Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information

New J. Chem.

"Links Between Through-Bond Interactions and Assembly Structure in Simple Piperidones"

Ling Yuan, Bobby G. Sumpter, Khalil A. Abboud, and Ronald K. Castellano*

General. First principles calculations based on many body perturbation theory (MBPT), coupled clusters (CC), configuration interactions (CI) on a defined active space (CASSCF) and density functional theory (DFT) were all performed using the NWChem suite of codes. In each case, all-electron calculations were performed along with atom-centered, contracted Gaussian basis sets. For all cases, a full geometry optimization was performed for each epimer. Tight convergence criteria were used for the MP2 calculations: converence for the SCF was 10^{-8}, the AO and MO integrals 10^{-11}, and the CPHF 10^{-5}; energy convergence for the geometry optimization was 10^{-7} with a maximun gradient of 10^{-5}. For the DFT, CASSF, and coupled cluster calculations, the NWChem default tolerances were used. The CASSF and CC were single-point calculatons based on the optimized geometry with the specified basis set using MP2. The SIC-DFT calculations are perturbation corrections to SIC for the optmized DFT structures.

Cartesian Coordinates and Energies (related to Tables 4 and 5 in manuscript)

Compound 6-*ax*, optimized Cartesian coordinates for MP2/6-311++G:**
Total Energy (Hartree) = –290.51465615

C	1.18661670	0.05764435	-1.31923214
C	1.57365386	0.09207432	0.16023073
H	1.66225000	-0.93206895	0.54210318
C	0.51452893	0.86123716	0.95830811
H	0.75715507	0.86518059	2.02664127
H	0.51177388	1.90636793	0.61939717
N	-0.84608263	0.35025861	0.80055838
C	-1.20729120	0.29800531	-0.61501698
H	-1.24045984	1.33318476	-0.98164836
H	-2.22135746	-0.10913324	-0.69486315
C	-0.22892557	-0.49749156	-1.48689717
H	-0.24587648	-1.55625518	-1.20149137
C	-1.04632340	-0.92294978	1.47544016
H	2.55189924	0.56855917	0.29406566
H	-0.82631022	-0.79626424	2.53955191
H	-0.43078281	-1.75640038	1.09990885
H	-2.09697735	-1.21166028	1.37884791
H	-0.54460424	-0.44425475	-2.53528087
H	1.21475282	1.08194030	-1.71675612
H	1.90707498	-0.53125986	-1.89693859

Compound 6-*eq*, optimized Cartesian coordinates for MP2/6-311++G:**
Total Energy (Hartree) = –290.52003435

C	1.33218881	-0.41002505	-1.29329121
C	1.68007058	-0.29373207	0.18890668
H	1.68520280	-1.28899307	0.64734383
C	0.64526390	0.56180074	0.90917239
H	0.86985447	0.61069817	1.98019797
H	0.68430931	1.59885140	0.51372748
N	-0.68991594	-0.00179273	0.74859395

C	-1.05829314	-0.01686156	-0.66226464
H	-1.04622680	1.01112218	-1.08235387
H	-2.08384548	-0.39248591	-0.74417903
C	-0.10455640	-0.89988821	-1.45729910
H	-0.19110393	-1.92621221	-1.08336745
H	2.67621289	0.14250496	0.32151705
H	-0.39704166	-0.90116722	-2.51314834
C	-1.65626055	0.76791308	1.51302147
H	-1.70983744	1.82211623	1.18275848
H	-1.38280447	0.75033643	2.57137480
H	-2.64797188	0.32056369	1.40444828
H	1.42728940	0.57891379	-1.76053843
H	2.03175124	-1.07873409	-1.80554890

Compound 7-*ax*, optimized Cartesian coordinates for MP2/6-311++G:**
Total Energy (Hartree) = –364.42110024

O	1.68633697	0.35028631	-1.97081545
C	0.97093621	-0.01732235	-1.05643661
C	1.37914085	0.07124935	0.39836002
H	1.46868926	-0.94285086	0.80564839
C	0.30090395	0.85030885	1.18719209
H	0.55160055	0.86595957	2.25236506
H	0.29431613	1.88923370	0.83568785
N	-1.04638722	0.32153438	1.03014018
C	-1.41248880	0.28975147	-0.37867620
H	-1.43170998	1.32466641	-0.74141107
H	-2.42790615	-0.10867129	-0.47008403
C	-0.44011542	-0.52368818	-1.26381384
H	-0.48442250	-1.58173902	-0.97914628
C	-1.23321559	-0.95991634	1.69328705
H	2.35364875	0.56164525	0.46608354
H	-1.01010829	-0.84301769	2.75734815
H	-0.60933485	-1.78123436	1.30425911
H	-2.28076422	-1.25845153	1.59662944
H	-0.69816803	-0.43646948	-2.32263354

Compound 7-*eq*, optimized Cartesian coordinates for MP2/6-311++G:**
Total Energy (Hartree) = –364.42468023

O	1.87460482	-0.21747164	-1.95234166
C	1.10157628	-0.42817950	-1.03663074
C	1.47504954	-0.24054585	0.41868525
H	1.49766373	-1.22316134	0.90444016
C	0.42390576	0.61904236	1.12371938
H	0.65169607	0.68229509	2.19236452
H	0.45511774	1.64883268	0.71442639
N	-0.90203712	0.03491291	0.96512271
C	-1.27556057	0.04183746	-0.44353671
H	-1.24784499	1.07046776	-0.85620738
H	-2.30393867	-0.32158386	-0.53366785
C	-0.33517185	-0.85545936	-1.25093811
H	-0.45181286	-1.88515487	-0.89373797
H	2.46771822	0.21238824	0.47436412
H	-0.56104507	-0.81619028	-2.31917978
C	-1.87689556	0.77958192	1.74794877
H	-1.94672637	1.83690672	1.43429985

H	-1.59722316	0.74827542	2.80383711
H	-2.86155982	0.31881903	1.63774162

Compound 8-*ax*, optimized Cartesian coordinates for MP2/6-311++G:**
Total Energy (Hartree) = –481.84971098

C	1.18879593	1.15986764	-2.48634533
C	1.94808759	1.01358064	-1.16524242
H	2.06671272	-0.04984073	-0.92770248
C	1.17213695	1.70450586	-0.03989497
H	1.68778911	1.63516096	0.92029480
H	1.08099867	2.77368497	-0.27135233
N	-0.19031261	1.19167507	0.09812833
C	-0.92102377	1.41718103	-1.15363432
H	-0.91544538	2.49947325	-1.33596492
H	-1.96399541	1.12200291	-1.04161329
C	-0.26028899	0.69333796	-2.32832872
H	-0.28758470	-0.38666240	-2.13537234
C	-0.34953748	-0.06769849	0.70795958
H	2.95153912	1.44846686	-1.24530644
H	-0.82819678	0.87958617	-3.24762995
C	-1.61583865	-0.69129311	0.73614847
C	-1.80775885	-1.91204571	1.38152261
C	-0.75097526	-2.55292659	2.03432005
C	0.50238056	-1.94066926	2.03065229
C	0.70619287	-0.72239969	1.37647818
H	-2.47045292	-0.21299955	0.27184250
H	-2.79918066	-2.35689850	1.38099460
H	-0.90306345	-3.50323949	2.53600706
H	1.34292640	-2.41409374	2.53103392
H	1.70048704	-0.29335348	1.39153755
H	1.19184956	2.21699780	-2.78715615
H	1.69045157	0.59861098	-3.28177398

Compound 8-*eq*, optimized Cartesian coordinates for MP2/6-311++G:**
Total Energy (Hartree)= –481.84969145

C	2.37566447	-1.29442146	-2.07893893
C	2.71062980	-1.04308214	-0.60983507
H	2.66015523	-1.98548466	-0.05208740
C	1.71667984	-0.06241215	0.00050473
H	1.91316088	0.08147948	1.06786593
H	1.82684365	0.92166596	-0.49589022
N	0.35070745	-0.57755363	-0.13820801
C	-0.00990214	-0.74192379	-1.55005928
H	0.04791871	0.22115671	-2.09410474
H	-1.04898067	-1.08410972	-1.59226544
C	0.92290543	-1.74687558	-2.21505243
H	0.79146100	-2.72101766	-1.72975708
H	3.72637701	-0.64506418	-0.50438492
H	0.64649248	-1.85765516	-3.26979901
C	-0.60012497	0.23958622	0.56295800
C	-0.82723741	1.58171909	0.22200453
C	-1.76230688	2.33975318	0.93177298
C	-2.47708718	1.76393944	1.98692007
C	-2.25316901	0.42701232	2.32942942
C	-1.31784381	-0.33138803	1.61923154

H	-0.27429282	2.03382473	-0.59698061
H	-1.93286573	3.37847452	0.66189007
H	-3.20349804	2.35429366	2.53763766
H	-2.80615213	-0.02459185	3.14832403
H	-1.12666908	-1.37183190	1.86645787
H	2.51637090	-0.36268411	-2.64419362
H	3.05479713	-2.03845704	-2.50908778

Compound 9-*ax*, optimized Cartesian coordinates for MP2/6-311++G:**
Total Energy (Hartree) = –555.76167066

O	1.47667602	1.27262226	-3.28147751
C	0.99829054	0.91180952	-2.21825781
C	1.80640781	0.83750696	-0.93994999
H	1.90256804	-0.21644342	-0.65031293
C	1.06739371	1.59624161	0.18148346
H	1.61446952	1.54138394	1.12384975
H	1.00228580	2.65788619	-0.08135948
N	-0.29887530	1.11680232	0.35915172
C	-1.04867470	1.36561265	-0.87078838
H	-0.98170266	2.43911289	-1.07933256
H	-2.10540970	1.13863165	-0.73437157
C	-0.46693615	0.56844444	-2.05469828
H	-0.56089684	-0.50137352	-1.82628900
C	-0.45849377	-0.15689320	0.94809918
H	2.80258610	1.25058833	-1.12079635
H	-0.99315684	0.78354460	-2.98875248
C	-1.70009387	-0.82414417	0.89323834
C	-1.88422501	-2.05939608	1.51461757
C	-0.84447128	-2.66899349	2.22076810
C	0.38522487	-2.01412950	2.29484608
C	0.58112108	-0.78095739	1.66793449
H	-2.54247431	-0.37750473	0.37846028
H	-2.85607760	-2.54059808	1.44888934
H	-0.99059190	-3.63014291	2.70301901
H	1.21145613	-2.46227130	2.83983607
H	1.55449390	-0.31336082	1.75336316

Compound 9-*eq*, optimized Cartesian coordinates for MP2/6-311++G:**
Total Energy (Hartree) = –555.76008186

O	2.92818912	-1.13860020	-2.76249273
C	2.14343510	-1.25795700	-1.83628543
C	2.50926714	-0.95138059	-0.40083311
H	2.45266442	-1.87841455	0.18163745
C	1.50525466	0.04783204	0.18191108
H	1.70529455	0.21390608	1.24446818
H	1.61888546	1.01811420	-0.33643194
N	0.14412078	-0.47710320	0.04777386
C	-0.21603010	-0.62978536	-1.36408851
H	-0.13258690	0.32819747	-1.91021278
H	-1.25959293	-0.95298326	-1.41840736
C	0.69888387	-1.66424227	-2.02639798
H	0.53878430	-2.63193123	-1.53650316
H	3.52813844	-0.55836296	-0.36248835
H	0.48589965	-1.75664570	-3.09416555
C	-0.81113399	0.33156142	0.75751248

C	-1.04310926	1.67352353	0.42219550
C	-1.98019545	2.42299611	1.13815222
C	-2.68975106	1.83770750	2.19159566
C	-2.45967709	0.50020929	2.52725822
C	-1.52242857	-0.25049689	1.81140244
H	-0.49379632	2.13243942	-0.39571621
H	-2.15595243	3.46193885	0.87413192
H	-3.41766132	2.42150736	2.74707881
H	-3.00908446	0.04242733	3.34487281
H	-1.32617929	-1.29107439	2.05290484

Compound 10-*ax*, optimized Cartesian coordinates for MP2/6-311++G:**
Total Energy (Hartree) = –830.04605435 (convergence on the optimization was 3.8×10^{-5}, max gradient 1.1×10^{-3})

C	0.81326605	0.59285498	-1.13329554
C	1.28952130	0.52779861	0.31979622
H	0.65227304	1.18343230	0.93187640
C	1.14622416	-0.91171905	0.83077579
H	1.84297779	-1.54481441	0.25808891
H	1.43942665	-0.97462963	1.88553421
N	-0.18832743	-1.48452492	0.68671506
C	-0.64351597	-1.39229336	-0.69764609
H	-1.65964257	-1.79788034	-0.75410016
H	0.00567947	-2.04044108	-1.30632372
C	-0.59740183	0.02168318	-1.29095930
H	-1.29816997	0.65858389	-0.73227463
C	-1.14667078	-0.92567164	1.62959037
C	2.74119618	1.01127515	0.47027512
H	3.40767097	0.29413152	-0.02724548
H	2.85346880	1.97161225	-0.04916631
C	3.13510238	1.16280735	1.91609172
C	2.64996638	2.24736486	2.66332405
H	2.04248698	3.00566971	2.17349045
C	2.94829328	2.37577471	4.02165313
H	2.56969288	3.22750321	4.58125137
C	3.73598261	1.41018281	4.65822330
H	3.97930101	1.51372345	5.71144820
C	4.22742250	0.32642147	3.92639464
H	4.84149848	-0.42699151	4.41367690
C	3.93003519	0.20836131	2.56521593
H	4.32109511	-0.63426449	1.99924295
C	-1.04933401	0.01296103	-2.75826786
H	-0.91273122	1.01839001	-3.18084502
H	-0.40153840	-0.66732702	-3.32800859
C	-2.48497638	-0.41558886	-2.90272655
C	-3.51991723	0.41871328	-2.45186399
H	-3.28054974	1.40362674	-2.05333154
C	-4.85459729	0.01166302	-2.52116663
H	-5.64287020	0.67531960	-2.17284175
C	-5.17454971	-1.24703951	-3.04236814
H	-6.21181989	-1.56196943	-3.10500653
C	-4.15547407	-2.08596438	-3.50153161
H	-4.39619335	-3.06200989	-3.91376302
C	-2.82257717	-1.66919550	-3.42901713
H	-2.03163361	-2.32513209	-3.78752427

H	-1.36952291	0.14490130	1.48457514
H	-0.75890667	-1.05484322	2.64377517
H	-2.08665166	-1.47689552	1.54667185
H	1.50485700	0.00308651	-1.75665724
H	0.85120224	1.62677436	-1.50272915

Compound 10-*eq*, optimized Cartesian coordinates for MP2/6-311++G:**
Total Energy (Hartree) = –830.04581103 (convergence on the optimization was 1.7×10^{-5}, max gradient 7.1×10^{-4})

C	0.84672152	0.34457526	-1.07028999
C	1.29757452	0.33381420	0.39036279
H	1.41554845	-0.70884681	0.72032553
C	0.22809628	1.01357642	1.25359271
H	0.50432067	0.96690615	2.31318109
H	0.18510658	2.07673901	0.96971884
N	-1.11654258	0.46482667	1.10386006
C	-1.52524204	0.48225050	-0.29787777
H	-1.60258951	1.53581902	-0.61154022
H	-2.52915688	0.04912262	-0.37190523
C	-0.55932186	-0.22727996	-1.25460838
H	-0.54346761	-1.30109705	-1.01667260
C	-1.25504233	-0.85032418	1.71336007
C	2.65449649	1.03518421	0.54244252
H	3.36315678	0.58305588	-0.16388033
H	2.53804117	2.08893691	0.25281068
C	3.20835972	0.95554510	1.94010422
C	3.12746195	2.04536473	2.81814498
H	2.67968234	2.97544371	2.47326051
C	3.62650771	1.95582278	4.12185733
H	3.56185667	2.81321037	4.78615399
C	4.21215627	0.76768226	4.56708609
H	4.61174830	0.69890993	5.57453172
C	4.29754389	-0.32820147	3.70146834
H	4.76238912	-1.25148873	4.03627064
C	3.79342620	-0.23362201	2.40237127
H	3.87203217	-1.08474427	1.72824000
C	-1.01727673	-0.06849568	-2.71101550
H	-1.05282778	1.00309370	-2.94936224
H	-0.26003502	-0.52011853	-3.36545865
C	-2.36162223	-0.68907506	-2.98208590
C	-3.52024425	0.09681387	-3.05799684
H	-3.43951115	1.17652601	-2.94979930
C	-4.77091661	-0.48701194	-3.28348652
H	-5.65711196	0.13834511	-3.34548428
C	-4.87961671	-1.87243554	-3.43362695
H	-5.84787423	-2.32766942	-3.62100241
C	-3.73183745	-2.66795424	-3.36075943
H	-3.80626542	-3.74408680	-3.48992170
C	-2.48564813	-2.07844473	-3.13074648
H	-1.59354306	-2.70047207	-3.08648759
H	-1.02397436	-0.77101228	2.77941449
H	-0.60725867	-1.63004781	1.28095091
H	-2.29241040	-1.17893580	1.60861066
H	0.84307972	1.38998034	-1.42185020
H	1.56778159	-0.19989367	-1.69697988

Compound 11-*ax*, optimized Cartesian coordinates for MP2/6-311++G:**
Total Energy (Hartree) = –1021.38071339

C	1.03570217	0.97600010	-1.57573681
C	1.57746067	0.84701337	-0.15161238
H	0.86417653	1.31631156	0.54341631
C	1.64596296	-0.63977672	0.20464780
H	2.31046460	-1.15527446	-0.50324697
H	2.06440382	-0.80635129	1.19946866
N	0.32572184	-1.26616817	0.09142685
C	-0.11972416	-1.20254932	-1.30343996
H	-1.02884205	-1.79153215	-1.44144205
H	0.65836256	-1.68265938	-1.91378625
C	-0.29760465	0.24906419	-1.75480047
H	-1.04450040	0.70849828	-1.08932294
C	-0.62453493	-0.87125277	1.05665316
C	-2.01028946	-0.96375868	0.80334055
H	-2.37804477	-1.29483499	-0.16053289
C	-2.94596492	-0.62095729	1.78120933
H	-4.00310074	-0.70553380	1.54615963
C	-2.54010001	-0.17086598	3.03975078
H	-3.27055613	0.09363412	3.79668096
C	-1.17159566	-0.06848291	3.30016086
H	-0.82418837	0.28373980	4.26719172
C	-0.22697080	-0.40864538	2.32997149
H	0.82170347	-0.29937435	2.57877890
C	2.93033882	1.54973549	0.00963977
H	3.66110992	1.10194072	-0.67771955
H	2.82071520	2.60161726	-0.28859142
C	3.42982441	1.46082293	1.42749513
C	2.77163453	2.16409909	2.44788784
H	1.94607554	2.82530387	2.19429903
C	3.17385628	2.04071086	3.78001677
H	2.65708920	2.59805841	4.55538312
C	4.23637941	1.19452735	4.11586802
H	4.55199343	1.09825134	5.14934686
C	4.90261148	0.49095133	3.10804845
H	5.73351422	-0.16114980	3.35967634
C	4.49581226	0.62152676	1.77677528
H	5.01659972	0.06992917	0.99717311
C	-0.81435750	0.35406274	-3.19424516
H	-0.89678278	1.41607645	-3.46424132
H	-0.08053962	-0.08935899	-3.88093571
C	-2.14818989	-0.32725439	-3.35047277
C	-3.28792452	0.21291409	-2.73592586
H	-3.21143726	1.16086111	-2.20765805
C	-4.52070715	-0.43981423	-2.80861203
H	-5.39356871	-0.00353272	-2.33245147
C	-4.62964682	-1.65829800	-3.48789893
H	-5.58623381	-2.16636120	-3.54783226
C	-3.50219320	-2.20555595	-4.10744126
H	-3.58048640	-3.14649153	-4.64336187
C	-2.27204109	-1.54511265	-4.03199672
H	-1.39776137	-1.97693564	-4.51377511
H	1.76939495	0.52703074	-2.26664266
H	0.92835419	2.03541899	-1.84551562

Compound 11-*eq*, optimized Cartesian coordinates for MP2/6-311++G:**
Total Energy (Hartree) = –1021.37752758

C	1.23709913	0.89500139	-1.74961938
C	1.85821965	0.60533060	-0.38500347
H	2.20427907	-0.43797232	-0.36697211
C	0.82382639	0.74627736	0.72860672
H	1.26826847	0.43087988	1.67584480
H	0.53613781	1.81459431	0.82661378
N	-0.33556139	-0.08956341	0.46013366
C	-0.98467762	0.30082132	-0.79243412
H	-1.28521236	1.36883804	-0.74393406
H	-1.89196554	-0.28845747	-0.92758356
C	-0.04240620	0.09422811	-1.96996142
H	0.20580672	-0.97639532	-1.99744446
C	-1.22969915	-0.28856700	1.53907859
C	-2.25773664	-1.24339376	1.39960675
H	-2.32560243	-1.82208742	0.48373072
C	-3.15326522	-1.48382728	2.43929129
H	-3.93388161	-2.22957450	2.30855023
C	-3.04055614	-0.78982987	3.65023381
H	-3.73544480	-0.98356847	4.46305682
C	-2.01398627	0.14356243	3.80398273
H	-1.90946900	0.68873091	4.73820887
C	-1.12183358	0.40352465	2.75693881
H	-0.34631953	1.14730358	2.90017972
C	3.06557205	1.52047778	-0.12719857
H	3.79028247	1.37451189	-0.93934771
H	2.73501960	2.56705278	-0.17137836
C	3.71977583	1.24956616	1.20119991
C	3.51109530	2.09576665	2.29926674
H	2.91482673	2.99680682	2.17134430
C	4.06967627	1.80190430	3.54788133
H	3.89995715	2.47064693	4.38819679
C	4.84203074	0.64860995	3.71321927
H	5.27613751	0.41706374	4.68170914
C	5.06126530	-0.20191605	2.62438006
H	5.66688904	-1.09679134	2.74373303
C	4.49803180	0.09660836	1.38066972
H	4.67592287	-0.56321353	0.53381815
C	-0.72202298	0.46504078	-3.29589219
H	-1.02430116	1.52066144	-3.26478064
H	0.01331717	0.36118602	-4.10495372
C	-1.91866616	-0.40550055	-3.57410834
C	-3.22479508	0.05996506	-3.36853005
H	-3.38060060	1.09199000	-3.06166475
C	-4.32489041	-0.78295217	-3.56050062
H	-5.33120944	-0.40483573	-3.39816462
C	-4.12860024	-2.10873665	-3.95820534
H	-4.98086596	-2.76578880	-4.10615276
C	-2.83020098	-2.58457344	-4.17025897
H	-2.66966679	-3.61227512	-4.48667496
C	-1.73607250	-1.73776189	-3.97450563
H	-0.72745195	-2.10841256	-4.14663202
H	1.96339510	0.67860531	-2.54501884
H	0.99901891	1.96909269	-1.81506388

Compound 2-*ax*, optimized Cartesian coordinates for MP2/6-311++G:**
Total Energy (Hartree) = –903.95933373 (convergence on optimization: energy was to 6.8×10^{-6}, max grad = 2.7×10^{-4})

O	1.50499798	0.78914029	-2.01257165
C	0.78051776	0.50084969	-1.07058663
C	1.25127502	0.51501342	0.36755774
H	0.57519993	1.17129889	0.93505303
C	1.08462321	-0.92511797	0.92359414
H	1.78702664	-1.57856045	0.38591324
H	1.36432674	-0.93884626	1.98230780
N	-0.25239682	-1.47587433	0.77885348
C	-0.67938564	-1.42874851	-0.60959331
H	-1.69590519	-1.82869608	-0.68596782
H	-0.01953521	-2.08498415	-1.19534442
C	-0.63195875	-0.01300877	-1.24440322
H	-1.30298495	0.63389280	-0.66081194
C	-1.21641040	-0.87746490	1.69197533
C	2.68828577	1.01606115	0.52092049
H	3.36630279	0.32780869	0.00310490
H	2.78345062	1.98586603	0.01997625
C	3.06106793	1.13143633	1.97521126
C	2.50688982	2.15386952	2.76099115
H	1.86104925	2.89475181	2.29311262
C	2.79034778	2.24603084	4.12554158
H	2.35777104	3.04879900	4.71653717
C	3.63042523	1.30490920	4.72972594
H	3.85228091	1.37467514	5.79047987
C	4.19515765	0.28563778	3.95806432
H	4.85583393	-0.44340784	4.41915817
C	3.90804322	0.20012181	2.59154157
H	4.35022548	-0.59386998	1.99330894
C	-1.08502459	-0.02598556	-2.70511181
H	-0.94668875	0.97496588	-3.12909919
H	-0.43685342	-0.69989930	-3.27705603
C	-2.52397334	-0.45490380	-2.81878252
C	-3.54874536	0.39642417	-2.37725196
H	-3.29565773	1.39091618	-2.01369769
C	-4.88592889	-0.00537217	-2.42217855
H	-5.66629726	0.66957697	-2.08204045
C	-5.21894649	-1.27561294	-2.90425313
H	-6.25796478	-1.58991969	-2.94077576
C	-4.20906934	-2.13055898	-3.35370301
H	-4.46155921	-3.11487398	-3.73823130
C	-2.87222748	-1.72117019	-3.30805051
H	-2.08846795	-2.38754384	-3.66219105
H	-1.37677290	0.20373455	1.54302442
H	-0.87409540	-1.02999970	2.71946020
H	-2.17957843	-1.38070630	1.56964638

Compound 2-*eq*, optimized Cartesian coordinates for MP2/6-311++G:**
Total Energy (Hartree) = –903.95896464 (convergence on the optimization was 1.8×10^{-5}, max gradient 1.7×10^{-4})

O	1.43702265	0.80119072	-1.89301033
C	0.78751327	0.29739212	-0.98708998
C	1.26744444	0.28910987	0.44976403

H	1.34348881	-0.75982318	0.77623648
C	0.18014651	0.97955518	1.31358183
H	0.46951696	0.93821843	2.36825890
H	0.14322638	2.03993389	1.02415745
N	-1.15523487	0.42859541	1.16318905
C	-1.56529441	0.46221994	-0.23091428
H	-1.62392482	1.51515635	-0.54231117
H	-2.57012119	0.03497435	-0.32038175
C	-0.60141382	-0.26925832	-1.20130695
H	-0.58187243	-1.33348418	-0.92380853
C	-1.31090953	-0.88467738	1.77402155
C	2.62538018	0.97571926	0.59240033
H	3.33172112	0.51819436	-0.10927075
H	2.51898472	2.02414496	0.29049577
C	3.15278829	0.89698621	1.99882481
C	3.07067507	1.99802825	2.86256970
H	2.63918857	2.92717343	2.49642906
C	3.54755406	1.91977081	4.17402375
H	3.48476484	2.78809217	4.82447794
C	4.11337863	0.72975761	4.64181069
H	4.49164121	0.66984983	5.65843294
C	4.20427582	-0.37638128	3.78978645
H	4.66177062	-1.29749453	4.14239312
C	3.72049083	-0.29203180	2.48064528
H	3.80416140	-1.15053631	1.81665787
C	-1.04731076	-0.12757992	-2.65900019
H	-1.07012429	0.93844190	-2.91348752
H	-0.29242830	-0.58488444	-3.30713141
C	-2.39758615	-0.74296347	-2.90472792
C	-3.54600629	0.05563864	-2.98462094
H	-3.44697036	1.13503234	-2.89520439
C	-4.80477997	-0.51457504	-3.19579446
H	-5.68056788	0.12390312	-3.26607195
C	-4.93083974	-1.89999214	-3.32559644
H	-5.90653255	-2.34339831	-3.49785520
C	-3.79268899	-2.70977326	-3.24651077
H	-3.88332534	-3.78593609	-3.36413133
C	-2.53830371	-2.13381920	-3.02932288
H	-1.65211521	-2.76550666	-2.98211188
H	-1.02865491	-0.81913856	2.82917566
H	-0.70880915	-1.68427842	1.30829669
H	-2.36313211	-1.17830577	1.71788636

Compound 3-*ax*, optimized Cartesian coordinates for MP2/6-311++G:**
Total Energy (Hartree) = –1095.29343297

O	1.55519133	1.50345813	-2.37959404
C	0.96759095	0.92445734	-1.47663195
C	1.53516232	0.80452229	-0.07396524
H	0.80224010	1.25426738	0.61351378
C	1.59049844	-0.69949539	0.27845532
H	2.26008549	-1.21605742	-0.42294293
H	2.01224820	-0.84799332	1.27431628
N	0.27371753	-1.31988115	0.17221386
C	-0.16281325	-1.25810120	-1.21895101
H	-1.07954689	-1.83249083	-1.36531146
H	0.60896580	-1.74287378	-1.83253857

C	-0.35119329	0.20302002	-1.68714239
H	-1.08227603	0.65456431	-0.99891389
C	-0.67921776	-0.92147612	1.13965185
C	-2.06473842	-1.01291036	0.88389135
H	-2.43264073	-1.34776844	-0.07981913
C	-3.00113753	-0.67131204	1.86335939
H	-4.05874708	-0.75737492	1.62807257
C	-2.59346757	-0.22438278	3.12221161
H	-3.32424888	0.04008601	3.87966703
C	-1.22550072	-0.11896843	3.38355269
H	-0.87764203	0.23177229	4.35166351
C	-0.27994506	-0.45780405	2.41203758
H	0.77004038	-0.35222676	2.66227753
C	2.88487873	1.50501985	0.08716752
H	3.60971520	1.05922051	-0.60438241
H	2.77484903	2.55323839	-0.21565544
C	3.37314185	1.40609386	1.51026105
C	2.71621590	2.11091335	2.53152626
H	1.89235813	2.77532379	2.27702445
C	3.11939638	1.98772435	3.86446400
H	2.60302123	2.54709751	4.63985754
C	4.18335211	1.14297105	4.19898224
H	4.49908690	1.04612243	5.23343079
C	4.84877915	0.43789163	3.19227825
H	5.68137335	-0.21379148	3.44270006
C	4.44107373	0.56741454	1.85964906
H	4.96292637	0.01763087	1.07892974
C	-0.86711130	0.30728769	-3.12286652
H	-0.94417266	1.36749393	-3.39232755
H	-0.12956365	-0.13100233	-3.80571785
C	-2.20122264	-0.38083486	-3.26453773
C	-3.34257199	0.16005784	-2.65129917
H	-3.26681148	1.11040473	-2.12586731
C	-4.57635049	-0.49334513	-2.72499454
H	-5.44992465	-0.05523177	-2.24989548
C	-4.68452270	-1.71061819	-3.40625422
H	-5.64182270	-2.21971466	-3.46576942
C	-3.55741049	-2.25898889	-4.02450457
H	-3.63474252	-3.19978214	-4.56263674
C	-2.32574783	-1.59864178	-3.94817909
H	-1.45106184	-2.02869358	-4.43197799

Compound 3-*eq*, optimized Cartesian coordinates for MP2/6-311++G:**
Total Energy (Hartree) = –1095.28806957

O	1.58439770	1.68034717	-2.42118569
C	1.15932711	0.84275790	-1.64111102
C	1.81547836	0.55979320	-0.29966991
H	2.13894600	-0.49210630	-0.31071706
C	0.76672135	0.68534405	0.81582570
H	1.22077498	0.37079836	1.75889651
H	0.47868006	1.75201861	0.91420425
N	-0.38489022	-0.15879282	0.53979290
C	-1.04080274	0.24602661	-0.70413069
H	-1.33920520	1.31288260	-0.65378015
H	-1.94719619	-0.34269676	-0.85179561
C	-0.10358523	0.04261353	-1.89994020

H	0.17276291	-1.02253631	-1.90556241
C	-1.28350029	-0.35362526	1.62179052
C	-2.30990615	-1.30712551	1.48380526
H	-2.38257936	-1.88481220	0.56693894
C	-3.20766570	-1.54540633	2.52308424
H	-3.99015042	-2.28805687	2.39313586
C	-3.09415625	-0.85020555	3.73284927
H	-3.78889048	-1.04210229	4.54587627
C	-2.06860140	0.08165672	3.88555618
H	-1.96332852	0.62905450	4.81837550
C	-1.17474544	0.33963998	2.83865019
H	-0.40047638	1.08424999	2.98263508
C	3.02247840	1.47185785	-0.05057655
H	3.74299470	1.32997634	-0.86291008
H	2.69811221	2.51705269	-0.10391742
C	3.66554674	1.19031723	1.28263959
C	3.45813030	2.03418453	2.38308246
H	2.86235478	2.93545062	2.25779953
C	4.01621242	1.73978785	3.63183042
H	3.84699960	2.40737565	4.47204990
C	4.78805223	0.58722796	3.79861800
H	5.22619162	0.35772790	4.76641320
C	5.00714484	-0.26140389	2.70898517
H	5.61235673	-1.15545471	2.82893892
C	4.44472797	0.03782004	1.46516114
H	4.62541053	-0.62276897	0.61991910
C	-0.77423242	0.41303308	-3.22629359
H	-1.06958121	1.46800588	-3.20025389
H	-0.03935546	0.31611320	-4.03225378
C	-1.97037580	-0.46509472	-3.49042202
C	-3.27797951	-0.00234971	-3.28567108
H	-3.43660491	1.02881045	-2.97878385
C	-4.37812398	-0.84551764	-3.47720093
H	-5.38396993	-0.46810791	-3.31605542
C	-4.18358250	-2.17076845	-3.87445499
H	-5.03648201	-2.82720434	-4.02627844
C	-2.88514610	-2.64510153	-4.08626862
H	-2.72558132	-3.67193848	-4.40288571
C	-1.79104845	-1.79788351	-3.89171883
H	-0.78395548	-2.17065979	-4.06616057

Compound 3-*ax*, optimized Cartesian coordinates for MP2/6-31G:**
Total Energy (Hartree) = –1094.45350778

O	1.54309346	1.51379630	-2.36984127
C	0.95748438	0.92272016	-1.46463683
C	1.52890286	0.80332162	-0.06569007
H	0.81032627	1.26094865	0.62413945
C	1.57386108	-0.69580949	0.29516665
H	2.23538277	-1.21743783	-0.40115185
H	1.99420918	-0.84063249	1.28608357
N	0.25558274	-1.30898733	0.19000649
C	-0.17743868	-1.25445520	-1.20081774
H	-1.09039558	-1.82440593	-1.34760679
H	0.59248435	-1.74209381	-1.80393922
C	-0.35790075	0.20096314	-1.67935563
H	-1.09544308	0.65385897	-1.00666869

C	-0.69672986	-0.91120302	1.15667806
C	-2.07838426	-1.01381713	0.90428284
H	-2.44474935	-1.33311935	-0.05941915
C	-3.01046140	-0.68463372	1.88517956
H	-4.06372488	-0.77265168	1.65324510
C	-2.60442414	-0.25214611	3.14531716
H	-3.33229507	0.00355523	3.90257555
C	-1.24017330	-0.14067639	3.40303762
H	-0.89513308	0.20049918	4.37029034
C	-0.29707491	-0.46666481	2.43180746
H	0.74760261	-0.35380150	2.67821909
C	2.88344628	1.49121279	0.08046131
H	3.59841319	1.03147991	-0.60441269
H	2.78609902	2.53172115	-0.23311410
C	3.37700764	1.40080039	1.49876639
C	2.72430824	2.10870549	2.51677834
H	1.89903788	2.76436027	2.26514993
C	3.13672502	1.99505215	3.84297195
H	2.62616987	2.55426750	4.61576282
C	4.20752551	1.16319263	4.17358540
H	4.52964653	1.07479966	5.20204687
C	4.86597524	0.45483264	3.16984461
H	5.69939056	-0.18898205	3.41752342
C	4.44854887	0.57041749	1.84369856
H	4.96495532	0.02057468	1.06611311
C	-0.85581564	0.29626587	-3.11900733
H	-0.92117268	1.34825798	-3.40058116
H	-0.11871878	-0.15338470	-3.78684080
C	-2.18897611	-0.38478341	-3.26878642
C	-3.32858037	0.15803417	-2.66050273
H	-3.25215281	1.10020162	-2.13023975
C	-4.56027063	-0.48784631	-2.74684921
H	-5.43182392	-0.05126071	-2.27719309
C	-4.67018875	-1.69440791	-3.43965663
H	-5.62557960	-2.19637161	-3.50879542
C	-3.54426690	-2.24390513	-4.05044866
H	-3.62207697	-3.17696795	-4.59259935
C	-2.31292387	-1.59459608	-3.95969277
H	-1.44065750	-2.02364756	-4.43828663

Compound 3-*eq*, optimized Cartesian coordinates for MP2/6-31G:**
Total Energy (Hartree) = –1094.44949313

O	1.58579549	1.66035555	-2.41167016
C	1.14640122	0.82769963	-1.62241508
C	1.80302234	0.54287724	-0.28599480
H	2.11540803	-0.50697209	-0.29485899
C	0.76262516	0.67825276	0.83282607
H	1.21056379	0.34512337	1.76687484
H	0.50359878	1.74476502	0.94807336
N	-0.40437681	-0.14138646	0.55120739
C	-1.05525496	0.27159128	-0.69129727
H	-1.34002456	1.33713086	-0.65420147
H	-1.96658349	-0.30181005	-0.83256695
C	-0.12148699	0.04508859	-1.88221238
H	0.13707979	-1.01956565	-1.87614442
C	-1.30014074	-0.34471624	1.63440220

C	-2.31812336	-1.30280332	1.49050596
H	-2.38401362	-1.87238985	0.57304779
C	-3.21397374	-1.54698820	2.52469878
H	-3.99136849	-2.28762457	2.39012952
C	-3.10053477	-0.86246880	3.73658235
H	-3.79290543	-1.05968406	4.54354169
C	-2.07929239	0.06908963	3.89501878
H	-1.97592419	0.60507908	4.82952512
C	-1.18764351	0.33617944	2.85445662
H	-0.42138133	1.08332531	3.00073254
C	3.01402262	1.44726195	-0.05308687
H	3.72118809	1.29888869	-0.87010118
H	2.69141985	2.48781016	-0.11359174
C	3.66816567	1.17816060	1.27259829
C	3.46978614	2.03276186	2.36228361
H	2.87651678	2.92951507	2.23017355
C	4.04019383	1.75224814	3.60355062
H	3.88080439	2.42692488	4.43412515
C	4.81433438	0.60552903	3.77280974
H	5.25657018	0.38589225	4.73493547
C	5.02486475	-0.25168994	2.69189071
H	5.63355036	-1.13779577	2.81433426
C	4.45315586	0.03295285	1.45363777
H	4.62616586	-0.62955057	0.61356737
C	-0.77299125	0.41245274	-3.21429784
H	-1.06651477	1.46364132	-3.19352560
H	-0.02919387	0.31653850	-4.00593104
C	-1.96193296	-0.46475925	-3.49185297
C	-3.26809449	-0.00205854	-3.30209851
H	-3.42782206	1.02700342	-3.00295776
C	-4.36098952	-0.84441469	-3.50712595
H	-5.36489414	-0.46976155	-3.35881676
C	-4.15951974	-2.16720690	-3.89839063
H	-5.00568410	-2.82147343	-4.05891730
C	-2.86102412	-2.64012392	-4.09268219
H	-2.69779128	-3.66386870	-4.40257386
C	-1.77330527	-1.79450029	-3.88727577
H	-0.76617853	-2.16244977	-4.04690458

Compound 3-*ax*, optimized Cartesian coordinates for MP2/cc-pvdz:
Total Energy (Hartree) = –1094.334050

O	1.55716164	1.50784320	-2.38360252
C	0.97109747	0.92441543	-1.48078227
C	1.53458153	0.80386992	-0.07401592
H	0.79729741	1.25570407	0.61725523
C	1.59113593	-0.70130603	0.27912437
H	2.26468615	-1.21841558	-0.42621016
H	2.01503268	-0.84932461	1.28059391
N	0.27569520	-1.32518491	0.17176378
C	-0.16291564	-1.26019061	-1.21889909
H	-1.08524394	-1.83647078	-1.36622116
H	0.61235483	-1.74561054	-1.83682955
C	-0.35072147	0.20273869	-1.68640030
H	-1.08585565	0.65646916	-0.99392132
C	-0.67689847	-0.92241356	1.13737706

C	-2.06643889	-1.01186848	0.88014961
H	-2.43588007	-1.34964567	-0.08856047
C	-3.00475221	-0.67267834	1.86288291
H	-4.06863111	-0.75765576	1.62560474
C	-2.59647295	-0.22333872	3.12548646
H	-3.33181074	0.04304985	3.88738459
C	-1.22446417	-0.11885299	3.38733956
H	-0.87435565	0.23552690	4.36045401
C	-0.27667213	-0.45524583	2.41238472
H	0.77917638	-0.35045276	2.66414137
C	2.88442021	1.50673074	0.08383428
H	3.61267483	1.05752633	-0.61081336
H	2.77263599	2.56045345	-0.21847115
C	3.37275438	1.40635868	1.50689293
C	2.71450071	2.11548613	2.53052351
H	1.88450239	2.78212284	2.27465244
C	3.11632163	1.98910087	3.86744238
H	2.59812141	2.55276242	4.64770652
C	4.18637279	1.14473535	4.20322589
H	4.50257375	1.04507883	5.24453061
C	4.85176503	0.43537398	3.19351361
H	5.68961780	-0.21991706	3.44508603
C	4.44405893	0.56558589	1.85713046
H	4.96786092	0.01257170	1.07109766
C	-0.86467373	0.31000239	-3.12360417
H	-0.94391469	1.37551173	-3.39299425
H	-0.12315954	-0.13163561	-3.80930429
C	-2.19823091	-0.37953525	-3.26496844
C	-3.34316292	0.16494893	-2.65119695
H	-3.26632370	1.11985359	-2.12093917
C	-4.57929925	-0.49207428	-2.72197191
H	-5.45881398	-0.05092998	-2.24540726
C	-4.68939824	-1.71137004	-3.40875519
H	-5.65207402	-2.22521833	-3.46653725
C	-3.55798571	-2.26263243	-4.02634436
H	-3.63553264	-3.20874220	-4.56809906
C	-2.32306809	-1.60055905	-3.95095366
H	-1.44240712	-2.03250872	-4.43671771

Compound 3-*eq*, optimized Cartesian coordinates for MP2/cc-pvdz:
Total Energy (Hartree) = –1094.329680

O	1.58808207	1.68364834	-2.42634830
C	1.16091673	0.84601818	-1.64382617
C	1.81750694	0.56161662	-0.30094935
H	2.13751933	-0.49759303	-0.31165634
C	0.76709402	0.68477967	0.81395104
H	1.22161302	0.37112862	1.76433059
H	0.47640735	1.75687484	0.91603887
N	-0.38024546	-0.16600217	0.53581091
C	-1.03923377	0.24701809	-0.70482207
H	-1.34106867	1.31962838	-0.65467549
H	-1.95288438	-0.34277029	-0.85196091
C	-0.10295033	0.04394891	-1.90271683
H	0.17495009	-1.02693904	-1.90201650
C	-1.28021871	-0.35561053	1.61983682

C	-2.31159445	-1.31041236	1.48158798
H	-2.38389691	-1.88882354	0.55735187
C	-3.21224890	-1.54848416	2.52344286
H	-3.99915818	-2.29525489	2.39160048
C	-3.09770874	-0.85142489	3.73738125
H	-3.79616281	-1.04304095	4.55488095
C	-2.06893583	0.08466054	3.88930258
H	-1.96132448	0.63525874	4.82764353
C	-1.17204121	0.34127770	2.84013974
H	-0.39306036	1.09075912	2.98436386
C	3.02474709	1.47439613	-0.05360178
H	3.74809745	1.33020852	-0.87152363
H	2.69620618	2.52493966	-0.11038143
C	3.66714343	1.19276463	1.28086566
C	3.45739495	2.03894378	2.38471721
H	2.85557257	2.94432293	2.25742561
C	4.01578528	1.74229395	3.63723096
H	3.84479390	2.41472740	4.48197892
C	4.79360807	0.58761580	3.80345056
H	5.23197020	0.35574323	4.77732825
C	5.00992408	-0.26572825	2.71041078
H	5.61909494	-1.16543690	2.83061974
C	4.44918680	0.03638013	1.46207058
H	4.62697363	-0.62997397	0.61160609
C	-0.77246491	0.41536411	-3.22958515
H	-1.06685199	1.47723345	-3.20057766
H	-0.03164817	0.31832284	-4.03838812
C	-1.96956118	-0.46271876	-3.49279615
C	-3.28105016	0.00145702	-3.28563734
H	-3.43897937	1.03888548	-2.97461502
C	-4.38386762	-0.84489115	-3.47722189
H	-5.39558256	-0.46431040	-3.31423526
C	-4.18849327	-2.17435397	-3.87740190
H	-5.04604908	-2.83462202	-4.02849387
C	-2.88501613	-2.65010574	-4.08804222
H	-2.72383045	-3.68351951	-4.40616053
C	-1.78806290	-1.79954750	-3.89556163
H	-0.77381613	-2.17487547	-4.06721982

Compound 3-*ax*, optimized Cartesian coordinates for B3LYP/cc-pvdz:
Total Energy (Hartree) = –1097.77581553

O	1.54191103	1.44110019	-2.33816561
C	0.97704149	0.83049964	-1.45031378
C	1.56108400	0.71617849	-0.03965671
H	0.86461094	1.25138469	0.63360239
C	1.52979118	-0.77481235	0.39694716
H	2.20841498	-1.35421844	-0.25256820
H	1.91721745	-0.88005715	1.41542074
N	0.19811252	-1.35277943	0.27762932
C	-0.22614657	-1.34318208	-1.11544253
H	-1.16932306	-1.88378704	-1.24525953
H	0.52874993	-1.89525938	-1.70147054
C	-0.34850859	0.09973667	-1.67867464
H	-1.10342995	0.61411372	-1.05397643
C	-0.75085116	-1.14579591	1.30031636
C	-2.13404397	-1.33237461	1.07313154

H	-2.50614250	-1.59419728	0.08467656
C	-3.06059928	-1.19097073	2.10636741
H	-4.11876565	-1.34776310	1.88572871
C	-2.65698069	-0.85137945	3.39861981
H	-3.38627133	-0.74033908	4.20216575
C	-1.29545841	-0.65268201	3.63401596
H	-0.94571563	-0.38051828	4.63229731
C	-0.35709182	-0.79089434	2.61127734
H	0.69071583	-0.62219046	2.85167452
C	2.95854656	1.35399107	0.05903762
H	3.66549291	0.76279251	-0.54545731
H	2.91280564	2.34418066	-0.41847034
C	3.47212387	1.48076749	1.47751223
C	2.96114424	2.46756455	2.33717838
H	2.19911978	3.15943060	1.96859287
C	3.41891164	2.58554163	3.65085153
H	3.00986879	3.36303327	4.29955318
C	4.40348573	1.71756052	4.13311621
H	4.76468937	1.81101096	5.15908366
C	4.92533121	0.73508589	3.28915369
H	5.69953603	0.05577521	3.65209852
C	4.46242428	0.62029527	1.97467970
H	4.88394880	-0.14659857	1.31970339
C	-0.78844600	0.14695020	-3.15296782
H	-0.68450252	1.18449180	-3.50405834
H	-0.08248250	-0.44579834	-3.75713513
C	-2.20253929	-0.34348857	-3.38041291
C	-3.30162636	0.45919351	-3.03165412
H	-3.12919684	1.45374353	-2.61169051
C	-4.61007292	0.01131437	-3.22286603
H	-5.44865724	0.65466855	-2.94808856
C	-4.84754860	-1.25266148	-3.77179478
H	-5.87019165	-1.60277650	-3.92487269
C	-3.76561381	-2.05986373	-4.12924714
H	-3.93831171	-3.04591739	-4.56568388
C	-2.45703725	-1.60698332	-3.93464085
H	-1.61738962	-2.24323972	-4.22618246

Compound 3-*eq*, optimized Cartesian coordinates for B3LYP/cc-pvdz:
Total Energy (Hartree) = –1097.77599556

O	1.66648554	1.41922128	-2.43875200
C	1.13058207	0.74966484	-1.57755097
C	1.72547950	0.58398201	-0.17839033
H	2.00000122	-0.48468460	-0.09379572
C	0.64500416	0.83458307	0.89744187
H	1.06222605	0.57268523	1.87783288
H	0.40364481	1.92166809	0.92072533
N	-0.53373832	0.02019423	0.64693858
C	-1.15139216	0.32537609	-0.64290568
H	-1.44574821	1.39853889	-0.69107234
H	-2.06925666	-0.26072664	-0.76159298
C	-0.19218395	0.01846760	-1.81000439
H	0.03946459	-1.06174543	-1.74900373
C	-1.39965585	-0.26791168	1.73068912
C	-2.36973148	-1.28307177	1.59146053
H	-2.44001985	-1.83437079	0.65258619

C	-3.21424043	-1.61536466	2.64738509
H	-3.95030614	-2.41052424	2.51081575
C	-3.11200030	-0.95795537	3.87869291
H	-3.76894037	-1.22697228	4.70729942
C	-2.15276716	0.04265751	4.02882773
H	-2.05867680	0.57282051	4.97903407
C	-1.31065602	0.39467117	2.96904158
H	-0.58994515	1.19863140	3.11431067
C	2.98182164	1.45330245	0.01497369
H	3.64589277	1.27898949	-0.84477675
H	2.69377499	2.51519560	-0.04036709
C	3.72036584	1.18430022	1.30891365
C	3.65583849	2.08291728	2.38428040
H	3.07492213	3.00281426	2.27922487
C	4.32858954	1.82440076	3.58238715
H	4.26587358	2.54057835	4.40450126
C	5.08149705	0.65729688	3.72596401
H	5.60866770	0.45331334	4.65981868
C	5.15991246	-0.24565382	2.66126954
H	5.75240421	-1.15775328	2.76025059
C	4.48753006	0.01804304	1.46653677
H	4.56577794	-0.69031011	0.63730114
C	-0.79239050	0.34124797	-3.19069596
H	-1.07736464	1.40519576	-3.21651796
H	0.00539772	0.22641756	-3.93933256
C	-1.98131851	-0.52130693	-3.55653217
C	-3.29172346	-0.02613259	-3.47935920
H	-3.45606562	1.00808834	-3.16625436
C	-4.38775759	-0.83096157	-3.80465255
H	-5.39819929	-0.42183780	-3.73988233
C	-4.19133423	-2.15093076	-4.21581105
H	-5.04547803	-2.78061784	-4.47256009
C	-2.89081134	-2.65705621	-4.30304241
H	-2.72519235	-3.68486115	-4.63285554
C	-1.79960316	-1.84895474	-3.97808990
H	-0.78676058	-2.25214324	-4.06263167

Compound 3-*ax*, optimized Cartesian coordinates for LDA/cc-pvdz:
Total Energy (Hartree) = –1087.93967213

O	1.48605389	1.58961606	-2.32959964
C	0.93901385	0.94347067	-1.44998090
C	1.52982740	0.79845082	-0.07157934
H	0.81079827	1.27444869	0.64655054
C	1.54121984	-0.68923578	0.31405504
H	2.22080684	-1.24808807	-0.37026364
H	1.95812114	-0.81413788	1.33557190
N	0.22317710	-1.25247941	0.20363422
C	-0.19848935	-1.24103649	-1.17038201
H	-1.14889634	-1.79732633	-1.31303456
H	0.56877923	-1.77377988	-1.77859668
C	-0.35106642	0.20047303	-1.68076969
H	-1.12076875	0.66292367	-1.00767896
C	-0.71490501	-0.91193699	1.17604178
C	-2.09791743	-1.00652434	0.92182766
H	-2.46524362	-1.31055501	-0.07242182
C	-3.02568277	-0.71705114	1.91605649

H	-4.09945012	-0.80868072	1.68190694
C	-2.61903261	-0.30928942	3.18381329
H	-3.35932474	-0.08169032	3.96683028
C	-1.25510440	-0.18200806	3.43438924
H	-0.90305261	0.15640728	4.42315438
C	-0.31403310	-0.46700665	2.45171666
H	0.75492698	-0.33827820	2.68909094
C	2.88828751	1.45671520	0.05676605
H	3.60468881	0.95615632	-0.63317116
H	2.80533451	2.50458250	-0.30763661
C	3.38618168	1.39463033	1.46429010
C	2.73260963	2.10681627	2.47751874
H	1.88218108	2.76153744	2.21461893
C	3.14202214	2.00330964	3.80352334
H	2.61710814	2.57706158	4.58547408
C	4.21595777	1.18095995	4.14245079
H	4.53961527	1.09535845	5.19252550
C	4.87823949	0.47120238	3.14430817
H	5.73122091	-0.17898251	3.40014835
C	4.46392597	0.57843594	1.81818987
H	4.98784483	0.01419015	1.02621636
C	-0.82175163	0.27235174	-3.11883535
H	-0.84587595	1.34086851	-3.42766383
H	-0.06496352	-0.21185769	-3.77656182
C	-2.15419884	-0.38417209	-3.28187540
C	-3.29037492	0.16121668	-2.67142222
H	-3.20080820	1.11253023	-2.11657200
C	-4.52497538	-0.47512257	-2.75829958
H	-5.40847611	-0.02531706	-2.27545186
C	-4.64605847	-1.67488985	-3.45843471
H	-5.62254690	-2.18121112	-3.52709528
C	-3.52510005	-2.22704941	-4.07248810
H	-3.60965215	-3.17422767	-4.63048287
C	-2.29138726	-1.58570062	-3.98212356
H	-1.40143277	-2.02503558	-4.46691553

Compound 3-*eq*, optimized Cartesian coordinates for LDA/cc-pvdz:
Total Energy (Hartree) = –1087.93469911

O	1.72409062	1.36430134	-2.48942074
C	1.16957681	0.72689553	-1.61163403
C	1.73405177	0.60814459	-0.21909306
H	2.02685716	-0.46692270	-0.10374852
C	0.66345024	0.87214117	0.83859892
H	1.08484361	0.59941867	1.82913863
H	0.45906228	1.98055231	0.86917575
N	-0.52941497	0.11904914	0.58858937
C	-1.09577452	0.39036399	-0.70475434
H	-1.34583651	1.48500140	-0.80439990
H	-2.04912217	-0.16046102	-0.83664166
C	-0.14035433	0.01596726	-1.83193624
H	0.06398075	-1.07898351	-1.72241409
C	-1.36693039	-0.22320512	1.64695184
C	-2.50079268	-1.02943430	1.43068547
H	-2.73006804	-1.39707655	0.41686447
C	-3.32117476	-1.40451044	2.48541874
H	-4.19610667	-2.04321245	2.27912333

C	-3.04613839	-0.99481220	3.78967101
H	-3.69962253	-1.29585728	4.62336747
C	-1.92958295	-0.19633990	4.01385625
H	-1.69318809	0.15066501	5.03360212
C	-1.10372283	0.19413414	2.96359133
H	-0.24684608	0.85268783	3.17532908
C	2.95452573	1.48954634	-0.02696348
H	3.63072688	1.33323698	-0.89557663
H	2.63584508	2.55540351	-0.08019797
C	3.64431801	1.21519984	1.26853963
C	3.47949839	2.05792901	2.37195942
H	2.86731622	2.97092470	2.26086749
C	4.08093952	1.76451616	3.59415608
H	3.94270056	2.44513262	4.45057474
C	4.85798081	0.61733408	3.73237998
H	5.33386774	0.38205811	4.69832080
C	5.03407158	-0.22934889	2.63909036
H	5.65491066	-1.13531361	2.73677091
C	4.43261372	0.06906561	1.42050060
H	4.57966942	-0.60081921	0.55405976
C	-0.71535360	0.29985969	-3.20717685
H	-0.98179758	1.37971718	-3.26622132
H	0.09241559	0.14883130	-3.95584268
C	-1.90766303	-0.54945862	-3.50126678
C	-3.20502221	-0.06259298	-3.31103852
H	-3.34040572	0.98481190	-2.98675105
C	-4.31568048	-0.87327592	-3.53531980
H	-5.32972914	-0.46670967	-3.38554402
C	-4.14485601	-2.19024563	-3.95442167
H	-5.02172519	-2.83297178	-4.13626221
C	-2.85748820	-2.68850484	-4.14877328
H	-2.71335956	-3.72761255	-4.48852714
C	-1.75154043	-1.87439945	-3.92305259
H	-0.73286056	-2.27072772	-4.08441624

Compound 3-*ax*, optimized Cartesian coordinates for LDA/6-311G:**
Total Energy (Hartree) = –1088.16664492

O	1.52155003	1.49392168	-2.34069887
C	0.95035123	0.89811197	-1.44807707
C	1.52267401	0.78051513	-0.06158410
H	0.80793566	1.27842108	0.63399604
C	1.50948271	-0.69830703	0.35619297
H	2.17458623	-1.28078332	-0.30993085
H	1.91979448	-0.80694372	1.37421510
N	0.17953691	-1.23419707	0.25423760
C	-0.23092276	-1.25226780	-1.12355138
H	-1.18290414	-1.79198376	-1.26095763
H	0.52724931	-1.80757936	-1.70811597
C	-0.35508879	0.18073572	-1.66417145
H	-1.11128486	0.66877857	-1.00651165
C	-0.75395433	-0.82562894	1.20071310
C	-2.13246923	-0.88486444	0.93661329
H	-2.50000145	-1.23061724	-0.03591437
C	-3.05562599	-0.50817919	1.89790842
H	-4.12306613	-0.57470742	1.65891845
C	-2.64872272	-0.04610008	3.14132681

H	-3.38340862	0.25107858	3.89551786
C	-1.28889017	0.04028257	3.40250906
H	-0.93769988	0.41350806	4.37105905
C	-0.35217129	-0.33190407	2.45257858
H	0.71079047	-0.23357140	2.69891484
C	2.88965513	1.41369004	0.06885396
H	3.59292206	0.91072468	-0.62139330
H	2.82964403	2.46027471	-0.28281669
C	3.39137793	1.33523714	1.47347169
C	2.68967249	1.95297575	2.50942691
H	1.78794957	2.53487269	2.27665104
C	3.11791891	1.84476165	3.82383673
H	2.55629292	2.34235945	4.62216754
C	4.25912555	1.11327904	4.12765780
H	4.59826029	1.02667239	5.16514263
C	4.96687175	0.49520305	3.10734649
H	5.86834063	-0.08321376	3.33671105
C	4.53289168	0.60539837	1.79302987
H	5.09076326	0.11369790	0.98626715
C	-0.81917193	0.22556283	-3.10258711
H	-0.85481684	1.28114979	-3.42986877
H	-0.05929835	-0.25625139	-3.74620948
C	-2.14351596	-0.44455630	-3.26984504
C	-3.26389942	0.02124637	-2.58015475
H	-3.17241970	0.91104089	-1.94332706
C	-4.48755338	-0.62135393	-2.69230641
H	-5.35654126	-0.23694582	-2.14729002
C	-4.61369667	-1.74593087	-3.49834380
H	-5.57939748	-2.25430020	-3.58768749
C	-3.50857007	-2.21828411	-4.19064801
H	-3.59822414	-3.10384679	-4.82928623
C	-2.28527060	-1.57245012	-4.07325695
H	-1.40990512	-1.94834589	-4.61790007

Compound 3-*eq*, optimized Cartesian coordinates for LDA/6-311G:**
Total Energy (Hartree) = –1088.16142780

O	1.70182783	1.39962045	-2.47284107
C	1.16671928	0.73308675	-1.61243862
C	1.74277688	0.58672043	-0.22879091
H	2.04096351	-0.48065936	-0.13169509
C	0.68124939	0.83238951	0.84257587
H	1.10630302	0.53363492	1.81649894
H	0.48264152	1.93391788	0.89786149
N	-0.51508194	0.08711217	0.58520746
C	-1.08764171	0.37442161	-0.70283756
H	-1.33399012	1.46421162	-0.78542455
H	-2.03555833	-0.17124105	-0.83610942
C	-0.13679051	0.01598391	-1.83817534
H	0.06652343	-1.07348205	-1.75029699
C	-1.35938404	-0.23702279	1.64291853
C	-2.45195504	-1.09335638	1.44119622
H	-2.63568189	-1.51719017	0.44799117
C	-3.27675631	-1.45013429	2.49161869
H	-4.11576419	-2.12870433	2.30334655
C	-3.04505446	-0.97263907	3.77625621
H	-3.69917659	-1.26085024	4.60507495

C	-1.96956159	-0.12498701	3.98544261
H	-1.77246547	0.27282071	4.98689721
C	-1.13929416	0.24770496	2.93798911
H	-0.31997429	0.94632667	3.13185911
C	2.95922693	1.47118064	-0.03002946
H	3.64300240	1.31490547	-0.88335153
H	2.64335048	2.53005577	-0.08835884
C	3.63931070	1.20170358	1.27036759
C	3.46655660	2.04573274	2.36474024
H	2.85592698	2.94996604	2.24814538
C	4.06145156	1.76127422	3.58661840
H	3.91648198	2.43884343	4.43498958
C	4.84055449	0.62308863	3.73290957
H	5.31187265	0.39700531	4.69545764
C	5.02281252	-0.22591071	2.64897646
H	5.64171466	-1.12340934	2.75524450
C	4.42719848	0.06272183	1.43093485
H	4.58059088	-0.60608680	0.57427507
C	-0.72533314	0.32139384	-3.20223759
H	-0.99310601	1.39434869	-3.24435010
H	0.06542423	0.18077383	-3.96035644
C	-1.91741480	-0.52739575	-3.49297845
C	-3.21019551	-0.04590640	-3.29766570
H	-3.34807064	0.99371411	-2.97448366
C	-4.31521517	-0.85781150	-3.51482369
H	-5.32345489	-0.45986210	-3.35804292
C	-4.14328445	-2.16922832	-3.93294346
H	-5.01360753	-2.81096368	-4.10765371
C	-2.86022559	-2.66108473	-4.13467193
H	-2.71712553	-3.69349926	-4.47197042
C	-1.75971635	-1.84657365	-3.91587150
H	-0.74769584	-2.23632235	-4.08390042

Compound 3-*ax*, optimized Cartesian coordinates for HF/6-311G:**
Total Energy (Hartree) = –1090.82450064

O	1.65391841	1.18382075	-2.41380619
C	1.03277290	0.72221528	-1.51177921
C	1.54646829	0.72027285	-0.07865139
H	0.84067558	1.30797124	0.50703712
C	1.48369085	-0.72532272	0.46239070
H	2.18293732	-1.34521141	-0.09485804
H	1.80750114	-0.73509598	1.48883347
N	0.16050280	-1.30844848	0.33525681
C	-0.27704689	-1.33756096	-1.04328542
H	-1.23543002	-1.82761754	-1.11802721
H	0.42798225	-1.95454720	-1.59698724
C	-0.32424306	0.05895649	-1.70531960
H	-1.03771090	0.66686695	-1.15250091
C	-0.77618449	-1.11942698	1.36905993
C	-2.11384325	-0.81045882	1.12651365
H	-2.47487272	-0.67015749	0.12701002
C	-3.01534720	-0.68009062	2.17262186
H	-4.04030184	-0.44364653	1.94622292
C	-2.61499642	-0.83749592	3.48334220
H	-3.31610948	-0.72962035	4.29064371
C	-1.28725302	-1.14826220	3.73372973

H	-0.94960055	-1.29247271	4.74518328
C	-0.38510307	-1.29614736	2.70095961
H	0.62435914	-1.57625058	2.93223370
C	2.94439478	1.34621437	0.02428801
H	3.64857168	0.73851127	-0.53444986
H	2.92513664	2.30975307	-0.47112693
C	3.43516926	1.51846305	1.44774013
C	2.88937617	2.49804033	2.27214058
H	2.11738969	3.14491793	1.89112395
C	3.32934060	2.66117739	3.57284583
H	2.89443406	3.42619151	4.19149174
C	4.33139901	1.84711316	4.07761380
H	4.67617442	1.97496971	5.08805858
C	4.88714066	0.87422646	3.26776253
H	5.67025309	0.24045014	3.64526777
C	4.44182591	0.71390257	1.96424572
H	4.88870912	-0.04274199	1.34241676
C	-0.73428247	0.01339895	-3.18389139
H	-0.58526162	0.99733098	-3.61157515
H	-0.06400872	-0.65055711	-3.72015452
C	-2.16966007	-0.42128438	-3.40186930
C	-3.21984327	0.45262526	-3.13438156
H	-3.00646243	1.44855845	-2.78424108
C	-4.53450681	0.06693202	-3.32375243
H	-5.32988521	0.76039623	-3.11493920
C	-4.82747403	-1.20498012	-3.79035191
H	-5.84891300	-1.50537792	-3.94097039
C	-3.79400617	-2.08059693	-4.06713892
H	-4.00817317	-3.06813686	-4.43623769
C	-2.47760814	-1.68967524	-3.87492950
H	-1.68304134	-2.37954807	-4.10182745

Compound 3-*eq*, optimized Cartesian coordinates for HF/6-311G:**
Total Energy (Hartree) = –1090.82754057

O	1.57028817	1.54139560	-2.34694624
C	1.09470711	0.81092157	-1.53964899
C	1.71850783	0.58446540	-0.16943105
H	2.00571704	-0.46486513	-0.13629033
C	0.64869909	0.77996863	0.91615683
H	1.06933897	0.51105173	1.87444810
H	0.37847139	1.84088581	0.95999041
N	-0.50000517	-0.06246231	0.65150161
C	-1.14771288	0.26631611	-0.61051152
H	-1.48750349	1.30807898	-0.61306855
H	-2.02259673	-0.35211401	-0.73609869
C	-0.19205794	0.03795419	-1.78943826
H	0.07829102	-1.01651008	-1.77274620
C	-1.38758477	-0.30532226	1.73213898
C	-2.19160182	-1.44465327	1.68675497
H	-2.10543823	-2.11257954	0.84892450
C	-3.07360630	-1.72847442	2.70809685
H	-3.68195124	-2.61378641	2.65065915
C	-3.16448768	-0.89301087	3.81311197
H	-3.84540889	-1.12037348	4.61332794
C	-2.36242678	0.22791045	3.87214650
H	-2.41748590	0.88600973	4.72136002

C	-1.48461524	0.52790242	2.83833910
H	-0.88193262	1.41339255	2.90833943
C	2.95912807	1.46487193	0.03822420
H	3.61489346	1.33356214	-0.81422209
H	2.66245264	2.50828367	0.02794256
C	3.72089458	1.16304906	1.31298738
C	3.71449171	2.04838207	2.38206743
H	3.16365376	2.96998041	2.30506969
C	4.41371658	1.76821164	3.54671906
H	4.39583982	2.47056909	4.36133655
C	5.13401708	0.59375099	3.65991657
H	5.67778771	0.37458775	4.56133458
C	5.15394729	-0.29678049	2.59764609
H	5.71716691	-1.21028349	2.67166047
C	4.45668900	-0.01225350	1.43801818
H	4.49096825	-0.70848745	0.61730322
C	-0.81222417	0.38742972	-3.14973293
H	-1.11591137	1.42887344	-3.14778708
H	-0.04196357	0.30235862	-3.90672211
C	-1.99004652	-0.48895972	-3.52509178
C	-3.29100103	-0.00638837	-3.48067636
H	-3.46995097	1.01215562	-3.18219571
C	-4.36533899	-0.81491906	-3.82044383
H	-5.36448759	-0.41844872	-3.77974267
C	-4.15411534	-2.12351863	-4.21337795
H	-4.98546580	-2.75163623	-4.47920454
C	-2.85973700	-2.61670003	-4.26815565
H	-2.68287558	-3.63068430	-4.58084222
C	-1.79153245	-1.80624084	-3.92931970
H	-0.79057912	-2.19927301	-3.98793164

Compound 3-*ax*, optimized Cartesian coordinates for B3LYP/6-311G:**
Total Energy (Hartree) = –1097.97936354

O	1.48567097	1.50873307	-2.29902503
C	0.92179328	0.90163838	-1.41439724
C	1.50948122	0.78592950	-0.00544675
H	0.82922066	1.32405754	0.66878031
C	1.46935829	-0.70470198	0.43348101
H	2.13169805	-1.28794438	-0.21557345
H	1.85929167	-0.81238885	1.44198640
N	0.13070444	-1.26772914	0.32157563
C	-0.29237469	-1.26966864	-1.07194729
H	-1.23360271	-1.79827405	-1.19617132
H	0.45233305	-1.83118278	-1.64676513
C	-0.40266782	0.17007074	-1.64739688
H	-1.16005807	0.68681249	-1.04235108
C	-0.81389797	-1.04014234	1.34094218
C	-2.19589922	-1.20963807	1.11636080
H	-2.56899204	-1.47792553	0.13834359
C	-3.11806072	-1.04282453	2.14392400
H	-4.17102903	-1.18646989	1.92672248
C	-2.71125078	-0.69405763	3.42810480
H	-3.43439114	-0.56410353	4.22404429
C	-1.35120895	-0.51321760	3.66175018
H	-1.00112985	-0.23710285	4.65051774
C	-0.41712889	-0.67637945	2.64451787

H	0.62559293	-0.52167057	2.88269346
C	2.91430219	1.40948799	0.07807126
H	3.58809937	0.85511688	-0.58181376
H	2.86184575	2.42006437	-0.33415613
C	3.48488226	1.44791404	1.47933771
C	2.99324710	2.35320215	2.42840293
H	2.20473713	3.04502545	2.14909184
C	3.50957215	2.38890723	3.72073715
H	3.11759108	3.10138967	4.43819071
C	4.53369069	1.51800416	4.09009197
H	4.94013882	1.54708146	5.09449366
C	5.03587912	0.61554804	3.15672962
H	5.83680672	-0.06192909	3.43140470
C	4.51461972	0.58336066	1.86423235
H	4.91800438	-0.11787341	1.14070487
C	-0.81997400	0.20356779	-3.12868083
H	-0.78037915	1.24111178	-3.46918842
H	-0.07054712	-0.33096724	-3.71990636
C	-2.19231293	-0.37992573	-3.39017748
C	-3.34958537	0.31069858	-3.00818828
H	-3.25985796	1.28332248	-2.53434635
C	-4.61410589	-0.22496853	-3.23764277
H	-5.49622281	0.33051459	-2.93884172
C	-4.74761782	-1.46620239	-3.85837475
H	-5.73144151	-1.88365217	-4.04108335
C	-3.60688812	-2.16227902	-4.24852051
H	-3.69902828	-3.12580010	-4.73736902
C	-2.34292393	-1.62173678	-4.01583945
H	-1.45993899	-2.16904056	-4.33041106

Compound 3-*eq*, optimized Cartesian coordinates for B3LYP/6-311G:**
Total Energy (Hartree) = –1097.97996339

O	1.65935611	1.41712640	-2.43396771
C	1.12942934	0.74471497	-1.57787286
C	1.72702269	0.57484293	-0.18132549
H	2.00435652	-0.48449753	-0.09681117
C	0.65058720	0.82479039	0.89909702
H	1.06925339	0.55548859	1.86803815
H	0.41593155	1.90476760	0.92838788
N	-0.53421630	0.01880511	0.64833543
C	-1.15067043	0.32467886	-0.64232155
H	-1.43774592	1.39112715	-0.68972257
H	-2.06340227	-0.25425121	-0.76090377
C	-0.19214862	0.01308701	-1.80890026
H	0.03244311	-1.06026987	-1.75033347
C	-1.39887599	-0.26982992	1.73051665
C	-2.38024271	-1.26780493	1.58501084
H	-2.45815631	-1.80853707	0.64950887
C	-3.22607774	-1.59527406	2.63536849
H	-3.96902464	-2.37252323	2.49400761
C	-3.11357586	-0.95202778	3.86862229
H	-3.77003813	-1.21608345	4.68914504
C	-2.14117569	0.02825823	4.02685302
H	-2.03812548	0.54322054	4.97582422
C	-1.29737260	0.37599944	2.97232233
H	-0.56836222	1.16098797	3.12334073

C	2.98027597	1.44897331	0.01173632
H	3.64234705	1.28114840	-0.84087556
H	2.69002272	2.50226961	-0.03971637
C	3.71869882	1.18081501	1.30507807
C	3.65063320	2.07624683	2.37720696
H	3.07125903	2.98816028	2.27247583
C	4.32228294	1.82042903	3.57180622
H	4.25771532	2.53068132	4.38872426
C	5.07749664	0.65969612	3.71404091
H	5.60188244	0.45893348	4.64129666
C	5.15967324	-0.23958465	2.65197014
H	5.75265574	-1.14217733	2.74973705
C	4.48819082	0.02115161	1.46095992
H	4.56922233	-0.68077037	0.63657228
C	-0.79537162	0.33861898	-3.18761270
H	-1.08285338	1.39380927	-3.21012935
H	-0.00634125	0.22924649	-3.93503220
C	-1.98166937	-0.52721194	-3.55263683
C	-3.28898140	-0.03529404	-3.48082289
H	-3.45492625	0.99176040	-3.17157620
C	-4.37920071	-0.83962244	-3.80972251
H	-5.38373508	-0.43545859	-3.75028847
C	-4.17894539	-2.15509902	-4.21895104
H	-5.02478331	-2.78123364	-4.47907546
C	-2.88137305	-2.65851511	-4.29951098
H	-2.71439553	-3.67890680	-4.62649511
C	-1.79623509	-1.85105533	-3.97060083
H	-0.78931226	-2.24948475	-4.04984223

Compound 3-*ax*, optimized Cartesian coordinates for HF/6-311++G:**
Total Energy (Hartree) = –1090.83525636

O	1.54659195	1.38932217	-2.32534609
C	0.97790519	0.82118815	-1.44865665
C	1.54455501	0.72425245	-0.03590232
H	0.85370151	1.26538712	0.60905982
C	1.51023676	-0.75685494	0.40061951
H	2.17089487	-1.33211446	-0.24283089
H	1.89895662	-0.86514373	1.39804950
N	0.18334954	-1.33231217	0.28623921
C	-0.23861383	-1.32069452	-1.10164214
H	-1.16312299	-1.85527330	-1.23346432
H	0.50752389	-1.86677762	-1.67308040
C	-0.35534791	0.11280427	-1.66462611
H	-1.08532410	0.64029663	-1.05233901
C	-0.76294336	-1.10592015	1.30220714
C	-2.13333720	-1.28569677	1.07944675
H	-2.50661839	-1.56114270	0.11448921
C	-3.05324446	-1.11971227	2.09987526
H	-4.09597097	-1.27214020	1.88244634
C	-2.65591635	-0.76409015	3.37586429
H	-3.37488688	-0.63542273	4.16399165
C	-1.30506565	-0.57657052	3.60604195
H	-0.95868157	-0.29739786	4.58577739
C	-0.37335196	-0.73947293	2.59608297
H	0.65693446	-0.58070035	2.84037419
C	2.93914840	1.35778799	0.06663708

H	3.63722203	0.78631278	-0.53657774
H	2.90115940	2.34559142	-0.37657235
C	3.45718790	1.46032015	1.48747644
C	2.92280473	2.39550368	2.37021307
H	2.14255383	3.05819379	2.03606834
C	3.38592547	2.49555019	3.67034823
H	2.96073882	3.22814069	4.33343338
C	4.39996192	1.66080126	4.11625332
H	4.76309077	1.73965394	5.12532961
C	4.94456989	0.73160699	3.24811680
H	5.73632181	0.08307831	3.57932677
C	4.47607923	0.63511164	1.94535278
H	4.91485053	-0.08778195	1.27917387
C	-0.79696826	0.15717664	-3.13424150
H	-0.72526065	1.18005411	-3.48383699
H	-0.09746327	-0.41409872	-3.73600805
C	-2.20460228	-0.35762815	-3.36047528
C	-3.30640547	0.39881240	-2.96910895
H	-3.15573762	1.36263996	-2.51308460
C	-4.59574990	-0.06342729	-3.16625793
H	-5.43184223	0.53988856	-2.85944658
C	-4.81140094	-1.29617517	-3.76433972
H	-5.81281339	-1.65529852	-3.92088736
C	-3.72619361	-2.05516223	-4.16433231
H	-3.87977763	-3.00983196	-4.63567989
C	-2.43523627	-1.58699350	-3.96402770
H	-1.60100015	-2.18569164	-4.28728933

Compound 3-*eq*, optimized Cartesian coordinates for HF/6-311++G:**
Total Energy (Hartree) = –1090.83912065

O	1.58242868	1.51104100	-2.36127668
C	1.10359563	0.78441749	-1.55094654
C	1.72944090	0.55776892	-0.18180637
H	2.01533825	-0.49218382	-0.15002935
C	0.66277261	0.75567397	0.90591850
H	1.08638308	0.48695718	1.86281769
H	0.39393639	1.81698652	0.95018418
N	-0.48891612	-0.08439494	0.64734089
C	-1.13943215	0.24311434	-0.61364380
H	-1.48065410	1.28450298	-0.61368497
H	-2.01396816	-0.37635330	-0.73728404
C	-0.18872145	0.01876089	-1.79779446
H	0.07954756	-1.03668326	-1.79035420
C	-1.37207504	-0.31831363	1.73342322
C	-2.18951577	-1.44888332	1.69496188
H	-2.12261721	-2.11610788	0.85496725
C	-3.06012605	-1.72809958	2.72828060
H	-3.67650894	-2.60819844	2.67716231
C	-3.12748048	-0.89563080	3.83817223
H	-3.79697661	-1.12078743	4.64854654
C	-2.31516275	0.21898724	3.88825184
H	-2.35240998	0.87533276	4.73983778
C	-1.44776864	0.51336984	2.84303281
H	-0.83563003	1.39257363	2.90923064
C	2.97246813	1.43608394	0.02380629
H	3.63952791	1.28239057	-0.81616173

H	2.68243101	2.48058672	-0.01314838
C	3.71484458	1.16028006	1.31602725
C	3.68545626	2.06533959	2.36887774
H	3.13190617	2.98280223	2.26570168
C	4.36473544	1.81034594	3.55177611
H	4.32856511	2.52745178	4.35287657
C	5.08926889	0.64139548	3.69963292
H	5.61839535	0.44207694	4.61428199
C	5.13258456	-0.26834947	2.65365061
H	5.69981976	-1.17680884	2.75344749
C	4.45381355	-0.00886422	1.47609227
H	4.50666673	-0.72048321	0.66959658
C	-0.81438621	0.38110799	-3.15289767
H	-1.11080935	1.42459966	-3.14171717
H	-0.04900663	0.29677586	-3.91487117
C	-2.00083464	-0.48279283	-3.53101463
C	-3.29809815	0.01000035	-3.47665300
H	-3.46798815	1.02708137	-3.16783290
C	-4.38122252	-0.78631168	-3.82042535
H	-5.37695889	-0.38217043	-3.77117965
C	-4.18228577	-2.09302300	-4.22867503
H	-5.01969918	-2.71158336	-4.49790715
C	-2.89135818	-2.59580323	-4.29493334
H	-2.72348255	-3.60707084	-4.62113735
C	-1.81463441	-1.79735941	-3.95090356
H	-0.81730256	-2.19813263	-4.01954360

Compound 3-*ax*, optimized Cartesian coordinates for HF/6-31G:**
Total Energy (Hartree) = –1090.62858708

O	1.65391841	1.18382075	-2.41380619
C	1.03277290	0.72221528	-1.51177921
C	1.54646829	0.72027285	-0.07865139
H	0.84067558	1.30797124	0.50703712
C	1.48369085	-0.72532272	0.46239070
H	2.18293732	-1.34521141	-0.09485804
H	1.80750114	-0.73509598	1.48883347
N	0.16050280	-1.30844848	0.33525681
C	-0.27704689	-1.33756096	-1.04328542
H	-1.23543002	-1.82761754	-1.11802721
H	0.42798225	-1.95454720	-1.59698724
C	-0.32424306	0.05895649	-1.70531960
H	-1.03771090	0.66686695	-1.15250091
C	-0.77618449	-1.11942698	1.36905993
C	-2.11384325	-0.81045882	1.12651365
H	-2.47487272	-0.67015749	0.12701002
C	-3.01534720	-0.68009062	2.17262186
H	-4.04030184	-0.44364653	1.94622292
C	-2.61499642	-0.83749592	3.48334220
H	-3.31610948	-0.72962035	4.29064371
C	-1.28725302	-1.14826220	3.73372973
H	-0.94960055	-1.29247271	4.74518328
C	-0.38510307	-1.29614736	2.70095961
H	0.62435914	-1.57625058	2.93223370
C	2.94439478	1.34621437	0.02428801
H	3.64857168	0.73851127	-0.53444986
H	2.92513664	2.30975307	-0.47112693

C	3.43516926	1.51846305	1.44774013
C	2.88937617	2.49804033	2.27214058
H	2.11738969	3.14491793	1.89112395
C	3.32934060	2.66117739	3.57284583
H	2.89443406	3.42619151	4.19149174
C	4.33139901	1.84711316	4.07761380
H	4.67617442	1.97496971	5.08805858
C	4.88714066	0.87422646	3.26776253
H	5.67025309	0.24045014	3.64526777
C	4.44182591	0.71390257	1.96424572
H	4.88870912	-0.04274199	1.34241676
C	-0.73428247	0.01339895	-3.18389139
H	-0.58526162	0.99733098	-3.61157515
H	-0.06400872	-0.65055711	-3.72015452
C	-2.16966007	-0.42128438	-3.40186930
C	-3.21984327	0.45262526	-3.13438156
H	-3.00646243	1.44855845	-2.78424108
C	-4.53450681	0.06693202	-3.32375243
H	-5.32988521	0.76039623	-3.11493920
C	-4.82747403	-1.20498012	-3.79035191
H	-5.84891300	-1.50537792	-3.94097039
C	-3.79400617	-2.08059693	-4.06713892
H	-4.00817317	-3.06813686	-4.43623769
C	-2.47760814	-1.68967524	-3.87492950
H	-1.68304134	-2.37954807	-4.10182745

Compound 3-*eq*, optimized Cartesian coordinates for HF/6-31G:**
Total Energy (Hartree) = –1090.63219729

O	1.59809821	1.48214167	-2.36288003
C	1.10158639	0.77456004	-1.53940139
C	1.72000530	0.56161459	-0.16487816
H	2.00059127	-0.48918849	-0.11615829
C	0.64940056	0.77781777	0.91620512
H	1.06454247	0.51571393	1.87886407
H	0.38819829	1.84104875	0.94891578
N	-0.50425749	-0.05903134	0.65555757
C	-1.15180037	0.26852737	-0.60611846
H	-1.48348589	1.31252178	-0.61651340
H	-2.03213982	-0.34400724	-0.72659066
C	-0.19863222	0.02281204	-1.78434970
H	0.05382260	-1.03634502	-1.76434585
C	-1.38731533	-0.30175086	1.74095111
C	-2.16796338	-1.45744836	1.71360599
H	-2.06920894	-2.13494728	0.88440477
C	-3.04118002	-1.74456388	2.74302385
H	-3.63140231	-2.64330622	2.70160225
C	-3.14416463	-0.89487666	3.83613944
H	-3.81660244	-1.12501177	4.64317812
C	-2.36581167	0.24497172	3.87582719
H	-2.43232539	0.91432793	4.71574889
C	-1.49843247	0.54759174	2.83434771
H	-0.91466339	1.44756858	2.88614498
C	2.96574006	1.43783243	0.03265505
H	3.62262279	1.28848183	-0.81599369
H	2.67413211	2.48242787	0.00237720

C	3.71929531	1.15316916	1.31622439
C	3.68796774	2.04367382	2.38191275
H	3.12379364	2.95663596	2.29452728
C	4.37975213	1.77978605	3.55484375
H	4.34285308	2.48562339	4.36615780
C	5.11747352	0.61660552	3.68039543
H	5.65644309	0.41068639	4.58820479
C	5.16121936	-0.27940352	2.62301154
H	5.73757472	-1.18412867	2.70744827
C	4.47078338	-0.01124644	1.45468496
H	4.52308995	-0.71074700	0.63722333
C	-0.81202351	0.37995361	-3.14620278
H	-1.10673888	1.42422442	-3.14123271
H	-0.03905010	0.29245151	-3.90013328
C	-1.99530552	-0.48659256	-3.52699304
C	-3.29567492	-0.00205159	-3.46187225
H	-3.46941027	1.01155964	-3.14296936
C	-4.37462900	-0.80197639	-3.80799860
H	-5.37300069	-0.40471231	-3.75108901
C	-4.16885363	-2.10368071	-4.22828535
H	-5.00398194	-2.72504308	-4.49946454
C	-2.87583842	-2.59894231	-4.30301987
H	-2.70386915	-3.60761284	-4.63608162
C	-1.80276877	-1.79706703	-3.95730561
H	-0.80255113	-2.19030960	-4.03121169

Compound 3-*ax*, optimized Cartesian coordinates for B3LYP/6-31G:**
Total Energy (Hartree) = –1097.73266852

O	1.47225035	1.52769059	-2.29381212
C	0.91762510	0.89799863	-1.40972436
C	1.51436795	0.77192220	-0.00543635
H	0.83258697	1.29817946	0.67965879
C	1.48371330	-0.72284497	0.42199441
H	2.14609212	-1.30038994	-0.23474289
H	1.88139223	-0.83569450	1.42934605
N	0.14531470	-1.29126308	0.31380417
C	-0.27823123	-1.28625848	-1.08148903
H	-1.21594395	-1.82431288	-1.21176745
H	0.47291657	-1.83756818	-1.66067598
C	-0.40170981	0.15767465	-1.64551710
H	-1.16379326	0.66039228	-1.03099608
C	-0.80268491	-1.02839931	1.32665799
C	-2.18712554	-1.18642254	1.09811935
H	-2.55910212	-1.46833625	0.12150734
C	-3.11357223	-0.98464384	2.11873333
H	-4.16910901	-1.11944594	1.89873192
C	-2.70715793	-0.61172354	3.39891703
H	-3.43342594	-0.45366629	4.18952527
C	-1.34377239	-0.44125760	3.63513937
H	-0.99415530	-0.14479521	4.62024242
C	-0.40537427	-0.63934319	2.62470084
H	0.63971019	-0.48726355	2.86289559
C	2.91626460	1.40376378	0.08170833
H	3.59441796	0.85547688	-0.58183817
H	2.85669937	2.41696411	-0.32851449
C	3.48282632	1.43632903	1.48632626

C	2.95273774	2.30451895	2.45329415
H	2.13758861	2.97223665	2.18376514
C	3.46264653	2.33164387	3.75082919
H	3.03953895	3.01417187	4.48245523
C	4.51935805	1.49077884	4.10780139
H	4.91859330	1.51282296	5.11753244
C	5.06111450	0.62728806	3.15597747
H	5.88814398	-0.02592259	3.41966478
C	4.54517383	0.60183230	1.85861506
H	4.97855878	-0.06932868	1.12096313
C	-0.82736512	0.20185702	-3.12483373
H	-0.79423652	1.24495428	-3.45537926
H	-0.07676486	-0.32296454	-3.72645680
C	-2.19854201	-0.38877741	-3.38057534
C	-3.35769673	0.27509582	-2.95034779
H	-3.26862380	1.23125736	-2.43969186
C	-4.62190753	-0.26755837	-3.17754992
H	-5.50611459	0.26554622	-2.83983148
C	-4.75289531	-1.48805775	-3.84410183
H	-5.73742693	-1.90921903	-4.02486594
C	-3.61017349	-2.15837974	-4.27972857
H	-3.69929223	-3.10609894	-4.80319013
C	-2.34638866	-1.61165374	-4.04827060
H	-1.46100111	-2.13704356	-4.39795007

Compound 3-*eq*, optimized Cartesian coordinates for B3LYP/6-31G:**
Total Energy (Hartree) = –1097.73283428

O	1.59809821	1.48214167	-2.36288003
C	1.10158639	0.77456004	-1.53940139
C	1.72000530	0.56161459	-0.16487816
H	2.00059127	-0.48918849	-0.11615829
C	0.64940056	0.77781777	0.91620512
H	1.06454247	0.51571393	1.87886407
H	0.38819829	1.84104875	0.94891578
N	-0.50425749	-0.05903134	0.65555757
C	-1.15180037	0.26852737	-0.60611846
H	-1.48348589	1.31252178	-0.61651340
H	-2.03213982	-0.34400724	-0.72659066
C	-0.19863222	0.02281204	-1.78434970
H	0.05382260	-1.03634502	-1.76434585
C	-1.38731533	-0.30175086	1.74095111
C	-2.16796338	-1.45744836	1.71360599
H	-2.06920894	-2.13494728	0.88440477
C	-3.04118002	-1.74456388	2.74302385
H	-3.63140231	-2.64330622	2.70160225
C	-3.14416463	-0.89487666	3.83613944
H	-3.81660244	-1.12501177	4.64317812
C	-2.36581167	0.24497172	3.87582719
H	-2.43232539	0.91432793	4.71574889
C	-1.49843247	0.54759174	2.83434771
H	-0.91466339	1.44756858	2.88614498
C	2.96574006	1.43783243	0.03265505
H	3.62262279	1.28848183	-0.81599369
H	2.67413211	2.48242787	0.00237720
C	3.71929531	1.15316916	1.31622439
C	3.68796774	2.04367382	2.38191275

H	3.12379364	2.95663596	2.29452728
C	4.37975213	1.77978605	3.55484375
H	4.34285308	2.48562339	4.36615780
C	5.11747352	0.61660552	3.68039543
H	5.65644309	0.41068639	4.58820479
C	5.16121936	-0.27940352	2.62301154
H	5.73757472	-1.18412867	2.70744827
C	4.47078338	-0.01124644	1.45468496
H	4.52308995	-0.71074700	0.63722333
C	-0.81202351	0.37995361	-3.14620278
H	-1.10673888	1.42422442	-3.14123271
H	-0.03905010	0.29245151	-3.90013328
C	-1.99530552	-0.48659256	-3.52699304
C	-3.29567492	-0.00205159	-3.46187225
H	-3.46941027	1.01155964	-3.14296936
C	-4.37462900	-0.80197639	-3.80799860
H	-5.37300069	-0.40471231	-3.75108901
C	-4.16885363	-2.10368071	-4.22828535
H	-5.00398194	-2.72504308	-4.49946454
C	-2.87583842	-2.59894231	-4.30301987
H	-2.70386915	-3.60761284	-4.63608162
C	-1.80276877	-1.79706703	-3.95730561
H	-0.80255113	-2.19030960	-4.03121169

Compound 3-*ax*, optimized Cartesian coordinates for LDA/6-31G:**
Total Energy (Hartree) = –1087.89102298

O	1.47419192	1.60905054	-2.32403215
C	0.93452228	0.94929849	-1.44684282
C	1.53086196	0.79722223	-0.07240954
H	0.81995389	1.25790325	0.65485583
C	1.55271775	-0.69417600	0.30228430
H	2.22722863	-1.24330354	-0.38549549
H	1.97681162	-0.82137354	1.31423464
N	0.23445359	-1.26144394	0.19513937
C	-0.18526477	-1.24637857	-1.18097506
H	-1.12575212	-1.80597075	-1.33139668
H	0.58313586	-1.76665315	-1.78781428
C	-0.34992091	0.19881304	-1.68016103
H	-1.12315140	0.64107850	-1.00709328
C	-0.70523103	-0.90798277	1.16346479
C	-2.08669809	-0.99414444	0.90515952
H	-2.45433994	-1.29869932	-0.08274492
C	-3.01385439	-0.69066462	1.89332565
H	-4.08214599	-0.77586526	1.65751463
C	-2.60844502	-0.27634103	3.15740796
H	-3.34564615	-0.03807883	3.93230997
C	-1.24623087	-0.15579467	3.41074023
H	-0.89650861	0.18722983	4.39254993
C	-0.30493419	-0.45490281	2.43486488
H	0.75809577	-0.32860242	2.67480813
C	2.88724690	1.46013434	0.05764746
H	3.60051187	0.96985530	-0.63369300
H	2.79896702	2.50440707	-0.29872768
C	3.37900691	1.38754066	1.46724135
C	2.71179915	2.08334698	2.48103116
H	1.86360400	2.73131485	2.21704744

C	3.10963891	1.96702064	3.80779480
H	2.57715879	2.52493191	4.58806866
C	4.18448637	1.14803012	4.14582842
H	4.49732110	1.05248467	5.19256890
C	4.85834816	0.45281871	3.14732256
H	5.70682503	-0.19371670	3.40277384
C	4.45560755	0.57224887	1.82025005
H	4.98389116	0.02002652	1.03055758
C	-0.82498899	0.27604801	-3.11679339
H	-0.85504662	1.34115008	-3.41673165
H	-0.07030278	-0.19674364	-3.77571357
C	-2.15511800	-0.38832458	-3.27103959
C	-3.28506432	0.14624459	-2.64293587
H	-3.19252217	1.09084293	-2.08800600
C	-4.51447416	-0.49848275	-2.71568806
H	-5.39045426	-0.06045018	-2.22138019
C	-4.63551344	-1.69488495	-3.41873513
H	-5.60414774	-2.20593849	-3.47472201
C	-3.52030483	-2.23653696	-4.04901804
H	-3.60503546	-3.17806693	-4.60550210
C	-2.29141919	-1.58735945	-3.97242466
H	-1.40782550	-2.01639966	-4.46509677

Compound 3-*eq*, optimized Cartesian coordinates for LDA/6-31G:**
Total Energy (Hartree) = –1087.88556896

O	1.70462613	1.40836380	-2.47857845
C	1.16829678	0.73430068	-1.61413949
C	1.74677376	0.58718606	-0.23014014
H	2.04554710	-0.48151759	-0.13044534
C	0.68291218	0.83123398	0.84265275
H	1.10898688	0.53232899	1.81776533
H	0.48537124	1.93373656	0.90115809
N	-0.51340363	0.08401157	0.58422327
C	-1.08661922	0.37597249	-0.70398605
H	-1.33405833	1.46625439	-0.78801689
H	-2.03718884	-0.16808213	-0.83928962
C	-0.13564868	0.01584220	-1.84155974
H	0.06460771	-1.07569912	-1.75197789
C	-1.36032720	-0.23774413	1.64426345
C	-2.45446812	-1.09649943	1.44071257
H	-2.63688905	-1.52162921	0.44550595
C	-3.28197167	-1.45372039	2.49371407
H	-4.12190814	-2.13331768	2.30180534
C	-3.04911223	-0.97503302	3.78140250
H	-3.70366623	-1.26283281	4.61218477
C	-1.97073171	-0.12470191	3.99123836
H	-1.77229465	0.27498159	4.99372885
C	-1.13882833	0.24976547	2.94153914
H	-0.32041351	0.95306635	3.13338000
C	2.96349448	1.47422081	-0.03327198
H	3.64399118	1.31828432	-0.89141359
H	2.64260179	2.53272784	-0.09488988
C	3.64329829	1.20476788	1.26911269
C	3.46655612	2.04967557	2.36703226
H	2.85234954	2.95362112	2.24785768
C	4.06185358	1.76370057	3.59219255

H	3.91598112	2.44311896	4.44119015
C	4.84325055	0.62211342	3.73771942
H	5.31519876	0.39534286	4.70144413
C	5.02582349	-0.23010247	2.65156424
H	5.64473246	-1.12993618	2.75634675
C	4.42996201	0.06061132	1.43017833
H	4.57889794	-0.60912047	0.57089433
C	-0.72359026	0.32279053	-3.20712215
H	-0.98807582	1.39796465	-3.24524026
H	0.07148372	0.18445988	-3.96347631
C	-1.91771671	-0.52632853	-3.49739532
C	-3.21342799	-0.04350653	-3.29805550
H	-3.34830944	0.99790050	-2.97265995
C	-4.32135664	-0.85746264	-3.51476138
H	-5.33070438	-0.45746013	-3.35741150
C	-4.14816485	-2.17239550	-3.93438628
H	-5.01970575	-2.81507640	-4.10853436
C	-2.86208456	-2.66683842	-4.13646155
H	-2.71747720	-3.70101464	-4.47321195
C	-1.75896593	-1.84978844	-3.91847732
H	-0.74358348	-2.23819819	-4.08281006

Compound 3-*ax*, optimized Cartesian coordinates for PBE0/6-31G:**
Total Energy (Hartree) = –1096.44865011

O	1.50149776	1.49381738	-2.31548672
C	0.93751618	0.88610747	-1.42711032
C	1.52198651	0.76630956	-0.02891961
H	0.82819656	1.28025062	0.65496486
C	1.50230100	-0.72167070	0.38909990
H	2.16640771	-1.29446433	-0.27073529
H	1.90508478	-0.83633461	1.39591292
N	0.17329789	-1.28824496	0.28176448
C	-0.24680295	-1.27976178	-1.10475474
H	-1.18185154	-1.82387141	-1.24199265
H	0.50855935	-1.82178736	-1.68787286
C	-0.37942749	0.16015534	-1.65069848
H	-1.13216467	0.65499924	-1.01684445
C	-0.77134107	-0.99180631	1.27707786
C	-2.15254046	-1.13312247	1.04304549
H	-2.52379055	-1.43297564	0.07004690
C	-3.07855883	-0.89169444	2.05067190
H	-4.13478026	-1.01536358	1.82773710
C	-2.67522243	-0.49407244	3.32059311
H	-3.40332806	-0.30431025	4.10251774
C	-1.31429829	-0.33919831	3.56027460
H	-0.96535968	-0.02350522	4.53977936
C	-0.37605084	-0.57643334	2.56314931
H	0.67060295	-0.43209058	2.80353847
C	2.90737667	1.40589279	0.07084536
H	3.59672397	0.87405377	-0.59470256
H	2.84377943	2.42575718	-0.32355967
C	3.44681900	1.41404471	1.47799245
C	2.85295987	2.21140349	2.46335257
H	2.01202369	2.84952481	2.20015764
C	3.32772333	2.20586932	3.77047399
H	2.85442453	2.83524137	4.51901339

C	4.41105183	1.40168635	4.11826978
H	4.78330895	1.39760927	5.13846550
C	5.01494092	0.60823326	3.14808427
H	5.86347201	-0.01902526	3.40652029
C	4.53428279	0.61563877	1.84070547
H	5.01289947	-0.00457697	1.08618892
C	-0.82273488	0.21577010	-3.11304020
H	-0.81101861	1.26249775	-3.43541839
H	-0.07569632	-0.29257436	-3.73320589
C	-2.18357573	-0.39165890	-3.33785728
C	-3.33203073	0.22308003	-2.82541593
H	-3.23924636	1.15924028	-2.27897044
C	-4.58966768	-0.34037969	-3.01316437
H	-5.46876933	0.15561099	-2.61124446
C	-4.72392861	-1.53300361	-3.72081850
H	-5.70594551	-1.97210051	-3.87042211
C	-3.59155752	-2.15380483	-4.23828658
H	-3.68438843	-3.08188467	-4.79529487
C	-2.33396259	-1.58652605	-4.04598868
H	-1.45315249	-2.07478909	-4.45681949

Compound 3-*eq*, optimized Cartesian coordinates for PBE0/6-31G:**
Total Energy (Hartree) = –1096.44722064

O	1.66564772	1.48508552	-2.46201186
C	1.15142780	0.78205441	-1.61706363
C	1.75358213	0.58329971	-0.23485269
H	2.03235284	-0.47973939	-0.17605018
C	0.69408639	0.81040268	0.85628097
H	1.12239560	0.49620523	1.81033561
H	0.48687245	1.89598677	0.92979008
N	-0.50288652	0.04718468	0.59169576
C	-1.10063929	0.39175669	-0.68546461
H	-1.33678794	1.47292380	-0.72866499
H	-2.04256696	-0.14062518	-0.81808893
C	-0.15659100	0.04599622	-1.84444995
H	0.06163141	-1.02886946	-1.75894220
C	-1.36277934	-0.25100103	1.66297198
C	-2.41467034	-1.16359823	1.47343372
H	-2.54963279	-1.63530846	0.50484319
C	-3.26035368	-1.50219344	2.51824811
H	-4.06132233	-2.21348759	2.33836520
C	-3.07826499	-0.95916340	3.78917347
H	-3.73759743	-1.23330856	4.60664223
C	-2.03349856	-0.06634699	3.98986550
H	-1.87117475	0.37117692	4.97122692
C	-1.19049178	0.29711493	2.94241442
H	-0.40537898	1.02112121	3.13001394
C	2.99414824	1.45368517	-0.01690829
H	3.68406639	1.28614535	-0.84998299
H	2.69885512	2.50747493	-0.07848544
C	3.67946557	1.18240068	1.29810871
C	3.52411748	2.04554455	2.38643756
H	2.91833195	2.94142776	2.27208437
C	4.13716425	1.77986663	3.60822345
H	4.00485861	2.46856532	4.43855533
C	4.92126552	0.64079987	3.76227068

H	5.40560921	0.43389270	4.71215375
C	5.08725402	-0.22804438	2.68611857
H	5.70549795	-1.11531034	2.79242082
C	4.47174612	0.04216294	1.46829896
H	4.61530413	-0.63850912	0.63203451
C	-0.76827539	0.34091446	-3.21635354
H	-1.04841114	1.39958322	-3.26317491
H	0.00725581	0.20246182	-3.97675282
C	-1.96308449	-0.52942967	-3.51357930
C	-3.26690672	-0.05060480	-3.35693270
H	-3.42097803	0.97963103	-3.04474376
C	-4.36791785	-0.86868772	-3.59928521
H	-5.37192719	-0.47278446	-3.47270708
C	-4.18117753	-2.18613815	-4.00669398
H	-5.03713086	-2.82518928	-4.20303519
C	-2.88765591	-2.67613804	-4.17183704
H	-2.73008020	-3.69988261	-4.50015471
C	-1.79233518	-1.85481216	-3.92678668
H	-0.78651525	-2.24535435	-4.06591107

Compound 3-*ax*, optimized Cartesian coordinates for PBE0/6-311G:**
Total Energy (Hartree) = –1096.66765845

O	1.50942262	1.49844096	-2.32987137
C	0.94154742	0.90715636	-1.44272353
C	1.51765167	0.79683131	-0.03857218
H	0.81917017	1.31983826	0.63352497
C	1.49198308	-0.68549978	0.39043056
H	2.15388356	-1.26546865	-0.26488935
H	1.89181912	-0.79433587	1.39770097
N	0.16204592	-1.24660687	0.28611514
C	-0.25621293	-1.24926834	-1.10050903
H	-1.19238555	-1.79045617	-1.23318702
H	0.49887657	-1.79905120	-1.67527013
C	-0.37784045	0.18415034	-1.65946906
H	-1.12788338	0.69243418	-1.03496296
C	-0.77911175	-0.95578268	1.28081212
C	-2.15906620	-1.09228529	1.04641781
H	-2.53037450	-1.38060712	0.07153800
C	-3.08329558	-0.86442589	2.05410583
H	-4.13954505	-0.98113809	1.83156690
C	-2.68044840	-0.48062065	3.32627192
H	-3.40416948	-0.29638318	4.11034492
C	-1.32105637	-0.32906349	3.56681735
H	-0.97230138	-0.02587101	4.54834879
C	-0.38463858	-0.55342497	2.56836722
H	0.66100544	-0.41247797	2.80964610
C	2.90534518	1.42681649	0.06633361
H	3.58933266	0.89008384	-0.59996875
H	2.85327425	2.44805145	-0.32122146
C	3.44289178	1.41937583	1.47241037
C	2.85406480	2.20576264	2.46624213
H	2.01953562	2.85536704	2.21113155
C	3.32406215	2.17446812	3.77309467
H	2.85589824	2.79862267	4.52838362
C	4.39511550	1.35658455	4.11304366
H	4.76382684	1.33434036	5.13394764

C	4.99311415	0.57279111	3.13515744
H	5.83349703	-0.06687133	3.38502452
C	4.51780562	0.60542881	1.82845296
H	4.99186771	-0.01155754	1.07031105
C	-0.81931181	0.21971575	-3.12109178
H	-0.81337721	1.25924082	-3.46275978
H	-0.07229732	-0.29555805	-3.73365845
C	-2.17527792	-0.39836409	-3.33754848
C	-3.32374244	0.20156084	-2.81269929
H	-3.23855625	1.13532420	-2.26354094
C	-4.57437594	-0.37585342	-2.98861208
H	-5.45383354	0.10698186	-2.57464922
C	-4.70295672	-1.56558229	-3.70025850
H	-5.67996446	-2.01859292	-3.83591802
C	-3.57153039	-2.16802028	-4.23166533
H	-3.65984260	-3.09158342	-4.79469713
C	-2.32077509	-1.58829461	-4.04923992
H	-1.43972219	-2.06415844	-4.47246089

Compound 3-*eq*, optimized Cartesian coordinates for PBE0/6-311G:**
Total Energy (Hartree) = –1096.66692033

O	1.65631205	1.43727308	-2.43135971
C	1.14211500	0.74509425	-1.58584466
C	1.73846028	0.56898211	-0.20143100
H	2.02699346	-0.48981664	-0.12597961
C	0.66999001	0.79772377	0.87783027
H	1.09607501	0.51464671	1.84193998
H	0.43337299	1.87803368	0.92582449
N	-0.50423774	-0.00334649	0.62025384
C	-1.11495519	0.30586290	-0.65974291
H	-1.40294796	1.37348856	-0.70596673
H	-2.02923160	-0.27281268	-0.78537217
C	-0.16030982	0.00074398	-1.81912357
H	0.07363581	-1.07181405	-1.75831178
C	-1.36549917	-0.29243912	1.69277115
C	-2.36455074	-1.26537238	1.53510403
H	-2.45905142	-1.78761977	0.58970016
C	-3.20824410	-1.59439930	2.58222085
H	-3.96666980	-2.35592125	2.43052672
C	-3.07835022	-0.97604430	3.82268929
H	-3.73593426	-1.24170475	4.64285389
C	-2.08991410	-0.01794098	3.99075433
H	-1.97288371	0.48084305	4.94777879
C	-1.24679002	0.32994024	2.94075677
H	-0.50147145	1.09992029	3.09925629
C	2.97253101	1.45103875	-0.00251803
H	3.65018056	1.28280788	-0.84449869
H	2.67311396	2.50212253	-0.06602174
C	3.68291963	1.19229887	1.29867567
C	3.58904451	2.08669895	2.36469932
H	3.01196862	2.99942283	2.24274048
C	4.22984367	1.83132904	3.57217599
H	4.14654086	2.54243109	4.38788863
C	4.97898971	0.67271041	3.73267665
H	5.48221923	0.47240891	4.67245446
C	5.08497232	-0.22602496	2.67656402

H	5.67447694	-1.13028577	2.78951620
C	4.44395855	0.03423633	1.47291691
H	4.54146359	-0.66834167	0.64937423
C	-0.76274220	0.32296593	-3.18629149
H	-1.02665370	1.38494827	-3.21864633
H	0.01511244	0.18680588	-3.94268128
C	-1.96525482	-0.51971169	-3.51757996
C	-3.25813446	-0.00515948	-3.42225500
H	-3.39726990	1.02942171	-3.12151007
C	-4.36567185	-0.79284851	-3.71608095
H	-5.36292792	-0.37193117	-3.63901728
C	-4.19708806	-2.11373389	-4.11221284
H	-5.05993177	-2.72785827	-4.34792745
C	-2.91365445	-2.63913927	-4.21420696
H	-2.77128190	-3.66696581	-4.53230107
C	-1.81105593	-1.84819357	-3.91971597
H	-0.81109066	-2.26349864	-4.01467176

Compound 3-*ax*, optimized Cartesian coordinates for B3LYP/cc-pvtz:
Total Energy (Hartree) = –1098.09417988

O	1.60712213	1.34089801	-2.37665402
C	1.01094346	0.79293453	-1.47583145
C	1.57171011	0.70852177	-0.05887158
H	0.87975133	1.25671804	0.59047953
C	1.52332966	-0.77401180	0.40045050
H	2.19653595	-1.36144319	-0.23030124
H	1.89908964	-0.86290690	1.41330513
N	0.19087389	-1.33896296	0.28029900
C	-0.22955908	-1.34122403	-1.10947207
H	-1.17227555	-1.86161110	-1.23456944
H	0.51126137	-1.90403530	-1.68440706
C	-0.32924728	0.09539948	-1.69005784
H	-1.06660452	0.62671353	-1.07773969
C	-0.75088712	-1.16397354	1.30635759
C	-2.12589502	-1.36712099	1.08604203
H	-2.49755277	-1.62179831	0.10655484
C	-3.04449633	-1.25393573	2.11997862
H	-4.09161783	-1.42283887	1.90487689
C	-2.64170924	-0.92680872	3.40784398
H	-3.36179101	-0.83842894	4.20894082
C	-1.28923835	-0.71192928	3.63784799
H	-0.94191689	-0.45047647	4.62892970
C	-0.35914858	-0.82225503	2.61408891
H	0.67728270	-0.64465821	2.85226726
C	2.97252525	1.32875560	0.04894844
H	3.67614360	0.71913700	-0.52136243
H	2.95223803	2.29966000	-0.44681447
C	3.46056571	1.48347384	1.46991530
C	2.93388562	2.47800946	2.29843712
H	2.17974803	3.15176575	1.90985132
C	3.37027424	2.62471938	3.60871123
H	2.95135705	3.40496034	4.23037479
C	4.34829393	1.77717689	4.11903352
H	4.69161660	1.89236314	5.13821154
C	4.88558541	0.78711533	3.30634991
H	5.65185938	0.12655525	3.69004720

C	4.44428533	0.64449785	1.99465038
H	4.87712761	-0.12447503	1.36661936
C	-0.77208181	0.12418746	-3.16030794
H	-0.64660852	1.14132555	-3.53242801
H	-0.09141065	-0.49362763	-3.74935041
C	-2.19588619	-0.33292552	-3.37211706
C	-3.26718341	0.49269911	-3.02063272
H	-3.07043487	1.47538729	-2.60918770
C	-4.58047268	0.07855654	-3.20096200
H	-5.39400121	0.73665129	-2.92563480
C	-4.85051736	-1.17477796	-3.74084155
H	-5.87281278	-1.49745837	-3.88451978
C	-3.79647850	-2.00474650	-4.10081432
H	-3.99412735	-2.97876139	-4.52855373
C	-2.48284877	-1.58475282	-3.91757271
H	-1.66857814	-2.23604817	-4.21061323

Compound 3-*eq*, optimized Cartesian coordinates for B3LYP/cc-pvtz:
Total Energy (Hartree) = –1098.09467560

O	1.65466675	1.42055215	-2.42737406
C	1.12738876	0.74716119	-1.57161435
C	1.72121932	0.58434060	-0.17623074
H	1.99841598	-0.47242065	-0.08915619
C	0.64263468	0.83571213	0.89763145
H	1.05783306	0.57491418	1.86744289
H	0.40509593	1.91273380	0.92060599
N	-0.53654342	0.02730363	0.65020846
C	-1.14779170	0.31819512	-0.64209488
H	-1.44080794	1.38041650	-0.69691258
H	-2.05579056	-0.26401786	-0.75872702
C	-0.18697020	0.00899005	-1.80367035
H	0.04399625	-1.06033285	-1.74256342
C	-1.39833743	-0.26252794	1.72950489
C	-2.37677697	-1.25991704	1.58672880
H	-2.45948146	-1.79990606	0.65382912
C	-3.21450512	-1.59117825	2.63804101
H	-3.95248623	-2.37008845	2.49946462
C	-3.09961172	-0.95009393	3.86906064
H	-3.74952775	-1.21846635	4.69016481
C	-2.13231733	0.03135335	4.02390805
H	-2.02749141	0.54480008	4.97104254
C	-1.29508643	0.38163318	2.96873842
H	-0.56799979	1.16514615	3.11876097
C	2.97110403	1.45737155	0.01973042
H	3.63172279	1.29411969	-0.83181067
H	2.68002276	2.50799726	-0.02660521
C	3.70940772	1.18581960	1.30862633
C	3.64645462	2.07780622	2.37968745
H	3.07208909	2.99030165	2.27747020
C	4.31611677	1.81870107	3.57118078
H	4.25400247	2.52602655	4.38775598
C	5.06404306	0.65677448	3.71144266
H	5.58520232	0.45255957	4.63668339
C	5.14223116	-0.23876102	2.65002650
H	5.72971412	-1.14201418	2.74600887
C	4.47318137	0.02609259	1.46217778

H	4.55240850	-0.67340461	0.63866957
C	-0.78846050	0.32653922	-3.18149934
H	-1.07026852	1.38054159	-3.20973401
H	-0.00256359	0.20907815	-3.92763252
C	-1.97671879	-0.53219954	-3.54332416
C	-3.27852891	-0.03608372	-3.46572541
H	-3.43900559	0.98720890	-3.14998537
C	-4.37091464	-0.83034409	-3.79738304
H	-5.37075527	-0.42250741	-3.73314160
C	-4.17906014	-2.14118991	-4.21498538
H	-5.02659182	-2.75917273	-4.47830570
C	-2.88708344	-2.64943117	-4.30071609
H	-2.72598944	-3.66574902	-4.63514929
C	-1.79959597	-1.85128356	-3.96875060
H	-0.79746288	-2.25396610	-4.05396687

Compound 3-*ax*, optimized Cartesian coordinates for LDA/6-31G*:
Total Energy (Hartree) = –1087.85830247

O	1.48514508	1.58857256	-2.32933520
C	0.93587115	0.94402349	-1.44669800
C	1.52799465	0.79816474	-0.06924262
H	0.81593777	1.26023292	0.65647822
C	1.55123819	-0.69410412	0.30400145
H	2.22416557	-1.24242901	-0.38624245
H	1.97731532	-0.82512168	1.31486036
N	0.23362627	-1.26326807	0.19750400
C	-0.18569911	-1.24678373	-1.17886017
H	-1.12352489	-1.81085788	-1.33032027
H	0.58578266	-1.76450640	-1.78462501
C	-0.35300761	0.19909517	-1.67682230
H	-1.12504213	0.64323529	-1.00290162
C	-0.70628877	-0.91256546	1.16681052
C	-2.08770961	-0.99906222	0.90933130
H	-2.45654509	-1.30424063	-0.07815799
C	-3.01548022	-0.69704197	1.89771328
H	-4.08426012	-0.78345237	1.66157501
C	-2.61047301	-0.28348451	3.16245968
H	-3.34826753	-0.04779828	3.93852396
C	-1.24803789	-0.16278384	3.41548483
H	-0.89775759	0.17934729	4.39824303
C	-0.30698562	-0.46035713	2.43863039
H	0.75590536	-0.33472619	2.68049290
C	2.88589209	1.46009512	0.05942782
H	3.59827410	0.96772340	-0.63270149
H	2.79863025	2.50547869	-0.29689301
C	3.38040300	1.38886485	1.46855082
C	2.71874942	2.09016171	2.48200150
H	1.87198495	2.74097560	2.21818234
C	3.12000518	1.97732533	3.80834136
H	2.59088769	2.53990010	4.58827891
C	4.19414793	1.15701680	4.14615686
H	4.51103440	1.06564869	5.19285177
C	4.86333621	0.45688367	3.14779955
H	5.71245962	-0.19007376	3.40330901
C	4.45625521	0.57222584	1.82138802
H	4.98311655	0.01625273	1.03247540

C	-0.82714094	0.27566544	-3.11446908
H	-0.85766356	1.34135075	-3.41539950
H	-0.07106921	-0.19792903	-3.77251183
C	-2.15739522	-0.38825721	-3.27185353
C	-3.28975065	0.14957332	-2.65098010
H	-3.19872772	1.09665425	-2.09822783
C	-4.52023915	-0.49285870	-2.72924800
H	-5.39818287	-0.05131493	-2.24006820
C	-4.64089982	-1.69011886	-3.43133541
H	-5.61160243	-2.19875485	-3.49324713
C	-3.52287984	-2.23490054	-4.05452155
H	-3.60714415	-3.17692604	-4.61141735
C	-2.29254990	-1.58837404	-3.97179207
H	-1.40778873	-2.02061409	-4.46138151

Compound 3-*eq*, optimized Cartesian coordinates for LDA/6-31G:**
Total Energy (Hartree) = –1087.85303497

O	1.70611033	1.40672817	-2.48091984
C	1.16906084	0.73342890	-1.61616159
C	1.74747745	0.58474946	-0.23196383
H	2.04565215	-0.48427556	-0.13149674
C	0.68370601	0.83082468	0.84025651
H	1.10921562	0.53156615	1.81594559
H	0.48599317	1.93384525	0.89817325
N	-0.51316404	0.08402644	0.58234354
C	-1.08624213	0.37598437	-0.70596092
H	-1.33457540	1.46654335	-0.78955155
H	-2.03693681	-0.16854385	-0.84150123
C	-0.13499279	0.01459030	-1.84286827
H	0.06399197	-1.07747754	-1.75355876
C	-1.35986254	-0.23803389	1.64248467
C	-2.45402871	-1.09642183	1.43896424
H	-2.63672151	-1.52225953	0.44375454
C	-3.28127604	-1.45477603	2.49190516
H	-4.12150866	-2.13480781	2.29944993
C	-3.04812360	-0.97695963	3.77997323
H	-3.70268464	-1.26454876	4.61157890
C	-1.96997070	-0.12585374	3.98980918
H	-1.77087813	0.27409161	4.99271722
C	-1.13819703	0.24878930	2.93985522
H	-0.31999620	0.95300146	3.13208168
C	2.96462362	1.47198171	-0.03485297
H	3.64591801	1.31473853	-0.89337848
H	2.64371822	2.53145557	-0.09709462
C	3.64360219	1.20268025	1.26795414
C	3.46665008	2.04776153	2.36553032
H	2.85149922	2.95178512	2.24714754
C	4.06222859	1.76225762	3.59086044
H	3.91634524	2.44195786	4.44031867
C	4.84460072	0.62097598	3.73648105
H	5.31715602	0.39448009	4.70058422
C	5.02731937	-0.23135027	2.65021730
H	5.64762632	-1.13082521	2.75485736
C	4.43106515	0.05946350	1.42895391
H	4.58077743	-0.61036710	0.56940955
C	-0.72316546	0.32212912	-3.20863180

H	-0.98803841	1.39809773	-3.24698039
H	0.07231141	0.18403489	-3.96585586
C	-1.91695777	-0.52734132	-3.49894702
C	-3.21256947	-0.04489164	-3.29933023
H	-3.34815022	0.99681467	-2.97348188
C	-4.32055638	-0.85908399	-3.51578515
H	-5.33055529	-0.45956493	-3.35794681
C	-4.14705859	-2.17415985	-3.93575748
H	-5.01878359	-2.81752047	-4.10966222
C	-2.86066405	-2.66806023	-4.13828136
H	-2.71595223	-3.70250715	-4.47569240
C	-1.75781030	-1.85034044	-3.92057008
H	-0.74207288	-2.23871980	-4.08558715

Compound 3-*ax*, Cartesian coordinates for CASSCF(10,10)/6-31G:**
Total Energy (Hartree) = –1090.718848263038

O	1.53645239	1.46508357	-2.34405761
C	0.95354945	0.88834454	-1.44750047
C	1.52516876	0.78209791	-0.04187214
H	0.82721166	1.30069502	0.63466642
C	1.49949940	-0.70504798	0.38044499
H	2.15967996	-1.28295227	-0.28005033
H	1.90280057	-0.82219890	1.38698547
N	0.16786315	-1.26528530	0.27542565
C	-0.24950055	-1.26158595	-1.11151554
H	-1.18622891	-1.80381291	-1.24679823
H	0.50463454	-1.81103192	-1.69034952
C	-0.37314765	0.17663678	-1.66560236
H	-1.12156251	0.68117837	-1.03404875
C	-0.77619307	-0.96725173	1.27181689
C	-2.15861532	-1.10660717	1.03983862
H	-2.53387973	-1.39592003	0.06450203
C	-3.08327123	-0.87791305	2.05227975
H	-4.14038814	-1.00450277	1.83057439
C	-2.67747648	-0.49160720	3.32538012
H	-3.40436589	-0.31630992	4.11284301
C	-1.31629197	-0.33070228	3.56162864
H	-0.96454597	-0.02124438	4.54305810
C	-0.37977011	-0.55568171	2.55930359
H	0.66694212	-0.40512987	2.79880840
C	2.91166258	1.41846642	0.06749503
H	3.60210559	0.89013957	-0.60066582
H	2.85230110	2.44262148	-0.31869331
C	3.44579008	1.41491255	1.47778820
C	2.85050846	2.20640208	2.46709616
H	2.01233819	2.84955930	2.20570808
C	3.31923189	2.18977195	3.77669431
H	2.84323693	2.81451455	4.52813200
C	4.39947102	1.38083616	4.12349558
H	4.76679356	1.36658520	5.14598245
C	5.00561045	0.59380004	3.14950168
H	5.85270772	-0.03678924	3.40671528
C	4.53015804	0.61175948	1.84012363
H	5.01221430	-0.00443050	1.08394669
C	-0.82025462	0.22557810	-3.12743229

H	-0.81474088	1.27177875	-3.45458962
H	-0.07183466	-0.28166412	-3.74768457
C	-2.17998336	-0.38959016	-3.34350526
C	-3.32858225	0.21910421	-2.82390673
H	-3.23830330	1.15934702	-2.28312626
C	-4.58402199	-0.35483881	-2.99582180
H	-5.46259268	0.13670985	-2.58610468
C	-4.71682060	-1.55164328	-3.69704408
H	-5.69682731	-2.00116881	-3.83241974
C	-3.58504791	-2.16469533	-4.22489713
H	-3.67659226	-3.09549082	-4.77851408
C	-2.32961676	-1.58752878	-4.04688616
H	-1.45010302	-2.07225511	-4.46581640

Compound 3-*eq*, Cartesian coordinates for CASSCF(10,10)/6-31G:**
Total Energy (Hartree) = –1090.724201869432

O	1.66185548	1.47312181	-2.44910773
C	1.15503091	0.76159221	-1.60677095
C	1.75306727	0.57648906	-0.22303315
H	2.04457873	-0.48271384	-0.15167538
C	0.67644073	0.79770593	0.85265069
H	1.10206195	0.52489303	1.82116651
H	0.42679609	1.87686599	0.89326801
N	-0.48734271	-0.02064919	0.59675684
C	-1.10165363	0.28871743	-0.68355977
H	-1.40885096	1.35270727	-0.72615585
H	-2.00732712	-0.30510056	-0.81233062
C	-0.13922347	0.00289963	-1.84557957
H	0.10468652	-1.06939347	-1.79253766
C	-1.35107353	-0.30177460	1.67475209
C	-2.32737957	-1.30307448	1.53704252
H	-2.39961571	-1.85615441	0.60466458
C	-3.17470312	-1.62121822	2.58869419
H	-3.91721955	-2.40411814	2.45456257
C	-3.06501392	-0.96652971	3.81497708
H	-3.72393339	-1.22339984	4.63957906
C	-2.09365830	0.01532355	3.96525610
H	-1.98938022	0.53832622	4.91262080
C	-1.25188584	0.35514156	2.90884204
H	-0.52334995	1.14598407	3.05275514
C	2.98423662	1.46152433	-0.00938778
H	3.67115035	1.30020714	-0.84746828
H	2.68255186	2.51412249	-0.06973552
C	3.67782446	1.19423261	1.30123090
C	3.56099631	2.08058645	2.37494508
H	2.98161086	2.99311515	2.25078685
C	4.18054242	1.81701012	3.59425546
H	4.07905088	2.52221686	4.41535531
C	4.93131697	0.65734897	3.75873604
H	5.41868370	0.45071595	4.70793127
C	5.06046583	-0.23378995	2.69556037
H	5.65102841	-1.13882018	2.81236519
C	4.44032640	0.03515667	1.48002206
H	4.55400429	-0.66158512	0.65142883
C	-0.74359269	0.32660873	-3.21456909

H	-0.99855298	1.39258840	-3.24874010
H	0.03222214	0.18048577	-3.97403939
C	-1.95682123	-0.50870502	-3.52922416
C	-3.24647339	0.01114815	-3.39282994
H	-3.37232977	1.04815079	-3.08688084
C	-4.36812064	-0.77433912	-3.64666265
H	-5.36185899	-0.34939557	-3.53439885
C	-4.21533729	-2.09856510	-4.04722444
H	-5.08807929	-2.71334785	-4.24872757
C	-2.93533877	-2.62809311	-4.19575531
H	-2.80656935	-3.65834870	-4.51802505
C	-1.81878999	-1.83900618	-3.93968305
H	-0.82189812	-2.25677089	-4.06631434

Compound 3-*ax*, Cartesian coordinates for CASSCF(10,10)/6-31G*:
Total Energy (Hartree) = –1090.677264723717

O	1.53645239	1.46508357	-2.34405761
C	0.95354945	0.88834454	-1.44750047
C	1.52516876	0.78209791	-0.04187214
H	0.82721166	1.30069502	0.63466642
C	1.49949940	-0.70504798	0.38044499
H	2.15967996	-1.28295227	-0.28005033
H	1.90280057	-0.82219890	1.38698547
N	0.16786315	-1.26528530	0.27542565
C	-0.24950055	-1.26158595	-1.11151554
H	-1.18622891	-1.80381291	-1.24679823
H	0.50463454	-1.81103192	-1.69034952
C	-0.37314765	0.17663678	-1.66560236
H	-1.12156251	0.68117837	-1.03404875
C	-0.77619307	-0.96725173	1.27181689
C	-2.15861532	-1.10660717	1.03983862
H	-2.53387973	-1.39592003	0.06450203
C	-3.08327123	-0.87791305	2.05227975
H	-4.14038814	-1.00450277	1.83057439
C	-2.67747648	-0.49160720	3.32538012
H	-3.40436589	-0.31630992	4.11284301
C	-1.31629197	-0.33070228	3.56162864
H	-0.96454597	-0.02124438	4.54305810
C	-0.37977011	-0.55568171	2.55930359
H	0.66694212	-0.40512987	2.79880840
C	2.91166258	1.41846642	0.06749503
H	3.60210559	0.89013957	-0.60066582
H	2.85230110	2.44262148	-0.31869331
C	3.44579008	1.41491255	1.47778820
C	2.85050846	2.20640208	2.46709616
H	2.01233819	2.84955930	2.20570808
C	3.31923189	2.18977195	3.77669431
H	2.84323693	2.81451455	4.52813200
C	4.39947102	1.38083616	4.12349558
H	4.76679356	1.36658520	5.14598245
C	5.00561045	0.59380004	3.14950168
H	5.85270772	-0.03678924	3.40671528
C	4.53015804	0.61175948	1.84012363
H	5.01221430	-0.00443050	1.08394669
C	-0.82025462	0.22557810	-3.12743229

H	-0.81474088	1.27177875	-3.45458962
H	-0.07183466	-0.28166412	-3.74768457
C	-2.17998336	-0.38959016	-3.34350526
C	-3.32858225	0.21910421	-2.82390673
H	-3.23830330	1.15934702	-2.28312626
C	-4.58402199	-0.35483881	-2.99582180
H	-5.46259268	0.13670985	-2.58610468
C	-4.71682060	-1.55164328	-3.69704408
H	-5.69682731	-2.00116881	-3.83241974
C	-3.58504791	-2.16469533	-4.22489713
H	-3.67659226	-3.09549082	-4.77851408
C	-2.32961676	-1.58752878	-4.04688616
H	-1.45010302	-2.07225511	-4.46581640

Compound 3-*eq*, Cartesian coordinates for CASSCF(10,10)/6-31G*:
Total Energy (Hartree) = –1090.682025200731

O	1.66185548	1.47312181	-2.44910773
C	1.15503091	0.76159221	-1.60677095
C	1.75306727	0.57648906	-0.22303315
H	2.04457873	-0.48271384	-0.15167538
C	0.67644073	0.79770593	0.85265069
H	1.10206195	0.52489303	1.82116651
H	0.42679609	1.87686599	0.89326801
N	-0.48734271	-0.02064919	0.59675684
C	-1.10165363	0.28871743	-0.68355977
H	-1.40885096	1.35270727	-0.72615585
H	-2.00732712	-0.30510056	-0.81233062
C	-0.13922347	0.00289963	-1.84557957
H	0.10468652	-1.06939347	-1.79253766
C	-1.35107353	-0.30177460	1.67475209
C	-2.32737957	-1.30307448	1.53704252
H	-2.39961571	-1.85615441	0.60466458
C	-3.17470312	-1.62121822	2.58869419
H	-3.91721955	-2.40411814	2.45456257
C	-3.06501392	-0.96652971	3.81497708
H	-3.72393339	-1.22339984	4.63957906
C	-2.09365830	0.01532355	3.96525610
H	-1.98938022	0.53832622	4.91262080
C	-1.25188584	0.35514156	2.90884204
H	-0.52334995	1.14598407	3.05275514
C	2.98423662	1.46152433	-0.00938778
H	3.67115035	1.30020714	-0.84746828
H	2.68255186	2.51412249	-0.06973552
C	3.67782446	1.19423261	1.30123090
C	3.56099631	2.08058645	2.37494508
H	2.98161086	2.99311515	2.25078685
C	4.18054242	1.81701012	3.59425546
H	4.07905088	2.52221686	4.41535531
C	4.93131697	0.65734897	3.75873604
H	5.41868370	0.45071595	4.70793127
C	5.06046583	-0.23378995	2.69556037
H	5.65102841	-1.13882018	2.81236519
C	4.44032640	0.03515667	1.48002206
H	4.55400429	-0.66158512	0.65142883
C	-0.74359269	0.32660873	-3.21456909

H	-0.99855298	1.39258840	-3.24874010
H	0.03222214	0.18048577	-3.97403939
C	-1.95682123	-0.50870502	-3.52922416
C	-3.24647339	0.01114815	-3.39282994
H	-3.37232977	1.04815079	-3.08688084
C	-4.36812064	-0.77433912	-3.64666265
H	-5.36185899	-0.34939557	-3.53439885
C	-4.21533729	-2.09856510	-4.04722444
H	-5.08807929	-2.71334785	-4.24872757
C	-2.93533877	-2.62809311	-4.19575531
H	-2.80656935	-3.65834870	-4.51802505
C	-1.81878999	-1.83900618	-3.93968305
H	-0.82189812	-2.25677089	-4.06631434

Compound 3-*ax*, Cartesian coordinates for CASSCF(12,12)/6-31G:**
Total Energy (Hartree) = –1090.746958652776

O	1.53645239	1.46508357	-2.34405761
C	0.95354945	0.88834454	-1.44750047
C	1.52516876	0.78209791	-0.04187214
H	0.82721166	1.30069502	0.63466642
C	1.49949940	-0.70504798	0.38044499
H	2.15967996	-1.28295227	-0.28005033
H	1.90280057	-0.82219890	1.38698547
N	0.16786315	-1.26528530	0.27542565
C	-0.24950055	-1.26158595	-1.11151554
H	-1.18622891	-1.80381291	-1.24679823
H	0.50463454	-1.81103192	-1.69034952
C	-0.37314765	0.17663678	-1.66560236
H	-1.12156251	0.68117837	-1.03404875
C	-0.77619307	-0.96725173	1.27181689
C	-2.15861532	-1.10660717	1.03983862
H	-2.53387973	-1.39592003	0.06450203
C	-3.08327123	-0.87791305	2.05227975
H	-4.14038814	-1.00450277	1.83057439
C	-2.67747648	-0.49160720	3.32538012
H	-3.40436589	-0.31630992	4.11284301
C	-1.31629197	-0.33070228	3.56162864
H	-0.96454597	-0.02124438	4.54305810
C	-0.37977011	-0.55568171	2.55930359
H	0.66694212	-0.40512987	2.79880840
C	2.91166258	1.41846642	0.06749503
H	3.60210559	0.89013957	-0.60066582
H	2.85230110	2.44262148	-0.31869331
C	3.44579008	1.41491255	1.47778820
C	2.85050846	2.20640208	2.46709616
H	2.01233819	2.84955930	2.20570808
C	3.31923189	2.18977195	3.77669431
H	2.84323693	2.81451455	4.52813200
C	4.39947102	1.38083616	4.12349558
H	4.76679356	1.36658520	5.14598245
C	5.00561045	0.59380004	3.14950168
H	5.85270772	-0.03678924	3.40671528
C	4.53015804	0.61175948	1.84012363
H	5.01221430	-0.00443050	1.08394669
C	-0.82025462	0.22557810	-3.12743229

H	-0.81474088	1.27177875	-3.45458962
H	-0.07183466	-0.28166412	-3.74768457
C	-2.17998336	-0.38959016	-3.34350526
C	-3.32858225	0.21910421	-2.82390673
H	-3.23830330	1.15934702	-2.28312626
C	-4.58402199	-0.35483881	-2.99582180
H	-5.46259268	0.13670985	-2.58610468
C	-4.71682060	-1.55164328	-3.69704408
H	-5.69682731	-2.00116881	-3.83241974
C	-3.58504791	-2.16469533	-4.22489713
H	-3.67659226	-3.09549082	-4.77851408
C	-2.32961676	-1.58752878	-4.04688616
H	-1.45010302	-2.07225511	-4.46581640

Compound 3-*eq*, Cartesian coordinates for CASSCF(12,12)/6-31G:**
Total Energy (Hartree) = –1090.750866672880

O	1.66185548	1.47312181	-2.44910773
C	1.15503091	0.76159221	-1.60677095
C	1.75306727	0.57648906	-0.22303315
H	2.04457873	-0.48271384	-0.15167538
C	0.67644073	0.79770593	0.85265069
H	1.10206195	0.52489303	1.82116651
H	0.42679609	1.87686599	0.89326801
N	-0.48734271	-0.02064919	0.59675684
C	-1.10165363	0.28871743	-0.68355977
H	-1.40885096	1.35270727	-0.72615585
H	-2.00732712	-0.30510056	-0.81233062
C	-0.13922347	0.00289963	-1.84557957
H	0.10468652	-1.06939347	-1.79253766
C	-1.35107353	-0.30177460	1.67475209
C	-2.32737957	-1.30307448	1.53704252
H	-2.39961571	-1.85615441	0.60466458
C	-3.17470312	-1.62121822	2.58869419
H	-3.91721955	-2.40411814	2.45456257
C	-3.06501392	-0.96652971	3.81497708
H	-3.72393339	-1.22339984	4.63957906
C	-2.09365830	0.01532355	3.96525610
H	-1.98938022	0.53832622	4.91262080
C	-1.25188584	0.35514156	2.90884204
H	-0.52334995	1.14598407	3.05275514
C	2.98423662	1.46152433	-0.00938778
H	3.67115035	1.30020714	-0.84746828
H	2.68255186	2.51412249	-0.06973552
C	3.67782446	1.19423261	1.30123090
C	3.56099631	2.08058645	2.37494508
H	2.98161086	2.99311515	2.25078685
C	4.18054242	1.81701012	3.59425546
H	4.07905088	2.52221686	4.41535531
C	4.93131697	0.65734897	3.75873604
H	5.41868370	0.45071595	4.70793127
C	5.06046583	-0.23378995	2.69556037
H	5.65102841	-1.13882018	2.81236519
C	4.44032640	0.03515667	1.48002206
H	4.55400429	-0.66158512	0.65142883

C	-0.74359269	0.32660873	-3.21456909
H	-0.99855298	1.39258840	-3.24874010
H	0.03222214	0.18048577	-3.97403939
C	-1.95682123	-0.50870502	-3.52922416
C	-3.24647339	0.01114815	-3.39282994
H	-3.37232977	1.04815079	-3.08688084
C	-4.36812064	-0.77433912	-3.64666265
H	-5.36185899	-0.34939557	-3.53439885
C	-4.21533729	-2.09856510	-4.04722444
H	-5.08807929	-2.71334785	-4.24872757
C	-2.93533877	-2.62809311	-4.19575531
H	-2.80656935	-3.65834870	-4.51802505
C	-1.81878999	-1.83900618	-3.93968305
H	-0.82189812	-2.25677089	-4.06631434

Compound 3-*ax*, Cartesian coordinates for CCSD(T)/STO-3G:
Total Energy (Hartree) = –1079.147266258

O	1.55716164	1.50784320	-2.38360252
C	0.97109747	0.92441543	-1.48078227
C	1.53458153	0.80386992	-0.07401592
H	0.79729741	1.25570407	0.61725523
C	1.59113593	-0.70130603	0.27912437
H	2.26468615	-1.21841558	-0.42621016
H	2.01503268	-0.84932461	1.28059391
N	0.27569520	-1.32518491	0.17176378
C	-0.16291564	-1.26019061	-1.21889909
H	-1.08524394	-1.83647078	-1.36622116
H	0.61235483	-1.74561054	-1.83682955
C	-0.35072147	0.20273869	-1.68640030
H	-1.08585565	0.65646916	-0.99392132
C	-0.67689847	-0.92241356	1.13737706
C	-2.06643889	-1.01186848	0.88014961
H	-2.43588007	-1.34964567	-0.08856047
C	-3.00475221	-0.67267834	1.86288291
H	-4.06863111	-0.75765576	1.62560474
C	-2.59647295	-0.22333872	3.12548646
H	-3.33181074	0.04304985	3.88738459
C	-1.22446417	-0.11885299	3.38733956
H	-0.87435565	0.23552690	4.36045401
C	-0.27667213	-0.45524583	2.41238472
H	0.77917638	-0.35045276	2.66414137
C	2.88442021	1.50673074	0.08383428
H	3.61267483	1.05752633	-0.61081336
H	2.77263599	2.56045345	-0.21847115
C	3.37275438	1.40635868	1.50689293
C	2.71450071	2.11548613	2.53052351
H	1.88450239	2.78212284	2.27465244
C	3.11632163	1.98910087	3.86744238
H	2.59812141	2.55276242	4.64770652
C	4.18637279	1.14473535	4.20322589
H	4.50257375	1.04507883	5.24453061
C	4.85176503	0.43537398	3.19351361
H	5.68961780	-0.21991706	3.44508603
C	4.44405893	0.56558589	1.85713046
H	4.96786092	0.01257170	1.07109766

C	-0.86467373	0.31000239	-3.12360417
H	-0.94391469	1.37551173	-3.39299425
H	-0.12315954	-0.13163561	-3.80930429
C	-2.19823091	-0.37953525	-3.26496844
C	-3.34316292	0.16494893	-2.65119695
H	-3.26632370	1.11985359	-2.12093917
C	-4.57929925	-0.49207428	-2.72197191
H	-5.45881398	-0.05092998	-2.24540726
C	-4.68939824	-1.71137004	-3.40875519
H	-5.65207402	-2.22521833	-3.46653725
C	-3.55798571	-2.26263243	-4.02634436
H	-3.63553264	-3.20874220	-4.56809906
C	-2.32306809	-1.60055905	-3.95095366
H	-1.44240712	-2.03250872	-4.43671771

Compound 3-*eq*, Cartesian coordinates for CCSD(T)/STO-3G:
Total Energy (Hartree) = –1079.148214919

O	1.58808207	1.68364834	-2.42634830
C	1.16091673	0.84601818	-1.64382617
C	1.81750694	0.56161662	-0.30094935
H	2.13751933	-0.49759303	-0.31165634
C	0.76709402	0.68477967	0.81395104
H	1.22161302	0.37112862	1.76433059
H	0.47640735	1.75687484	0.91603887
N	-0.38024546	-0.16600217	0.53581091
C	-1.03923377	0.24701809	-0.70482207
H	-1.34106867	1.31962838	-0.65467549
H	-1.95288438	-0.34277029	-0.85196091
C	-0.10295033	0.04394891	-1.90271683
H	0.17495009	-1.02693904	-1.90201650
C	-1.28021871	-0.35561053	1.61983682
C	-2.31159445	-1.31041236	1.48158798
H	-2.38389691	-1.88882354	0.55735187
C	-3.21224890	-1.54848416	2.52344286
H	-3.99915818	-2.29525489	2.39160048
C	-3.09770874	-0.85142489	3.73738125
H	-3.79616281	-1.04304095	4.55488095
C	-2.06893583	0.08466054	3.88930258
H	-1.96132448	0.63525874	4.82764353
C	-1.17204121	0.34127770	2.84013974
H	-0.39306036	1.09075912	2.98436386
C	3.02474709	1.47439613	-0.05360178
H	3.74809745	1.33020852	-0.87152363
H	2.69620618	2.52493966	-0.11038143
C	3.66714343	1.19276463	1.28086566
C	3.45739495	2.03894378	2.38471721
H	2.85557257	2.94432293	2.25742561
C	4.01578528	1.74229395	3.63723096
H	3.84479390	2.41472740	4.48197892
C	4.79360807	0.58761580	3.80345056
H	5.23197020	0.35574323	4.77732825
C	5.00992408	-0.26572825	2.71041078
H	5.61909494	-1.16543690	2.83061974
C	4.44918680	0.03638013	1.46207058
H	4.62697363	-0.62997397	0.61160609

C	-0.77246491	0.41536411	-3.22958515
H	-1.06685199	1.47723345	-3.20057766
H	-0.03164817	0.31832284	-4.03838812
C	-1.96956118	-0.46271876	-3.49279615
C	-3.28105016	0.00145702	-3.28563734
H	-3.43897937	1.03888548	-2.97461502
C	-4.38386762	-0.84489115	-3.47722189
H	-5.39558256	-0.46431040	-3.31423526
C	-4.18849327	-2.17435397	-3.87740190
H	-5.04604908	-2.83462202	-4.02849387
C	-2.88501613	-2.65010574	-4.08804222
H	-2.72383045	-3.68351951	-4.40616053
C	-1.78806290	-1.79954750	-3.89556163
H	-0.77381613	-2.17487547	-4.06721982

Compound 3-*ax*, Cartesian coordinates for CCSD/cc-pvdz:
Total Energy (Hartree) = –1094.486710

O	1.55716164	1.50784320	-2.38360252
C	0.97109747	0.92441543	-1.48078227
C	1.53458153	0.80386992	-0.07401592
H	0.79729741	1.25570407	0.61725523
C	1.59113593	-0.70130603	0.27912437
H	2.26468615	-1.21841558	-0.42621016
H	2.01503268	-0.84932461	1.28059391
N	0.27569520	-1.32518491	0.17176378
C	-0.16291564	-1.26019061	-1.21889909
H	-1.08524394	-1.83647078	-1.36622116
H	0.61235483	-1.74561054	-1.83682955
C	-0.35072147	0.20273869	-1.68640030
H	-1.08585565	0.65646916	-0.99392132
C	-0.67689847	-0.92241356	1.13737706
C	-2.06643889	-1.01186848	0.88014961
H	-2.43588007	-1.34964567	-0.08856047
C	-3.00475221	-0.67267834	1.86288291
H	-4.06863111	-0.75765576	1.62560474
C	-2.59647295	-0.22333872	3.12548646
H	-3.33181074	0.04304985	3.88738459
C	-1.22446417	-0.11885299	3.38733956
H	-0.87435565	0.23552690	4.36045401
C	-0.27667213	-0.45524583	2.41238472
H	0.77917638	-0.35045276	2.66414137
C	2.88442021	1.50673074	0.08383428
H	3.61267483	1.05752633	-0.61081336
H	2.77263599	2.56045345	-0.21847115
C	3.37275438	1.40635868	1.50689293
C	2.71450071	2.11548613	2.53052351
H	1.88450239	2.78212284	2.27465244
C	3.11632163	1.98910087	3.86744238
H	2.59812141	2.55276242	4.64770652
C	4.18637279	1.14473535	4.20322589
H	4.50257375	1.04507883	5.24453061
C	4.85176503	0.43537398	3.19351361
H	5.68961780	-0.21991706	3.44508603
C	4.44405893	0.56558589	1.85713046
H	4.96786092	0.01257170	1.07109766

C	-0.86467373	0.31000239	-3.12360417
H	-0.94391469	1.37551173	-3.39299425
H	-0.12315954	-0.13163561	-3.80930429
C	-2.19823091	-0.37953525	-3.26496844
C	-3.34316292	0.16494893	-2.65119695
H	-3.26632370	1.11985359	-2.12093917
C	-4.57929925	-0.49207428	-2.72197191
H	-5.45881398	-0.05092998	-2.24540726
C	-4.68939824	-1.71137004	-3.40875519
H	-5.65207402	-2.22521833	-3.46653725
C	-3.55798571	-2.26263243	-4.02634436
H	-3.63553264	-3.20874220	-4.56809906
C	-2.32306809	-1.60055905	-3.95095366
H	-1.44240712	-2.03250872	-4.43671771

Compound 3-*eq*, optimized Cartesian coordinates for CCSD/cc-pvdz:
Total Energy (Hartree) = –1094.486130

O	1.58808207	1.68364834	-2.42634830
C	1.16091673	0.84601818	-1.64382617
C	1.81750694	0.56161662	-0.30094935
H	2.13751933	-0.49759303	-0.31165634
C	0.76709402	0.68477967	0.81395104
H	1.22161302	0.37112862	1.76433059
H	0.47640735	1.75687484	0.91603887
N	-0.38024546	-0.16600217	0.53581091
C	-1.03923377	0.24701809	-0.70482207
H	-1.34106867	1.31962838	-0.65467549
H	-1.95288438	-0.34277029	-0.85196091
C	-0.10295033	0.04394891	-1.90271683
H	0.17495009	-1.02693904	-1.90201650
C	-1.28021871	-0.35561053	1.61983682
C	-2.31159445	-1.31041236	1.48158798
H	-2.38389691	-1.88882354	0.55735187
C	-3.21224890	-1.54848416	2.52344286
H	-3.99915818	-2.29525489	2.39160048
C	-3.09770874	-0.85142489	3.73738125
H	-3.79616281	-1.04304095	4.55488095
C	-2.06893583	0.08466054	3.88930258
H	-1.96132448	0.63525874	4.82764353
C	-1.17204121	0.34127770	2.84013974
H	-0.39306036	1.09075912	2.98436386
C	3.02474709	1.47439613	-0.05360178
H	3.74809745	1.33020852	-0.87152363
H	2.69620618	2.52493966	-0.11038143
C	3.66714343	1.19276463	1.28086566
C	3.45739495	2.03894378	2.38471721
H	2.85557257	2.94432293	2.25742561
C	4.01578528	1.74229395	3.63723096
H	3.84479390	2.41472740	4.48197892
C	4.79360807	0.58761580	3.80345056
H	5.23197020	0.35574323	4.77732825
C	5.00992408	-0.26572825	2.71041078
H	5.61909494	-1.16543690	2.83061974
C	4.44918680	0.03638013	1.46207058
H	4.62697363	-0.62997397	0.61160609

C	-0.77246491	0.41536411	-3.22958515
H	-1.06685199	1.47723345	-3.20057766
H	-0.03164817	0.31832284	-4.03838812
C	-1.96956118	-0.46271876	-3.49279615
C	-3.28105016	0.00145702	-3.28563734
H	-3.43897937	1.03888548	-2.97461502
C	-4.38386762	-0.84489115	-3.47722189
H	-5.39558256	-0.46431040	-3.31423526
C	-4.18849327	-2.17435397	-3.87740190
H	-5.04604908	-2.83462202	-4.02849387
C	-2.88501613	-2.65010574	-4.08804222
H	-2.72383045	-3.68351951	-4.40616053
C	-1.78806290	-1.79954750	-3.89556163
H	-0.77381613	-2.17487547	-4.06721982

Compound 3-*ax*, Cartesian coordinates for CCSD(T)/cc-pvdz:
Total Energy (Hartree) = –1094.65650

O	1.55716164	1.50784320	-2.38360252
C	0.97109747	0.92441543	-1.48078227
C	1.53458153	0.80386992	-0.07401592
H	0.79729741	1.25570407	0.61725523
C	1.59113593	-0.70130603	0.27912437
H	2.26468615	-1.21841558	-0.42621016
H	2.01503268	-0.84932461	1.28059391
N	0.27569520	-1.32518491	0.17176378
C	-0.16291564	-1.26019061	-1.21889909
H	-1.08524394	-1.83647078	-1.36622116
H	0.61235483	-1.74561054	-1.83682955
C	-0.35072147	0.20273869	-1.68640030
H	-1.08585565	0.65646916	-0.99392132
C	-0.67689847	-0.92241356	1.13737706
C	-2.06643889	-1.01186848	0.88014961
H	-2.43588007	-1.34964567	-0.08856047
C	-3.00475221	-0.67267834	1.86288291
H	-4.06863111	-0.75765576	1.62560474
C	-2.59647295	-0.22333872	3.12548646
H	-3.33181074	0.04304985	3.88738459
C	-1.22446417	-0.11885299	3.38733956
H	-0.87435565	0.23552690	4.36045401
C	-0.27667213	-0.45524583	2.41238472
H	0.77917638	-0.35045276	2.66414137
C	2.88442021	1.50673074	0.08383428
H	3.61267483	1.05752633	-0.61081336
H	2.77263599	2.56045345	-0.21847115
C	3.37275438	1.40635868	1.50689293
C	2.71450071	2.11548613	2.53052351
H	1.88450239	2.78212284	2.27465244
C	3.11632163	1.98910087	3.86744238
H	2.59812141	2.55276242	4.64770652
C	4.18637279	1.14473535	4.20322589
H	4.50257375	1.04507883	5.24453061
C	4.85176503	0.43537398	3.19351361
H	5.68961780	-0.21991706	3.44508603
C	4.44405893	0.56558589	1.85713046
H	4.96786092	0.01257170	1.07109766

C	-0.86467373	0.31000239	-3.12360417
H	-0.94391469	1.37551173	-3.39299425
H	-0.12315954	-0.13163561	-3.80930429
C	-2.19823091	-0.37953525	-3.26496844
C	-3.34316292	0.16494893	-2.65119695
H	-3.26632370	1.11985359	-2.12093917
C	-4.57929925	-0.49207428	-2.72197191
H	-5.45881398	-0.05092998	-2.24540726
C	-4.68939824	-1.71137004	-3.40875519
H	-5.65207402	-2.22521833	-3.46653725
C	-3.55798571	-2.26263243	-4.02634436
H	-3.63553264	-3.20874220	-4.56809906
C	-2.32306809	-1.60055905	-3.95095366
H	-1.44240712	-2.03250872	-4.43671771

Compound 3-*eq*, optimized Cartesian coordinates for CCSD(T)/cc-pvdz:
Total Energy (Hartree) = –1094.65442

O	1.58808207	1.68364834	-2.42634830
C	1.16091673	0.84601818	-1.64382617
C	1.81750694	0.56161662	-0.30094935
H	2.13751933	-0.49759303	-0.31165634
C	0.76709402	0.68477967	0.81395104
H	1.22161302	0.37112862	1.76433059
H	0.47640735	1.75687484	0.91603887
N	-0.38024546	-0.16600217	0.53581091
C	-1.03923377	0.24701809	-0.70482207
H	-1.34106867	1.31962838	-0.65467549
H	-1.95288438	-0.34277029	-0.85196091
C	-0.10295033	0.04394891	-1.90271683
H	0.17495009	-1.02693904	-1.90201650
C	-1.28021871	-0.35561053	1.61983682
C	-2.31159445	-1.31041236	1.48158798
H	-2.38389691	-1.88882354	0.55735187
C	-3.21224890	-1.54848416	2.52344286
H	-3.99915818	-2.29525489	2.39160048
C	-3.09770874	-0.85142489	3.73738125
H	-3.79616281	-1.04304095	4.55488095
C	-2.06893583	0.08466054	3.88930258
H	-1.96132448	0.63525874	4.82764353
C	-1.17204121	0.34127770	2.84013974
H	-0.39306036	1.09075912	2.98436386
C	3.02474709	1.47439613	-0.05360178
H	3.74809745	1.33020852	-0.87152363
H	2.69620618	2.52493966	-0.11038143
C	3.66714343	1.19276463	1.28086566
C	3.45739495	2.03894378	2.38471721
H	2.85557257	2.94432293	2.25742561
C	4.01578528	1.74229395	3.63723096
H	3.84479390	2.41472740	4.48197892
C	4.79360807	0.58761580	3.80345056
H	5.23197020	0.35574323	4.77732825
C	5.00992408	-0.26572825	2.71041078
H	5.61909494	-1.16543690	2.83061974
C	4.44918680	0.03638013	1.46207058
H	4.62697363	-0.62997397	0.61160609

C	-0.77246491	0.41536411	-3.22958515
H	-1.06685199	1.47723345	-3.20057766
H	-0.03164817	0.31832284	-4.03838812
C	-1.96956118	-0.46271876	-3.49279615
C	-3.28105016	0.00145702	-3.28563734
H	-3.43897937	1.03888548	-2.97461502
C	-4.38386762	-0.84489115	-3.47722189
H	-5.39558256	-0.46431040	-3.31423526
C	-4.18849327	-2.17435397	-3.87740190
H	-5.04604908	-2.83462202	-4.02849387
C	-2.88501613	-2.65010574	-4.08804222
H	-2.72383045	-3.68351951	-4.40616053
C	-1.78806290	-1.79954750	-3.89556163
H	-0.77381613	-2.17487547	-4.06721982

Compound 3-*ax*, Cartesian coordinates for SIC-PBE0/6-311G:**
Total Energy (Hartree) = –1096.17877637

O	1.51183798	1.49637574	-2.33230048
C	0.94396278	0.90509114	-1.44515264
C	1.52006703	0.79476609	-0.04100129
H	0.82158553	1.31777304	0.63109586
C	1.49439844	-0.68756500	0.38800145
H	2.15629892	-1.26753387	-0.26731846
H	1.89423448	-0.79640109	1.39527186
N	0.16446128	-1.24867209	0.28368603
C	-0.25379757	-1.25133356	-1.10293814
H	-1.18997019	-1.79252139	-1.23561613
H	0.50129193	-1.80111642	-1.67769924
C	-0.37542509	0.18208512	-1.66189817
H	-1.12546802	0.69036896	-1.03739207
C	-0.77669639	-0.95784790	1.27838301
C	-2.15665084	-1.09435051	1.04398870
H	-2.52795914	-1.38267234	0.06910889
C	-3.08088022	-0.86649111	2.05167672
H	-4.13712969	-0.98320331	1.82913779
C	-2.67803304	-0.48268587	3.32384281
H	-3.40175412	-0.29844840	4.10791581
C	-1.31864101	-0.33112871	3.56438824
H	-0.96988602	-0.02793623	4.54591968
C	-0.38222322	-0.55549019	2.56593811
H	0.66342080	-0.41454319	2.80721699
C	2.90776054	1.42475127	0.06390450
H	3.59174802	0.88801862	-0.60239786
H	2.85568961	2.44598623	-0.32365057
C	3.44530714	1.41731061	1.46998126
C	2.85648016	2.20369742	2.46381302
H	2.02195098	2.85330182	2.20870244
C	3.32647751	2.17240290	3.77066556
H	2.85831360	2.79655745	4.52595451
C	4.39753086	1.35451933	4.11061455
H	4.76624220	1.33227514	5.13151853
C	4.99552951	0.57072589	3.13272833
H	5.83591239	-0.06893655	3.38259541
C	4.52022098	0.60336359	1.82602385
H	4.99428307	-0.01362276	1.06788194

C	-0.81689645	0.21765053	-3.12352089
H	-0.81096185	1.25717560	-3.46518889
H	-0.06988196	-0.29762327	-3.73608756
C	-2.17286256	-0.40042931	-3.33997759
C	-3.32132708	0.19949562	-2.81512840
H	-3.23614089	1.13325898	-2.26597005
C	-4.57196058	-0.37791864	-2.99104119
H	-5.45141818	0.10491664	-2.57707833
C	-4.70054136	-1.56764751	-3.70268761
H	-5.67754910	-2.02065814	-3.83834713
C	-3.56911503	-2.17008550	-4.23409444
H	-3.65742724	-3.09364864	-4.79712624
C	-2.31835973	-1.59035983	-4.05166903
H	-1.43730683	-2.06622366	-4.47489000

Compound 3-*eq*, Cartesian coordinates for SIC-PBE0/6-311G:**
Total Energy (Hartree) = –1096.18590236

O	1.65749786	1.43941228	-2.43311800
C	1.14326381	0.74759007	-1.58734025
C	1.73953725	0.57187020	-0.20281712
H	2.02795452	-0.48695218	-0.12724235
C	0.67095500	0.80107875	0.87626769
H	1.09667985	0.51815073	1.84063116
H	0.43423789	1.88135925	0.92367864
N	-0.50330486	0.00014780	0.61870373
C	-1.11383327	0.30846803	-0.66145592
H	-1.40213908	1.37585634	-0.70791251
H	-2.02797432	-0.27042506	-0.78698174
C	-0.15900674	0.00322043	-1.82055803
H	0.07495422	-1.06931078	-1.75931221
C	-1.36442482	-0.28925789	1.69108648
C	-2.36222902	-1.26360522	1.53400846
H	-2.45642506	-1.78646681	0.58889119
C	-3.20564197	-1.59296571	2.58126134
H	-3.96311483	-2.35558836	2.43023686
C	-3.07665291	-0.97356508	3.82127142
H	-3.73360260	-1.24001925	4.64169952
C	-2.08913956	-0.01442849	3.98877778
H	-1.97276954	0.48475870	4.94563405
C	-1.24634460	0.33397686	2.93867038
H	-0.50213357	1.10521036	3.09664418
C	2.97369795	1.45374400	-0.00400212
H	3.65125713	1.28525912	-0.84599518
H	2.67460024	2.50487320	-0.06796507
C	3.68369674	1.19507774	1.29753918
C	3.58924782	2.08935157	2.36370400
H	3.01206658	3.00198390	2.24162311
C	4.22930951	1.83394737	3.57159884
H	4.14504895	2.54481715	4.38754438
C	4.97844848	0.67533700	3.73221018
H	5.48135118	0.47522765	4.67218462
C	5.08511979	-0.22336647	2.67607289
H	5.67449511	-1.12774845	2.78935778
C	4.44483771	0.03706458	1.47204445
H	4.54311860	-0.66540651	0.64845400

C	-0.76112137	0.32520550	-3.18801061
H	-1.02456800	1.38730603	-3.22086909
H	0.01664273	0.18802464	-3.94436120
C	-1.96416643	-0.51685852	-3.51891991
C	-3.25689023	-0.00205055	-3.42236514
H	-3.39539193	1.03235274	-3.12069054
C	-4.36494771	-0.78932942	-3.71534668
H	-5.36197607	-0.36795737	-3.63720772
C	-4.19700044	-2.11006527	-4.11227452
H	-5.06027287	-2.72377941	-4.34758146
C	-2.91374381	-2.63572180	-4.21560409
H	-2.77204341	-3.66347255	-4.53430413
C	-1.81063042	-1.84528351	-3.92158947
H	-0.81088866	-2.26099069	-4.01751388

Compound 3-*ax*, Cartesian coordinates for SIC-B3LYP/6-311G:**
Total Energy (Hartree) = –1096.705815

O	1.60178618	1.33674775	-2.39452347
C	1.00738629	0.79185511	-1.48957739
C	1.56242640	0.72844828	-0.06683632
H	0.86161595	1.28008366	0.57434242
C	1.52713703	-0.74803878	0.42491832
H	2.22636704	-1.34251976	-0.17451812
H	1.87824388	-0.79342114	1.45176450
N	0.20009747	-1.33612116	0.29688597
C	-0.22822486	-1.34545547	-1.09237668
H	-1.17362299	-1.87406534	-1.19669898
H	0.51138909	-1.91582000	-1.66651742
C	-0.33116646	0.08354765	-1.69860719
H	-1.07275900	0.62919336	-1.10031908
C	-0.74540128	-1.17282506	1.32785717
C	-2.12577903	-1.06848194	1.06633738
H	-2.49798660	-1.06085229	0.05149418
C	-3.04684053	-0.96542507	2.10552134
H	-4.10128414	-0.88883643	1.86239628
C	-2.63415760	-0.94809958	3.43333186
H	-3.35484927	-0.86323574	4.23744642
C	-1.27082946	-1.04620049	3.70474000
H	-0.91939810	-1.04426336	4.73079507
C	-0.34163382	-1.16002783	2.67847894
H	0.70278491	-1.26503165	2.93789618
C	2.95990951	1.36504873	0.03546883
H	3.66960063	0.76029349	-0.53725633
H	2.92771339	2.33601332	-0.46456629
C	3.45068839	1.52847337	1.45787159
C	2.92160385	2.52823070	2.28356186
H	2.16482525	3.20052463	1.89063170
C	3.35862499	2.68069564	3.59621865
H	2.93731534	3.46396077	4.21685136
C	4.33971732	1.83442039	4.11073281
H	4.68328104	1.95423701	5.13180919
C	4.87912574	0.83908434	3.30069431
H	5.64851966	0.17991731	3.68799705
C	4.43734428	0.69007715	1.98675373
H	4.87140520	-0.08248401	1.35969206

C	-0.76423903	0.08462007	-3.17535028
H	-0.62608536	1.09386334	-3.56960121
H	-0.08396540	-0.55434760	-3.74650673
C	-2.19375797	-0.36642883	-3.38441167
C	-3.26123616	0.48428320	-3.06848551
H	-3.05500908	1.48131895	-2.69153554
C	-4.58043893	0.07624029	-3.24345446
H	-5.39103979	0.75328126	-2.99745756
C	-4.85993394	-1.19535159	-3.74182932
H	-5.88670645	-1.51366409	-3.88152480
C	-3.80994362	-2.04995549	-4.06576128
H	-4.01621213	-3.03869313	-4.46107069
C	-2.49042804	-1.63691354	-3.88829296
H	-1.67883408	-2.30751451	-4.15258049

Compound 3-*eq*, Cartesian coordinates for SIC-B3LYP/6-311G:**
Total Energy (Hartree) = –1096.7155345

O	1.67036015	1.42555149	-2.44565379
C	1.14209581	0.75123068	-1.58996673
C	1.73840948	0.58056081	-0.19380689
H	2.02648501	-0.47675944	-0.11774900
C	0.66293240	0.81315143	0.89164083
H	1.08536672	0.52873776	1.85426234
H	0.42838870	1.89235094	0.93889296
N	-0.52537416	0.01441711	0.63432783
C	-1.13595795	0.33170396	-0.65605836
H	-1.41128696	1.40121162	-0.69855663
H	-2.05394336	-0.23655732	-0.78200941
C	-0.17625695	0.01509864	-1.82088582
H	0.05000629	-1.05740030	-1.75443719
C	-1.38845631	-0.28311992	1.71424103
C	-2.40727177	-1.24034708	1.54831641
H	-2.51940969	-1.74473998	0.59681870
C	-3.25094841	-1.57502242	2.59827959
H	-4.02343407	-2.31921589	2.43846506
C	-3.10112548	-0.98140914	3.85208004
H	-3.75739416	-1.25017079	4.67114887
C	-2.09174889	-0.04289820	4.03103278
H	-1.95717873	0.43289078	4.99648573
C	-1.24979430	0.31271631	2.97809973
H	-0.49220475	1.06527820	3.14910573
C	2.98335608	1.46528010	0.00747178
H	3.65366584	1.30385100	-0.84019406
H	2.68364433	2.51586665	-0.04550628
C	3.71149984	1.20182574	1.30757108
C	3.63528189	2.10147075	2.37558691
H	3.06345732	3.01684552	2.26022814
C	4.28903037	1.84522924	3.57996170
H	4.21772143	2.55827795	4.39400126
C	5.03456860	0.67983191	3.73631015
H	5.54315944	0.47742067	4.67183067
C	5.12725543	-0.22220195	2.67731927
H	5.71371553	-1.12792039	2.78542796
C	4.47405386	0.03926278	1.47633279
H	4.56394413	-0.66465437	0.65453516

C	-0.77713617	0.33014756	-3.20271298
H	-1.04965364	1.38881016	-3.24034930
H	0.00797374	0.19806651	-3.95090381
C	-1.97662492	-0.52523825	-3.54843779
C	-3.27633740	-0.01382666	-3.47815589
H	-3.42572299	1.02212670	-3.19158054
C	-4.38006948	-0.81069544	-3.77848915
H	-5.37846670	-0.39174346	-3.71944040
C	-4.20114962	-2.13849958	-4.15776661
H	-5.05757946	-2.76002432	-4.39336409
C	-2.91095496	-2.66023557	-4.23974268
H	-2.75994501	-3.68962469	-4.54534730
C	-1.81220718	-1.85985645	-3.93952444
H	-0.81123414	-2.27321158	-4.01901010