

Supplementary Material

Tunable Aromaticity in Bicalicenes

Marcos Mandado,* Nicolás Ramos-Berdullas

*Department of Physical Chemistry, University of Vigo, Lagoas-Marcosende s/n,
36310.Vigo, Spain*

*corresponding author email: mandado@uvigo.es

Table S1. Cartesian coordinates of the structures **0-20** obtained at the HF/6-311G(d,p) level

0			
C	-1.854312490441	0.721261361088	0.000000000000
C	-1.854312490441	-0.721261361088	0.000000000000
C	-0.700501721000	-1.510463347164	0.000000000000
C	0.700501721000	-1.510463347164	0.000000000000
C	1.854312490441	-0.721261361088	0.000000000000
C	1.854312490441	0.721261361088	0.000000000000
C	0.700501721000	1.510463347164	0.000000000000
C	-0.700501721000	1.510463347164	0.000000000000
C	0.000000000000	2.668245583082	0.000000000000
C	0.000000000000	-2.668245583082	0.000000000000
C	-3.187840650171	1.132921475046	0.000000000000
C	-4.001637033832	0.000000000000	0.000000000000
C	-3.187840650171	-1.132921475046	0.000000000000
C	3.187840650171	-1.132921475046	0.000000000000
C	4.001637033832	0.000000000000	0.000000000000
C	3.187840650171	1.132921475046	0.000000000000
H	0.000000000000	3.735654423154	0.000000000000
H	-3.525566937451	2.151978559554	0.000000000000
H	-5.074089785411	0.000000000000	0.000000000000
H	-3.525566937451	-2.151978559554	0.000000000000
H	0.000000000000	-3.735654423154	0.000000000000
H	3.525566937451	-2.151978559554	0.000000000000
H	5.074089785411	0.000000000000	0.000000000000
H	3.525566937451	2.151978559554	0.000000000000
1			
C	0.000000000000	0.714252825724	1.861189844694
C	0.000000000000	-0.725062742891	1.856638687319
C	0.000000000000	-1.519456587619	0.693696117640
C	0.000000000000	-1.515251512401	-0.700822627089
C	0.000000000000	-0.714252825724	-1.861189844694
C	0.000000000000	0.725062742891	-1.856638687319
C	0.000000000000	1.519456587619	-0.693696117640
C	0.000000000000	1.515251512401	0.700822627089
C	0.000000000000	2.671721134674	0.003853710600
C	0.000000000000	-2.671721134674	-0.003853710600
C	0.000000000000	1.128214621300	3.185307761766

C	0.000000000000	-0.014718589736	3.994532244890
C	0.000000000000	-1.151269975137	3.177175839094
C	0.000000000000	-1.128214621300	-3.185307761766
C	0.000000000000	0.014718589736	-3.994532244890
C	0.000000000000	1.151269975137	-3.177175839094
H	0.000000000000	2.139990363563	3.541357406593
H	0.000000000000	-2.167815173174	3.517891886500
H	0.000000000000	-2.139990363563	-3.541357406593
H	0.000000000000	2.167815173174	-3.517891886500
C	0.000000000000	-0.015979361599	5.424040670425
N	0.000000000000	-0.012640428079	6.555635141196
C	0.000000000000	0.015979361599	-5.424040670425
N	0.000000000000	0.012640428079	-6.555635141196
O	0.000000000000	-3.970939569134	0.047811256755
H	0.000000000000	-4.349031945287	-0.817958867353
O	0.000000000000	3.970939569134	-0.047811256755
H	0.000000000000	4.349031945287	0.817958867353

2

C	-0.017211320326	0.733624625527	1.846381214113
C	-0.017341938493	-0.710850440209	1.860181327851
C	-0.006587526580	-1.500436541644	0.706431033695
C	0.006564621594	-1.495010544924	-0.704410074771
C	0.017211341993	-0.733597819416	-1.846381214113
C	0.017341960160	0.710877246320	-1.860181327851
C	0.006587548246	1.500463347755	-0.706431033695
C	-0.006564599928	1.495037351035	0.704410074771
C	0.000170484098	2.656721739038	-0.017897987047
C	-0.000170462431	-2.656694932927	0.017897987047
C	-0.029794534831	1.154946454897	3.196254790037
C	-0.037207804415	0.028801608721	3.991317583704
C	-0.029674880815	-1.120888033405	3.183086324562
C	0.029794556497	-1.154919648786	-3.196254790037
C	0.037207826082	-0.028774802610	-3.991317583704
C	0.029674902482	1.120914839516	-3.183086324562
H	-0.032945483940	2.173963695534	3.534408866775
H	-0.033057273155	-2.129807992537	3.545770711196
H	0.032945505607	-2.173936889423	-3.534408866775
H	0.033057294822	2.129834798648	-3.545770711196
C	-0.000263135753	-4.067729051722	0.027632619874
N	-0.000275271876	-5.196879674352	0.028769215195
C	0.000263157420	4.067755857833	-0.027632619874
N	0.000275293542	5.196906480463	-0.028769215195
O	-0.049763265147	-0.047149236095	5.338141211057
H	-0.053302868832	0.813080466113	5.717963348943
O	0.049763286814	0.047176042206	-5.338141211057
H	0.053302890499	-0.813053660002	-5.717963348943

3

C	0.000000000000	0.722062483291	1.854780723962
C	0.000000000000	-0.722062483291	1.854780723962
C	0.000000000000	-1.513978945419	0.697839403290
C	0.000000000000	-1.513978945419	-0.697839403290
C	0.000000000000	-0.722062483291	-1.854780723962
C	0.000000000000	0.722062483291	-1.854780723962
C	0.000000000000	1.513978945419	-0.697839403290
C	0.000000000000	1.513978945419	0.697839403290
C	0.000000000000	2.672076956166	0.000000000000
C	0.000000000000	-2.672076956166	0.000000000000
C	0.000000000000	1.140179268284	3.178265367089

C	0.000000000000	0.000000000000	3.990529993707
C	0.000000000000	-1.140179268284	3.178265367089
C	0.000000000000	-1.140179268284	-3.178265367089
C	0.000000000000	0.000000000000	-3.990529993707
C	0.000000000000	1.140179268284	-3.178265367089
H	0.000000000000	2.154524267731	3.525699090749
H	0.000000000000	-2.154524267731	3.525699090749
H	0.000000000000	-2.154524267731	-3.525699090749
H	0.000000000000	2.154524267731	-3.525699090749
C	0.000000000000	0.000000000000	5.420957348514
N	0.000000000000	0.000000000000	6.552330510865
C	0.000000000000	0.000000000000	-5.420957348514
N	0.000000000000	0.000000000000	-6.552330510865
H	0.000000000000	3.739743849783	0.000000000000
H	0.000000000000	-3.739743849783	0.000000000000

4

C	0.000000000000	0.724889298622	1.848597758074
C	0.000000000000	-0.724889298622	1.848597758074
C	0.000000000000	-1.508363374550	0.705496018814
C	0.000000000000	-1.508363374550	-0.705496018814
C	0.000000000000	-0.724889298622	-1.848597758074
C	0.000000000000	0.724889298622	-1.848597758074
C	0.000000000000	1.508363374550	-0.705496018814
C	0.000000000000	1.508363374550	0.705496018814
C	0.000000000000	2.666298543216	0.000000000000
C	0.000000000000	-2.666298543216	0.000000000000
C	0.000000000000	1.132876608731	3.185133088400
C	0.000000000000	0.000000000000	3.997107264484
C	0.000000000000	-1.132876608731	3.185133088400
C	0.000000000000	-1.132876608731	-3.185133088400
C	0.000000000000	0.000000000000	-3.997107264484
C	0.000000000000	1.132876608731	-3.185133088400
H	0.000000000000	2.150936661356	3.524577734419
H	0.000000000000	-2.150936661356	3.524577734419
H	0.000000000000	-2.150936661356	-3.524577734419
H	0.000000000000	2.150936661356	-3.524577734419
H	0.000000000000	0.000000000000	5.068866420809
H	0.000000000000	0.000000000000	-5.068866420809
C	0.000000000000	4.078023185241	0.000000000000
N	0.000000000000	5.207037993562	0.000000000000
C	0.000000000000	-4.078023185241	0.000000000000
N	0.000000000000	-5.207037993562	0.000000000000

5

C	0.000000000000	0.712663857510	1.860335833130
C	0.000000000000	-0.724004794216	1.857637417427
C	0.000000000000	-1.516697498595	0.697955549880
C	0.000000000000	-1.510332867618	-0.703376226636
C	0.000000000000	-0.712663857510	-1.860335833130
C	0.000000000000	0.724004794216	-1.857637417427
C	0.000000000000	1.516697498595	-0.697955549880
C	0.000000000000	1.510332867618	0.703376226636
C	0.000000000000	2.664735344789	0.004412488462
C	0.000000000000	-2.664735344789	-0.004412488462
C	0.000000000000	1.122252108976	3.195384455174
C	0.000000000000	-0.012192791081	4.006757176286
C	0.000000000000	-1.142629230703	3.188775045249
C	0.000000000000	-1.122252108976	-3.195384455174
C	0.000000000000	0.012192791081	-4.006757176286

C	0.000000000000	1.142629230703	-3.188775045249
H	0.000000000000	2.139863357521	3.539651550142
H	0.000000000000	-2.163545967154	3.520485388273
H	0.000000000000	-2.139863357521	-3.539651550142
H	0.000000000000	2.163545967154	-3.520485388273
O	0.000000000000	-3.971529761391	0.036918138881
H	0.000000000000	-4.331165593381	-0.835708512210
O	0.000000000000	3.971529761391	-0.036918138881
H	0.000000000000	4.331165593381	0.835708512210
H	0.000000000000	0.015038988519	-5.079223801787
H	0.000000000000	-0.015038988519	5.079223801787

6

C	-0.017363214342	0.705804314663	1.863006545859
C	-0.017261836292	-0.729379458232	1.851240143067
C	-0.006502631536	-1.501329041327	0.696611733770
C	0.006554490926	-1.500015923132	-0.704035902196
C	0.017363244175	-0.705772147829	-1.863006545859
C	0.017261866125	0.729411625065	-1.851240143067
C	0.006502661370	1.501361208161	-0.696611733770
C	-0.006554461093	1.500048089965	0.704035902196
C	-0.000151284605	2.659083748167	0.017881762154
C	0.000151314439	-2.659051581333	-0.017881762154
C	-0.029731787358	1.120492520516	3.190051314618
C	-0.037231386662	-0.024727274008	3.993828229609
C	-0.029784768072	-1.154315144452	3.194321555543
C	0.029731817191	-1.120460353683	-3.190051314618
C	0.037231416495	0.024759440842	-3.993828229609
C	0.029784797906	1.154347311285	-3.194321555543
H	-0.033093817420	2.130166858004	3.551326272943
H	-0.032943210308	-2.173954504469	3.532496926457
H	0.033093847254	-2.130134691171	-3.551326272943
H	0.032943240141	2.173986671302	-3.532496926457
H	-0.000239597898	3.726341523039	0.028018152594
H	0.000239627732	-3.726309356206	-0.028018152594
O	-0.049854742230	0.039185190606	5.347985844239
H	-0.053251535079	-0.827557766256	5.711824259584
O	0.049854772064	-0.039153023773	-5.347985844239
H	0.053251564912	0.827589933089	-5.711824259584

7

C	0.000000000000	0.713336917741	1.858995999307
C	0.000000000000	-0.713336917741	1.858995999307
C	0.000000000000	-1.495396281887	0.680137937878
C	0.000000000000	-1.495396281887	-0.680137937878
C	0.000000000000	-0.713336917741	-1.858995999307
C	0.000000000000	0.713336917741	-1.858995999307
C	0.000000000000	1.495396281887	-0.680137937878
C	0.000000000000	1.495396281887	0.680137937878
C	0.000000000000	2.698184185767	0.000000000000
C	0.000000000000	-2.698184185767	0.000000000000
C	0.000000000000	1.143710838375	3.192201844210
C	0.000000000000	0.000000000000	3.973434661843
C	0.000000000000	-1.143710838375	3.192201844210
C	0.000000000000	-1.143710838375	-3.192201844210
C	0.000000000000	0.000000000000	-3.973434661843
C	0.000000000000	1.143710838375	-3.192201844210
H	0.000000000000	2.154446611620	3.550955211383
H	0.000000000000	-2.154446611620	3.550955211383
H	0.000000000000	-2.154446611620	-3.550955211383

H	0.000000000000	2.154446611620	-3.550955211383
Li	0.000000000000	4.656386406897	0.000000000000
Li	0.000000000000	-4.656386406897	0.000000000000
F	0.000000000000	0.000000000000	-5.309471847493
F	0.000000000000	0.000000000000	5.309471847493

8

C	0.000000000000	0.721229685706	1.856002173615
C	0.000000000000	-0.721229685706	1.856002173615
C	0.000000000000	-1.522746536322	0.716603588526
C	0.000000000000	-1.522746536322	-0.716603588526
C	0.000000000000	-0.721229685706	-1.856002173615
C	0.000000000000	0.721229685706	-1.856002173615
C	0.000000000000	1.522746536322	-0.716603588526
C	0.000000000000	1.522746536322	0.716603588526
C	0.000000000000	2.652659867235	0.000000000000
C	0.000000000000	-2.652659867235	0.000000000000
C	0.000000000000	1.113633818018	3.199371079467
C	0.000000000000	0.000000000000	4.072519591581
C	0.000000000000	-1.113633818018	3.199371079467
C	0.000000000000	-1.113633818018	-3.199371079467
C	0.000000000000	0.000000000000	-4.072519591581
C	0.000000000000	1.113633818018	-3.199371079467
H	0.000000000000	2.147161574063	3.506651539915
H	0.000000000000	-2.147161574063	3.506651539915
H	0.000000000000	-2.147161574063	-3.506651539915
H	0.000000000000	2.147161574063	-3.506651539915
F	0.000000000000	3.943343156101	0.000000000000
F	0.000000000000	-3.943343156101	0.000000000000
Li	0.000000000000	0.000000000000	-6.021324200079
Li	0.000000000000	0.000000000000	6.021324200079

9

C	0.000000000000	0.718482711823	1.856384278462
C	0.000000000000	-0.718482711823	1.856384278462
C	0.000000000000	-1.503812279721	0.699446686605
C	0.000000000000	-1.503812279721	-0.699446686605
C	0.000000000000	-0.718482711823	-1.856384278462
C	0.000000000000	0.718482711823	-1.856384278462
C	0.000000000000	1.503812279721	-0.699446686605
C	0.000000000000	1.503812279721	0.699446686605
C	0.000000000000	2.661879956875	0.000000000000
C	0.000000000000	-2.661879956875	0.000000000000
C	0.000000000000	1.142643615079	3.189549197294
C	0.000000000000	0.000000000000	3.971055847559
C	0.000000000000	-1.142643615079	3.189549197294
C	0.000000000000	-1.142643615079	-3.189549197294
C	0.000000000000	0.000000000000	-3.971055847559
C	0.000000000000	1.142643615079	-3.189549197294
H	0.000000000000	2.152963943434	3.547509692492
H	0.000000000000	-2.152963943434	3.547509692492
H	0.000000000000	-2.152963943434	-3.547509692492
H	0.000000000000	2.152963943434	-3.547509692492
F	0.000000000000	0.000000000000	-5.297636260008
F	0.000000000000	0.000000000000	5.297636260008
H	0.000000000000	3.729279281128	0.000000000000
H	0.000000000000	-3.729279281128	0.000000000000

10

C	0.000000000000	0.720446274085	1.856670582257
C	0.000000000000	-0.720446274085	1.856670582257

C	0.000000000000	-1.521964505788	0.711884650383
C	0.000000000000	-1.521964505788	-0.711884650383
C	0.000000000000	-0.720446274085	-1.856670582257
C	0.000000000000	0.720446274085	-1.856670582257
C	0.000000000000	1.521964505788	-0.711884650383
C	0.000000000000	1.521964505788	0.711884650383
C	0.000000000000	2.654439654185	0.000000000000
C	0.000000000000	-2.654439654185	0.000000000000
C	0.000000000000	1.131999110918	3.191121621504
C	0.000000000000	0.000000000000	4.005029406997
C	0.000000000000	-1.131999110918	3.191121621504
C	0.000000000000	-1.131999110918	-3.191121621504
C	0.000000000000	0.000000000000	-4.005029406997
C	0.000000000000	1.131999110918	-3.191121621504
H	0.000000000000	2.151325394935	3.527564394155
H	0.000000000000	-2.151325394935	3.527564394155
H	0.000000000000	-2.151325394935	-3.527564394155
H	0.000000000000	2.151325394935	-3.527564394155
F	0.000000000000	3.936681129700	0.000000000000
F	0.000000000000	-3.936681129700	0.000000000000
H	0.000000000000	0.000000000000	5.077150278624
H	0.000000000000	0.000000000000	-5.077150278624

11

C	0.000000000000	0.716938810205	1.858003821261
C	0.000000000000	-0.716938810205	1.858003821261
C	0.000000000000	-1.501323667059	0.681187056126
C	0.000000000000	-1.501323667059	-0.681187056126
C	0.000000000000	-0.716938810205	-1.858003821261
C	0.000000000000	0.716938810205	-1.858003821261
C	0.000000000000	1.501323667059	-0.681187056126
C	0.000000000000	1.501323667059	0.681187056126
C	0.000000000000	2.703841978269	0.000000000000
C	0.000000000000	-2.703841978269	0.000000000000
C	0.000000000000	1.134030140229	3.189799959786
C	0.000000000000	0.000000000000	4.006299952989
C	0.000000000000	-1.134030140229	3.189799959786
C	0.000000000000	-1.134030140229	-3.189799959786
C	0.000000000000	0.000000000000	-4.006299952989
C	0.000000000000	1.134030140229	-3.189799959786
H	0.000000000000	2.154401932082	3.527702681094
H	0.000000000000	-2.154401932082	3.527702681094
H	0.000000000000	-2.154401932082	-3.527702681094
H	0.000000000000	2.154401932082	-3.527702681094
H	0.000000000000	0.000000000000	5.080291165448
H	0.000000000000	0.000000000000	-5.080291165448
Li	0.000000000000	4.657154664153	0.000000000000
Li	0.000000000000	-4.657154664153	0.000000000000

12

C	0.000000000000	0.722220114596	1.853000650247
C	0.000000000000	-0.722220114596	1.853000650247
C	0.000000000000	-1.510602627344	0.704076794335
C	0.000000000000	-1.510602627344	-0.704076794335
C	0.000000000000	-0.722220114596	-1.853000650247
C	0.000000000000	0.722220114596	-1.853000650247
C	0.000000000000	1.510602627344	-0.704076794335
C	0.000000000000	1.510602627344	0.704076794335
C	0.000000000000	2.668726100150	0.000000000000
C	0.000000000000	-2.668726100150	0.000000000000

C	0.000000000000	1.114760828278	3.195123139305
C	0.000000000000	0.000000000000	4.068508440438
C	0.000000000000	-1.114760828278	3.195123139305
C	0.000000000000	-1.114760828278	-3.195123139305
C	0.000000000000	0.000000000000	-4.068508440438
C	0.000000000000	1.114760828278	-3.195123139305
H	0.000000000000	2.147976060282	3.504269128929
H	0.000000000000	-2.147976060282	3.504269128929
H	0.000000000000	-2.147976060282	-3.504269128929
H	0.000000000000	2.147976060282	-3.504269128929
H	0.000000000000	3.736157661156	0.000000000000
H	0.000000000000	-3.736157661156	0.000000000000
Li	0.000000000000	0.000000000000	6.015437393282
Li	0.000000000000	0.000000000000	-6.015437393282

13

C	-1.57558452	3.41595654	0.00000000
C	1.15712917	3.58332188	0.00000000
C	2.78232411	1.48425419	0.00000000
C	2.93569973	-1.15179373	0.00000000
C	1.57558452	-3.41595654	0.00000000
C	-1.15712917	-3.58332188	0.00000000
C	-2.78232411	-1.48425419	0.00000000
C	-2.93569973	1.15179373	0.00000000
C	-5.04282766	-0.30401848	0.00000000
C	5.04282766	0.30401848	0.00000000
C	-2.50104712	5.87687306	0.00000000
C	-0.44889303	7.54115919	0.00000000
C	1.79501892	6.11815570	0.00000000
C	2.50104712	-5.87687306	0.00000000
C	0.44889303	-7.54115919	0.00000000
C	-1.79501892	-6.11815570	0.00000000
H	-4.46057244	6.40578129	0.00000000
H	3.66465907	6.89913058	0.00000000
H	4.46057244	-6.40578129	0.00000000
H	-3.66465907	-6.89913058	0.00000000
H	-7.05635568	-0.43036718	0.00000000
H	7.05635568	0.43036718	0.00000000
C	0.60675494	-10.30111186	0.00000000
O	-1.15712917	-11.69187230	0.00000000
H	2.53752898	-11.06216286	0.00000000
C	-0.60675494	10.30111186	0.00000000
O	1.15712917	11.69187230	0.00000000
H	-2.53752898	11.06216286	0.00000000

14

C	3.74338899	0.35112042	0.00000000
C	2.49399021	2.78645276	0.00000000
C	-0.10187978	3.14407057	0.00000000
C	-2.49399021	1.95907074	0.00000000
C	-3.74338899	-0.35112042	0.00000000
C	-2.49399021	-2.78645276	0.00000000
C	0.10187978	-3.14407057	0.00000000
C	2.49399021	-1.95907074	0.00000000
C	2.26852062	-4.51503060	0.00000000
C	-2.26852062	4.51503060	0.00000000
C	6.34046819	0.82306979	0.00000000
C	6.72833762	3.43033819	0.00000000
C	4.38430872	4.63102162	0.00000000
C	-6.34046819	-0.82306979	0.00000000

C	-6.72833762	-3.43033819	0.00000000
C	-4.38430872	-4.63102162	0.00000000
H	7.79444286	-0.59182125	0.00000000
H	4.05784135	6.63237233	0.00000000
H	-7.79444286	0.59182125	0.00000000
H	-4.05784135	-6.63237233	0.00000000
H	8.53049416	4.35574658	0.00000000
H	-8.53049416	-4.35574658	0.00000000
C	3.45574408	-7.03498547	0.00000000
O	2.26031772	-8.91816764	0.00000000
H	5.51730683	-7.04147218	0.00000000
C	-3.45574408	7.03498547	0.00000000
O	-2.26031772	8.91816764	0.00000000
H	-5.51730683	7.04147218	0.00000000

15

C	1.36222875	-3.50130692	0.00000000
C	-1.35900929	-3.50591728	0.00000000
C	-2.85479874	-1.32028009	0.00000000
C	-2.84718322	1.32862524	0.00000000
C	-1.36222875	3.50130692	0.00000000
C	1.35900929	3.50591728	0.00000000
C	2.85479874	1.32028009	0.00000000
C	2.84718322	-1.32862524	0.00000000
C	5.03920093	0.00266477	0.00000000
C	-5.03920093	-0.00266477	0.00000000
C	2.13230504	-6.03486247	0.00000000
C	0.00751071	-7.58391896	0.00000000
C	-2.13230504	-6.01929717	0.00000000
C	-2.13230504	6.03486247	0.00000000
C	-0.00751071	7.58391896	0.00000000
C	2.13230504	6.01929717	0.00000000
H	4.05856966	-6.67667785	0.00000000
H	-4.06084176	-6.65555869	0.00000000
H	-4.05856966	6.67667785	0.00000000
H	4.06084176	6.65555869	0.00000000
H	7.05625178	0.00456709	0.00000000
H	-7.05625178	-0.00456709	0.00000000
C	-0.00130774	-10.42840790	0.00000000
C	0.00130774	10.42840790	0.00000000
H	-0.95452221	-11.18121290	1.65651639
H	-0.95452221	-11.18121290	-1.65651639
H	1.91333323	-11.16181875	0.00000000
H	-1.91333323	11.16181875	0.00000000
H	0.95452221	11.18121290	-1.65651639
H	0.95452221	11.18121290	1.65651639

16

C	-1.36356557	3.50756213	0.00000000
C	1.35838692	3.50452490	0.00000000
C	2.85174400	1.31894568	0.00000000
C	2.85934035	-1.31649472	0.00000000
C	1.36356557	-3.50756213	0.00000000
C	-1.35838692	-3.50452490	0.00000000
C	-2.85174400	-1.31894568	0.00000000
C	-2.85934035	1.31649472	0.00000000
C	-5.05099298	-0.00205008	0.00000000
C	5.05099298	0.00205008	0.00000000
C	-2.14051030	6.02588033	0.00000000
C	0.00297971	7.56596053	0.00000000

C	2.14051030	6.02675862	0.00000000
C	2.14051030	-6.02588033	0.00000000
C	-0.00297971	-7.56596053	0.00000000
C	-2.14051030	-6.02675862	0.00000000
H	-4.06562308	6.66696385	0.00000000
H	4.06708169	6.66350511	0.00000000
H	4.06562308	-6.66696385	0.00000000
H	-4.06708169	-6.66350511	0.00000000
H	0.00317509	9.59282332	0.00000000
H	-0.00317509	-9.59282332	0.00000000
C	-7.85303595	-0.03436266	0.00000000
C	7.85303595	0.03436266	0.00000000
H	8.53843226	1.02710678	1.65742736
H	8.53843226	1.02710678	-1.65742736
H	8.60603740	-1.86602693	0.00000000
H	-8.53843226	-1.02710678	1.65742736
H	-8.60603740	1.86602693	0.00000000
H	-8.53843226	-1.02710678	-1.65742736

17

C	0.00000000	1.36797946	3.50610351
C	0.00000000	-1.36797946	3.50610351
C	0.00000000	-2.86448898	1.31760365
C	0.00000000	-2.86448898	-1.31760365
C	0.00000000	-1.36797946	-3.50610351
C	0.00000000	1.36797946	-3.50610351
C	0.00000000	2.86448898	-1.31760365
C	0.00000000	2.86448898	1.31760365
C	0.00000000	5.05291113	0.00000000
C	0.00000000	-5.05291113	0.00000000
C	0.00000000	2.16967491	6.00086493
C	0.00000000	0.00000000	7.49357562
C	0.00000000	-2.16967491	6.00086493
C	0.00000000	-2.16967491	-6.00086493
C	0.00000000	0.00000000	-7.49357562
C	0.00000000	2.16967491	-6.00086493
H	0.00000000	4.07358690	6.68332470
H	0.00000000	-4.07358690	6.68332470
H	0.00000000	-4.07358690	-6.68332470
H	0.00000000	4.07358690	-6.68332470
H	0.00000000	7.07067765	0.00000000
H	0.00000000	-7.07067765	0.00000000
N	0.00000000	0.00000000	10.19882951
O	0.00000000	-1.99477173	11.24031591
O	0.00000000	1.99477173	11.24031591
N	0.00000000	0.00000000	-10.19882951
O	0.00000000	1.99477173	-11.24031591
O	0.00000000	-1.99477173	-11.24031591

18

C	0.00000000	3.49338493	1.37245568
C	0.00000000	3.49338493	-1.37245568
C	0.00000000	1.35845778	-2.86804294
C	0.00000000	-1.35845778	-2.86804294
C	0.00000000	-3.49338493	-1.37245568
C	0.00000000	-3.49338493	1.37245568
C	0.00000000	-1.35845778	2.86804294
C	0.00000000	1.35845778	2.86804294
C	0.00000000	0.00000000	5.01571644
C	0.00000000	0.00000000	-5.01571644

C	0.00000000	6.02286712	2.14056060
C	0.00000000	7.55634825	0.00000000
C	0.00000000	6.02286712	-2.14056060
C	0.00000000	-6.02286712	-2.14056060
C	0.00000000	-7.55634825	0.00000000
C	0.00000000	-6.02286712	2.14056060
H	0.00000000	6.65397051	4.06739883
H	0.00000000	6.65397051	-4.06739883
H	0.00000000	-6.65397051	-4.06739883
H	0.00000000	-6.65397051	4.06739883
H	0.00000000	9.58134034	0.00000000
H	0.00000000	-9.58134034	0.00000000
N	0.00000000	0.00000000	-7.70625346
O	0.00000000	2.00515905	-8.70471331
O	0.00000000	-2.00515905	-8.70471331
N	0.00000000	0.00000000	7.70625346
O	0.00000000	2.00515905	8.70471331
O	0.00000000	-2.00515905	8.70471331

19

C	1.19507572	-3.56452594	0.00000000
C	-1.51636933	-3.44717793	0.00000000
C	-2.90708458	-1.17432162	0.00000000
C	-2.75944609	1.47046753	0.00000000
C	-1.19507572	3.56452594	0.00000000
C	1.51636933	3.44717793	0.00000000
C	2.90708458	1.17432162	0.00000000
C	2.75944609	-1.47046753	0.00000000
C	5.02115367	-0.22894016	0.00000000
C	-5.02115367	0.22894016	0.00000000
C	1.86997635	-6.15181751	0.00000000
C	-0.33865089	-7.54422392	0.00000000
C	-2.42634176	-5.89846206	0.00000000
C	-1.86997635	6.15181751	0.00000000
C	0.33865089	7.54422392	0.00000000
C	2.42634176	5.89846206	0.00000000
H	3.76506400	-6.86520977	0.00000000
H	-4.36641919	-6.48321292	0.00000000
H	-3.76506400	6.86520977	0.00000000
H	4.36641919	6.48321292	0.00000000
H	7.03618675	-0.31545450	0.00000000
H	-7.03618675	0.31545450	0.00000000
O	0.65587002	10.07427855	0.00000000
C	-1.51636933	11.56863985	0.00000000
H	-2.65802970	11.22727861	1.67414195
H	-0.89409024	13.51397044	0.00000000
H	-2.65802970	11.22727861	-1.67414195
O	-0.65587002	-10.07427855	0.00000000
C	1.51636933	-11.56863985	0.00000000
H	0.89409024	-13.51397044	0.00000000
H	2.65802970	-11.22727861	-1.67414195
H	2.65802970	-11.22727861	1.67414195

20

C	3.74993675	0.40795091	0.00000000
C	2.49460766	2.81410927	0.00000000
C	-0.13968986	3.14281754	0.00000000
C	-2.49460766	1.93888892	0.00000000
C	-3.74993675	-0.40795091	0.00000000
C	-2.49460766	-2.81410927	0.00000000

C	0.13968986	-3.14281754	0.00000000
C	2.49460766	-1.93888892	0.00000000
C	2.30540386	-4.48600390	0.00000000
C	-2.30540386	4.48600390	0.00000000
C	6.34382161	0.88382424	0.00000000
C	6.71723232	3.49544805	0.00000000
C	4.36285853	4.67789329	0.00000000
C	-6.34382161	-0.88382424	0.00000000
C	-6.71723232	-3.49544805	0.00000000
C	-4.36285853	-4.67789329	0.00000000
H	7.80764662	-0.52171537	0.00000000
H	4.02797131	6.67867025	0.00000000
H	-7.80764662	0.52171537	0.00000000
H	-4.02797131	-6.67867025	0.00000000
H	8.51410307	4.43338997	0.00000000
H	-8.51410307	-4.43338997	0.00000000
O	3.34858235	-6.70561695	0.00000000
O	-3.34858235	6.70561695	0.00000000
C	6.03369769	-6.75659409	0.00000000
H	6.75868859	-5.83774549	1.67838659
H	6.55773748	-8.72555506	0.00000000
H	6.75868859	-5.83774549	-1.67838659
C	-6.03369769	6.75659409	0.00000000
H	-6.75868859	5.83774549	1.67838659
H	-6.55773748	8.72555506	0.00000000
H	-6.75868859	5.83774549	-1.67838659

Table S2. Cartesian coordinates of the structures **0-20** obtained at the B3LYP/6-311G(d,p) level

0			
C	-1.861442772299	0.727828103563	0.000000000000
C	-1.861442772299	-0.727828103563	0.000000000000
C	-0.711431170766	-1.509165785109	0.000000000000
C	0.711431170766	-1.509165785109	0.000000000000
C	1.861442772299	-0.727828103563	0.000000000000
C	1.861442772299	0.727828103563	0.000000000000
C	0.711431170766	1.509165785109	0.000000000000
C	-0.711431170766	1.509165785109	0.000000000000
C	0.000000000000	2.682379521418	0.000000000000
C	0.000000000000	-2.682379521418	0.000000000000
C	-3.210426435687	1.141026546227	0.000000000000
C	-4.025977309764	0.000000000000	0.000000000000
C	-3.210426435687	-1.141026546227	0.000000000000
C	3.210426435687	-1.141026546227	0.000000000000
C	4.025977309764	0.000000000000	0.000000000000
C	3.210426435687	1.141026546227	0.000000000000
H	0.000000000000	3.759234639902	0.000000000000
H	-3.549999218248	2.167667019495	0.000000000000
H	-5.106901814985	0.000000000000	0.000000000000
H	-3.549999218248	-2.167667019495	0.000000000000
H	0.000000000000	-3.759234639902	0.000000000000
H	3.549999218248	-2.167667019495	0.000000000000
H	5.106901814985	0.000000000000	0.000000000000

H	3.549999218248	2.167667019495	0.000000000000
1			
C	0.000000000000	0.720097714295	1.868474220600
C	0.000000000000	-0.731147619196	1.863606167773
C	0.000000000000	-1.519387485418	0.707832493742
C	0.000000000000	-1.514365946988	-0.716096497506
C	0.000000000000	-0.720097714295	-1.868474220600
C	0.000000000000	0.731147619196	-1.863606167773
C	0.000000000000	1.519387485418	-0.707832493742
C	0.000000000000	1.514365946988	0.716096497506
C	0.000000000000	2.684647128617	0.002906503835
C	0.000000000000	-2.684647128617	-0.002906503835
C	0.000000000000	1.135421744344	3.209361709824
C	0.000000000000	-0.015363115427	4.026875631880
C	0.000000000000	-1.159550759060	3.199750624588
C	0.000000000000	-1.135421744344	-3.209361709824
C	0.000000000000	0.015363115427	-4.026875631880
C	0.000000000000	1.159550759060	-3.199750624588
H	0.000000000000	2.154281245079	3.568720267342
H	0.000000000000	-2.183614035299	3.542754638897
H	0.000000000000	-2.154281245079	-3.568720267342
H	0.000000000000	2.183614035299	-3.542754638897
C	0.000000000000	-0.017490101162	5.445680517919
N	0.000000000000	-0.015516504113	6.601747126962
C	0.000000000000	0.017490101162	-5.445680517919
N	0.000000000000	0.015516504113	-6.601747126962
O	0.000000000000	-4.001261423478	0.063037248425
H	0.000000000000	-4.377693146019	-0.827329551109
O	0.000000000000	4.001261423478	-0.063037248425
H	0.000000000000	4.377693146019	0.827329551109
2			
C	-0.017296839286	0.737484749639	1.855555469168
C	-0.017388459965	-0.722999094917	1.865169946932
C	-0.006682549094	-1.493776376818	0.716625152831
C	0.006558302274	-1.495963808136	-0.703732335501
C	0.017296860952	-0.737457943528	-1.855555469168
C	0.017388481632	0.723025901029	-1.865169946932
C	0.006682570761	1.493803182929	-0.716625152831
C	-0.006558280607	1.495990614247	0.703732335501
C	0.000122685713	2.683595974056	-0.012766681342
C	-0.000122664047	-2.683569167945	0.012766681342
C	-0.029858102212	1.162186892009	3.203074775688
C	-0.037426589632	0.017541118417	4.014785208374
C	-0.029934153692	-1.135466373926	3.210896608624
C	0.029858123878	-1.162160085898	-3.203074775688
C	0.037426611299	-0.017514312306	-4.014785208374
C	0.029934175358	1.135493180037	-3.210896608624
H	-0.033016501609	2.189281587122	3.542029233240
H	-0.033333180892	-2.151926729526	3.575364327102
H	0.033016523276	-2.189254781011	-3.542029233240
H	0.033333202559	2.151953535637	-3.575364327102
C	-0.000148790644	-4.075198809540	0.015365631406
N	-0.000116271498	-5.232810346208	0.011707853448
C	0.000148812310	4.075225615651	-0.015365631406
N	0.000116293164	5.232837152319	-0.011707853448
O	-0.050061173380	-0.046103457883	5.370098228684
H	-0.053458318615	0.844839728096	5.734643224928
O	0.050061195047	0.046130263994	-5.370098228684

H	0.053458340282	-0.844812921985	-5.734643224928
		3	
C	0.000000000000	0.728016050269	1.861716759469
C	0.000000000000	-0.728016050269	1.861716759469
C	0.000000000000	-1.511182824799	0.709180555446
C	0.000000000000	-1.511182824799	-0.709180555446
C	0.000000000000	-0.728016050269	-1.861716759469
C	0.000000000000	0.728016050269	-1.861716759469
C	0.000000000000	1.511182824799	-0.709180555446
C	0.000000000000	1.511182824799	0.709180555446
C	0.000000000000	2.684142831124	0.000000000000
C	0.000000000000	-2.684142831124	0.000000000000
C	0.000000000000	1.148420261040	3.200923633443
C	0.000000000000	0.000000000000	4.021146613669
C	0.000000000000	-1.148420261040	3.200923633443
C	0.000000000000	-1.148420261040	-3.200923633443
C	0.000000000000	0.000000000000	-4.021146613669
C	0.000000000000	1.148420261040	-3.200923633443
H	0.000000000000	2.170296692746	3.550627414433
H	0.000000000000	-2.170296692746	3.550627414433
H	0.000000000000	-2.170296692746	-3.550627414433
H	0.000000000000	2.170296692746	-3.550627414433
C	0.000000000000	0.000000000000	5.440872937193
N	0.000000000000	0.000000000000	6.596490016160
C	0.000000000000	0.000000000000	-5.440872937193
N	0.000000000000	0.000000000000	-6.596490016160
H	0.000000000000	3.761162523269	0.000000000000
H	0.000000000000	-3.761162523269	0.000000000000
		4	
C	0.000000000000	0.731041976534	1.856541367619
C	0.000000000000	-0.731041976534	1.856541367619
C	0.000000000000	-1.504009970908	0.711037634331
C	0.000000000000	-1.504009970908	-0.711037634331
C	0.000000000000	-0.731041976534	-1.856541367619
C	0.000000000000	0.731041976534	-1.856541367619
C	0.000000000000	1.504009970908	-0.711037634331
C	0.000000000000	1.504009970908	0.711037634331
C	0.000000000000	2.689948249849	0.000000000000
C	0.000000000000	-2.689948249849	0.000000000000
C	0.000000000000	1.141739492429	3.207086556192
C	0.000000000000	0.000000000000	4.020598127705
C	0.000000000000	-1.141739492429	3.207086556192
C	0.000000000000	-1.141739492429	-3.207086556192
C	0.000000000000	0.000000000000	-4.020598127705
C	0.000000000000	1.141739492429	-3.207086556192
H	0.000000000000	2.167581351753	3.547926871363
H	0.000000000000	-2.167581351753	3.547926871363
H	0.000000000000	-2.167581351753	-3.547926871363
H	0.000000000000	2.167581351753	-3.547926871363
H	0.000000000000	0.000000000000	5.101070173109
H	0.000000000000	0.000000000000	-5.101070173109
C	0.000000000000	4.083347149134	0.000000000000
N	0.000000000000	5.240331653079	0.000000000000
C	0.000000000000	-4.083347149134	0.000000000000
N	0.000000000000	-5.240331653079	0.000000000000
		5	
C	0.000000000000	0.718845886287	1.868225975827
C	0.000000000000	-0.730947601170	1.864917714224

C	0.000000000000	-1.518093345281	0.712504928299
C	0.000000000000	-1.510814719148	-0.718808037369
C	0.000000000000	-0.718845886287	-1.868225975827
C	0.000000000000	0.730947601170	-1.864917714224
C	0.000000000000	1.518093345281	-0.712504928299
C	0.000000000000	1.510814719148	0.718808037369
C	0.000000000000	2.678929818772	0.003938308823
C	0.000000000000	-2.678929818772	-0.003938308823
C	0.000000000000	1.128912477275	3.220216183856
C	0.000000000000	-0.013487628618	4.033282391867
C	0.000000000000	-1.151053729161	3.212461323230
C	0.000000000000	-1.128912477275	-3.220216183856
C	0.000000000000	0.013487628618	-4.033282391867
C	0.000000000000	1.151053729161	-3.212461323230
H	0.000000000000	2.153837991653	3.566846184357
H	0.000000000000	-2.179743078360	3.545455809155
H	0.000000000000	-2.153837991653	-3.566846184357
H	0.000000000000	2.179743078360	-3.545455809155
O	0.000000000000	-4.004127396412	0.051274050827
H	0.000000000000	-4.360658982101	-0.846311154184
O	0.000000000000	4.004127396412	-0.051274050827
H	0.000000000000	4.360658982101	0.846311154184
H	0.000000000000	0.016956296665	-5.114097168379
H	0.000000000000	-0.016956296665	5.114097168379

6

C	-0.017405050427	0.717698775096	1.867501726273
C	-0.017334205541	-0.734961202143	1.858999785719
C	-0.006583436234	-1.504611897399	0.705277682058
C	0.006680651938	-1.499779260904	-0.717569152475
C	0.017405080261	-0.717666608263	-1.867501726273
C	0.017334235374	0.734993368977	-1.858999785719
C	0.006583466067	1.504644064233	-0.705277682059
C	-0.006680622104	1.499811427737	0.717569152475
C	-0.000116892350	2.676694161377	0.014203415197
C	0.000116922183	-2.676661994544	-0.014203415197
C	-0.029958526046	1.133742669737	3.214381994028
C	-0.037464677719	-0.016399073314	4.018858729736
C	-0.029914073145	-1.160496051602	3.208188379508
C	0.029958555879	-1.133710502904	-3.214381994028
C	0.037464707552	0.016431240147	-4.018858729736
C	0.029914102979	1.160528218435	-3.208188379508
H	-0.033331463735	2.151140802266	3.576831820328
H	-0.033094650969	-2.187519939756	3.548733666384
H	0.033331493568	-2.151108635432	-3.576831820328
H	0.033094680802	2.187552106589	-3.548733666384
H	-0.000183190504	3.753167156054	0.021983947526
H	0.000183220337	-3.753134989220	-0.021983947526
O	-0.050177875219	0.044080095007	5.382651630903
H	-0.053464214210	-0.851118408622	5.734623892820
O	0.050177905053	-0.044047928174	-5.382651630903
H	0.053464244044	0.851150575455	-5.734623892820

7

C	0.000000000000	0.724681764520	1.858338734811
C	0.000000000000	-0.724681764520	1.858338734811
C	0.000000000000	-1.500500975519	0.690575866951
C	0.000000000000	-1.500500975519	-0.690575866951
C	0.000000000000	-0.724681764520	-1.858338734811
C	0.000000000000	0.724681764520	-1.858338734811

C	0.000000000000	1.500500975519	-0.690575866951
C	0.000000000000	1.500500975519	0.690575866951
C	0.000000000000	2.722899101336	0.000000000000
C	0.000000000000	-2.722899101336	0.000000000000
C	0.000000000000	1.153633319607	3.204992516960
C	0.000000000000	0.000000000000	3.990595826715
C	0.000000000000	-1.153633319607	3.204992516960
C	0.000000000000	-1.153633319607	-3.204992516960
C	0.000000000000	0.000000000000	-3.990595826715
C	0.000000000000	1.153633319607	-3.204992516960
H	0.000000000000	2.171097672474	3.567631390337
H	0.000000000000	-2.171097672474	3.567631390337
H	0.000000000000	-2.171097672474	-3.567631390337
H	0.000000000000	2.171097672474	-3.567631390337
Li	0.000000000000	4.649731694768	0.000000000000
Li	0.000000000000	-4.649731694768	0.000000000000
F	0.000000000000	0.000000000000	-5.346967656461
F	0.000000000000	0.000000000000	5.346967656461

8

C	0.000000000000	0.726597643051	1.868592638709
C	0.000000000000	-0.726597643051	1.868592638709
C	0.000000000000	-1.523435106369	0.733843271173
C	0.000000000000	-1.523435106369	-0.733843271173
C	0.000000000000	-0.726597643051	-1.868592638709
C	0.000000000000	0.726597643051	-1.868592638709
C	0.000000000000	1.523435106369	-0.733843271173
C	0.000000000000	1.523435106369	0.733843271173
C	0.000000000000	2.664264118699	0.000000000000
C	0.000000000000	-2.664264118699	0.000000000000
C	0.000000000000	1.121118293375	3.228255635277
C	0.000000000000	0.000000000000	4.102576995917
C	0.000000000000	-1.121118293375	3.228255635277
C	0.000000000000	-1.121118293375	-3.228255635277
C	0.000000000000	0.000000000000	-4.102576995917
C	0.000000000000	1.121118293375	-3.228255635277
H	0.000000000000	2.162947765195	3.535038522011
H	0.000000000000	-2.162947765195	3.535038522011
H	0.000000000000	-2.162947765195	-3.535038522011
H	0.000000000000	2.162947765195	-3.535038522011
F	0.000000000000	3.985791653169	0.000000000000
F	0.000000000000	-3.985791653169	0.000000000000
Li	0.000000000000	0.000000000000	-6.040432821484
Li	0.000000000000	0.000000000000	6.040432821484

9

C	0.000000000000	0.727083764382	1.862563939900
C	0.000000000000	-0.727083764382	1.862563939900
C	0.000000000000	-1.504702541022	0.710664529909
C	0.000000000000	-1.504702541022	-0.710664529909
C	0.000000000000	-0.727083764382	-1.862563939900
C	0.000000000000	0.727083764382	-1.862563939900
C	0.000000000000	1.504702541022	-0.710664529909
C	0.000000000000	1.504702541022	0.710664529909
C	0.000000000000	2.678486020298	0.000000000000
C	0.000000000000	-2.678486020298	0.000000000000
C	0.000000000000	1.153003907112	3.209344433265
C	0.000000000000	0.000000000000	3.995068981346
C	0.000000000000	-1.153003907112	3.209344433265
C	0.000000000000	-1.153003907112	-3.209344433265

C	0.000000000000	0.000000000000	-3.995068981346
C	0.000000000000	1.153003907112	-3.209344433265
H	0.000000000000	2.170595641658	3.570040294964
H	0.000000000000	-2.170595641658	3.570040294964
H	0.000000000000	-2.170595641658	-3.570040294964
H	0.000000000000	2.170595641658	-3.570040294964
F	0.000000000000	0.000000000000	-5.340447813972
F	0.000000000000	0.000000000000	5.340447813972
H	0.000000000000	3.755142155944	0.000000000000
H	0.000000000000	-3.755142155944	0.000000000000

10

C	0.000000000000	0.726330266303	1.866726783000
C	0.000000000000	-0.726330266303	1.866726783000
C	0.000000000000	-1.523082696786	0.728419918174
C	0.000000000000	-1.523082696786	-0.728419918174
C	0.000000000000	-0.726330266303	-1.866726783000
C	0.000000000000	0.726330266303	-1.866726783000
C	0.000000000000	1.523082696786	-0.728419918174
C	0.000000000000	1.523082696786	0.728419918174
C	0.000000000000	2.667252276677	0.000000000000
C	0.000000000000	-2.667252276677	0.000000000000
C	0.000000000000	1.139837001615	3.217547744096
C	0.000000000000	0.000000000000	4.033205656069
C	0.000000000000	-1.139837001615	3.217547744096
C	0.000000000000	-1.139837001615	-3.217547744096
C	0.000000000000	0.000000000000	-4.033205656069
C	0.000000000000	1.139837001615	-3.217547744096
H	0.000000000000	2.166998621638	3.554986736793
H	0.000000000000	-2.166998621638	3.554986736793
H	0.000000000000	-2.166998621638	-3.554986736793
H	0.000000000000	2.166998621638	-3.554986736793
F	0.000000000000	3.978861069357	0.000000000000
F	0.000000000000	-3.978861069357	0.000000000000
H	0.000000000000	0.000000000000	5.113756829334
H	0.000000000000	0.000000000000	-5.113756829334

11

C	0.000000000000	0.725961134813	1.857961307467
C	0.000000000000	-0.725961134813	1.857961307467
C	0.000000000000	-1.504323476857	0.691430817773
C	0.000000000000	-1.504323476857	-0.691430817773
C	0.000000000000	-0.725961134813	-1.857961307467
C	0.000000000000	0.725961134813	-1.857961307467
C	0.000000000000	1.504323476857	-0.691430817773
C	0.000000000000	1.504323476857	0.691430817773
C	0.000000000000	2.726361046034	0.000000000000
C	0.000000000000	-2.726361046034	0.000000000000
C	0.000000000000	1.141662620362	3.205587519689
C	0.000000000000	0.000000000000	4.024373832123
C	0.000000000000	-1.141662620362	3.205587519689
C	0.000000000000	-1.141662620362	-3.205587519689
C	0.000000000000	0.000000000000	-4.024373832123
C	0.000000000000	1.141662620362	-3.205587519689
H	0.000000000000	2.169017235921	3.546501234450
H	0.000000000000	-2.169017235921	3.546501234450
H	0.000000000000	-2.169017235921	-3.546501234450
H	0.000000000000	2.169017235921	-3.546501234450
H	0.000000000000	0.000000000000	5.106497342718
H	0.000000000000	0.000000000000	-5.106497342718

Li	0.000000000000	4.649939778177	0.000000000000
Li	0.000000000000	-4.649939778177	0.000000000000

12

C	0.000000000000	0.728084987203	1.862269827027
C	0.000000000000	-0.728084987203	1.862269827027
C	0.000000000000	-1.508208715342	0.714763888499
C	0.000000000000	-1.508208715342	-0.714763888499
C	0.000000000000	-0.728084987203	-1.862269827027
C	0.000000000000	0.728084987203	-1.862269827027
C	0.000000000000	1.508208715342	-0.714763888499
C	0.000000000000	1.508208715342	0.714763888499
C	0.000000000000	2.682400787558	0.000000000000
C	0.000000000000	-2.682400787558	0.000000000000
C	0.000000000000	1.122741761515	3.220130578133
C	0.000000000000	0.000000000000	4.094639555383
C	0.000000000000	-1.122741761515	3.220130578133
C	0.000000000000	-1.122741761515	-3.220130578133
C	0.000000000000	0.000000000000	-4.094639555383
C	0.000000000000	1.122741761515	-3.220130578133
H	0.000000000000	2.163787010617	3.530465347084
H	0.000000000000	-2.163787010617	3.530465347084
H	0.000000000000	-2.163787010617	-3.530465347084
H	0.000000000000	2.163787010617	-3.530465347084
H	0.000000000000	3.759545054065	0.000000000000
H	0.000000000000	-3.759545054065	0.000000000000
Li	0.000000000000	0.000000000000	6.031466087317
Li	0.000000000000	0.000000000000	-6.031466087317

13

C	0.84748494	-1.81185126	0.00000000
C	-0.61038893	-1.90650804	0.00000000
C	-1.46509042	-0.80371266	0.00000000
C	-1.55442166	0.61336078	0.00000000
C	-0.84748494	1.81185126	0.00000000
C	0.61038893	1.90650804	0.00000000
C	1.46509042	0.80371266	0.00000000
C	1.55442166	-0.61336078	0.00000000
C	2.68002025	0.17270639	0.00000000
C	-2.68002025	-0.17270639	0.00000000
C	1.34630012	-3.12530029	0.00000000
C	0.25481936	-4.01728213	0.00000000
C	-0.94240559	-3.26673882	0.00000000
C	-1.34630012	3.12530029	0.00000000
C	-0.25481936	4.01728213	0.00000000
C	0.94240559	3.26673882	0.00000000
H	2.39169285	-3.40388136	0.00000000
H	-1.93640451	-3.68984340	0.00000000
H	-2.39169285	3.40388136	0.00000000
H	1.93640451	3.68984340	0.00000000
H	3.75468272	0.24435306	0.00000000
H	-3.75468272	-0.24435306	0.00000000
C	-0.34178894	5.47621029	0.00000000
O	0.61038893	6.22780640	0.00000000
H	-1.37916765	5.87822185	0.00000000
C	0.34178894	-5.47621029	0.00000000
O	-0.61038893	-6.22780640	0.00000000
H	1.37916765	-5.87822185	0.00000000

14

C	-1.99473502	0.17283845	0.00000000
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C	-1.32663487	1.47329580	0.00000000
C	0.04230994	1.65919585	0.00000000
C	1.32663487	1.03877237	0.00000000
C	1.99473502	-0.17283845	-0.00000000
C	1.32663487	-1.47329580	-0.00000000
C	-0.04230994	-1.65919585	0.00000000
C	-1.32663487	-1.03877237	0.00000000
C	-1.19590736	-2.41641008	-0.00000000
C	1.19590736	2.41641008	0.00000000
C	-3.38303861	0.42914905	0.00000000
C	-3.58353167	1.81747869	0.00000000
C	-2.33669513	2.45895469	-0.00000000
C	3.38303861	-0.42914905	-0.00000000
C	3.58353167	-1.81747869	-0.00000000
C	2.33669513	-2.45895469	0.00000000
H	-4.15807580	-0.32470369	-0.00000000
H	-2.15674089	3.52484204	0.00000000
H	4.15807580	0.32470369	-0.00000000
H	2.15674089	-3.52484204	-0.00000000
H	-4.54415181	2.31232909	0.00000000
H	4.54415181	-2.31232909	-0.00000000
C	-1.77503407	-3.75428654	-0.00000000
O	-1.09876369	-4.75988091	-0.00000000
H	-2.88022112	-3.79258178	-0.00000000
C	1.77503407	3.75428654	-0.00000000
O	1.09876369	4.75988091	0.00000000
H	2.88022112	3.79258178	0.00000000

15

C	0.72767579	-1.86070514	0.00000000
C	-0.72670570	-1.86181192	0.00000000
C	-1.50840613	-0.71157889	0.00000000
C	-1.50738067	0.71221926	0.00000000
C	-0.72767579	1.86070514	0.00000000
C	0.72670570	1.86181192	0.00000000
C	1.50840613	0.71157889	0.00000000
C	1.50738067	-0.71221926	0.00000000
C	2.68166933	0.00120703	0.00000000
C	-2.68166933	-0.00120703	0.00000000
C	1.13677406	-3.21241482	0.00000000
C	0.00176678	-4.03919797	0.00000000
C	-1.13677406	-3.21030986	0.00000000
C	-1.13677406	3.21241482	0.00000000
C	-0.00176678	4.03919797	0.00000000
C	1.13677406	3.21030986	0.00000000
H	2.16329464	-3.55543191	0.00000000
H	-2.16460098	-3.54974972	0.00000000
H	-2.16329464	3.55543191	0.00000000
H	2.16460098	3.54974972	0.00000000
H	3.75848513	0.00212925	0.00000000
H	-3.75848513	-0.00212925	0.00000000
C	0.00149176	-5.54208317	0.00000000
C	-0.00149176	5.54208317	0.00000000
H	-0.50865357	-5.94528353	0.88095128
H	-0.50865357	-5.94528353	-0.88095128
H	1.02066343	-5.93497611	0.00000000
H	-1.02066343	5.93497611	0.00000000
H	0.50865357	5.94528353	-0.88095128
H	0.50865357	5.94528353	0.88095128

16

C	-0.72829874	1.86253437	0.00000000
C	0.72536672	1.86111702	0.00000000
C	1.50882303	0.70944911	0.00000000
C	1.51246354	-0.70885363	-0.00000000
C	0.72829874	-1.86253437	0.00000000
C	-0.72536672	-1.86111702	-0.00000000
C	-1.50882303	-0.70944911	0.00000000
C	-1.51246354	0.70885363	-0.00000000
C	-2.68854366	-0.00098328	-0.00000000
C	2.68854366	0.00098328	0.00000000
C	-1.14063546	3.21133659	0.00000000
C	0.00127872	4.02771930	0.00000000
C	1.14063546	3.21105973	0.00000000
C	1.14063546	-3.21133659	-0.00000000
C	-0.00127872	-4.02771930	-0.00000000
C	-1.14063546	-3.21105973	-0.00000000
H	-2.16663146	3.55348730	0.00000000
H	2.16751580	3.55054667	0.00000000
H	2.16663146	-3.55348730	-0.00000000
H	-2.16751580	-3.55054667	0.00000000
H	0.00152359	5.10874907	0.00000000
H	-0.00152359	-5.10874907	-0.00000000
C	-4.16686024	-0.01768387	0.00000000
C	4.16686024	0.01768387	0.00000000
H	4.54037186	0.54969378	0.88033656
H	4.54037186	0.54969378	-0.88033656
H	4.57648112	-0.99268411	-0.00000000
H	-4.54037186	-0.54969378	0.88033656
H	-4.57648112	0.99268411	-0.00000000
H	-4.54037186	-0.54969378	-0.88033656

17

C	-0.00000000	0.73023821	1.86277252
C	-0.00000000	-0.73023821	1.86277252
C	0.00000000	-1.51249980	0.70887608
C	0.00000000	-1.51249980	-0.70887608
C	-0.00000000	-0.73023821	-1.86277252
C	0.00000000	0.73023821	-1.86277252
C	0.00000000	1.51249980	-0.70887608
C	0.00000000	1.51249980	0.70887608
C	-0.00000000	2.68509698	0.00000000
C	-0.00000000	-2.68509698	0.00000000
C	0.00000000	1.15528945	3.19986410
C	0.00000000	0.00000000	3.99396639
C	-0.00000000	-1.15528945	3.19986410
C	-0.00000000	-1.15528945	-3.19986410
C	0.00000000	0.00000000	-3.99396639
C	0.00000000	1.15528945	-3.19986410
H	-0.00000000	2.16852018	3.56926001
H	-0.00000000	-2.16852018	3.56926001
H	-0.00000000	-2.16852018	-3.56926001
H	0.00000000	2.16852018	-3.56926001
H	-0.00000000	3.76212529	0.00000000
H	-0.00000000	-3.76212529	0.00000000
N	0.00000000	0.00000000	5.43759157
O	0.00000000	-1.08924574	6.00482809
O	0.00000000	1.08924574	6.00482809
N	0.00000000	-0.00000000	-5.43759157

O	0.00000000	1.08924574	-6.00482809
O	0.00000000	-1.08924574	-6.00482809

18

C	0.00000000	1.85930331	0.73126182
C	0.00000000	1.85930331	-0.73126182
C	-0.00000000	0.72506084	-1.51358155
C	-0.00000000	-0.72506084	-1.51358155
C	-0.00000000	-1.85930331	-0.73126182
C	-0.00000000	-1.85930331	0.73126182
C	-0.00000000	-0.72506084	1.51358155
C	-0.00000000	0.72506084	1.51358155
C	0.00000000	-0.00000000	2.67296693
C	0.00000000	0.00000000	-2.67296693
C	-0.00000000	3.21087846	1.14209177
C	0.00000000	4.02387972	-0.00000000
C	0.00000000	3.21087846	-1.14209177
C	-0.00000000	-3.21087846	-1.14209177
C	-0.00000000	-4.02387972	0.00000000
C	-0.00000000	-3.21087846	1.14209177
H	-0.00000000	3.54378915	2.17035225
H	0.00000000	3.54378915	-2.17035225
H	-0.00000000	-3.54378915	-2.17035225
H	-0.00000000	-3.54378915	2.17035225
H	-0.00000000	5.10419684	-0.00000000
H	-0.00000000	-5.10419684	0.00000000
N	0.00000000	0.00000000	-4.09691211
O	0.00000000	1.09682735	-4.64815962
O	-0.00000000	-1.09682735	-4.64815962
N	-0.00000000	-0.00000000	4.09691211
O	-0.00000000	1.09682735	4.64815962
O	-0.00000000	-1.09682735	4.64815962

19

C	0.56875311	-1.91618602	0.00000000
C	-0.87891722	-1.79764549	0.00000000
C	-1.55874777	-0.58163051	0.00000000
C	-1.43538626	0.83611152	0.00000000
C	-0.56875311	1.91618602	0.00000000
C	0.87891722	1.79764549	0.00000000
C	1.55874777	0.58163051	0.00000000
C	1.43538626	-0.83611152	0.00000000
C	2.66785733	-0.22025903	0.00000000
C	-2.66785733	0.22025903	0.00000000
C	0.87891722	-3.29935841	0.00000000
C	-0.33287527	-4.00658015	0.00000000
C	-1.40989956	-3.09953517	0.00000000
C	-0.87891722	3.29935841	0.00000000
C	0.33287527	4.00658015	0.00000000
C	1.40989956	3.09953517	0.00000000
H	1.87498388	-3.71503653	0.00000000
H	-2.45441961	-3.37434535	0.00000000
H	-1.87498388	3.71503653	0.00000000
H	2.45441961	3.37434535	0.00000000
H	3.74094260	-0.30655535	0.00000000
H	-3.74094260	0.30655535	0.00000000
O	0.53904371	5.35032892	0.00000000
C	-0.62178367	6.16684370	0.00000000
H	-1.23267048	5.99135418	0.89333341
H	-0.27068716	7.19751937	0.00000000

H	-1.23267048	5.99135418	-0.89333341
O	-0.53904371	-5.35032892	0.00000000
C	0.62178367	-6.16684370	0.00000000
H	0.27068716	-7.19751937	0.00000000
H	1.23267048	-5.99135418	-0.89333341
H	1.23267048	-5.99135418	0.89333341

20

C	1.99435782	0.20523038	0.00000000
C	1.32954286	1.49312416	0.00000000
C	-0.05493990	1.67082845	0.00000000
C	-1.32954286	1.02483696	0.00000000
C	-1.99435782	-0.20523038	0.00000000
C	-1.32954286	-1.49312416	0.00000000
C	0.05493990	-1.67082845	0.00000000
C	1.32954286	-1.02483696	0.00000000
C	1.21604723	-2.39208311	0.00000000
C	-1.21604723	2.39208311	0.00000000
C	3.38354433	0.45786180	0.00000000
C	3.58559507	1.84647609	0.00000000
C	2.33638453	2.48341128	0.00000000
C	-3.38354433	-0.45786180	0.00000000
C	-3.58559507	-1.84647609	0.00000000
C	-2.33638453	-2.48341128	0.00000000
H	4.15968201	-0.29562104	0.00000000
H	2.16191514	3.55048955	0.00000000
H	-4.15968201	0.29562104	0.00000000
H	-2.16191514	-3.55048955	0.00000000
H	4.54586042	2.34277583	0.00000000
H	-4.54586042	-2.34277583	0.00000000
O	1.75911729	-3.59102126	0.00000000
O	-1.75911729	3.59102126	0.00000000
C	3.20365360	-3.61328016	0.00000000
H	3.58903678	-3.12238453	0.89572180
H	3.48075688	-4.66453038	0.00000000
H	3.58903678	-3.12238453	-0.89572180
C	-3.20365360	3.61328016	0.00000000
H	-3.58903678	3.12238453	0.89572180
H	-3.48075688	4.66453038	0.00000000
H	-3.58903678	3.12238453	-0.89572180