The anomeric effect: the dominance of exchange effects in closed-shell systems

Glauco F. Bauerfeldt[†], *Thiago M. Cardozo*[‡], *Márcio S. Pereira*[†], *Clarissa O da Silva*[†]*
* e-mail:clarissa-dq@ufrrj.br
[†]Dep. Química, Universidade Federal Rural do Rio de Janeiro, Rodovia BR 465, km 47, Seropédica – RJ . BRAZIL, 23890-000
[‡]Instituto de Química da UFRJ, CT, bloco A, sala 409 – Cidade Universitária, Ilha do Fundão, Rio de Janeiro, RJ. BRAZIL, 21949-900

Supplementary Information

Table of Contents:

1. HF/6-31G(d,p) energy values for Cy derivatives (in hartree):

	T	VNe	V_{NN}	J	K	Total E
OH(A)60°	308.8302233	-1395.406967	336.39016	484.922227	-43.818822	-309.083176
OH(A)180°	308.830720	-1395.411089	336.391529	484.924574	-43.818903	-309.083170
OH(A)300°	308.829729	-1393.783899	335.724277	483.966850	-43.817880	-309.080923
OH(E)60°	308.834809	-1384.455152	331.034971	479.317994	-43.815907	-309.083285
OH(E)180°	308.840521	-1385.107591	331.306050	479.696312	-43.818894	-309.083602
OH(E)300°	308.840423	-1385.108103	331.306646	479.696316	-43.818884	-309.083603
NH_2(A)60°	289.067852	-1345.474030	335.663211	474.036288	-42.546606	-289.253285
NH_2(A)180°	289.068155	-1344.113254	335.103572	473.235389	-42.544976	-289.251114
NH_2(A)300°	289.068242	-1344.111410	335.102230	473.234821	-42.544998	-289.251114
NH_2(E)60°	289.075172	-1335.624585	330.850603	468.988502	-42.543824	-289.254132
NH_2(E)180°	289.075135	-1336.372663	331.190074	469.398832	-42.545771	-289.254394
NH_2(E)300°	289.075202	-1335.620545	330.848468	468.986574	-42.543819	-289.254121
F(A)	332.819077	-1452.501538	335.289892	496.607439	-45.296007	-333.081137
F(E)	332.829392	-1441.305605	329.763831	490.927842	-45.296280	-333.080820
CN(A)	325.702998	-1497.217530	369.141114	523.360301	-46.946482	-325.959599
CN(E)	325.702702	-1483.425649	362.308241	516.400135	-46.945707	-325.960278

2. HF/6-31G(d,p) energy values for 2-THP derivatives (in hartree):

	T	V_{Ne}	V_{NN}	J	K	Total E
OH(A)60°	344.499740	-1496.705584	343.622847	509.850804	-46.171375	-344.903569
OH(A)180°	344.491551	-1497.032698	343.801634	510.010898	-46.168604	-344.897219
OH(A)300°	344.490410	-1495.371999	343.120616	509.031222	-46.167320	-344.897072
OH(E)60°	344.505304	-1487.172800	338.982073	504.952535	-46.167661	-344.900548
OH(E)180°	344.501091	-1487.296553	339.017169	505.048346	-46.164153	-344.894099
OH(E)300°	344.505707	-1487.738078	339.220729	505.279079	-46.169034	-344.901596
NH_2(A)60°	324.737123	-1446.274151	342.603147	498.763056	-44.897215	-325.068040
NH_2(A)180°	324.730202	-1444.710893	341.997765	497.813697	-44.891422	-325.060651
NH_2(A)300°	324.734973	-1444.742694	341.962448	497.873243	-44.896642	-325.068673
NH_2(E)60°	324.739703	-1437.374766	338.291768	494.168709	-44.890685	-325.065270
NH_2(E)180°	324.740406	-1437.933187	338.527685	494.491289	-44.892712	-325.066520
NH_2(E)300°	324.746132	-1437.604909	338.369152	494.311910	-44.895366	-325.073080
F(A)	368.477376	-1554.328332	342.856451	521.741345	-47.645838	-368.898999
F(E)	368.482768	-1544.325443	337.951589	516.638205	-47.641424	-368.894305
CN(A)	361.356993	-1597.422499	375.872199	547.716332	-49.285431	-361.762406
CN(E)	361.355745	-1584.587723	369.506841	541.247797	-49.283982	-361.761322

3. Geometric and energetic data for Cy derivatives

F_axial(Cy) HF 6-31g**

atom	x	y	z
	angstroms		
C1	0.2250606595	1.3211450920	-0.5323278344
C2	-0.9952049454	1.1622313121	0.3801135671
C3	-1.7377606354	-0.1475154770	0.0974864619
C4	-0.7989541370	-1.3529391515	0.2092975676
C5	1.1478455715	0.1148481200	-0.4553953518
H6	-2.5717978068	-0.2591600595	0.7849387350
H7	-0.6666014794	1.1749895456	1.4157653925
H8	-1.6620371752	2.0101202405	0.2508260976
H9	-0.0963559203	1.4374400122	-1.5658601929
H10	0.7866064158	2.2126078692	-0.2699179380
H11	-0.4605161715	-1.4534667309	1.2369428132
H12	-1.3283446969	-2.2686268086	-0.0389437277
H13	-2.1638320901	-0.1126436028	-0.9051053963
H15	1.9808224271	0.2265174167	-1.1410240631
F16	1.6917549577	0.0702153863	0.8174717875
C16	0.4208397750	-1.1973614411	-0.7043620998
H17	1.1156847112	-2.0191621380	-0.5599884940
H18	0.1092272394	-1.2201851376	-1.7471836903

Energy components, in hartrees:

(A)	Nuclear repulsion.....	335.28989161011	
(E)	Total one-electron terms.....	-1119.68246043921	
(F)	Electron-nuclear.....	-1452.50153793788	
(H)	Kinetic.....	332.81907749866	
(I)	Total two-electron terms.....	451.31143181271	
(J)	Coulomb.....	496.60743859137	
(K)	Exchange.....	-45.29600677866	
(L)	Electronic energy.....	-668.37102862651	(E+I)
(M)	-V/T.....	2.00078739332	(-(A+F+I)/H)
(N)	Total energy.....	-333.08113701639	(A+L)

SCFE: SCF energy: HF -333.08113701639 hartrees iterations: 2

F_equat(Cy) HF 6-31g**

		angstroms	
atom	x	y	z
C1	0.2063851007	1.2851187419	-0.5631118616
C2	-1.0118665911	1.1363255437	0.3545404183
C3	-1.7588769145	-0.1745776076	0.0861358089
C4	-0.8200964656	-1.3815940224	0.1860641631
C5	1.1229702996	0.0805597735	-0.4409380145
H6	-2.5834184106	-0.2843286458	0.7850808480
H7	-0.6866774557	1.1584063805	1.3939798434
H8	-1.6769342780	1.9844315566	0.2224191683
H9	-0.1140275110	1.3649220728	-1.5996588040
H10	0.7609649855	2.1890623410	-0.3300074068
H11	-0.4842974560	-1.4918513216	1.2164844565
H12	-1.3510638833	-2.2952718539	-0.0637359254
H13	-2.1961020040	-0.1412220567	-0.9106124458
F14	2.1664513902	0.2200082385	-1.3308525672
H15	1.5627793434	0.0471897475	0.5522431527
C16	0.3967231688	-1.2210692143	-0.7312461138
H17	1.0838577182	-2.0537690550	-0.6154984739
H18	0.0806257687	-1.2093185302	-1.7721880771

Energy components, in hartrees:

(A)	Nuclear repulsion.....	329.76383059416	
(E)	Total one-electron terms.....	-1108.47621277264	
(F)	Electron-nuclear.....	-1441.30560493956	
(H)	Kinetic.....	332.82939216692	
(I)	Total two-electron terms.....	445.63156199641	
(J)	Coulomb.....	490.92784186306	
(K)	Exchange.....	-45.29627986665	
(L)	Electronic energy.....	-662.84465077623	(E+I)
(M)	-V/T.....	2.00075542612	(-(A+F+I)/H)
(N)	Total energy.....	-333.08082018207	(A+L)

SCFE: SCF energy: HF -333.08082018207 hartrees iterations: 2

O_axial approximately 60°(Cy) HF 6-31g**

angstroms

atom	x	y	z
C1	0.2344312627	1.3247779805	-0.5049482749
C2	-1.0003097313	1.1789806458	0.3894539640
C3	-1.7556333848	-0.1197065270	0.0913473731
C4	-0.8334889808	-1.3374715438	0.2048324071
C5	1.1571207404	0.1129751462	-0.4120800717
H6	-2.5990624172	-0.2264285909	0.7685738309
H7	-0.6883362208	1.1864001420	1.4296499646
H8	-1.6561197239	2.0344071455	0.2490413445
H9	-0.0755428199	1.4408181460	-1.5423061172
H10	0.7964507290	2.2137257334	-0.2361737849
H11	-0.5114336232	-1.4492118913	1.2366488687
H12	-1.3721405342	-2.2441581036	-0.0583534718
H13	-2.1696547156	-0.0745718320	-0.9160043707
H14	1.9580626184	0.2226742576	-1.1431342782
O15	1.7082483359	0.1122950924	0.8861558346
H16	2.3000383636	-0.6158625529	0.9805509467
C17	0.3971591204	-1.1856685877	-0.6939662100
H18	1.0667826916	-2.0356882643	-0.5679432543
H19	0.0924212399	-1.1881466097	-1.7393626210

Energy components, in hartrees:

(A)	Nuclear repulsion.....	336.39016321171	
(E)	Total one-electron terms.....	-1086.57674358463	
(F)	Electron-nuclear.....	-1395.40696689886	
(H)	Kinetic.....	308.83022331423	
(I)	Total two-electron terms.....	441.10340485459	
(J)	Coulomb.....	484.92222686402	
(K)	Exchange.....	-43.81882200943	
(L)	Electronic energy.....	-645.47333873004	(E+I)
(M)	-V/T.....	2.00081906557	(-(A+F+I)/H)
(N)	Total energy.....	-309.08317551833	(A+L)

SCFE: SCF energy: HF -309.08317551833 hartrees iterations: 2

O_axial_ approximately 180°(Cy) HF 6-31g**

angstroms

atom	x	y	z
C1	2.3725895787	0.2851192619	-1.4014915755
C2	3.1053450599	1.6183884524	-1.2257900096
C3	2.1388155634	2.8007987063	-1.3423689203
C4	0.9747149185	2.6664048568	-0.3560125773
C5	1.2008063819	0.1412563546	-0.4269836653
H6	2.6689508272	3.7340702652	-1.1710749883
H7	3.5818911723	1.6388360849	-0.2493902749
H8	3.8968348441	1.7039059478	-1.9658882045
H9	1.9890752689	0.2066757327	-2.4176140685
H10	3.0622201068	-0.5477444359	-1.2690348826
H11	1.3504908106	2.7381953756	0.6603725700
H12	0.2718104549	3.4842162114	-0.4926730244
H13	1.7482463351	2.8473453157	-2.3590023922
H14	0.6528091490	-0.7712934439	-0.6613675932
O15	1.6497130914	0.0848811290	0.9088481865
H16	2.2300143353	-0.6502647467	1.0190549866
C17	0.2483398673	1.3290656411	-0.5282898107
H18	-0.5292561623	1.2186690983	0.2210429604
H19	-0.2363206890	1.2976266984	-1.5028513030

Energy components, in hartrees:

(A)	Nuclear repulsion.....	336.39152903533	
(E)	Total one-electron terms.....	-1086.58036941061	
(F)	Electron-nuclear.....	-1395.41108943630	
(H)	Kinetic.....	308.83072002569	
(I)	Total two-electron terms.....	441.10567050013	
(J)	Coulomb.....	484.92457367867	
(K)	Exchange.....	-43.81890317854	
(L)	Electronic energy.....	-645.47469891047	(E+I)
(M)	-V/T.....	2.00081743762	(-(A+F+I)/H)
(N)	Total energy.....	-309.08316987514	(A+L)

SCFE: SCF energy: HF -309.08316987514 hartrees iterations: 2

O_axial_ approximately 300° HF(Cy) 6-31g**

angstroms

atom	x	y	z
C1	0.4408692024	-1.1027373482	-0.9095414018
C2	1.3101226850	-2.3628208663	-0.9983294664
C3	2.5539650443	-2.1246155131	-1.8606321985
C4	3.3580914985	-0.9206089348	-1.3594624785
C5	1.2277584130	0.1180433437	-0.4234593984
H6	3.1780395570	-3.0142311292	-1.8747799223
H7	1.6149904054	-2.6742500749	0.0006964805
H8	0.7253603153	-3.1854782031	-1.3999258670
H9	0.0347723919	-0.8825632997	-1.8955290425
H10	-0.4022223544	-1.2655408649	-0.2451010150
H11	3.7823873748	-1.1489836920	-0.3817418631
H12	4.2049846258	-0.7344833244	-2.0137618955
H13	2.2454248545	-1.9440811953	-2.8896498924
H14	0.5963327084	0.9956952475	-0.4995502095
O15	1.5337641976	0.0261492359	0.9493843306
H16	2.0947638629	-0.7129074628	1.1133020438
C17	2.4855517885	0.3372119460	-1.2694973485
H18	3.0503422500	1.1656676931	-0.8529312190
H19	2.1808157736	0.6290063827	-2.2732104000

Energy components, in hartrees:

(A)	Nuclear repulsion.....	335.72427716563	
(E)	Total one-electron terms.....	-1084.95417045645	
(F)	Electron-nuclear.....	-1393.78389939668	
(H)	Kinetic.....	308.82972894024	
(I)	Total two-electron terms.....	440.14896979685	
(J)	Coulomb.....	483.96684996376	
(K)	Exchange.....	-43.81788016691	
(L)	Electronic energy.....	-644.80520065960	(E+I)
(M)	-V/T.....	2.00081337556	(-(A+F+I)/H)
(N)	Total energy.....	-309.08092349397	(A+L)

SCFE: SCF energy: HF -309.08092349397 hartrees iterations: 2

O_equat_ approximately 60°(Cy) HF 6-31g**

angstroms

atom	x	y	z
C1	0.4791768379	-1.2286157401	-0.3566163066
C2	-0.9836965395	-1.4589231903	0.0371626975
C3	-1.1544590435	-1.5003281507	1.5590538966
C4	-0.5821404769	-0.2404520438	2.2164792970
C5	1.0473041887	0.0302250590	0.2975849420
H6	-2.2047907378	-1.6119534123	1.8150431861
H7	-1.5965173932	-0.6562016483	-0.3715472578
H8	-1.3468030106	-2.3808867087	-0.4084463266
H9	1.0773354276	-2.0868289598	-0.0446525795
H10	0.5827758946	-1.1484955775	-1.4346400130
H11	-1.1749662277	0.6227791895	1.9159330347
H12	-0.6637549765	-0.3087189138	3.2977198766
H13	0.5109981872	0.8936998414	-0.0862874972
H14	-0.6425276857	-2.3769791748	1.9548773326
O15	2.3862642192	0.2462419728	-0.0702077859
H16	2.9176448259	-0.4686445552	0.2423471054
C17	0.8794685342	-0.0137928833	1.8159178849
H18	1.2604442798	0.9085273349	2.2442963314
H19	1.4932812266	-0.8242277634	2.2136875341

Energy components, in hartrees:

(A)	Nuclear repulsion.....	331.03497091030	
(E)	Total one-electron terms.....	-1075.62034262378	
(F)	Electron-nuclear.....	-1384.45515204987	
(H)	Kinetic.....	308.83480942610	
(I)	Total two-electron terms.....	435.50208653123	
(J)	Coulomb.....	479.31799355063	
(K)	Exchange.....	-43.81590701940	
(L)	Electronic energy.....	-640.11825609255	(E+I)
(M)	-V/T.....	2.00080455878	(-(A+F+I)/H)
(N)	Total energy.....	-309.08328518225	(A+L)

SCFE: SCF energy: HF -309.08328518225 hartrees iterations: 2

O_equat_ approximately 180°(Cy) HF 6-31G**

angstroms

atom	x	y	z
C1	0.7936817170	-0.1411096741	1.7743443400
C2	-0.6908816528	-0.3515047292	2.0877140446
C3	-1.5454104959	0.7822628739	1.5131831868
C4	-1.2983239909	0.9571615593	0.0116835463
C5	1.0333664091	0.0246509633	0.2743955218
H6	-2.5983619646	0.5885607993	1.7000604935
H7	-1.0200797378	-1.2998208483	1.6642694123
H8	-0.8356506016	-0.4267117570	3.1617898644
H9	1.1589688545	0.7522405360	2.2769199109
H10	1.3798502399	-0.9780563594	2.1517667798
H11	-1.6615053723	0.0761980137	-0.5165587447
H12	-1.8692037686	1.8001233915	-0.3673859117
H13	0.7504605782	-0.9030561385	-0.2284025236
H14	-1.3021083365	1.7107514797	0.0278621603
O15	2.3784191694	0.3219443001	-0.0067565712
H16	2.9301436569	-0.3811380992	0.2943943815
C17	0.1891128930	1.1577876708	-0.2934314506
H18	0.3591376149	1.2267254809	-1.3634568637
H19	0.5377288872	2.0912975899	0.1433338700

Energy components, in hartrees:

(A)	Nuclear repulsion.....	331.30605019964	
(E)	Total one-electron terms.....	-1076.26707020417	
(F)	Electron-nuclear.....	-1385.10759094104	
(H)	Kinetic.....	308.84052073687	
(I)	Total two-electron terms.....	435.87741783426	
(J)	Coulomb.....	479.69631155476	
(K)	Exchange.....	-43.81889372050	
(L)	Electronic energy.....	-640.38965236991	(E+I)
(M)	-V/T.....	2.00078707753	(-(A+F+I)/H)
(N)	Total energy.....	-309.08360217027	(A+L)

SCFE: SCF energy: HF -309.08360217027 hartrees iterations: 2

O_equat_ approximately 300°(Cy) HF 6-31G**

angstroms

atom	x	y	z
C1	0.1651539634	1.1339698850	-0.2868233747
C2	-1.3255947450	0.7992045307	-0.1795304808
C3	-1.6579405075	-0.5188697381	-0.8855170098
C4	-0.7811270174	-1.6624629387	-0.3667470970
C5	1.0320597035	-0.0036563644	0.2360599737
H6	-2.7085065123	-0.7622930366	-0.7505838227
H7	-1.6059803232	0.7241667105	0.8706027635
H8	-1.9161749349	1.6091259426	-0.5983689293
H9	0.4340418219	1.3143764994	-1.3255319669
H10	0.3988667603	2.0409968727	0.2620854367
H11	-1.0304653354	-1.8626093777	0.6747614188
H12	-0.9896363024	-2.5769788859	-0.9148726715
H13	0.8327375556	-0.1283137642	1.3029340232
H14	-1.4989310289	-0.4027473670	-1.9566886423
O15	2.3740220455	0.3708811983	0.0478635289
H16	2.9430827653	-0.2961220272	0.3952777858
C17	0.7066914385	-1.3151890965	-0.4772216825
H18	1.3123449890	-2.1206547612	-0.0637534745
H19	0.9898966940	-1.2120030746	-1.5228060198

Energy components, in hartrees:

(A)	Nuclear repulsion.....	331.30664563721	
(E)	Total one-electron terms.....	-1076.26767995411	
(F)	Electron-nuclear.....	-1385.10810259095	
(H)	Kinetic.....	308.84042263684	
(I)	Total two-electron terms.....	435.87743138887	
(J)	Coulomb.....	479.69631557779	
(K)	Exchange.....	-43.81888418891	
(L)	Electronic energy.....	-640.39024856523	(E+I)
(M)	-V/T.....	2.00078739787	(-(A+F+I)/H)
(N)	Total energy.....	-309.08360292802	(A+L)

SCFE: SCF energy: HF -309.08360292802 hartrees iterations: 2

NH2_axial_ approximately 60°(Cy) HF 6-31G**

angstroms

atom	x	y	z
C1	2.2267101665	0.1922160733	-1.6008982102
C2	2.8835870117	1.5728343722	-1.6902214896
C3	1.8344324900	2.6761561780	-1.8539396842
C4	0.7911140650	2.6214928052	-0.7343223027
C5	1.1711296062	0.1109940638	-0.4913961881
H6	2.3157587511	3.6506936361	-1.8694111283
H7	3.4606950127	1.7556495833	-0.7891203907
H8	3.5802233277	1.5918395659	-2.5249299426
H9	1.7458680932	-0.0428064960	-2.5491825566
H10	2.9824389353	-0.5752367919	-1.4426322596
H11	1.2670855311	2.8551619868	0.2129512839
H12	0.0241241679	3.3741525823	-0.9005028184
H13	1.3365931126	2.5605273161	-2.8168717233
H14	0.6448074163	-0.8412361734	-0.5988483853
H15	1.1503085199	0.1504010083	1.5503348720
H16	2.4836326143	-0.5184614799	0.9410121677
N17	1.8208092939	0.2201259546	0.8104335596
C18	0.1420085102	1.2369964323	-0.6482895807
H19	-0.5653712097	1.2030268785	0.1785093858
H20	-0.4350625913	1.0500210146	-1.5525646803

Energy components, in hartrees:

(A)	Nuclear repulsion.....	335.66321105192	
(E)	Total one-electron terms.....	-1056.40617796355	
(F)	Electron-nuclear.....	-1345.47402966495	
(H)	Kinetic.....	289.06785170140	
(I)	Total two-electron terms.....	431.48968183707	
(J)	Coulomb.....	474.03628805244	
(K)	Exchange.....	-42.54660621537	
(L)	Electronic energy.....	-624.91649612647	(E+I)
(M)	-V/T.....	2.00064148736	(-(A+F+I)/H)
(N)	Total energy.....	-289.25328507456	(A+L)

SCFE: SCF energy: HF -289.25328507456 hartrees iterations: 2

NH2_axial_ approximately 180°(Cy) HF 6-31G**

angstroms

atom	x	y	z
C1	0.4652822080	-1.2636479341	-0.6885987673
C2	1.4103636850	-2.4699160992	-0.7165459970
C3	2.5134225563	-2.2881654109	-1.7638786092
C4	3.2764394304	-0.9770212762	-1.5501045961
C5	1.2087469976	0.0673687517	-0.4722910714
H6	3.1986126261	-3.1315862257	-1.7386141087
H7	1.8626656725	-2.6084721190	0.2644849332
H8	0.8459994433	-3.3763191009	-0.9185307677
H9	-0.0712201195	-1.2144768455	-1.6354330514
H10	-0.2875788831	-1.3919660285	0.0867101093
H11	3.8434035958	-1.0328399767	-0.6221426360
H12	4.0092086739	-0.8377279968	-2.3404015712
H13	2.0643585581	-2.2818690145	-2.7564550663
H14	0.4992952798	0.8768893034	-0.6210408804
H15	1.0157619018	0.2281443683	1.5526565712
H16	2.3975922226	-0.4697265500	1.1151260694
N17	1.7484547592	0.2505361862	0.8712569001
C18	2.3252633066	0.2250853509	-1.5124018481
H19	2.8735436630	1.1378924693	-1.3046240588
H20	1.8691747154	0.3385055453	-2.4945880031

Energy components, in hartrees:

(A)	Nuclear repulsion.....	335.10357244731	
(E)	Total one-electron terms.....	-1055.04509939468	
(F)	Electron-nuclear.....	-1344.11325424638	
(H)	Kinetic.....	289.06815485170	
(I)	Total two-electron terms.....	430.69041248648	
(J)	Coulomb.....	473.23538863128	
(K)	Exchange.....	-42.54497614480	
(L)	Electronic energy.....	-624.35468690820	(E+I)
(M)	-V/T.....	2.00063292897	(-(A+F+I)/H)
(N)	Total energy.....	-289.25111446089	(A+L)

SCFE: SCF energy: HF -289.25111446089 hartrees iterations: 2

NH2_axial_ approximately 300°(Cy) HF 6-31G**

angstroms

atom	x	y	z
C1	0.2077745852	1.3170222643	-0.5283757044
C2	-1.0138531396	1.1843238366	0.3887584614
C3	-1.7755958223	-0.1177187555	0.1215716164
C4	-0.8530024987	-1.3361977829	0.2255492023
C5	1.1480563422	0.1078377112	-0.4445447958
H6	-2.6081382655	-0.2162717549	0.8134104492
H7	-0.7020554405	1.2163902965	1.4315552558
H8	-1.6711346583	2.0379594319	0.2466667111
H9	-0.1380374625	1.4154610052	-1.5561502356
H10	0.7672954097	2.2152452969	-0.2893975021
H11	-0.5244401038	-1.4538178620	1.2572487824
H12	-1.3985491815	-2.2428830923	-0.0217804954
H13	-2.2052464691	-0.0808671273	-0.8789019829
H14	1.8911078776	0.2095543613	-1.2308786128
H15	1.2896705462	0.0184036857	1.6033445697
H16	2.5649368451	-0.5997795186	0.8420561883
N17	1.8892953590	0.1379482264	0.8122892180
C18	0.3637395942	-1.1933491705	-0.6954446982
H19	1.0271476865	-2.0482165772	-0.5795063234
H20	0.0249198178	-1.2030874420	-1.7307460909

Energy components, in hartrees:

(A)	Nuclear repulsion.....	335.10223001748	
(E)	Total one-electron terms.....	-1055.04316770723	
(F)	Electron-nuclear.....	-1344.11140955714	
(H)	Kinetic.....	289.06824184991	
(I)	Total two-electron terms.....	430.68982352116	
(J)	Coulomb.....	473.23482114647	
(K)	Exchange.....	-42.54499762531	
(L)	Electronic energy.....	-624.35334418607	(E+I)
(M)	-V/T.....	2.00063262681	(-(A+F+I)/H)
(N)	Total energy.....	-289.25111416859	(A+L)

SCFE: SCF energy: HF -289.25111416859 hartrees iterations: 2

NH2_equat_ approximately 60°(Cy) HF 6-31G**

angstroms

atom	x	y	z
C1	0.4420736631	-1.2213694069	-0.3653244927
C2	-1.0387962141	-1.4145786905	-0.0245998586
C3	-1.2618146791	-1.4409478053	1.4898353264
C4	-0.6834802753	-0.1896914258	2.1564703468
C5	1.0275837553	0.0354309303	0.2943281279
H6	-2.3223716962	-1.5280066006	1.7113808002
H7	-1.6171349173	-0.5996244782	-0.4586404624
H8	-1.4093016450	-2.3308788861	-0.4766130669
H9	1.0082565839	-2.0902733043	-0.0268978939
H10	0.5753758332	-1.1644628447	-1.4441727432
H11	-1.2479234983	0.6832297056	1.8304807708
H12	-0.8036209135	-0.2492178045	3.2349469304
H13	-0.7824926438	-2.3255775942	1.9078543008
H14	0.5012626627	0.9009107136	-0.1062305749
H15	2.9844224475	-0.5278700386	0.3524337997
H16	2.6103222598	0.3312036173	-0.9579574934
N17	2.4421884749	0.2489252192	0.0256057617
C18	0.7944723106	0.0060776889	1.8060462242
H19	1.1755916999	0.9244765609	2.2407435541
H20	1.3778518752	-0.8097925967	2.2356093486

Energy components, in hartrees:

(A)	Nuclear repulsion.....	330.85060278447	
(E)	Total one-electron terms.....	-1046.54941307782	
(F)	Electron-nuclear.....	-1335.62458524585	
(H)	Kinetic.....	289.07517216803	
(I)	Total two-electron terms.....	426.44467872163	
(J)	Coulomb.....	468.98850237259	
(K)	Exchange.....	-42.54382365096	
(L)	Electronic energy.....	-620.10473435619	(E+I)
(M)	-V/T.....	2.00061907566	(-(A+F+I)/H)
(N)	Total energy.....	-289.25413157173	(A+L)

SCFE: SCF energy: HF -289.25413157173 hartrees iterations: 2

NH2_equat_ approximately 180°(Cy) HF 6-31G**

atom	x	y	z
	angstroms		
C1	0.9144930138	-0.1067079302	1.8475691039
C2	-0.5365819752	-0.2844239232	2.3030377677
C3	-1.4275833122	0.8464276458	1.7812177128
C4	-1.3197633349	0.9804265622	0.2595619106
C5	1.0218714680	0.0128134897	0.3264430349
H6	-2.4610792126	0.6737293805	2.0704159575
H7	-0.9170849033	-1.2384853139	1.9397083536
H8	-0.5811526855	-0.3274692402	3.3880092533
H9	1.3381883623	0.7919036632	2.2907371356
H10	1.5191854054	-0.9429398765	2.1944699412
H11	-1.7410044207	0.0922041572	-0.2101430118
H12	-1.9127421096	1.8229445979	-0.0861626944
H13	-1.1255165826	1.7841106998	2.2458269547
H14	0.6463970632	-0.9207843966	-0.1075996183
H15	3.0006552770	-0.4768744785	0.2617042759
H16	2.5017679564	0.3275177212	-1.0412515943
N17	2.4059504863	0.2673772467	-0.0464045481
C18	0.1360150689	1.1506765435	-0.1836254749
H19	0.1915852406	1.2016038357	-1.2697154985
H20	0.5349544501	2.0891520005	0.1952192892

Energy components, in hartrees:

(A)	Nuclear repulsion.....	331.19007350479	
(E)	Total one-electron terms.....	-1047.29752843985	
(F)	Electron-nuclear.....	-1336.37266328984	
(H)	Kinetic.....	289.07513484999	
(I)	Total two-electron terms.....	426.85306129307	
(J)	Coulomb.....	469.39883213899	
(K)	Exchange.....	-42.54577084592	
(L)	Electronic energy.....	-620.44446714678	(E+I)
(M)	-V/T.....	2.00062011142	(-(A+F+I)/H)
(N)	Total energy.....	-289.25439364199	(A+L)

SCFE: SCF energy: HF -289.25439364199 hartrees iterations: 2

NH2_equat_ approximately 300°(Cy) HF 6-31G**

angstroms

atom	x	y	z
C1	0.2450697980	1.2829547590	-0.1344182971
C2	-1.2354074113	1.1929549798	0.2471091393
C3	-1.8777152788	-0.0937958270	-0.2785026286
C4	-1.0992624197	-1.3291190524	0.1818778964
C5	1.0321198865	0.0533818586	0.3230141321
H6	-2.9118959468	-0.1582450885	0.0497475000
H7	-1.3284427489	1.2223944403	1.3321594847
H8	-1.7688402410	2.0608080243	-0.1315255471
H9	0.3331372370	1.3731738048	-1.2182028243
H10	0.6995400817	2.1721331829	0.2904286381
H11	-1.1814429579	-1.4226158155	1.2642449744
H12	-1.5372064651	-2.2299755186	-0.2398561474
H13	-1.8975468440	-0.0672879730	-1.3675221852
H14	0.9981806138	0.0232619230	1.4113371436
H15	2.9783299868	-0.5568021882	0.2982263960
H16	2.5357421400	0.2212604059	-1.0411048697
N17	2.4319999198	0.2090521361	-0.0444396682
C18	0.3792893101	-1.2315024173	-0.2064744392
H19	0.9233562268	-2.0983530748	0.1642819672
H20	0.4704801808	-1.2480497784	-1.2934310847

Energy components, in hartrees:

(A)	Nuclear repulsion.....	330.84846800774	
(E)	Total one-electron terms.....	-1046.54534310055	
(F)	Electron-nuclear.....	-1335.62054521709	
(H)	Kinetic.....	289.07520211655	
(I)	Total two-electron terms.....	426.44275451975	
(J)	Coulomb.....	468.98657369073	
(K)	Exchange.....	-42.54381917098	
(L)	Electronic energy.....	-620.10258858079	(E+I)
(M)	-V/T.....	2.00061893395	(-(A+F+I)/H)
(N)	Total energy.....	-289.25412057305	(A+L)

SCFE: SCF energy: HF -289.25412057305 hartrees iterations: 2

CN(axial) (Cy) HF 6-31G**

		angstroms	
atom	x	y	z
C1	0.1976004282	1.3238696170	-0.5214969883
C2	-1.0357313736	1.1614046471	0.3712005067
C3	-1.7728300862	-0.1486922064	0.0768444031
C4	-0.8393796348	-1.3568293352	0.1998855577
C5	1.1465809412	0.1131922675	-0.4273728112
H6	-2.6160467287	-0.2603543927	0.7522117861
H7	-0.7327036576	1.1822507262	1.4156260182
H8	-1.7002752236	2.0077479620	0.2236417827
H9	-0.1130832039	1.4112947714	-1.5600543921
H10	0.7339653071	2.2338349997	-0.2730161388
H11	-0.5254363850	-1.4708070786	1.2350365236
H12	-1.3669438025	-2.2680014827	-0.0667979056
H13	-2.1837381563	-0.1122651481	-0.9315154180
H15	1.9406595696	0.2250976240	-1.1589454940
C16	0.3942952636	-1.2051878599	-0.6942681226
H17	1.0669654611	-2.0469199951	-0.5661759194
H18	0.0891521320	-1.1978580896	-1.7380864308
C18	1.8139013583	0.0754686761	0.8921640643
N19	2.3240354878	0.0473250510	1.9065449967

Energy components, in hartrees:

(A)	Nuclear repulsion.....	369.14111449502	
(E)	Total one-electron terms.....	-1171.51453222366	
(F)	Electron-nuclear.....	-1497.21753045220	
(H)	Kinetic.....	325.70299822854	
(I)	Total two-electron terms.....	476.41381841062	
(J)	Coulomb.....	523.36030080326	
(K)	Exchange.....	-46.94648239264	
(L)	Electronic energy.....	-695.10071381305	(E+I)
(M)	-V/T.....	2.00078783766	(-(A+F+I)/H)
(N)	Total energy.....	-325.95959931803	(A+L)

CN(equat) (Cy) HF 6-31G**

atom	x	y	z
	angstroms		
C1	0.1768771470	1.2715644968	-0.5999783722
C2	-1.0133883650	1.1323325108	0.3522808049
C3	-1.7789910826	-0.1719901688	0.1128332982
C4	-0.8527392899	-1.3879576887	0.2044768091
C5	1.1044312855	0.0473700923	-0.4933184007
H6	-2.5887965785	-0.2657260011	0.8306522996
H7	-0.6562892942	1.1590797493	1.3808402562
H8	-1.6749286852	1.9850354594	0.2318761731
H9	-0.1774476891	1.3565492496	-1.6244919497
H10	0.7357131611	2.1759635216	-0.3823995039
H11	-0.4875739207	-1.4889745686	1.2255741088
H12	-1.4019849402	-2.2977049022	-0.0192717898
H13	-2.2383959531	-0.1433206974	-0.8740682611
H15	1.5255175880	0.0152347545	0.5087966022
C16	0.3386633248	-1.2636238756	-0.7485662191
H17	1.0093606699	-2.1090959463	-0.6333111014
H18	-0.0094969933	-1.2725081858	-1.7787732579
C18	2.2454327217	0.1739474278	-1.4201106438
N19	3.1162544403	0.2689467156	-2.1427551115

Energy components, in hartrees:

(A)	Nuclear repulsion.....	362.30824100755	
(E)	Total one-electron terms.....	-1157.72294721448	
(F)	Electron-nuclear.....	-1483.42564941325	
(H)	Kinetic.....	325.70270219877	
(I)	Total two-electron terms.....	469.45442842294	
(J)	Coulomb.....	516.40013518955	
(K)	Exchange.....	-46.94570676661	
(L)	Electronic energy.....	-688.26851879154	(E+I)
(M)	-V/T.....	2.00079083036	(-(A+F+I)/H)
(N)	Total energy.....	-325.96027778399	(A+L)

4. Geometric and energetic data for 2-THP derivatives

F_axial(THP) HF 6-31G**

atom	x	y	z
	angstroms		
C1	0.2297411971	1.3039749822	-0.5285775670
C2	-1.0018077314	1.1782180797	0.3716670206
C3	-1.7121754324	-0.1479457732	0.0889415629
C4	-0.7242479480	-1.3013192340	0.1929084732
C5	1.0945847591	0.0608094205	-0.4356690026
H6	-2.5310557364	-0.3079745048	0.7849947282
H7	-0.6925166699	1.2127914258	1.4126722698
H8	-1.6717322150	2.0167817504	0.2101778192
H9	-0.0761001859	1.4145273306	-1.5655923563
H10	0.8271622361	2.1706329904	-0.2659495690
H11	-0.3865700668	-1.4265221859	1.2170388783
H12	-1.1657935165	-2.2329747301	-0.1338780697
H13	-2.1355748711	-0.1327956900	-0.9127210621
O14	0.3944537065	-1.0953933052	-0.6488477665
H15	1.9057151449	0.0682079199	-1.1494247847
F16	1.6624725473	0.0262040564	0.8143455822

Energy components, in hartrees:

(A)	Nuclear repulsion.....	342.85645063385	
(E)	Total one-electron terms.....	-1185.85095573152	
(F)	Electron-nuclear.....	-1554.32833206543	
(H)	Kinetic.....	368.47737633391	
(I)	Total two-electron terms.....	474.09550656154	
(J)	Coulomb.....	521.74134457714	
(K)	Exchange.....	-47.64583801560	
(L)	Electronic energy.....	-711.75544916997	(E+I)
(M)	-V/T.....	2.00114422819	(-(A+F+I)/H)
(N)	Total energy.....	-368.89899853613	(A+L)

SCFE: SCF energy: HF -368.89899853613 hartrees iterations: 2

F_equat(THP) HF 6-31G**

		angstroms	
atom	x	y	z
C1	0.1743765961	1.1915605400	-0.2371316753
C2	-1.3242157439	0.9121733982	-0.0844448698
C3	-1.6762641939	-0.4287890096	-0.7348839182
C4	-0.7405334797	-1.5175907491	-0.2239829951
C5	0.9692696671	-0.0023805582	0.2478003438
H6	-2.7065803157	-0.7033931153	-0.5258827261
H7	-1.5827712305	0.8805897500	0.9732051179
H8	-1.9040605301	1.7180076634	-0.5219536495
H9	0.4287729536	1.3482544384	-1.2813713520
H10	0.4721005687	2.0768362275	0.3158859814
H11	-0.9241364787	-1.7079329638	0.8345208785
H12	-0.8804069961	-2.4477283790	-0.7574020756
H13	0.8636150525	-0.1413148787	1.3231571464
H14	-1.5700445210	-0.3534643875	-1.8138821667
O15	0.6059006663	-1.1559463278	-0.4144947283
F16	2.2824795251	0.1862602768	-0.0061055109

Energy components, in hartrees:

(A)	Nuclear repulsion.....	337.95158880418	
(E)	Total one-electron terms.....	-1175.84267520449	
(F)	Electron-nuclear.....	-1544.32544271802	
(H)	Kinetic.....	368.48276751353	
(I)	Total two-electron terms.....	468.99678148828	
(J)	Coulomb.....	516.63820541607	
(K)	Exchange.....	-47.64142392779	
(L)	Electronic energy.....	-706.84589371622	(E+I)
(M)	-V/T.....	2.00111684300	(-(A+F+I)/H)
(N)	Total energy.....	-368.89430491203	(A+L)

SCFE: SCF energy: HF -368.89430491203 hartrees iterations: 2

O_axial_ approximately 60°(THP) HF 6-31g**

atom	x	y	z
			angstroms
C1	0.2261547382	1.2985656152	-0.5248604266
C2	-1.0095321821	1.1726567923	0.3687846916
C3	-1.7209026132	-0.1510794497	0.0787470317
C4	-0.7369023297	-1.3074678035	0.1865967899
C5	1.1035069171	0.0599815182	-0.4247051192
H6	-2.5456330731	-0.3105586043	0.7686657098
H7	-0.7073468972	1.2057767222	1.4114949760
H8	-1.6784664456	2.0117902014	0.2021900059
H9	-0.0800137198	1.4038128003	-1.5625840367
H10	0.8163254452	2.1702619905	-0.2633115147
H11	-0.4120516841	-1.4291246689	1.2164653399
H12	-1.1850679796	-2.2381595256	-0.1372157470
H13	-2.1370042571	-0.1332917725	-0.9261558784
O14	0.3831377514	-1.1103224054	-0.6493971802
H15	1.8637485032	0.0670855501	-1.1989151942
O16	1.6995981723	0.0538961333	0.8333728219
H17	2.2344514018	-0.7202917939	0.9130318704

Energy components, in hartrees:

(A)	Nuclear repulsion.....	343.62284652278	
(E)	Total one-electron terms.....	-1152.20584457100	
(F)	Electron-nuclear.....	-1496.70558414102	
(H)	Kinetic.....	344.49973957002	
(I)	Total two-electron terms.....	463.67942912374	
(J)	Coulomb.....	509.85080447713	
(K)	Exchange.....	-46.17137535339	
(L)	Electronic energy.....	-688.52641544726	(E+I)
(M)	-V/T.....	2.00117221962	(-(A+F+I)/H)
(N)	Total energy.....	-344.90356892449	(A+L)

SCFE: SCF energy: HF -344.90356892449 hartrees iterations: 2

O_axial_ approximately 180° HF(THP) 6-31g**

angstroms

atom	x	y	z
C1	2.2788640412	0.1542184501	-1.4570061155
C2	3.0184555203	1.4897305653	-1.3494251131
C3	2.0111400599	2.6405035411	-1.4171943274
C4	0.9037363758	2.4292407500	-0.3931532891
C5	1.1405271820	0.0793051401	-0.4411452260
H6	2.4988337168	3.5948864354	-1.2361330463
H7	3.5558642534	1.5319616642	-0.4060293431
H8	3.7559821623	1.5770237440	-2.1417922574
H9	1.8478494927	0.0473186843	-2.4493802706
H10	2.9576710061	-0.6839740262	-1.3124074631
H11	1.2909555916	2.5244101220	0.6159258713
H12	0.1082866848	3.1519116689	-0.5209112594
H13	1.5711803425	2.6840660124	-2.4110725261
O14	0.2966002954	1.1648985887	-0.5539116379
H15	0.5195677364	-0.7910833009	-0.6298910413
O16	1.6256381303	0.0408858282	0.8721759260
H17	2.1573807179	-0.7277739407	0.9970450733

Energy components, in hartrees:

(A)	Nuclear repulsion.....	343.80163438989	
(E)	Total one-electron terms.....	-1152.54114714202	
(F)	Electron-nuclear.....	-1497.03269819221	
(H)	Kinetic.....	344.49155105019	
(I)	Total two-electron terms.....	463.84229349981	
(J)	Coulomb.....	510.01089777554	
(K)	Exchange.....	-46.16860427573	
(L)	Electronic energy.....	-688.69885364221	(E+I)
(M)	-V/T.....	2.00117758535	(-(A+F+I)/H)
(N)	Total energy.....	-344.89721925231	(A+L)

SCFE: SCF energy: HF -344.89721925231 hartrees iterations: 2

O_axial_ approximately 300° HF(THP) 6-31g**

angstroms

atom	x	y	z
C1	0.7770850920	-1.3082629319	-0.9854200521
C2	2.0024839170	-2.2091109900	-1.1799944683
C3	3.0687015414	-1.4658596821	-1.9886314932
C4	3.3467763279	-0.1058003325	-1.3600760281
C5	1.1679165313	0.0613697771	-0.4316459417
H6	3.9883518842	-2.0421885915	-2.0458277584
H7	2.4167770780	-2.5049074032	-0.2156502584
H8	1.7134768249	-3.1311387332	-1.6742082244
H9	0.2958201323	-1.1521417220	-1.9466809763
H10	0.0480203017	-1.7666449181	-0.3245600469
H11	3.8383889933	-0.2245922287	-0.3950925979
H12	4.0021635193	0.4878430352	-1.9838167730
H13	2.7141490183	-1.3162154596	-3.0054058242
O14	2.1659021086	0.6406147918	-1.2139054768
H15	0.3353038657	0.7464471957	-0.4883260549
O16	1.5148434632	0.0112111057	0.9143734647
H17	2.0458168474	-0.7433737963	1.1057086672

Energy components, in hartrees:

(A)	Nuclear repulsion.....	343.12061552984	
(E)	Total one-electron terms.....	-1150.88158901927	
(F)	Electron-nuclear.....	-1495.37199891264	
(H)	Kinetic.....	344.49040989336	
(I)	Total two-electron terms.....	462.86390169202	
(J)	Coulomb.....	509.03122151106	
(K)	Exchange.....	-46.16731981904	
(L)	Electronic energy.....	-688.01768732725	(E+I)
(M)	-V/T.....	2.00118047380	(-(A+F+I)/H)
(N)	Total energy.....	-344.89707179742	(A+L)

SCFE: SCF energy: HF -344.89707179742 hartrees iterations: 2

O_equat_ approximately 60°(THP) HF 6-31g**

atom	x	y	z
		angstroms	
C1	0.1624008630	-0.8682581618	-0.6168779122
C2	-1.2542218322	-1.0314567875	-0.0585881696
C3	-1.1917072254	-1.4916336696	1.3997211714
C4	-0.2659269300	-0.5779311020	2.1928972706
C5	1.0018360783	0.0156059762	0.2968697817
H6	-2.1804699797	-1.4941470326	1.8509178716
H7	-1.7776263982	-0.0778059957	-0.1146006185
H8	-1.8219884019	-1.7333113843	-0.6613477716
H9	0.6483383071	-1.8403041942	-0.6849793720
H10	0.1486957199	-0.4388246232	-1.6136513636
H11	-0.6989913420	0.4205444721	2.2696318331
H12	-0.1083026514	-0.9477086375	3.1977423875
H13	0.6039930596	1.0288149430	0.3050827648
H14	-0.8087316238	-2.5081623459	1.4487773005
O15	1.0035411691	-0.4978518753	1.5966216662
O16	2.3102252049	0.1219415510	-0.1208706232
H17	2.7494195158	-0.6967991982	0.0508225306

Energy components, in hartrees:

(A)	Nuclear repulsion.....	338.98207292205	
(E)	Total one-electron terms.....	-1142.66749523129	
(F)	Electron-nuclear.....	-1487.17279951366	
(H)	Kinetic.....	344.50530428237	
(I)	Total two-electron terms.....	458.78487390980	
(J)	Coulomb.....	504.95253461601	
(K)	Exchange.....	-46.16766070621	
(L)	Electronic energy.....	-683.88262132149	(E+I)
(M)	-V/T.....	2.00114728021	(-(A+F+I)/H)
(N)	Total energy.....	-344.90054839944	(A+L)

SCFE: SCF energy: HF -344.90054839944 hartrees iterations: 2

O_equat_ approximately 180° HF(THP) 6-31g**

angstroms

atom	x	y	z
C1	0.8075617673	-0.1345486583	1.7924854496
C2	-0.6794796707	-0.1615690502	2.1570203068
C3	-1.3906177272	1.0365570427	1.5235121499
C4	-1.0666789372	1.1048406155	0.0362358482
C5	0.9855455958	0.0070270647	0.2855192117
H6	-2.4664244123	0.9695583765	1.6630890460
H7	-1.1287541422	-1.0839322184	1.7905520808
H8	-0.8060335416	-0.1609083357	3.2350802362
H9	1.2988391869	0.7155319228	2.2571725735
H10	1.3072962322	-1.0367218078	2.1397473277
H11	-1.5097966856	0.2536050187	-0.4839736778
H12	-1.4585431690	2.0075264589	-0.4135502507
H13	0.5864908799	-0.8807342275	-0.2176069349
H14	-1.0557610572	1.9556562345	1.9975528577
O15	0.3192284192	1.1280926680	-0.1824551207
O16	2.3099496126	0.2021077733	-0.0714605995
H17	2.8015408764	-0.5853154025	0.0932728838

Energy components, in hartrees:

(A)	Nuclear repulsion.....	339.01716918115	
(E)	Total one-electron terms.....	-1142.79546228386	
(F)	Electron-nuclear.....	-1487.29655318729	
(H)	Kinetic.....	344.50109090343	
(I)	Total two-electron terms.....	458.88419373387	
(J)	Coulomb.....	505.04834631119	
(K)	Exchange.....	-46.16415257732	
(L)	Electronic energy.....	-683.91126854999	(E+I)
(M)	-V/T.....	2.00114080471	(-(A+F+I)/H)
(N)	Total energy.....	-344.89409936884	(A+L)

SCFE: SCF energy: HF -344.89409936884 hartrees iterations: 2

O_equat_ approximately 300° HF(THP) 6-31g**

angstroms

atom	x	y	z
C1	0.1743205760	1.1877483475	-0.2343967802
C2	-1.3237265936	0.9074901480	-0.0829196214
C3	-1.6790373909	-0.4325831526	-0.7331857415
C4	-0.7494207433	-1.5254092018	-0.2202336546
C5	0.9802441104	-0.0035926664	0.2472613044
H6	-2.7117147787	-0.7026607222	-0.5280793968
H7	-1.5839434461	0.8757974090	0.9744119112
H8	-1.9044437451	1.7128231163	-0.5214455032
H9	0.4287524916	1.3512828739	-1.2774151986
H10	0.4697475478	2.0716832538	0.3217800430
H11	-0.9344173692	-1.7095053331	0.8397078686
H12	-0.9016539121	-2.4571652476	-0.7493506155
H13	0.8203010023	-0.1536704901	1.3198614922
H14	-1.5686597298	-0.3583722068	-1.8120636899
O15	0.5958318348	-1.1729270727	-0.4160871258
O16	2.3132479427	0.2172163053	-0.0157141067
H17	2.7895435872	-0.5838469828	0.1371396455

Energy components, in hartrees:

(A)	Nuclear repulsion.....	339.22072880473	
(E)	Total one-electron terms.....	-1143.23237010431	
(F)	Electron-nuclear.....	-1487.73807758041	
(H)	Kinetic.....	344.50570747610	
(I)	Total two-electron terms.....	459.11004482440	
(J)	Coulomb.....	505.27907876030	
(K)	Exchange.....	-46.16903393589	
(L)	Electronic energy.....	-684.12232527991	(E+I)
(M)	-V/T.....	2.00114915077	(-(A+F+I)/H)
(N)	Total energy.....	-344.90159647518	(A+L)

SCFE: SCF energy: HF -344.90159647518 hartrees iterations: 2

NH2_axial_ approximately 60°(THP) HF 6-31g**

angstroms

atom	x	y	z
C1	-4.3488513100	-0.8937150411	0.3572349047
C2	-4.2158023371	0.2163455110	-0.6876795819
C3	-3.6590086045	1.4788374353	-0.0257878182
C4	-2.3761507106	1.1539460915	0.7273893252
C5	-3.0446753335	-1.0939993634	1.1287334366
H6	-3.4616736197	2.2508109540	-0.7653527867
H7	-3.5457560146	-0.1052245817	-1.4790410489
H8	-5.1809407064	0.4174000344	-1.1441177000
H9	-5.1205639752	-0.6279032770	1.0752714893
H10	-4.6523865829	-1.8312252503	-0.1030343426
H11	-1.5892874319	0.8851731605	0.0299103274
H12	-2.0396866780	2.0030364764	1.3094360000
H13	-4.3894308306	1.8791636921	0.6740360788
O14	-2.5765147105	0.1122039173	1.6560089657
H15	-3.2399261922	-1.7072263661	2.0062818018
H16	-1.1877213220	-1.8190382853	0.7931166333
H17	-2.3238038482	-2.5469584069	-0.1045505578
N18	-2.0283639208	-1.6683975339	0.2713585172

Energy components, in hartrees:

(A)	Nuclear repulsion.....	342.60314737127	
(E)	Total one-electron terms.....	-1121.53702763296	
(F)	Electron-nuclear.....	-1446.27415096366	
(H)	Kinetic.....	324.73712333070	
(I)	Total two-electron terms.....	453.86584068135	
(J)	Coulomb.....	498.76305569454	
(K)	Exchange.....	-44.89721501319	
(L)	Electronic energy.....	-667.67118695160	(E+I)
(M)	-V/T.....	2.00101902809	(-(A+F+I)/H)
(N)	Total energy.....	-325.06803958034	(A+L)

SCFE: SCF energy: HF -325.06803958034 hartrees iterations: 2

NH2_axial_ approximately 180°(THP) HF 6-31g**

atom	x	y	z
	angstroms		
C1	-3.4237254020	-2.1080223897	2.3213927993
C2	-4.1994537029	-3.3333063566	1.8324376632
C3	-5.3312443173	-2.8861656568	0.9042188925
C4	-4.7818640476	-1.9946706964	-0.2015495975
C5	-2.9867325957	-1.2218732709	1.1551697064
H6	-5.8350253148	-3.7435325647	0.4648795702
H7	-3.5308081380	-3.9996907396	1.2960001966
H8	-4.5951117888	-3.8870740816	2.6792622011
H9	-4.0583348238	-1.5098820463	2.9703421444
H10	-2.5560852495	-2.4013258284	2.9081447505
H11	-4.1438034120	-2.5693200400	-0.8652025557
H12	-5.5830027491	-1.5628299553	-0.7887049208
H13	-6.0736987439	-2.3297762728	1.4723926093
O14	-4.0680243538	-0.9011231597	0.3296730702
H15	-2.6572826251	-0.2596749457	1.5423335003
H16	-1.6489881127	-1.2735831520	-0.3611067614
H17	-1.1728557440	-2.1241808792	0.9341768716
N18	-1.9623274269	-1.8795846499	0.3709995221

Energy components, in hartrees:

(A)	Nuclear repulsion.....	342.59168840921	
(E)	Total one-electron terms.....	-1121.51703234477	
(F)	Electron-nuclear.....	-1446.25207593061	
(H)	Kinetic.....	324.73504358584	
(I)	Total two-electron terms.....	453.85731403963	
(J)	Coulomb.....	498.75410536718	
(K)	Exchange.....	-44.89679132755	
(L)	Electronic energy.....	-667.65971830514	(E+I)
(M)	-V/T.....	2.00102540923	(-(A+F+I)/H)
(N)	Total energy.....	-325.06802989593	(A+L)

SCFE: SCF energy: HF -325.06802989593 hartrees iterations: 2

NH2_axial_ approximately 300°(THP) HF 6-31g**

angstroms

atom	x	y	z
C1	-2.8554735235	0.2498668565	1.7099425069
C2	-1.9370730846	0.2320422894	2.9364121149
C3	-2.4257909172	-0.8214279782	3.9328983221
C4	-2.5947782878	-2.1633931984	3.2321349528
C5	-3.0420269308	-1.1459343856	1.1139951177
H6	-1.7341393707	-0.9248443267	4.7651884618
H7	-0.9125203849	0.0099750692	2.6413735419
H8	-1.9129223354	1.2151284936	3.3967275802
H9	-3.8333871638	0.6145278719	2.0123139951
H10	-2.4776568553	0.9168243414	0.9429727513
H11	-1.6203374223	-2.5571257900	2.9405231249
H12	-3.0510913916	-2.8932400895	3.8892303398
H13	-3.3856212017	-0.5170082635	4.3432560291
O14	-3.4377431226	-2.0609046217	2.1160468949
H15	-3.8797263753	-1.1360880760	0.4296693162
H16	-1.0439137258	-1.5324331282	0.8917808198
H17	-2.0111804491	-2.4811415629	0.0056869619
N18	-1.8891200534	-1.5537688209	0.3597684057

Energy components, in hartrees:

(A)	Nuclear repulsion.....	341.96244761751	
(E)	Total one-electron terms.....	-1120.00772084121	
(F)	Electron-nuclear.....	-1444.74269385901	
(H)	Kinetic.....	324.73497301780	
(I)	Total two-electron terms.....	452.97660060706	
(J)	Coulomb.....	497.87324250872	
(K)	Exchange.....	-44.89664190166	
(L)	Electronic energy.....	-667.03112023415	(E+I)
(M)	-V/T.....	2.00102760598	(-(A+F+I)/H)
(N)	Total energy.....	-325.06867261664	(A+L)

SCFE: SCF energy: HF -325.06867261664 hartrees iterations: 2

NH2_equat_ approximately 60°(THP) HF 6-31g**

atom	x	y	z
	angstroms		
C1	-4.5132559518	-0.8386358999	0.3180277152
C2	-4.2635429230	0.2668532297	-0.7119211508
C3	-3.7006861034	1.5075445879	-0.0155409927
C4	-2.5106830659	1.1195497801	0.8532216924
C5	-3.2622493323	-1.0911472991	1.1640149430
H6	-3.3981376962	2.2589049787	-0.7404252864
H7	-3.5494194118	-0.0855349501	-1.4551932902
H8	-5.1779118074	0.5048702836	-1.2470014053
H9	-5.3212318698	-0.5459356080	0.9863191284
H10	-4.8141724375	-1.7616444610	-0.1726758819
H11	-1.6796080469	0.7935538422	0.2253897644
H12	-2.1666286980	1.9567867193	1.4471045042
H13	-4.4656654449	1.9533959719	0.6156081201
O14	-2.8470277838	0.1040735458	1.7592655984
H15	-2.4688817947	-1.4672022277	0.5146435337
H16	-4.1037868278	-1.6929739126	2.8922880294
H17	-3.7404309247	-2.9182135456	1.8913454912
N18	-3.4269936030	-2.0338872737	2.2380494031

Energy components, in hartrees:

(A)	Nuclear repulsion.....	338.29176847692	
(E)	Total one-electron terms.....	-1112.63506259127	
(F)	Electron-nuclear.....	-1437.37476571929	
(H)	Kinetic.....	324.73970312802	
(I)	Total two-electron terms.....	449.27802401664	
(J)	Coulomb.....	494.16870875738	
(K)	Exchange.....	-44.89068474075	
(L)	Electronic energy.....	-663.35703857464	(E+I)
(M)	-V/T.....	2.00100254748	(-(A+F+I)/H)
(N)	Total energy.....	-325.06527009772	(A+L)

SCFE: SCF energy: HF -325.06527009772 hartrees iterations: 2

NH2_equat_ approximately 180°(THP) HF 6-31g**

angstroms

atom	x	y	z
C1	-2.3805155234	0.0778378843	1.5420283622
C2	-2.0647985937	0.9512385116	0.3244212746
C3	-1.4986804937	0.0880912519	-0.8063803397
C4	-2.4147628208	-1.1018328047	-1.0651232958
C5	-3.2436710579	-1.1097549799	1.1336908972
H6	-1.3828442622	0.6682143362	-1.7184016751
H7	-2.9739389958	1.4441300543	-0.0179836765
H8	-1.3666339627	1.7381094875	0.5929493480
H9	-1.4666289647	-0.3160688300	1.9759132462
H10	-2.8882501721	0.6572587794	2.3100162923
H11	-3.3679124292	-0.7589130589	-1.4725503420
H12	-1.9777647904	-1.7875777331	-1.7798025302
H13	-0.5154718511	-0.2825008071	-0.5279133690
O14	-2.6324355244	-1.8382638152	0.1077105089
H15	-4.2011099810	-0.7319172136	0.7498385984
H16	-3.9338406753	-1.6095105355	2.9690125407
H17	-3.8997042762	-2.8429426404	1.9159907800
N18	-3.4092245002	-2.0285996361	2.2276964483

Energy components, in hartrees:

(A)	Nuclear repulsion.....	338.52768453360	
(E)	Total one-electron terms.....	-1113.19278110678	
(F)	Electron-nuclear.....	-1437.93318734784	
(H)	Kinetic.....	324.74040624106	
(I)	Total two-electron terms.....	449.59857701197	
(J)	Coulomb.....	494.49128863479	
(K)	Exchange.....	-44.89271162282	
(L)	Electronic energy.....	-663.59420409481	(E+I)
(M)	-V/T.....	2.00100422773	(-(A+F+I)/H)
(N)	Total energy.....	-325.06651956122	(A+L)

SCFE: SCF energy: HF -325.06651956122 hartrees iterations: 2

NH2_equat_ approximately 300°(THP) HF 6-31g**

angstroms

atom	x	y	z
C1	-2.1952221368	-1.6594233252	0.1909823292
C2	-2.1064171784	-0.7933722407	-1.0688110528
C3	-3.4916845132	-0.6259818436	-1.6971517535
C4	-4.4864476056	-0.1582614409	-0.6425675360
C5	-3.2693449056	-1.1350773186	1.1362457085
H6	-3.4627130241	0.0846001862	-2.5193884149
H7	-1.7095257342	0.1863462831	-0.8055509895
H8	-1.4111744428	-1.2294910636	-1.7798748182
H9	-2.4516159915	-2.6814397394	-0.0834491876
H10	-1.2453093006	-1.6909716220	0.7139801448
H11	-4.2351193909	0.8527316858	-0.3147262631
H12	-5.4958853855	-0.1352756758	-1.0344869939
H13	-3.8306160416	-1.5773457090	-2.1004592077
O14	-4.5030440331	-1.0271030377	0.4576415409
H15	-2.9861789183	-0.1426517842	1.4886814636
H16	-4.1120312974	-1.6155182776	2.8904357071
H17	-3.7078747125	-2.8931521536	1.9935393303
N18	-3.4102966075	-1.9798997881	2.2770678847

Energy components, in hartrees:

(A)	Nuclear repulsion.....	338.36915204106	
(E)	Total one-electron terms.....	-1112.85877703669	
(F)	Electron-nuclear.....	-1437.60490924429	
(H)	Kinetic.....	324.74613220760	
(I)	Total two-electron terms.....	449.41654491842	
(J)	Coulomb.....	494.31191042595	
(K)	Exchange.....	-44.89536550753	
(L)	Electronic energy.....	-663.44223211826	(E+I)
(M)	-V/T.....	2.00100677987	(-(A+F+I)/H)
(N)	Total energy.....	-325.07308007721	(A+L)

SCFE: SCF energy: HF -325.07308007721 hartrees iterations: 2

CN axial(THP) HF 6-31g**

atom	x	y	z
		angstroms	
C1	0.2021016861	1.3171693406	-0.5242133848
C2	-1.0426068646	1.1869281327	0.3564613912
C3	-1.7442278284	-0.1431857797	0.0691621767
C4	-0.7576337872	-1.2960136361	0.1910307531
C5	1.0845957482	0.0690299592	-0.4170872951
H6	-2.5712919236	-0.3007073475	0.7554963792
H7	-0.7572728293	1.2330893684	1.4049775862
H8	-1.7120577891	2.0215645553	0.1754688729
H9	-0.0927316943	1.4063865661	-1.5656838905
H10	0.7799877212	2.1992940687	-0.2686168645
H11	-0.4311228222	-1.4132116414	1.2224189049
H12	-1.1961807560	-2.2309693315	-0.1292972939
H13	-2.1538701376	-0.1334327057	-0.9378786182
O14	0.3666082346	-1.1004522216	-0.6432275216
H15	1.8611501409	0.0968635081	-1.1702070496
C16	1.7820456155	0.0175373355	0.9029379585
N17	2.3124691823	-0.0109260303	1.9058440805

Energy components, in hartrees:

(A)	Nuclear repulsion.....	375.87219865514	
(E)	Total one-electron terms.....	-1236.06550599656	
(F)	Electron-nuclear.....	-1597.42249890551	
(H)	Kinetic.....	361.35699290895	
(I)	Total two-electron terms.....	498.43090094856	
(J)	Coulomb.....	547.71633234399	
(K)	Exchange.....	-49.28543139543	
(L)	Electronic energy.....	-737.63460504800	(E+I)
(M)	-V/T.....	2.00112191958	(-(A+F+I)/H)
(N)	Total energy.....	-361.76240639286	(A+L)

CN equat(THP) HF 6-31g**

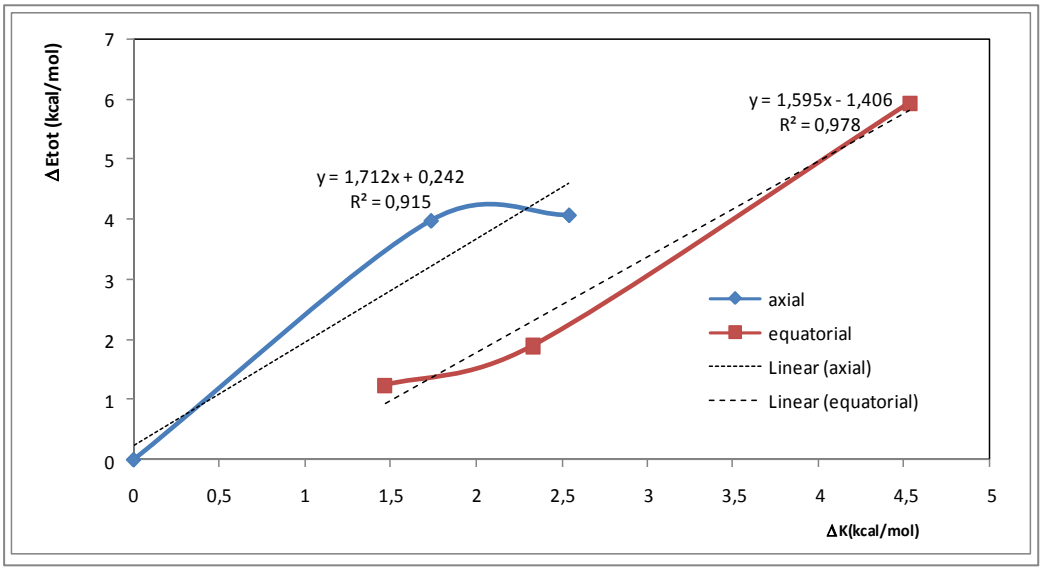
		angstroms	
atom	x	y	z
C1	0.1535511119	1.2065720809	-0.2543023328
C2	-1.3389575452	0.9118251884	-0.0817613977
C3	-1.6918582267	-0.4286895682	-0.7320242354
C4	-0.7566047601	-1.5196356111	-0.2285717298
C5	0.9667346803	0.0017417392	0.2264051043
H6	-2.7210360793	-0.7031844659	-0.5185786881
H7	-1.5813852394	0.8772647816	0.9793218010
H8	-1.9286232639	1.7147776311	-0.5115263844
H9	0.3834367121	1.3800240743	-1.3010289319
H10	0.4476973885	2.0917867569	0.3003026698
H11	-0.9259883169	-1.7074916065	0.8323251384
H12	-0.9040814691	-2.4491707184	-0.7608431970
H13	0.8366234767	-0.1192742807	1.3018663646
H14	-1.5916998993	-0.3517043487	-1.8114296508
O15	0.5919253264	-1.1672464447	-0.4340959216
C16	2.4136084541	0.1982199737	-0.0110846996
N17	3.5201403845	0.3821977421	-0.1784832677

Energy components, in hartrees:

(A)	Nuclear repulsion.....	369.50684074829	
(E)	Total one-electron terms.....	-1223.23197806183	
(F)	Electron-nuclear.....	-1584.58772322373	
(H)	Kinetic.....	361.35574516189	
(I)	Total two-electron terms.....	491.96381505752	
(J)	Coulomb.....	541.24779703975	
(K)	Exchange.....	-49.28398198223	
(L)	Electronic energy.....	-731.26816300432	(E+I)
(M)	-V/T.....	2.00112237622	(-(A+F+I)/H)
(N)	Total energy.....	-361.76132225602	(A+L)

5. Linear correlation for ΔK and ΔE_{tot} in (A and E) rotameric families of 2-OH-THP

Linear correlation between ΔE_{tot} and ΔK, for rotameric family of axial and equatorial anomers of 2-OH THP. The reference is the corresponding absolute values for 2-OH THP rotamer of A anomer with φ=55.5°.



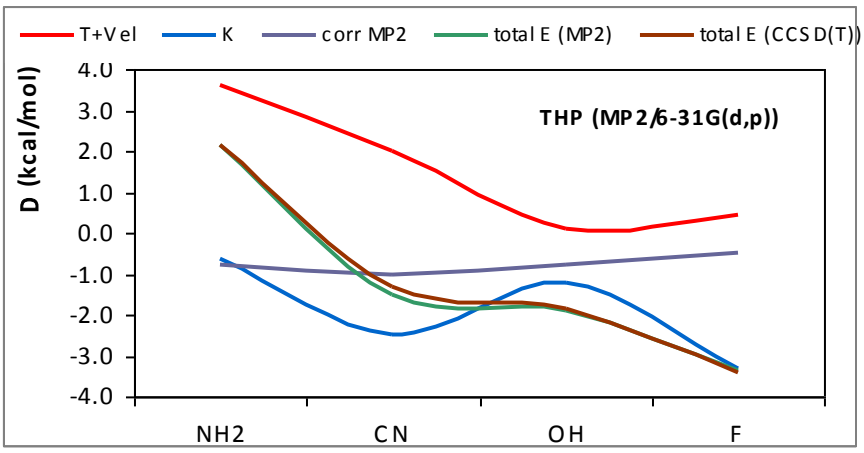
6. K and the anomeric effect (MP2 results)

All quantities are in kcal/mol

Ax - Eq	F-THP		CN-THP		OH-THP		NH2-THP	
	HF	MP2	HF	MP2	HF	MP2	HF	MP2
T	-3,15	-1,09	0,94	8,10	-3,72	-4,22	-6,88	-5,65
Vel	3,00	1,53	-0,69	-6,08	3,96	4,33	10,47	9,23
T+Vel	-0,15	0,44	0,25	2,02	0,24	0,11	3,59	3,59
K	-2,79	-3,31	-0,93	-2,47	-1,48	-1,22	-0,82	-0,63
corrMP2	-	-0,50	-	-1,04	-	-0,79	-	-0,80
total E0	-2,94	-2,88	-0,68	-0,45	-1,24	-1,10	2,77	2,95
total E (MP2)	-	-3,38	-	-1,49	-	-1,89		2,15
total E (CCSD(T))	-	-3,41	-	-1,30	-	-1,85		2,16

Ax - Eq	F-THP		CN-THP		OH-THP		NH2-THP	
	HF	MP2	HF	MP2	HF	MP2	HF	MP2
T	-0,61	-2,49	0,61	5,66	0,78	-1,51	-4,22	-6,26
Vel	0,69	2,14	0,17	-3,28	0,92	2,56	8,77	10,31
T+Vel	0,08	-0,34	0,78	2,38	1,70	1,05	4,56	4,05
K	-2,94	-2,45	-1,31	-2,69	-2,58	-1,82	-1,58	-0,98
corrMP2	-	-0,62	-	-1,01	-	-0,55	-	-0,35
total E0	-2,85	-2,79	-0,53	-0,31	-0,88	-0,77	2,98	3,07
total E (MP2)	-	-3,41	-	-1,32	-	-1,32		2,73
total E (CCSD(T))	-	-3,44	-	-1,08	-	-1,30		2,73

ΔE_{tot} (MP2) (yellow line) is governed by ΔK values (cyan lines).



ΔK, $\Delta T+\Delta V_{el}$ and ΔE_{tot} anomeric difference, as a function of the substituent in 2-THP rings.

6. Influence on the basis set type on the anomeric effect calculations

2F-THP

		T	VNe	V_{NN}	J	K	Total E
4-31G(d,p)	F(A)	366.419780	-1552.976427	343.394182	522.179166	-47.563231	-368.546530
	F(E)	366.419363	-1542.418193	338.214888	516.800036	-47.557745	-368.541650
6-31G(d,p)	F(A)	368.477376	-1554.328332	342.856451	521.741345	-47.645838	-368.898999
	F(E)	368.482768	-1544.325443	337.951589	516.638205	-47.641424	-368.894305
6-311G(d,p)	F(A)	368.995713	-1555.243816	343.027655	521.911706	-47.671732	-368.980475
	F(E)	368.996509	-1545.345153	338.174021	516.867480	-47.668629	-368.975771
cc-vDZP	F(A)	368.909229	-1554.696056	342.865721	521.663932	-47.652190	-368.909363
	F(E)	368.920798	-1545.115892	338.167869	516.770706	-47.648038	-368.904558
cc-vTZP	F(A)	368.888863	-1556.687801	343.766692	522.702912	-47.691779	-369.021114
	F(E)	368.884650	-1546.783484	338.907443	517.661020	-47.687037	-369.017408

2-OH THP

		T	VNe	V_{NN}	J	K	Total E
4-31G(d,p)	OH(A)	342.418392	-1495.068181	344.025040	510.136188	-46.083726	-344.572288
	OH(E)	342.417704	-1485.846648	339.500562	505.439240	-46.080915	-344.570058
6-31G(d,p)	OH(A)	344.499740	-1496.705584	343.622847	509.850804	-46.171375	-344.903569
	OH(E)	344.505707	-1487.738078	339.220729	505.279079	-46.169034	-344.901596
6-311G(d,p)	OH(A)	345.002118	-1497.522406	343.732185	510.014110	-46.202776	-344.976768
	OH(E)	345.003136	-1488.673457	339.389485	505.505819	-46.199943	-344.974961
cc-vDZP	OH(A)	344.899446	-1497.317060	343.737216	509.951280	-46.183413	-344.912531
	OH(E)	344.911400	-1488.538618	339.421948	505.476716	-46.182094	-344.910647
cc-vTZP	OH(A)	344.882335	-1498.444073	344.221617	510.544197	-46.218575	-345.014499
	OH(E)	344.886855	-1489.782015	339.967951	506.129035	-46.215349	-345.013523

All values were obtained from geometry optimization calculations performed for each basis set. Only the most stable rotamers of each anomer were considered for 2-OH THP compound.

8. Absolute values for C5-O5, O5-C1 and C1-X bond lengths in 2-F, 2-CN and 2-OH THP compounds, in Å.

	C5-O5 (in THF)		O5-C1 (in THF)		C1-X (in THF)	
X substituent	A	E	A	E	A	E
F	1.415	1.407	1.368	1.379	1.373	1.351
CN	1.414	1.409	1.391	1.394	1.494	1.479
OH	1.411	1.404	1.393	1.398	1.392	1.377
NH_2	1.402	1.402	1.413	1.412	1.437	1.427