Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Formation and Reactivity of NHC-Boryl Radicals: Insight into Substituent Effect from Theoretical Calculations

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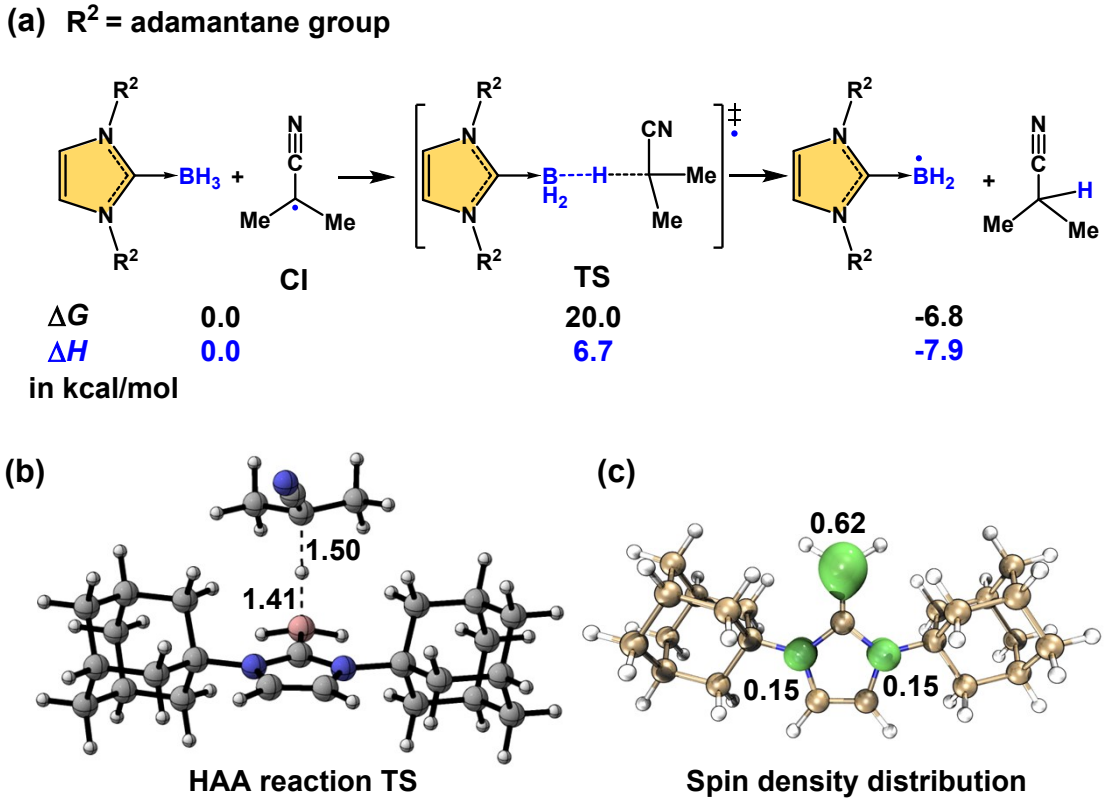

Figure S1. (a) Computed ΔG^{TS}, ΔG^{R}, ΔH^{TS} and ΔH^{R} (in kcal/mol) of the HAA reaction for the bulky adamantly substituted NHC-borane at the M06-2X/cc-PVTZ/SMD//B3LYP-D3(BJ)/6-31++G(d,p)/SMD level, (b) the transition-state structure of the HAA reaction and selected bond lengths (in Å), (c) the spin density (in a.u.) of the corresponding boryl radial.

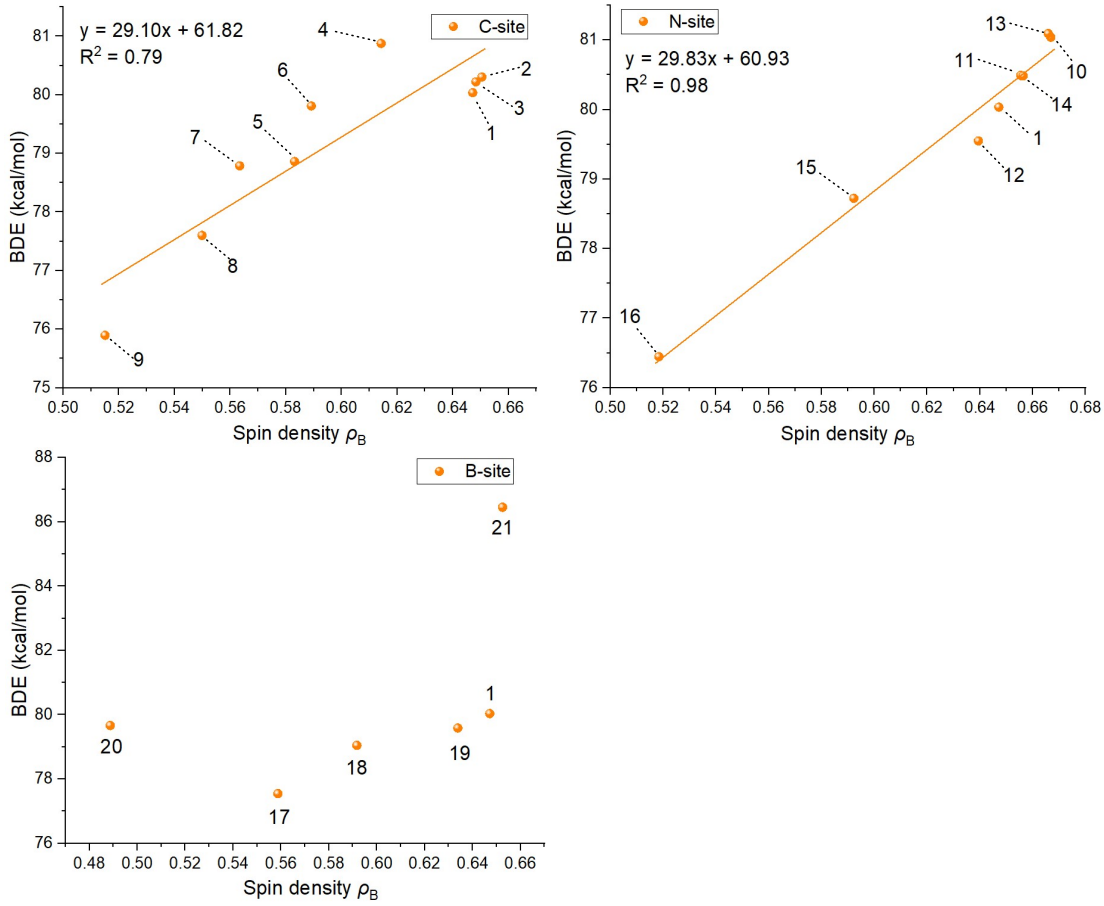

Figure S2. Correlations between the B–H BDE of the NHC-boranes and the spin density of the B site of their corresponding NHC-boryl radicals for the C-, N-, B-site substitutions predicted at the M06-2X/cc-PVTZ/SMD level.

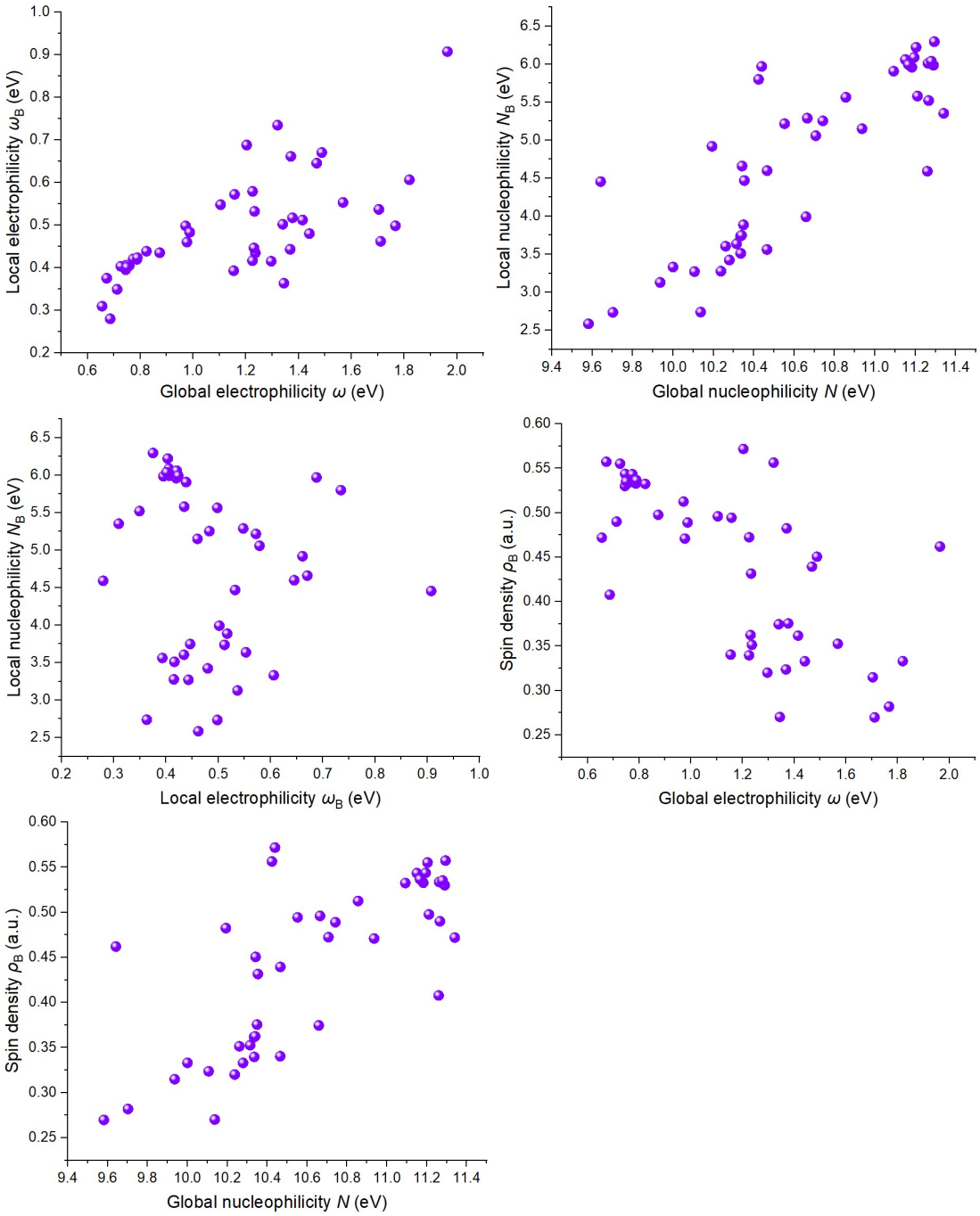

Figure S3. Correlations among the indices of electrophilicity and nucleophilicity, as well as between the indice and the spin density of the B atom for the NHC-boryl radicals calculated at the M06-2X/cc-PVTZ/SMD level.

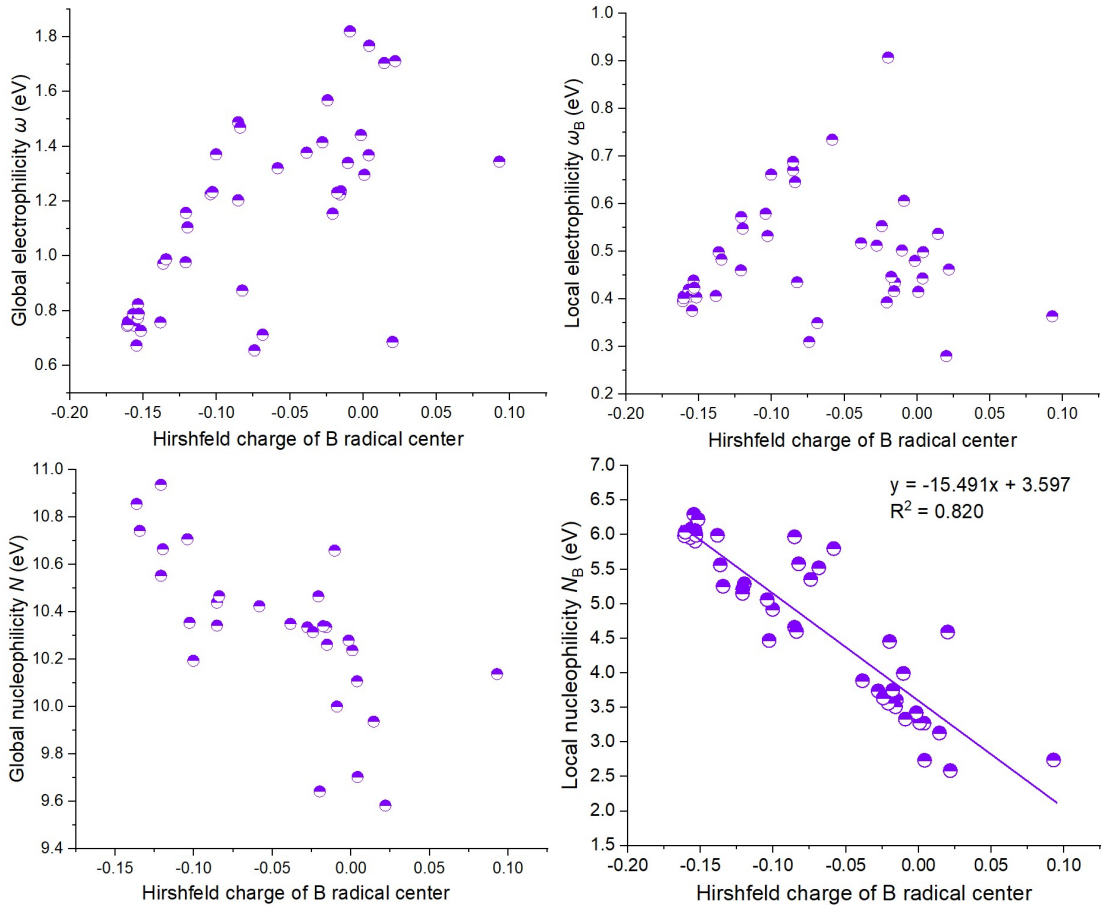

Figure S4. Correlations between the Hirshfeld charge (a.u.) of the B center and indices of ω, ω_B, N and N_B for the studied NHC-boryl radicals.

Generally, the solvent effect can affect the bond dissociation energy notably. Herein the B–H bond dissociation energies of the single-site-modified NHC-boranes (**1**–**21**) were calculated in organic solvents with different static dielectric constants (ε) covering the range from non-polarity to strong-polarity, such as dimethyl sulfoxide (DMSO, ε = 46.83), *N*, *N*-dimethylformamide (DMF, ε=37.22), acetonitrile (ε=35.69), tetrahydrofuran (THF, ε=7.43), and toluene (ε=2.37). As shown in Figure S5, the B–H BDE values for the discussed NHC-boranes generally increase with the increasing solvent polarity. However, the differences of the BDEs for the selected NHC-boranes are small, which suggests that the solvent effect on the B–H BDEs is less notable. Solvents may have remarkably influence on the subsequent reactions involving the NHC-boryl radicals after the B–H bond homolytic cleavage.

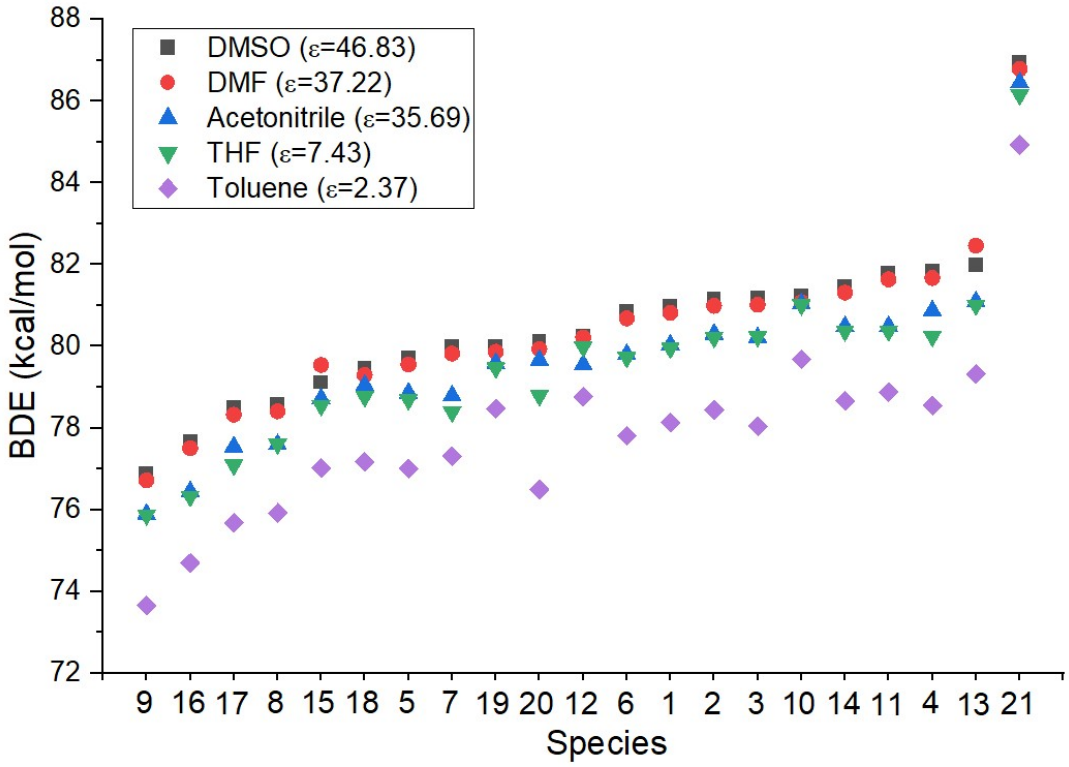

Figure S5. The effect of different solvents on the B–H bond dissociation energy of the selected NHC-boranes **1**–**21**. The BDE values of selected NHC-boranes in DMSO are in ascending order.

Table S1. Hirshfeld charges (a.u.) of the B atom for studied NHC-boryl radicals calculated at the M06-2X/cc-PVTZ level.

Radicals	Hirshfeld Charge	Radicals	Hirshfeld Charge	Radicals	Hirshfeld Charge
1'	-0.15363	**16'**	-0.10276	**31'**	-0.01988
2'	-0.16047	**17'**	-0.07416	**32'**	-0.02081
3'	-0.15700	**18'**	-0.08252	**33'**	0.021883
4'	-0.13642	**19'**	-0.05835	**34'**	0.004139
5'	-0.11979	**20'**	0.020049	**35'**	-0.024279
6'	-0.12094	**21'**	-0.08529	**36'**	-0.038578
7'	-0.10032	**22'**	0.00381	**37'**	-0.017747
8'	-0.10411	**23'**	0.000812	**38'**	-0.160978
9'	-0.08533	**24'**	-0.00153	**39'**	-0.153104
10'	-0.15464	**25'**	0.014377	**40'**	-0.160433
11'	-0.15606	**26'**	-0.01525	**41'**	-0.083886
12'	-0.13835	**27'**	-0.02777	**42'**	-0.121032
13'	-0.15164	**28'**	-0.01582	**43'**	-0.06859
14'	-0.15375	**29'**	0.092948	**44'**	-0.010401
15'	-0.13445	**30'**	-0.00900		

Table S2. The calculated absolute electronic energies (*E*, in a.u.), thermal free energies (*G*, in a.u.) calculated at the M06-2X/cc-PVTZ/SMD//B3LYP-D3(BJ)/6-31++G(d,p)/SMD level.

Boranes	*E*	*G*corr	*G*	*H*
1	-331.4510363	0.169332	-331.2817043	-331.4510363
2	-410.071	0.227943	-409.843057	-410.071
3	-370.7604091	0.19763	-370.5627791	-370.7604091
4	-791.0412109	0.158013	-790.8831979	-791.0412109
5	-1250.6317	0.152926	-1250.478774	-1250.6317
6	-668.4943631	0.17532	-668.3190431	-668.4943631
7	-1005.524481	0.182241	-1005.34224	-1005.524481
8	-485.077611	0.218897	-484.858714	-485.077611
9	-501.1155611	0.20721	-500.9083511	-501.1155611
10	-722.0976855	0.423478	-721.6742075	-722.0976855
11	-526.7747643	0.296248	-526.4785163	-526.7747643
12	-449.3664314	0.258866	-449.1075654	-449.3664314
13	-488.6789276	0.28711	-488.3918176	-488.6789276
14	-410.064826	0.228121	-409.836705	-410.064826
15	-751.6936484	0.129494	-751.5641544	-751.6936484
16	-629.1823979	0.146249	-629.0361489	-629.1823979
17	-370.7569384	0.199456	-370.5574824	-370.7569384
18	-562.4795654	0.256625	-562.2229404	-562.4795654
19	-423.7310196	0.172406	-423.5586136	-423.7310196
20	-430.7552445	0.164589	-430.5906555	-430.7552445
21	-668.5294217	0.179468	-668.3499537	-668.5294217
22	-1044.839779	0.214899	-1044.62488	-1044.839779
23	-1128.068377	0.167155	-1127.901222	-1128.068377
24	-822.1177331	0.227243	-821.8904901	-822.1177331
25	-838.1543186	0.215504	-837.9388146	-838.1543186

26	-1044.840359	0.21512	-1044.625239	-1044.840359
27	-1319.787904	0.224212	-1319.563692	-1319.787904
28	-1128.08193	0.169244	-1127.912686	-1128.08193
29	-1188.067982	0.132204	-1187.935778	-1188.067982
30	-1029.872723	0.27262	-1029.600103	-1029.872723
31	-1181.037587	0.139782	-1180.897805	-1181.037587
32	-1167.392145	0.198878	-1167.193267	-1167.392145
33	-1425.904252	0.147078	-1425.757174	-1425.904252
34	-1617.640958	0.204263	-1617.436695	-1617.640958
35	-1013.935272	0.28434	-1013.650932	-1013.935272
36	-1319.894423	0.226426	-1319.667997	-1319.894423
37	-1167.455491	0.199059	-1167.256432	-1167.455491
38	-487.5290694	0.26617	-487.2628994	-487.5290694
39	-410.1025842	0.226806	-409.8757782	-410.1025842
40	-488.7253284	0.287122	-488.4382064	-488.7253284
41	-501.1713726	0.207028	-500.9643446	-501.1713726
42	-714.9453403	0.280258	-714.6650823	-714.9453403
43	-410.1012271	0.22933	-409.8718971	-410.1012271
44	-579.7890005	0.267219	-579.5217815	-579.7890005
adamantyl substituted	-1031.856245	0.503827	-1031.352418	-1031.284969

Radicals	***E***	***G*corr**	***G***	***H***
1'	-330.817629	0.158856	-330.658773	-330.817629
2'	-409.4371046	0.217406	-409.2196986	-409.4371046
3'	-370.1276031	0.18805	-369.9395531	-370.1276031
4'	-790.4094586	0.150532	-790.2589266	-790.4094586
5'	-1249.99999	0.142277	-1249.857713	-1249.99999
6'	-667.8632757	0.166803	-667.6964727	-667.8632757

7'	-1004.896138	0.174843	-1004.721295	-1004.896138
8'	-484.4483448	0.208684	-484.2396608	-484.4483448
9'	-500.4889555	0.196939	-500.2920165	-500.4889555
10'	-721.4623565	0.412682	-721.0496745	-721.4623565
11'	-526.1395717	0.284712	-525.8548597	-526.1395717
12'	-448.7323341	0.246925	-448.4854091	-448.7323341
13'	-488.04366	0.27646	-487.7672	-488.04366
14'	-409.4306006	0.217542	-409.2130586	-409.4306006
15'	-751.0624467	0.119133	-750.9433137	-751.0624467
16'	-628.5554938	0.136553	-628.4189408	-628.5554938
17'	-370.1263778	0.18786	-369.9385178	-370.1263778
18'	-561.8478206	0.246237	-561.6015836	-561.8478206
19'	-423.0982028	0.161805	-422.9363978	-423.0982028
20'	-430.122103	0.15379	-429.968313	-430.122103
21'	-667.8852167	0.168425	-667.7167917	-667.8852167
22'	-1044.21627	0.203979	-1044.012291	-1044.21627
23'	-1127.448413	0.158528	-1127.289885	-1127.448413
24'	-821.4962447	0.216711	-821.2795337	-821.4962447
25'	-837.5363692	0.204999	-837.3313702	-837.5363692
26'	-1044.215159	0.204439	-1044.01072	-1044.215159
27'	-1319.167213	0.215742	-1318.951471	-1319.167213
28'	-1127.456731	0.158489	-1127.298242	-1127.456731
29'	-1187.445107	0.123559	-1187.321548	-1187.445107
30'	-1029.253303	0.262346	-1028.990957	-1029.253303
31'	-1180.411244	0.13098	-1180.280264	-1180.411244
32'	-1166.765883	0.188146	-1166.577737	-1166.765883
33'	-1425.286545	0.136408	-1425.150137	-1425.286545
34'	-1617.017903	0.193452	-1616.824451	-1617.017903
35'	-1013.311602	0.274015	-1013.037587	-1013.311602

36'	-1319.267135	0.215831	-1319.051304	-1319.267135
37'	-1166.828855	0.188867	-1166.639988	-1166.828855
38'	-486.894907	0.255767	-486.63914	-486.894907
39'	-409.4681411	0.218156	-409.2499851	-409.4681411
40'	-488.0910519	0.277548	-487.8135039	-488.0910519
41'	-500.5434864	0.195753	-500.3477334	-500.5434864
42'	-714.3110945	0.269765	-714.0413295	-714.3110945
43'	-409.4672679	0.219106	-409.2481619	-409.4672679
44'	-579.1640253	0.256866	-578.9071593	-579.1640253
adamantyl substituted	-1031.221911	0.492997	-1030.728914	-1030.660773

Compounds	***E***	***G*corr**	***G***
TS1	-542.1902439	0.263624	-541.9266199
TS2	-620.8177018	0.322427	-620.4952748
TS3	-581.5042865	0.293156	-581.2111305
TS4	-1001.791743	0.255502	-1001.536241
TS5	-1461.390679	0.247331	-1461.143348
TS6	-879.2654794	0.271618	-878.9938614
TS7	-1216.328423	0.279711	-1216.048712
TS8	-695.8329586	0.313225	-695.5197336
TS9	-711.8717109	0.301507	-711.5702039
TS10	-932.8724151	0.517732	-932.3546831
TS11	-737.5314521	0.390754	-737.1406981
TS12	-660.1169515	0.352035	-659.7649165
TS13	-699.4323618	0.381701	-699.0506608
TS14	-620.811828	0.322843	-620.488985
TS15	-962.4412761	0.22489	-962.2163861
TS16	-839.9531594	0.241258	-839.7119014

TS17	-581.5027403	0.293826	-581.2089143
TS18	-773.2421774	0.350664	-772.8915134
TS19	-634.4762449	0.266325	-634.2099199
TS20	-641.5017697	0.259019	-641.2427507
TS21	-879.2907716	0.273516	-879.0172556
TS22	-1255.646582	0.30887	-1255.337712
TS23	-1338.85717	0.263199	-1338.593971
TS24	-1032.905621	0.321355	-1032.584266
TS25	-1048.943588	0.309682	-1048.633906
TS26	-1255.647614	0.309486	-1255.338128
TS27	-1530.5959	0.320101	-1530.275799
TS28	-1338.86391	0.263481	-1338.600429
TS29	-1398.855969	0.228203	-1398.627766
TS30	-1240.681997	0.366541	-1240.315456
TS31	-1391.827736	0.235697	-1391.592039
TS32	-1378.177228	0.293099	-1377.884129
TS33	-1636.612215	0.240909	-1636.371306
TS34	-1828.346998	0.297836	-1828.049162

Table S3. The predicted B–H bond dissociation energies (kcal/mol) of the selected NHC-boranes **1**–**21** in different solvents at the M06-2X/cc-PVTZ/SMD level.

Species	DMSO	DMF	Acetonitrile	THF	Toluene
1	80.97961	80.81839	80.03579	79.94931	78.13082
2	81.15017	80.99049	80.30382	80.21523	78.44274
3	81.17992	81.01844	80.22072	80.24018	78.04549
4	81.82554	81.67018	80.87669	80.24303	78.54716
5	79.71592	79.55608	78.86172	78.68985	77.01033
6	80.85182	80.68376	79.80934	79.72488	77.81047
7	79.98766	79.82225	78.78892	78.39445	77.30609
8	78.56058	78.40522	77.60228	77.60697	75.9215
9	76.87493	76.71449	75.89629	75.87001	73.65717
10	81.21585	81.07852	81.04093	81.01279	79.67732
11	81.77726	81.63729	80.49098	80.37343	78.87382
12	80.24133	80.21391	79.54944	79.98775	78.76767
13	81.99168	82.46352	81.094	81.00727	79.3204
14	81.44852	81.31321	80.48453	80.3776	78.662
15	79.11504	79.54263	78.72395	78.55014	77.01608
16	77.67585	77.50557	76.44447	76.32201	74.69371
17	78.49439	78.32508	77.54666	76.09204	75.67786
18	79.44928	79.29512	79.04781	78.7633	77.16883
19	79.99961	79.86853	79.58684	79.47034	78.46889
20	80.11208	79.92953	79.66631	78.79309	76.49023
21	86.94107	86.78445	86.45568	86.15665	84.93203

Table S4. The calculated absolute electronic energies (*E*, in a.u.), thermal free energies (*G*, in a.u.) calculated at the G4(MP2)-6X level.

Boranes	***G***	***H***
1	-331.0017148	-330.9620706
2	-409.5057556	-409.4590319
3	-370.2542208	-370.2102626
4	-790.1785104	-790.1356169
5	-1249.355713	-1249.309213
6	-667.822797	-667.7748975
7	-1004.630845	-1004.576921
8	-484.4244742	-484.3789427
9	-500.4635497	-500.4181297
10	-721.0660751	-721.003719
11	-526.035967	-525.9817261
12	-448.7433418	-448.6934949
13	-487.9948687	-487.943056
14	-409.4986129	-409.4528332
15	-750.8896192	-750.8486894
16	-628.5714305	-628.5259495
17	-370.2499075	-370.2068549
18	-561.7163228	-561.6627953
19	-423.1852834	-423.1416183
20	-430.2445127	-430.2022848
21	-667.8503866	-667.8022771
22	-1043.88453	-1043.825646
23	-1126.98226	-1126.930606
24	-821.2423907	-821.1870091
25	-837.2794861	-837.2247034
26	-1043.8881	-1043.826235

27	-1318.447513	-1318.38677
28	-1126.997717	-1126.946439
29	-1186.981602	-1186.932245
30	-1028.74018	-1028.679063
31	-1179.915728	-1179.863279
32	-1166.246932	-1166.191442
33	-1424.55279	-1424.494833
34	-1616.011718	-1615.948763

Radicals	***G***	***H***
1'	-330.3792664	-330.3392122
2'	-408.8816087	-408.8337823
3'	-369.6305538	-369.586746
4'	-789.5565693	-789.5131855
5'	-1248.734861	-1248.68757
6'	-667.2029982	-667.1549641
7'	-1004.016518	-1003.959527
8'	-483.8060757	-483.7597559
9'	-499.8463932	-499.8005881
10'	-720.4458065	-720.3792884
11'	-525.4120809	-525.3586131
12'	-448.1195113	-448.0692437
13'	-487.3709521	-487.3168194
14'	-408.8762524	-408.8275324
15'	-750.2707607	-750.2288117
16'	-627.9550784	-627.9076048
17'	-369.616722	-369.571032
18'	-561.066408	-561.0121097
19'	-422.5603968	-422.5158651
20'	-429.6283658	-429.5865481

21'	-667.2165594	-667.1642759
22'	-1043.272745	-1043.211846
23'	-1126.373279	-1126.321628
24'	-820.6284189	-820.5746871
25'	-836.6698232	-836.6138988
26'	-1043.272458	-1043.212947
27'	-1317.836592	-1317.773419
28'	-1126.383028	-1126.329648
29'	-1186.3733	-1186.32187
30'	-1028.130868	-1028.067485
31'	-1179.298353	-1179.244766
32'	-1165.632282	-1165.576896
33'	-1423.947209	-1423.890757
34'	-1615.404394	-1615.337801

Table S5. The one-electron energies of the frontier molecular orbitals α-HOMO and β-LUMO of all the studied radicals at the M06-2X/cc-PVTZ level.

	$E_{\alpha\text{-HOMO}}$	$E_{\beta\text{-LUMO}}$	μ	η	ω	N	spin density
1'	-4.67032	-0.54353	-2.60692	4.126789	0.823406	11.09264	0.53254
2'	-4.50011	-0.45424	-2.47717	4.045864	0.758354	11.26285	0.533679
3'	-4.58003	-0.49302	-2.53653	4.087009	0.787125	11.18293	0.532859
4'	-4.90717	-0.76628	-2.83672	4.140898	0.97165	10.85579	0.512517
5'	-5.09798	-0.95332	-3.02565	4.14466	1.104381	10.66498	0.49595
6'	-5.2103	-1.01876	-3.11453	4.191542	1.157128	10.55266	0.494343
7'	-5.56957	-1.28456	-3.42706	4.285009	1.370447	10.19339	0.482493
8'	-5.05588	-1.14006	-3.09797	3.915819	1.225464	10.70709	0.472445
9'	-5.42079	-1.45223	-3.43651	3.968554	1.487895	10.34218	0.45058
10'	-4.46858	-0.27938	-2.37398	4.189198	0.672656	11.29438	0.557382
11'	-4.56851	-0.41078	-2.48965	4.157729	0.745401	11.19445	0.543787
12'	-4.59251	-0.42924	-2.51087	4.163273	0.757154	11.17045	0.536291
13'	-4.55907	-0.37252	-2.46579	4.186549	0.726152	11.20389	0.555259
14'	-4.6123	-0.45808	-2.53519	4.154229	0.773571	11.15066	0.543461
15'	-5.02081	-0.77242	-2.89661	4.248386	0.987478	10.74215	0.488996
16'	-5.40936	-1.10614	-3.25775	4.30322	1.233135	10.35361	0.431557
17'	-4.42211	-0.25316	-2.33763	4.168944	0.655385	11.34086	0.472034
18'	-4.55213	-0.66222	-2.60717	3.889907	0.873717	11.21083	0.497665
19'	-5.33902	-1.24029	-3.28966	4.098731	1.320145	10.42394	0.556393
20'	-4.50306	-0.29954	-2.4013	4.203521	0.685881	11.2599	0.407749
21'	-5.32395	-1.07272	-3.19834	4.251237	1.203103	10.43901	0.571789
22'	-5.65623	-1.27119	-3.46371	4.385043	1.367979	10.10673	0.323735
23'	-5.52563	-1.18414	-3.35488	4.341489	1.296243	10.23733	0.320124
24'	-5.48387	-1.38787	-3.43587	4.095994	1.441068	10.27909	0.332974
25'	-5.82672	-1.68645	-3.75658	4.140273	1.704226	9.93624	0.314925
26'	-5.50223	-1.09739	-3.29981	4.404837	1.235998	10.26073	0.351381
27'	-5.42841	-1.35903	-3.39372	4.069379	1.41512	10.33455	0.36173
28'	-5.42755	-1.09124	-3.25939	4.336313	1.224961	10.33541	0.339642
29'	-5.62578	-1.24099	-3.43338	4.384788	1.344205	10.13719	0.270212
30'	-5.76268	-1.81683	-3.78975	3.94585	1.819915	10.00028	0.333091
31'	-6.12152	-1.96223	-4.04187	4.159291	1.963883	9.641443	0.46203
32'	-5.29731	-1.00095	-3.14913	4.296356	1.154118	10.46566	0.34033
33'	-6.18149	-1.67381	-3.92765	4.507678	1.71113	9.58147	0.269804
34'	-6.06048	-1.74781	-3.90415	4.312673	1.767158	9.702478	0.281907
35'	-5.44808	-1.54754	-3.49781	3.900541	1.568331	10.31488	0.352577
36'	-5.41366	-1.30968	-3.36167	4.103985	1.376812	10.3493	0.375534
37'	-5.42326	-1.10064	-3.26195	4.322619	1.230769	10.33971	0.362449
38'	-4.47281	-0.43347	-2.45314	4.03934	0.74491	11.29015	0.530103
39'	-4.5971	-0.49199	-2.54454	4.105104	0.788616	11.16587	0.536767

40'	-4.4833	-0.43996	-2.46163	4.04334	0.749335	11.27966	0.535302
41'	-5.29676	-1.43713	-3.36694	3.859635	1.468572	10.4662	0.439415
42'	-4.82652	-0.78981	-2.80817	4.036711	0.976761	10.93644	0.470973
43'	-4.49711	-0.35901	-2.42806	4.138104	0.712341	11.26585	0.490017
44'	-5.1042	-1.28992	-3.19706	3.814274	1.339862	10.65876	0.374578

Table S6. Cartesian coordinates of all the studied molecules.

Structure----------

1

C	0.009649000	0.589902000	-0.000088000
C	-0.725915000	-1.542463000	0.000061000
C	0.634541000	-1.578900000	0.000008000
H	-1.459558000	-2.332961000	0.000104000
H	1.325784000	-2.406822000	-0.000034000
N	-1.089546000	-0.204431000	-0.000010000
B	0.095468000	2.188127000	0.000040000
H	0.717942000	2.547822000	0.992563000
H	0.718193000	2.548037000	-0.992276000
H	-1.019284000	2.674010000	-0.000041000
N	1.065145000	-0.262712000	-0.000103000
C	2.461753000	0.160927000	0.000038000
H	2.670378000	0.758175000	-0.890129000
H	2.670606000	0.756992000	0.890952000
H	3.092170000	-0.727960000	-0.000631000
C	-2.473490000	0.267567000	-0.000002000
H	-2.666987000	0.867037000	0.890965000
H	-2.667053000	0.866873000	-0.891067000
H	-3.127950000	-0.604031000	0.000082000

END----------

Structure----------

2

C	0.321057000	1.153033000	-0.009992000
C	-0.927093000	-0.744412000	0.001232000
C	0.386900000	-1.118151000	-0.004680000
N	-0.939846000	0.653889000	-0.002901000
B	0.817414000	2.681780000	0.005615000
H	1.480825000	2.870466000	1.019437000
H	1.537017000	2.879328000	-0.966695000
H	-0.124533000	3.450113000	-0.018439000
N	1.129256000	0.063777000	-0.016458000
C	2.586345000	0.108107000	0.009527000
H	2.987981000	-0.589330000	-0.727977000
H	2.912639000	1.116485000	-0.235112000
H	2.956544000	-0.163389000	1.002363000
C	-2.175326000	1.429762000	-0.000954000
H	-1.926889000	2.487597000	-0.007822000
H	-2.766318000	1.187325000	-0.887698000
H	-2.757516000	1.196899000	0.894150000
C	1.026569000	-2.463181000	-0.001257000

H 0.261391000 -3.240519000 0.049645000
H 1.619834000 -2.629425000 -0.908016000
H 1.695019000 -2.586180000 0.858574000
C -2.179379000 -1.550807000 0.007459000
H -2.793126000 -1.332879000 0.889107000
H -2.791504000 -1.349441000 -0.879332000
H -1.938746000 -2.615713000 0.017242000
END----------

Structure----------
3
C -0.721450000 0.635285000 -0.009514000
C -0.018796000 -1.508644000 0.003250000
C 1.097316000 -0.728338000 -0.003602000
N -1.118267000 -0.659840000 -0.001552000
B -1.606002000 1.975853000 0.003549000
H -1.322465000 2.624808000 1.003601000
H -1.327590000 2.647152000 -0.982897000
H -2.793590000 1.714874000 0.002616000
N 0.638239000 0.587438000 -0.016679000
C 1.511636000 1.755323000 0.006951000
H 2.319155000 1.622769000 -0.715294000
H 0.930667000 2.634964000 -0.261416000
H 1.936773000 1.890122000 1.005596000
C -2.491649000 -1.155593000 0.003737000
H -3.175272000 -0.311025000 -0.022947000
H -2.653836000 -1.787748000 -0.872683000
H -2.665747000 -1.740517000 0.910385000
C 2.542115000 -1.086767000 0.002572000
H 2.649183000 -2.173255000 0.038564000
H 3.050390000 -0.720439000 -0.896582000
H 3.055722000 -0.660003000 0.871389000
H -0.128218000 -2.581742000 0.009174000
END----------

Structure----------
4
C -1.141135000 0.552602000 -0.000022000
C -0.053002000 -1.430777000 0.000004000
C 0.875091000 -0.439420000 -0.000006000
N -1.284421000 -0.796184000 -0.000004000
B -2.264821000 1.700966000 -0.000008000
H -2.109705000 2.397487000 0.994507000
H -2.109006000 2.398217000 -0.993892000

H -3.377863000 1.215571000 -0.000572000
N 0.203562000 0.772059000 -0.000016000
C 0.849163000 2.082073000 0.000004000
H 1.468008000 2.189632000 -0.893500000
H 0.074022000 2.843944000 0.000034000
H 1.468035000 2.189587000 0.893494000
C -2.541914000 -1.543342000 0.000024000
H -3.369983000 -0.839918000 0.000102000
H -2.588704000 -2.171073000 -0.892651000
H -2.588604000 -2.171154000 0.892647000
Cl 2.590719000 -0.541852000 -0.000002000
H 0.052474000 -2.503577000 0.000022000
END----------

Structure----------
5
C -1.584169000 -0.247773000 -0.000006000
C 0.639841000 -0.595035000 0.000000000
C 0.434423000 0.749891000 0.000004000
N -0.609873000 -1.196582000 0.000004000
B -3.180212000 -0.434256000 -0.000014000
H -3.631693000 0.116029000 0.994328000
H -3.631717000 0.116521000 -0.994059000
H -3.475697000 -1.610771000 -0.000274000
N -0.935467000 0.947770000 -0.000002000
C -1.580182000 2.259972000 0.000031000
H -1.287619000 2.813988000 -0.894274000
H -2.655985000 2.107416000 0.000076000
H -1.287559000 2.813963000 0.894334000
C -0.803519000 -2.647006000 -0.000020000
H -1.871138000 -2.845607000 0.000065000
H -0.347143000 -3.076492000 -0.893992000
H -0.346990000 -3.076539000 0.893850000
Cl 1.573837000 2.025017000 -0.000023000
Cl 2.109435000 -1.470066000 0.000019000
END----------

Structure----------
6
C 1.711550000 0.469465000 0.000064000
C 0.403529000 -1.363948000 -0.000081000
C -0.410135000 -0.270646000 -0.000011000
N 1.694790000 -0.890563000 0.000006000
B 2.973298000 1.450467000 0.000148000

H	2.906005000	2.164092000	-0.992104000
H	2.906082000	2.163813000	0.992607000
H	4.003932000	0.808526000	0.000024000
N	0.411842000	0.851402000	0.000012000
C	-0.003120000	2.255995000	0.000007000
H	0.390530000	2.747434000	0.891195000
H	0.390120000	2.747338000	-0.891418000
H	-1.087840000	2.323267000	0.000259000
C	2.881010000	-1.749830000	0.000043000
H	3.478422000	-1.556872000	-0.891706000
H	3.478184000	-1.557137000	0.892012000
H	2.544755000	-2.786020000	-0.000157000
C	-1.892089000	-0.239326000	-0.000037000
F	-2.409123000	0.400255000	1.086640000
F	-2.409059000	0.400554000	-1.086566000
F	-2.397301000	-1.492568000	-0.000223000
H	0.171774000	-2.417083000	-0.000146000

END----------

Structure----------

7

C	-0.086914000	2.089489000	0.000009000
C	0.693161000	-0.024366000	0.000005000
C	-0.679402000	-0.085674000	-0.000012000
N	1.029480000	1.323233000	0.000013000
B	-0.207012000	3.682978000	0.000017000
H	-0.844415000	4.007581000	-0.990980000
H	-0.844446000	4.007570000	0.990997000
H	0.889764000	4.196203000	0.000040000
N	-1.131025000	1.225668000	-0.000002000
C	-2.520772000	1.703317000	0.000012000
H	-2.681594000	2.310222000	0.891696000
H	-2.681721000	2.309977000	-0.891816000
H	-3.211498000	0.867474000	0.000181000
C	2.383423000	1.902518000	0.000018000
H	2.505058000	2.515496000	-0.892445000
H	2.505231000	2.515138000	0.892707000
H	3.128651000	1.115079000	-0.000221000
C	-1.672091000	-1.211065000	-0.000113000
C	1.777615000	-1.062310000	0.000098000
F	-2.482851000	-1.139809000	1.090154000
F	-2.483378000	-1.139111000	-1.089942000
F	-1.123247000	-2.431457000	-0.000650000
F	1.331036000	-2.323723000	0.000598000

F 2.580033000 -0.925570000 1.090299000
F 2.579599000 -0.926263000 -1.090508000
END----------

Structure----------
8
C -0.491033000 -0.706803000 -0.006434000
C -0.516954000 0.696056000 -0.002377000
C -1.716487000 1.408152000 0.001996000
C -2.893825000 0.656292000 0.004555000
C -2.867917000 -0.752633000 0.003111000
C -1.664408000 -1.461689000 -0.001927000
C 1.644730000 0.036805000 -0.005669000
H -1.733910000 2.492428000 0.004001000
H -3.850203000 1.169582000 0.008744000
H -3.804966000 -1.300501000 0.006962000
H -1.642433000 -2.545884000 -0.000807000
C 1.193836000 2.520229000 -0.000477000
H 0.793531000 3.007547000 -0.893296000
H 0.788404000 3.006557000 0.890524000
H 2.277752000 2.594456000 0.002666000
C 1.317906000 -2.449638000 0.005987000
H 1.139574000 -2.890776000 0.990853000
H 0.777468000 -3.021961000 -0.751258000
H 2.382112000 -2.468813000 -0.216533000
N 0.812800000 1.112582000 -0.002070000
N 0.852142000 -1.068932000 -0.014346000
B 3.247628000 0.008966000 0.008396000
H 3.607576000 -0.593948000 1.010341000
H 3.629405000 -0.611581000 -0.974230000
H 3.707874000 1.131894000 0.002384000
END----------

Structure----------
9
C -0.494428000 -0.704572000 -0.009478000
C -0.528591000 0.696620000 -0.002724000
C -1.747710000 1.369641000 0.003461000
C -2.881732000 0.556775000 0.006318000
C -1.682380000 -1.432584000 -0.002929000
C 1.630550000 0.047801000 -0.008290000
H -1.824586000 2.450461000 0.007191000
H -3.867000000 1.013982000 0.011894000
H -1.691009000 -2.518332000 -0.001672000

C	1.165642000	2.534271000	0.000063000
H	0.763743000	3.018478000	-0.893241000
H	0.758167000	3.016219000	0.892034000
H	2.249350000	2.610314000	0.003584000
C	1.334601000	-2.438014000	0.010513000
H	1.351614000	-2.807637000	1.039453000
H	0.671419000	-3.061198000	-0.591143000
H	2.338556000	-2.468944000	-0.407711000
N	0.789916000	1.123210000	-0.002520000
N	0.848212000	-1.062718000	-0.021298000
B	3.230637000	0.027000000	0.010050000
H	3.582605000	-0.591796000	1.004212000
H	3.610625000	-0.584049000	-0.978464000
H	3.688084000	1.149923000	0.019526000
N	-2.861052000	-0.795071000	0.004173000

END----------

Structure----------

10

C	-0.003160000	-0.153787000	0.552249000
C	0.691154000	0.432389000	-1.514073000
C	-0.667032000	0.423701000	-1.527429000
H	1.402896000	0.653951000	-2.292244000
H	-1.366881000	0.640459000	-2.317863000
N	1.083819000	0.079562000	-0.229506000
B	-0.071659000	-0.597663000	2.097247000
H	-0.696466000	-1.647845000	2.178497000
H	1.042942000	-0.747946000	2.557898000
H	-0.670893000	0.261711000	2.732184000
N	-1.076055000	0.061763000	-0.253302000
C	2.492981000	-0.025791000	0.187134000
C	3.170862000	-1.245591000	-0.474226000
C	3.266948000	1.263302000	-0.103185000
H	2.457871000	-0.170507000	1.265643000
C	4.705360000	-1.079501000	-0.531893000
H	2.774188000	-1.375686000	-1.486849000
H	2.901801000	-2.143066000	0.094340000
C	4.653055000	1.201320000	0.578748000
H	3.383914000	1.379144000	-1.186841000
H	2.699379000	2.128456000	0.254742000
C	5.212229000	-0.239798000	0.646690000
H	4.988840000	-0.583359000	-1.468858000
H	5.183112000	-2.065075000	-0.542394000
H	4.582340000	1.613247000	1.591964000

H 5.346238000 1.843377000 0.023634000
H 4.897676000 -0.718527000 1.583245000
H 6.307432000 -0.216123000 0.661110000
C -2.482147000 -0.058850000 0.164067000
C -3.168936000 1.324279000 0.185905000
C -3.250851000 -1.046317000 -0.718642000
H -2.442569000 -0.461246000 1.175985000
C -4.703409000 1.198175000 0.061147000
H -2.780263000 1.933500000 -0.637095000
H -2.898329000 1.832736000 1.117980000
C -4.637174000 -1.332926000 -0.096942000
H -3.365014000 -0.617199000 -1.720927000
H -2.677785000 -1.972801000 -0.827423000
C -5.199894000 -0.116124000 0.675046000
H -4.991937000 1.226275000 -0.997363000
H -5.184332000 2.058056000 0.539711000
H -4.565362000 -2.192329000 0.579436000
H -5.329187000 -1.617239000 -0.897695000
H -4.880667000 -0.159595000 1.724543000
H -6.294901000 -0.150212000 0.680476000
END----------

Structure----------
11
C -1.635719000 0.625083000 0.003696000
C -1.046663000 -1.553136000 -0.058403000
C -2.405088000 -1.494746000 -0.045103000
H -0.376362000 -2.396573000 -0.084896000
H -3.151079000 -2.273582000 -0.060807000
N -0.593015000 -0.243147000 -0.031286000
B -1.555415000 2.227706000 0.046515000
H -2.670229000 2.694306000 0.185071000
H -0.837308000 2.570888000 0.976073000
H -1.060974000 2.633303000 -0.999552000
N -2.748335000 -0.152013000 -0.006710000
C -4.126836000 0.335449000 0.015405000
H -4.312623000 0.902697000 0.928806000
H -4.316938000 0.969638000 -0.851821000
H -4.790191000 -0.528986000 -0.015545000
C 0.824882000 0.151812000 -0.028002000
C 1.488142000 -0.198436000 1.322007000
C 1.591079000 -0.469953000 -1.198954000
H 0.814867000 1.234073000 -0.159632000
C 3.021363000 -0.325985000 1.185017000

H 1.070089000 -1.140082000 1.693968000
H 1.228878000 0.578825000 2.049400000
C 2.993257000 0.173258000 -1.302398000
H 1.680902000 -1.550433000 -1.036580000
H 1.031828000 -0.327880000 -2.129338000
C 3.553018000 0.591771000 0.077862000
H 3.286125000 -1.363265000 0.943499000
H 3.497909000 -0.096260000 2.144078000
H 2.947015000 1.050067000 -1.958369000
H 3.673417000 -0.542416000 -1.777817000
H 3.258308000 1.625110000 0.302681000
H 4.648278000 0.577468000 0.057408000
END----------

Structure----------
12
C 0.852873000 0.525812000 0.000083000
C 0.243526000 -1.646229000 0.000051000
C 1.600764000 -1.605239000 -0.000001000
H -0.415943000 -2.494986000 0.000059000
H 2.335783000 -2.394629000 -0.000045000
N -0.209831000 -0.330855000 0.000069000
B 0.984463000 2.131649000 0.000052000
H 1.631726000 2.450362000 -0.991660000
H -0.078876000 2.704496000 0.001195000
N 1.954841000 -0.270209000 0.000016000
C 3.331777000 0.213519000 -0.000052000
H 3.516839000 0.819049000 -0.889515000
H 3.517296000 0.818078000 0.889981000
H 3.996417000 -0.650268000 -0.000695000
C -1.666984000 0.052644000 -0.000003000
C -1.969296000 0.849946000 1.276440000
H -1.395977000 1.775733000 1.321309000
H -3.034344000 1.100499000 1.298485000
H -1.738501000 0.247137000 2.160925000
C -1.968975000 0.850700000 -1.276046000
H -3.034019000 1.101254000 -1.298184000
H -1.395661000 1.776523000 -1.320249000
H -1.737975000 0.248418000 -2.160835000
C -2.529799000 -1.215454000 -0.000507000
H -2.361644000 -1.826030000 -0.892603000
H -2.362084000 -1.826481000 0.891365000
H -3.577498000 -0.904286000 -0.000674000
H 1.633746000 2.450142000 0.990499000

END----------

Structure----------

13

C	0.002823000	0.706094000	-0.076241000
C	-0.698259000	-1.430488000	0.116096000
C	0.659845000	-1.446261000	0.107611000
H	-1.413119000	-2.233521000	0.191437000
H	1.356667000	-2.265820000	0.175466000
N	-1.086198000	-0.102215000	0.001928000
B	0.078194000	2.308605000	-0.202844000
H	0.715835000	2.747793000	0.746117000
H	0.669516000	2.599369000	-1.235487000
H	-1.033656000	2.799820000	-0.212292000
N	1.072853000	-0.128819000	-0.013388000
C	2.487005000	0.300394000	-0.046668000
H	2.451876000	1.376879000	-0.211640000
C	-2.501476000	0.328296000	-0.030886000
H	-2.465477000	1.411046000	-0.139060000
C	-3.188012000	-0.021952000	1.289114000
H	-4.210126000	0.369040000	1.282540000
H	-3.239986000	-1.105866000	1.436920000
H	-2.653033000	0.421137000	2.134980000
C	-3.207627000	-0.274420000	-1.245332000
H	-3.269332000	-1.365290000	-1.171059000
H	-4.226799000	0.119545000	-1.305383000
H	-2.681122000	-0.015720000	-2.169383000
C	3.151069000	0.019822000	1.301314000
H	3.190834000	-1.055578000	1.505538000
H	4.176004000	0.403286000	1.291461000
H	2.604918000	0.510398000	2.112974000
C	3.214072000	-0.360986000	-1.216955000
H	2.699369000	-0.156044000	-2.160866000
H	4.231434000	0.036389000	-1.283366000
H	3.282005000	-1.445643000	-1.082777000

END----------

Structure----------

14

C	-0.735410000	0.605915000	-0.008703000
C	0.121123000	-1.482219000	0.003017000
C	-1.233632000	-1.596036000	0.007499000
H	0.893302000	-2.233961000	0.006234000
H	-1.876062000	-2.462475000	0.014661000

N 0.409195000 -0.124096000 -0.006915000
B -0.957982000 2.194334000 -0.015060000
H -1.550867000 2.506611000 1.011514000
H 0.096744000 2.794239000 -0.086294000
N -1.740675000 -0.307715000 0.000527000
C -3.161121000 0.027276000 0.002770000
H -3.400191000 0.635211000 0.877778000
H -3.416706000 0.582999000 -0.901946000
H -3.732611000 -0.899945000 0.035596000
C 1.785515000 0.418359000 -0.004893000
C 2.506480000 0.014649000 1.281079000
H 3.492446000 0.488659000 1.309371000
H 1.941652000 0.336826000 2.161503000
H 2.649142000 -1.069909000 1.333816000
C 2.527249000 -0.024296000 -1.265809000
H 2.672887000 -1.109593000 -1.282736000
H 1.976251000 0.269303000 -2.164811000
H 3.512791000 0.450612000 -1.292908000
H -1.671289000 2.480294000 -0.969025000
H 1.661568000 1.500238000 -0.022498000
END----------

Structure----------
15
C -0.301229000 0.591293000 -0.000011000
C -1.109809000 -1.524613000 -0.000001000
C 0.243899000 -1.635627000 -0.000001000
H -1.876197000 -2.283766000 -0.000001000
H 0.903626000 -2.487900000 -0.000015000
N -1.418516000 -0.171308000 0.000005000
B -0.153069000 2.182636000 0.000020000
H 0.479176000 2.509921000 0.994234000
H 0.479516000 2.509947000 -0.993964000
H -1.252786000 2.696341000 -0.000159000
N 0.706510000 -0.325589000 -0.000030000
C -2.787512000 0.350448000 0.000019000
H -2.955965000 0.954776000 0.892105000
H -2.955998000 0.954735000 -0.892089000
H -3.467945000 -0.500716000 0.000051000
Cl 2.360227000 0.089574000 -0.000007000
END----------

Structure----------
16

C -0.807218000 0.562700000 -0.000078000
C -1.598150000 -1.557422000 -0.000088000
C -0.250397000 -1.661285000 -0.000102000
H -2.362019000 -2.318633000 -0.000109000
H 0.400787000 -2.518764000 -0.000128000
N -1.913156000 -0.202661000 -0.000102000
B -0.720383000 2.163660000 -0.000072000
H -0.108699000 2.521881000 0.992403000
H -0.110444000 2.521994000 -0.993582000
H -1.843452000 2.620120000 0.000935000
N 0.227689000 -0.345606000 -0.000099000
C 1.613461000 0.003849000 0.000110000
C -3.289913000 0.301516000 -0.000182000
H -3.464905000 0.903301000 0.891895000
H -3.464797000 0.903317000 -0.892269000
H -3.958255000 -0.558760000 -0.000231000
F 2.360854000 -1.111805000 -0.000634000
F 1.947680000 0.724570000 1.085840000
F 1.947606000 0.726010000 -1.084663000
END----------

Structure----------
17
C -0.055902000 -0.261887000 0.012670000
C 1.011064000 1.730146000 -0.019560000
C 1.962617000 0.759476000 -0.023814000
H 1.090829000 2.805463000 -0.030625000
H 3.039449000 0.816689000 -0.039913000
N -0.218134000 1.087140000 0.002553000
B -1.118538000 -1.481212000 0.049345000
H -0.784702000 -2.230668000 -0.871738000
N 1.291164000 -0.450751000 -0.003601000
C 1.946577000 -1.754615000 0.004196000
H 1.639131000 -2.321701000 0.885066000
H 1.678911000 -2.315055000 -0.893961000
H 3.024559000 -1.595952000 0.029532000
C -1.490130000 1.811173000 0.032420000
H -2.099489000 1.543124000 -0.830112000
H -2.032673000 1.584736000 0.950665000
H -1.269201000 2.878003000 -0.000874000
H -0.873959000 -2.095620000 1.092796000
C -2.704132000 -1.114100000 -0.053766000
H -3.078904000 -0.498782000 0.775611000
H -2.980522000 -0.596730000 -0.983496000

H -3.292523000 -2.043330000 -0.035220000
END----------

Structure----------
18
C 1.323462000 0.033593000 0.509140000
C 3.172493000 -0.101229000 -0.774940000
C 2.695218000 1.169659000 -0.876138000
H 4.031919000 -0.577282000 -1.219700000
H 3.053209000 2.023852000 -1.428907000
N 2.315992000 -0.782117000 0.075807000
B 0.073136000 -0.318707000 1.459374000
H 0.039809000 0.505622000 2.365140000
H 0.255917000 -1.426580000 1.941021000
N 1.564216000 1.231704000 -0.080284000
C 0.708987000 2.407572000 0.051617000
H -0.163759000 2.313842000 -0.599167000
H 0.378839000 2.502071000 1.086137000
H 1.285413000 3.288394000 -0.231847000
C 2.480535000 -2.187323000 0.446805000
H 2.700095000 -2.274404000 1.512377000
H 1.571755000 -2.743872000 0.215473000
H 3.311631000 -2.592557000 -0.130110000
C -1.310529000 -0.275803000 0.610539000
C -2.479270000 0.323992000 1.118468000
C -1.411710000 -0.853304000 -0.672555000
C -3.681452000 0.342008000 0.400182000
H -2.447874000 0.793705000 2.099822000
C -2.603439000 -0.840480000 -1.404897000
H -0.534108000 -1.323545000 -1.113608000
C -3.749430000 -0.241379000 -0.869058000
H -4.561853000 0.815804000 0.828113000
H -2.639327000 -1.295721000 -2.391885000
H -4.677976000 -0.226756000 -1.433363000
END----------

Structure----------
19
C 0.115483000 -0.152303000 0.314914000
C 2.188390000 0.299228000 -0.428433000
C 1.518249000 1.481227000 -0.335402000
H 3.197576000 0.074685000 -0.735115000
H 1.823613000 2.493330000 -0.548602000
N 1.308355000 -0.691944000 -0.027704000

B -1.189736000 -0.916552000 0.857254000
H -1.527236000 -0.431177000 1.920243000
H -0.962668000 -2.096432000 0.987735000
N 0.249206000 1.181827000 0.126562000
C -0.812904000 2.164293000 0.333267000
H -1.489499000 2.173386000 -0.524602000
H -1.370700000 1.909528000 1.234781000
H -0.355855000 3.146704000 0.450697000
C 1.642398000 -2.116453000 0.023177000
H 1.612691000 -2.472742000 1.054067000
H 0.936917000 -2.686168000 -0.582542000
H 2.648603000 -2.240723000 -0.376118000
C -2.394022000 -0.740645000 -0.162676000
N -3.287607000 -0.618414000 -0.903985000
END----------

Structure----------
20
C 0.047470000 -0.283945000 0.001325000
C -0.709790000 1.834885000 -0.001386000
C -1.794152000 1.013264000 -0.001773000
H -0.629638000 2.910249000 -0.002225000
H -2.851636000 1.224962000 -0.003057000
N 0.412737000 1.019531000 0.000586000
B 0.939343000 -1.634176000 0.004863000
H 0.654669000 -2.273755000 1.012017000
N -1.307044000 -0.282843000 -0.000108000
C -2.132930000 -1.487634000 -0.000108000
H -1.924459000 -2.081676000 -0.892512000
H -1.920611000 -2.084152000 0.889711000
H -3.179886000 -1.186125000 0.002634000
C 1.783808000 1.535819000 0.002392000
H 2.312471000 1.196837000 0.893468000
H 2.314209000 1.198924000 -0.888427000
H 1.727947000 2.624048000 0.003629000
H 0.642236000 -2.287174000 -0.989868000
F 2.361299000 -1.322489000 -0.006193000
END----------

Structure----------
21
C -0.682003000 -0.021202000 0.445249000
C -2.682078000 -0.560607000 -0.435411000
C -2.595819000 0.798022000 -0.411827000

H	-3.467749000	-1.218783000	-0.770906000
H	-3.289095000	1.561828000	-0.726517000
N	-1.498462000	-1.044175000	0.091640000
B	0.777805000	-0.144212000	1.101431000
H	0.970294000	0.766449000	1.878476000
N	-1.363146000	1.108880000	0.133485000
C	-0.869871000	2.476644000	0.285002000
H	-0.115555000	2.500258000	1.069222000
H	-0.432938000	2.823130000	-0.654422000
H	-1.707099000	3.119950000	0.558746000
C	-1.194146000	-2.466331000	0.255935000
H	-0.256850000	-2.707694000	-0.245654000
H	-1.117046000	-2.713471000	1.316205000
H	-2.005293000	-3.037964000	-0.194118000
H	0.895793000	-1.217292000	1.649003000
C	1.928134000	-0.054429000	-0.033226000
F	1.947467000	1.125295000	-0.759349000
F	1.872068000	-1.038992000	-1.006338000
F	3.207406000	-0.157511000	0.477088000

END----------

Structure----------

22

C	1.460256000	0.295131000	-0.279239000
C	-0.275944000	1.741879000	-0.001658000
C	-0.801270000	0.482556000	0.029235000
N	1.094375000	1.588612000	-0.192715000
B	2.962893000	-0.254021000	-0.514079000
H	2.902572000	-1.393397000	-0.932875000
H	3.434660000	0.463118000	-1.387997000
N	0.293170000	-0.406796000	-0.119920000
C	0.271955000	-1.845689000	-0.077482000
C	2.018763000	2.722504000	-0.273470000
H	2.116159000	3.183621000	0.711292000
H	2.983897000	2.354986000	-0.609656000
H	1.631116000	3.449717000	-0.987665000
C	-2.241645000	0.091862000	0.085211000
F	-2.575940000	-0.787416000	-0.895349000
F	-2.610702000	-0.476922000	1.263426000
F	-3.037810000	1.170921000	-0.080801000
C	3.831855000	-0.146265000	0.871119000
H	3.887604000	0.877819000	1.266667000
H	3.425303000	-0.776114000	1.674803000
H	4.866024000	-0.476622000	0.700322000

F 0.445146000 -2.377436000 -1.301406000
F 1.233673000 -2.319625000 0.725706000
F -0.900308000 -2.283584000 0.398887000
C -0.879269000 3.096433000 0.123721000
H -1.899630000 3.044644000 0.494380000
H -0.288540000 3.701001000 0.817666000
H -0.881182000 3.604708000 -0.846909000
END----------

Structure----------
23
C 1.139942000 -0.052183000 -0.000086000
C 0.212504000 2.025748000 0.000112000
C -0.814358000 1.153731000 0.000179000
N 1.379633000 1.273321000 -0.000068000
B 2.165576000 -1.320811000 -0.000272000
H 1.854780000 -1.975028000 0.988267000
H 1.854505000 -1.974952000 -0.988777000
N -0.251013000 -0.135648000 0.000024000
C -1.075073000 -1.311748000 0.000025000
C 2.676275000 1.961129000 -0.000218000
H 3.479626000 1.238289000 -0.000241000
H 2.736646000 2.586567000 -0.892996000
H 2.736787000 2.586661000 0.892484000
Cl -2.494989000 1.487834000 0.000375000
H 0.219097000 3.104100000 0.000164000
C 3.770149000 -1.037753000 -0.000479000
H 4.144053000 -0.505970000 -0.886818000
H 4.144304000 -0.506117000 0.885843000
H 4.276180000 -2.014181000 -0.000630000
F -0.379626000 -2.438668000 -0.000197000
F -1.877904000 -1.315319000 -1.087603000
F -1.877583000 -1.315540000 1.087888000
END----------

Structure----------
24
C 0.990309000 -0.518892000 -0.017247000
C 1.421186000 0.811125000 0.070884000
C 2.766770000 1.164427000 -0.013131000
C 3.681120000 0.125356000 -0.180686000
C 3.253577000 -1.211689000 -0.259298000
C 1.903974000 -1.561884000 -0.180382000
C -0.833531000 0.861143000 0.277592000

H 3.082967000 2.199144000 0.050085000
H 4.739787000 0.353073000 -0.249874000
H 3.989104000 -1.999517000 -0.385657000
H 1.600113000 -2.596923000 -0.242412000
C 0.346454000 3.059206000 0.364567000
H 1.074955000 3.322095000 1.134051000
H 0.653463000 3.484960000 -0.593502000
H -0.634889000 3.433181000 0.642384000
C -1.322738000 -1.552398000 0.085834000
N 0.284402000 1.603516000 0.250040000
N -0.419052000 -0.447312000 0.101266000
B -2.338143000 1.424618000 0.429601000
H -3.064150000 0.522736000 0.798981000
H -2.291521000 2.283763000 1.300473000
F -2.325902000 -1.365222000 -0.789317000
F -1.871952000 -1.774350000 1.298317000
F -0.677916000 -2.673906000 -0.273778000
C -2.830419000 2.062144000 -1.000699000
H -2.181869000 2.875993000 -1.354489000
H -2.871011000 1.314409000 -1.805239000
H -3.841971000 2.480642000 -0.903552000
END----------

Structure----------
25
C 0.984979000 -0.520956000 -0.016362000
C 1.427423000 0.802729000 0.074929000
C 2.780468000 1.110619000 -0.015694000
C 3.631125000 0.021156000 -0.191133000
C 1.914431000 -1.548028000 -0.188324000
C -0.821620000 0.866688000 0.283208000
H 3.154482000 2.125293000 0.045594000
H 4.702076000 0.182543000 -0.270043000
H 1.630192000 -2.589939000 -0.257278000
C 0.379967000 3.060621000 0.372380000
H 1.131952000 3.315312000 1.121259000
H 0.660737000 3.485417000 -0.593849000
H -0.591192000 3.437999000 0.680006000
C -1.327335000 -1.548560000 0.086348000
N 0.305741000 1.604167000 0.257106000
N -0.419766000 -0.442439000 0.106794000
B -2.319045000 1.441303000 0.427965000
H -3.055785000 0.541727000 0.777916000
H -2.269914000 2.292047000 1.305670000

N 3.219526000 -1.260908000 -0.272416000
C -2.784928000 2.096124000 -1.003997000
H -2.124621000 2.906160000 -1.343436000
H -2.824720000 1.354737000 -1.814104000
H -3.793003000 2.523383000 -0.912053000
F -1.893533000 -1.756919000 1.290175000
F -2.312038000 -1.366761000 -0.807875000
F -0.668932000 -2.668463000 -0.252080000
END----------

Structure----------
26
C -0.751939000 0.963259000 0.293313000
C 1.202792000 -0.130197000 0.028289000
C 0.242743000 -1.095209000 -0.055432000
N 0.579123000 1.103543000 0.247288000
B -1.828639000 2.154292000 0.496807000
H -2.884267000 1.673484000 0.856880000
H -1.386391000 2.854472000 1.399157000
N -0.967065000 -0.386409000 0.091990000
C 1.274081000 2.389558000 0.384255000
H 0.571581000 3.104800000 0.802655000
H 2.120500000 2.274631000 1.060675000
H 1.615312000 2.729744000 -0.594060000
C -1.982117000 3.009498000 -0.893554000
H -1.034683000 3.447434000 -1.238015000
H -2.371657000 2.402146000 -1.722834000
H -2.684051000 3.843600000 -0.753749000
C 2.687975000 -0.241541000 -0.059967000
C -2.296809000 -0.937796000 0.060297000
C 0.359625000 -2.572336000 -0.222095000
H -0.189894000 -3.093578000 0.565193000
H -0.035002000 -2.893861000 -1.189786000
H 1.404343000 -2.865149000 -0.158636000
F -3.077409000 -0.259375000 -0.794979000
F -2.281945000 -2.215306000 -0.337879000
F -2.871837000 -0.898294000 1.276819000
F 3.209882000 0.660280000 -0.933521000
F 3.094294000 -1.459640000 -0.468527000
F 3.295337000 -0.003279000 1.136190000
END----------

Structure----------
27

C	0.142564000	0.081396000	-0.000277000
C	1.237844000	2.073097000	-0.000121000
C	2.188804000	1.118902000	-0.000038000
N	0.011577000	1.422027000	-0.000269000
B	-0.978606000	-1.102637000	-0.000299000
H	-0.737739000	-1.771585000	-0.992511000
H	-0.737462000	-1.771817000	0.991687000
N	1.519942000	-0.118774000	-0.000129000
C	2.242939000	-1.360769000	-0.000104000
C	-1.219975000	2.222421000	-0.000379000
H	-2.084024000	1.572034000	-0.000762000
H	-1.224042000	2.849352000	0.893183000
H	-1.223579000	2.849769000	-0.893649000
Cl	3.890965000	1.312155000	0.000188000
H	1.321308000	3.148082000	-0.000082000
F	1.453346000	-2.424373000	-0.000399000
F	3.041180000	-1.431762000	1.087674000
F	3.041636000	-1.431522000	-1.087563000
C	-2.525168000	-0.647054000	-0.000000000
C	-3.242596000	-0.456862000	-1.198077000
C	-3.242009000	-0.456428000	1.198350000
C	-4.586717000	-0.068834000	-1.206656000
H	-2.732786000	-0.606299000	-2.147992000
C	-4.586129000	-0.068387000	1.207445000
H	-2.731747000	-0.605523000	2.148077000
C	-5.264625000	0.133554000	0.000526000
H	-5.105608000	0.073731000	-2.151487000
H	-5.104549000	0.074521000	2.152482000
H	-6.308822000	0.434205000	0.000720000

END----------

Structure----------

28

C	0.108664000	0.782659000	0.298594000
C	-1.609038000	-0.637077000	-0.040699000
C	-0.489315000	-1.386004000	-0.157800000
N	-1.234601000	0.675751000	0.236385000
B	0.960064000	2.133743000	0.537144000
H	0.417926000	2.725980000	1.462144000
H	2.086959000	1.818930000	0.871412000
N	0.562964000	-0.490034000	0.051550000
C	1.944519000	-0.872738000	0.027236000
C	-2.179129000	1.779932000	0.414095000
H	-1.621102000	2.653323000	0.739710000

H -2.681031000 1.987029000 -0.532991000
H -2.912595000 1.506793000 1.174061000
C 0.958640000 3.037046000 -0.831337000
H 1.437852000 2.522800000 -1.676643000
H -0.051363000 3.318708000 -1.161419000
H 1.513154000 3.972755000 -0.673115000
F 2.519287000 -0.746005000 1.235910000
F 2.646212000 -0.134388000 -0.846580000
F 2.043508000 -2.160340000 -0.341149000
H -0.351459000 -2.433291000 -0.365184000
Cl -3.248489000 -1.111651000 -0.190201000
END----------

Structure----------
29
C 1.139308000 -0.107819000 -0.000703000
C 0.327315000 2.006511000 -0.000236000
C -0.743654000 1.186129000 -0.000221000
N 1.455432000 1.196931000 -0.000167000
B 2.123068000 -1.421825000 -0.000387000
H 1.880025000 -2.063897000 1.005677000
H 1.881308000 -2.063193000 -1.007287000
N -0.244180000 -0.128420000 0.000037000
C -1.099950000 -1.281609000 0.000019000
C 2.797175000 1.799444000 0.000006000
H 3.542980000 1.013510000 -0.000124000
H 2.895827000 2.419583000 -0.892865000
H 2.895900000 2.419340000 0.893039000
Cl -2.407075000 1.588134000 0.000272000
H 0.389626000 3.083025000 -0.000033000
F -0.407791000 -2.414315000 -0.001506000
F -1.899251000 -1.270965000 -1.085966000
F -1.897368000 -1.272618000 1.087390000
F 3.517670000 -1.019108000 0.000818000
END----------

Structure----------
30
C -2.126152000 0.133088000 -0.177529000
C -2.011714000 -1.201396000 0.223786000
C -3.033861000 -2.111916000 -0.020444000
C -4.150402000 -1.593393000 -0.672815000
C -3.287420000 0.561849000 -0.823270000
C -0.108668000 -0.174852000 0.871237000

H -2.974876000 -3.152150000 0.275509000
H -4.991462000 -2.242236000 -0.897889000
H -3.434080000 1.583824000 -1.148117000
C -0.306221000 -2.620361000 1.385162000
H -0.977888000 -2.939792000 2.184842000
H -0.306801000 -3.360032000 0.582370000
H 0.700471000 -2.491556000 1.771393000
C -0.573840000 2.118394000 0.057469000
N -0.776278000 -1.342600000 0.847829000
N -0.917426000 0.738657000 0.227208000
B 1.348060000 0.085355000 1.507201000
H 1.404805000 1.241738000 1.867735000
H 1.430315000 -0.637049000 2.487035000
N -4.277917000 -0.306704000 -1.058931000
F -0.639887000 2.798649000 1.218508000
F 0.663564000 2.262158000 -0.436581000
F -1.430744000 2.694533000 -0.799978000
C 2.530031000 -0.249884000 0.446407000
C 2.394158000 -1.146733000 -0.631213000
C 3.794167000 0.354988000 0.603390000
C 3.455286000 -1.432709000 -1.499212000
H 1.440976000 -1.639673000 -0.808858000
C 4.864069000 0.074989000 -0.252442000
H 3.943273000 1.063937000 1.415381000
C 4.699287000 -0.823428000 -1.312968000
H 3.308126000 -2.129761000 -2.320628000
H 5.823764000 0.561846000 -0.096454000
H 5.525687000 -1.041221000 -1.983957000
END----------

Structure----------
31
C 0.942562000 0.040716000 -0.000098000
C -0.090378000 2.056401000 0.000121000
C -1.067626000 1.127516000 0.000212000
N 1.117385000 1.372983000 -0.000092000
B 2.007978000 -1.176904000 -0.000255000
H 1.813007000 -1.847569000 0.988540000
H 1.812878000 -1.847446000 -0.989116000
N -0.433273000 -0.127141000 0.000017000
C -1.184352000 -1.356202000 -0.000011000
C 2.376361000 2.129942000 -0.000303000
H 3.220533000 1.451857000 -0.000339000
H 2.402014000 2.755368000 -0.894176000

H 2.402213000 2.755520000 0.893457000
Cl -2.762721000 1.360614000 0.000494000
H -0.144518000 3.133306000 0.000183000
F -0.408111000 -2.430674000 -0.000496000
F -1.980313000 -1.409828000 -1.086966000
F -1.979647000 -1.410295000 1.087410000
C 3.538387000 -0.788763000 -0.000296000
N 4.693481000 -0.624050000 -0.000346000
END----------

Structure----------
32
C 0.217359000 0.961354000 0.282582000
C -1.620832000 -0.302786000 0.010889000
C -0.587437000 -1.177816000 -0.086478000
N -1.125618000 0.978948000 0.233193000
B 1.176553000 2.249473000 0.482726000
H 2.269399000 1.869990000 0.857088000
N 0.555228000 -0.359686000 0.076843000
C -1.966260000 2.168556000 0.374339000
H -1.327602000 3.006986000 0.636037000
H -2.477470000 2.367895000 -0.569402000
H -2.697492000 2.001475000 1.166753000
C 1.267846000 3.097289000 -0.918170000
H 1.718920000 2.516538000 -1.735400000
H 0.287468000 3.441934000 -1.277174000
H 1.889485000 3.994052000 -0.785214000
C 1.919834000 -0.804690000 0.078149000
C -0.627210000 -2.649428000 -0.302582000
H -0.152081000 -2.933835000 -1.245272000
H -0.135317000 -3.189229000 0.511018000
H -1.672329000 -2.962371000 -0.337736000
F 2.474983000 -0.694236000 1.300866000
F 2.001798000 -2.091612000 -0.285666000
F 2.666227000 -0.092055000 -0.782059000
Cl -3.303816000 -0.615770000 -0.112206000
H 0.664990000 2.918714000 1.372281000
END----------

Structure----------
33
C 0.407548000 0.604674000 0.223227000
C -0.796939000 -1.318483000 -0.109131000
C 0.502889000 -1.665025000 -0.143912000

N	-0.851531000	0.074122000	0.115740000
B	0.884967000	2.138949000	0.420357000
H	2.048389000	2.092578000	0.758525000
N	1.216979000	-0.480296000	0.056688000
C	-2.109374000	0.786395000	0.195600000
C	0.710179000	2.957207000	-0.990981000
H	1.325584000	2.535438000	-1.797671000
H	-0.323728000	2.989610000	-1.357837000
H	1.034569000	3.998055000	-0.854874000
C	2.663605000	-0.446406000	0.085591000
F	3.123406000	-0.117702000	1.299388000
F	3.127346000	-1.667766000	-0.216349000
F	3.150574000	0.417711000	-0.810926000
Cl	-2.166137000	-2.323983000	-0.291702000
H	0.224412000	2.616871000	1.323212000
H	0.967940000	-2.625338000	-0.287828000
F	-2.796290000	0.617103000	-0.949323000
F	-2.850468000	0.283854000	1.199452000
F	-1.943818000	2.082223000	0.400456000

END----------

Structure----------

34

C	-0.409243000	0.382107000	-0.577661000
C	-2.142455000	-0.721221000	0.433416000
C	-2.394542000	0.595683000	0.558907000
N	-0.923403000	-0.846918000	-0.264222000
B	0.976728000	0.768114000	-1.319531000
H	0.930939000	1.957455000	-1.540577000
N	-1.325173000	1.246923000	-0.060852000
C	-0.341977000	-2.137771000	-0.571558000
C	-1.236213000	2.691829000	-0.134563000
F	-1.292189000	3.119615000	-1.401499000
F	-2.274344000	3.218549000	0.529224000
F	-0.109619000	3.141136000	0.426704000
Cl	-3.079963000	-2.037208000	0.986978000
H	1.003373000	0.169288000	-2.375660000
H	-3.219954000	1.109725000	1.021384000
F	-0.118522000	-2.813054000	0.569481000
F	-1.203799000	-2.853857000	-1.315101000
F	0.798197000	-2.029429000	-1.232072000
C	2.247132000	0.398341000	-0.384499000
C	3.456946000	-0.037709000	-0.959003000
C	2.226456000	0.530038000	1.018202000

C	4.587405000	-0.317681000	-0.183591000
H	3.514713000	-0.164791000	-2.038018000
C	3.347154000	0.246058000	1.806864000
H	1.316238000	0.863140000	1.513478000
C	4.537187000	-0.178814000	1.207695000
H	5.504316000	-0.650773000	-0.663808000
H	3.291021000	0.357052000	2.887023000
H	5.410502000	-0.400954000	1.814826000

END----------

Structure----------

35

C	-2.119350000	-0.190716000	0.104358000
C	-1.583764000	-1.427528000	-0.280504000
C	-2.271735000	-2.625787000	-0.097491000
C	-3.534474000	-2.543093000	0.486767000
C	-4.078080000	-1.303643000	0.868581000
C	-3.385658000	-0.105051000	0.686345000
C	-0.029727000	0.128723000	-0.807331000
H	-1.840001000	-3.574476000	-0.394388000
H	-4.106417000	-3.450582000	0.650194000
H	-5.064272000	-1.271309000	1.320138000
H	-3.824507000	0.834340000	0.989673000
C	0.558746000	-2.232360000	-1.325198000
H	1.053948000	-2.719547000	-0.481942000
H	-0.038732000	-2.961246000	-1.874587000
H	1.300187000	-1.791132000	-1.986313000
C	-1.185200000	2.168272000	-0.039420000
N	-0.325723000	-1.178641000	-0.833040000
N	-1.121270000	0.754402000	-0.237450000
B	1.370711000	0.765101000	-1.292397000
H	1.301171000	1.975021000	-1.263162000
F	-1.114044000	2.840385000	-1.204634000
F	-0.186888000	2.608199000	0.749458000
F	-2.343229000	2.503097000	0.549539000
C	2.570930000	0.213696000	-0.349862000
C	3.823756000	-0.132875000	-0.891903000
C	2.430625000	0.076757000	1.046178000
C	4.882315000	-0.578576000	-0.091860000
H	3.974421000	-0.055419000	-1.966814000
C	3.477223000	-0.373934000	1.858037000
H	1.480772000	0.326605000	1.515461000
C	4.712994000	-0.703382000	1.291021000
H	5.835487000	-0.835000000	-0.548084000

H	3.328490000	-0.468566000	2.931014000
H	5.529402000	-1.054518000	1.916240000
H	1.531280000	0.401861000	-2.447593000

END----------

Structure----------

36

C	-0.454840000	-0.055092000	0.672671000
C	-1.912797000	1.464987000	-0.122437000
C	-2.435499000	0.257171000	-0.436753000
N	-0.712537000	1.262473000	0.553005000
B	0.861548000	-0.706688000	1.339171000
H	0.943238000	-0.252459000	2.470017000
N	-1.517622000	-0.670774000	0.062097000
C	-1.674328000	-2.091767000	-0.067208000
C	0.168067000	2.332485000	1.024072000
H	0.907587000	1.895741000	1.689560000
H	0.663453000	2.798945000	0.170076000
H	-0.422642000	3.071953000	1.565569000
F	-1.774286000	-2.690480000	1.131059000
F	-0.643533000	-2.644646000	-0.725333000
F	-2.796090000	-2.353852000	-0.756107000
C	2.176008000	-0.322816000	0.470857000
C	3.405934000	-0.044119000	1.098326000
C	2.164397000	-0.274553000	-0.937882000
C	4.562585000	0.252980000	0.368334000
H	3.459696000	-0.057200000	2.185153000
C	3.311061000	0.026261000	-1.681206000
H	1.237882000	-0.476941000	-1.472345000
C	4.520149000	0.291179000	-1.029340000
H	5.493861000	0.461311000	0.889632000
H	3.260997000	0.054587000	-2.767060000
H	5.413733000	0.526386000	-1.601092000
H	-3.343976000	-0.014626000	-0.946696000
Cl	-2.533817000	3.027847000	-0.446620000
H	0.705197000	-1.909048000	1.404979000

END----------

Structure----------

37

C	-0.820830000	0.374611000	-0.492395000
C	0.492591000	2.129395000	0.067315000
C	1.273016000	1.028719000	0.157324000
N	-0.764435000	1.707421000	-0.330748000

B	-2.139429000	-0.468029000	-0.899224000
H	-1.822266000	-1.610104000	-1.164336000
N	0.454572000	-0.068334000	-0.187060000
C	0.830161000	-1.453074000	-0.302026000
C	-1.882965000	2.633257000	-0.525598000
H	-2.388692000	2.805941000	0.426182000
H	-1.484588000	3.572401000	-0.909972000
H	-2.576841000	2.201632000	-1.243809000
Cl	2.926978000	0.984500000	0.607485000
H	0.729511000	3.165626000	0.248967000
F	0.715824000	-1.881528000	-1.572021000
F	0.059918000	-2.230901000	0.473505000
F	2.100967000	-1.636778000	0.074066000
C	-3.249108000	-0.415503000	0.309545000
H	-3.581196000	0.616189000	0.497241000
H	-4.146644000	-0.948310000	-0.040803000
C	-2.796711000	-1.033106000	1.641773000
H	-3.579361000	-0.989517000	2.411646000
H	-2.517745000	-2.086896000	1.518117000
H	-1.916806000	-0.514513000	2.045144000
H	-2.575116000	0.074658000	-1.910425000

END----------

Structure----------

38

C	-0.374080000	-0.686139000	-0.019850000
C	-0.404620000	0.673901000	0.016667000
C	-1.637764000	1.515035000	0.029681000
C	-2.838560000	0.625336000	-0.355947000
C	-2.808662000	-0.736402000	0.358860000
C	-1.572820000	-1.576688000	-0.028570000
C	1.767779000	0.046118000	-0.001513000
H	-1.791177000	1.950381000	1.026869000
H	-3.769380000	1.151099000	-0.119882000
H	-2.800535000	-0.571057000	1.444090000
H	-1.446259000	-2.409791000	0.672023000
C	1.293010000	2.516784000	0.054243000
H	0.971554000	3.001423000	-0.871547000
H	0.813743000	3.009287000	0.903572000
H	2.373058000	2.594918000	0.149263000
C	1.458409000	-2.426301000	-0.054608000
H	1.695094000	-2.759570000	0.959962000
H	0.690220000	-3.073341000	-0.477813000
H	2.355094000	-2.483865000	-0.671298000

N 0.918941000 1.107017000 0.032376000
N 0.967696000 -1.052804000 -0.040669000
B 3.371915000 0.012449000 0.007765000
H 3.744033000 -0.716096000 0.920026000
H 3.765947000 -0.467217000 -1.050881000
H 3.835679000 1.127882000 0.150258000
H -1.545737000 2.354671000 -0.668714000
H -2.825906000 0.460694000 -1.441242000
H -3.716779000 -1.301491000 0.125316000
H -1.710837000 -2.019528000 -1.024563000
END----------

Structure----------
39
C -0.001917000 0.786415000 0.000000000
C 0.699266000 -1.354236000 -0.000128000
C -0.661503000 -1.368778000 -0.000086000
H 1.402537000 -2.169144000 -0.000167000
H -1.348875000 -2.197429000 -0.000096000
N 1.087812000 -0.022924000 -0.000090000
B -0.066510000 2.386948000 0.000004000
H -0.685967000 2.754490000 -0.991870000
H -0.685931000 2.754506000 0.991889000
H 1.051051000 2.864233000 -0.000016000
N -1.074299000 -0.046597000 -0.000055000
C -2.466214000 0.437968000 -0.000218000
H -2.590797000 1.072817000 0.881122000
H -2.591138000 1.071463000 -0.882495000
C 2.480714000 0.469961000 -0.000106000
H 2.606074000 1.101667000 -0.882219000
H 2.606155000 1.101492000 0.882123000
C 3.509704000 -0.649494000 -0.000267000
H 4.505447000 -0.196337000 -0.000268000
H 3.426914000 -1.280684000 0.889952000
H 3.426827000 -1.280502000 -0.890606000
C -3.491146000 -0.684598000 0.000851000
H -4.489446000 -0.237277000 0.000769000
H -3.404388000 -1.316075000 -0.888843000
H -3.403923000 -1.314748000 0.891442000
END----------

Structure----------
40
C 0.160233000 1.600725000 -0.007526000

C	-0.726586000	-0.482439000	-0.159808000
C	0.596445000	-0.620962000	0.158859000
N	-0.969033000	0.892677000	-0.256318000
B	0.391783000	3.188455000	0.008181000
H	0.698643000	3.530432000	1.146133000
H	1.326800000	3.458925000	-0.736332000
H	-0.608906000	3.783298000	-0.341922000
N	1.116128000	0.672808000	0.246023000
C	2.503745000	1.011507000	0.545125000
H	3.050814000	1.231668000	-0.375466000
H	2.527513000	1.886067000	1.195251000
H	2.978237000	0.174927000	1.055611000
C	-2.275838000	1.474672000	-0.550325000
H	-2.877397000	1.541609000	0.359956000
H	-2.135819000	2.470381000	-0.964062000
H	-2.793807000	0.850923000	-1.279156000
C	1.413180000	-1.858999000	0.346498000
H	2.014254000	-1.772532000	1.259300000
H	0.723555000	-2.691557000	0.511964000
C	2.326092000	-2.181816000	-0.848385000
H	3.041613000	-1.375250000	-1.037526000
H	2.892954000	-3.099098000	-0.656253000
H	1.733662000	-2.328502000	-1.757766000
C	-1.781146000	-1.525686000	-0.349246000
H	-2.367351000	-1.301046000	-1.247904000
H	-1.277513000	-2.477354000	-0.542089000
C	-2.722068000	-1.683522000	0.857230000
H	-3.262683000	-0.756160000	1.070978000
H	-3.460820000	-2.468380000	0.662294000
H	-2.156675000	-1.959891000	1.753617000

END----------

Structure----------

41

C	-0.516200000	-0.686474000	-0.000077000
C	-0.529540000	0.718819000	0.000022000
C	-1.744665000	1.393193000	0.000124000
C	-2.883596000	0.581763000	0.000086000
C	1.618604000	0.039902000	-0.000085000
H	-1.808854000	2.475665000	0.000236000
H	-3.872503000	1.026730000	0.000163000
C	1.198678000	2.528774000	-0.000123000
H	0.802560000	3.019235000	-0.892738000
H	0.802581000	3.019525000	0.892344000

H	2.283790000	2.585531000	-0.000128000
C	1.298947000	-2.442328000	0.000105000
H	1.900608000	-2.626997000	0.892058000
H	0.430356000	-3.099655000	-0.000378000
H	1.901545000	-2.626953000	-0.891213000
N	0.798302000	1.125141000	0.000092000
N	0.819607000	-1.064510000	-0.000159000
B	3.214606000	-0.024294000	0.000091000
H	3.559461000	-0.653988000	0.990551000
H	3.559760000	-0.654634000	-0.989858000
H	3.709174000	1.083096000	-0.000234000
C	-2.761498000	-0.817463000	-0.000043000
H	-3.652737000	-1.438095000	-0.000061000
N	-1.585501000	-1.472790000	-0.000112000

END----------

Structure----------

42

C	0.000076000	0.231625000	0.143104000
C	-0.677469000	-1.679537000	-0.878567000
C	0.677280000	-1.679454000	-0.878924000
H	-1.391660000	-2.382112000	-1.276344000
H	1.391389000	-2.382089000	-1.276738000
N	-1.076967000	-0.499312000	-0.255836000
B	0.000577000	1.602035000	0.977085000
H	1.005056000	1.639280000	1.665149000
H	0.000855000	2.555716000	0.210243000
H	-1.003529000	1.639971000	1.665581000
N	1.076902000	-0.499222000	-0.256272000
C	-2.451362000	-0.137495000	-0.073354000
C	-2.920592000	1.081735000	-0.564592000
C	-3.306214000	-1.035239000	0.568861000
C	-4.267276000	1.409472000	-0.397417000
H	-2.240761000	1.758342000	-1.069624000
C	-4.653985000	-0.702236000	0.723023000
H	-2.917618000	-1.974790000	0.948197000
C	-5.135280000	0.519931000	0.244139000
H	-4.637735000	2.357409000	-0.775103000
H	-5.323022000	-1.395173000	1.223696000
H	-6.182524000	0.777772000	0.368891000
C	2.451341000	-0.137574000	-0.073704000
C	2.920992000	1.080990000	-0.566146000
C	3.305617000	-1.034772000	0.569975000
C	4.267670000	1.408628000	-0.398659000

H	2.241451000	1.757212000	-1.072111000
C	4.653389000	-0.701893000	0.724419000
H	2.916546000	-1.973747000	0.950254000
C	5.135169000	0.519606000	0.244327000
H	4.638551000	2.356063000	-0.777190000
H	5.322028000	-1.394385000	1.226242000
H	6.182404000	0.777385000	0.369283000

END----------

Structure----------

43

C	0.279352000	-0.000030000	0.306549000
C	2.330311000	-0.680225000	-0.348571000
C	2.330138000	0.680736000	-0.348543000
H	3.101084000	-1.392709000	-0.596097000
H	3.100658000	1.393513000	-0.595998000
N	1.064334000	-1.077164000	0.051166000
B	-1.267852000	-0.000344000	0.747722000
H	-1.466421000	0.998097000	1.435705000
H	-1.466142000	-0.999239000	1.435075000
N	1.064019000	1.077297000	0.051211000
C	0.642773000	2.470020000	0.188447000
H	-0.285855000	2.633975000	-0.359122000
H	0.492230000	2.717554000	1.241394000
H	1.425635000	3.104863000	-0.226759000
C	0.643508000	-2.470021000	0.188319000
H	0.493289000	-2.717768000	1.241269000
H	-0.285208000	-2.634183000	-0.359033000
H	1.426465000	-3.104566000	-0.227150000
C	-2.250436000	0.000019000	-0.567770000
H	-2.040791000	0.875757000	-1.203378000
H	-2.040666000	-0.875225000	-1.204013000
C	-3.743563000	-0.000230000	-0.207030000
H	-4.004578000	0.881770000	0.392902000
H	-4.396976000	0.000024000	-1.090734000
H	-4.004438000	-0.882698000	0.392281000

END----------

Structure----------

44

C	-0.949769000	0.095471000	-0.620334000
C	1.140948000	0.728711000	-0.058215000
C	1.114310000	-0.674489000	-0.137650000
N	-0.141185000	1.160476000	-0.363984000

B	-2.525980000	0.152246000	-0.928516000
H	-2.857014000	-0.914261000	-1.426038000
H	-2.715902000	1.053532000	-1.739405000
N	-0.186022000	-1.024382000	-0.482505000
C	-0.545881000	2.562510000	-0.358584000
H	0.198318000	3.149833000	-0.900700000
H	-1.511162000	2.651606000	-0.851363000
H	-0.618944000	2.925771000	0.669774000
C	-0.640525000	-2.400556000	-0.671666000
H	-1.481853000	-2.610276000	-0.011816000
H	-0.937185000	-2.559321000	-1.709638000
H	0.191929000	-3.058610000	-0.424789000
C	-3.352375000	0.439570000	0.464082000
H	-4.420137000	0.543208000	0.216693000
H	-3.056352000	1.409053000	0.894618000
C	-3.196840000	-0.645305000	1.541475000
H	-2.147510000	-0.764048000	1.842382000
H	-3.770738000	-0.422514000	2.451680000
H	-3.536411000	-1.621360000	1.171798000
C	2.325573000	1.374041000	0.277052000
C	3.421890000	0.538066000	0.510473000
C	3.290393000	-0.856276000	0.403643000
H	2.396823000	2.453218000	0.355242000
H	4.148185000	-1.496276000	0.588290000
H	4.384395000	0.960125000	0.777873000
N	2.143938000	-1.483432000	0.080249000

END--------------------------