0.864281	3.724871	-0.874111
H	1.052700	4.120366	-2.382625
H	2.174448	3.671702	-1.090639
H	1.950258	6.138874	-1.206256
H	0.196006	6.018661	-1.038969
H	2.278153	5.208287	1.064674
H	1.194060	6.601215	1.152110
H	0.359193	4.664109	2.530306
H	-0.783519	5.103221	1.256817
H	-0.484144	2.624400	1.378092
H	1.252895	2.810610	1.137291
H	-2.342485	2.611069	0.012660
H	-5.493543	-0.728910	0.177215
H	-2.509272	-2.096411	-1.527210
H	-0.472314	-0.765317	-1.897232
H	2.280577	1.539640	-2.826745
H	4.357294	0.298319	-2.326659
H	4.816341	-1.615590	0.800990

9-conf06

- Electronic Energy (Eh): -6896.16066195

- Cartesian Coordinates:

Br	2.952324	-2.421706	-1.334888
C	2.812133	-0.630659	-0.721076
C	1.603757	0.031009	-0.882251
C	1.433890	1.352396	-0.449644
C	0.095357	2.041976	-0.709105
C	-0.062216	3.435025	-0.050354
C	-0.186355	3.411988	1.478737
C	-0.236382	4.827772	2.054748
C	-1.382497	5.634521	1.444519
C	-1.304255	5.642802	-0.082247
C	-1.234401	4.224070	-0.649174
C	-1.081011	1.129432	-0.403300
C	-2.154372	1.043958	-1.290898
C	-3.260859	0.251721	-1.001957
Br	-4.680939	0.190238	-2.260149
C	-3.333758	-0.491240	0.187838
N	-4.467740	-1.277863	0.439129
C	-4.721529	-2.050330	1.525759
C	-6.088838	-2.779219	1.461002
F	-5.903170	-4.089151	1.522789
F	-6.845141	-2.406340	2.482729
F	-6.759730	-2.509435	0.330178
O	-4.023672	-2.219513	2.494392
C	-2.250290	-0.413200	1.074416
C	-1.150928	0.381410	0.776094
C	2.533455	1.976302	0.141751
C	3.750408	1.320248	0.311167
C	3.915070	-0.000726	-0.115826
N	5.116162	-0.709843	0.033575
C	6.275860	-0.272843	0.585543
C	7.402920	-1.337812	0.583540

F	7.016819	-2.491087	0.016021
F	8.449895	-0.882835	-0.088313
F	7.775254	-1.599933	1.827722
O	6.508740	0.811895	1.058480
H	0.773112	-0.498524	-1.352363
H	0.070312	2.229570	-1.797149
H	0.849597	4.003938	-0.306635
H	0.640394	2.843644	1.933132
H	-1.114144	2.881780	1.753800
H	-0.338006	4.785080	3.150326
H	0.721178	5.339721	1.850105
H	-2.342913	5.185775	1.754823
H	-1.378572	6.664640	1.833924
H	-2.168280	6.176530	-0.508025
H	-0.405618	6.202786	-0.397058
H	-1.142776	4.259502	-1.747744
H	-2.180158	3.698351	-0.428936
H	-2.135018	1.605258	-2.227062
H	-5.180980	-1.259147	-0.283985
H	-2.286457	-0.986926	1.997547
H	-0.318476	0.409320	1.482104
H	2.465816	3.007065	0.489682
H	4.589750	1.828325	0.780140
H	5.106968	-1.662972	-0.318071

9-conf07

- Electronic Energy (Eh): -6896.16055941

- Cartesian Coordinates:

Br	-4.891014	0.192003	2.319566
C	-3.433549	0.143685	1.104255
C	-2.289387	0.872009	1.413668
C	-1.187902	0.876346	0.556958
C	0.031065	1.724917	0.880550
C	-0.036530	3.119814	0.210403
C	-1.156620	3.987220	0.800731
C	-1.135467	5.402697	0.222100
C	-1.212698	5.387080	-1.304641
C	-0.120221	4.503577	-1.906861
C	-0.161904	3.092532	-1.318922
C	1.330489	0.955756	0.652010
C	2.449154	1.506192	0.025480
C	3.624770	0.773557	-0.116707
Br	5.093741	1.596805	-0.994811
C	3.735464	-0.538041	0.367956
N	4.939697	-1.237484	0.200054
C	5.234346	-2.497512	0.608759
C	6.678934	-2.939299	0.258429
F	7.355182	-3.184186	1.371651
F	6.647779	-4.042253	-0.473261
F	7.347317	-2.002575	-0.432600
O	4.521101	-3.272271	1.196101
C	2.615419	-1.089654	1.006598
C	1.447134	-0.352681	1.138069
C	-1.268829	0.112422	-0.611212
C	-2.405783	-0.619009	-0.929640
C	-3.517461	-0.614494	-0.075207
N	-4.690076	-1.334466	-0.348018
C	-4.963513	-2.100004	-1.434742
C	-6.373545	-2.744448	-1.398361
F	-7.056746	-2.418446	-0.289888
F	-7.078409	-2.341552	-2.445136
F	-6.265991	-4.063933	-1.438244
O	-4.253662	-2.319961	-2.384288
H	-2.262521	1.447071	2.341245
H	-0.003311	1.919937	1.966880
H	0.909239	3.632403	0.463814
H	-1.063801	4.025904	1.899035
H	-2.133620	3.520793	0.583321
H	-1.964107	5.993879	0.642253

H	-0.203256	5.906844	0.533710
H	-2.199563	4.998287	-1.612750
H	-1.142403	6.411626	-1.702340
H	-0.223892	4.458140	-3.002139
H	0.868154	4.954820	-1.705543
H	0.624654	2.467364	-1.770152
H	-1.122031	2.620917	-1.589335
H	2.431440	2.522368	-0.366173
H	5.674129	-0.731963	-0.286923
H	2.679029	-2.103621	1.394715
H	0.593236	-0.818281	1.635328
H	-0.416209	0.077399	-1.292397
H	-2.450390	-1.205927	-1.844090
H	-5.419482	-1.264159	0.355571

9-conf08

- Electronic Energy (Eh): -6896.16102261

- Cartesian Coordinates:

Br	2.784685	-2.442711	-1.447866
C	2.665671	-0.621624	-0.924737
C	1.484276	0.061674	-1.172352
C	1.330526	1.405783	-0.808800
C	0.021747	2.113298	-1.156822
C	-0.128220	3.538893	-0.569877
C	-0.313538	3.591086	0.952492
C	-0.352802	5.033262	1.459648
C	-1.455050	5.834318	0.766778
C	-1.316405	5.768800	-0.754302
C	-1.256643	4.323927	-1.252025
C	-1.188680	1.242643	-0.862718
C	-1.311822	0.563962	0.353743
C	-2.440249	-0.193694	0.634878
Br	-2.535583	-1.084053	2.308747
C	-3.493777	-0.309325	-0.290993
N	-4.612845	-1.088948	0.037150
C	-5.714597	-1.322623	-0.719598
C	-6.750489	-2.251148	-0.034435
F	-6.383462	-2.597545	1.209150
F	-7.922614	-1.640103	0.040569
F	-6.892819	-3.362865	-0.741817
O	-5.956374	-0.905391	-1.824950
C	-3.365891	0.362590	-1.512049
C	-2.230200	1.120099	-1.782892
C	2.419073	2.029561	-0.197226
C	3.608923	1.352051	0.058595
C	3.756551	0.008404	-0.298084
N	4.929294	-0.723072	-0.058695
C	6.070150	-0.292618	0.536066
C	7.163947	-1.386595	0.641786
F	7.453577	-1.609832	1.915391
F	6.778163	-2.550363	0.095810
F	8.261929	-0.987099	0.018227
O	6.308321	0.805186	0.974954
H	0.661656	-0.468224	-1.656049
H	0.044438	2.249214	-2.252467
H	0.806781	4.074587	-0.814143
H	0.480810	3.027185	1.466576
H	-1.264331	3.095863	1.214063
H	-0.498154	5.044749	2.551088
H	0.623788	5.514052	1.269973
H	-2.437025	5.421135	1.058442
H	-1.442763	6.881334	1.107946
H	-2.150494	6.299909	-1.238905
H	-0.393488	6.294488	-1.057857
H	-1.119833	4.305799	-2.346192
H	-2.222068	3.828463	-1.047770
H	-0.509735	0.616085	1.091765
H	-4.587010	-1.525385	0.954257
H	-4.165990	0.278790	-2.243763

H	-2.159911	1.630595	-2.746291
H	2.364179	3.077110	0.098831
H	4.439634	1.860713	0.542117
H	4.912286	-1.690012	-0.370137

9-conf09

- Electronic Energy (Eh): -6896.16066205

- Cartesian Coordinates:

Br	2.952357	-2.421583	-1.335159
C	2.812157	-0.630561	-0.721284
C	1.603761	0.031092	-0.882392
C	1.433889	1.352460	-0.449733
C	0.095332	2.042018	-0.709143
C	-0.062241	3.435031	-0.050317
C	-0.186318	3.411867	1.478780
C	-0.236339	4.827607	2.054900
C	-1.382495	5.634384	1.444777
C	-1.304300	5.642785	-0.081992
C	-1.234458	4.224096	-0.649029
C	-1.081012	1.129452	-0.403317
C	-2.154487	1.044137	-1.290796
C	-3.260953	0.251884	-1.001830
Br	-4.681194	0.190609	-2.259848
C	-3.333724	-0.491250	0.187864
N	-4.467694	-1.277881	0.439168
C	-4.721378	-2.050515	1.525708
C	-6.088613	-2.779534	1.460883
F	-6.759965	-2.508937	0.330531
F	-5.902718	-4.089503	1.521518
F	-6.844573	-2.407621	2.483195
O	-4.023451	-2.219811	2.494271
C	-2.250146	-0.413365	1.074317
C	-1.150801	0.381265	0.775976
C	2.533468	1.976370	0.141637
C	3.750440	1.320336	0.310970
C	3.915107	-0.000626	-0.116069
N	5.116224	-0.709710	0.033243
C	6.275779	-0.272875	0.585646
C	7.402833	-1.337851	0.583610
F	7.774682	-1.600500	1.827833
F	7.016936	-2.490879	0.015464
F	8.450073	-0.882611	-0.087639
O	6.508530	0.811717	1.058975
H	0.773103	-0.498441	-1.352484
H	0.070250	2.229647	-1.797179
H	0.849558	4.003968	-0.306580
H	0.640466	2.843493	1.933076
H	-1.114079	2.881617	1.753847
H	-0.337898	4.784837	3.150480
H	0.721200	5.339588	1.850242
H	-2.342890	5.185586	1.755074
H	-1.378593	6.664469	1.834266
H	-2.168333	6.176543	-0.507715
H	-0.405671	6.202796	-0.396780
H	-1.142875	4.259604	-1.747600
H	-2.180201	3.698357	-0.428784
H	-2.135232	1.605572	-2.226881
H	-5.181037	-1.259011	-0.283839
H	-2.286205	-0.987230	1.997366
H	-0.318259	0.409053	1.481885
H	2.465819	3.007117	0.489614
H	4.589789	1.828401	0.779942
H	5.107125	-1.662739	-0.318675

9-conf10

- Electronic Energy (Eh): -6896.16089684

- Cartesian Coordinates:

Br	-4.954575	1.641448	-0.771429
----	-----------	----------	-----------

C	-3.490930	0.819840	0.117111
C	-2.342683	1.577680	0.331495
C	-1.228251	1.030458	0.968771
C	0.040324	1.825420	1.271884
C	0.099672	3.238140	0.639190
C	0.274014	3.253528	-0.885548
C	0.220183	4.678485	-1.438074
C	1.273787	5.568371	-0.778687
C	1.148147	5.542096	0.744671
C	1.181486	4.112665	1.287317
C	1.294589	1.016838	0.983696
C	1.433137	0.298411	-0.207801
C	2.601032	-0.397619	-0.487469
Br	2.715445	-1.347149	-2.127274
C	3.680382	-0.408952	0.415481
N	4.840129	-1.127987	0.090032
C	5.978606	-1.243507	0.819159
C	7.065285	-2.114389	0.137094
F	6.654869	-2.618330	-1.037104
F	8.148159	-1.384643	-0.088693
F	7.390208	-3.127438	0.925471
O	6.222304	-0.755576	1.894768
C	3.537067	0.301906	1.612601
C	2.361816	0.996779	1.882119
C	-1.322417	-0.301474	1.391966
C	-2.463591	-1.064178	1.187856
C	-3.577964	-0.515800	0.536910
N	-4.753987	-1.241055	0.294925
C	-5.015675	-2.533610	0.614980
C	-6.424115	-3.007238	0.171380
F	-7.143400	-2.020936	-0.386757
F	-6.309211	-3.981756	-0.719674
F	-7.096718	-3.462188	1.216913
O	-4.293880	-3.318947	1.177260
H	-2.342541	2.611086	-0.012670
H	0.025780	1.993186	2.363165
H	-0.864248	3.724972	0.874172
H	-0.484291	2.624455	-1.378041
H	1.252765	2.810666	-1.137365
H	0.358993	4.664158	-2.530338
H	-0.783645	5.103285	-1.256791
H	2.278043	5.208381	-1.064830
H	1.193918	6.601286	-1.152183
H	1.950276	6.138939	1.206131
H	0.196015	6.018723	1.038946
H	1.052835	4.120423	2.382551
H	2.174474	3.671777	1.090460
H	0.613174	0.270601	-0.927244
H	4.816225	-1.615769	-0.800856
H	4.357247	0.298357	2.326691
H	2.280539	1.539680	2.826737
H	-0.472272	-0.765246	1.897202
H	-2.509207	-2.096407	1.527191
H	-5.493489	-0.729019	-0.177279

9-conf11

- Electronic Energy (Eh): -6896.16284381

- Cartesian Coordinates:

Br	2.870861	-0.937631	2.294575
C	2.632599	-0.189266	0.566124
C	1.502147	0.580703	0.329698
C	1.277697	1.155863	-0.923826
C	0.052181	2.021098	-1.177491
C	0.102667	3.355377	-0.400817
C	-1.095899	4.251365	-0.741878
C	-1.050110	5.585190	0.003370
C	0.260476	6.327233	-0.253164
C	1.462447	5.446424	0.083652
C	1.413397	4.110841	-0.658661

C	-1.212934	1.206220	-0.953456
C	-1.849996	1.140016	0.287815
C	-2.969462	0.336927	0.473294
Br	-3.780264	0.305300	2.189874
C	-3.499976	-0.433292	-0.575326
N	-4.631767	-1.228354	-0.340916
C	-5.283848	-2.027908	-1.222287
C	-6.499983	-2.766017	-0.605042
F	-6.318434	-4.075837	-0.685188
F	-6.686521	-2.453063	0.686898
F	-7.602621	-2.446615	-1.265630
O	-5.024178	-2.216243	-2.384686
C	-2.862928	-0.363572	-1.821223
C	-1.744207	0.442217	-1.994839
C	2.220158	0.924460	-1.925171
C	3.355694	0.151952	-1.700175
C	3.584653	-0.421202	-0.444107
N	4.709915	-1.209215	-0.158888
C	5.732442	-1.530494	-0.990744
C	6.815368	-2.419481	-0.326257
F	7.978376	-1.784188	-0.325070
F	6.513756	-2.730562	0.944053
F	6.947371	-3.549797	-1.003276
O	5.880640	-1.205618	-2.142682
H	0.785499	0.723988	1.140083
H	0.070517	2.284247	-2.248284
H	0.068420	3.132564	0.682962
H	-2.041679	3.731920	-0.526369
H	-1.088882	4.440687	-1.831262
H	-1.910253	6.207582	-0.288798
H	-1.155901	5.397387	1.086933
H	0.309995	6.617169	-1.317973
H	0.293907	7.262525	0.327312
H	2.402488	5.970033	-0.150245
H	1.477063	5.252637	1.171137
H	2.275167	3.490375	-0.369938
H	1.509670	4.290866	-1.745827
H	-1.487265	1.727603	1.132391
H	-5.001640	-1.194359	0.604614
H	-3.260189	-0.949559	-2.646819
H	-1.268006	0.470387	-2.977992
H	2.073148	1.362399	-2.915323
H	4.080044	-0.016661	-2.493695
H	4.755435	-1.579707	0.785945

9-conf12

- Electronic Energy (Eh): -6896.16284389

- Cartesian Coordinates:

Br	2.870572	-0.937973	2.294471
C	2.632449	-0.189367	0.566105
C	1.502011	0.580631	0.329687
C	1.277659	1.155940	-0.923782
C	0.052198	2.021257	-1.177415
C	0.102793	3.355517	-0.400686
C	-1.095699	4.251599	-0.741727
C	-1.049794	5.585425	0.003513
C	0.260849	6.327361	-0.253044
C	1.462745	5.446452	0.083789
C	1.413584	4.110872	-0.658521
C	-1.212973	1.206459	-0.953428
C	-1.849972	1.140119	0.287879
C	-2.969464	0.337064	0.473314
Br	-3.780216	0.305229	2.189911
C	-3.500073	-0.432982	-0.575375
N	-4.631932	-1.227981	-0.341053
C	-5.283666	-2.027946	-1.222308
C	-6.499818	-2.766076	-0.605161
F	-6.687048	-2.452424	0.686515
F	-7.602233	-2.447426	-1.266453

F	-6.317774	-4.075887	-0.684455
O	-5.023811	-2.216510	-2.384635
C	-2.863115	-0.363118	-1.821305
C	-1.744353	0.442626	-1.994878
C	2.220196	0.924656	-1.925090
C	3.355711	0.152123	-1.700103
C	3.584575	-0.421176	-0.444076
N	4.709814	-1.209226	-0.158874
C	5.732398	-1.530421	-0.990685
C	6.815208	-2.419612	-0.326273
F	6.513657	-2.730607	0.944073
F	6.946937	-3.549970	-1.003274
F	7.978345	-1.784557	-0.325199
O	5.880680	-1.205433	-2.142584
H	0.785306	0.723817	1.140041
H	0.070559	2.284469	-2.248193
H	0.068546	3.132655	0.683081
H	-2.041516	3.732230	-0.526201
H	-1.088689	4.440927	-1.831109
H	-1.909898	6.207875	-0.288642
H	-1.155574	5.397645	1.087082
H	0.310391	6.617267	-1.317861
H	0.294357	7.262666	0.327405
H	2.402838	5.969970	-0.150098
H	1.477328	5.252678	1.171278
H	2.275291	3.490326	-0.369793
H	1.509882	4.290898	-1.745686
H	-1.487172	1.727573	1.132517
H	-5.001894	-1.193988	0.604446
H	-3.260447	-0.949002	-2.646941
H	-1.268209	0.470904	-2.978056
H	2.073251	1.362719	-2.915197
H	4.080127	-0.016415	-2.493579
H	4.755309	-1.579770	0.785940

9-conf13

- Electronic Energy (Eh): -6896.16280389

- Cartesian Coordinates:

Br	2.960580	-1.009390	2.471900
C	2.653320	-0.173358	0.795403
C	1.527695	0.626141	0.652167
C	1.254605	1.265966	-0.559688
C	0.036764	2.165176	-0.710599
C	0.157053	3.463424	0.117748
C	-1.036307	4.397578	-0.124659
C	-0.922673	5.697606	0.671278
C	0.390096	6.422476	0.379000
C	1.586870	5.503396	0.618063
C	1.470240	4.201676	-0.175079
C	-1.232868	1.368103	-0.449411
C	-1.823203	0.664766	-1.501854
C	-2.948637	-0.123334	-1.295696
Br	-3.692011	-1.045806	-2.778476
C	-3.532932	-0.240870	-0.022424
N	-4.669543	-1.046730	0.141424
C	-5.366123	-1.280032	1.282112
C	-6.572896	-2.233877	1.086275
F	-6.420675	-3.311481	1.841658
F	-7.692557	-1.620211	1.438762
F	-6.705257	-2.636910	-0.187030
O	-5.151188	-0.841300	2.384771
C	-2.943398	0.466640	1.032412
C	-1.817098	1.252538	0.814238
C	2.142668	1.067445	-1.616272
C	3.272567	0.265664	-1.484877
C	3.551037	-0.371486	-0.270370
N	4.673989	-1.190578	-0.078807
C	5.647347	-1.489731	-0.975240
C	6.745027	-2.426323	-0.407498

F	6.822253	-3.525849	-1.141469
F	7.918386	-1.811091	-0.435579
F	6.500530	-2.791352	0.860682
O	5.743945	-1.114472	-2.117369
H	0.852715	0.741567	1.501826
H	0.005865	2.475012	-1.768634
H	0.170983	3.194401	1.191143
H	-1.981235	3.888663	0.117916
H	-1.079601	4.632746	-1.204327
H	-1.781904	6.349510	0.449115
H	-0.978404	5.466651	1.750174
H	0.393140	6.755704	-0.674254
H	0.473816	7.331693	0.994759
H	2.525921	6.016662	0.358587
H	1.651004	5.263632	1.694511
H	2.330878	3.551738	0.043851
H	1.516564	4.425503	-1.257439
H	-1.395764	0.725609	-2.504828
H	-5.003696	-1.507475	-0.700189
H	-3.384126	0.392559	2.023852
H	-1.399316	1.795018	1.664590
H	1.956846	1.556121	-2.575738
H	3.954151	0.123745	-2.320338
H	4.760004	-1.605327	0.844642

9-conf14

- Electronic Energy (Eh): -6896.162575290001
- Cartesian Coordinates:

Br	-4.407154	-0.015667	2.397763
C	-3.205402	0.172914	0.940568
C	-2.099073	1.002184	1.097791
C	-1.183927	1.178466	0.060503
C	0.009106	2.106433	0.233916
C	-0.089074	3.362134	-0.660100
C	1.077099	4.326806	-0.405497
C	0.981604	5.587137	-1.265185
C	-0.354438	6.301575	-1.068555
C	-1.524367	5.352110	-1.321292
C	-1.426017	4.089832	-0.464582
C	1.302512	1.320307	0.076692
C	1.853301	0.687074	1.192982
C	3.000713	-0.088813	1.084182
Br	3.686212	-0.915297	2.649332
C	3.648010	-0.263199	-0.151388
N	4.804519	-1.054547	-0.216996
C	5.564026	-1.328584	-1.307434
C	6.772128	-2.251950	-1.003518
F	6.666852	-3.373352	-1.701093
F	7.899225	-1.643700	-1.340696
F	6.851329	-2.579411	0.295719
O	5.400788	-0.946430	-2.439548
C	3.098132	0.374672	-1.270270
C	1.948931	1.148193	-1.149615
C	-1.411498	0.492075	-1.135217
C	-2.513807	-0.335339	-1.304011
C	-3.437520	-0.511456	-0.263464
N	-4.566589	-1.336313	-0.379272
C	-4.964431	-2.056712	-1.458146
C	-6.272349	-2.855427	-1.220991
F	-6.042462	-4.150676	-1.376854
F	-6.769635	-2.669375	0.011796
F	-7.194057	-2.477400	-2.093997
O	-4.428058	-2.136444	-2.535218
H	-1.958114	1.523165	2.046871
H	-0.017755	2.466813	1.276024
H	-0.047070	3.043305	-1.718825
H	2.039908	3.823586	-0.580194
H	1.065936	4.611578	0.663039
H	1.819257	6.263357	-1.033495

H	1.092071	5.308281	-2.328400
H	-0.412836	6.681970	-0.033016
H	-0.422400	7.180430	-1.728724
H	-2.482431	5.860282	-1.130284
H	-1.533294	5.062788	-2.387333
H	-2.264679	3.415441	-0.694718
H	-1.528030	4.361661	0.602981
H	1.377556	0.794075	2.170026
H	5.102880	-1.466771	0.662326
H	3.587992	0.256048	-2.233935
H	1.562640	1.634587	-2.047337
H	-0.709143	0.595731	-1.964912
H	-2.676235	-0.860403	-2.242435
H	-5.153866	-1.390541	0.447930

9-conf15

- Electronic Energy (Eh): -6896.162681349999
- Cartesian Coordinates:

Br	-4.556886	-0.164791	2.538911
C	-3.282712	0.087312	1.154819
C	-2.172945	0.885930	1.413576
C	-1.205398	1.105733	0.433740
C	-0.006684	1.997786	0.720403
C	-0.031430	3.299987	-0.109878
C	1.140050	4.222257	0.254120
C	1.115567	5.527797	-0.540684
C	-0.213590	6.262306	-0.373801
C	-1.388523	5.355478	-0.736065
C	-1.361220	4.047967	0.055659
C	1.278167	1.192495	0.597176
C	1.972402	1.072433	-0.608853
C	3.112177	0.281927	-0.700139
Br	4.002532	0.175644	-2.373657
C	3.605890	-0.422180	0.411374
N	4.759755	-1.207853	0.271700
C	5.384896	-1.944371	1.224563
C	6.640494	-2.691357	0.704784
F	6.875307	-2.454654	-0.595368
F	7.707564	-2.306376	1.388776
F	6.482438	-3.997373	0.859697
O	5.076723	-2.072351	2.383403
C	2.911191	-0.298510	1.621556
C	1.773064	0.494932	1.700989
C	-1.385346	0.495170	-0.810279
C	-2.490474	-0.301063	-1.080364
C	-3.465922	-0.521568	-0.097234
N	-4.599665	-1.318701	-0.315620
C	-4.952026	-1.972285	-1.451226
C	-6.279904	-2.762742	-1.322541
F	-6.056950	-4.052338	-1.528064
F	-6.839866	-2.628222	-0.110097
F	-7.149206	-2.330926	-2.223763
O	-4.363417	-2.001481	-2.503369
H	-2.070168	1.347373	2.397683
H	-0.083470	2.303404	1.777290
H	0.058280	3.036124	-1.180979
H	2.100113	3.706606	0.101847
H	1.080018	4.450583	1.334425
H	1.954117	6.170895	-0.231096
H	1.274897	5.302464	-1.610414
H	-0.317477	6.588965	0.676388
H	-0.228860	7.176071	-0.988329
H	-2.344297	5.875472	-0.566693
H	-1.348425	5.122945	-1.815239
H	-2.200655	3.406417	-0.252335
H	-1.512666	4.265864	1.129632
H	1.638502	1.607474	-1.498958
H	5.170543	-1.220260	-0.657317
H	3.279437	-0.832308	2.494581

H	1.252527	0.567031	2.659146
H	-0.643029	0.634692	-1.598925
H	-2.614998	-0.767159	-2.055036
H	-5.228993	-1.409578	0.476770

9-conf16

- Electronic Energy (Eh): -6896.16284389

- Cartesian Coordinates:

Br	2.869969	-0.939235	2.294058
C	2.632223	-0.189899	0.565956
C	1.501778	0.580102	0.329583
C	1.277692	1.155932	-0.923695
C	0.052266	2.021335	-1.177238
C	0.102922	3.355480	-0.400328
C	-1.095510	4.251686	-0.741281
C	-1.049578	5.585382	0.004192
C	0.261113	6.327298	-0.252173
C	1.462955	5.446274	0.084545
C	1.413762	4.110819	-0.657987
C	-1.212953	1.206573	-0.953374
C	-1.850024	1.140178	0.287887
C	-2.969555	0.337144	0.473211
Br	-3.780351	0.305207	2.189791
C	-3.500139	-0.432814	-0.575562
N	-4.631977	-1.227839	-0.341295
C	-5.283859	-2.027560	-1.222665
C	-6.499865	-2.765875	-0.605409
F	-7.602447	-2.447222	-1.266423
F	-6.317752	-4.075670	-0.684911
F	-6.686862	-2.452425	0.686341
O	-5.024128	-2.215839	-2.385061
C	-2.863107	-0.362871	-1.821459
C	-1.744308	0.442846	-1.994914
C	2.220503	0.925164	-1.924864
C	3.356038	0.152644	-1.699917
C	3.584627	-0.421188	-0.444087
N	4.709795	-1.209368	-0.158969
C	5.733255	-1.529067	-0.990276
C	6.815399	-2.419394	-0.326312
F	7.979260	-1.785792	-0.325917
F	6.514100	-2.729968	0.944195
F	6.945380	-3.550023	-1.003319
O	5.882531	-1.202367	-2.141564
H	0.784851	0.722887	1.139810
H	0.070653	2.284679	-2.247984
H	0.068626	3.132471	0.683408
H	-2.041371	3.732332	-0.525907
H	-1.088419	4.441198	-1.830628
H	-1.909629	6.207931	-0.287910
H	-1.155431	5.397421	1.087721
H	0.310710	6.617410	-1.316931
H	0.294643	7.262487	0.328462
H	2.403074	5.969795	-0.149233
H	1.477503	5.252315	1.172001
H	2.275438	3.490198	-0.369322
H	1.510116	4.291017	-1.745117
H	-1.487236	1.727555	1.132584
H	-5.001861	-1.193942	0.604235
H	-3.260432	-0.948656	-2.647167
H	-1.268100	0.471165	-2.978059
H	2.073779	1.363644	-2.914819
H	4.080721	-0.015387	-2.493257
H	4.754849	-1.580689	0.785561

9-conf17

- Electronic Energy (Eh): -6896.16268164

- Cartesian Coordinates:

Br	4.001956	0.174836	2.373941
----	----------	----------	----------

C	3.111923	0.281584	0.700274
C	1.972165	1.072106	0.608999
C	1.278143	1.192491	-0.597126
C	-0.006665	1.997840	-0.720327
C	-0.031299	3.300024	0.109991
C	-1.361011	4.048129	-0.055590
C	-1.388236	5.355619	0.736173
C	-0.213200	6.262346	0.373993
C	1.115884	5.527709	0.540897
C	1.140282	4.222186	-0.253941
C	-1.205432	1.105860	-0.433673
C	-2.172889	0.885973	-1.413584
C	-3.282677	0.087377	-1.154866
Br	-4.556706	-0.164863	-2.539070
C	-3.466017	-0.521392	0.097228
N	-4.599768	-1.318539	0.315539
C	-4.952311	-1.971921	1.451206
C	-6.279973	-2.762711	1.322316
F	-6.840249	-2.627575	0.110078
F	-6.056510	-4.052398	1.526890
F	-7.149202	-2.331843	2.224016
O	-4.363922	-2.000851	2.503478
C	-2.490672	-0.300791	1.080432
C	-1.385516	0.495418	0.810381
C	1.773251	0.495244	-1.701036
C	2.911380	-0.298203	-1.621617
C	3.605859	-0.422209	-0.411345
N	4.759734	-1.207878	-0.271673
C	5.385139	-1.944010	-1.224648
C	6.640686	-2.691072	-0.704873
F	6.874875	-2.455239	0.595550
F	6.482989	-3.997025	-0.860786
F	7.707952	-2.305357	-1.388133
O	5.077275	-2.071558	-2.383625
H	1.638100	1.606904	1.499188
H	-0.083448	2.303500	-1.777201
H	0.058359	3.036126	1.181089
H	-2.200524	3.406645	-0.252327
H	-1.512368	4.266078	-1.129566
H	-2.343951	5.875708	0.566765
H	-1.348219	5.123051	1.815343
H	-0.317014	6.589062	-0.676184
H	-0.228406	7.176084	0.988562
H	1.954502	6.170739	0.231353
H	1.275160	5.302334	1.610627
H	2.100289	3.706441	-0.101635
H	1.080318	4.450547	-1.334245
H	-2.070013	1.347323	-2.397723
H	-5.229030	-1.409450	-0.476898
H	-2.615294	-0.766776	2.055143
H	-0.643296	0.635013	1.599105
H	1.252904	0.567614	-2.659276
H	3.279795	-0.831757	-2.494718
H	5.170227	-1.220672	0.657471

9-conf18

- Electronic Energy (Eh): -6896.16257559

- Cartesian Coordinates:

Br	-3.686333	-0.914661	2.649440
C	-3.000693	-0.088526	1.084163
C	-1.853325	0.687432	1.192913
C	-1.302451	1.320431	0.076533
C	-0.009085	2.106636	0.233711
C	0.088994	3.362314	-0.660339
C	1.425860	4.090134	-0.464803
C	1.524091	5.352402	-1.321538
C	0.354076	6.301767	-1.068814
C	-0.981901	5.587200	-1.265447
C	-1.077278	4.326863	-0.405754

C	1.184010	1.178744	0.060303
C	2.099004	1.002309	1.097698
C	3.205356	0.173059	0.940524
Br	4.406898	-0.015711	2.397868
C	3.437685	-0.511101	-0.263579
N	4.566772	-1.335911	-0.379364
C	4.964413	-2.056730	-1.458049
C	6.272099	-2.855768	-1.220677
F	7.193628	-2.478920	-2.094352
F	6.769918	-2.668877	0.011753
F	6.041571	-4.151072	-1.375333
O	4.428013	-2.136626	-2.535088
C	2.514146	-0.334797	-1.304252
C	1.411784	0.492547	-1.135495
C	-1.948753	1.148042	-1.149799
C	-3.097906	0.374448	-1.270403
C	-3.647865	-0.263207	-0.151433
N	-4.804323	-1.054632	-0.216952
C	-5.563558	-1.329225	-1.307444
C	-6.771692	-2.252522	-1.003422
F	-6.851238	-2.579402	0.295955
F	-7.898734	-1.644533	-1.341191
F	-6.666164	-3.374256	-1.700430
O	-5.400037	-0.947597	-2.439698
H	-1.377681	0.794668	2.169980
H	0.017767	2.467043	1.275810
H	0.047028	3.043437	-1.719049
H	2.264584	3.415816	-0.694916
H	1.527826	4.361993	0.602755
H	2.482114	5.860656	-1.130540
H	1.533039	5.063068	-2.387575
H	0.412433	6.682170	-0.033275
H	0.421963	7.180627	-1.728984
H	-1.819625	6.263338	-1.033774
H	-1.092328	5.308326	-2.328662
H	-2.040031	3.823541	-0.580465
H	-1.066157	4.611643	0.662778
H	1.957896	1.523114	2.046852
H	5.154152	-1.389962	0.447781
H	2.676744	-0.859714	-2.242735
H	0.709577	0.596328	-1.965298
H	-1.562387	1.634268	-2.047580
H	-3.587677	0.255562	-2.234082
H	-5.102876	-1.466463	0.662487

9-conf19

- Electronic Energy (Eh): -6896.1626814

- Cartesian Coordinates:

Br	-4.556624	-0.164865	2.539060
C	-3.282648	0.087456	1.154825
C	-2.172862	0.886063	1.413537
C	-1.205449	1.106018	0.433601
C	-0.006685	1.997998	0.720265
C	-0.031300	3.300194	-0.110033
C	1.140280	4.222347	0.253917
C	1.115907	5.527861	-0.540935
C	-0.213174	6.262513	-0.374071
C	-1.388222	5.355791	-0.736235
C	-1.361007	4.048309	0.055543
C	1.278137	1.192652	0.597107
C	1.972139	1.072183	-0.609023
C	3.111909	0.281677	-0.700258
Br	4.001919	0.174815	-2.373926
C	3.605879	-0.422005	0.411418
N	4.759735	-1.207716	0.271788
C	5.385189	-1.943752	1.224814
C	6.640333	-2.691387	0.704893
F	7.707442	-2.308141	1.389700
F	6.480904	-3.997452	0.858464

F	6.875888	-2.453695	-0.594941
O	5.077439	-2.071118	2.383841
C	2.911436	-0.297908	1.621695
C	1.773281	0.495512	1.701065
C	-1.385577	0.495644	-0.810485
C	-2.490733	-0.300565	-1.080531
C	-3.466025	-0.521246	-0.097290
N	-4.599783	-1.318378	-0.315625
C	-4.952125	-1.972055	-1.451178
C	-6.279707	-2.762965	-1.322268
F	-6.840263	-2.627429	-0.110209
F	-7.148802	-2.332560	-2.224330
F	-6.056024	-4.052697	-1.526298
O	-4.363605	-2.001165	-2.503376
H	-2.069954	1.347361	2.397697
H	-0.083492	2.303659	1.777137
H	0.058368	3.036326	-1.181137
H	2.100289	3.706594	0.101638
H	1.080300	4.450716	1.334218
H	1.954518	6.170892	-0.231374
H	1.275213	5.302472	-1.610657
H	-0.316998	6.589268	0.676093
H	-0.228361	7.176228	-0.988674
H	-2.343927	5.875896	-0.566823
H	-1.348216	5.123209	-1.815402
H	-2.200527	3.406828	-0.252364
H	-1.512361	4.266268	1.129517
H	1.638042	1.606902	-1.499246
H	5.170343	-1.220410	-0.657308
H	3.279896	-0.831358	2.494842
H	1.252949	0.567948	2.659308
H	-0.643404	0.635308	-1.599240
H	-2.615388	-0.766502	-2.055262
H	-5.229123	-1.409175	0.476765

9-conf20

- Electronic Energy (Eh): -6896.1608970199995

- Cartesian Coordinates:

Br	2.715241	-1.347355	2.127195
C	2.600963	-0.397671	0.487467
C	1.433064	0.298335	0.207738
C	1.294604	1.016843	-0.983717
C	0.040352	1.825439	-1.271941
C	0.099688	3.238168	-0.639274
C	1.181366	4.112747	-1.287565
C	1.148051	5.542179	-0.744921
C	1.273902	5.568471	0.778420
C	0.220427	4.678548	1.437961
C	0.274237	3.253586	0.885442
C	-1.228226	1.030489	-0.968828
C	-2.342558	1.577660	-0.331333
C	-3.490799	0.819825	-0.116891
Br	-4.954315	1.641358	0.771933
C	-3.577919	-0.515756	-0.536858
N	-4.753926	-1.241020	-0.294802
C	-5.015776	-2.533443	-0.615261
C	-6.424180	-3.007122	-0.171589
F	-7.143252	-2.021015	0.387174
F	-7.097046	-3.461495	-1.217199
F	-6.309206	-3.982086	0.718973
O	-4.294151	-3.318629	-1.177968
C	-2.463650	-1.064078	-1.188023
C	-1.322483	-0.301379	-1.392197
C	2.361931	0.996916	-1.882030
C	3.537180	0.302074	-1.612451
C	3.680397	-0.408887	-0.415376
N	4.840134	-1.127922	-0.089892
C	5.978658	-1.243360	-0.818954
C	7.065191	-2.114531	-0.137037

F	8.148334	-1.385140	0.088509
F	6.654816	-2.618291	1.037251
F	7.389615	-3.127742	-0.925447
O	6.222469	-0.755222	-1.894444
H	0.613051	0.270476	0.927123
H	0.025816	1.993164	-2.363228
H	-0.864298	3.724936	-0.874127
H	1.052541	4.120496	-2.382778
H	2.174406	3.671907	-1.090862
H	1.950090	6.139051	-1.206500
H	0.195859	6.018767	-1.039064
H	2.278212	5.208525	1.064426
H	1.194042	6.601384	1.151922
H	0.359393	4.664231	2.530206
H	-0.783442	5.103310	1.256819
H	-0.483984	2.624503	1.378050
H	1.253030	2.810754	1.137143
H	-2.342341	2.611024	0.012963
H	-5.493304	-0.729078	0.177693
H	-2.509328	-2.096256	-1.527500
H	-0.472413	-0.765111	-1.897596
H	2.280722	1.539903	-2.826605
H	4.357451	0.298639	-2.326438
H	4.816198	-1.615720	0.800987

9-conf21

- Electronic Energy (Eh): -6896.1608963

- Cartesian Coordinates:

Br	2.716311	-1.346121	2.127820
C	2.601479	-0.397024	0.487788
C	1.433475	0.298847	0.208180
C	1.294617	1.016927	-0.983489
C	0.040225	1.825313	-1.271644
C	0.099366	3.238057	-0.638964
C	1.181413	4.112537	-1.286762
C	1.147931	5.541993	-0.744192
C	1.273020	5.568333	0.779212
C	0.219122	4.678533	1.438245
C	0.273121	3.253529	0.885831
C	-1.228245	1.030194	-0.968499
C	-2.343126	1.577669	-0.332177
C	-3.491276	0.819742	-0.117697
Br	-4.955535	1.641718	0.769513
C	-3.577818	-0.516266	-0.536461
N	-4.753785	-1.241573	-0.294442
C	-5.015145	-2.534337	-0.613875
C	-6.423801	-3.007877	-0.170873
F	-7.143106	-2.021635	0.387349
F	-7.096135	-3.462346	-1.216796
F	-6.309353	-3.982712	0.719878
O	-4.292981	-3.319892	-1.175386
C	-2.463021	-1.064895	-1.186444
C	-1.321917	-0.302086	-1.390650
C	2.361671	0.996730	-1.882116
C	3.537025	0.302012	-1.612667
C	3.680633	-0.408535	-0.415390
N	4.840492	-1.127392	-0.089990
C	5.978466	-1.243805	-0.819762
C	7.065376	-2.114354	-0.137639
F	7.390479	-3.127423	-0.925883
F	8.148091	-1.384294	0.088003
F	6.655116	-2.618188	1.036661
O	6.221613	-0.756791	-1.895909
H	0.613670	0.271174	0.927809
H	0.025636	1.993084	-2.362922
H	-0.864470	3.724881	-0.874317
H	1.053129	4.120247	-2.382036
H	2.174324	3.671636	-1.089555
H	1.950239	6.138785	-1.205403

H	0.195921	6.018644	-1.038825
H	2.277150	5.208298	1.065741
H	1.193077	6.601265	1.152637
H	0.357493	4.664260	2.530563
H	-0.784616	5.103366	1.256539
H	-0.485404	2.624525	1.378068
H	1.251770	2.810695	1.138089
H	-2.343403	2.611362	0.011118
H	-5.493521	-0.729402	0.177252
H	-2.508241	-2.097408	-1.524966
H	-0.471455	-0.766118	-1.895105
H	2.280158	1.539395	-2.826849
H	4.357052	0.298287	-2.326934
H	4.816938	-1.614661	0.801188

10-conf01

- Electronic Energy (Eh): -6779.416268370001

- Cartesian Coordinates:

Br	-2.876080	-0.485694	2.291027
C	-2.641823	0.273604	0.566859
C	-1.507002	1.037025	0.329720
C	-1.284777	1.619239	-0.921025
C	-0.054211	2.477299	-1.175500
C	-0.097509	3.816943	-0.400854
C	-1.402756	4.566891	-0.669894
C	1.106116	4.694338	-0.747995
C	1.205341	1.653788	-0.951887
C	1.845464	1.585601	0.287656
C	2.958252	0.772758	0.472326
Br	3.772945	0.737578	2.186942
C	3.478862	-0.005078	-0.575564
N	4.603837	-0.809955	-0.342181
C	5.245974	-1.617944	-1.223274
C	6.456649	-2.366134	-0.607409
F	6.262460	-3.674327	-0.684203
F	6.649337	-2.052087	0.683342
F	7.560541	-2.058596	-1.271468
O	4.981347	-1.806658	-2.384470
C	2.838986	0.067004	-1.819974
C	1.726932	0.881969	-1.992646
C	-2.234214	1.401389	-1.918965
C	-3.374148	0.635624	-1.693261
C	-3.600815	0.055565	-0.439911
N	-4.730146	-0.726348	-0.154326
C	-5.759598	-1.033914	-0.982941
C	-6.844759	-1.921080	-0.319622
F	-6.543033	-2.236059	0.949685
F	-6.980525	-3.049516	-0.999189
F	-8.005774	-1.282447	-0.316141
O	-5.911507	-0.699418	-2.131611
H	-0.784575	1.168350	1.137026
H	-0.071299	2.739978	-2.246756
H	-0.066009	3.590810	0.680458
H	-1.412826	5.527672	-0.134306
H	-1.514691	4.783422	-1.745410
H	-2.283682	3.992516	-0.350082
H	2.062496	4.199772	-0.527242
H	1.100997	4.947983	-1.820795
H	1.075331	5.637684	-0.182757
H	1.490199	2.177989	1.132069
H	4.976513	-0.777104	0.602281
H	3.228637	-0.524804	-2.645039
H	1.247884	0.911096	-2.974401
H	-2.089039	1.844343	-2.907174
H	-4.103664	0.477519	-2.484208
H	-4.773931	-1.102445	0.788369

10-conf02

- Electronic Energy (Eh): -6779.41627266

- Cartesian Coordinates:

Br	2.980590	-1.173342	-2.292898
C	2.670782	0.079808	-0.901011
C	1.538712	0.879970	-0.971992
C	1.262851	1.819100	0.025339
C	0.036439	2.715212	-0.063792
C	0.143697	3.752440	-1.207943
C	1.447577	4.545607	-1.111534
C	-1.059224	4.696827	-1.210478
C	-1.224385	1.863824	-0.097767
C	-1.800917	1.455132	1.107179
C	-2.916075	0.626847	1.124201
Br	-3.640706	0.118723	2.803117
C	-3.503466	0.170551	-0.068877
N	-4.628742	-0.664794	-0.006336
C	-5.323402	-1.202999	-1.040112
C	-6.513265	-2.089849	-0.590541
F	-6.648111	-2.126263	0.744312
F	-6.333640	-3.331619	-1.016303
F	-7.641467	-1.622049	-1.102518
O	-5.116745	-1.070469	-2.220873
C	-2.928210	0.582912	-1.277033
C	-1.812194	1.412748	-1.281958
C	2.155416	1.917856	1.092221
C	3.291795	1.118770	1.175180
C	3.572752	0.181373	0.174732
N	4.702034	-0.650732	0.204861
C	5.677287	-0.694652	1.147017
C	6.778490	-1.745122	0.849840
F	6.834505	-2.628573	1.835256
F	7.955186	-1.145311	0.746910
F	6.553734	-2.413184	-0.292305
O	5.771170	-0.028766	2.148184
H	0.860293	0.757449	-1.817941
H	0.003566	3.294855	0.874304
H	0.161418	3.205359	-2.167682
H	1.501923	5.296747	-1.913352
H	1.510080	5.080279	-0.148990
H	2.332676	3.899071	-1.194005
H	-2.012089	4.160608	-1.321802
H	-1.103710	5.266548	-0.267668
H	-0.981933	5.422188	-2.034041
H	-1.370188	1.782663	2.055632
H	-4.955569	-0.889110	0.929145
H	-3.371480	0.244628	-2.210731
H	-1.405426	1.716611	-2.248454
H	1.967706	2.643928	1.886916
H	3.976344	1.211088	2.015135
H	4.792208	-1.293827	-0.576476

10-conf03

- Electronic Energy (Eh): -6779.41604839

- Cartesian Coordinates:

Br	3.639792	-0.558470	-2.545364
C	2.970561	-0.694450	-0.774433
C	1.830831	-1.457575	-0.553639
C	1.292742	-1.596038	0.727856
C	0.007566	-2.390585	0.909039
C	-0.075807	-3.186593	2.233964
C	1.100773	-4.153994	2.370004
C	-1.403449	-3.937906	2.340814
C	-1.194455	-1.481281	0.701288
C	-2.115661	-1.748665	-0.311062
C	-3.228925	-0.934758	-0.497001
Br	-4.437850	-1.363752	-1.896205
C	-3.462292	0.179049	0.325779
N	-4.597666	0.972914	0.104156
C	-4.992634	2.072461	0.794429

C	-6.308033	2.697956	0.262033
F	-6.815359	2.016435	-0.777125
F	-6.085226	3.941759	-0.135710
F	-7.219052	2.713831	1.223364
O	-4.448678	2.590774	1.737585
C	-2.533204	0.447539	1.341471
C	-1.423962	-0.369452	1.516183
C	1.943381	-0.942455	1.777012
C	3.084993	-0.176379	1.567889
C	3.622642	-0.035725	0.282526
N	4.771956	0.723004	0.015577
C	5.537606	1.411930	0.898910
C	6.744618	2.130804	0.242426
F	6.679482	3.431204	0.483249
F	6.781477	1.957395	-1.088002
F	7.875773	1.659192	0.746462
O	5.384070	1.514009	2.090677
H	1.350994	-1.949729	-1.402140
H	-0.017936	-3.139921	0.099652
H	-0.036116	-2.466933	3.071115
H	1.041737	-4.706652	3.319437
H	1.088360	-4.893528	1.552392
H	2.071046	-3.638670	2.339426
H	-2.266169	-3.256756	2.333619
H	-1.523117	-4.642487	1.500740
H	-1.442155	-4.521787	3.272286
H	-1.973466	-2.609262	-0.967733
H	-5.191370	0.680148	-0.666316
H	-2.696553	1.308217	1.985937
H	-0.717384	-0.120918	2.310842
H	1.566617	-1.031106	2.797757
H	3.578421	0.321793	2.399235
H	5.058400	0.754062	-0.958626

10-conf04

- Electronic Energy (Eh): -6779.414579240001

- Cartesian Coordinates:

Br	-2.649933	-0.820818	2.279051
C	-2.518611	0.237697	0.708743
C	-1.367600	0.988410	0.513042
C	-1.216680	1.786105	-0.625721
C	0.019756	2.647284	-0.822685
C	-0.092487	4.004779	-0.076629
C	-0.261222	3.873210	1.438392
C	-1.211362	4.866984	-0.663197
C	1.306729	1.867046	-0.559031
C	1.416959	0.562834	-1.058772
C	2.578994	-0.176436	-0.893940
Br	2.639319	-1.937528	-1.600397
C	3.693213	0.354031	-0.218187
N	4.845296	-0.431833	-0.067834
C	6.004500	-0.096719	0.552351
C	7.068896	-1.224027	0.526126
F	8.159656	-0.798007	-0.093187
F	6.634714	-2.323023	-0.110179
F	7.388458	-1.568951	1.764598
O	6.279053	0.943095	1.098127
C	3.588962	1.657950	0.275143
C	2.418307	2.392575	0.101804
C	-2.255046	1.789632	-1.557758
C	-3.413279	1.040737	-1.372164
C	-3.568553	0.249250	-0.228337
N	-4.711649	-0.527206	0.012666
C	-5.817347	-0.643118	-0.765359
C	-6.894115	-1.589273	-0.173776
F	-6.507744	-2.141737	0.986694
F	-7.150390	-2.568757	-1.027324
F	-8.011761	-0.913135	0.048553
O	-6.039649	-0.105418	-1.821635

H	-0.569531	0.938703	1.255429
H	0.048549	2.904446	-1.896132
H	0.852124	4.539041	-0.273206
H	-0.178725	4.860512	1.917053
H	-1.252184	3.466411	1.692002
H	0.496070	3.217489	1.893002
H	-1.088245	5.009180	-1.748117
H	-2.200376	4.414287	-0.490977
H	-1.215920	5.861764	-0.193320
H	0.575822	0.109028	-1.585953
H	4.796007	-1.361592	-0.474524
H	4.438271	2.090110	0.799138
H	2.397545	3.405521	0.503654
H	-2.163853	2.394905	-2.462775
H	-4.210112	1.056645	-2.112017
H	-4.701249	-1.063687	0.875448

10-conf05

- Electronic Energy (Eh): -6779.414395

- Cartesian Coordinates:

Br	-4.942825	1.868619	0.940594
C	-3.453839	1.146450	0.008849
C	-2.325791	1.947324	-0.150177
C	-1.194969	1.472899	-0.816441
C	0.051967	2.319506	-1.063999
C	0.080759	3.690360	-0.334620
C	1.155083	4.606782	-0.922407
C	0.244686	3.587743	1.183489
C	1.326768	1.525544	-0.831137
C	1.490559	0.742100	0.315447
C	2.675538	0.056828	0.545801
Br	2.823355	-0.985608	2.125363
C	3.747663	0.121880	-0.363476
N	4.924556	-0.590019	-0.088239
C	6.056944	-0.644613	-0.833863
C	7.164440	-1.535270	-0.213570
F	6.785126	-2.087901	0.949136
F	8.248998	-0.809405	0.014248
F	7.474202	-2.514839	-1.049509
O	6.280151	-0.094148	-1.883375
C	3.579594	0.898449	-1.515733
C	2.387492	1.581871	-1.735924
C	-1.252046	0.169102	-1.325777
C	-2.372675	-0.635586	-1.177190
C	-3.503532	-0.160777	-0.497469
N	-4.660499	-0.931248	-0.309691
C	-4.889989	-2.202773	-0.724715
C	-6.293923	-2.735938	-0.337959
F	-6.172104	-3.825441	0.405046
F	-6.975910	-3.039548	-1.432535
F	-7.008608	-1.838093	0.358341
O	-4.147222	-2.927662	-1.338493
H	-2.355527	2.955610	0.260673
H	0.030903	2.560175	-2.141332
H	-0.889936	4.169782	-0.546307
H	1.101419	5.605274	-0.463587
H	2.165778	4.210540	-0.737589
H	1.033042	4.730144	-2.009709
H	-0.476426	2.895699	1.643185
H	1.255072	3.240286	1.448308
H	0.103257	4.574778	1.648711
H	0.676967	0.652090	1.036905
H	4.919470	-1.124825	0.775668
H	4.393671	0.954680	-2.234562
H	2.287084	2.176755	-2.646821
H	-0.388517	-0.238031	-1.856436
H	-2.389427	-1.644296	-1.583384
H	-5.410929	-0.474959	0.200898

10-conf06

- Electronic Energy (Eh): -6779.41421857

- Cartesian Coordinates:

Br	2.790895	-1.778893	1.629235
C	2.718132	-0.150061	0.656701
C	1.527455	0.561681	0.647588
C	1.406259	1.769210	-0.051942
C	0.087672	2.536996	0.028671
C	-0.030409	3.747010	-0.938001
C	-1.200867	4.652113	-0.550337
C	-0.123500	3.359451	-2.414968
C	-1.114952	1.613151	-0.069144
C	-2.182615	1.751492	0.818902
C	-3.311215	0.944883	0.713490
Br	-4.720745	1.196023	1.959873
C	-3.413386	-0.037259	-0.285470
N	-4.568492	-0.830059	-0.355136
C	-4.850298	-1.814553	-1.245923
C	-6.234609	-2.476106	-1.019705
F	-6.884969	-1.955256	0.032601
F	-6.082501	-3.773891	-0.804136
F	-6.993495	-2.307291	-2.092437
O	-4.165076	-2.208701	-2.156379
C	-2.336363	-0.182622	-1.171444
C	-1.214676	0.628518	-1.057237
C	2.536135	2.228644	-0.730949
C	3.735522	1.520720	-0.730607
C	3.851402	0.312440	-0.036804
N	5.032910	-0.443040	-0.006903
C	6.217562	-0.156450	-0.602893
C	7.312676	-1.224535	-0.349122
F	6.867057	-2.246855	0.397488
F	8.338609	-0.674259	0.283707
F	7.737301	-1.716221	-1.503220
O	6.494073	0.803700	-1.278271
H	0.672694	0.162079	1.196102
H	0.065972	2.971309	1.043797
H	0.887238	4.341705	-0.794465
H	-1.211606	5.555651	-1.177907
H	-2.166993	4.141733	-0.688057
H	-1.134636	4.974826	0.500445
H	0.674493	2.666939	-2.720930
H	-1.088078	2.877709	-2.636829
H	-0.049555	4.255990	-3.048608
H	-2.140740	2.501845	1.610776
H	-5.274310	-0.636331	0.349324
H	-2.395075	-0.942902	-1.946845
H	-0.387864	0.477713	-1.754115
H	2.507366	3.166497	-1.285495
H	4.599198	1.899269	-1.272276
H	4.986188	-1.306244	0.526893

10-conf07

- Electronic Energy (Eh): -6779.414035800001

- Cartesian Coordinates:

Br	5.107220	1.728347	-1.280116
C	3.598574	1.063185	-0.337573
C	2.440002	1.835543	-0.321151
C	1.294169	1.399260	0.345502
C	0.013376	2.225600	0.443648
C	-0.023592	3.503119	-0.438783
C	-1.148735	4.443565	-0.003684
C	-0.117081	3.223515	-1.940286
C	-1.225704	1.366788	0.250555
C	-2.317947	1.503873	1.108364
C	-3.478304	0.761446	0.914224
Br	-4.920326	1.005837	2.124275
C	-3.589173	-0.152440	-0.146710

N	-4.777435	-0.880795	-0.305311
C	-5.074979	-1.789144	-1.268867
C	-6.497161	-2.392324	-1.132559
F	-6.417254	-3.707563	-1.000821
F	-7.208098	-2.113800	-2.215348
F	-7.158129	-1.909171	-0.068923
O	-4.377939	-2.156793	-2.181429
C	-2.487501	-0.297588	-1.001836
C	-1.333946	0.448883	-0.798696
C	1.366776	0.164252	1.002393
C	2.517628	-0.610935	0.996646
C	3.664595	-0.175360	0.317727
N	4.852527	-0.919752	0.271445
C	5.102926	-2.123761	0.845307
C	6.538214	-2.648026	0.580892
F	7.257947	-1.807549	-0.178963
F	6.482875	-3.815513	-0.041997
F	7.177262	-2.807145	1.730442
O	4.356878	-2.797188	1.511485
H	2.457796	2.791021	-0.843746
H	-0.017244	2.588601	1.486026
H	0.922349	4.036191	-0.243985
H	-1.102086	5.385897	-0.569535
H	-2.138830	3.997030	-0.185601
H	-1.079901	4.691692	1.066956
H	0.643400	2.508278	-2.286834
H	-1.103970	2.813788	-2.204281
H	0.016356	4.155615	-2.509611
H	-2.270528	2.201985	1.946339
H	-5.497596	-0.697507	0.387444
H	-2.552692	-1.006115	-1.824318
H	-0.489448	0.299693	-1.474411
H	0.491681	-0.211551	1.537145
H	2.546374	-1.565900	1.516251
H	5.611660	-0.499525	-0.256999

10-conf08

- Electronic Energy (Eh): -6779.41457856

- Cartesian Coordinates:

Br	-2.650353	-0.820748	2.279001
C	-2.518767	0.237506	0.708544
C	-1.367721	0.988208	0.512947
C	-1.216598	1.785762	-0.625886
C	0.019825	2.646963	-0.822714
C	-0.092482	4.004405	-0.076593
C	-0.261034	3.872772	1.438440
C	-1.211482	4.866552	-0.663035
C	1.306777	1.866728	-0.558970
C	1.416912	0.562298	-1.058146
C	2.579026	-0.176842	-0.893300
Br	2.639201	-1.938268	-1.598932
C	3.693410	0.353974	-0.218084
N	4.845598	-0.431763	-0.067808
C	6.004989	-0.096295	0.551790
C	7.069549	-1.223421	0.525496
F	7.389999	-1.567633	1.763930
F	8.159808	-0.797507	-0.094780
F	6.635163	-2.322850	-0.109937
O	6.279643	0.943726	1.097124
C	3.589215	1.658061	0.274773
C	2.418473	2.392563	0.101414
C	-2.254776	1.789098	-1.558139
C	-3.413015	1.040176	-1.372677
C	-3.568511	0.248896	-0.228747
N	-4.711644	-0.527548	0.012142
C	-5.817449	-0.643060	-0.765759
C	-6.894639	-1.588559	-0.173918
F	-6.507733	-2.142433	0.985709
F	-7.152971	-2.566970	-1.027985

F	-8.011295	-0.911258	0.050191
O	-6.039622	-0.105382	-1.822072
H	-0.569781	0.938580	1.255482
H	0.048778	2.904162	-1.896156
H	0.852049	4.538793	-0.273232
H	-0.178645	4.860083	1.917110
H	-1.251922	3.465830	1.692140
H	0.496425	3.217159	1.892935
H	-1.088564	5.008644	-1.748000
H	-2.200481	4.413885	-0.490612
H	-1.215924	5.861380	-0.193252
H	0.575641	0.108218	-1.584890
H	4.796065	-1.361833	-0.473772
H	4.438615	2.090479	0.798416
H	2.397723	3.405649	0.502925
H	-2.163429	2.394255	-2.463222
H	-4.209693	1.055926	-2.112709
H	-4.701317	-1.064047	0.874922

10-conf09

- Electronic Energy (Eh): -6779.4142184

- Cartesian Coordinates:

Br	2.790828	-1.778483	1.629922
C	2.718017	-0.149879	0.657004
C	1.527408	0.561915	0.647877
C	1.406193	1.769325	-0.051921
C	0.087643	2.537126	0.028679
C	-0.030302	3.747191	-0.937970
C	-1.200592	4.652463	-0.550264
C	-0.123497	3.359578	-2.414915
C	-1.115007	1.613354	-0.069264
C	-2.182873	1.751916	0.818497
C	-3.311482	0.945322	0.712961
Br	-4.721302	1.196760	1.958952
C	-3.413455	-0.037005	-0.285822
N	-4.568529	-0.829812	-0.355593
C	-4.850008	-1.814680	-1.246086
C	-6.233751	-2.477152	-1.019243
F	-6.991067	-2.314462	-2.093906
F	-6.886575	-1.952543	0.029665
F	-6.079992	-3.773781	-0.797433
O	-4.164555	-2.208971	-2.156318
C	-2.336229	-0.182557	-1.171528
C	-1.214542	0.628555	-1.057219
C	2.535979	2.228531	-0.731165
C	3.735340	1.520495	-0.730834
C	3.851248	0.312388	-0.036800
N	5.032636	-0.443244	-0.007020
C	6.217463	-0.156416	-0.602568
C	7.312382	-1.224782	-0.349281
F	7.735103	-1.717806	-1.503537
F	6.867230	-2.246161	0.398901
F	8.339479	-0.674464	0.281552
O	6.494085	0.803985	-1.277558
H	0.672676	0.162544	1.196603
H	0.065917	2.971408	1.043821
H	0.887445	4.341735	-0.794457
H	-1.211259	5.555970	-1.177885
H	-2.166816	4.142239	-0.687866
H	-1.134203	4.975233	0.500489
H	0.674359	2.666898	-2.720844
H	-1.088168	2.877992	-2.636703
H	-0.049405	4.256045	-3.048638
H	-2.141168	2.502408	1.610243
H	-5.274777	-0.635586	0.348299
H	-2.394768	-0.942973	-1.946809
H	-0.387589	0.477630	-1.753904
H	2.507254	3.166258	-1.285936
H	4.598930	1.898942	-1.272710

H 4.985962 -1.306320 0.526989

10-conf10

- Electronic Energy (Eh): -6779.41439409

- Cartesian Coordinates:

Br	-4.944789	1.869539	0.937321
C	-3.454844	1.147091	0.007324
C	-2.326624	1.947894	-0.150766
C	-1.195065	1.473273	-0.815680
C	0.051918	2.320117	-1.062315
C	0.080541	3.690376	-0.331775
C	1.155420	4.607068	-0.918130
C	0.243442	3.586514	1.186348
C	1.326755	1.526107	-0.829965
C	1.490695	0.742140	0.316237
C	2.675714	0.056761	0.546134
Br	2.823697	-0.986454	2.125161
C	3.747717	0.122248	-0.363233
N	4.924594	-0.589906	-0.088580
C	6.057137	-0.643482	-0.834020
C	7.164542	-1.534869	-0.214653
F	8.249641	-0.809697	0.012629
F	7.473183	-2.514436	-1.051049
F	6.785668	-2.087601	0.948167
O	6.280462	-0.091875	-1.882907
C	3.579536	0.899396	-1.515078
C	2.387407	1.582908	-1.734820
C	-1.251647	0.169331	-1.324684
C	-2.372452	-0.635299	-1.177003
C	-3.504001	-0.160305	-0.498609
N	-4.661092	-0.930806	-0.311645
C	-4.889581	-2.202877	-0.725485
C	-6.292391	-2.737502	-0.336758
F	-6.167709	-3.816863	0.420783
F	-6.969293	-3.058501	-1.429280
F	-7.013506	-1.834298	0.345872
O	-4.146102	-2.927887	-1.338267
H	-2.356763	2.956261	0.259852
H	0.030969	2.561747	-2.139453
H	-0.889900	4.170216	-0.543706
H	1.101492	5.605262	-0.458682
H	2.165938	4.210596	-0.732833
H	1.034233	4.731176	-2.005453
H	-0.478251	2.894402	1.645032
H	1.253545	3.238518	1.451570
H	0.102076	4.573254	1.652224
H	0.677182	0.651744	1.037738
H	4.919650	-1.125113	0.775088
H	4.393564	0.956033	-2.233940
H	2.286915	2.178281	-2.645391
H	-0.387621	-0.238029	-1.854344
H	-2.388760	-1.644135	-1.582915
H	-5.412598	-0.473878	0.196793

10-conf11

- Electronic Energy (Eh): -6779.4140357

- Cartesian Coordinates:

Br	5.107400	-1.728445	1.279635
C	3.598595	-1.063213	0.337415
C	2.440083	-1.835688	0.320946
C	1.294130	-1.399349	-0.345450
C	0.013384	-2.225788	-0.443583
C	-0.023415	-3.503378	0.438751
C	-1.148633	-4.443792	0.003780
C	-0.116621	-3.223860	1.940284
C	-1.225739	-1.367087	-0.250385
C	-2.317874	-1.503940	-1.108366
C	-3.478225	-0.761506	-0.914213
Br	-4.920111	-1.005594	-2.124480
C	-3.589190	0.152161	0.146892

N	-4.777381	0.880634	0.305401
C	-5.075088	1.788590	1.269267
C	-6.496929	2.392429	1.132510
F	-6.416188	3.707449	0.998775
F	-7.207739	2.116000	2.215872
F	-7.158483	1.908157	0.069746
O	-4.378288	2.155661	2.182253
C	-2.487653	0.297033	1.002235
C	-1.334107	-0.449454	0.799096
C	1.366567	-0.164199	-1.002111
C	2.517343	0.611089	-0.996303
C	3.664418	0.175479	-0.317584
N	4.852246	0.920012	-0.271220
C	5.102488	2.124102	-0.844964
C	6.537807	2.648371	-0.580814
F	6.482585	3.816146	0.041516
F	7.176861	2.806881	-1.730457
F	7.257482	1.808179	0.179411
O	4.356251	2.797612	-1.510856
H	2.458086	-2.791310	0.843264
H	-0.017256	-2.588713	-1.485990
H	0.922496	-4.036419	0.243746
H	-1.101886	-5.386176	0.569539
H	-2.138689	-3.997260	0.185911
H	-1.079994	-4.691828	-1.066894
H	0.643856	-2.508534	2.286672
H	-1.103507	-2.814289	2.204534
H	0.017080	-4.155966	2.509538
H	-2.270383	-2.201892	-1.946471
H	-5.497533	0.697379	-0.387378
H	-2.552942	1.005353	1.824890
H	-0.489730	-0.300513	1.475018
H	0.491394	0.211624	-1.536720
H	2.545956	1.566171	-1.515708
H	5.611506	0.499729	0.257002

10-conf12

- Electronic Energy (Eh): -6779.41626772

- Cartesian Coordinates:

Br	-2.875940	-0.486231	2.290984
C	-2.641882	0.273426	0.566944
C	-1.506937	1.036691	0.329777
C	-1.284840	1.619142	-0.920850
C	-0.054261	2.477185	-1.175389
C	-0.097626	3.816861	-0.400830
C	-1.402906	4.566760	-0.669844
C	1.105949	4.694308	-0.748050
C	1.205309	1.653693	-0.951779
C	1.845651	1.585699	0.287668
C	2.958423	0.772827	0.472285
Br	3.773406	0.737869	2.186765
C	3.478792	-0.005260	-0.575528
N	4.603763	-0.810130	-0.342182
C	5.245796	-1.618246	-1.223248
C	6.456844	-2.365967	-0.607547
F	7.560535	-2.057809	-1.271657
F	6.263249	-3.674245	-0.684519
F	6.649463	-2.052017	0.683227
O	4.980973	-1.807201	-2.384353
C	2.838674	0.066602	-1.819825
C	1.726662	0.881625	-1.992478
C	-2.234512	1.401696	-1.918698
C	-3.374518	0.636092	-1.692977
C	-3.601063	0.055780	-0.439694
N	-4.730510	-0.725976	-0.154137
C	-5.759840	-1.033648	-0.982851
C	-6.845001	-1.920854	-0.319611
F	-6.980870	-3.049145	-0.999447
F	-8.005963	-1.282160	-0.315857

F	-6.543106	-2.236163	0.949581
O	-5.911692	-0.699169	-2.131536
H	-0.784295	1.167655	1.136952
H	-0.071385	2.739778	-2.246666
H	-0.066127	3.590808	0.680502
H	-1.412967	5.527537	-0.134243
H	-1.514906	4.783296	-1.745354
H	-2.283805	3.992371	-0.349980
H	2.062359	4.199823	-0.527237
H	1.100815	4.947845	-1.820876
H	1.075113	5.637706	-0.182896
H	1.490564	2.178283	1.132017
H	4.976496	-0.777216	0.602259
H	3.228111	-0.525439	-2.644830
H	1.247443	0.910575	-2.974155
H	-2.089405	1.844860	-2.906824
H	-4.104212	0.478242	-2.483815
H	-4.774190	-1.102357	0.788454

10-conf13

- Electronic Energy (Eh): -6779.41611035

- Cartesian Coordinates:

Br	-4.005752	0.111442	2.485039
C	-3.107693	0.552063	0.871386
C	-1.971895	1.350281	0.945687
C	-1.271965	1.709856	-0.208266
C	0.009486	2.528703	-0.162827
C	0.029618	3.640328	0.914226
C	-1.142928	4.605329	0.733021
C	1.356986	4.399484	0.895403
C	1.211122	1.600855	-0.061210
C	2.186820	1.596887	-1.057634
C	3.299572	0.766538	-0.964587
Br	4.584728	0.818374	-2.360442
C	3.477594	-0.092558	0.131957
N	4.613737	-0.914001	0.185846
C	4.960952	-1.791593	1.160785
C	6.292166	-2.535284	0.878766
F	7.151877	-2.305222	1.859631
F	6.862967	-2.145099	-0.271660
F	6.070445	-3.839196	0.802395
O	4.365011	-2.043130	2.178555
C	2.494143	-0.088545	1.131730
C	1.386272	0.742148	1.027223
C	-1.756971	1.241974	-1.431506
C	-2.891148	0.443738	-1.517932
C	-3.591770	0.080049	-0.360532
N	-4.742346	-0.722136	-0.386104
C	-5.356511	-1.261755	-1.469127
C	-6.612617	-2.099187	-1.114682
F	-6.853329	-2.126838	0.205480
F	-6.451269	-3.347724	-1.526334
F	-7.677657	-1.586607	-1.712908
O	-5.039117	-1.160764	-2.628121
H	-1.645639	1.698780	1.926535
H	0.086303	3.042643	-1.135965
H	-0.060750	3.161641	1.905974
H	-1.127728	5.385200	1.508846
H	-1.080738	5.107754	-0.246308
H	-2.115744	4.096521	0.785326
H	2.212038	3.742844	1.109842
H	1.527632	4.864338	-0.090060
H	1.352207	5.203648	1.645969
H	2.087998	2.254680	-1.923383
H	5.248815	-0.833363	-0.602949
H	2.614429	-0.749705	1.986803
H	0.637361	0.707847	1.821258
H	-1.231339	1.503992	-2.353079
H	-3.251486	0.091546	-2.481671

H	-5.159112	-0.917515	0.519546
---	-----------	-----------	----------

10-conf14

- Electronic Energy (Eh): -6779.41604863

- Cartesian Coordinates:

Br	3.639806	0.558553	2.545312
C	2.970664	0.694707	0.774363
C	1.830858	1.457721	0.553611
C	1.292822	1.596295	-0.727900
C	0.007553	2.390701	-0.909007
C	-0.075997	3.186632	-2.233974
C	1.100412	4.154236	-2.370087
C	-1.403761	3.937728	-2.340849
C	-1.194362	1.481281	-0.701150
C	-2.115653	1.748705	0.311106
C	-3.228853	0.934712	0.497069
Br	-4.437910	1.363751	1.896141
C	-3.462045	-0.179232	-0.325578
N	-4.597324	-0.973211	-0.103873
C	-4.992693	-2.072296	-0.794642
C	-6.307842	-2.698090	-0.261979
F	-6.815493	-2.016278	0.776834
F	-6.084480	-3.941603	0.136430
F	-7.218817	-2.714887	-1.223307
O	-4.449119	-2.590160	-1.738272
C	-2.532855	-0.447778	-1.341161
C	-1.423695	0.369315	-1.515912
C	1.943606	0.942957	-1.777110
C	3.085328	0.177020	-1.568033
C	3.622910	0.036239	-0.282661
N	4.772361	-0.722299	-0.015749
C	5.537320	-1.412242	-0.898885
C	6.744388	-2.131019	-0.242399
F	7.875485	-1.660028	-0.747127
F	6.678814	-3.431554	-0.482388
F	6.781778	-1.956795	1.087916
O	5.383206	-1.515203	-2.090504
H	1.350897	1.949681	1.402153
H	-0.017962	3.140065	-0.099647
H	-0.036204	2.466930	-3.071083
H	1.041258	4.706834	-3.319546
H	1.087879	4.893805	-1.552511
H	2.070779	3.639091	-2.339503
H	-2.266377	3.256449	-2.333612
H	-1.523537	4.642341	-1.500819
H	-1.442559	4.521543	-3.272357
H	-1.973597	2.609406	0.967671
H	-5.190897	-0.680597	0.666758
H	-2.696098	-1.308530	-1.985552
H	-0.717017	0.120758	-2.310475
H	1.566885	1.031689	-2.797863
H	3.578820	-0.321013	-2.399423
H	5.059151	-0.752851	0.958367

10-conf15

- Electronic Energy (Eh): -6779.41611023

- Cartesian Coordinates:

Br	4.584783	0.818495	2.360392
C	3.299588	0.766549	0.964578
C	2.186836	1.596899	1.057595
C	1.211091	1.600764	0.061217
C	0.009486	2.528659	0.162775
C	0.029674	3.640206	-0.914369
C	1.357077	4.399300	-0.895634
C	-1.142818	4.605280	-0.733224
C	-1.272002	1.709883	0.208234
C	-1.971893	1.350234	-0.945720
C	-3.107730	0.552074	-0.871396

Br	-4.005739	0.111352	-2.485049
C	-3.591889	0.080195	0.360541
N	-4.742490	-0.721953	0.386123
C	-5.356710	-1.261470	1.469166
C	-6.612610	-2.099209	1.114721
F	-6.853645	-2.126437	-0.205391
F	-7.677683	-1.587325	1.713425
F	-6.450645	-3.347871	1.525826
O	-5.039470	-1.160219	2.628185
C	-2.891316	0.443976	1.517942
C	-1.757093	1.242144	1.431495
C	1.386185	0.741941	-1.027133
C	2.494057	-0.088755	-1.131612
C	3.477562	-0.092657	-0.131892
N	4.613699	-0.914103	-0.185756
C	4.961006	-1.791611	-1.160746
C	6.292217	-2.535292	-0.878679
F	7.151968	-2.305236	-1.859505
F	6.070497	-3.839207	-0.802303
F	6.862958	-2.145104	0.271773
O	4.365145	-2.043058	-2.178588
H	2.088047	2.254775	1.923285
H	0.086312	3.042664	1.135877
H	-0.060735	3.161429	-1.906070
H	1.352301	5.203441	-1.646225
H	1.527793	4.864183	0.089805
H	2.212091	3.742620	-1.110094
H	-2.115664	4.096525	-0.785482
H	-1.080590	5.107774	0.246067
H	-1.127582	5.385095	-1.509105
H	-1.645568	1.698631	-1.926582
H	-5.159197	-0.917440	-0.519531
H	-3.251729	0.091909	2.481698
H	-1.231498	1.504232	2.353069
H	0.637225	0.707544	-1.821117
H	2.614306	-0.750001	-1.986623
H	5.248723	-0.833512	0.603088

10-conf16

- Electronic Energy (Eh): -6779.41626839

- Cartesian Coordinates:

Br	-2.875920	-0.486040	2.291038
C	-2.641864	0.273606	0.566991
C	-1.506945	1.036901	0.329831
C	-1.284848	1.619353	-0.920800
C	-0.054251	2.477371	-1.175373
C	-0.097514	3.817039	-0.400797
C	-1.402773	4.566983	-0.669806
C	1.106100	4.694420	-0.748022
C	1.205295	1.653812	-0.951845
C	1.845592	1.585749	0.287628
C	2.958361	0.772875	0.472238
Br	3.773312	0.737804	2.186719
C	3.478762	-0.005111	-0.575633
N	4.603766	-0.809964	-0.342283
C	5.245675	-1.618235	-1.223272
C	6.456473	-2.366294	-0.607466
F	6.262513	-3.674498	-0.684361
F	6.649174	-2.052316	0.683298
F	7.560314	-2.058515	-1.271544
O	4.980933	-1.807090	-2.384418
C	2.838741	0.066868	-1.819971
C	1.726715	0.881885	-1.992604
C	-2.234528	1.401909	-1.918634
C	-3.374535	0.636294	-1.692912
C	-3.601053	0.055947	-0.439647
N	-4.730469	-0.725847	-0.154082
C	-5.759772	-1.033598	-0.982804
C	-6.844692	-1.921182	-0.319669

F	-6.979729	-3.049742	-0.999255
F	-8.005980	-1.283115	-0.316466
F	-6.543017	-2.235984	0.949707
O	-5.911617	-0.699168	-2.131504
H	-0.784325	1.167886	1.137018
H	-0.071428	2.739989	-2.246641
H	-0.066015	3.590996	0.680534
H	-1.412829	5.527758	-0.134204
H	-1.514759	4.783533	-1.745314
H	-2.283683	3.992606	-0.349954
H	2.062474	4.199905	-0.527123
H	1.101037	4.947888	-1.820864
H	1.075269	5.637856	-0.182936
H	1.490469	2.178300	1.131984
H	4.976401	-0.777138	0.602196
H	3.228282	-0.525059	-2.645002
H	1.247558	0.910967	-2.974305
H	-2.089454	1.845097	-2.906753
H	-4.104233	0.478467	-2.483749
H	-4.774219	-1.102082	0.788563

10-conf17

- Electronic Energy (Eh): -6779.41604871

- Cartesian Coordinates:

Br	3.640001	0.558970	2.545179
C	2.970703	0.694765	0.774261
C	1.830927	1.457815	0.553441
C	1.292785	1.596138	-0.728046
C	0.007562	2.390602	-0.909243
C	-0.075911	3.186481	-2.234247
C	1.100588	4.153964	-2.370408
C	-1.403609	3.937690	-2.341131
C	-1.194391	1.481238	-0.701345
C	-2.115527	1.748614	0.311069
C	-3.228739	0.934661	0.497126
Br	-4.437578	1.363649	1.896397
C	-3.462104	-0.179198	-0.325582
N	-4.597383	-0.973148	-0.103766
C	-4.992952	-2.072112	-0.794619
C	-6.308064	-2.697876	-0.261826
F	-6.815351	-2.016326	0.777347
F	-6.084790	-3.941556	0.136104
F	-7.219282	-2.714206	-1.222924
O	-4.449596	-2.589882	-1.738422
C	-2.533078	-0.447697	-1.341324
C	-1.423901	0.369361	-1.516173
C	1.943433	0.942520	-1.777174
C	3.085104	0.176536	-1.568028
C	3.622797	0.036006	-0.282668
N	4.772210	-0.722563	-0.015697
C	5.537167	-1.412569	-0.898787
C	6.744341	-2.131142	-0.242276
F	6.781528	-1.957103	1.088071
F	7.875370	-1.659750	-0.746809
F	6.679141	-3.431645	-0.482482
O	5.383017	-1.515672	-2.090387
H	1.351089	1.950006	1.401919
H	-0.017941	3.140010	-0.099924
H	-0.036186	2.466753	-3.071336
H	1.041480	4.706535	-3.319886
H	1.088141	4.893565	-1.552858
H	2.070903	3.638720	-2.339816
H	-2.266279	3.256478	-2.333871
H	-1.523316	4.642325	-1.501110
H	-1.442374	4.521495	-3.272648
H	-1.973331	2.609256	0.967682
H	-5.190777	-0.680633	0.667038
H	-2.696444	-1.308379	-1.985777
H	-0.717379	0.120847	-2.310888

H	1.566630	1.031063	-2.797913
H	3.578494	-0.321717	-2.399347
H	5.058990	-0.753071	0.958424

10-conf18

- Electronic Energy (Eh): -6779.416110509999

- Cartesian Coordinates:

Br	-4.005340	0.111171	2.485109
C	-3.107516	0.552096	0.871408
C	-1.971722	1.350321	0.945685
C	-1.271948	1.710091	-0.208303
C	0.009485	2.528962	-0.162854
C	0.029542	3.640596	0.914186
C	-1.143077	4.605508	0.732996
C	1.356860	4.399837	0.895317
C	1.211120	1.601123	-0.061177
C	2.186647	1.596854	-1.057762
C	3.299368	0.766457	-0.964703
Br	4.584279	0.817873	-2.360802
C	3.477522	-0.092375	0.132020
N	4.613618	-0.913886	0.185925
C	4.960890	-1.791341	1.160969
C	6.291956	-2.535253	0.878829
F	6.862590	-2.145305	-0.271756
F	6.070037	-3.839143	0.802694
F	7.151872	-2.305154	1.859518
O	4.365096	-2.042598	2.178895
C	2.494257	-0.088034	1.131982
C	1.386428	0.742705	1.027463
C	-1.757110	1.242408	-1.431556
C	-2.891289	0.444175	-1.517961
C	-3.591742	0.080270	-0.360523
N	-4.742299	-0.721942	-0.386076
C	-5.356424	-1.261637	-1.469086
C	-6.612293	-2.099410	-1.114587
F	-6.450333	-3.348061	-1.525699
F	-7.677395	-1.587525	-1.713268
F	-6.853292	-2.126635	0.205531
O	-5.039142	-1.160502	-2.628098
H	-1.645346	1.698670	1.926547
H	0.086333	3.042883	-1.135999
H	-0.060784	3.161911	1.905940
H	-1.127877	5.385416	1.508783
H	-1.080980	5.107889	-0.246361
H	-2.115853	4.096635	0.785386
H	2.211963	3.743239	1.109678
H	1.527413	4.864731	-0.090143
H	1.352085	5.203977	1.645908
H	2.087717	2.254437	-1.923658
H	5.248564	-0.833466	-0.603000
H	2.614675	-0.748972	1.987207
H	0.637670	0.708668	1.821653
H	-1.231606	1.504590	-2.353155
H	-3.251763	0.092139	-2.481706
H	-5.158999	-0.917397	0.519586

10-conf19

- Electronic Energy (Eh): -6779.41611063

- Cartesian Coordinates:

Br	4.585259	0.818871	2.360031
C	3.299756	0.766563	0.964512
C	2.187016	1.596903	1.057540
C	1.211056	1.600526	0.061343
C	0.009500	2.528463	0.162938
C	0.029764	3.640010	-0.914233
C	1.357214	4.399019	-0.895540
C	-1.142657	4.605166	-0.733064
C	-1.272014	1.709740	0.208359

C	-1.972109	1.350390	-0.945564
C	-3.107957	0.552245	-0.871284
Br	-4.006262	0.111991	-2.484898
C	-3.591925	0.080028	0.360623
N	-4.742538	-0.722036	0.386199
C	-5.356641	-1.261750	1.469191
C	-6.612700	-2.099275	1.114655
F	-7.677654	-1.587401	1.713618
F	-6.450859	-3.348054	1.525432
F	-6.853910	-2.126148	-0.205430
O	-5.039253	-1.160766	2.628183
C	-2.891130	0.443493	1.518002
C	-1.756922	1.241680	1.431575
C	1.385957	0.741461	-1.026830
C	2.493820	-0.089257	-1.131326
C	3.477509	-0.092918	-0.131792
N	4.613643	-0.914381	-0.185688
C	4.960805	-1.792045	-1.160600
C	6.292344	-2.535318	-0.878801
F	7.152543	-2.303153	-1.858814
F	6.071489	-3.839466	-0.804565
F	6.862161	-2.146455	0.272546
O	4.364799	-2.043692	-2.178292
H	2.088383	2.254986	1.923089
H	0.086339	3.042455	1.136045
H	-0.060685	3.161176	-1.905902
H	1.352456	5.203153	-1.646134
H	1.527970	4.863913	0.089887
H	2.212191	3.742298	-1.109995
H	-2.115534	4.096467	-0.785190
H	-1.080300	5.107715	0.246190
H	-1.127446	5.384940	-1.508983
H	-1.645935	1.699005	-1.926398
H	-5.159353	-0.917284	-0.519449
H	-3.251354	0.091160	2.481727
H	-1.231189	1.503541	2.353134
H	0.636847	0.706848	-1.820666
H	2.613942	-0.750677	-1.986218
H	5.248638	-0.833924	0.603185

11-conf01

- Electronic Energy (Eh): -7737.93455342

- Cartesian Coordinates:

Br	3.016464	-2.461491	0.618210
C	2.721389	-0.641660	0.201711
C	1.529165	-0.047640	0.600736
C	1.282506	1.300826	0.329940
C	0.024354	2.027917	0.786710
C	0.088756	2.550697	2.270670
C	-1.197569	3.339215	2.554140
C	0.247696	1.444777	3.322164
C	1.290410	3.501188	2.389915
C	-1.253993	1.297437	0.399886
C	-1.695056	0.117069	1.007724
C	-2.881127	-0.486624	0.605122
Br	-3.438593	-2.066923	1.478932
C	-3.667680	0.041807	-0.426744
N	-4.869340	-0.576389	-0.822271
C	-6.087097	0.005956	-0.622269
C	-7.269368	-0.855998	-1.126557
F	-7.672626	-0.417526	-2.313854
F	-6.921750	-2.146184	-1.263284
F	-8.280945	-0.789152	-0.280788
O	-6.285302	1.092121	-0.150654
C	-3.205115	1.209578	-1.049216
C	-2.030029	1.827799	-0.633685
C	2.247535	2.014269	-0.385243
C	3.429911	1.411630	-0.801557
C	3.702966	0.069659	-0.500632

N	4.909349	-0.541029	-0.893557
C	6.112272	-0.181891	-0.359401
C	7.302482	-0.995339	-0.922124
F	7.948890	-0.277429	-1.833489
F	6.895519	-2.132544	-1.509606
F	8.142312	-1.310417	0.047133
O	6.300939	0.695874	0.437921
H	0.800810	-0.658336	1.130034
H	0.002872	2.954361	0.193541
H	-1.153952	3.790604	3.556929
H	-2.089615	2.696686	2.513956
H	-1.336204	4.154055	1.825601
H	1.116521	0.801337	3.118045
H	-0.649381	0.816630	3.410921
H	0.408639	1.902656	4.310004
H	1.304620	3.966654	3.386873
H	1.239723	4.312151	1.645752
H	2.246908	2.974671	2.255225
H	-1.137658	-0.342643	1.820428
H	-4.845490	-1.565013	-1.046587
H	-1.716919	2.739760	-1.144264
H	2.083634	3.063188	-0.636129
H	4.856960	-1.415097	-1.404962
Cl	-4.078628	1.885864	-2.382530
Cl	4.553974	2.336255	-1.740142

11-conf02

- Electronic Energy (Eh): -7737.93458622

- Cartesian Coordinates:

Br	4.640125	2.347644	-1.384591
C	3.382465	1.229911	-0.525446
C	2.194747	1.783689	-0.060891
C	1.245110	0.997246	0.598139
C	-0.011002	1.672152	1.132829
C	0.018881	1.962490	2.679836
C	0.063826	0.705094	3.556685
C	1.265196	2.808549	2.981395
C	-1.234413	2.775868	3.033288
C	-1.298320	1.045368	0.615422
C	-1.740732	-0.234546	0.966147
C	-2.941952	-0.729173	0.470247
Br	-3.500989	-2.455057	0.998839
C	-3.742925	0.014286	-0.406370
N	-4.961406	-0.494463	-0.895895
C	-6.165760	0.036331	-0.536799
C	-7.373230	-0.687143	-1.179777
F	-7.830268	0.022329	-2.205202
F	-7.038008	-1.903557	-1.640137
F	-8.343894	-0.834365	-0.296424
O	-6.337577	0.992785	0.168482
C	-3.279162	1.284678	-0.774982
C	-2.087963	1.790237	-0.264236
C	1.510077	-0.366853	0.740594
C	2.689403	-0.922364	0.255158
C	3.663451	-0.133792	-0.374186
N	4.870385	-0.690183	-0.839761
C	5.821521	-1.173774	0.010305
C	7.069210	-1.730475	-0.716401
F	7.000197	-3.055530	-0.779342
F	8.168462	-1.390717	-0.068644
F	7.162447	-1.265362	-1.972967
O	5.740393	-1.230989	1.206951
H	2.017903	2.851086	-0.201422
H	0.002475	2.678647	0.688826
H	0.165609	1.001799	4.611715
H	0.924739	0.063105	3.318624
H	-0.857969	0.111124	3.483679
H	1.291690	3.722052	2.365737
H	2.194800	2.248853	2.799735

H	1.264070	3.119307	4.037001
H	-1.212488	3.066737	4.094447
H	-2.156819	2.201127	2.862070
H	-1.295870	3.698763	2.434450
H	-1.172844	-0.862910	1.647888
H	-4.955532	-1.406138	-1.339802
H	-1.774568	2.788279	-0.574219
H	0.800794	-1.038604	1.218277
H	5.133135	-0.523436	-1.804835
Cl	-4.173316	2.238382	-1.910673
Cl	2.927123	-2.631560	0.408555

11-conf03

- Electronic Energy (Eh): -7737.93447713

- Cartesian Coordinates:

Br	-4.273306	-2.071662	-1.826260
C	-3.249617	-1.042048	-0.617560
C	-2.058908	-1.565592	-0.125891
C	-1.278349	-0.847201	0.784768
C	0.003029	-1.491461	1.295336
C	0.067739	-1.738411	2.848961
C	1.268945	-2.653063	3.135385
C	0.227965	-0.461897	3.684393
C	-1.219236	-2.461914	3.269875
C	1.258816	-0.855539	0.714038
C	2.213114	-1.682322	0.114208
C	3.398965	-1.155788	-0.385341
Br	4.665226	-2.324248	-1.160813
C	3.672078	0.216839	-0.330488
N	4.877196	0.744148	-0.833128
C	5.825077	1.292450	-0.019324
C	7.075438	1.792481	-0.781900
F	7.164965	1.245355	-2.005317
F	7.015406	3.110782	-0.931251
F	8.173110	1.488219	-0.113646
O	5.740405	1.440494	1.169238
C	2.691829	1.043327	0.238149
C	1.514428	0.516708	0.759115
C	-1.720684	0.424050	1.162694
C	-2.901186	0.954418	0.652370
C	-3.703981	0.227198	-0.238383
N	-4.914453	0.750439	-0.731909
C	-5.998683	0.953527	0.071367
C	-7.221461	1.526235	-0.684610
F	-7.142309	1.292739	-2.005010
F	-7.284251	2.841691	-0.509456
F	-8.337121	0.982147	-0.235609
O	-6.047380	0.770707	1.256992
H	-1.744524	-2.558924	-0.450081
H	-0.016085	-2.509812	0.878974
H	1.286465	-2.929586	4.200292
H	2.224898	-2.159934	2.904485
H	1.215571	-3.585631	2.550785
H	-0.661954	0.181118	3.644668
H	1.107445	0.124641	3.379848
H	0.371024	-0.734821	4.741008
H	-1.173892	-2.729390	4.336453
H	-1.361229	-3.392294	2.696707
H	-2.109809	-1.833846	3.119476
H	2.041573	-2.757767	0.048783
H	5.145038	0.502075	-1.780720
H	0.795659	1.214301	1.183591
H	-1.159162	1.038439	1.862461
H	-5.058636	0.755247	-1.735717
Cl	2.918652	2.760373	0.266945
Cl	-3.354128	2.562036	1.111385

11-conf04

- Electronic Energy (Eh): -7737.93437588

- Cartesian Coordinates:

Br	-2.707107	-2.027991	-1.524378
C	-2.517467	-0.477306	-0.461206
C	-1.399052	0.328138	-0.644192
C	-1.234751	1.494655	0.106984
C	-0.061429	2.447251	-0.084344
C	-0.264947	3.487157	-1.248738
C	-1.509242	4.328512	-0.922400
C	0.960558	4.410942	-1.284954
C	-0.468334	2.856182	-2.632644
C	1.279749	1.727410	-0.054702
C	1.767568	0.937120	-1.100841
C	2.986583	0.278831	-0.982241
Br	3.583384	-0.792809	-2.420133
C	3.780548	0.391830	0.166532
N	5.012494	-0.281184	0.274477
C	5.213928	-1.293858	1.167162
C	6.639769	-1.892249	1.102887
F	7.238599	-1.625314	-0.069534
F	7.390588	-1.372779	2.068014
F	6.596284	-3.202773	1.254684
O	4.422933	-1.694376	1.976429
C	3.298208	1.208650	1.198856
C	2.068396	1.850454	1.091922
C	-2.200202	1.799637	1.069196
C	-3.306545	0.979810	1.265567
C	-3.500438	-0.171649	0.489368
N	-4.631342	-0.992623	0.662101
C	-5.888967	-0.572111	0.342209
C	-6.977959	-1.641004	0.600023
F	-6.455715	-2.876027	0.673225
F	-7.872913	-1.628881	-0.370786
F	-7.591147	-1.391637	1.751829
O	-6.191804	0.517944	-0.060485
H	-0.661138	0.027930	-1.385539
H	-0.056476	3.076083	0.818606
H	-1.625820	5.132500	-1.664594
H	-1.428788	4.801171	0.069612
H	-2.429164	3.725553	-0.938916
H	1.876611	3.864658	-1.554409
H	1.128749	4.890310	-0.307218
H	0.814297	5.208963	-2.028700
H	-0.726464	3.643654	-3.357023
H	-1.292908	2.128020	-2.637309
H	0.439556	2.367946	-3.012589
H	1.207169	0.814923	-2.024795
H	5.681648	-0.172154	-0.479595
H	1.733183	2.468339	1.926394
H	-2.096065	2.688863	1.692425
H	-4.482297	-1.985437	0.805533
Cl	4.253761	1.465489	2.619791
Cl	-4.431172	1.380455	2.520139

11-conf05

- Electronic Energy (Eh): -7737.9342719

- Cartesian Coordinates:

Br	-3.216620	-1.709667	-1.920634
C	-2.858032	-0.177885	-0.873038
C	-1.627451	0.454510	-1.011328
C	-1.317492	1.582260	-0.245788
C	0.006328	2.329230	-0.344997
C	0.122961	3.288767	-1.587138
C	1.438484	4.070386	-1.461174
C	0.094608	2.572404	-2.942860
C	-1.051414	4.277804	-1.536870
C	1.216267	1.438426	-0.098010
C	1.631837	0.425683	-0.968843
C	2.762756	-0.332020	-0.685576

Br	3.291006	-1.669489	-1.911540
C	3.515714	-0.130750	0.478401
N	4.663875	-0.899188	0.751022
C	5.916534	-0.359262	0.741719
C	7.030314	-1.386045	1.057781
F	7.406505	-1.267817	2.326111
F	6.610852	-2.648169	0.870890
F	8.078310	-1.180915	0.281040
O	6.189843	0.795266	0.556722
C	3.077377	0.867602	1.359304
C	1.957700	1.640525	1.068757
C	-2.285015	2.055334	0.644129
C	-3.524265	1.434637	0.763396
C	-3.835363	0.290633	0.015054
N	-5.077204	-0.359790	0.146386
C	-5.442756	-1.010335	1.289105
C	-6.844006	-1.661640	1.201576
F	-7.231592	-1.838924	-0.072350
F	-7.741856	-0.880808	1.792496
F	-6.842624	-2.838542	1.799501
O	-4.808380	-1.069285	2.306527
H	-0.913078	0.035992	-1.716388
H	-0.001987	3.023684	0.508125
H	1.520114	4.811634	-2.270581
H	2.314991	3.408379	-1.522819
H	1.492460	4.612829	-0.503681
H	-0.813402	1.964971	-3.072292
H	0.976599	1.935332	-3.097569
H	0.100092	3.321045	-3.749802
H	-0.947522	5.029073	-2.334261
H	-1.085689	4.815311	-0.575677
H	-2.018715	3.772731	-1.677499
H	1.099403	0.219607	-1.894142
H	4.578969	-1.909558	0.734991
H	1.661051	2.410258	1.782812
H	-2.087281	2.938059	1.253981
H	-5.605758	-0.549646	-0.697884
Cl	3.911598	1.132440	2.853064
Cl	-4.703305	2.121131	1.829886

11-conf06

- Electronic Energy (Eh): -7737.93436063

- Cartesian Coordinates:

Br	4.361778	1.587480	-2.266418
C	3.305213	1.185384	-0.752685
C	2.096137	1.850003	-0.578897
C	1.274209	1.573816	0.517710
C	-0.055850	2.307690	0.619678
C	-0.280060	3.162199	1.923083
C	0.965428	4.031167	2.146983
C	-1.488426	4.082064	1.685096
C	-0.557406	2.332771	3.183936
C	-1.236937	1.418243	0.253087
C	-1.439794	0.154448	0.813053
C	-2.564522	-0.592419	0.480665
Br	-2.807319	-2.282475	1.289362
C	-3.515464	-0.126440	-0.437064
N	-4.654339	-0.888561	-0.761389
C	-5.912980	-0.497214	-0.410665
C	-7.012422	-1.492490	-0.852669
F	-7.614874	-1.041749	-1.947291
F	-6.505325	-2.703756	-1.133497
F	-7.913824	-1.634676	0.102198
O	-6.209202	0.524328	0.146974
C	-3.282252	1.125625	-1.023282
C	-2.169601	1.884706	-0.676083
C	1.721153	0.628660	1.445764
C	2.941894	-0.017920	1.281658
C	3.757134	0.231823	0.168186

N	4.980522	-0.440607	-0.014141
C	5.044811	-1.779923	-0.268760
C	6.491106	-2.300205	-0.449289
F	6.543270	-3.183535	-1.429041
F	6.905623	-2.878245	0.672573
F	7.345760	-1.304490	-0.736527
O	4.116224	-2.539310	-0.315843
H	1.786134	2.586541	-1.321922
H	-0.013474	3.066581	-0.176039
H	0.805941	4.714057	2.995264
H	1.189186	4.644942	1.259635
H	1.854526	3.422516	2.368648
H	-2.422412	3.512396	1.570053
H	-1.353339	4.701911	0.784207
H	-1.618212	4.762756	2.539872
H	-0.813852	3.008211	4.014289
H	0.316564	1.753258	3.511174
H	-1.407225	1.647658	3.048336
H	-0.728302	-0.268440	1.519672
H	-4.518495	-1.849409	-1.055936
H	-2.034456	2.856461	-1.153083
H	1.141822	0.384399	2.333063
H	5.807810	0.116798	-0.196770
Cl	-4.365452	1.734564	-2.229949
Cl	3.467120	-1.120778	2.510148

11-conf07

- Electronic Energy (Eh): -7737.93429908

- Cartesian Coordinates:

Br	4.575020	1.553135	-2.156072
C	3.275989	0.932387	-0.932820
C	2.165715	1.726278	-0.668013
C	1.192121	1.313707	0.246126
C	0.025558	2.247061	0.543558
C	0.215597	3.116569	1.842212
C	0.347944	2.301135	3.135021
C	1.493142	3.953689	1.672030
C	-0.985658	4.064961	1.961092
C	-1.326312	1.562891	0.394686
C	-1.828984	0.618148	1.295710
C	-3.060623	0.012576	1.073022
Br	-3.678137	-1.272615	2.313583
C	-3.853452	0.332077	-0.037194
N	-5.098216	-0.289933	-0.250194
C	-5.325077	-1.128430	-1.303186
C	-6.759640	-1.708898	-1.324823
F	-6.737684	-2.976715	-1.691923
F	-7.345661	-1.631594	-0.118576
F	-7.509307	-1.026203	-2.183220
O	-4.549570	-1.393244	-2.180322
C	-3.356631	1.302057	-0.919086
C	-2.113674	1.891802	-0.711486
C	1.346669	0.064919	0.851722
C	2.447472	-0.736706	0.568334
C	3.448991	-0.314004	-0.317846
N	4.577918	-1.112308	-0.585250
C	5.532974	-1.357003	0.357231
C	6.687666	-2.250273	-0.156169
F	7.845378	-1.817640	0.308899
F	6.751666	-2.258708	-1.497607
F	6.503632	-3.502074	0.248307
O	5.515786	-0.983302	1.498371
H	2.070083	2.689034	-1.172184
H	0.047076	2.992880	-0.265150
H	1.154277	1.555385	3.073041
H	-0.586905	1.793720	3.410377
H	0.595098	2.977040	3.967814
H	1.463516	4.553363	0.748092
H	2.394876	3.324379	1.641228

H	1.602691	4.650444	2.516655
H	-0.847864	4.749619	2.811741
H	-1.925285	3.515604	2.121134
H	-1.103307	4.677775	1.052912
H	-1.271001	0.331521	2.183927
H	-5.756892	-0.309535	0.520674
H	-1.767589	2.634996	-1.431423
H	0.604129	-0.326865	1.543619
H	4.795909	-1.323300	-1.552818
Cl	-4.309897	1.816705	-2.269908
Cl	2.548819	-2.300793	1.305645

11-conf08

- Electronic Energy (Eh): -7737.93430162

- Cartesian Coordinates:

Br	-3.964924	0.902802	2.760644
C	-3.028524	0.686634	1.134622
C	-1.909474	1.475319	0.890778
C	-1.196763	1.362841	-0.306586
C	0.009615	2.269156	-0.510842
C	-0.071942	3.246730	-1.741810
C	0.072983	2.559224	-3.105528
C	-1.421187	3.976839	-1.682870
C	1.057668	4.279419	-1.603714
C	1.331661	1.522150	-0.389499
C	1.627880	0.368102	-1.119911
C	2.854778	-0.268172	-0.968674
Br	3.196829	-1.835659	-1.967503
C	3.840125	0.221889	-0.100949
N	5.077444	-0.434114	0.045986
C	5.439805	-1.054997	1.205945
C	6.833808	-1.723421	1.133840
F	7.220390	-1.933056	-0.135405
F	7.739819	-0.939941	1.708502
F	6.818804	-2.886904	1.757535
O	4.807900	-1.078032	2.226432
C	3.541366	1.391038	0.612773
C	2.305977	2.016910	0.480595
C	-1.630118	0.413904	-1.237194
C	-2.736425	-0.389532	-0.981151
C	-3.473344	-0.261613	0.204978
N	-4.610911	-1.053566	0.452730
C	-5.760810	-0.918739	-0.268945
C	-6.884448	-1.882544	0.181904
F	-6.933135	-2.930505	-0.633151
F	-8.053495	-1.269419	0.158581
F	-6.676256	-2.341457	1.426709
O	-5.931859	-0.179337	-1.199501
H	-1.598116	2.198908	1.645816
H	-0.008775	2.949972	0.353266
H	-0.778664	1.906386	-3.340735
H	1.001658	1.973610	-3.176426
H	0.109862	3.323938	-3.896350
H	-1.555520	4.491447	-0.717880
H	-2.266632	3.285960	-1.816784
H	-1.478772	4.735641	-2.477979
H	0.974479	5.038272	-2.396278
H	2.051134	3.814663	-1.690451
H	1.010184	4.803339	-0.635591
H	0.901930	-0.067462	-1.803206
H	5.602006	-0.653490	-0.793634
H	2.116736	2.919187	1.063888
H	-1.119038	0.270096	-2.186136
H	-4.653571	-1.568080	1.325595
Cl	4.730583	2.101640	1.652259
Cl	-3.175323	-1.591931	-2.148435

11-conf09

- Electronic Energy (Eh): -7737.93419918

- Cartesian Coordinates:

Br	4.007116	1.097798	-2.603726
C	3.076176	0.712550	-1.005960
C	1.937493	1.447526	-0.694710
C	1.227500	1.209288	0.485690
C	0.002674	2.067405	0.771493
C	0.090292	2.963201	2.062832
C	1.411217	3.744059	2.011823
C	-1.078312	3.960284	2.030027
C	0.017667	2.180792	3.380065
C	-1.305105	1.300341	0.625809
C	-2.296177	1.819807	-0.212153
C	-3.509366	1.160813	-0.375778
Br	-4.804231	1.901041	-1.535862
C	-3.791719	-0.034120	0.298565
N	-5.021472	-0.698167	0.127685
C	-5.115177	-1.915020	-0.483395
C	-6.566051	-2.447823	-0.563532
F	-7.465598	-1.455531	-0.459532
F	-6.766749	-3.068126	-1.711003
F	-6.788827	-3.300838	0.430689
O	-4.200936	-2.575626	-0.894139
C	-2.799142	-0.537786	1.152038
C	-1.575858	0.107923	1.300543
C	1.683940	0.190952	1.327568
C	2.811155	-0.557003	1.003502
C	3.544849	-0.303865	-0.164436
N	4.702455	-1.040994	-0.479549
C	5.848734	-0.939410	0.252929
C	6.999739	-1.826290	-0.279387
F	6.792146	-2.201320	-1.552055
F	7.098002	-2.927353	0.456769
F	8.146074	-1.172749	-0.224385
O	6.000223	-0.280132	1.245122
H	1.608805	2.228925	-1.381694
H	-0.012704	2.804967	-0.044857
H	1.469865	4.448693	2.855215
H	1.495658	4.327615	1.080955
H	2.283424	3.076380	2.071537
H	-2.051475	3.454222	2.116075
H	-1.081671	4.548324	1.098171
H	-0.995045	4.667699	2.868829
H	-0.006627	2.888566	4.222716
H	0.894881	1.537724	3.535074
H	-0.892231	1.566061	3.446611
H	-2.120567	2.749371	-0.755709
H	-5.872523	-0.159595	0.245689
H	-0.845253	-0.347933	1.964970
H	1.174801	-0.052970	2.256825
H	4.756520	-1.477838	-1.393139
Cl	-3.099422	-1.970365	2.078623
Cl	3.282326	-1.846569	2.059490

11-conf10

- Electronic Energy (Eh): -7737.9333905

- Cartesian Coordinates:

Br	2.794311	-1.151970	2.313848
C	2.619624	0.057526	0.871937
C	1.457641	0.813982	0.770089
C	1.285435	1.711375	-0.286924
C	0.042905	2.578520	-0.448093
C	0.082112	3.917817	0.379154
C	-1.199397	4.706852	0.076120
C	0.211588	3.719585	1.895254
C	1.290582	4.738927	-0.098152
C	-1.246152	1.774139	-0.350128

C	-1.764718	1.269535	0.847111
C	-2.934698	0.518379	0.851535
Br	-3.575372	-0.153087	2.498273
C	-3.649623	0.253390	-0.323933
N	-4.835296	-0.504800	-0.303491
C	-4.932368	-1.728841	-0.900825
C	-6.328574	-2.376882	-0.739251
F	-6.214074	-3.677797	-0.549600
F	-6.998779	-1.857966	0.303256
F	-7.053897	-2.163999	-1.832002
O	-4.076983	-2.277805	-1.538830
C	-3.138203	0.785748	-1.516031
C	-1.954672	1.517430	-1.526365
C	2.314373	1.827691	-1.224182
C	3.486638	1.087919	-1.105988
C	3.661011	0.171173	-0.059306
N	4.832372	-0.600456	0.057973
C	5.174571	-1.557510	-0.853969
C	6.494370	-2.286975	-0.505368
F	6.792231	-2.177863	0.800164
F	7.498893	-1.755772	-1.194423
F	6.404695	-3.569648	-0.802242
O	4.583123	-1.820692	-1.864473
H	0.681015	0.670994	1.518837
H	0.072833	2.924221	-1.492261
H	-1.165846	5.691457	0.566938
H	-2.096937	4.182561	0.435940
H	-1.318430	4.875173	-1.006222
H	1.075845	3.090886	2.156454
H	-0.692053	3.283878	2.342966
H	0.360877	4.696776	2.379429
H	1.292361	5.725537	0.389269
H	1.261354	4.906108	-1.186757
H	2.243545	4.246130	0.144991
H	-1.267877	1.447716	1.797869
H	-5.550152	-0.248979	0.368742
H	-1.593799	1.902763	-2.481205
H	2.221232	2.519908	-2.062120
H	5.293883	-0.623848	0.960741
Cl	-4.003017	0.577217	-3.000963
Cl	4.755625	1.348619	-2.255231

11-conf11

- Electronic Energy (Eh): -7737.93317322

- Cartesian Coordinates:

Br	3.818484	-0.223888	2.541910
C	3.080741	0.455903	0.939818
C	1.881424	1.156519	1.001902
C	1.292767	1.666097	-0.160354
C	-0.027074	2.424648	-0.184302
C	-0.059498	3.762938	0.645047
C	1.164143	4.601165	0.248865
C	-1.331596	4.534386	0.259767
C	-0.065043	3.562014	2.166091
C	-1.231665	1.520284	0.044727
C	-2.307520	1.598554	-0.843885
C	-3.453260	0.828275	-0.666765
Br	-4.895608	1.072122	-1.852350
C	-3.549678	-0.082918	0.393309
N	-4.682261	-0.896623	0.589136
C	-5.008732	-1.912670	-0.262934
C	-6.278102	-2.684323	0.171162
F	-6.511303	-2.552240	1.487768
F	-7.337476	-2.209909	-0.476044
F	-6.153206	-3.969652	-0.099224
O	-4.445828	-2.191573	-1.285527
C	-2.462143	-0.158230	1.274595
C	-1.327843	0.628097	1.115219
C	1.960633	1.465257	-1.370737

C	3.172914	0.784583	-1.427005
C	3.756187	0.248541	-0.270104
N	4.973162	-0.457118	-0.316442
C	5.096897	-1.663266	-0.944405
C	6.525149	-2.253123	-0.856926
F	7.188106	-1.997227	-1.979503
F	6.474219	-3.559958	-0.679691
F	7.221934	-1.718603	0.159942
O	4.239024	-2.236115	-1.557640
H	1.418013	1.291524	1.976315
H	-0.127681	2.769187	-1.224371
H	1.130849	5.582711	0.745767
H	1.193710	4.776444	-0.838512
H	2.105754	4.110667	0.536725
H	-2.243645	4.004918	0.572669
H	-1.390409	4.699610	-0.827925
H	-1.335802	5.521503	0.746165
H	-0.214523	4.533399	2.661774
H	0.886946	3.162054	2.541310
H	-0.882000	2.901272	2.492353
H	-2.266140	2.288445	-1.688013
H	-5.091911	-0.914019	1.516658
H	-0.519622	0.507537	1.833502
H	1.544258	1.856368	-2.300277
H	5.704312	-0.183806	0.330928
Cl	-2.541270	-1.265662	2.614078
Cl	3.982016	0.646462	-2.951192

11-conf12

- Electronic Energy (Eh): -7737.93339566

- Cartesian Coordinates:

Br	3.741574	0.304203	-2.906788
C	2.981125	0.747973	-1.235393
C	1.844687	1.548199	-1.203369
C	1.238299	1.887208	0.009730
C	-0.045357	2.706123	-0.040483
C	-0.139636	3.959691	0.906759
C	-0.478779	3.626537	2.366671
C	1.187763	4.728337	0.841736
C	-1.256220	4.870064	0.368106
C	-1.268729	1.799853	0.014541
C	-1.406467	0.793699	0.974195
C	-2.539695	-0.010275	0.993278
Br	-2.672820	-1.368567	2.299885
C	-3.583064	0.161729	0.071836
N	-4.723463	-0.663089	0.099634
C	-5.021712	-1.534131	-0.908505
C	-6.310011	-2.351406	-0.648282
F	-6.155855	-3.597038	-1.056715
F	-6.629768	-2.374092	0.656207
F	-7.329297	-1.807499	-1.304826
O	-4.416078	-1.666732	-1.936292
C	-3.443145	1.187602	-0.873289
C	-2.298600	1.978691	-0.910356
C	1.827567	1.420014	1.187174
C	2.980205	0.641362	1.153802
C	3.575285	0.269553	-0.060190
N	4.725115	-0.541352	-0.099441
C	4.713487	-1.844976	0.306094
C	6.085533	-2.544580	0.153865
F	6.716288	-2.559489	1.323299
F	6.873530	-1.906520	-0.727316
F	5.925397	-3.787423	-0.260357
O	3.781884	-2.432052	0.783700
H	1.416367	1.896746	-2.144631
H	-0.052525	3.144010	-1.050083
H	-0.587491	4.561248	2.937704
H	0.301623	3.040534	2.870164
H	-1.428282	3.077856	2.449942

H	1.463287	4.958048	-0.199955
H	2.016457	4.161759	1.289770
H	1.101729	5.682078	1.384382
H	-1.317814	5.789892	0.969006
H	-2.240402	4.380321	0.411539
H	-1.066684	5.166348	-0.675965
H	-0.620509	0.608479	1.705584
H	-5.186280	-0.798745	0.991826
H	-2.227947	2.755616	-1.672934
H	1.418276	1.667120	2.164021
H	5.505333	-0.230229	-0.667736
Cl	-4.720524	1.517889	-1.995540
Cl	3.703030	0.167637	2.655436

11-conf13

- Electronic Energy (Eh): -7737.93318745

- Cartesian Coordinates:

Br	3.779499	0.360488	-2.853135
C	3.049524	0.731200	-1.150625
C	1.875731	1.471805	-1.067315
C	1.291324	1.755657	0.170407
C	-0.027810	2.517121	0.178452
C	-0.121167	3.777687	1.117182
C	-1.308795	4.630581	0.640414
C	-0.351614	3.448355	2.598749
C	1.164544	4.601989	0.961718
C	-1.211661	1.566794	0.304485
C	-2.293471	1.702530	-0.568358
C	-3.410776	0.877492	-0.467657
Br	-4.868479	1.189912	-1.618161
C	-3.467550	-0.141040	0.492451
N	-4.568769	-1.011897	0.604482
C	-4.860867	-1.945859	-0.347854
C	-6.095437	-2.809516	0.005944
F	-5.919554	-4.053897	-0.396014
F	-6.327353	-2.823917	1.329059
F	-7.176563	-2.314930	-0.588297
O	-4.294483	-2.094019	-1.395711
C	-2.372434	-0.270220	1.359443
C	-1.266953	0.566223	1.277466
C	1.939377	1.294647	1.319324
C	3.127802	0.576099	1.234664
C	3.703270	0.260300	-0.004533
N	4.891990	-0.487805	-0.096229
C	4.961440	-1.798421	0.280335
C	6.363127	-2.420690	0.071972
F	7.032689	-2.417820	1.219808
F	7.085909	-1.728743	-0.824255
F	6.255889	-3.664364	-0.356290
O	4.077206	-2.443601	0.772737
H	1.401984	1.817754	-1.987517
H	-0.104826	2.943573	-0.833044
H	-1.371966	5.556072	1.232377
H	-2.265691	4.099529	0.753050
H	-1.199771	4.918665	-0.417373
H	0.491894	2.916962	3.059313
H	-1.261258	2.848204	2.747012
H	-0.479193	4.384053	3.164227
H	1.073285	5.555185	1.504463
H	1.361650	4.835513	-0.096805
H	2.043779	4.073689	1.357477
H	-2.279291	2.475946	-1.337778
H	-4.969187	-1.142913	1.526966
H	-0.443995	0.405478	1.972585
H	1.548968	1.501096	2.313192
H	5.635057	-0.124487	-0.683066
Cl	-2.406289	-1.512312	2.576229
Cl	3.919451	0.109207	2.703197

11-conf14

- Electronic Energy (Eh): -7737.92998291

- Cartesian Coordinates:

Br	3.278201	-2.265077	1.131504
C	2.739851	-0.572476	0.486624
C	1.489852	-0.084982	0.851929
C	1.058901	1.171372	0.412498
C	-0.283970	1.787766	0.778134
C	-0.510120	2.064966	2.312351
C	-0.676531	0.800062	3.164260
C	0.691010	2.868697	2.830083
C	-1.781211	2.915485	2.463500
C	-1.463104	1.105193	0.098819
C	-1.687509	-0.273023	0.154780
C	-2.822013	-0.832108	-0.424136
Br	-3.062760	-2.698686	-0.328856
C	-3.776921	-0.040525	-1.077493
N	-4.947660	-0.597742	-1.639797
C	-6.178318	-0.726312	-1.063932
C	-6.303051	-0.257487	0.413930
F	-6.023090	1.043178	0.537263
F	-7.531886	-0.459363	0.842586
F	-5.464249	-0.929917	1.206629
O	-7.134898	-1.181315	-1.632266
C	-3.514325	1.333803	-1.173138
C	-2.382700	1.896392	-0.594763
C	1.912580	1.899172	-0.420342
C	3.153677	1.399470	-0.801865
C	3.604290	0.153938	-0.342674
N	4.870844	-0.347515	-0.699022
C	6.028471	0.225179	-0.258587
C	7.301184	-0.498071	-0.760551
F	7.822337	0.166179	-1.785824
F	7.032730	-1.746966	-1.175508
F	8.200340	-0.568571	0.203803
O	6.118406	1.214807	0.415248
H	0.873449	-0.698355	1.504762
H	-0.252685	2.797211	0.341669
H	0.251579	0.216264	3.234628
H	-1.481584	0.150218	2.789922
H	-0.945323	1.087649	4.192075
H	0.829142	3.798140	2.254741
H	1.626144	2.292448	2.768713
H	0.536988	3.147045	3.883631
H	-1.905917	3.221281	3.513109
H	-2.685177	2.361716	2.168951
H	-1.729656	3.832414	1.854704
H	-0.982398	-0.937922	0.648400
H	-4.917482	-0.922690	-2.602622
H	-2.230473	2.972937	-0.682338
H	1.611383	2.877938	-0.796793
H	4.921363	-1.278974	-1.096721
Cl	-4.618285	2.355354	-2.033831
Cl	4.129107	2.327192	-1.890798

11-conf15

- Electronic Energy (Eh): -7737.929925689999

- Cartesian Coordinates:

Br	-4.578921	-2.543749	-0.975649
C	-3.288891	-1.307444	-0.361952
C	-2.037141	-1.774380	0.022792
C	-1.059947	-0.896932	0.502177
C	0.271234	-1.475834	0.962258
C	0.400559	-1.643073	2.522876
C	1.733104	-2.347479	2.816437
C	0.346138	-0.324675	3.304461
C	-0.753158	-2.537323	3.001922
C	1.475391	-0.839915	0.282701

C	1.897122	0.474025	0.512905
C	3.030673	0.978539	-0.115479
Br	3.532217	2.763362	0.221008
C	3.794939	0.193878	-0.990743
N	4.962179	0.693012	-1.611761
C	6.254526	0.593415	-1.183952
C	6.479494	-0.117620	0.180827
F	6.069482	-1.388066	0.138088
F	7.761352	-0.105051	0.483064
F	5.809252	0.492366	1.162204
O	7.193397	1.024590	-1.798503
C	3.341163	-1.108018	-1.245629
C	2.209146	-1.616150	-0.618109
C	-1.366611	0.465124	0.544510
C	-2.611986	0.932284	0.136803
C	-3.611079	0.054581	-0.308646
N	-4.882236	0.522443	-0.692766
C	-5.759104	1.060569	0.203786
C	-7.097910	1.499185	-0.436508
F	-8.106053	1.223292	0.369632
F	-7.314905	0.878538	-1.607723
F	-7.079306	2.807086	-0.668941
O	-5.554786	1.244603	1.372515
H	-1.829977	-2.843923	-0.036457
H	0.265919	-2.513885	0.597897
H	2.596037	-1.731146	2.522835
H	1.822561	-2.557745	3.892949
H	1.805979	-3.307618	2.280631
H	-0.571192	0.244773	3.094093
H	1.218062	0.314814	3.108632
H	0.350644	-0.542024	4.383401
H	-0.638204	-2.759816	4.073405
H	-0.770333	-3.498145	2.462719
H	-1.731415	-2.052759	2.865659
H	1.361466	1.127070	1.197289
H	4.870226	1.168185	-2.505814
H	1.906136	-2.640739	-0.838343
H	-0.641180	1.202765	0.879587
H	-5.240521	0.240755	-1.598659
Cl	4.201133	-2.107014	-2.370377
Cl	-2.904217	2.639439	0.151828

11-conf16

- Electronic Energy (Eh): -7737.92997275

- Cartesian Coordinates:

Br	3.519876	-2.584508	0.363715
C	2.880813	-0.808926	0.267004
C	1.615148	-0.525955	0.768618
C	1.109858	0.778107	0.733208
C	-0.254417	1.177998	1.276945
C	-0.448263	0.984797	2.828316
C	-1.761621	1.670523	3.236330
C	-0.511970	-0.480597	3.277246
C	0.719509	1.680853	3.541459
C	-1.413905	0.650440	0.443407
C	-2.391115	1.554045	0.014385
C	-3.508170	1.120511	-0.691039
Br	-4.781460	2.389714	-1.253728
C	-3.694784	-0.235376	-0.994212
N	-4.838519	-0.692474	-1.687184
C	-6.010774	-1.156853	-1.164895
C	-6.127156	-1.153394	0.386057
F	-5.958929	0.074838	0.883954
F	-7.318246	-1.586825	0.743914
F	-5.206346	-1.946003	0.941347
O	-6.927314	-1.552033	-1.834915
C	-2.683249	-1.125152	-0.603927
C	-1.566269	-0.695799	0.104086
C	1.906828	1.771044	0.157835

C	3.164533	1.481205	-0.361531
C	3.688673	0.182243	-0.305263
N	4.972216	-0.114894	-0.802130
C	6.106759	0.358929	-0.210422
C	7.405440	-0.102774	-0.914039
F	7.875716	0.875139	-1.679716
F	7.192984	-1.171696	-1.699063
F	8.322840	-0.423912	-0.020241
O	6.158234	1.096848	0.735293
H	1.045617	-1.341873	1.206955
H	-0.292239	2.270469	1.152490
H	-2.640164	1.169493	2.803058
H	-1.781767	2.726149	2.921265
H	-1.872494	1.649105	4.330871
H	0.449489	-0.998384	3.155531
H	-1.292963	-1.044030	2.745146
H	-0.757950	-0.521492	4.349246
H	0.582230	1.632715	4.632320
H	0.785441	2.743722	3.258743
H	1.684237	1.208519	3.303642
H	-2.289056	2.616085	0.241871
H	-4.814384	-0.713583	-2.703315
H	-0.822657	-1.441015	0.376724
H	1.547113	2.799360	0.098158
H	5.063794	-0.873278	-1.469051
Cl	-2.819034	-2.803130	-1.017219
Cl	4.069067	2.749000	-1.118084

11-conf17

- Electronic Energy (Eh): -7737.9299322

- Cartesian Coordinates:

Br	4.215359	2.635499	-0.856615
C	3.158706	1.221110	-0.184766
C	1.900893	1.506670	0.334813
C	1.092005	0.494127	0.859280
C	-0.265673	0.883482	1.426674
C	-0.485307	0.563361	2.953368
C	-0.634443	-0.930414	3.269386
C	0.708826	1.130501	3.733812
C	-1.765411	1.279644	3.412165
C	-1.426811	0.458454	0.538734
C	-2.387982	1.412945	0.192334
C	-3.503929	1.064949	-0.560716
Br	-4.754817	2.400487	-1.008823
C	-3.705236	-0.252617	-0.994932
N	-4.848479	-0.624770	-1.737824
C	-6.032658	-1.118178	-1.272113
C	-6.166274	-1.256694	0.271251
F	-5.990626	-0.081712	0.882263
F	-7.365980	-1.707240	0.575180
F	-5.260483	-2.107944	0.760341
O	-6.947155	-1.435859	-1.984795
C	-2.708828	-1.190020	-0.684784
C	-1.592579	-0.846465	0.069539
C	1.578502	-0.815912	0.819462
C	2.828105	-1.101763	0.278881
C	3.656690	-0.087349	-0.222079
N	4.933525	-0.370628	-0.743080
C	5.956469	-0.815423	0.043127
C	7.274436	-1.045128	-0.734741
F	7.279675	-0.393089	-1.908931
F	7.427594	-2.339582	-0.989453
F	8.305640	-0.624612	-0.025336
O	5.892806	-1.064278	1.215948
H	1.554501	2.541378	0.342084
H	-0.273350	1.983316	1.395638
H	-0.894639	-1.052405	4.331806
H	0.297422	-1.489683	3.109103
H	-1.438887	-1.399400	2.683382

H	0.837186	2.207869	3.541566
H	1.649136	0.625623	3.467122
H	0.553129	0.999697	4.815373
H	-1.892234	1.163348	4.498951
H	-2.663601	0.869111	2.927117
H	-1.724626	2.359411	3.196392
H	-2.274109	2.446402	0.522571
H	-4.812362	-0.555769	-2.751466
H	-0.859180	-1.623033	0.275204
H	0.998983	-1.651230	1.205167
H	5.161738	-0.013246	-1.664256
Cl	-2.863450	-2.818108	-1.259270
Cl	3.337689	-2.755193	0.198854

11-conf18

- Electronic Energy (Eh): -7737.92969221

- Cartesian Coordinates:

Br	-2.277351	-1.757365	-1.720265
C	-2.148651	-0.299401	-0.525668
C	-1.022701	0.513753	-0.578249
C	-0.903040	1.613166	0.275449
C	0.285626	2.564214	0.218767
C	0.127003	3.716424	-0.842517
C	-1.035960	4.613990	-0.387560
C	1.415211	4.551306	-0.852611
C	-0.188911	3.232112	-2.264659
C	1.601614	1.798176	0.219125
C	2.158535	1.199790	-0.915680
C	3.335435	0.463622	-0.827819
Br	4.049908	-0.291002	-2.399857
C	3.999789	0.285426	0.393779
N	5.189349	-0.471486	0.490986
C	5.329234	-1.794513	0.796865
C	4.015944	-2.595087	1.024483
F	3.228444	-2.548894	-0.053152
F	4.301308	-3.855972	1.277023
F	3.323740	-2.105138	2.056003
O	6.393437	-2.346232	0.887411
C	3.451745	0.918450	1.518839
C	2.275072	1.654613	1.434865
C	-1.918788	1.843084	1.205198
C	-3.034205	1.013793	1.270069
C	-3.183613	-0.068254	0.391121
N	-4.322283	-0.895488	0.432215
C	-5.560886	-0.443340	0.081894
C	-6.662640	-1.524461	0.191606
F	-7.504096	-1.427992	-0.821340
F	-7.336490	-1.367579	1.325679
F	-6.145543	-2.763775	0.190690
O	-5.841078	0.678177	-0.243206
H	-0.241143	0.277120	-1.298858
H	0.277078	3.097803	1.181139
H	-1.135761	5.475236	-1.065053
H	-0.869199	5.007182	0.628068
H	-1.995655	4.076251	-0.393588
H	2.273061	3.981119	-1.237635
H	1.671129	4.901146	0.160332
H	1.288446	5.438271	-1.491769
H	-0.371018	4.103232	-2.912245
H	-1.094159	2.608331	-2.294140
H	0.636146	2.670578	-2.723260
H	1.688329	1.300591	-1.891003
H	6.077250	0.003139	0.349765
H	1.882694	2.117688	2.341494
H	-1.848199	2.676163	1.905998
H	-4.181348	-1.897780	0.496186
Cl	4.261781	0.795508	3.045454
Cl	-4.226879	1.313492	2.489539

11-conf19

- Electronic Energy (Eh): -7737.929781130001

- Cartesian Coordinates:

Br	-2.362792	-1.797798	-1.699325
C	-2.198321	-0.325221	-0.527078
C	-1.063934	0.474281	-0.610262
C	-0.916362	1.584077	0.225411
C	0.277677	2.526789	0.143327
C	0.122743	3.662962	-0.935674
C	-0.107953	3.154760	-2.365488
C	-1.086639	4.526428	-0.541372
C	1.384632	4.536356	-0.898905
C	1.598254	1.769360	0.147233
C	2.113702	1.092712	-0.963416
C	3.307326	0.384125	-0.875321
Br	3.963080	-0.477393	-2.417712
C	4.031006	0.311698	0.323340
N	5.240537	-0.412953	0.420354
C	5.425333	-1.706566	0.815241
C	4.143352	-2.513438	1.165297
F	4.469558	-3.745799	1.496848
F	3.489275	-1.960612	2.189849
F	3.305380	-2.564070	0.126668
O	6.505224	-2.228848	0.893827
C	3.522232	1.019735	1.421732
C	2.328831	1.728693	1.337516
C	-1.914905	1.837359	1.168354
C	-3.038445	1.022763	1.263717
C	-3.215075	-0.069939	0.402962
N	-4.362106	-0.883414	0.474651
C	-5.600902	-0.422186	0.137030
C	-6.713173	-1.488769	0.278807
F	-7.567838	-1.397619	-0.723536
F	-7.368916	-1.307180	1.419768
F	-6.210405	-2.733900	0.289220
O	-5.873238	0.697719	-0.200039
H	-0.299601	0.215195	-1.340768
H	0.273000	3.078179	1.095584
H	-0.331489	4.008988	-3.022526
H	-0.963478	2.466024	-2.425646
H	0.775835	2.659242	-2.789797
H	-0.986545	4.918759	0.483341
H	-2.030102	3.963954	-0.601104
H	-1.171283	5.388474	-1.219911
H	1.269024	5.400869	-1.570122
H	2.277708	3.980062	-1.219745
H	1.573767	4.922214	0.115695
H	1.597971	1.109807	-1.920542
H	6.109711	0.066738	0.201144
H	1.970331	2.254555	2.223637
H	-1.824183	2.679618	1.855648
H	-4.231266	-1.886074	0.552237
Cl	4.402941	1.026959	2.913782
Cl	-4.207302	1.353946	2.497969

11-conf20

- Electronic Energy (Eh): -7737.92964981

- Cartesian Coordinates:

Br	-4.344934	1.430074	2.200877
C	-3.005620	0.940135	0.961868
C	-1.883163	1.749677	0.826903
C	-0.879974	1.433062	-0.093248
C	0.302768	2.381132	-0.245090
C	0.153630	3.407863	-1.429339
C	-0.001499	2.762940	-2.813063
C	-1.095918	4.261629	-1.160346
C	1.386672	4.322297	-1.427920
C	1.637652	1.655579	-0.149431

C	2.164505	0.852593	-1.166849
C	3.376525	0.191498	-0.997067
Br	4.047366	-0.846779	-2.419143
C	4.108195	0.294712	0.194604
N	5.337679	-0.378749	0.374325
C	5.560801	-1.602353	0.937011
C	4.303362	-2.391448	1.398690
F	4.665255	-3.561238	1.884158
F	3.639284	-1.728200	2.348770
F	3.462230	-2.598385	0.382589
O	6.655611	-2.078433	1.078034
C	3.586592	1.126272	1.195996
C	2.374743	1.787911	1.030204
C	-1.017041	0.260981	-0.839720
C	-2.130761	-0.558082	-0.686833
C	-3.161774	-0.228068	0.205167
N	-4.303481	-1.041284	0.339819
C	-5.222683	-1.170870	-0.659781
C	-6.399839	-2.106720	-0.294770
F	-6.205324	-3.306178	-0.831146
F	-7.536950	-1.614502	-0.751162
F	-6.515333	-2.266038	1.033770
O	-5.159798	-0.671370	-1.749987
H	-1.801329	2.649223	1.438773
H	0.271934	3.020612	0.649822
H	-0.222244	3.544973	-3.555414
H	-0.832846	2.043297	-2.843352
H	0.915314	2.261501	-3.151876
H	-1.048852	4.747375	-0.172425
H	-2.018148	3.663475	-1.203239
H	-1.179908	5.055934	-1.917170
H	1.274578	5.113951	-2.184236
H	2.307887	3.766857	-1.658236
H	1.521987	4.810057	-0.449168
H	1.644196	0.731617	-2.113955
H	6.192125	0.091899	0.087957
H	2.007642	2.416278	1.843003
H	-0.250214	-0.056189	-1.543736
H	-4.560249	-1.355366	1.269151
Cl	4.474361	1.350758	2.666884
Cl	-2.211915	-2.029331	-1.596572

11-conf21

- Electronic Energy (Eh): -7737.9295986100005

- Cartesian Coordinates:

Br	3.342747	-1.016561	2.351423
C	2.646833	-0.064721	0.874995
C	1.477377	0.668445	1.043272
C	0.938258	1.402609	-0.018186
C	-0.323701	2.248267	0.086016
C	-0.221244	3.495636	1.040155
C	1.020100	4.302295	0.633090
C	-1.471767	4.361862	0.826042
C	-0.123880	3.145612	2.530056
C	-1.585418	1.414921	0.267929
C	-2.627777	1.577675	-0.649832
C	-3.807888	0.850735	-0.533254
Br	-5.186496	1.143867	-1.783063
C	-3.989214	-0.080039	0.499163
N	-5.181203	-0.828899	0.626139
C	-5.459573	-2.072918	0.137914
C	-4.345165	-2.750253	-0.708270
F	-3.239473	-2.942828	0.015332
F	-4.765830	-3.920132	-1.143748
F	-4.016307	-2.000973	-1.763445
O	-6.501390	-2.642231	0.327025
C	-2.946667	-0.218381	1.427597
C	-1.764959	0.505495	1.313283
C	1.597407	1.351121	-1.248854

C	2.755743	0.599828	-1.420137
C	3.317434	-0.116380	-0.354000
N	4.503488	-0.858830	-0.510504
C	5.709803	-0.261934	-0.734103
C	6.877558	-1.268781	-0.866058
F	6.568020	-2.461947	-0.333013
F	7.952440	-0.809369	-0.252024
F	7.164752	-1.460326	-2.148659
O	5.904522	0.915234	-0.868604
H	1.012210	0.667614	2.025980
H	-0.432104	2.703467	-0.909508
H	1.082248	5.228954	1.223522
H	0.983573	4.585154	-0.431139
H	1.948340	3.735646	0.799117
H	-2.387818	3.846249	1.151160
H	-1.595259	4.637760	-0.233494
H	-1.389920	5.294145	1.404909
H	-0.128635	4.073474	3.122205
H	0.808933	2.619205	2.775929
H	-0.977194	2.540980	2.871116
H	-2.523479	2.286596	-1.472526
H	-5.944782	-0.431729	1.167238
H	-0.994158	0.333773	2.060749
H	1.203735	1.897102	-2.107467
H	4.498367	-1.832819	-0.228032
Cl	-3.135614	-1.305559	2.764551
Cl	3.481151	0.529231	-2.990436

11-conf22

- Electronic Energy (Eh): -7737.9296587

- Cartesian Coordinates:

Br	-4.339828	1.423936	2.206788
C	-3.003486	0.936599	0.963615
C	-1.881048	1.746059	0.828007
C	-0.879962	1.431220	-0.095046
C	0.302822	2.379248	-0.246765
C	0.153978	3.406487	-1.430516
C	0.002922	2.762387	-2.815048
C	-1.097562	4.257799	-1.163192
C	1.385540	4.322901	-1.426098
C	1.637875	1.653973	-0.151307
C	2.163498	0.848990	-1.167792
C	3.375921	0.188557	-0.998294
Br	4.044995	-0.852662	-2.419044
C	4.109278	0.294515	0.192102
N	5.339180	-0.378272	0.371530
C	5.563390	-1.600525	0.936702
C	4.306786	-2.388770	1.402018
F	4.669568	-3.557315	1.889797
F	3.643780	-1.723436	2.351398
F	3.464401	-2.598294	0.387479
O	6.658481	-2.076187	1.077011
C	3.588892	1.128068	1.192458
C	2.376600	1.788985	1.026996
C	-1.019226	0.261054	-0.844152
C	-2.133070	-0.557781	-0.690908
C	-3.161772	-0.229663	0.204401
N	-4.303636	-1.042648	0.339524
C	-5.226154	-1.167065	-0.657490
C	-6.405441	-2.100287	-0.292696
F	-6.502403	-2.285812	1.033888
F	-6.230247	-3.289814	-0.856593
F	-7.545146	-1.588635	-0.721200
O	-5.166063	-0.663350	-1.745964
H	-1.797561	2.644178	1.441755
H	0.271874	3.018448	0.648341
H	-0.217226	3.544676	-3.557308
H	-0.827393	2.041670	-2.847900
H	0.921318	2.262547	-3.151965

H	-1.053213	4.742822	-0.174788
H	-2.018630	3.658002	-1.208205
H	-1.181579	5.052561	-1.919535
H	1.273876	5.114579	-2.182450
H	2.308119	3.768925	-1.654535
H	1.517930	4.810621	-0.446923
H	1.641970	0.725888	-2.113953
H	6.193048	0.091614	0.082201
H	2.010491	2.418979	1.838984
H	-0.254240	-0.054719	-1.550762
H	-4.556332	-1.362774	1.267886
Cl	4.478680	1.355963	2.661596
Cl	-2.217488	-2.026354	-1.604683

11-conf23

- Electronic Energy (Eh): -7737.92961432

- Cartesian Coordinates:

Br	4.104923	1.518936	-2.263986
C	2.915225	0.953942	-0.909719
C	1.775912	1.709493	-0.655207
C	0.881005	1.336337	0.351207
C	-0.323904	2.225612	0.629210
C	-0.121555	3.223111	1.830007
C	0.176008	2.545901	3.174197
C	1.063456	4.139879	1.486906
C	-1.388966	4.079501	1.959465
C	-1.630876	1.444894	0.617212
C	-2.471399	1.589511	-0.490787
C	-3.665866	0.882632	-0.585898
Br	-4.766354	1.150134	-2.091085
C	-4.065964	-0.007030	0.420490
N	-5.274318	-0.735025	0.334789
C	-5.474251	-1.994503	-0.152455
C	-4.228411	-2.715413	-0.739858
F	-4.574316	-3.901839	-1.195703
F	-3.695801	-2.016197	-1.745132
F	-3.282418	-2.879948	0.188158
O	-6.543082	-2.544720	-0.150904
C	-3.231550	-0.121607	1.542324
C	-2.036258	0.582000	1.640110
C	1.142401	0.164216	1.063803
C	2.272342	-0.600248	0.793208
C	3.195844	-0.213897	-0.189449
N	4.354514	-0.972025	-0.446352
C	5.374523	-1.063383	0.454465
C	6.555107	-1.934717	-0.037195
F	6.522120	-2.114807	-1.367663
F	6.501430	-3.131507	0.535425
F	7.705776	-1.364701	0.272495
O	5.397721	-0.574562	1.551131
H	1.595194	2.611320	-1.242018
H	-0.393429	2.891665	-0.243754
H	0.406189	3.316238	3.925860
H	1.048276	1.878346	3.116320
H	-0.681080	1.978005	3.561176
H	0.911020	4.654402	0.524538
H	2.009801	3.581866	1.429524
H	1.179843	4.912373	2.261813
H	-1.247788	4.855183	2.727356
H	-2.262250	3.476328	2.248891
H	-1.628200	4.586229	1.010705
H	-2.193283	2.265896	-1.300540
H	-6.121255	-0.309074	0.702068
H	-1.440248	0.441548	2.538655
H	0.463064	-0.194585	1.834424
H	4.529111	-1.272144	-1.399038
Cl	-3.703509	-1.153625	2.852536
Cl	2.509895	-2.073659	1.671592

11-conf24

- Electronic Energy (Eh): -7737.929676850001

- Cartesian Coordinates:

Br	-3.161974	-2.121234	-1.416967
C	-2.743368	-0.382415	-0.806428
C	-1.451590	0.098312	-0.989959
C	-1.097474	1.373931	-0.541629
C	0.294982	1.968079	-0.708999
C	0.593700	2.541540	-2.144465
C	0.564638	1.491442	-3.261847
C	-0.463608	3.611048	-2.457879
C	1.978743	3.203983	-2.113626
C	1.395202	1.093451	-0.124567
C	1.782827	-0.137222	-0.665312
C	2.819541	-0.869841	-0.097340
Br	3.275709	-2.532035	-0.858815
C	3.518907	-0.402972	1.024520
N	4.587950	-1.132518	1.592105
C	5.922328	-1.017966	1.329327
C	6.327174	0.010962	0.235663
F	7.632602	-0.014423	0.062217
F	5.741845	-0.266378	-0.932804
F	5.972502	1.250930	0.582809
O	6.768161	-1.663637	1.888555
C	3.098270	0.813233	1.581090
C	2.061937	1.548218	1.015922
C	-2.082326	2.147325	0.077812
C	-3.380051	1.672874	0.239255
C	-3.738105	0.386229	-0.187351
N	-5.041090	-0.114416	-0.003311
C	-5.549334	-0.385422	1.234028
C	-6.990985	-0.947022	1.195552
F	-7.127445	-1.922859	2.074454
F	-7.305247	-1.429349	-0.018113
F	-7.858297	0.016243	1.485334
O	-5.002249	-0.190577	2.284658
H	-0.726686	-0.552678	-1.473022
H	0.292331	2.866987	-0.074905
H	0.697652	1.990973	-4.233620
H	-0.395439	0.955864	-3.302125
H	1.378898	0.759240	-3.170099
H	-0.491790	4.391214	-1.680381
H	-1.471695	3.178214	-2.541059
H	-0.231605	4.103278	-3.414340
H	2.187813	3.693335	-3.076953
H	2.779012	2.471817	-1.929011
H	2.037634	3.973599	-1.327306
H	1.295986	-0.545573	-1.547389
H	4.377434	-1.816957	2.313878
H	1.780261	2.494641	1.479634
H	-1.850392	3.151980	0.434205
H	-5.519736	-0.503697	-0.808107
Cl	3.877132	1.413813	3.007219
Cl	-4.568178	2.715619	0.946195

11-conf25

- Electronic Energy (Eh): -7737.92974334

- Cartesian Coordinates:

Br	3.362300	-1.395305	2.167134
C	2.796626	0.014204	1.042387
C	1.511774	0.521260	1.202425
C	1.045796	1.553201	0.380882
C	-0.355677	2.141877	0.462313
C	-0.748046	2.804239	1.836324
C	-0.960913	1.806611	2.982447
C	0.362598	3.791064	2.222378
C	-2.057041	3.584073	1.633910
C	-1.421386	1.206073	-0.091718

C	-1.556887	-0.122902	0.318136
C	-2.592162	-0.913874	-0.168695
Br	-2.716676	-2.702441	0.410459
C	-3.531152	-0.411005	-1.080401
N	-4.601638	-1.200602	-1.557915
C	-5.871305	-1.283839	-1.064866
C	-6.173211	-0.451851	0.214202
F	-5.368928	-0.803158	1.221189
F	-6.003010	0.855371	-0.003765
F	-7.419997	-0.650113	0.589935
O	-6.734499	-1.959387	-1.558551
C	-3.353178	0.907278	-1.524513
C	-2.321730	1.701859	-1.037962
C	1.921007	2.067811	-0.578863
C	3.214176	1.574571	-0.721178
C	3.678445	0.520745	0.078558
N	4.976561	-0.002487	-0.072080
C	5.365655	-0.677737	-1.193040
C	6.830585	-1.173169	-1.130906
F	6.935033	-2.370976	-1.675258
F	7.276719	-1.246446	0.133973
F	7.619459	-0.331364	-1.789860
O	4.703055	-0.860953	-2.176979
H	0.884572	0.089142	1.978551
H	-0.337834	2.994374	-0.233079
H	-1.347135	2.342224	3.863009
H	-0.027282	1.320216	3.296697
H	-1.698577	1.031875	2.725762
H	0.531043	4.535075	1.427326
H	1.316996	3.277592	2.411564
H	0.086992	4.335848	3.138105
H	-2.304129	4.147792	2.546027
H	-2.903970	2.916477	1.416080
H	-1.972960	4.308639	0.808107
H	-0.855942	-0.567826	1.021123
H	-4.453708	-1.767700	-2.388703
H	-2.233260	2.726033	-1.402593
H	1.604472	2.883171	-1.231094
H	5.551425	-0.091464	0.758624
Cl	-4.434917	1.562123	-2.709367
Cl	4.266223	2.313244	-1.880860

11-conf26

- Electronic Energy (Eh): -7737.92968705

- Cartesian Coordinates:

Br	4.409308	2.187931	-1.636607
C	3.227234	1.382418	-0.402701
C	1.953114	1.916071	-0.242530
C	1.039400	1.343598	0.647480
C	-0.348735	1.960774	0.744663
C	-0.750451	2.534026	2.155542
C	-1.005203	1.463627	3.224646
C	0.375557	3.464142	2.628111
C	-2.037760	3.356730	1.987190
C	-1.427107	1.096288	0.105982
C	-1.618145	-0.249540	0.429840
C	-2.664901	-0.973062	-0.131946
Br	-2.866376	-2.787278	0.333544
C	-3.559883	-0.383547	-1.036156
N	-4.642242	-1.104749	-1.589128
C	-5.927553	-1.172862	-1.135979
C	-6.238409	-0.407821	0.182180
F	-7.502096	-0.582039	0.510404
F	-5.477501	-0.847812	1.187851
F	-6.016186	0.903053	0.048703
O	-6.797983	-1.788024	-1.692022
C	-3.325439	0.951932	-1.394022
C	-2.283029	1.679339	-0.831740
C	1.458106	0.234348	1.388234

C	2.740995	-0.283793	1.242557
C	3.652678	0.267536	0.330541
N	4.942475	-0.271070	0.162955
C	5.150965	-1.507622	-0.375983
C	6.647694	-1.887830	-0.477436
F	6.974749	-2.700862	0.520530
F	7.441908	-0.807051	-0.402151
F	6.890372	-2.498447	-1.622638
O	4.302651	-2.286240	-0.715273
H	1.667014	2.787300	-0.833955
H	-0.296123	2.860167	0.113016
H	-0.089973	0.927250	3.510325
H	-1.763032	0.732592	2.906204
H	-1.384837	1.946124	4.138164
H	0.574918	4.258182	1.890599
H	1.314281	2.915342	2.795496
H	0.096618	3.949461	3.575704
H	-2.289586	3.859602	2.932983
H	-2.894875	2.726231	1.707406
H	-1.922268	4.136059	1.216874
H	-0.953887	-0.760358	1.123554
H	-4.488455	-1.630087	-2.445881
H	-2.150850	2.720330	-1.129480
H	0.806385	-0.245145	2.114715
H	5.734209	0.359663	0.223787
Cl	-4.349518	1.714690	-2.565768
Cl	3.216747	-1.611795	2.247777

11-conf27

- Electronic Energy (Eh): -7737.929544

- Cartesian Coordinates:

Br	3.743782	-1.640103	1.768101
C	2.997126	-0.134058	0.918898
C	1.685095	0.215850	1.225487
C	1.093181	1.358735	0.678091
C	-0.337210	1.795449	0.961300
C	-0.670408	2.126374	2.464912
C	0.387765	3.111954	2.980026
C	-2.047575	2.807306	2.510682
C	-0.712884	0.901395	3.387760
C	-1.372432	0.905298	0.287190
C	-2.373774	1.508298	-0.480008
C	-3.384278	0.750414	-1.061155
Br	-4.695405	1.619676	-2.097841
C	-3.435910	-0.640459	-0.894850
N	-4.473550	-1.418633	-1.456215
C	-5.648281	-1.799702	-0.875905
C	-5.905196	-1.285389	0.569365
F	-5.879466	0.049370	0.623443
F	-7.086699	-1.694408	0.983775
F	-4.980181	-1.743458	1.417236
O	-6.466666	-2.491386	-1.420916
C	-2.397297	-1.239655	-0.166925
C	-1.385226	-0.485164	0.416044
C	1.862737	2.142388	-0.186044
C	3.164818	1.778622	-0.507272
C	3.763399	0.631349	0.029550
N	5.082742	0.284338	-0.320474
C	5.367027	-0.808035	-1.088378
C	6.879150	-0.978292	-1.370014
F	7.401354	-1.851296	-0.515524
F	7.542757	0.180959	-1.227269
F	7.073049	-1.416131	-2.599790
O	4.577735	-1.619460	-1.487945
H	1.142155	-0.418806	1.921778
H	-0.433452	2.770739	0.461017
H	0.144551	3.430660	4.004989
H	0.434000	4.014982	2.350257
H	1.391003	2.660758	2.998245

H	-2.855072	2.122920	2.210864
H	-2.085592	3.688817	1.850722
H	-2.264269	3.149260	3.533865
H	-1.070413	1.208377	4.382425
H	0.278240	0.451162	3.536030
H	-1.404713	0.129344	3.019552
H	-2.376063	2.589976	-0.621514
H	-4.351377	-1.784341	-2.396935
H	-0.609564	-1.014163	0.965438
H	1.446686	3.047038	-0.631986
H	5.796999	0.999283	-0.236358
Cl	-2.366121	-2.963199	0.009072
Cl	4.081092	2.774632	-1.599020

11-conf28

- Electronic Energy (Eh): -7737.929687509999

- Cartesian Coordinates:

Br	4.408980	2.187671	-1.637132
C	3.227025	1.382330	-0.403014
C	1.952925	1.916014	-0.242784
C	1.039323	1.343671	0.647415
C	-0.348794	1.960845	0.744743
C	-0.750397	2.533867	2.155727
C	-1.004766	1.463340	3.224817
C	0.375499	3.464165	2.628208
C	-2.037916	3.356328	1.987675
C	-1.427164	1.096366	0.106044
C	-1.617990	-0.249543	0.429662
C	-2.664770	-0.973064	-0.132102
Br	-2.866060	-2.787357	0.333148
C	-3.559894	-0.383469	-1.036096
N	-4.642261	-1.104699	-1.589081
C	-5.927489	-1.173063	-1.135777
C	-6.238437	-0.407788	0.182229
F	-7.502122	-0.582087	0.510468
F	-5.477479	-0.847666	1.187923
F	-6.016332	0.903090	0.048686
O	-6.797782	-1.788745	-1.691463
C	-3.325609	0.952081	-1.393836
C	-2.283233	1.679492	-0.831504
C	1.458075	0.234494	1.388256
C	2.740943	-0.283675	1.242537
C	3.652528	0.267553	0.330345
N	4.942367	-0.270988	0.162756
C	5.151025	-1.507510	-0.376155
C	6.647826	-1.887575	-0.477034
F	6.890815	-2.499351	-1.621544
F	6.974881	-2.699518	0.521864
F	7.441789	-0.806568	-0.402714
O	4.302840	-2.286116	-0.715795
H	1.666727	2.787122	-0.834343
H	-0.296258	2.860333	0.113218
H	-0.089373	0.927198	3.510423
H	-1.762428	0.732109	2.906416
H	-1.384467	1.945730	4.138363
H	0.574517	4.258380	1.890787
H	1.314392	2.915550	2.795280
H	0.096653	3.949235	3.575954
H	-2.289592	3.859174	2.933522
H	-2.894982	2.725661	1.708115
H	-1.922787	4.135660	1.217303
H	-0.953512	-0.760408	1.123142
H	-4.488171	-1.630913	-2.445243
H	-2.151162	2.720541	-1.129096
H	0.806330	-0.244920	2.114772
H	5.734055	0.359794	0.223801
Cl	-4.349736	1.714864	-2.565491
Cl	3.216821	-1.611500	2.247907

11-conf29

- Electronic Energy (Eh): -7737.92972468

- Cartesian Coordinates:

Br	3.626276	-2.178484	1.478580
C	2.948855	-0.485535	0.982331
C	1.651322	-0.150165	1.353268
C	1.104216	1.085752	0.992486
C	-0.317421	1.517915	1.323256
C	-0.680245	1.587400	2.854291
C	-0.805471	0.219552	3.538104
C	0.403734	2.411807	3.562656
C	-2.027268	2.314654	2.993474
C	-1.361628	0.800244	0.478906
C	-2.326249	1.563864	-0.185054
C	-3.341547	0.956285	-0.915528
Br	-4.601326	2.040122	-1.802659
C	-3.434489	-0.439352	-1.007986
N	-4.477135	-1.069545	-1.724335
C	-5.675060	-1.517327	-1.248357
C	-5.956027	-1.270946	0.261494
F	-5.064667	-1.904030	1.029142
F	-5.898516	0.029605	0.561573
F	-7.157504	-1.714733	0.568881
O	-6.496250	-2.072607	-1.928464
C	-2.431419	-1.193072	-0.380711
C	-1.415412	-0.589348	0.351484
C	1.911918	1.972357	0.275948
C	3.217662	1.643295	-0.073999
C	3.763120	0.395256	0.258388
N	5.074296	0.042384	-0.113260
C	5.435868	-0.147875	-1.415635
C	6.922378	-0.542714	-1.587249
F	7.048047	-1.465907	-2.522407
F	7.443005	-1.026588	-0.447380
F	7.634360	0.522775	-1.937021
O	4.732694	0.003105	-2.376734
H	1.078133	-0.876896	1.924073
H	-0.367869	2.569517	1.003577
H	0.159157	-0.299339	3.623249
H	-1.520272	-0.437850	3.021253
H	-1.177781	0.359319	4.564393
H	0.509098	3.409588	3.107283
H	1.385302	1.916729	3.521001
H	0.143371	2.552986	4.622649
H	-2.259729	2.475619	4.056888
H	-2.854581	1.735792	2.556614
H	-2.006668	3.301937	2.504798
H	-2.295094	2.652765	-0.127052
H	-4.342092	-1.255217	-2.714777
H	-0.668542	-1.232947	0.811327
H	1.530699	2.952880	-0.013308
H	5.696917	-0.305002	0.607833
Cl	-2.449375	-2.920227	-0.523840
Cl	4.183579	2.820612	-0.897735

11-conf30

- Electronic Energy (Eh): -7737.92967248

- Cartesian Coordinates:

Br	4.325463	2.395977	-1.289179
C	3.235806	1.344330	-0.159788
C	1.944880	1.776222	0.124416
C	1.097438	1.022876	0.942258
C	-0.314126	1.540213	1.180907
C	-0.689954	1.852250	2.678419
C	-0.864373	0.608065	3.558975
C	0.411944	2.742474	3.269784
C	-2.014882	2.631371	2.685739
C	-1.371917	0.733489	0.440428

C	-2.302897	1.415775	-0.348446
C	-3.330351	0.735322	-0.992507
Br	-4.543225	1.708940	-2.055660
C	-3.469612	-0.654076	-0.870020
N	-4.525275	-1.353930	-1.497111
C	-5.743563	-1.682659	-0.977770
C	-6.034365	-1.193111	0.469685
F	-7.251364	-1.551021	0.824323
F	-5.170216	-1.719325	1.341932
F	-5.943589	0.136740	0.560835
O	-6.575246	-2.310738	-1.577001
C	-2.499857	-1.333559	-0.117815
C	-1.471575	-0.656627	0.528349
C	1.599788	-0.163777	1.484505
C	2.899425	-0.581984	1.217080
C	3.744871	0.153619	0.373818
N	5.051420	-0.280898	0.080772
C	5.297555	-1.406346	-0.651507
C	6.805643	-1.683316	-0.861537
F	7.218727	-2.605261	0.000953
F	7.545912	-0.579555	-0.666495
F	7.027276	-2.116717	-2.088586
O	4.474699	-2.169321	-1.077791
H	1.592590	2.712034	-0.312374
H	-0.329286	2.532184	0.705031
H	-1.235157	0.913157	4.549371
H	0.081452	0.075702	3.728861
H	-1.599636	-0.095167	3.140604
H	0.554904	3.654920	2.668787
H	1.377318	2.217384	3.321126
H	0.143800	3.052708	4.291119
H	-2.254229	2.956990	3.709202
H	-2.854846	2.017867	2.327420
H	-1.957874	3.532983	2.054955
H	-2.235889	2.499094	-0.457888
H	-4.383748	-1.699931	-2.442566
H	-0.752592	-1.244683	1.094654
H	1.001866	-0.785645	2.146491
H	5.811742	0.377582	0.209748
Cl	-2.576832	-3.059984	0.008261
Cl	3.480515	-2.021903	1.984741

11-conf31

- Electronic Energy (Eh): -7737.929671980001

- Cartesian Coordinates:

Br	-4.325760	-2.396078	-1.289049
C	-3.235916	-1.344438	-0.159817
C	-1.945020	-1.776426	0.124338
C	-1.097456	-1.023059	0.942040
C	0.314107	-1.540405	1.180613
C	0.689960	-1.852640	2.678055
C	0.863532	-0.608579	3.558980
C	-0.411540	-2.743605	3.269068
C	2.015306	-2.631040	2.685355
C	1.371884	-0.733490	0.440280
C	2.302905	-1.415644	-0.348682
C	3.330388	-0.735108	-0.992597
Br	4.543252	-1.708567	-2.055928
C	3.469665	0.654280	-0.869897
N	4.525355	1.354210	-1.496819
C	5.743707	1.682686	-0.977467
C	6.034445	1.192838	0.469883
F	7.251435	1.550666	0.824664
F	5.170216	1.718900	1.342140
F	5.943643	-0.137037	0.560745
O	6.575394	2.310850	-1.576582
C	2.499856	1.333625	-0.117662
C	1.471521	0.656618	0.528348
C	-1.599662	0.163674	1.484239

C	-2.899296	0.581949	1.216884
C	-3.744856	-0.153629	0.373709
N	-5.051361	0.280942	0.080652
C	-5.297550	1.406601	-0.651248
C	-6.805616	1.683533	-0.861361
F	-7.218545	2.606129	0.000519
F	-7.545979	0.579983	-0.665496
F	-7.027264	2.116084	-2.088710
O	-4.474751	2.169757	-1.077331
H	-1.592839	-2.712315	-0.312377
H	0.329352	-2.532295	0.704555
H	1.234921	-0.913644	4.549156
H	-0.082751	-0.077176	3.729310
H	1.598048	0.095455	3.140638
H	-0.553607	-3.656207	2.668097
H	-0.143563	-3.053560	4.290533
H	-1.377299	-2.219186	3.320017
H	2.254585	-2.956915	3.708752
H	2.855025	-2.016961	2.327441
H	1.958950	-3.532453	2.054228
H	2.235907	-2.498943	-0.458324
H	4.383704	1.700701	-2.442079
H	0.752483	1.244659	1.094593
H	-1.001605	0.785541	2.146101
H	-5.811777	-0.377411	0.209742
Cl	2.576800	3.060057	0.008644
Cl	-3.480244	2.021908	1.984600

11-conf32

- Electronic Energy (Eh): -7737.9288794

- Cartesian Coordinates:

Br	2.221120	-1.009787	2.319023
C	2.142907	0.243390	0.907150
C	0.971782	0.966325	0.716526
C	0.873474	1.891461	-0.325937
C	-0.392048	2.705631	-0.564814
C	-0.461933	4.031415	0.280462
C	-1.830900	4.690916	0.059930
C	-0.206923	3.839604	1.782651
C	0.624485	4.980858	-0.253076
C	-1.613692	1.795452	-0.556588
C	-2.305248	1.421980	0.599371
C	-3.371269	0.530423	0.534639
Br	-4.286249	0.097992	2.124422
C	-3.781717	-0.034792	-0.680509
N	-4.857156	-0.948973	-0.750583
C	-4.815863	-2.312710	-0.699389
C	-3.414577	-2.955696	-0.499051
F	-3.531100	-4.266210	-0.437469
F	-2.596308	-2.651187	-1.508497
F	-2.844389	-2.529676	0.631337
O	-5.790474	-3.009848	-0.795817
C	-3.100120	0.369964	-1.837984
C	-2.036305	1.262955	-1.777423
C	1.978990	2.073806	-1.157787
C	3.159113	1.365902	-0.948554
C	3.262923	0.420629	0.081601
N	4.441648	-0.322460	0.281858
C	4.887147	-1.243719	-0.622038
C	6.191025	-1.951476	-0.181238
F	6.380203	-1.863361	1.145788
F	7.235034	-1.384735	-0.776756
F	6.154876	-3.229395	-0.508812
O	4.391448	-1.491751	-1.686634
H	0.126484	0.780864	1.378772
H	-0.320663	3.061594	-1.603750
H	-1.848552	5.691005	0.519190
H	-2.650648	4.106672	0.501182
H	-2.045245	4.810854	-1.014028

H	0.776966	3.386988	1.973806
H	-0.967486	3.223198	2.280239
H	-0.221060	4.820374	2.282071
H	0.579239	5.944162	0.276896
H	0.489761	5.184881	-1.327278
H	1.634529	4.570343	-0.106247
H	-2.030476	1.823515	1.571758
H	-5.795515	-0.581634	-0.884959
H	-1.529711	1.536455	-2.704296
H	1.939599	2.787676	-1.981780
H	4.826634	-0.356070	1.219465
Cl	-3.600592	-0.241908	-3.379233
Cl	4.522008	1.700845	-1.963055

11-conf33

- Electronic Energy (Eh): -7737.9288752600005

- Cartesian Coordinates:

Br	3.277965	0.299567	2.524924
C	2.624045	0.757516	0.811876
C	1.421110	1.448663	0.719472
C	0.892389	1.794721	-0.528544
C	-0.430647	2.523352	-0.722112
C	-0.523302	3.959292	-0.083383
C	0.709661	4.758829	-0.527564
C	-1.783050	4.645609	-0.634404
C	-0.606392	3.966862	1.448535
C	-1.635294	1.634909	-0.438393
C	-1.789896	0.915046	0.749436
C	-2.919536	0.132330	0.964504
Br	-3.090448	-0.780678	2.603825
C	-3.931096	0.024015	-0.000760
N	-5.080583	-0.770539	0.211377
C	-5.295388	-2.070378	-0.147115
C	-4.111708	-2.802602	-0.839377
F	-3.784930	-2.208943	-1.990001
F	-3.027554	-2.809584	-0.060983
F	-4.449064	-4.049779	-1.095973
O	-6.329384	-2.650424	0.052309
C	-3.773280	0.765010	-1.181079
C	-2.644850	1.547217	-1.400169
C	1.624177	1.445111	-1.665939
C	2.839566	0.774468	-1.569810
C	3.362009	0.399016	-0.324062
N	4.579157	-0.299332	-0.214646
C	4.731940	-1.577867	-0.669406
C	6.150343	-2.147574	-0.426383
F	6.871796	-2.050154	-1.537706
F	6.082100	-3.416927	-0.071503
F	6.796766	-1.475552	0.540811
O	3.905987	-2.229423	-1.246864
H	0.907364	1.704820	1.642996
H	-0.477820	2.724739	-1.802708
H	0.638848	5.797786	-0.171299
H	0.794852	4.785704	-1.625741
H	1.640155	4.329230	-0.127894
H	-2.703054	4.144246	-0.298963
H	-1.786000	4.661091	-1.736068
H	-1.826980	5.688986	-0.287478
H	-0.779882	4.995994	1.798404
H	0.324944	3.627642	1.922415
H	-1.439572	3.352634	1.821008
H	-1.029241	0.943535	1.526584
H	-5.884918	-0.342872	0.662649
H	-2.564018	2.097360	-2.338573
H	1.256354	1.707464	-2.659060
H	5.276114	0.060409	0.428192
Cl	-5.014147	0.720593	-2.389836
Cl	3.727091	0.445592	-3.019287

11-conf34

- Electronic Energy (Eh): -7737.92880674

- Cartesian Coordinates:

Br	4.524029	1.472300	-1.940534
C	3.130058	1.155318	-0.705081
C	1.962538	1.903956	-0.800368
C	0.902964	1.693822	0.086780
C	-0.348730	2.551164	-0.052890
C	-0.387484	3.798855	0.906546
C	-0.353948	3.449657	2.400134
C	0.834326	4.677005	0.593674
C	-1.661707	4.598445	0.600390
C	-1.621741	1.718085	-0.109843
C	-2.176697	1.064171	0.995477
C	-3.332297	0.300920	0.865509
Br	-4.047660	-0.524825	2.400606
C	-3.976736	0.149253	-0.370508
N	-5.149782	-0.626671	-0.508403
C	-5.262882	-1.941001	-0.861161
C	-3.933083	-2.710306	-1.098400
F	-4.192911	-3.966733	-1.395921
F	-3.239283	-2.172915	-2.104611
F	-3.160905	-2.684424	-0.009869
O	-6.317011	-2.505734	-0.983952
C	-3.428386	0.831621	-1.465972
C	-2.272359	1.594337	-1.340039
C	1.055042	0.716599	1.072384
C	2.233071	-0.015991	1.179062
C	3.295595	0.176850	0.283887
N	4.481371	-0.576471	0.374989
C	4.515552	-1.918209	0.124510
C	5.928767	-2.532698	0.268527
F	6.039798	-3.136962	1.446184
F	6.888980	-1.595687	0.197465
F	6.145265	-3.417238	-0.687273
O	3.574995	-2.614972	-0.140394
H	1.877947	2.656473	-1.585754
H	-0.270828	3.003944	-1.052695
H	-0.263259	4.375418	2.988618
H	0.507525	2.815363	2.656491
H	-1.273745	2.952867	2.737845
H	0.870391	4.954785	-0.471948
H	1.777980	4.170645	0.845363
H	0.789612	5.608182	1.178323
H	-1.679607	5.527540	1.190139
H	-2.570159	4.028338	0.845013
H	-1.713683	4.876014	-0.464664
H	-1.724802	1.141750	1.981365
H	-6.047820	-0.173127	-0.362402
H	-1.880903	2.098084	-2.224975
H	0.262622	0.501750	1.786336
H	5.362064	-0.074000	0.386734
Cl	-4.212587	0.739779	-3.008090
Cl	2.387827	-1.154103	2.475317

11-conf35

- Electronic Energy (Eh): -7737.92881993

- Cartesian Coordinates:

Br	2.491346	-1.018637	2.374792
C	2.251266	0.237051	0.983510
C	1.069465	0.966138	0.934506
C	0.852428	1.894168	-0.087250
C	-0.427017	2.716887	-0.174328
C	-0.395179	4.035040	0.684736
C	0.007490	3.826682	2.151706
C	0.640815	4.978992	0.051075
C	-1.773491	4.707439	0.610766
C	-1.648812	1.817267	-0.038258

C	-2.232531	1.330796	-1.212018
C	-3.308671	0.450692	-1.168175
Br	-4.067336	-0.144171	-2.785894
C	-3.841833	0.014353	0.052949
N	-4.929584	-0.885861	0.112170
C	-4.899265	-2.246539	0.220639
C	-3.492770	-2.909128	0.227755
F	-2.812444	-2.608459	-0.880328
F	-2.770864	-2.498427	1.274023
F	-3.618220	-4.218408	0.298190
O	-5.886596	-2.927689	0.300446
C	-3.271346	0.535368	1.223284
C	-2.193033	1.412521	1.183400
C	1.852218	2.072332	-1.044420
C	3.044934	1.357766	-0.978636
C	3.266036	0.410318	0.030851
N	4.457072	-0.337556	0.090098
C	4.792035	-1.257261	-0.861914
C	6.136450	-1.968810	-0.576518
F	7.105917	-1.402414	-1.287214
F	6.060012	-3.245804	-0.900814
F	6.477681	-1.884433	0.720036
O	4.175839	-1.501178	-1.862564
H	0.308915	0.783138	1.692921
H	-0.469159	3.083183	-1.211174
H	0.053792	4.802741	2.658364
H	1.000705	3.362945	2.240214
H	-0.707466	3.213692	2.716446
H	0.399151	5.194551	-1.001937
H	1.656033	4.556849	0.089934
H	0.660248	5.937588	0.591070
H	-1.736786	5.701707	1.081390
H	-2.548876	4.122484	1.125507
H	-2.094007	4.842213	-0.434605
H	-1.839192	1.635988	-2.183084
H	-5.872416	-0.505706	0.104271
H	-1.798824	1.773579	2.130335
H	1.719182	2.788632	-1.856390
H	4.946552	-0.377964	0.977408
Cl	-3.929750	0.089528	2.763873
Cl	4.278078	1.687330	-2.149051

11-conf36

- Electronic Energy (Eh): -7737.92883402

- Cartesian Coordinates:

Br	3.540409	0.198062	2.539504
C	2.772961	0.700455	0.887039
C	1.544022	1.350818	0.892268
C	0.932169	1.727390	-0.307915
C	-0.419710	2.422665	-0.394122
C	-0.491803	3.851729	0.262526
C	-0.427940	3.845892	1.794970
C	0.672871	4.687302	-0.287259
C	-1.815392	4.506441	-0.162175
C	-1.581448	1.507403	-0.029325
C	-2.644831	1.388366	-0.929305
C	-3.741296	0.582244	-0.642142
Br	-5.159323	0.498125	-1.879391
C	-3.812211	-0.150664	0.550826
N	-4.920571	-0.973296	0.854659
C	-5.080712	-2.308331	0.617458
C	-3.917988	-3.023777	-0.125836
F	-2.786306	-2.964256	0.579430
F	-4.224334	-4.290651	-0.316150
F	-3.688312	-2.461695	-1.315002
O	-6.057765	-2.927090	0.945857
C	-2.748061	-0.009753	1.454028
C	-1.649929	0.794677	1.169970
C	1.607845	1.450059	-1.498697

C	2.849386	0.821891	-1.500106
C	3.455761	0.415532	-0.302986
N	4.700703	-0.240796	-0.292327
C	4.873726	-1.490285	-0.815720
C	6.323952	-2.013500	-0.679827
F	6.324367	-3.301870	-0.394168
F	6.995843	-1.368466	0.288361
F	6.979241	-1.825864	-1.820305
O	4.040591	-2.146212	-1.377658
H	1.076706	1.550809	1.853463
H	-0.553576	2.631346	-1.465965
H	-0.582041	4.869270	2.169893
H	0.549798	3.516003	2.172501
H	-1.212900	3.216159	2.239294
H	0.654030	4.725119	-1.388262
H	1.647581	4.279775	0.019460
H	0.608789	5.721217	0.084562
H	-1.854755	5.546034	0.196512
H	-2.686293	3.977542	0.252662
H	-1.921764	4.528547	-1.258572
H	-2.624806	1.936305	-1.872451
H	-5.711462	-0.556124	1.338340
H	-0.852824	0.841390	1.908380
H	1.174269	1.738604	-2.457410
H	5.418230	0.114432	0.330128
Cl	-2.804329	-0.842800	2.973002
Cl	3.662962	0.587386	-3.010057

11-conf37

- Electronic Energy (Eh): -7737.92878476

- Cartesian Coordinates:

Br	3.696456	0.594581	-2.794695
C	2.788293	0.902228	-1.166983
C	1.595967	1.617564	-1.185752
C	0.881736	1.856280	-0.008128
C	-0.437059	2.610659	-0.111676
C	-0.564820	3.918273	0.756384
C	-0.779024	3.666537	2.255037
C	0.705027	4.756738	0.553670
C	-1.770215	4.717539	0.235124
C	-1.638060	1.679039	-0.009659
C	-1.780564	0.739451	1.014706
C	-2.904313	-0.077998	1.076644
Br	-3.062002	-1.295751	2.505274
C	-3.920202	-0.001035	0.112437
N	-5.064038	-0.829435	0.169096
C	-5.276418	-2.031379	-0.442450
C	-4.094811	-2.603693	-1.274801
F	-4.428969	-3.776105	-1.774040
F	-3.778413	-1.790405	-2.286090
F	-3.005053	-2.760139	-0.520892
O	-6.306504	-2.645481	-0.357258
C	-3.773917	0.958662	-0.899796
C	-2.650980	1.775982	-0.966604
C	1.418189	1.374016	1.189053
C	2.624373	0.680940	1.208587
C	3.331527	0.412114	0.027519
N	4.540968	-0.307415	0.040054
C	4.604662	-1.625638	0.391376
C	6.037089	-2.207343	0.319917
F	6.828212	-1.480383	-0.486549
F	6.009979	-3.445544	-0.135298
F	6.584394	-2.206331	1.530814
O	3.690641	-2.303903	0.771804
H	1.213304	1.981855	-2.140511
H	-0.456696	2.989331	-1.144639
H	-0.963532	4.625902	2.762124
H	0.098642	3.220246	2.741577
H	-1.651494	3.024132	2.444912

H	0.886136	4.954734	-0.514970
H	1.596056	4.255007	0.958477
H	0.605683	5.727538	1.062659
H	-1.839445	5.681941	0.760477
H	-2.717888	4.182809	0.397119
H	-1.678404	4.931410	-0.841814
H	-1.012794	0.622567	1.777419
H	-5.865052	-0.508011	0.706269
H	-2.577476	2.499831	-1.779294
H	0.924794	1.543750	2.143222
H	5.331360	0.087853	-0.457524
Cl	-5.022724	1.145818	-2.086853
Cl	3.270905	0.188866	2.738304

11-conf38

- Electronic Energy (Eh): -7737.92879574

- Cartesian Coordinates:

Br	3.666688	0.680870	-2.787354
C	2.821907	0.912930	-1.113642
C	1.598242	1.571569	-1.062545
C	0.928583	1.752356	0.151031
C	-0.424132	2.451039	0.125620
C	-0.536598	3.771333	0.975978
C	-1.825609	4.497185	0.558781
C	-0.588030	3.545117	2.492630
C	0.664643	4.664237	0.634868
C	-1.581258	1.480935	0.326274
C	-2.643411	1.504684	-0.582254
C	-3.731926	0.651491	-0.433652
Br	-5.151476	0.762968	-1.667381
C	-3.794025	-0.271098	0.619930
N	-4.893681	-1.144481	0.780282
C	-5.040845	-2.421702	0.320849
C	-3.874736	-2.987874	-0.537074
F	-3.664358	-2.234989	-1.620037
F	-2.737346	-3.027500	0.159709
F	-4.165257	-4.210911	-0.930914
O	-6.009853	-3.098027	0.542170
C	-2.730306	-0.273281	1.535189
C	-1.640281	0.577663	1.389776
C	1.541220	1.271518	1.311802
C	2.777278	0.634983	1.261243
C	3.441205	0.424150	0.043822
N	4.680670	-0.240022	-0.014408
C	4.817477	-1.562014	0.299814
C	6.268548	-2.078186	0.147091
F	6.871814	-2.084194	1.331038
F	6.989020	-1.296728	-0.674549
F	6.272831	-3.304313	-0.340505
O	3.952249	-2.288878	0.703827
H	1.155849	1.937128	-1.990632
H	-0.530115	2.808032	-0.909728
H	-1.891554	5.471332	1.066329
H	-2.724894	3.922141	0.825027
H	-1.850467	4.685373	-0.526529
H	0.357801	3.157222	2.894547
H	-1.401889	2.863507	2.780939
H	-0.773164	4.505398	2.997769
H	0.570693	5.638138	1.138912
H	0.728131	4.851956	-0.449006
H	1.614511	4.210887	0.954433
H	-2.628776	2.202285	-1.420890
H	-5.684751	-0.825871	1.333641
H	-0.839487	0.509180	2.123238
H	1.084866	1.397377	2.290826
H	5.430812	0.202012	-0.534405
Cl	-2.778086	-1.349572	2.892271
Cl	3.514199	0.140270	2.748688

11-conf39

- Electronic Energy (Eh): -7737.92876548

- Cartesian Coordinates:

Br	3.620906	0.592906	-2.816853
C	2.799787	0.884573	-1.140660
C	1.577478	1.546103	-1.095444
C	0.925409	1.770059	0.120488
C	-0.429624	2.464136	0.088989
C	-0.550060	3.794795	0.922081
C	-0.627470	3.587321	2.440491
C	0.657828	4.681479	0.588356
C	-1.830934	4.518808	0.476868
C	-1.579446	1.488937	0.306378
C	-2.652066	1.500960	-0.589798
C	-3.732981	0.641276	-0.423412
Br	-5.167972	0.736710	-1.640554
C	-3.776134	-0.275948	0.635714
N	-4.867795	-1.155977	0.813657
C	-5.011866	-2.436318	0.362084
C	-3.852324	-2.998925	-0.507033
F	-2.705871	-3.025716	0.175336
F	-4.138476	-4.226516	-0.889783
F	-3.661447	-2.251160	-1.597161
O	-5.973655	-3.117981	0.598073
C	-2.701607	-0.266272	1.538397
C	-1.619266	0.591131	1.375372
C	1.554598	1.330391	1.288617
C	2.789626	0.691485	1.243039
C	3.435404	0.436300	0.024352
N	4.673380	-0.230870	-0.028439
C	4.814650	-1.540316	0.333137
C	6.263074	-2.062771	0.176728
F	6.887581	-2.017484	1.348807
F	6.967908	-1.317380	-0.690704
F	6.259650	-3.308762	-0.257391
O	3.955894	-2.250582	0.778337
H	1.121867	1.878959	-2.029439
H	-0.539381	2.806158	-0.951036
H	-0.814387	4.554929	2.930766
H	0.308192	3.198074	2.864046
H	-1.450270	2.914316	2.723405
H	0.740733	4.851437	-0.497118
H	1.601673	4.233326	0.931901
H	0.555419	5.663455	1.074787
H	-1.904322	5.497199	0.975121
H	-2.735393	3.947187	0.732770
H	-1.836921	4.698004	-0.610222
H	-2.651703	2.193727	-1.432554
H	-5.654316	-0.839961	1.374929
H	-0.808251	0.532483	2.098711
H	1.112052	1.491679	2.268818
H	5.413558	0.188810	-0.580379
Cl	-2.726058	-1.336100	2.901077
Cl	3.548598	0.250809	2.736366

12-conf01

- Electronic Energy (Eh): -6935.47406035

- Cartesian Coordinates:

C	0.539199	2.849682	2.212012
C	0.133680	3.333636	0.814382
C	0.067100	2.170510	-0.248209
C	-1.198721	1.325060	-0.268056
C	-1.748718	0.698910	0.855028
C	-2.889458	-0.088855	0.753262
Br	-3.564271	-0.898220	2.332859
C	-3.536654	-0.289599	-0.477305
N	-4.684967	-1.093155	-0.529951
C	-5.441527	-1.391198	-1.616429

C	-6.642691	-2.318865	-1.298159
F	-7.774798	-1.720992	-1.637215
F	-6.714842	-2.633013	0.004833
F	-6.533211	-3.446799	-1.984247
O	-5.280555	-1.025681	-2.754164
C	-2.990713	0.335942	-1.604441
C	-1.849868	1.121131	-1.488617
C	1.320563	1.305880	-0.280826
C	2.353284	1.600547	-1.174514
C	3.525634	0.854015	-1.223821
C	3.705249	-0.238573	-0.367657
N	4.863851	-1.029545	-0.371453
C	5.967790	-0.882819	-1.146366
C	7.062129	-1.946897	-0.873110
F	6.701201	-2.819305	0.080830
F	7.309785	-2.631339	-1.979732
F	8.178863	-1.351994	-0.480250
O	6.176066	-0.045021	-1.988493
C	2.662849	-0.546425	0.524471
Br	2.823151	-2.021159	1.709826
C	1.496730	0.206748	0.564043
C	1.192874	4.368739	0.359096
C	0.830134	5.142388	-0.909925
C	-0.544992	5.800427	-0.795034
C	-1.618478	4.792568	-0.384184
C	-1.227096	4.060156	0.899339
H	1.525098	2.362695	2.204565
H	0.601534	3.710174	2.895412
H	-0.184857	2.150783	2.652824
H	0.057361	2.679373	-1.220357
H	-1.302286	0.821612	1.839877
H	-4.979644	-1.494215	0.355688
H	-3.474266	0.197322	-2.568599
H	-1.451862	1.591371	-2.391359
H	2.244974	2.442014	-1.862833
H	4.314828	1.104778	-1.928740
H	4.867909	-1.801340	0.289208
H	0.715564	-0.083861	1.265961
H	1.311948	5.094960	1.181835
H	2.173868	3.879781	0.247442
H	0.844180	4.476134	-1.790091
H	1.602275	5.903105	-1.104325
H	-0.496214	6.598321	-0.032686
H	-0.816597	6.291433	-1.742623
H	-1.787138	4.067656	-1.199242
H	-2.582031	5.304214	-0.235001
H	-1.154593	4.801302	1.714937
H	-2.019910	3.357511	1.197370

12-conf02

- Electronic Energy (Eh): -6935.47403924

- Cartesian Coordinates:

C	0.642419	2.613312	-2.730004
C	0.162813	3.177492	-1.387275
C	0.059582	2.081864	-0.258242
C	1.322434	1.244268	-0.106686
C	1.562144	0.101055	-0.873923
C	2.736105	-0.626099	-0.726132
Br	2.985904	-2.164030	-1.811278
C	3.722469	-0.246463	0.201409
N	4.891873	-1.012999	0.314842
C	5.948143	-0.800967	1.139361
C	7.074431	-1.855552	0.985328
F	8.197099	-1.261539	0.607872
F	7.282305	-2.464319	2.143067
F	6.776080	-2.793087	0.072517
O	6.095178	0.086460	1.942739
C	3.478708	0.890713	0.980048
C	2.299279	1.610676	0.822628

C	-1.193720	1.216708	-0.253215
C	-1.684528	0.499479	-1.349511
C	-2.819788	-0.298439	-1.262148
C	-3.521603	-0.414163	-0.056180
N	-4.671315	-1.204858	0.085680
C	-5.284811	-1.957228	-0.862395
C	-6.537502	-2.708469	-0.341860
F	-7.601811	-2.346875	-1.042351
F	-6.363823	-4.015269	-0.472831
F	-6.786908	-2.452208	0.951753
O	-4.967512	-2.096478	-2.017487
C	-3.035689	0.303706	1.048871
Br	-3.928185	0.209516	2.721096
C	-1.899883	1.097834	0.947935
C	-1.202428	3.873562	-1.583018
C	-1.666152	4.679619	-0.369554
C	-0.627820	5.729035	0.027324
C	0.748461	5.102157	0.250733
C	1.184067	4.256384	-0.947348
H	-0.048156	1.872094	-3.154646
H	0.721880	3.428995	-3.464710
H	1.635380	2.148421	-2.645222
H	-0.006557	2.651440	0.677310
H	0.825465	-0.244226	-1.598748
H	4.945846	-1.821316	-0.298320
H	4.223808	1.197444	1.710330
H	2.140106	2.489316	1.452141
H	-1.186432	0.556950	-2.316321
H	-3.179564	-0.843132	-2.131924
H	-5.087733	-1.208430	1.012337
H	-1.556782	1.636092	1.834029
H	-1.101251	4.562554	-2.440173
H	-1.969296	3.139315	-1.872594
H	-1.865113	4.005654	0.481715
H	-2.627987	5.164781	-0.597608
H	-0.552039	6.477527	-0.781493
H	-0.952415	6.274851	0.927087
H	0.727407	4.492675	1.171055
H	1.499820	5.886073	0.434109
H	1.334272	4.931305	-1.807791
H	2.164676	3.791519	-0.756973

12-conf03

- Electronic Energy (Eh): -6935.47380053

- Cartesian Coordinates:

C	0.507183	2.246004	-3.081098
C	0.114344	2.863903	-1.734112
C	0.008863	1.800629	-0.574407
C	1.239490	0.912026	-0.449417
C	2.254101	1.273946	0.440703
C	3.406713	0.507551	0.570573
Br	4.736340	1.077318	1.800141
C	3.590677	-0.663558	-0.182382
N	4.768019	-1.408892	-0.020385
C	5.128948	-2.545775	-0.667357
C	6.514954	-3.090532	-0.234865
F	6.388366	-4.323834	0.230507
F	7.334624	-3.108918	-1.275851
F	7.082698	-2.342597	0.724331
O	4.510676	-3.147413	-1.509846
C	2.568366	-1.035748	-1.065379
C	1.421581	-0.260548	-1.187842
C	-1.280832	0.994077	-0.502033
C	-1.832916	0.257233	-1.555391
C	-3.004194	-0.477327	-1.408742
C	-3.681553	-0.506756	-0.183562
N	-4.866122	-1.230072	0.017758
C	-5.543930	-1.983474	-0.884684
C	-6.820443	-2.645049	-0.303789

F	-7.883207	-2.248305	-0.987583
F	-7.017536	-2.330596	0.986108
F	-6.723384	-3.963152	-0.392240
O	-5.265980	-2.182777	-2.041020
C	-3.132879	0.229531	0.878955
Br	-3.987343	0.249160	2.573541
C	-1.961702	0.960038	0.718921
C	-1.225149	3.617748	-1.890115
C	-1.598943	4.475547	-0.681160
C	-0.497087	5.483837	-0.355253
C	0.856747	4.797762	-0.172058
C	1.201479	3.904423	-1.365240
H	-0.240909	1.536144	-3.459312
H	0.599975	3.040343	-3.837360
H	1.475828	1.728474	-3.025867
H	0.000660	2.395509	0.347563
H	2.150440	2.173624	1.050253
H	5.424629	-1.044500	0.663667
H	2.687737	-1.943584	-1.652125
H	0.649400	-0.596534	-1.880253
H	-1.355210	0.248137	-2.534001
H	-3.411773	-1.038557	-2.246343
H	-5.257152	-1.176316	0.953936
H	-1.570840	1.516140	1.573661
H	-1.130756	4.278787	-2.769750
H	-2.036008	2.912108	-2.126227
H	-1.793436	3.833822	0.195586
H	-2.545724	5.000320	-0.882917
H	-0.420489	6.207638	-1.186131
H	-0.757646	6.066513	0.542211
H	0.845395	4.212125	0.763898
H	1.650817	5.549155	-0.039362
H	1.344142	4.551442	-2.248070
H	2.168202	3.400439	-1.205630

12-conf04

- Electronic Energy (Eh): -6935.474060239999

- Cartesian Coordinates:

C	0.538901	2.849255	2.212408
C	0.133504	3.333424	0.814808
C	0.067020	2.170423	-0.247962
C	-1.198807	1.324992	-0.267904
C	-1.748471	0.698246	0.855024
C	-2.889283	-0.089401	0.753202
Br	-3.563584	-0.899633	2.332573
C	-3.536940	-0.289394	-0.477250
N	-4.685358	-1.092798	-0.529899
C	-5.442320	-1.390114	-1.616280
C	-6.643120	-2.318326	-1.298274
F	-6.716310	-2.631201	0.004969
F	-7.775310	-1.721766	-1.639113
F	-6.532016	-3.446951	-1.983072
O	-5.281729	-1.023851	-2.753836
C	-2.991331	0.336731	-1.604216
C	-1.850368	1.121749	-1.488351
C	1.320535	1.305876	-0.280677
C	2.353141	1.600608	-1.174488
C	3.525534	0.854162	-1.223933
C	3.705326	-0.238426	-0.367792
N	4.863963	-1.029337	-0.371704
C	5.967835	-0.882568	-1.146713
C	7.062199	-1.946663	-0.873615
F	6.701551	-2.818838	0.080650
F	8.179118	-1.351768	-0.481313
F	7.309379	-2.631384	-1.980179
O	6.176011	-0.044791	-1.988883
C	2.663038	-0.546350	0.524432
Br	2.823585	-2.021083	1.709758
C	1.496864	0.206738	0.564140

C	1.192743	4.368599	0.359778
C	0.830079	5.142495	-0.909107
C	-0.545027	5.800562	-0.794143
C	-1.618567	4.792636	-0.383594
C	-1.227286	4.059907	0.899779
H	1.524833	2.362332	2.204988
H	0.601112	3.709644	2.895951
H	-0.185146	2.150239	2.653051
H	0.057266	2.679416	-1.220045
H	-1.301701	0.820397	1.839790
H	-4.979936	-1.494035	0.355694
H	-3.475261	0.198722	-2.568273
H	-1.452613	1.592406	-2.390988
H	2.244689	2.442066	-1.862798
H	4.314621	1.104971	-1.928954
H	4.868168	-1.801077	0.289023
H	0.715791	-0.083965	1.266123
H	1.311773	5.094658	1.182663
H	2.173734	3.879644	0.248096
H	0.844112	4.476393	-1.789394
H	1.602257	5.903215	-1.103360
H	-0.496264	6.598279	-0.031602
H	-0.816557	6.291805	-1.741631
H	-1.787191	4.067935	-1.198846
H	-2.582118	5.304267	-0.234347
H	-1.154867	4.800866	1.715554
H	-2.020116	3.357181	1.197587

12-conf05

- Electronic Energy (Eh): -6935.4738581

- Cartesian Coordinates:

C	-0.416716	2.477192	2.623358
C	-0.089846	3.042161	1.235760
C	-0.015053	1.931685	0.118454
C	-1.229108	1.012000	0.095111
C	-2.301287	1.317213	-0.747428
C	-3.440477	0.521081	-0.781786
Br	-4.852222	1.014026	-1.951287
C	-3.552473	-0.624608	0.022689
N	-4.718548	-1.401633	-0.043748
C	-5.012196	-2.523155	0.661211
C	-6.404485	-3.117877	0.325887
F	-7.055895	-2.402770	-0.604695
F	-7.155105	-3.147104	1.417099
F	-6.267346	-4.353532	-0.131062
O	-4.331215	-3.079928	1.486120
C	-2.472596	-0.940448	0.857689
C	-1.340094	-0.135699	0.884829
C	1.285705	1.148094	0.012156
C	1.904765	1.042692	-1.237156
C	3.077238	0.322137	-1.431449
C	3.689535	-0.335244	-0.357943
N	4.872480	-1.077119	-0.490038
C	5.605334	-1.279237	-1.614112
C	6.857989	-2.164229	-1.385496
F	6.772665	-3.261704	-2.122707
F	7.948449	-1.498861	-1.735044
F	6.993938	-2.537194	-0.103363
O	5.389297	-0.861344	-2.724425
C	3.074751	-0.233449	0.901247
Br	3.840302	-1.092337	2.411752
C	1.901541	0.489817	1.081442
C	1.240554	3.824712	1.302998
C	1.548487	4.632568	0.042264
C	0.416531	5.608000	-0.280393
C	-0.931823	4.893729	-0.374679
C	-1.209765	4.048691	0.870007
H	0.357560	1.796640	3.003314
H	-0.493439	3.302203	3.347870

H	-1.377056	1.941630	2.629727
H	-0.064447	2.484104	-0.828361
H	-2.253960	2.194606	-1.395201
H	-5.423532	-1.076314	-0.699011
H	-2.536088	-1.828135	1.482725
H	-0.521579	-0.428840	1.542817
H	1.455295	1.540978	-2.099838
H	3.534382	0.259768	-2.416217
H	5.215161	-1.509836	0.362831
H	1.481314	0.535854	2.084186
H	1.169149	4.523139	2.155541
H	2.074068	3.145153	1.536508
H	1.717234	3.954547	-0.812151
H	2.493574	5.180592	0.179932
H	0.362543	6.367362	0.519993
H	0.628824	6.153409	-1.213251
H	-0.950407	4.267647	-1.283932
H	-1.743699	5.626262	-0.505074
H	-1.325633	4.731620	1.729407
H	-2.173654	3.523456	0.774850

12-conf06

- Electronic Energy (Eh): -6935.47380074

- Cartesian Coordinates:

C	0.507040	2.245719	-3.081237
C	0.114221	2.863675	-1.734265
C	0.008858	1.800462	-0.574519
C	1.239550	0.911916	-0.449526
C	2.254035	1.273842	0.440768
C	3.406729	0.507597	0.570623
Br	4.736185	1.077332	1.800410
C	3.590936	-0.663379	-0.182508
N	4.768387	-1.408530	-0.020527
C	5.129560	-2.545192	-0.667713
C	6.515233	-3.090310	-0.234656
F	6.387499	-4.322360	0.233890
F	7.334300	-3.112187	-1.275966
F	7.084248	-2.340645	0.722449
O	4.511479	-3.146700	-1.510442
C	2.568753	-1.035582	-1.065627
C	1.421860	-0.260521	-1.188080
C	-1.280790	0.993839	-0.502044
C	-1.832670	0.256653	-1.555268
C	-3.003903	-0.477973	-1.408568
C	-3.681427	-0.507097	-0.183475
N	-4.866000	-1.230400	0.017885
C	-5.543649	-1.984100	-0.884425
C	-6.820562	-2.645050	-0.303687
F	-7.016416	-2.332343	0.986819
F	-6.725252	-3.963092	-0.394303
F	-7.883303	-2.245834	-0.986160
O	-5.265450	-2.183861	-2.040623
C	-3.132958	0.229538	0.878912
Br	-3.987668	0.249590	2.573377
C	-1.961817	0.960091	0.718831
C	-1.225330	3.617432	-1.890278
C	-1.599137	4.475386	-0.681431
C	-0.497291	5.483707	-0.355598
C	0.856542	4.797652	-0.172357
C	1.201304	3.904294	-1.365497
H	-0.240912	1.535612	-3.459265
H	0.599567	3.039989	-3.837597
H	1.475810	1.728406	-3.026057
H	0.000689	2.395383	0.347428
H	2.150162	2.173373	1.050495
H	5.425095	-1.043899	0.663302
H	2.688321	-1.943301	-1.652518
H	0.649812	-0.596510	-1.880636
H	-1.354804	0.247319	-2.533798

H	-3.411309	-1.039497	-2.246057
H	-5.257016	-1.176620	0.954065
H	-1.571104	1.516455	1.573468
H	-1.130990	4.278357	-2.770003
H	-2.036174	2.911732	-2.126273
H	-1.793662	3.833766	0.195381
H	-2.545908	5.000143	-0.883272
H	-0.420694	6.207469	-1.186513
H	-0.757846	6.066428	0.541837
H	0.845178	4.211994	0.763586
H	1.650594	5.549060	-0.039652
H	1.343895	4.551237	-2.248393
H	2.168073	3.400390	-1.205885

12-conf07

- Electronic Energy (Eh): -6935.47385916

- Cartesian Coordinates:

C	-0.414654	2.476011	-2.624438
C	-0.089475	3.041535	-1.236678
C	-0.014954	1.931347	-0.119057
C	1.285811	1.147805	-0.012558
C	1.901251	0.488600	-1.081504
C	3.074593	-0.234427	-0.901137
Br	3.839531	-1.094657	-2.411194
C	3.689906	-0.335047	0.357879
N	4.872962	-1.076693	0.490162
C	5.606314	-1.277738	1.614098
C	6.859169	-2.162519	1.385699
F	6.993969	-2.537711	0.104104
F	7.949674	-1.495951	1.732882
F	6.775232	-3.258697	2.124971
O	5.390666	-0.858920	2.724139
C	3.077995	0.323249	1.431056
C	1.905401	1.043548	1.236599
C	-1.229097	1.011779	-0.095499
C	-1.340293	-0.136076	-0.884982
C	-2.472853	-0.940732	-0.857540
C	-3.552608	-0.624646	-0.022478
N	-4.718742	-1.401570	0.044275
C	-5.012567	-2.523211	-0.660424
C	-6.404906	-3.117708	-0.324885
F	-7.055870	-2.402798	0.606147
F	-6.267947	-4.353571	0.131547
F	-7.155868	-3.146338	-1.415889
O	-4.331737	-3.080194	-1.485314
C	-3.440425	0.521199	0.781732
Br	-4.851994	1.014514	1.951297
C	-2.301169	1.317232	0.747086
C	-1.210246	4.047539	-0.872143
C	-0.933794	4.893079	0.372534
C	0.414216	5.608110	0.279111
C	1.547001	4.633211	-0.042250
C	1.240605	3.824736	-1.302950
H	-1.374170	1.938980	-2.631431
H	-0.492166	3.300873	-3.349038
H	0.361036	1.796744	-3.003813
H	-0.064362	2.484051	0.827591
H	1.480608	0.533642	-2.084125
H	5.215199	-1.510307	-0.362433
H	3.535568	0.261773	2.415684
H	1.456247	1.542568	2.099021
H	-0.521894	-0.429451	-1.543004
H	-2.536471	-1.828546	-1.482385
H	-5.423554	-1.076124	0.699656
H	-2.253737	2.194757	1.394668
H	-1.325736	4.730194	-1.731812
H	-2.173946	3.521836	-0.777666
H	-0.952694	4.267247	1.281950
H	-1.746206	5.625168	0.502087

H	0.360451	6.367152	-0.521594
H	0.625418	6.153976	1.211950
H	1.715407	3.955599	0.812559
H	2.491899	5.181715	-0.179308
H	1.169652	4.522804	-2.155828
H	2.074642	3.145458	-1.535438

12-conf08

- Electronic Energy (Eh): -6935.47405989

- Cartesian Coordinates:

C	0.539327	2.849353	2.212187
C	0.133671	3.333473	0.814647
C	0.067089	2.170461	-0.248091
C	-1.198737	1.325023	-0.267998
C	-1.748521	0.698526	0.855000
C	-2.889288	-0.089195	0.753216
Br	-3.563799	-0.899080	2.332670
C	-3.536737	-0.289513	-0.477284
N	-4.685055	-1.093057	-0.529971
C	-5.442114	-1.390326	-1.616309
C	-6.642927	-2.318501	-1.298213
F	-6.715404	-2.632297	0.004849
F	-7.775205	-1.721392	-1.637910
F	-6.532549	-3.446627	-1.983894
O	-5.281664	-1.023986	-2.753856
C	-2.991017	0.336375	-1.604331
C	-1.850114	1.121482	-1.488498
C	1.320568	1.305855	-0.280804
C	2.353280	1.600614	-1.174488
C	3.525636	0.854113	-1.223861
C	3.705288	-0.238541	-0.367770
N	4.863875	-1.029524	-0.371705
C	5.968143	-0.882198	-1.146035
C	7.062169	-1.946742	-0.873417
F	8.179819	-1.352311	-0.482611
F	7.307768	-2.632257	-1.979885
F	6.701910	-2.818165	0.081684
O	6.176733	-0.043851	-1.987538
C	2.662897	-0.546489	0.524321
Br	2.823225	-2.021319	1.709556
C	1.496745	0.206648	0.563946
C	1.192790	4.368692	0.359448
C	0.829904	5.142540	-0.909403
C	-0.545225	5.800528	-0.794274
C	-1.618651	4.792557	-0.383538
C	-1.227141	4.059894	0.899804
H	1.525367	2.362647	2.204630
H	0.601424	3.709734	2.895749
H	-0.184486	2.150132	2.652888
H	0.057327	2.679436	-1.220183
H	-1.301881	0.820928	1.839796
H	-4.979576	-1.494384	0.355600
H	-3.474808	0.198099	-2.568421
H	-1.452264	1.591975	-2.391176
H	2.244934	2.442135	-1.862736
H	4.314835	1.104965	-1.928743
H	4.867934	-1.801444	0.288815
H	0.715562	-0.084074	1.265800
H	1.311913	5.094766	1.182308
H	2.173790	3.879788	0.247620
H	0.843867	4.476414	-1.789672
H	1.602009	5.903303	-1.103775
H	-0.496409	6.598272	-0.031767
H	-0.816909	6.291720	-1.741744
H	-1.787356	4.067817	-1.198738
H	-2.582208	5.304145	-0.234170
H	-1.154637	4.800890	1.715539
H	-2.019895	3.357146	1.197759

12-conf09

- Electronic Energy (Eh): -6935.47385724

- Cartesian Coordinates:

C	-0.417627	2.478074	2.622627
C	-0.090043	3.042651	1.235031
C	-0.015119	1.931897	0.117992
C	-1.229131	1.012192	0.094834
C	-2.301299	1.317070	-0.747842
C	-3.440435	0.520858	-0.781955
Br	-4.852170	1.013278	-1.951694
C	-3.552399	-0.624564	0.022915
N	-4.718432	-1.401683	-0.043325
C	-5.012003	-2.522917	0.662085
C	-6.404214	-3.117922	0.326978
F	-7.155299	-3.145654	1.417903
F	-7.055162	-2.403923	-0.604793
F	-6.267040	-4.354180	-0.128319
O	-4.331011	-3.079246	1.487298
C	-2.472533	-0.940051	0.858053
C	-1.340069	-0.135239	0.884943
C	1.285585	1.148176	0.011901
C	1.904023	1.041545	-1.237622
C	3.076352	0.320739	-1.431808
C	3.689152	-0.335637	-0.357971
N	4.872078	-1.077575	-0.489931
C	5.603984	-1.281292	-1.614340
C	6.857241	-2.165345	-1.385384
F	7.947384	-1.498580	-1.733476
F	6.773641	-3.262257	-2.123524
F	6.992508	-2.539151	-0.103422
O	5.387019	-0.864973	-2.725058
C	3.074996	-0.232620	0.901417
Br	3.841249	-1.090100	2.412359
C	1.901904	0.490894	1.081505
C	1.240479	3.824955	1.302565
C	1.549067	4.632316	0.041678
C	0.417472	5.607931	-0.281692
C	-0.931034	4.893977	-0.376219
C	-1.209601	4.049324	0.868595
H	0.356005	1.796928	3.002824
H	-0.493885	3.303222	3.347036
H	-1.378379	1.943253	2.628836
H	-0.064443	2.484093	-0.828955
H	-2.253987	2.194250	-1.395910
H	-5.423307	-1.076769	-0.698906
H	-2.536001	-1.827505	1.483428
H	-0.521545	-0.428085	1.543065
H	1.454147	1.539039	-2.100551
H	3.532966	0.257363	-2.416759
H	5.215081	-1.509683	0.363115
H	1.482198	0.537926	2.084421
H	1.168847	4.523691	2.154839
H	2.073782	3.145342	1.536652
H	1.717948	3.953968	-0.812457
H	2.494246	5.180142	0.179501
H	0.363398	6.367567	0.518429
H	0.630230	6.152982	-1.214653
H	-0.949500	4.267666	-1.285320
H	-1.742686	5.626680	-0.507060
H	-1.325653	4.732508	1.727770
H	-2.173569	3.524269	0.773217

12-conf10

- Electronic Energy (Eh): -6935.47380045

- Cartesian Coordinates:

C	0.507061	2.246711	-3.081179
C	0.114320	2.864479	-1.734109
C	0.008898	1.801093	-0.574539

C	1.239475	0.912404	-0.449639
C	2.253958	1.274028	0.440765
C	3.406471	0.507506	0.570677
Br	4.735868	1.076802	1.800697
C	3.590499	-0.663422	-0.182554
N	4.767771	-1.408879	-0.020547
C	5.128612	-2.545708	-0.667640
C	6.514387	-3.090823	-0.234920
F	6.387378	-4.324087	0.230470
F	7.334216	-3.109471	-1.275770
F	7.082151	-2.343005	0.724336
O	4.510381	-3.147073	-1.510367
C	2.568340	-1.035289	-1.065852
C	1.421621	-0.259979	-1.188329
C	-1.280796	0.994527	-0.502199
C	-1.832857	0.257735	-1.555600
C	-3.004138	-0.476840	-1.409000
C	-3.681492	-0.506348	-0.183826
N	-4.866029	-1.229711	0.017471
C	-5.543565	-1.983522	-0.884837
C	-6.819372	-2.646113	-0.303559
F	-7.882197	-2.253598	-0.989563
F	-7.018478	-2.328572	0.985264
F	-6.719356	-3.964309	-0.388242
O	-5.265577	-2.182894	-2.041155
C	-3.132847	0.229927	0.878724
Br	-3.987352	0.249517	2.573282
C	-1.961691	0.960470	0.718736
C	-1.225208	3.618285	-1.889985
C	-1.598998	4.475965	-0.680946
C	-0.497141	5.484241	-0.354985
C	0.856683	4.798135	-0.171862
C	1.201445	3.904963	-1.365164
H	-0.241042	1.536819	-3.459299
H	0.599722	3.041088	-3.837415
H	1.475754	1.729250	-3.026073
H	0.000736	2.395869	0.347494
H	2.150246	2.173562	1.050520
H	5.424255	-1.044736	0.663758
H	2.687773	-1.942968	-1.652827
H	0.649581	-0.595747	-1.881001
H	-1.355162	0.248708	-2.534217
H	-3.411699	-1.038031	-2.246636
H	-5.257322	-1.175599	0.953518
H	-1.570857	1.516561	1.573494
H	-1.130893	4.279408	-2.769562
H	-2.036017	2.912599	-2.126140
H	-1.793453	3.834183	0.195765
H	-2.545797	5.000731	-0.882631
H	-0.420560	6.208116	-1.185802
H	-0.757667	6.066845	0.542532
H	0.845286	4.212342	0.763996
H	1.650757	5.549495	-0.039022
H	1.344114	4.552083	-2.247917
H	2.168162	3.400961	-1.205594

12-conf11

- Electronic Energy (Eh): -6935.473857659999

- Cartesian Coordinates:

C	0.417177	2.477627	2.622986
C	0.089940	3.042423	1.235398
C	0.015099	1.931800	0.118209
C	-1.285629	1.148149	0.012015
C	-1.901692	0.490319	1.081434
C	-3.074864	-0.233035	0.901281
Br	-3.840744	-1.091270	2.411999
C	-3.689368	-0.335389	-0.357990
N	-4.872298	-1.077302	-0.490011
C	-5.604829	-1.280064	-1.614177

C	-6.857617	-2.164833	-1.385400
F	-7.947995	-1.499314	-1.734956
F	-6.772544	-3.262389	-2.122495
F	-6.993589	-2.537645	-0.103224
O	-5.388490	-0.862784	-2.724663
C	-3.076830	0.321540	-1.431644
C	-1.904421	1.042195	-1.237394
C	1.229145	1.012114	0.094981
C	1.340111	-0.135434	0.884928
C	2.472587	-0.940215	0.857929
C	3.552461	-0.624559	0.022851
N	4.718529	-1.401626	-0.043455
C	5.012087	-2.523109	0.661604
C	6.404349	-3.117939	0.326363
F	7.155052	-3.146815	1.417529
F	7.055681	-2.403136	-0.604495
F	6.267159	-4.353748	-0.130172
O	4.331071	-3.079753	1.486571
C	3.440493	0.520980	-0.781832
Br	4.852240	1.013683	-1.951437
C	2.301315	1.317149	-0.747622
C	1.209667	4.049043	0.869319
C	0.931398	4.893908	-0.375415
C	-0.417040	5.607999	-0.281007
C	-1.548800	4.632450	0.041990
C	-1.240520	3.824845	1.302797
H	1.377756	1.942492	2.629273
H	0.493596	3.302686	3.347477
H	-0.356724	1.796700	3.003032
H	0.064472	2.484100	-0.828677
H	-1.481721	0.536784	2.084265
H	-5.215113	-1.509700	0.362967
H	-3.533746	0.258733	-2.416491
H	-1.454764	1.540127	-2.100184
H	0.521596	-0.428398	1.543000
H	2.536060	-1.827788	1.483130
H	5.423496	-1.076453	-0.698807
H	2.254002	2.194422	-1.395560
H	1.325626	4.732079	1.728624
H	2.173604	3.523913	0.774036
H	0.949924	4.267715	-1.284596
H	1.743154	5.626536	-0.506030
H	-0.363030	6.367491	0.519256
H	-0.629564	6.153237	-1.213914
H	-1.717591	3.954268	-0.812292
H	-2.493945	5.180354	0.179735
H	-1.168986	4.523438	2.155197
H	-2.073925	3.145264	1.536620

13-conf01

- Electronic Energy (Eh): -6700.78194995

- Cartesian Coordinates:

Br	4.414573	1.848984	1.467453
C	3.205753	1.287447	0.115323
C	2.085899	2.076990	-0.137951
C	1.163834	1.711963	-1.117577
C	-0.089102	2.521508	-1.417198
C	-0.132951	3.895334	-0.742270
C	-1.346677	1.730837	-1.085755
C	-1.456187	1.038017	0.122614
C	-2.623524	0.359941	0.447343
Br	-2.700661	-0.565248	2.103128
C	-3.727942	0.345677	-0.424731
N	-4.884626	-0.357396	-0.055835
C	-6.041894	-0.479432	-0.753599
C	-7.116053	-1.329998	-0.027436
F	-8.188286	-0.589040	0.211947
F	-6.678715	-1.814377	1.145307
F	-7.467205	-2.355660	-0.787777

O	-6.310027	-0.010734	-1.831969
C	-3.614216	1.039263	-1.635577
C	-2.440591	1.717042	-1.950951
C	1.405553	0.533353	-1.832858
C	2.518594	-0.257748	-1.590511
C	3.446690	0.106627	-0.602700
N	4.587979	-0.655632	-0.313106
C	4.985840	-1.814704	-0.896410
C	6.309880	-2.375743	-0.315935
F	6.107363	-3.589465	0.173770
F	7.224461	-2.447719	-1.271635
F	6.801577	-1.608656	0.669710
O	4.440090	-2.424811	-1.781702
H	1.949680	2.985799	0.448182
H	-0.098261	2.690288	-2.506936
H	0.748691	4.499393	-1.004064
H	-1.030346	4.442296	-1.063701
H	-0.181426	3.803969	0.353804
H	-0.615472	1.014618	0.819090
H	-4.841219	-0.828794	0.843074
H	-4.456798	1.035301	-2.323170
H	-2.382592	2.248491	-2.904283
H	0.695256	0.217771	-2.601267
H	2.688818	-1.169443	-2.158525
H	5.182602	-0.288878	0.424599

13-conf02

- Electronic Energy (Eh): -6700.782051609999

- Cartesian Coordinates:

Br	-2.983862	0.323200	-2.584323
C	-2.662244	-0.652411	-0.988278
C	-1.524360	-1.440603	-0.911075
C	-1.237162	-2.182658	0.240859
C	0.038942	-3.011469	0.273023
C	0.158817	-3.935288	1.488356
C	1.272457	-2.127700	0.157995
C	1.393976	-0.969777	0.930723
C	2.540899	-0.190239	0.863285
Br	2.636242	1.372574	1.936503
C	3.612107	-0.536304	0.018489
N	4.748961	0.285039	-0.019163
C	5.870447	0.119037	-0.764535
C	6.928806	1.231411	-0.547546
F	7.167293	1.853903	-1.692322
F	8.058605	0.696803	-0.108939
F	6.530950	2.149229	0.347158
O	6.117159	-0.766760	-1.544935
C	3.486315	-1.695863	-0.755808
C	2.333234	-2.471224	-0.679793
C	-2.133682	-2.101113	1.304969
C	-3.279171	-1.309701	1.238310
C	-3.566441	-0.568418	0.088540
N	-4.703485	0.244030	-0.032807
C	-5.676293	0.455351	0.889160
C	-6.786157	1.424856	0.406722
F	-7.959497	0.810543	0.426631
F	-6.841968	2.478010	1.208347
F	-6.571759	1.866800	-0.842286
O	-5.761100	-0.012885	1.997273
H	-0.840030	-1.471403	-1.761757
H	0.021896	-3.651277	-0.625167
H	-0.702847	-4.615458	1.561432
H	1.070285	-4.544016	1.407528
H	0.229841	-3.360434	2.424455
H	0.577976	-0.662023	1.587996
H	4.719947	1.099048	0.588129
H	4.302933	-1.975885	-1.417244
H	2.265236	-3.370678	-1.297077
H	-1.954085	-2.662585	2.222562

H	-3.965757	-1.258315	2.080146
H	-4.801037	0.729742	-0.919861

13-conf03

- Electronic Energy (Eh): -6700.78161222

- Cartesian Coordinates:

Br	-4.936953	-1.403791	-1.962751
C	-3.477637	-1.099819	-0.787467
C	-2.341241	-1.891490	-0.923912
C	-1.238683	-1.706145	-0.090236
C	-0.017925	-2.606788	-0.209202
C	-0.054962	-3.697596	0.864604
C	1.263611	-1.785879	-0.230295
C	2.233619	-1.869392	0.767201
C	3.382124	-1.082437	0.711126
Br	4.656305	-1.250691	2.108682
C	3.604537	-0.185834	-0.344675
N	4.776287	0.585148	-0.359806
C	5.165368	1.491362	-1.292164
C	6.528629	2.158798	-0.974460
F	7.078085	1.687475	0.155845
F	6.366654	3.466241	-0.834904
F	7.379138	1.937211	-1.965142
O	4.584026	1.818013	-2.296776
C	2.627349	-0.104341	-1.348760
C	1.486259	-0.889801	-1.282140
C	-1.310361	-0.703823	0.880710
C	-2.440638	0.089853	1.026498
C	-3.551697	-0.094224	0.190639
N	-4.715838	0.682283	0.291687
C	-4.977170	1.680438	1.173257
C	-6.377648	2.319796	0.986597
F	-6.249469	3.608328	0.707396
F	-7.072693	1.748146	-0.009300
F	-7.081802	2.192369	2.101175
O	-4.262730	2.103207	2.047794
H	-2.322150	-2.663512	-1.696113
H	-0.081737	-3.108360	-1.189279
H	-0.978521	-4.285771	0.769898
H	0.799573	-4.384061	0.768674
H	-0.044494	-3.266143	1.877330
H	2.113881	-2.550798	1.609386
H	5.405464	0.439082	0.424330
H	2.782130	0.584491	-2.175980
H	0.738648	-0.796239	-2.073903
H	-0.455854	-0.526295	1.538298
H	-2.480480	0.867001	1.786277
H	-5.447739	0.461682	-0.377368

13-conf04

- Electronic Energy (Eh): -6700.78167861

- Cartesian Coordinates:

Br	-4.750840	-1.981021	-1.175925
C	-3.343103	-1.304844	-0.096893
C	-2.227251	-2.108798	0.116579
C	-1.162581	-1.658139	0.896427
C	0.036090	-2.555807	1.165550
C	-0.076456	-3.194000	2.552623
C	1.340835	-1.809241	0.923204
C	1.601718	-1.319402	-0.362031
C	2.767159	-0.621305	-0.638104
Br	3.049730	0.009797	-2.405820
C	3.726992	-0.378308	0.363758
N	4.891149	0.334010	0.039646
C	5.923816	0.655524	0.859008
C	7.056371	1.441349	0.148871
F	7.256792	2.596699	0.763563
F	6.771314	1.699965	-1.136860

F	8.179446	0.738468	0.183877
O	6.047524	0.397863	2.030604
C	3.465427	-0.866927	1.647091
C	2.291620	-1.569740	1.913808
C	-1.250985	-0.379511	1.453537
C	-2.361078	0.429258	1.248502
C	-3.433763	-0.020497	0.464641
N	-4.575520	0.757180	0.220167
C	-4.845518	2.007006	0.675000
C	-6.212887	2.557863	0.193500
F	-6.874776	1.680942	-0.577682
F	-6.976874	2.840631	1.237817
F	-6.028049	3.663430	-0.512433
O	-4.160630	2.702618	1.382783
H	-2.194241	-3.101872	-0.336677
H	-0.000132	-3.372388	0.424976
H	0.758619	-3.883808	2.745498
H	-0.088948	-2.431367	3.346227
H	-1.014187	-3.762213	2.628401
H	0.875259	-1.478190	-1.161960
H	4.960051	0.642341	-0.925963
H	4.194840	-0.689540	2.434042
H	2.134079	-1.932445	2.930195
H	-0.425175	0.004768	2.057324
H	-2.414166	1.422894	1.687494
H	-5.280820	0.324399	-0.369215

13-conf05

- Electronic Energy (Eh): -6700.781950109999

- Cartesian Coordinates:

Br	-2.701111	-0.563897	-2.103674
C	-2.623693	0.360334	-0.447373
C	-1.456364	1.038330	-0.122494
C	-1.346649	1.730450	1.086269
C	-0.089062	2.521013	1.417851
C	-0.132911	3.895027	0.743291
C	1.163848	1.711530	1.117948
C	2.085971	2.076887	0.138498
C	3.205828	1.287425	-0.115000
Br	4.414652	1.849383	-1.466949
C	3.446712	0.106337	0.602610
N	4.587957	-0.655893	0.312763
C	4.986191	-1.814730	0.896275
C	6.309937	-2.375943	0.315271
F	6.106822	-3.589282	-0.175195
F	7.224618	-2.448947	1.270776
F	6.801832	-1.608460	-0.669958
O	4.440828	-2.424639	1.781941
C	2.518551	-0.258386	1.590228
C	1.405512	0.532650	1.832799
C	-2.440362	1.716017	1.951696
C	-3.613981	1.038273	1.636195
C	-3.727911	0.345415	0.424960
N	-4.884589	-0.357603	0.055912
C	-6.041739	-0.480069	0.753793
C	-7.116020	-1.330162	0.027246
F	-8.188094	-0.588875	-0.211930
F	-6.678715	-1.814174	-1.145654
F	-7.467441	-2.356024	0.787178
O	-6.309718	-0.012025	1.832483
H	-0.615794	1.015439	-0.819165
H	-0.098140	2.689511	2.507634
H	-1.030341	4.441874	1.064822
H	0.748696	4.499042	1.005302
H	-0.181313	3.803956	-0.352811
H	1.949788	2.985891	-0.447343
H	5.182356	-0.289153	-0.425131
H	2.688760	-1.170257	2.157968
H	0.695161	0.216774	2.601039

H	-2.382210	2.246897	2.905337
H	-4.456403	1.033803	2.323980
H	-4.841294	-0.828506	-0.843261

13-conf06

- Electronic Energy (Eh): -6700.78167856

- Cartesian Coordinates:

Br	-3.049756	0.010100	-2.405678
C	-2.767262	-0.621163	-0.638013
C	-1.601748	-1.319110	-0.361901
C	-1.340869	-1.808996	0.923320
C	-0.036087	-2.555509	1.165633
C	0.076571	-3.193609	2.552753
C	1.162567	-1.657906	0.896350
C	2.227223	-2.108688	0.116543
C	3.343100	-1.304809	-0.097029
Br	4.750801	-1.981155	-1.175998
C	3.433791	-0.020383	0.464338
N	4.575512	0.757304	0.219649
C	4.846156	2.006581	0.675579
C	6.213203	2.557682	0.193445
F	6.977601	2.840683	1.237388
F	6.027781	3.663173	-0.512499
F	6.874908	1.680857	-0.577996
O	4.161895	2.701710	1.384438
C	2.361138	0.429507	1.248150
C	1.251029	-0.379218	1.453309
C	-2.291742	-1.569656	1.913876
C	-3.465647	-0.867010	1.647119
C	-3.727211	-0.378386	0.363793
N	-4.891487	0.333734	0.039593
C	-5.924098	0.655366	0.858959
C	-7.056640	1.441154	0.148771
F	-7.256799	2.596695	0.763192
F	-6.771739	1.699372	-1.137069
F	-8.179823	0.738445	0.184134
O	-6.047798	0.397848	2.030590
H	-0.875198	-1.477722	-1.161787
H	0.000047	-3.372169	0.425135
H	-0.758459	-3.883445	2.745720
H	1.014337	-3.761773	2.628504
H	0.089073	-2.430910	3.346292
H	2.194165	-3.101817	-0.336596
H	5.280483	0.324727	-0.370275
H	2.414310	1.423155	1.687108
H	0.425246	0.005160	2.057074
H	-2.134216	-1.932322	2.930280
H	-4.195132	-0.689784	2.434038
H	-4.960378	0.641983	-0.926044

13-conf07

- Electronic Energy (Eh): -6700.78195031

- Cartesian Coordinates:

Br	2.701527	-0.562196	2.104351
C	2.623807	0.360921	0.447443
C	1.456491	1.038857	0.122397
C	1.346587	1.730212	-1.086786
C	0.088980	2.520651	-1.418582
C	0.132764	3.894851	-0.744411
C	-1.163871	1.711160	-1.118415
C	-2.086098	2.076860	-0.139191
C	-3.205892	1.287393	0.114574
Br	-4.414931	1.849865	1.466120
C	-3.446595	0.105973	-0.602543
N	-4.587816	-0.656221	-0.312463
C	-4.985810	-1.815418	-0.895408
C	-6.309758	-2.376318	-0.314578
F	-6.107129	-3.589896	0.175458

F	-7.224466	-2.448618	-1.270130
F	-6.801357	-1.608973	0.670909
O	-4.440204	-2.425770	-1.780622
C	-2.518336	-0.259096	-1.589934
C	-1.405357	0.531947	-1.832771
C	2.440090	1.715073	-1.952464
C	3.613704	1.037398	-1.636792
C	3.727825	0.345315	-0.425131
N	4.884545	-0.357498	-0.055819
C	6.041239	-0.481255	-0.754229
C	7.115838	-1.330375	-0.027003
F	8.187081	-0.588034	0.212845
F	6.678262	-1.814718	1.145663
F	7.468726	-2.355900	-0.786632
O	6.308741	-0.014656	-1.833664
H	0.616071	1.016505	0.819268
H	0.098039	2.688831	-2.508413
H	1.030148	4.441662	-1.066125
H	-0.748894	4.498728	-1.006561
H	0.181210	3.804101	0.351716
H	-1.950061	2.986161	0.446221
H	-5.182323	-0.289184	0.425196
H	-2.688402	-1.171244	-2.157271
H	-0.694924	0.215825	-2.600833
H	2.381772	2.245338	-2.906436
H	4.455953	1.032326	-2.324785
H	4.841429	-0.827687	0.843735

13-conf08

- Electronic Energy (Eh): -6700.78161213

- Cartesian Coordinates:

Br	-4.656050	-1.250087	2.109141
C	-3.382075	-1.082049	0.711377
C	-2.233471	-1.868854	0.767509
C	-1.263633	-1.785537	-0.230171
C	0.017966	-2.606313	-0.209045
C	0.055145	-3.696973	0.864916
C	1.238713	-1.705629	-0.090217
C	2.341647	-1.891821	-0.923217
C	3.478106	-1.100227	-0.786859
Br	4.937913	-1.405385	-1.961221
C	3.551869	-0.093871	0.190488
N	4.716061	0.682550	0.291453
C	4.977199	1.681335	1.172356
C	6.377746	2.320504	0.985602
F	7.081173	2.195010	2.100829
F	6.249577	3.608587	0.704199
F	7.073513	1.747346	-0.008903
O	4.262508	2.104882	2.046310
C	2.440437	0.091045	1.025654
C	1.310084	-0.702552	0.879957
C	-1.486537	-0.889774	-1.282232
C	-2.627728	-0.104459	-1.348896
C	-3.604765	-0.185788	-0.344652
N	-4.776632	0.585006	-0.359835
C	-5.165995	1.490939	-1.292353
C	-6.529576	2.157825	-0.974892
F	-6.368382	3.465432	-0.836284
F	-7.380112	1.935026	-1.965309
F	-7.078623	1.686952	0.155805
O	-4.584700	1.817712	-2.296949
H	-2.113502	-2.549986	1.609886
H	0.081784	-3.107994	-1.189070
H	-0.799332	-4.383538	0.769128
H	0.978756	-4.285080	0.770253
H	0.044689	-3.265363	1.877580
H	2.322813	-2.664449	-1.694823
H	5.448253	0.461252	-0.377062
H	2.480041	0.868786	1.784846

H	0.455293	-0.524362	1.536998
H	-0.739053	-0.796351	-2.074135
H	-2.782691	0.584145	-2.176273
H	-5.405848	0.438805	0.424251

13-conf09

- Electronic Energy (Eh): -6700.781612089999

- Cartesian Coordinates:

Br	-4.937655	-1.404818	-1.961511
C	-3.477983	-1.100477	-0.786772
C	-2.341559	-1.892077	-0.923440
C	-1.238748	-1.706473	-0.090163
C	-0.017960	-2.607036	-0.209361
C	-0.054818	-3.697949	0.864343
C	1.263531	-1.786076	-0.230468
C	2.233344	-1.869257	0.767243
C	3.381799	-1.082223	0.711197
Br	4.655677	-1.249989	2.109075
C	3.604340	-0.185863	-0.344778
N	4.776084	0.585141	-0.359907
C	5.165224	1.491291	-1.292300
C	6.528763	2.158274	-0.974885
F	7.077190	1.688482	0.156565
F	6.367773	3.466046	-0.837756
F	7.379734	1.934232	-1.964672
O	4.583851	1.818025	-2.296865
C	2.627319	-0.104649	-1.349037
C	1.486277	-0.890195	-1.282460
C	-1.310200	-0.703978	0.880620
C	-2.440500	0.089625	1.026623
C	-3.551809	-0.094691	0.191153
N	-4.715934	0.681828	0.292344
C	-4.976941	1.680335	1.173602
C	-6.376534	2.321202	0.985614
F	-7.077962	2.204679	2.102918
F	-6.246072	3.607208	0.695364
F	-7.075466	1.743094	-0.003825
O	-4.262341	2.103211	2.047960
H	-2.322658	-2.664243	-1.695506
H	-0.081838	-3.108499	-1.189492
H	-0.978346	-4.286185	0.769663
H	0.799758	-4.384347	0.768263
H	-0.044285	-3.266604	1.877117
H	2.113465	-2.550435	1.609596
H	5.405098	0.439289	0.424403
H	2.782139	0.584065	-2.176351
H	0.738795	-0.796852	-2.074374
H	-0.455503	-0.526265	1.537912
H	-2.480159	0.866893	1.786290
H	-5.448416	0.460376	-0.375799

13-conf10

- Electronic Energy (Eh): -6700.78195019

- Cartesian Coordinates:

Br	4.414871	1.849480	1.466734
C	3.205875	1.287428	0.114979
C	2.086037	2.076929	-0.138515
C	1.163840	1.711532	-1.117873
C	-0.089044	2.521064	-1.417775
C	-0.132862	3.895064	-0.743192
C	-1.346653	1.730531	-1.086216
C	-1.456363	1.038368	0.122523
C	-2.623704	0.360392	0.447400
Br	-2.701138	-0.563873	2.103678
C	-3.727940	0.345554	-0.424908
N	-4.884648	-0.357406	-0.055832
C	-6.041701	-0.480105	-0.753823
C	-7.115980	-1.330193	-0.027273

F	-8.187986	-0.588870	0.212075
F	-6.678601	-1.814345	1.145555
F	-7.467524	-2.355960	-0.787264
O	-6.309632	-0.012205	-1.832590
C	-3.614020	1.038461	-1.636117
C	-2.440379	1.716163	-1.951625
C	1.405396	0.532579	-1.832649
C	2.518413	-0.258485	-1.590087
C	3.446650	0.106280	-0.602551
N	4.587893	-0.655969	-0.312718
C	4.986018	-1.814877	-0.896151
C	6.309820	-2.376067	-0.315262
F	6.106787	-3.589445	0.175123
F	7.224449	-2.448955	-1.270832
F	6.801732	-1.608626	0.669997
O	4.440548	-2.424857	-1.781703
H	1.949953	2.985999	0.447245
H	-0.098108	2.689584	-2.507556
H	0.748784	4.499042	-1.005153
H	-1.030252	4.441956	-1.064756
H	-0.181321	3.803981	0.352907
H	-0.615777	1.015424	0.819174
H	-4.841365	-0.828281	0.843356
H	-4.456461	1.034050	-2.323879
H	-2.382225	2.247077	-2.905247
H	0.694980	0.216693	-2.600824
H	2.688552	-1.170414	-2.157754
H	5.182408	-0.289148	0.425042

13-conf11

- Electronic Energy (Eh): -6700.7816781

- Cartesian Coordinates:

Br	3.050769	0.008970	2.406054
C	2.767658	-0.621456	0.638185
C	1.602126	-1.319399	0.362175
C	1.340815	-1.808673	-0.923201
C	0.036005	-2.555146	-1.165399
C	-0.076741	-3.193294	-2.552495
C	-1.162646	-1.657542	-0.896120
C	-2.227640	-2.108656	-0.116951
C	-3.343578	-1.304862	0.096556
Br	-4.751792	-1.981767	1.174519
C	-3.434035	-0.020141	-0.464215
N	-4.575762	0.757493	-0.219565
C	-4.846118	2.007052	-0.674875
C	-6.213130	2.558143	-0.192659
F	-6.977185	2.842240	-1.236544
F	-6.027573	3.662993	0.514240
F	-6.875284	1.680871	0.577893
O	-4.161599	2.702431	-1.383253
C	-2.361055	0.430050	-1.247421
C	-1.250880	-0.378601	-1.452520
C	2.291264	-1.568707	-1.913999
C	3.465185	-0.866037	-1.647345
C	3.727193	-0.378038	-0.363877
N	4.891482	0.334091	-0.039779
C	5.924187	0.655425	-0.859161
C	7.056794	1.441213	-0.149074
F	8.179978	0.738524	-0.184534
F	7.256876	2.596764	-0.763493
F	6.772000	1.699431	1.136804
O	6.047894	0.397705	-2.030743
H	0.875901	-1.478527	1.162255
H	-0.000111	-3.371765	-0.424854
H	0.758332	-3.883063	-2.745529
H	-1.014472	-3.761529	-2.628151
H	-0.089387	-2.430604	-3.346042
H	-2.194794	-3.101995	0.335749
H	-5.280985	0.324683	0.369899

H	-2.414086	1.423907	-1.685935
H	-0.424893	0.006047	-2.055835
H	2.133385	-1.930883	-2.930525
H	4.194374	-0.688403	-2.434446
H	4.960414	0.642494	0.925804

13-conf12

- Electronic Energy (Eh): -6700.78205152

- Cartesian Coordinates:

Br	-2.635976	1.373363	1.935736
C	-2.540792	-0.189889	0.863138
C	-1.393876	-0.969423	0.930765
C	-1.272469	-2.127650	0.158481
C	-0.038972	-3.011433	0.273706
C	-0.158847	-3.934935	1.489275
C	1.237160	-2.182673	0.241307
C	1.524348	-1.440847	-0.910777
C	2.662259	-0.652709	-0.988155
Br	2.983876	0.322574	-2.584404
C	3.566487	-0.568542	0.088627
N	4.703535	0.243869	-0.032890
C	5.676298	0.455443	0.889068
C	6.786086	1.424970	0.406513
F	6.841408	2.478498	1.207712
F	6.571926	1.866336	-0.842743
F	7.959549	0.810962	0.427022
O	5.761092	-0.012583	1.997272
C	3.279239	-1.309619	1.238533
C	2.133722	-2.100973	1.305371
C	-2.333341	-2.471481	-0.679061
C	-3.486420	-1.696134	-0.755252
C	-3.612107	-0.536267	0.018605
N	-4.748962	0.285060	-0.019200
C	-5.870513	0.118836	-0.764431
C	-6.928951	1.231154	-0.547556
F	-8.058360	0.696598	-0.107865
F	-6.530723	2.149666	0.346269
F	-7.168289	1.852800	-1.692606
O	-6.117289	-0.767213	-1.544526
H	-0.577802	-0.661422	1.587828
H	-0.021988	-3.651463	-0.624326
H	-1.070363	-4.543619	1.408660
H	0.702768	-4.615151	1.562478
H	-0.229779	-3.359842	2.425235
H	0.840002	-1.471796	-1.761437
H	4.801140	0.729318	-0.920083
H	3.965860	-1.258106	2.080335
H	1.954131	-2.662294	2.223056
H	-2.265428	-3.371180	-1.295996
H	-4.303108	-1.976397	-1.416496
H	-4.719836	1.099314	0.587758

13-conf13

- Electronic Energy (Eh): -6700.78205157

- Cartesian Coordinates:

Br	2.983778	-0.323002	-2.584361
C	2.662220	0.652560	-0.988273
C	1.524329	1.440742	-0.911002
C	1.237177	2.182765	0.240961
C	-0.038946	3.011548	0.273230
C	-0.158821	3.935245	1.488651
C	-1.272440	2.127744	0.158145
C	-1.393907	0.969736	0.930747
C	-2.540804	0.190166	0.863224
Br	-2.636090	-1.372765	1.936284
C	-3.612035	0.536278	0.018476
N	-4.748842	-0.285112	-0.019247
C	-5.870424	-0.119004	-0.764455

C	-6.928751	-1.231417	-0.547516
F	-7.167388	-1.853714	-1.692371
F	-8.058487	-0.696871	-0.108679
F	-6.530780	-2.149383	0.346975
O	-6.117249	0.766936	-1.544657
C	-3.486291	1.695933	-0.755691
C	-2.333236	2.471323	-0.679598
C	2.133755	2.101217	1.305027
C	3.279246	1.309822	1.238298
C	3.566460	0.568548	0.088505
N	4.703493	-0.243902	-0.032883
C	5.676237	-0.455380	0.889117
C	6.785997	-1.425006	0.406686
F	7.959490	-0.811047	0.427175
F	6.841252	-2.478466	1.207978
F	6.571855	-1.866475	-0.842530
O	5.761032	0.012784	1.997261
H	0.839969	1.471562	-1.761657
H	-0.021954	3.651432	-0.624905
H	0.702805	4.615460	1.561757
H	-1.070324	4.543933	1.407925
H	-0.229771	3.360300	2.424700
H	-0.577897	0.661936	1.587984
H	-4.719763	-1.099193	0.587947
H	-4.302927	1.976003	-1.417081
H	-2.265276	3.370853	-1.296776
H	1.954192	2.662693	2.222624
H	3.965880	1.258416	2.080095
H	4.801079	-0.729521	-0.919985

13-conf14

- Electronic Energy (Eh): -6700.78161212

- Cartesian Coordinates:

Br	-4.656106	-1.250332	2.108962
C	-3.382057	-1.082207	0.711277
C	-2.233510	-1.869103	0.767360
C	-1.263612	-1.785708	-0.230252
C	0.017937	-2.606577	-0.209174
C	0.054995	-3.697372	0.864649
C	1.238709	-1.705954	-0.090214
C	2.341363	-1.891560	-0.923705
C	3.477803	-1.099949	-0.787269
Br	4.937257	-1.404310	-1.962276
C	3.551812	-0.094152	0.190632
N	4.715990	0.682304	0.291651
C	4.977265	1.680664	1.172991
C	6.377720	2.320007	0.986233
F	6.249427	3.608080	0.704883
F	7.073526	1.746951	-0.008336
F	7.081189	2.194524	2.101431
O	4.262719	2.103782	2.047277
C	2.440643	0.090197	1.026279
C	1.310321	-0.703426	0.880518
C	-1.486398	-0.889784	-1.282202
C	-2.627531	-0.104384	-1.348820
C	-3.604625	-0.185782	-0.344638
N	-4.776447	0.585090	-0.359795
C	-5.165539	1.491358	-1.292094
C	-6.529120	2.158259	-0.974701
F	-6.368024	3.465942	-0.836693
F	-7.379799	1.934946	-1.964880
F	-7.077938	1.687825	0.156292
O	-4.584081	1.818297	-2.296544
H	-2.113643	-2.550365	1.609647
H	0.081751	-3.108144	-1.189256
H	-0.799550	-4.383838	0.768759
H	0.978545	-4.285566	0.769922
H	0.044560	-3.265905	1.877372
H	2.322321	-2.663741	-1.695753

H	5.448109	0.461255	-0.377021
H	2.480433	0.867524	1.785882
H	0.455738	-0.525685	1.537950
H	-0.738862	-0.796292	-2.074048
H	-2.782406	0.584343	-2.176112
H	-5.405659	0.438926	0.424301

13-conf15

- Electronic Energy (Eh): -6700.78167738

- Cartesian Coordinates:

Br	-4.751613	-1.981604	-1.175211
C	-3.343579	-1.304919	-0.096871
C	-2.227577	-2.108665	0.116516
C	-1.162690	-1.657640	0.895885
C	0.036014	-2.555174	1.165086
C	-0.076707	-3.193439	2.552144
C	1.340831	-1.808674	0.922948
C	1.601945	-1.318765	-0.362202
C	2.767563	-0.620896	-0.638159
Br	3.050300	0.010467	-2.405769
C	3.727424	-0.378260	0.363747
N	4.891942	0.333529	0.039755
C	5.924262	0.655602	0.859399
C	7.057380	1.440427	0.149026
F	8.179677	0.736144	0.183309
F	7.259476	2.595278	0.764050
F	6.772133	1.699789	-1.136463
O	6.047334	0.398982	2.031266
C	3.465557	-0.866807	1.647066
C	2.291575	-1.569331	1.913655
C	-1.251073	-0.378837	1.452582
C	-2.361304	0.429769	1.247594
C	-3.434170	-0.020360	0.464227
N	-4.576053	0.757197	0.219807
C	-4.846218	2.006849	0.675002
C	-6.213501	2.557783	0.193340
F	-6.977529	2.840702	1.237602
F	-6.028445	3.663279	-0.512669
F	-6.875417	1.680873	-0.577821
O	-4.161478	2.702374	1.382987
H	-2.194591	-3.101900	-0.336412
H	-0.000054	-3.371762	0.424493
H	-1.014482	-3.761616	2.627786
H	0.758308	-3.883316	2.745072
H	-0.089224	-2.430824	3.345768
H	0.875507	-1.477275	-1.162219
H	4.961000	0.641705	-0.925891
H	4.194873	-0.689574	2.434150
H	2.133835	-1.931856	2.930081
H	-0.425129	0.005733	2.056013
H	-2.414407	1.423513	1.686353
H	-5.281203	0.324485	-0.369808

13-conf16

- Electronic Energy (Eh): -6700.78205157

- Cartesian Coordinates:

Br	-2.636594	-1.369159	-1.939563
C	-2.541049	0.192006	-0.863960
C	-1.394098	0.971599	-0.930354
C	-1.272429	2.128323	-0.155868
C	-0.038834	3.012146	-0.269638
C	-0.158435	3.937478	-1.483839
C	1.237174	2.183148	-0.238328
C	1.524205	1.439727	0.912765
C	2.661993	0.651306	0.989122
Br	2.983402	-0.326172	2.584064
C	3.566242	0.568457	-0.087738
N	4.703178	-0.244271	0.032746

C	5.675980	-0.454702	-0.889418
C	6.785680	-1.424916	-0.408014
F	6.571368	-1.867918	0.840630
F	7.959178	-0.810926	-0.427584
F	6.841080	-2.477385	-1.210590
O	5.760876	0.014775	-1.996998
C	3.279135	1.311111	-1.236667
C	2.133750	2.102735	-1.302479
C	-2.333087	2.470623	0.682573
C	-3.486196	1.695205	0.757545
C	-3.612128	0.536817	-0.018490
N	-4.748968	-0.284584	0.018148
C	-5.870164	-0.119920	0.764258
C	-6.927699	-1.233068	0.547249
F	-6.532923	-2.145654	-0.354149
F	-7.158680	-1.861867	1.690251
F	-8.060817	-0.698498	0.117615
O	-6.116804	0.764767	1.545936
H	-0.578192	0.664796	-1.588189
H	-0.021859	3.650821	0.629357
H	-1.069831	4.546230	-1.402377
H	0.703335	4.617614	-1.555966
H	-0.229421	3.363803	-2.420666
H	0.839834	1.469638	1.763444
H	4.800695	-0.730870	0.919318
H	3.965786	1.260584	-2.078505
H	1.954264	2.665311	-2.219419
H	-2.264967	3.369140	1.301208
H	-4.302728	1.974265	1.419493
H	-4.720361	-1.097318	-0.590867

13-conf17

- Electronic Energy (Eh): -6700.78161256

- Cartesian Coordinates:

Br	-4.937688	-1.404897	-1.961412
C	-3.477982	-1.100448	-0.786740
C	-2.341577	-1.892093	-0.923343
C	-1.238743	-1.706390	-0.090133
C	-0.017969	-2.607001	-0.209264
C	-0.054948	-3.697902	0.864450
C	1.263549	-1.786074	-0.230403
C	2.233317	-1.869226	0.767356
C	3.381790	-1.082231	0.711323
Br	4.655691	-1.250001	2.109165
C	3.604392	-0.185961	-0.344725
N	4.776093	0.585126	-0.359770
C	5.165525	1.490806	-1.292522
C	6.528712	2.158402	-0.974891
F	7.379856	1.935092	-1.964679
F	7.077393	1.688653	0.156480
F	6.367004	3.466043	-0.837424
O	4.584533	1.816949	-2.297504
C	2.627476	-0.104853	-1.349097
C	1.486393	-0.890347	-1.282497
C	-1.310159	-0.703794	0.880556
C	-2.440451	0.089829	1.026504
C	-3.551783	-0.094556	0.191071
N	-4.715914	0.681946	0.292218
C	-4.976748	1.680861	1.173073
C	-6.376681	2.321123	0.985613
F	-7.074559	1.744755	-0.005580
F	-7.078758	2.201431	2.102214
F	-6.247025	3.607875	0.698479
O	-4.261930	2.104202	2.047029
H	-2.322729	-2.664370	-1.695298
H	-0.081877	-3.108495	-1.189376
H	-0.978455	-4.286150	0.769633
H	0.799647	-4.384296	0.768491
H	-0.044570	-3.266573	1.877230

H	2.113345	-2.550371	1.609720
H	5.405155	0.439334	0.424502
H	2.782370	0.583669	-2.176543
H	0.738968	-0.797104	-2.074472
H	-0.455454	-0.526032	1.537820
H	-2.480067	0.867199	1.786068
H	-5.448419	0.460379	-0.375868

13-conf18

- Electronic Energy (Eh): -6700.7820515

- Cartesian Coordinates:

Br	-2.983941	-0.322773	2.584377
C	-2.662291	0.652547	0.988159
C	-1.524393	1.440723	0.910842
C	-1.237174	2.182576	-0.241208
C	0.038947	3.011363	-0.273538
C	0.158823	3.934975	-1.489026
C	1.272462	2.127595	-0.158353
C	1.393947	0.969467	-0.930778
C	2.540873	0.189947	-0.863162
Br	2.636199	-1.373152	-1.935969
C	3.612115	0.536239	-0.018504
N	4.748972	-0.285090	0.019272
C	5.870456	-0.118957	0.764631
C	6.929015	-1.231123	0.547566
F	7.169490	-1.852021	1.692752
F	8.057916	-0.696496	0.106604
F	6.530321	-2.150250	-0.345420
O	6.117163	0.767009	1.544848
C	3.486360	1.696020	0.755473
C	2.333272	2.471350	0.679298
C	-2.133696	2.100873	-1.305315
C	-3.279193	1.309497	-1.238536
C	-3.566477	0.568392	-0.088647
N	-4.703513	-0.244043	0.032789
C	-5.676417	-0.455342	-0.889089
C	-6.786239	-1.424849	-0.406559
F	-7.959707	-0.810842	-0.427257
F	-6.841468	-2.478451	-1.207663
F	-6.572199	-1.866084	0.842752
O	-5.761267	0.012854	-1.997215
H	-0.840089	1.471665	1.761537
H	0.021945	3.651317	0.624544
H	-0.702842	4.615127	-1.562216
H	1.070291	4.543716	-1.408312
H	0.229849	3.359959	-2.425024
H	0.577923	0.661524	-1.587929
H	4.719809	-1.099384	-0.587627
H	4.303020	1.976201	1.416787
H	2.265314	3.370984	1.296321
H	-1.954088	2.662225	-2.222977
H	-3.965785	1.257984	-2.080359
H	-4.801260	-0.729373	0.920032

13-conf19

- Electronic Energy (Eh): -6700.78195013

- Cartesian Coordinates:

Br	4.414738	1.849408	1.466921
C	3.205847	1.287380	0.115058
C	2.085983	2.076823	-0.138441
C	1.163863	1.711442	-1.117896
C	-0.089051	2.520921	-1.417801
C	-0.132902	3.894933	-0.743226
C	-1.346649	1.730391	-1.086237
C	-1.456367	1.038161	0.122463
C	-2.623741	0.360230	0.447326
Br	-2.701161	-0.564131	2.103567
C	-3.728020	0.345509	-0.424939

N	-4.884762	-0.357366	-0.055817
C	-6.041791	-0.480109	-0.753860
C	-7.116194	-1.329974	-0.027216
F	-7.468119	-2.355568	-0.787270
F	-8.187967	-0.588364	0.212337
F	-6.678797	-1.814331	1.145502
O	-6.309602	-0.012374	-1.832727
C	-3.614073	1.038490	-1.636111
C	-2.440406	1.716127	-1.951617
C	1.405542	0.532580	-1.832750
C	2.518608	-0.258433	-1.590188
C	3.446756	0.106308	-0.602579
N	4.588113	-0.655801	-0.312822
C	4.985900	-1.815106	-0.895703
C	6.310200	-2.375752	-0.315419
F	7.224772	-2.447038	-1.271230
F	6.801639	-1.608741	0.670399
F	6.108250	-3.589697	0.173915
O	4.439958	-2.425623	-1.780593
H	1.949787	2.985839	0.447378
H	-0.098113	2.689427	-2.507582
H	0.748730	4.498931	-1.005189
H	-1.030310	4.441795	-1.064790
H	-0.181363	3.803844	0.352870
H	-0.615762	1.015077	0.819084
H	-4.841463	-0.828194	0.843393
H	-4.456555	1.034119	-2.323825
H	-2.382249	2.247068	-2.905223
H	0.695198	0.216692	-2.600992
H	2.688792	-1.170329	-2.157895
H	5.182794	-0.288725	0.424676

13-conf20

- Electronic Energy (Eh): -6700.78168793

- Cartesian Coordinates:

Br	-4.755162	-2.002011	-1.127538
C	-3.344312	-1.301851	-0.068027
C	-2.230531	-2.103171	0.165166
C	-1.163831	-1.635542	0.932162
C	0.031849	-2.529996	1.224790
C	-0.083722	-3.132461	2.627560
C	1.338691	-1.793337	0.965147
C	1.613957	-1.359155	-0.336877
C	2.780588	-0.669414	-0.628843
Br	3.083531	-0.115815	-2.419006
C	3.726763	-0.378839	0.373267
N	4.891834	0.324470	0.033141
C	5.906507	0.697749	0.853049
C	7.032125	1.479986	0.128077
F	7.115987	2.706679	0.622820
F	6.815490	1.581493	-1.192514
F	8.192476	0.867815	0.306175
O	6.013668	0.497559	2.037426
C	3.451025	-0.812469	1.673355
C	2.276530	-1.507760	1.955904
C	-1.247914	-0.342519	1.455638
C	-2.355941	0.463817	1.230784
C	-3.430861	-0.003153	0.460209
N	-4.570902	0.771054	0.197263
C	-4.839409	2.030810	0.624775
C	-6.206388	2.572430	0.131807
F	-6.972035	2.872744	1.170074
F	-6.021260	3.665698	-0.592853
F	-6.866669	1.681809	-0.624917
O	-4.153793	2.740849	1.317357
H	-2.200932	-3.107861	-0.261972
H	-0.006180	-3.364830	0.505057
H	-1.020592	-3.700414	2.715184
H	0.752489	-3.814965	2.840545

H	-0.100572	-2.349788	3.401281
H	0.898003	-1.555380	-1.137994
H	4.978094	0.579456	-0.946568
H	4.169936	-0.598101	2.460747
H	2.107653	-1.827116	2.984976
H	-0.420453	0.055091	2.048423
H	-2.405798	1.468561	1.644105
H	-5.276752	0.326420	-0.382555