ELECTRONIC SUPPLEMENTARY INFORMATION

DFT investigation of hydrogen atom–abstraction reactions of NHC–boranes by various carbon–centered radicals: barriers and correlation analyses

Hong-jie Qu,[a,b], Lang Yuan,[a] Cai-xin Jia,[a] Hai-tao Yu,[*a] Hui Xu[*a]

[a]*Key Laboratory of Functional Inorganic Material Chemistry (Ministry of Education) and School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, P. R. China*
[b]*College of Science, Heilongjiang Bayi Agricultural University, Daqing, 163319, P. R. China*

List of Content

Comparison and explanation of methods

The theoretical methods often used in the available computations of NHC-boranes (H-abstraction, addition, cyclization, complexation, *etc.*) are B3LYP[1] and M06-2X[2] with the 6-31+G(d) – 6-311++G(d,p) basis sets. Another example involved the B3PW91 method[3]. Considering of the possible existence of weak interaction or other non-covalent interactions in transition states, we employed the two methods, B3LYP and M06-2X, combined with the 6-311++G(d,p) basis set to obtain the data and results in the original manuscript. Based on the referee's review report, we further tested another two levels of theory, B3LYP-D3BJ/6-311++G(2d,2p) and ωB97DX/6-311++G(2d,2p). The results were analyzed along with the B3LYP- and M06-2X-computed results.

As shown in Fig. S19, the results at the B3LYP level have high linear correlations with those at the M06-2X ((a) and (b)), B3LYP-D3BJ ((c) and (d)), and ωB97DX ((e) and (f)) levels, R^2 varies in the ranges of 0.88–0.97 for kinetic barriers and 0.98–1.00 for thermodynamic reaction energies, reaction enthalpies, and reaction Gibbs free energies. Clearly, the transition states are more method-dependent than the minimum structures. A similar pattern was reflected in the correlation analysis among the B3LYP-D3BJ-, ωB97DX-, and M06-2X-computed results, as shown in Fig. S20.

The results indicate that the M06-2X, B3LYP-D3BJ, and ωB97DX methods gave a slightly different ordering of barriers to the H-atom abstractions by those reactant radicals with close nucleophilicity or electrophilicity index from the B3LYP method. Although this difference, we found that the results at the four levels of theory keep good consistence in predicting the statistical correlations of different physical quantities investigated in this study. Furthermore, the B3LYP-D3BJ and ωB97DX methods, the newly tested methods, did not improve those correlations relative to the B3LYP and M06-2X methods, but keep consistence with the B3LYP and M06-2X methods. It seems that such a result is closely related to the statistical nature of correlation analysis. Based on the assessment of different methods to the statistical correlations investigated in this study, we described the results using the B3LYP-computed data.

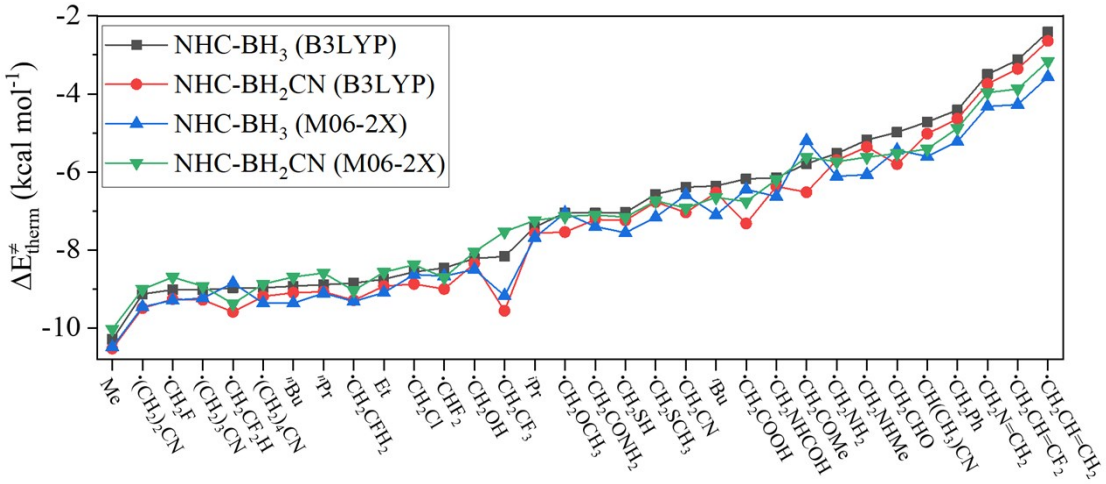

Figure S1 Thermal contributions ($\Delta E^{\neq}_{therm}$) of the H-abstraction reactions by various radical reactants.

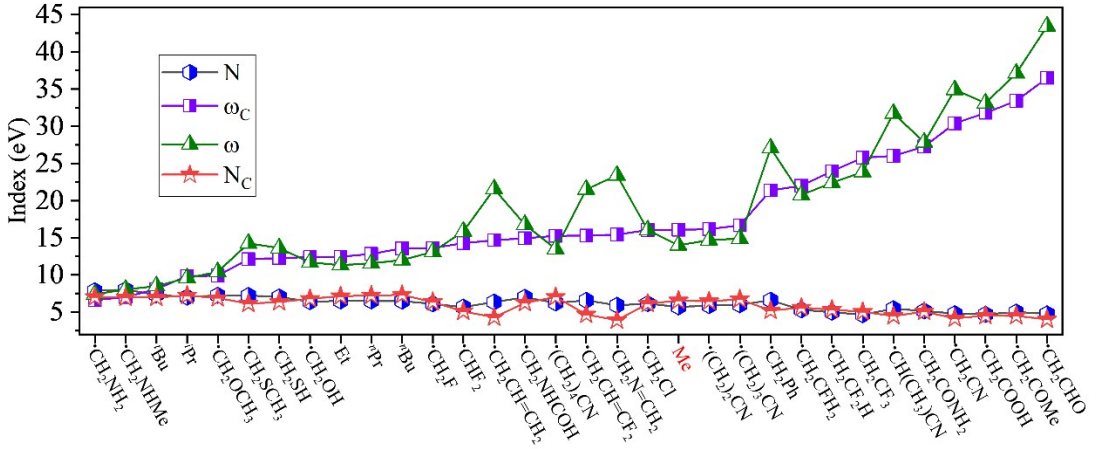

Figure S2 Global nucleophilic (N) and electrophilic (ω), and local nucleophilic (N_C) and electrophilic (ω_C) indexes of radical reactants..

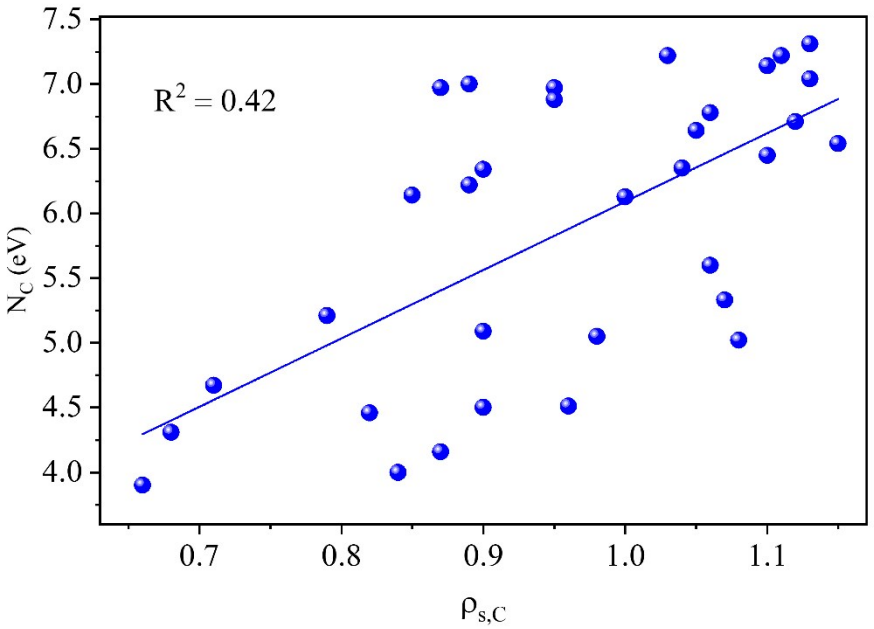

Figure S3 Plot of local nucleophilic index (N_C) vs spin density (ρ_C) for the attacking radicals.

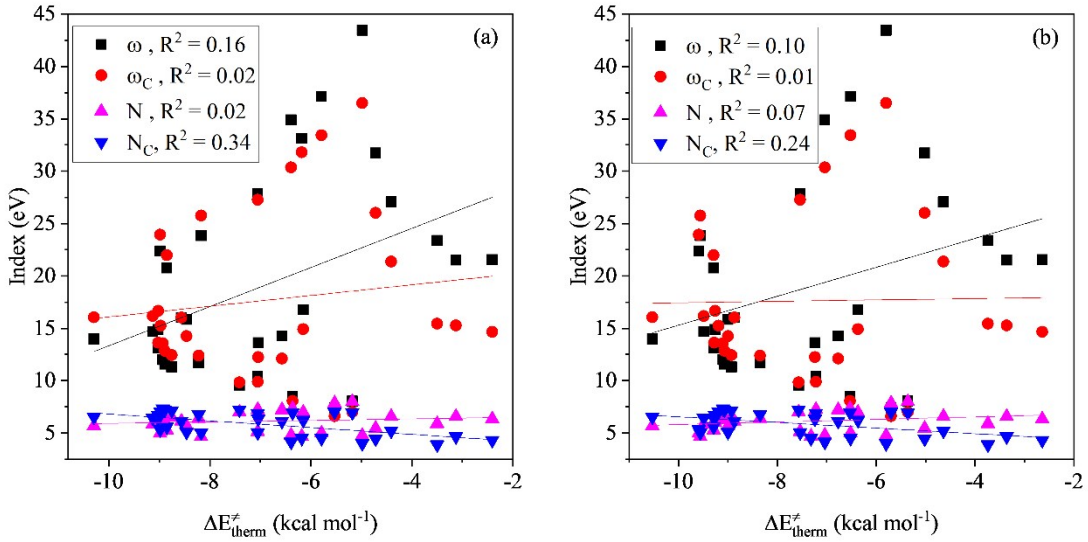

Figure S4 Global nucleophilic (N) and electrophilic (ω) and local nucleophilic (N) and electrophilic (ω_C) indexes of radical reactants vs thermal contribution ($\Delta E^{\neq}_{therm}$) for the H-abstraction reactions of NHC-BH_3 (a) and NHC-BH_2CN (b) by different radicals.

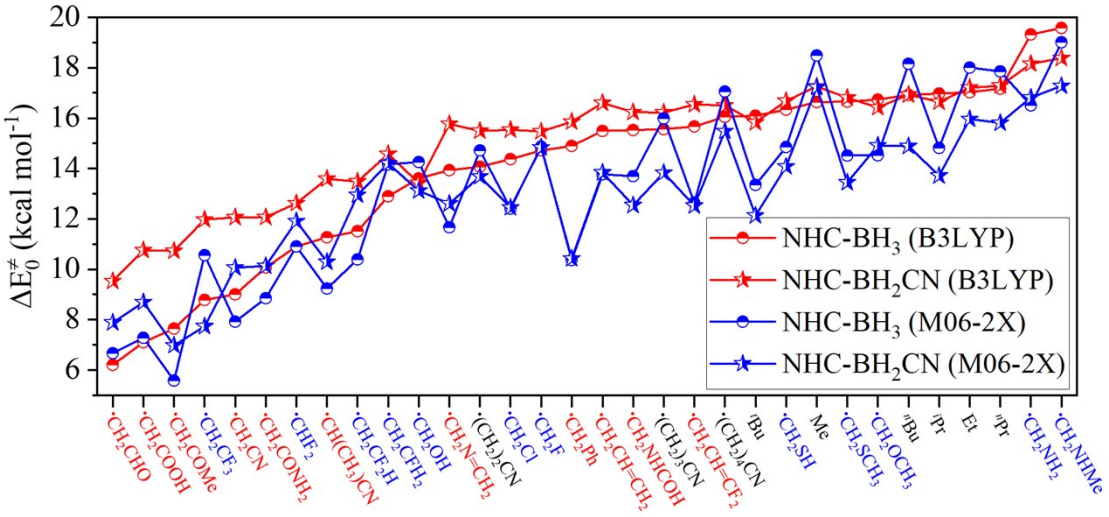

Figure S5 Intrinsic barrier distribution of the H-abstraction reactions by various radical reactants..

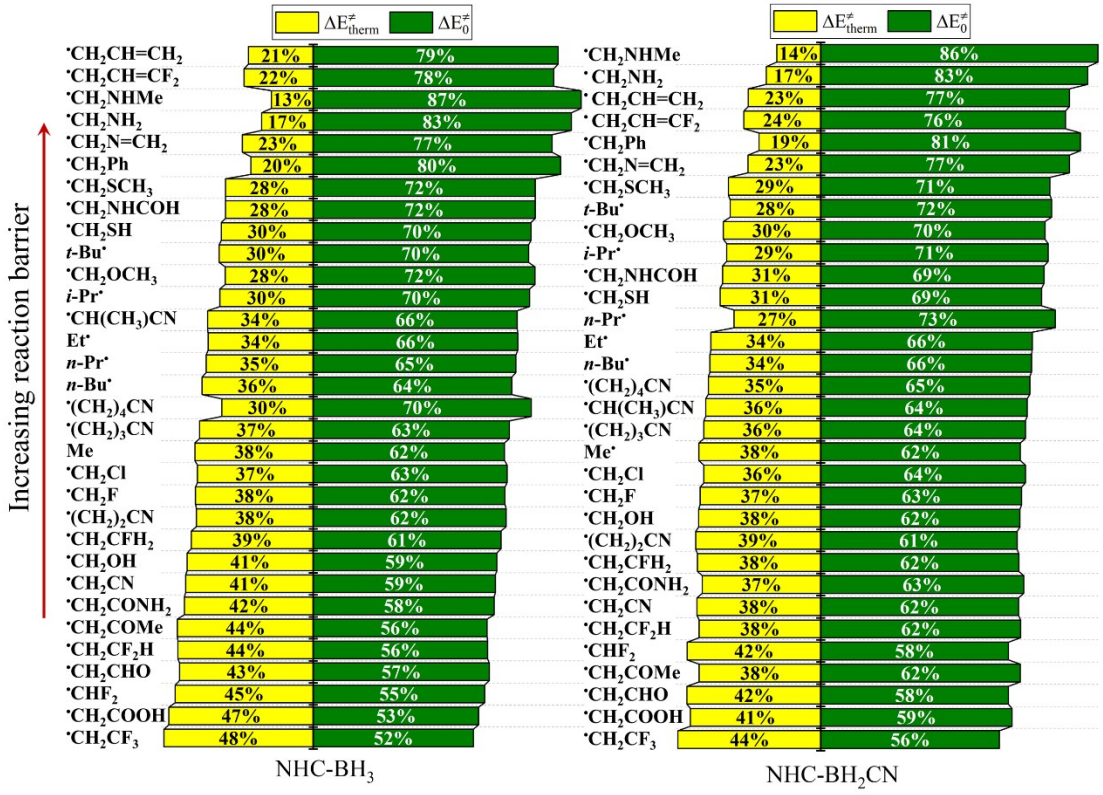

Figure S6 Change of percentages of intrinsic barrier ($\Delta E_0^{\neq}$) and thermal contribution ($\Delta E_{therm}^{\neq}$) in activation barrier ($\Delta E^{\neq}$) with increasing activation barrier for the H-abstraction reactions of NHC-BH_3 (a) and NHC-BH_2CN (b) by different radicals.

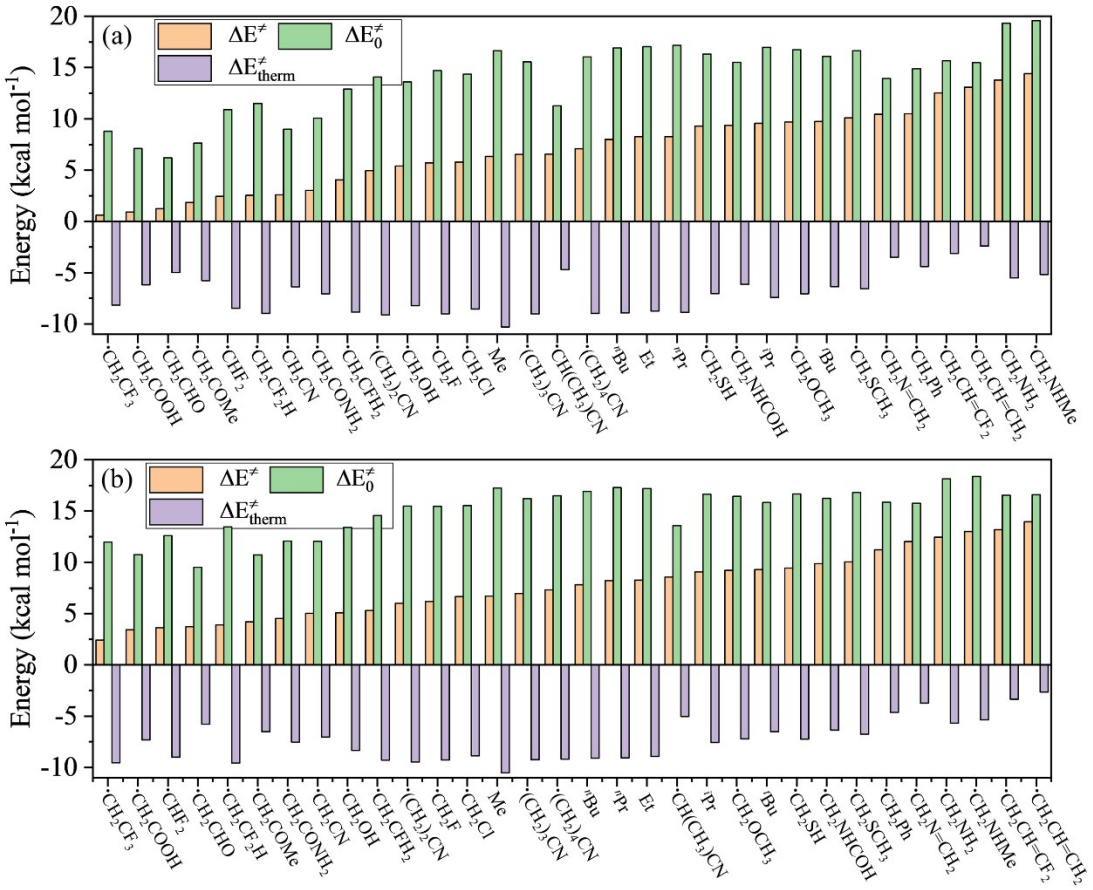

Figure S7 Histograms of activation barrier ($\Delta E^{\neq}$) and its two components, intrinsic barrier ($\Delta E_0^{\neq}$) and thermal contribution ($\Delta E_{therm}^{\neq}$) for the H-abstraction reactions of NHC-BH_3 (a) and NHC-BH_2CN (b) by different radicals.

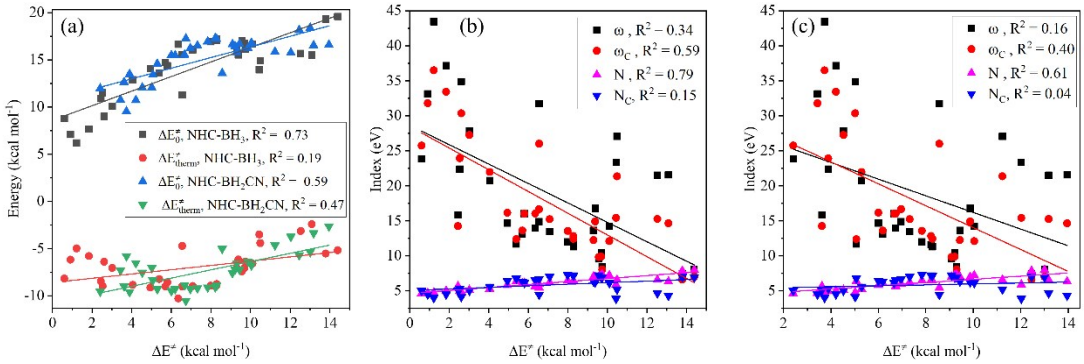

Figure S8 Linear dependences of activation barrier ($\Delta E^{\neq}$) on intrinsic barrier ($\Delta E_0^{\neq}$) and thermal contribution ($\Delta E_{therm}^{\neq}$) (a) and plots of nucleophilic/electrophilic indexes vs activation barrier ($\Delta E^{\neq}$) for the H-abstraction reactions of NHC-BH_3 (b) and NHC-BH_2CN (c).

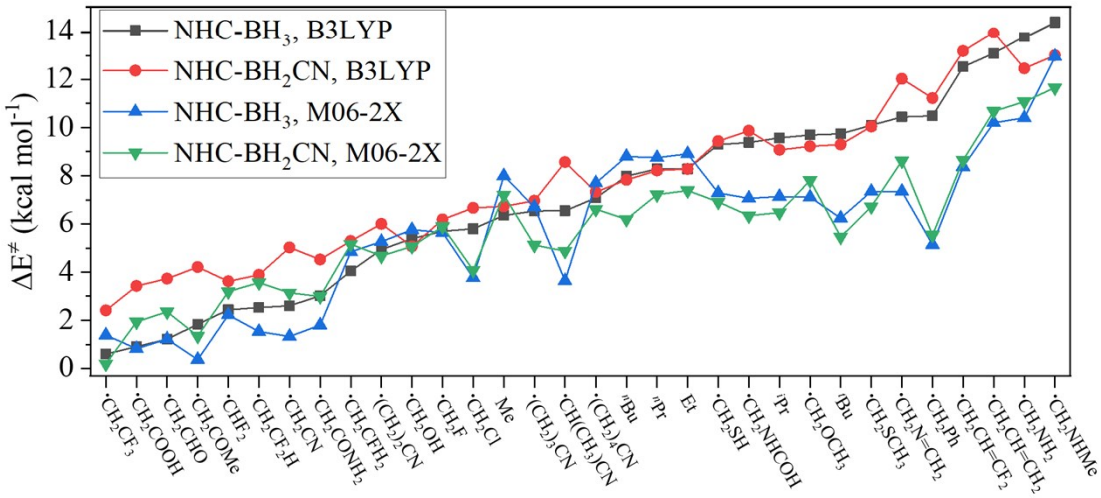

Figure S9 Activation barriers ($\Delta E^{\neq}$) of the H-abstraction reactions by various radical reactants..

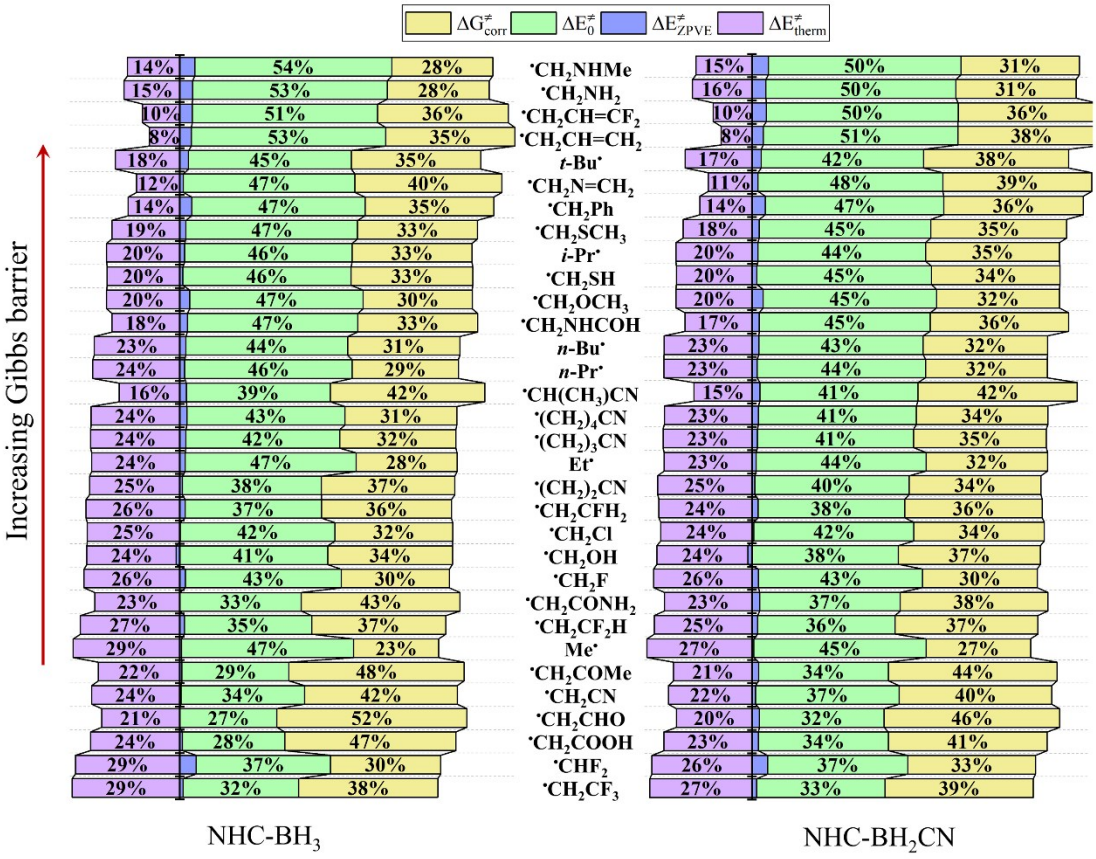

Figure S10 Percentage stacked column chart of four components, intrinsic barrier ($\Delta E^{\neq}_{0}$), thermal contribution ($\Delta E^{\neq}_{therm}$), activation ZPVE correction ($\Delta E^{\neq}_{ZPVE}$) and activation Gibbs free energy thermal correction ($\Delta G^{\neq}_{corr}$), that make up free energy barrier for the H-abstraction reactions of NHC-BH_3 (a) and NHC-BH_2CN (b).

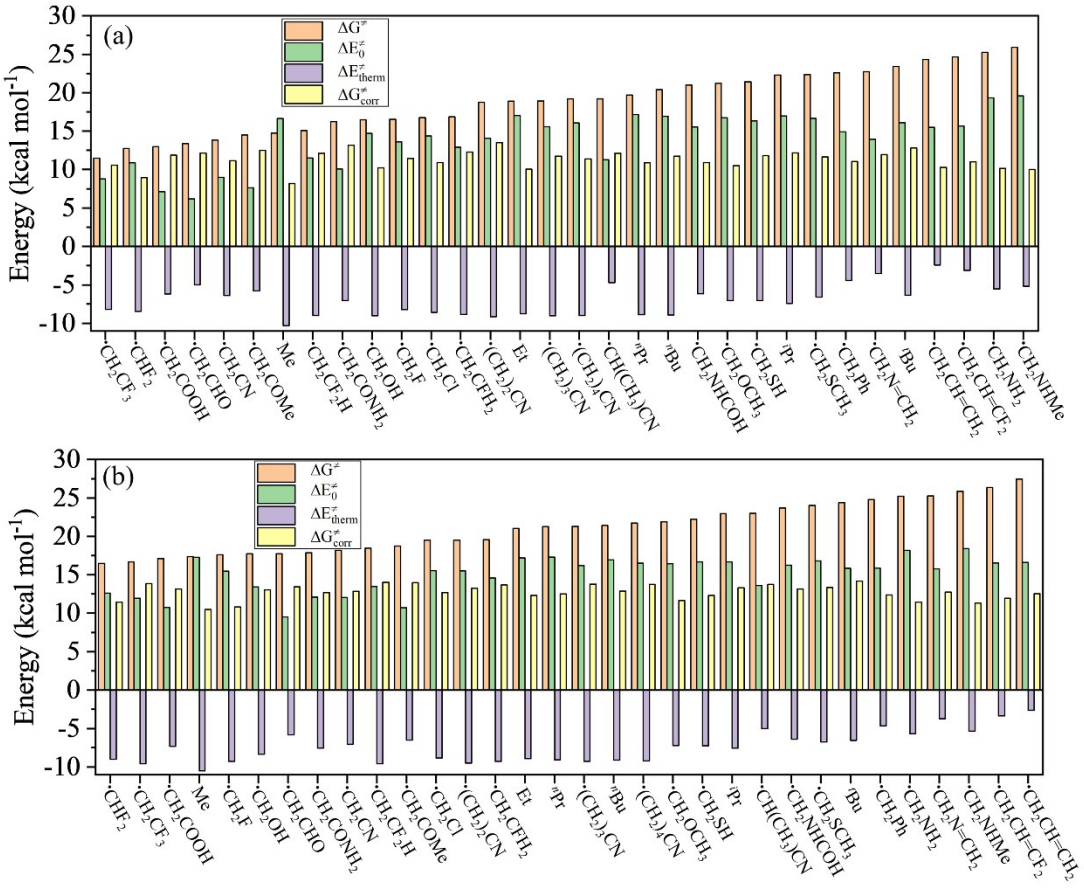

Figure S11 Bar chart of free energy barrier ($\Delta G^{\neq}$) and its three components, intrinsic barrier ($\Delta E_0^{\neq}$), thermal contribution ($\Delta E_{therm}^{\neq}$), and activation Gibbs free energy thermal correction ($\Delta G_{corr}^{\neq}$) for the H-abstraction reactions of NHC-BH_3 (a) and NHC-BH_2CN (b).

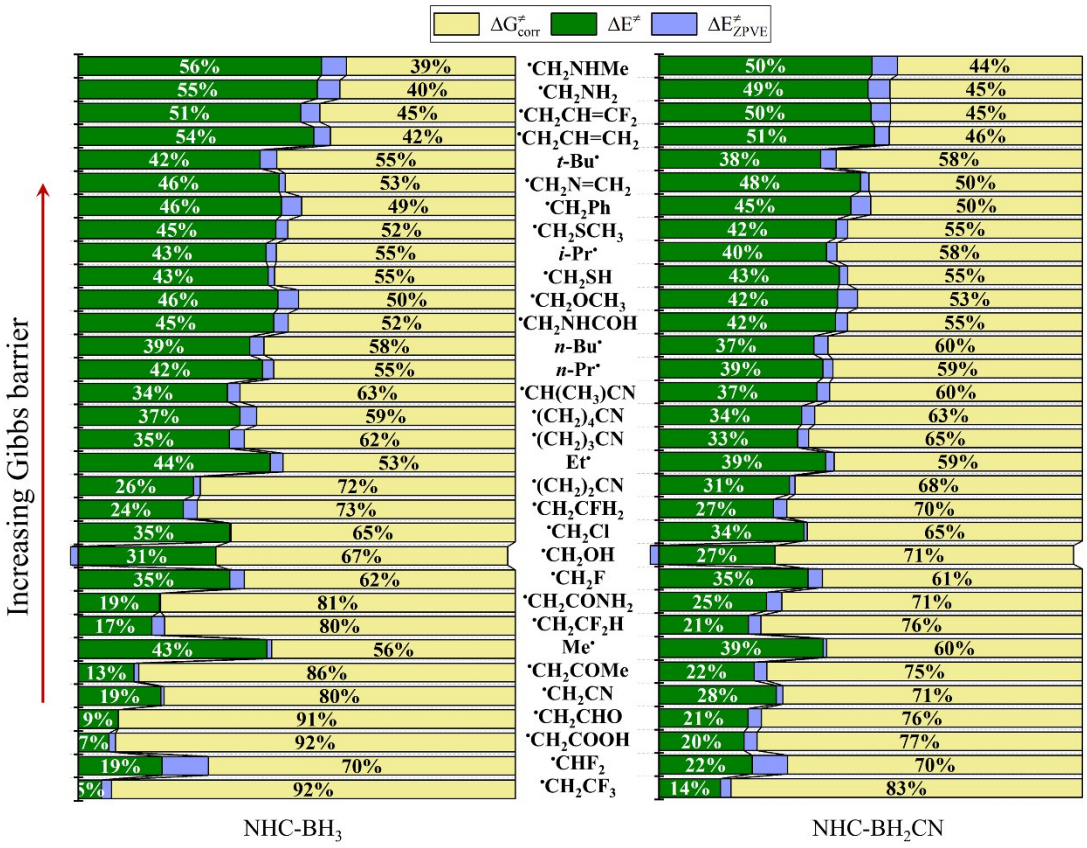

Figure S12 Percentage stacked column chart of three components, activation barrier ($\Delta E^{\neq}$), activation ZPVE correction ($\Delta E^{\neq}_{ZPVE}$) and activation Gibbs free energy thermal correction ($\Delta G^{\neq}_{corr}$), that make up free energy barrier for the H-abstraction reactions of $NHC\text{-}BH_3$ (a) and $NHC\text{-}BH_2CN$ (b).

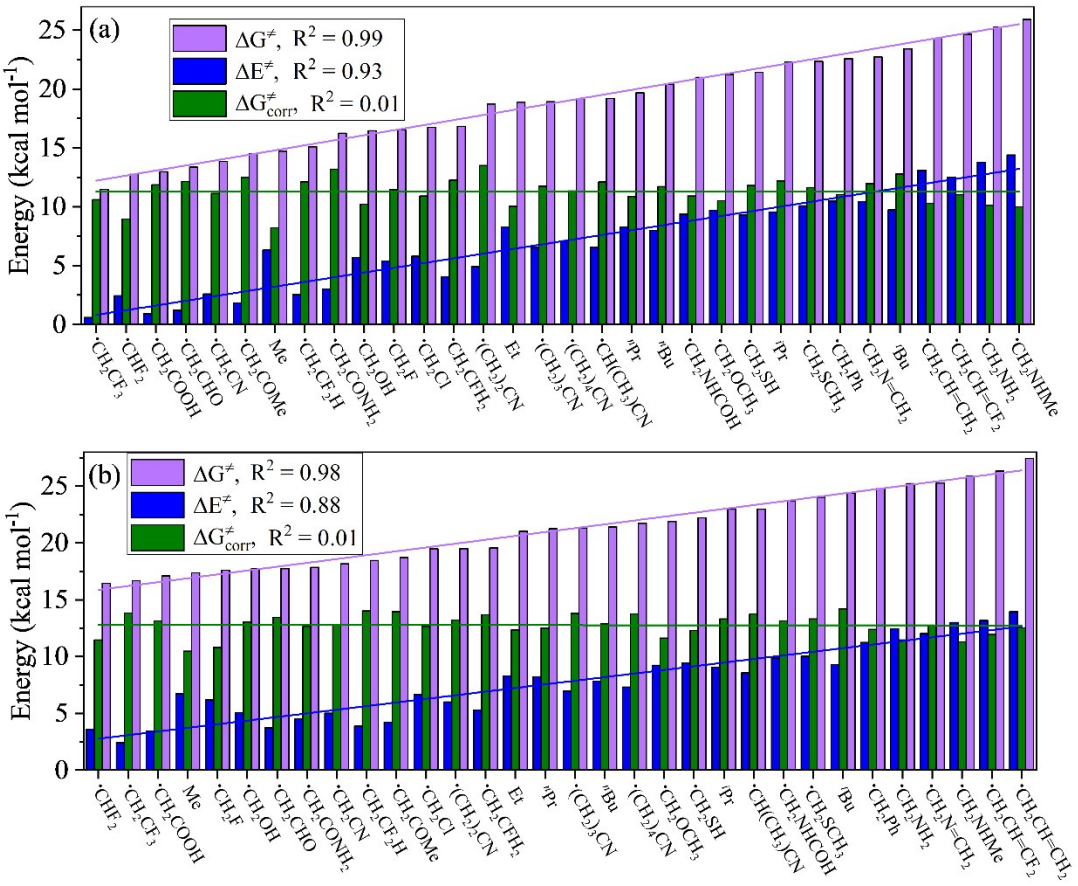

Figure S13 Bar chart of free energy barrier ($\Delta G^{\neq}$) and its components, activation barrier ($\Delta E^{\neq}$) and activation Gibbs free energy thermal correction ($\Delta G^{\neq}_{corr}$), for the H-abstraction reactions of NHC-BH_3 (a) and NHC-BH_2CN (b).

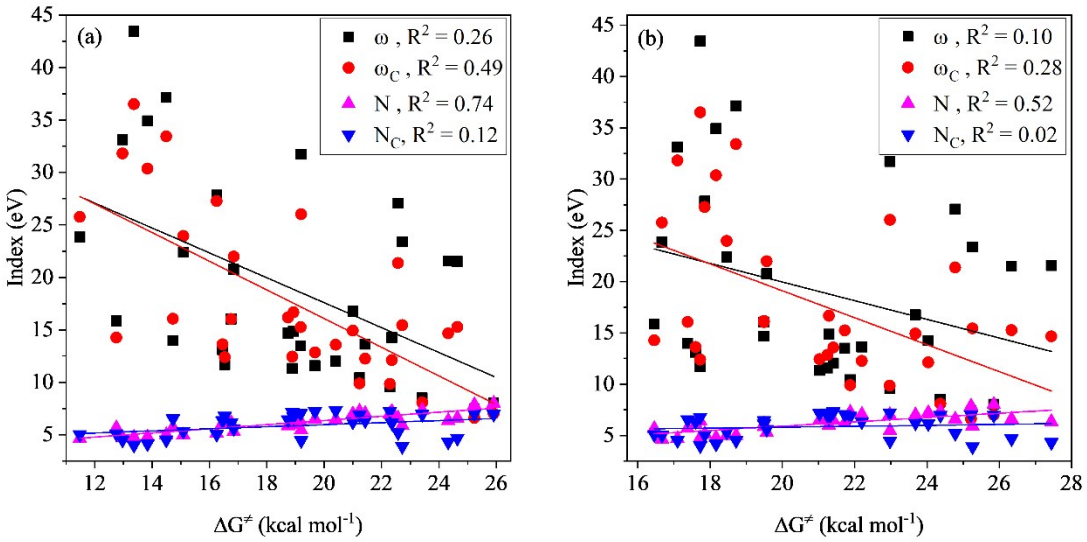

Figure S14 Plots of global/local nucleophilic and electrophilic indexes of radical reactants vs free energy barriers ($\Delta G^{\neq}$) of H-abstraction reactions of NHC-BH_3 (a) and NHC-BH_2CN (b).

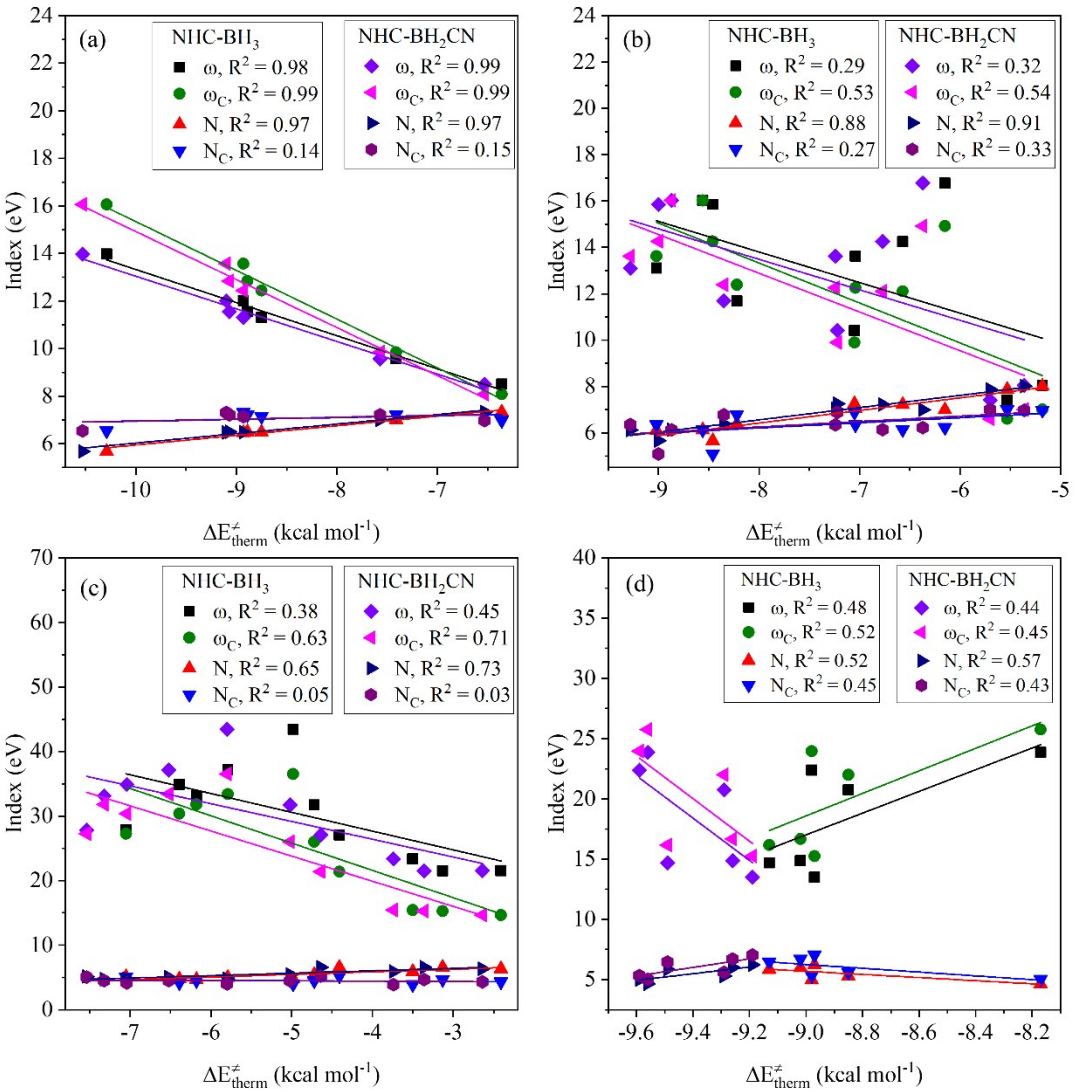

Figure S15 Analysis of linear dependences of thermal contribution ($\Delta E^{\neq}_{therm}$) on global nucleophilic (N), global electrophilic (ω), local nucleophilic (N_C), and local electrophilic (ω_C) indexes for the radicals of types **I** (a), **II** (b), **III** (c), and **IV** (d).

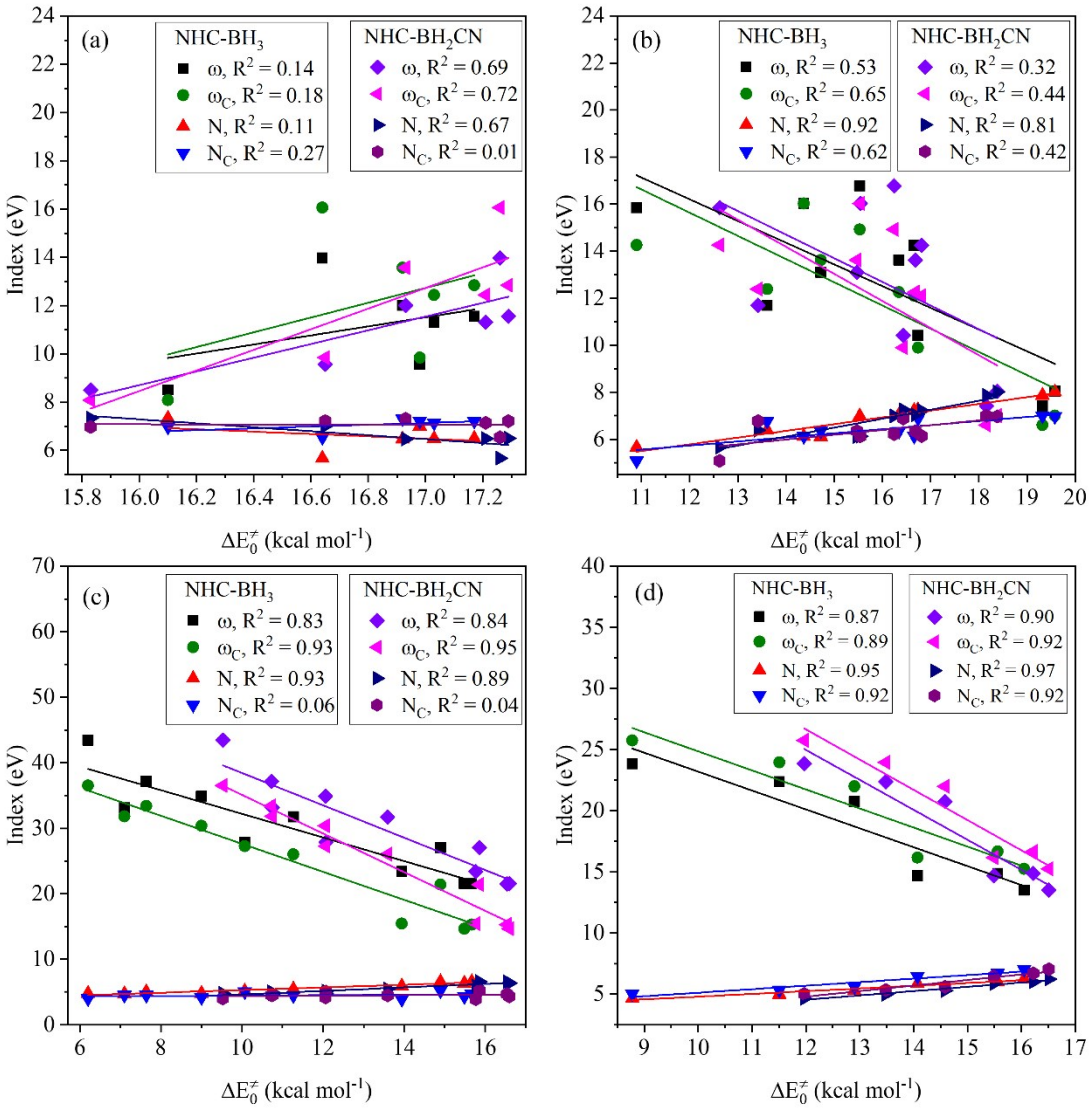

Figure S16 Analysis of linear dependences of intrinsic barrier ($\Delta E_0^{\neq}$) with global nucleophilic (N), global electrophilic (ω), local nucleophilic (N_C), and local electrophilic (ω_C) indexes for the radicals of types **I** (a), **II** (b), **III** (c), and **IV** (d).

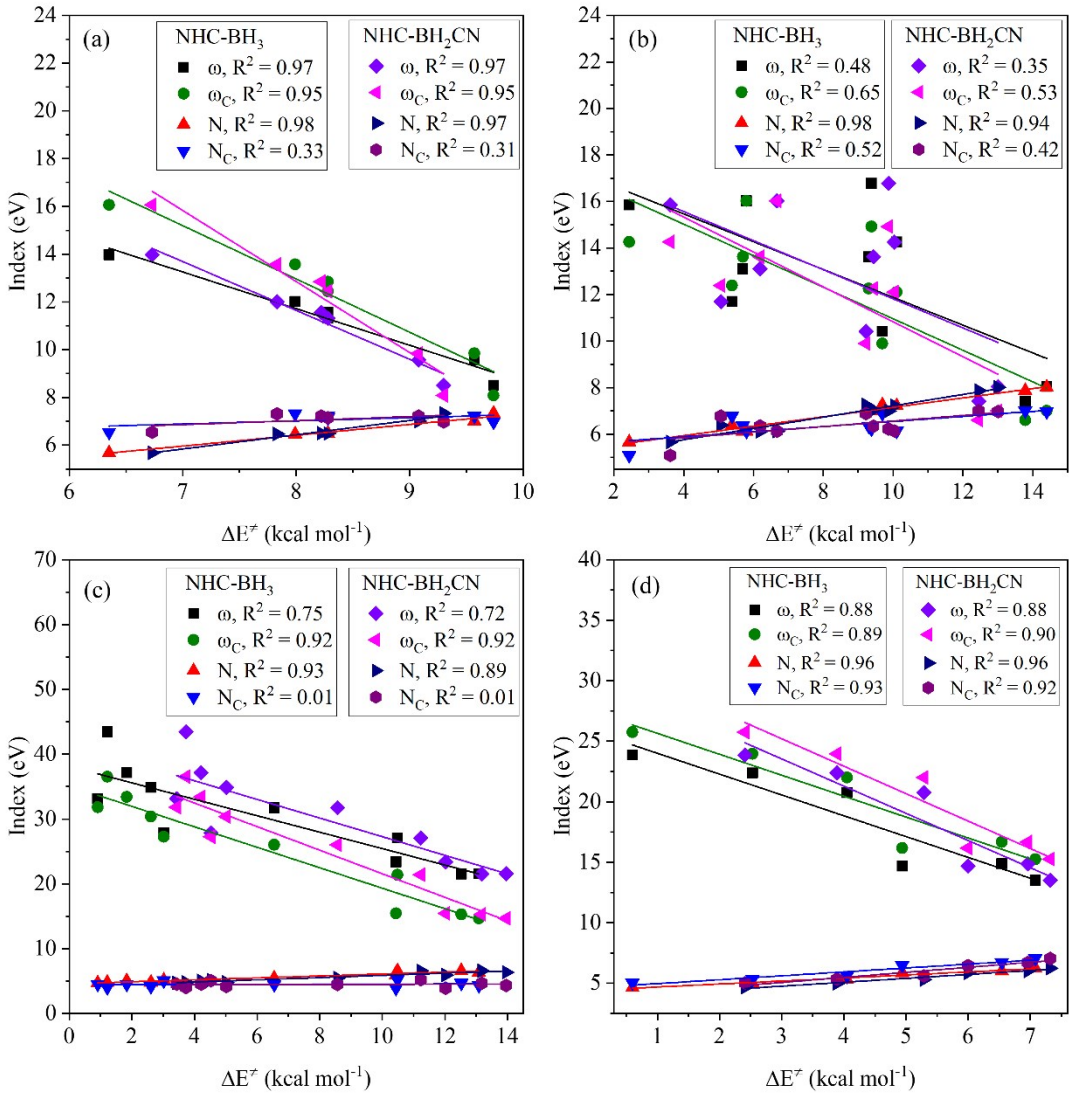

Figure S17 Analysis of linear dependences of activation barrier ($\Delta E^{\neq}$) with global nucleophilic (N), global electrophilic (ω), local nucleophilic (N_C), and local electrophilic (ω_C) indexes for the radicals of types **I** (a), **II** (b), **III** (c), and **IV** (d).

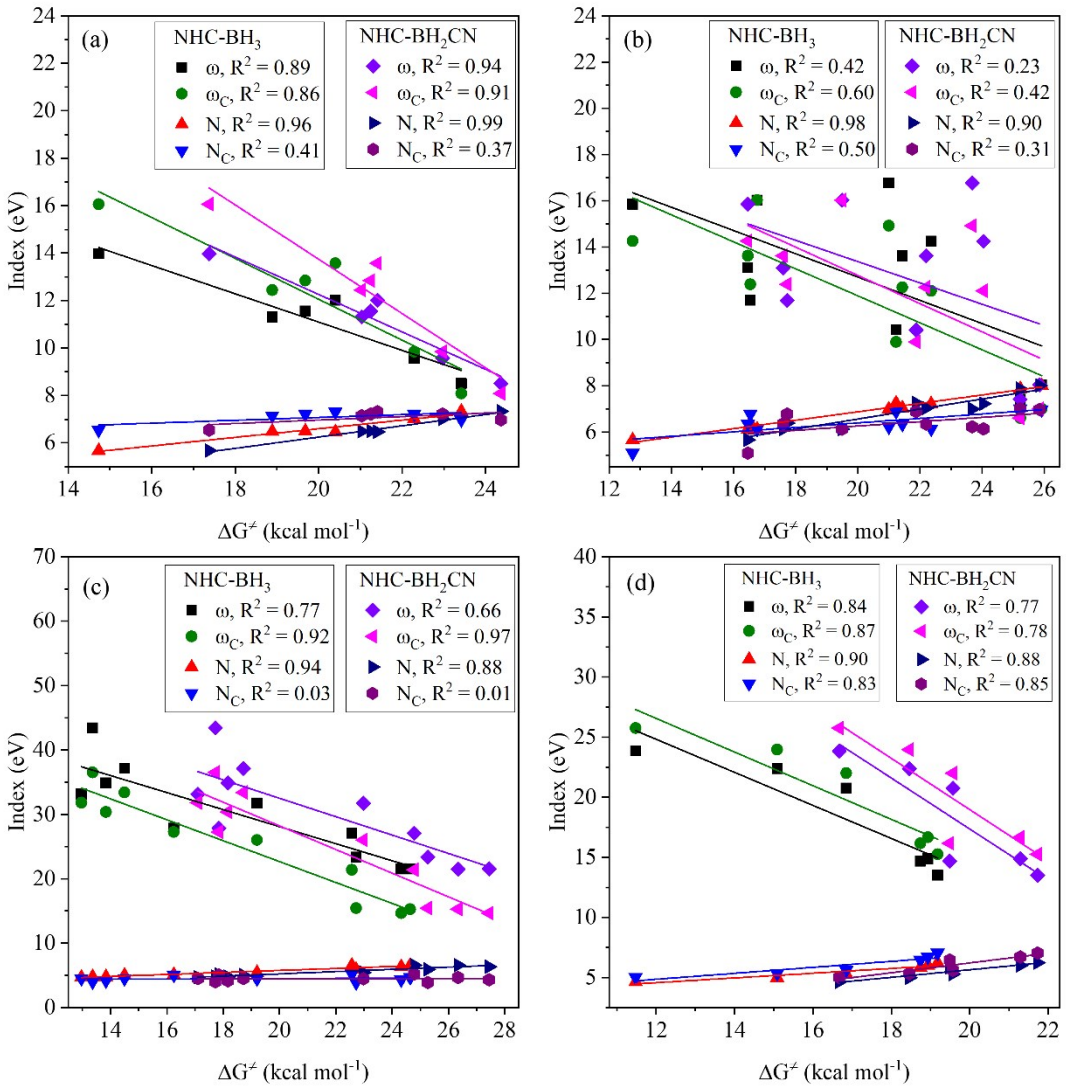

Figure S18 Analysis of linear dependences of free energy barrier ($\Delta G^{\neq}$) with global nucleophilic (N), global electrophilic (ω), local nucleophilic (N_C), and local electrophilic (ω_C) indexes for the radicals of types **I** (a), **II** (b), **III** (c), and **IV** (d).

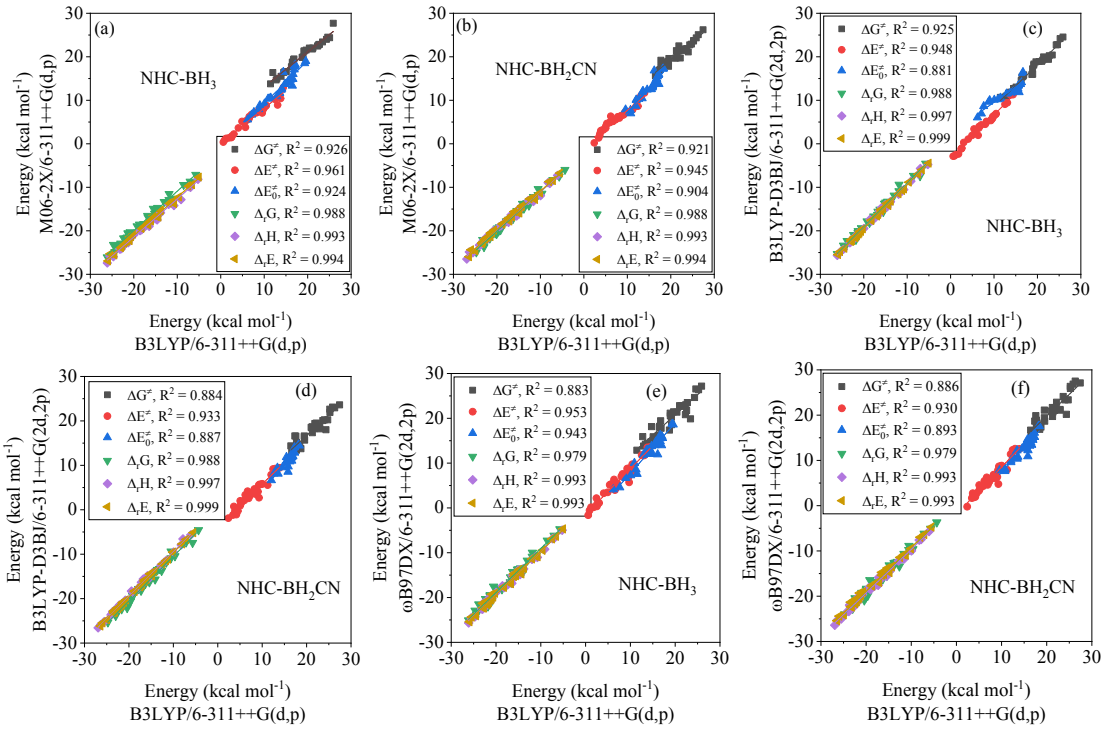

Figure S19 Correlation analysis of the kinetic and thermodynamic quantities of the H-abstraction reactions computed at the B3LYP/6-311++G(d,p) level with those computed at the B3LYP-D3BJ/6-311++G(2d,2p), ωB97DX/6-311++G(2d,2p), and M06-2X/6-311++G(d,p) levels of theory.

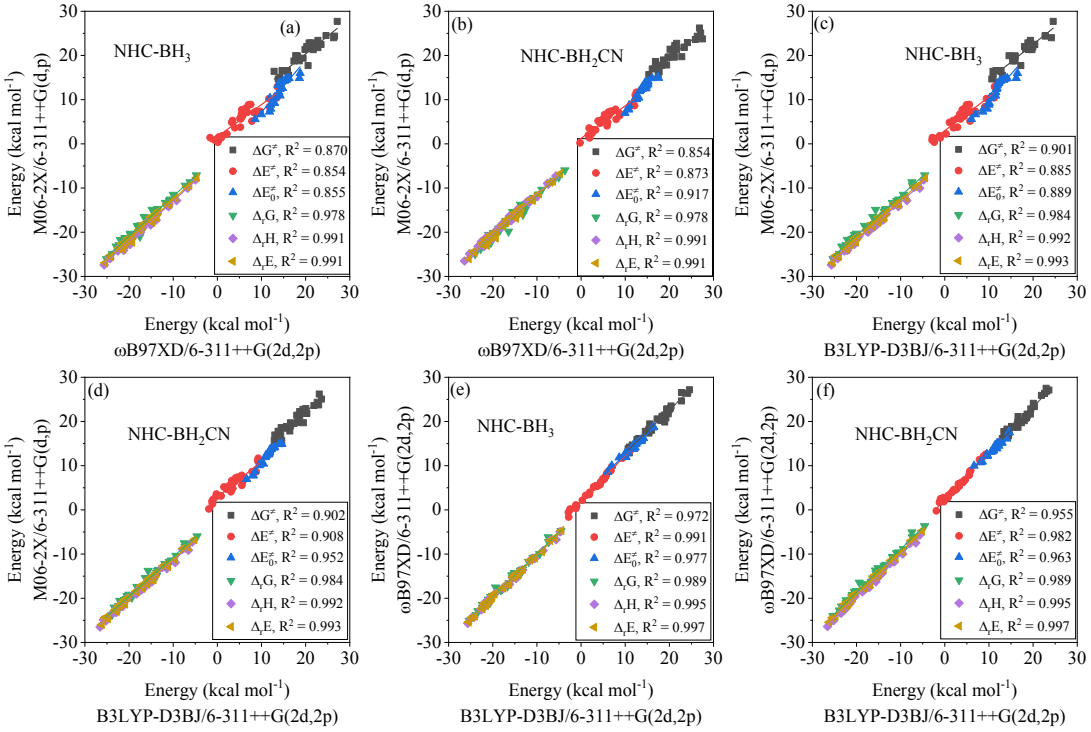

Figure S20 Correlation analysis of the kinetic and thermodynamic quantities of the H-abstraction reactions computed at the B3LYP-D3BJ/6-311++G(2d,2p), ωB97DX/6-311++G(2d,2p), and M06-2X/6-311++G(d,p).

Table S1 Total electronic energies (E, hartree), zero-point vibrational energies (ZPVE, hartree/particle), Gibbs free energies (G, hartree), enthalpies (H, hartree), thermal corrections to Gibbs free energy (G_{corr}, hartree), and thermal corrections to enthalpy (H_{corr}, hartree) of the structures of NHC-boranes, NHC-boryl radicals, and RH optimized at the B3LYP/6-311++G(d,p) in BTF at 376 K.

Species	E	ZPVE	G	H	G_{coor}	H_{coor}
NHC-BH_3	-331.598609	0.158913	-331.484030	-331.425269	0.114579	0.173340
NHC-BH_2CN	-423.905043	0.160229	-423.795270	-423.727771	0.109773	0.177272
NHC-$^{\bullet}BH_2$	-330.964966	0.148261	-330.862962	-330.802167	0.102004	0.162799
NHC-B(•)HCN	-423.272422	0.149815	-423.171992	-423.106003	0.100429	0.166419
CH_3NH_2	-95.897929	0.063749	-95.864445	-95.828249	0.033484	0.069680
$CH_3CH{=}CF_2$	-316.484166	0.064019	-316.457081	-316.412112	0.027085	0.072054
$CH_3CH{=}CH_2$	-117.943653	0.078694	-117.897366	-117.858640	0.046287	0.085013
$CH(CH_3)_3$	-158.506768	0.130566	-158.413172	-158.366466	0.093596	0.140302
$CH_3N{=}CH_2$	-133.987655	0.067831	-133.952565	-133.913130	0.035090	0.074525
CH_3Ph	-271.641327	0.127177	-271.555484	-271.503397	0.085843	0.137930
$CH_2(CH_3)_2$	-119.181329	0.102610	-119.112854	-119.070887	0.068475	0.110441
CH_3SH	-438.746659	0.045838	-438.732807	-438.694630	0.013852	0.052029
$CH_3(CH_2)_2CH_3$	-158.505777	0.131047	-158.412155	-158.365013	0.093622	0.140764
$CH_3CH_2CH_3$	-119.181329	0.102610	-119.112854	-119.070887	0.068475	0.110441
$CH_2(CH_3)CN$	-172.127753	0.074022	-172.089132	-172.045820	0.038621	0.081933
$CH_3(CH_2)_3CN$	-250.777106	0.130729	-250.688464	-250.634495	0.088642	0.142611
$CH_3(CH_2)_2CN$	-211.452603	0.102318	-211.389053	-211.340395	0.063550	0.112208
CH_3CH_3	-79.856731	0.074104	-79.813149	-79.776540	0.043582	0.080192
CH_3CH_2CN	-172.127753	0.074022	-172.089132	-172.045820	0.038621	0.081933
CH_3F	-139.794816	0.038960	-139.784071	-139.750795	0.010745	0.044021
CH_3OH	-115.770082	0.051011	-115.749106	-115.713333	0.020976	0.056749
CH_4	-40.534131	0.044375	-40.512734	-40.484839	0.021397	0.049292
CH_3CN	-132.803769	0.045139	-132.790282	-132.752464	0.013486	0.051305
CH_3CHO	-153.886044	0.054893	-153.863150	-153.825413	0.022894	0.060631
CH_3COOH	-229.170954	0.061207	-229.144045	-229.103078	0.026909	0.067876
CH_2F_2	-239.070606	0.032416	-239.070483	-239.032706	0.000123	0.037900
CH_3CF_3	-377.690108	0.051636	-377.675409	-377.630156	0.014699	0.059952
CH_3Cl	-500.154807	0.037606	-500.146974	-500.111927	0.007833	0.042880
CH_3OCH_3	-155.080308	0.079196	-155.034880	-154.993756	0.045428	0.086552
CH_3SCH_3	-478.070095	0.075381	-478.030670	-477.986537	0.039425	0.083558
CH_3NHMe	-135.212683	0.091900	-135.154595	-135.113244	0.058088	0.099439
CH_3NHCOH	-209.280668	0.073937	-209.242695	-209.198591	0.037973	0.082077
CH_3COMe	-193.223673	0.083020	-193.176150	-193.132895	0.047523	0.090778
CH_3CONH_2	-209.299005	0.073290	-209.262444	-209.217257	0.036561	0.081748
CH_3CF_2H	-278.407490	0.059916	-278.382939	-278.340122	0.024551	0.067368
CH_3CFH_2	-179.126891	0.067463	-179.092678	-179.052737	0.034213	0.074154

Table S2 Total electronic energies (E, hartree), zero-point vibrational energies (ZPVE, hartree/particle), Gibbs free energies (G, hartree), enthalpies (H, hartree), thermal corrections to Gibbs free energy (G_{corr}, hartree), and thermal corrections to enthalpy (H_{corr}, hartree) of the structures of the attacking radical R• optimized at the B3LYP/6-311++G(d,p) in BTF at 376 K.

Species	E	ZPVE	G	H	G_{coor}	H_{coor}
$^{\bullet}CH_2NH_2$	-95.241889	0.049797	-95.222676	-95.186061	0.019213	0.055828
$^{\bullet}CH_2CH{=}CF_2$	-315.837554	0.050937	-315.824789	-315.777889	0.012765	0.072054
$^{\bullet}CH_2CH{=}CH_2$	-117.299714	0.065741	-117.267183	-117.227178	0.032531	0.072536
^{t}Bu	-157.846072	0.115648	-157.769752	-157.720047	0.076321	0.126026
$^{\bullet}CH_2N{=}CH_2$	-133.338363	0.053481	-133.317900	-133.278244	0.020463	0.060119
$^{\bullet}CH_2Ph$	-270.989971	0.114088	-270.915484	-270.865727	0.074488	0.124245
^{i}Pr	-118.515994	0.087250	-118.465036	-118.420183	0.050958	0.095811
$^{\bullet}CH_2SH$	-438.083398	0.031135	-438.085822	-438.045451	-0.002420	0.037947
^{n}Bu	-157.834182	0.116177	-157.757574	-157.707679	0.076608	0.126503
^{n}Pr	-118.509910	0.087605	-118.457793	-118.414023	0.052118	0.095888
$^{\bullet}CH(CH_3)CN$	-171.473467	0.059786	-171.450504	-171.405552	0.022963	0.067915
$^{\bullet}(CH_2)_4CN$	-250.104950	0.115937	-250.033139	-249.976589	0.071811	0.128361
$^{\bullet}(CH_2)_3CN$	-210.779804	0.087401	-210.733808	-210.681898	0.045996	0.097906
Et	-79.185621	0.058826	-79.158902	-79.120105	0.026720	0.065516
$^{\bullet}(CH_2)_2CN$	-171.452840	0.058623	-171.431393	-171.385732	0.021447	0.067109
$^{\bullet}CH_2F$	-139.121735	0.024305	-139.127406	-139.092110	-0.005671	0.029625
$^{\bullet}CH_2OH$	-115.099005	0.035103	-115.094104	-115.058418	0.004901	0.040587
Me	-39.855770	0.029550	-39.852370	-39.821029	0.003401	0.034741
$^{\bullet}CH_2CN$	-132.139999	0.030847	-132.141013	-132.103102	-0.001014	0.036897
$^{\bullet}CH_2CHO$	-153.228686	0.042493	-153.218992	-153.180050	0.009694	0.048636
$^{\bullet}CH_2COOH$	-228.505685	0.047944	-228.493222	-228.450361	0.012463	0.055324
$^{\bullet}CHF_2$	-238.397362	0.018751	-238.411431	-238.373203	-0.014069	0.024159
$^{\bullet}CH_2CF_3$	-377.011042	0.036845	-377.012725	-376.965454	-0.001683	0.045588
$^{\bullet}CH_2Cl$	-499.483265	0.022436	-499.493153	-499.454860	-0.009890	0.042880
$^{\bullet}CH_2OCH_3$	-154.417897	0.065290	-154.387158	-154.345045	0.030739	0.072852
$^{\bullet}CH_2SCH_3$	-477.409204	0.061023	-477.385380	-477.339551	0.023824	0.069653
$^{\bullet}CH_2NHMe$	-134.558203	0.078186	-134.514558	-134.472272	0.043645	0.085931
$^{\bullet}CH_2NHCOH$	-208.621437	0.059738	-208.597847	-208.553471	0.023590	0.067966
$^{\bullet}CH_2COMe$	-192.562982	0.070095	-192.530397	-192.484412	0.032585	0.078570
$^{\bullet}CH_2CONH_2$	-208.632887	0.059205	-208.610732	-208.565140	0.022155	0.067747
$^{\bullet}CH_2CF_2H$	-277.730770	0.045151	-277.723055	-277.677649	0.007715	0.053121
$^{\bullet}CH_2CFH_2$	-179.126891	0.067463	-179.092678	-179.052737	0.034213	0.060035

Table S3 Spin densities ($\rho_{s,C}$, *e*) on the central C atoms, global nucleophilic (N, eV) and electrophilic indices (ω, eV), and local nucleophilic (N_C, eV) and electrophilic indices (ω_C, eV) of the attacking radical R$^{\bullet}$ and NHC-boranes computed at the mpwpw91/6-311+G(d,p) in BTF.

Species	$\rho_{s,C}$	ω	ω_C	N	N_C
$^{\bullet}CH_2NH_2$	0.89	7.41	6.60	7.87	7.00
$^{\bullet}CH_2CH=CF_2$	0.71	21.50	15.27	6.58	4.67
$^{\bullet}CH_2CH=CH_2$	0.68	21.56	14.66	6.34	4.31
^{t}Bu	0.95	8.50	8.08	7.33	6.97
$^{\bullet}CH_2N=CH_2$	0.66	23.38	15.43	5.91	3.90
$^{\bullet}CH_2Ph$	0.79	27.05	21.37	6.59	5.21
^{i}Pr	1.03	9.57	9.85	7.01	7.22
$^{\bullet}CH_2SH$	0.90	13.62	12.26	7.04	6.34
^{n}Bu	1.13	12.01	13.57	6.47	7.31
^{n}Pr	1.11	11.56	12.84	6.50	7.22
$^{\bullet}CH(CH_3)CN$	0.82	31.72	26.01	5.44	4.46
$^{\bullet}(CH_2)_4CN$	1.13	13.49	15.24	6.23	7.04
$^{\bullet}(CH_2)_3CN$	1.12	14.88	16.66	5.99	6.71
Et	1.10	11.31	12.44	6.49	7.14
$^{\bullet}(CH_2)_2CN$	1.10	14.69	16.16	5.86	6.45
$^{\bullet}CH_2F$	1.04	13.10	13.62	6.11	6.35
$^{\bullet}CH_2OH$	1.06	11.69	12.39	6.39	6.78
Me	1.15	13.97	16.06	5.68	6.54
$^{\bullet}CH_2CN$	0.87	34.90	30.37	4.78	4.16
$^{\bullet}CH_2CHO$	0.84	43.45	36.50	4.77	4.00
$^{\bullet}CH_2COOH$	0.96	33.13	31.81	4.69	4.51
$^{\bullet}CHF_2$	0.90	15.85	14.26	5.66	5.09
$^{\bullet}CH_2CF_3$	1.08	23.85	25.76	4.65	5.02
$^{\bullet}CH_2Cl$	1.00	16.03	16.03	6.13	6.13
$^{\bullet}CH_2OCH_3$	0.95	10.42	9.90	7.25	6.88
$^{\bullet}CH_2SCH_3$	0.85	14.25	12.11	7.22	6.14
$^{\bullet}CH_2NHMe$	0.87	8.04	7.00	8.01	6.97
$^{\bullet}CH_2NHCOH$	0.89	16.77	14.92	6.99	6.22
$^{\bullet}CH_2COMe$	0.90	37.13	33.42	5.00	4.50
$^{\bullet}CH_2CONH_2$	0.98	27.83	27.27	5.15	5.05
$^{\bullet}CH_2CF_2H$	1.07	22.38	23.95	4.98	5.33
$^{\bullet}CH_2CFH_2$	1.06	20.75	21.99	5.29	5.60
NHC-BH_3	/	4.61	/	5.39	/
NHC-BH_2CN	/	6.14	/	4.84	/

Table S4 Total electronic energies (E, hartree), zero-point vibrational energies (ZPVE, hartree/particle), Gibbs free energies (G, hartree), enthalpies (H, hartree), thermal corrections to Gibbs free energy (G_{corr}, hartree), and thermal corrections to enthalpy (H_{corr}, hartree) of the transition states (**TS**) of the H-atom abstraction reactions of NHC-BH_3 by R$^{\bullet}$ optimized at the B3LYP/6-311++G(d,p) in BTF at 376 K.

TS	R$^{\bullet}$	E	ZPVE	G	H	G_{coor}	H_{coor}
TS1	$^{\bullet}CH_2NH_2$	-426.816451	0.206641	-426.666498	-426.588998	0.149953	0.227453
TS2	$^{\bullet}CH_2CH=CF_2$	-647.414469	0.208130	-647.269559	-647.182587	0.144910	0.231882
TS3	$^{\bullet}CH_2CH=CH_2$	-448.875976	0.223163	-448.712458	-448.631106	0.163518	0.244870
TS4	^{t}Bu	-489.427749	0.273155	-489.216453	-489.129628	0.211296	0.298120
TS5	$^{\bullet}CH_2N=CH_2$	-464.919843	0.211902	-464.765727	-464.686783	0.154116	0.233060
TS6	$^{\bullet}CH_2Ph$	-602.570213	0.271349	-602.363553	-602.273572	0.206660	0.296641
TS7	^{i}Pr	-450.098514	0.245329	-449.913550	-449.830261	0.184964	0.268253
TS8	$^{\bullet}CH_2SH$	-769.666686	0.189545	-769.535709	-769.456322	0.130977	0.210364
TS9	^{n}Bu	-489.418979	0.274016	-489.209102	-489.120144	0.209877	0.298835
TS10	^{n}Pr	-450.094485	0.245685	-449.910453	-449.825982	0.184032	0.268503
TS11	$^{\bullet}CH(CH_3)CN$	-503.060776	0.217839	-502.903934	-502.820144	0.156842	0.240632
TS12	$^{\bullet}(CH_2)_4CN$	-581.691095	0.273669	-581.486598	-581.390428	0.204497	0.300667
TS13	$^{\bullet}(CH_2)_3CN$	-542.366977	0.245301	-542.187677	-542.096651	0.179300	0.270326
TS14	Et	-410.770134	0.216844	-410.612824	-410.532177	0.157310	0.237957
TS15	$^{\bullet}(CH_2)_2CN$	-503.043135	0.217095	-502.885557	-502.804212	0.157577	0.238922
TS16	$^{\bullet}CH_2F$	-470.710394	0.182348	-470.585206	-470.508367	0.125188	0.202027
TS17	$^{\bullet}CH_2OH$	-446.689513	0.194501	-446.551776	-446.474732	0.137737	0.214781
TS18	Me	-371.443995	0.188197	-371.312926	-371.236539	0.131069	0.207456
TS19	$^{\bullet}CH_2CN$	-463.734286	0.189598	-463.602989	-463.524024	0.131297	0.210262
TS20	$^{\bullet}CH_2CHO$	-484.825349	0.201410	-484.681719	-484.603283	0.143630	0.222066
TS21	$^{\bullet}CH_2COOH$	-560.102537	0.206555	-559.956590	-559.873860	0.145947	0.228677
TS22	$^{\bullet}CHF_2$	-569.989924	0.175505	-569.875130	-569.793906	0.114794	0.196018
TS23	$^{\bullet}CH_2CF_3$	-708.608259	0.195327	-708.478465	-708.389448	0.129794	0.218811
TS24	$^{\bullet}CH_2Cl$	-831.072538	0.181262	-830.950469	-830.871258	0.122069	0.201280
TS25	$^{\bullet}CH_2OCH_3$	-485.999459	0.222603	-485.837356	-485.754702	0.162103	0.244757
TS26	$^{\bullet}CH_2SCH_3$	-808.990728	0.218940	-808.833774	-808.748789	0.156954	0.241939
TS27	$^{\bullet}CH_2NHMe$	-466.131480	0.234713	-465.957303	-465.874083	0.174177	0.257397
TS28	$^{\bullet}CH_2NHCOH$	-540.203977	0.217536	-540.048413	-539.963665	0.155564	0.240312
TS29	$^{\bullet}CH_2COMe$	-524.158408	0.228758	-523.991320	-523.906571	0.167088	0.251837
TS30	$^{\bullet}CH_2CONH_2$	-540.226637	0.218068	-540.068869	-539.985794	0.157768	0.240843
TS31	$^{\bullet}CH_2CF_2H$	-609.324635	0.203358	-609.183038	-609.098829	0.141597	0.225806
TS32	$^{\bullet}CH_2CFH_2$	-510.044323	0.210797	-509.894053	-509.811809	0.150270	0.232514

Table S5 Total electronic energies (E, hartree), zero-point vibrational energies (ZPVE, hartree/particle), Gibbs free energies (G, hartree), enthalpies (H, hartree), thermal corrections to Gibbs free energy (G_{corr}, hartree), and thermal corrections to enthalpy (H_{corr}, hartree) of the transition states (**TS**) of the H-atom abstraction reactions of NHC-BH_2CN by R• optimized at the B3LYP/6-311++G(d,p) in BTF at 376 K.

TS	R•	E	ZPVE	G	H	G_{coor}	H_{coor}
TS33	•CH_2NH_2	-519.125015	0.207962	-518.977746	-518.893853	0.147269	0.231162
TS34	•$CH_2CH{=}CF_2$	-739.719650	0.209222	-739.578081	-739.484207	0.141569	0.235443
TS35	•$CH_2CH{=}CH_2$	-541.180978	0.224435	-541.018726	-540.932483	0.162252	0.248495
TS36	^{t}Bu	-581.734877	0.274458	-581.526187	-581.432960	0.208690	0.301917
TS37	•$CH_2N{=}CH_2$	-557.223429	0.212907	-557.072909	-556.986858	0.150520	0.236571
TS38	•CH_2Ph	-694.875263	0.272455	-694.671260	-694.575075	0.204003	0.300187
TS39	^{i}Pr	-542.405651	0.246565	-542.223707	-542.133730	0.181944	0.271922
TS40	•CH_2SH	-861.972673	0.190635	-861.845716	-861.758754	0.126957	0.213919
TS41	^{n}Bu	-581.725623	0.275282	-581.518726	-581.423130	0.206897	0.302493
TS42	^{n}Pr	-542.401037	0.247025	-542.219205	-542.128820	0.181832	0.272217
TS43	•$CH(CH_3)CN$	-595.363769	0.218935	-595.209157	-595.119649	0.154612	0.244120
TS44	•$(CH_2)_4CN$	-673.997262	0.275096	-673.793775	-673.692873	0.203487	0.304389
TS45	•$(CH_2)_3CN$	-634.672876	0.246742	-634.495149	-634.398858	0.177727	0.274018
TS46	Et	-503.076804	0.218388	-502.920661	-502.835111	0.156142	0.241693
TS47	•$(CH_2)_2CN$	-595.347909	0.218434	-595.195599	-595.104170	0.152309	0.243738
TS48	•CH_2F	-563.015949	0.183576	-562.894630	-562.810329	0.121319	0.205620
TS49	•CH_2OH	-538.996589	0.195951	-538.861122	-538.778019	0.135467	0.218570
TS50	Me	-463.749830	0.189518	-463.619946	-463.538794	0.129884	0.211036
TS51	•CH_2CN	-556.036572	0.190610	-555.907333	-555.823012	0.129239	0.213560
TS52	•CH_2CHO	-577.126905	0.201845	-576.986001	-576.901966	0.140904	0.224939
TS53	•CH_2COOH	-652.404420	0.207333	-652.261248	-652.172624	0.143172	0.231796
TS54	•CHF_2	-662.294432	0.176776	-662.180464	-662.094908	0.113968	0.199524
TS55	•CH_2CF_3	-800.911570	0.196397	-800.781436	-800.689513	0.130134	0.222057
TS56	•CH_2Cl	-923.377425	0.182407	-923.257367	-923.172672	0.120058	0.204753
TS57	•CH_2OCH_3	-578.306604	0.223870	-578.147563	-578.058139	0.159041	0.248465
TS58	•CH_2SCH_3	-901.297163	0.220172	-901.142345	-901.051595	0.154818	0.245568
TS59	•CH_2NHMe	-558.440044	0.235952	-558.268637	-558.178875	0.171407	0.261169
TS60	•CH_2NHCOH	-632.509691	0.218903	-632.355387	-632.265700	0.154304	0.243991
TS61	•CH_2COMe	-616.460429	0.229441	-616.295831	-616.205469	0.164598	0.254960
TS62	•CH_2CONH_2	-632.529673	0.218396	-632.377556	-632.285622	0.152117	0.244051
TS63	•CH_2CF_2H	-701.628736	0.204503	-701.488902	-701.399456	0.139834	0.229280
TS64	•CH_2CFH_2	-602.348647	0.211989	-602.200958	-602.112573	0.147689	0.236074

Table S6 Activation barrier ($\Delta E^{\neq}$), activation zero-point vibrational energy correction ($\Delta E^{\neq}_{ZPVE}$), intrinsic barrier ($\Delta E^{\neq}_{0}$), thermal contribution ($\Delta E^{\neq}_{therm}$), activation Gibbs free energy correction ($\Delta G^{\neq}_{corr}$), and Gibbs free energy barrier ($\Delta G^{\neq}$) of the H-atom abstraction reactions of NHC-BH_3 by R$^{\bullet}$ computed at the B3LYP/6-311++G(d,p) in BTF at 376 K. All units are in kcal mol^{-1}.

R$^{\bullet}$	$\Delta E^{\neq}$	$\Delta E^{\neq}_{ZPVE}$	$\Delta E^{\neq}_{0}$	$\Delta E^{\neq}_{therm}$	$\Delta G^{\neq}_{corr}$	$\Delta G^{\neq}$
$^{\bullet}CH_2NH_2$	13.79	-1.30	19.32	-5.53	10.14	25.23
$^{\bullet}CH_2CH=CF_2$	12.53	-1.08	15.67	-3.13	11.02	24.64
$^{\bullet}CH_2CH=CH_2$	13.09	-0.94	15.49	-2.41	10.30	24.32
^{t}Bu	9.74	-0.88	16.10	-6.36	12.80	23.42
$^{\bullet}CH_2N=CH_2$	10.44	-0.31	13.94	-3.50	11.97	22.72
$^{\bullet}CH_2Ph$	10.49	-1.04	14.90	-4.41	11.04	22.57
^{i}Pr	9.57	-0.52	16.98	-7.41	12.19	22.29
$^{\bullet}CH_2SH$	9.30	-0.32	16.34	-7.04	11.81	21.43
^{n}Bu	7.99	-0.67	16.92	-8.93	11.73	20.40
^{n}Pr	8.28	-0.52	17.17	-8.89	10.88	19.68
$^{\bullet}CH(CH_3)CN$	6.55	-0.54	11.27	-4.72	12.11	19.20
$^{\bullet}(CH_2)_4CN$	7.08	-0.74	16.05	-8.97	11.36	19.18
$^{\bullet}(CH_2)_3CN$	6.54	-0.64	15.56	-9.02	11.75	18.93
Et	8.28	-0.56	17.03	-8.75	10.05	18.89
$^{\bullet}(CH_2)_2CN$	4.94	-0.28	14.07	-9.13	13.52	18.74
$^{\bullet}CH_2F$	5.70	-0.55	14.72	-9.02	10.22	16.46
$^{\bullet}CH_2OH$	5.39	0.30	13.61	-8.22	11.46	16.54
Me	6.35	-0.17	16.64	-10.29	8.21	14.73
$^{\bullet}CH_2CN$	2.61	-0.10	9.00	-6.39	11.13	13.84
$^{\bullet}CH_2CHO$	1.22	0.00	6.20	-4.98	12.15	13.37
$^{\bullet}CH_2COOH$	0.91	-0.19	7.10	-6.18	11.86	12.97
$^{\bullet}CHF_2$	2.44	-1.35	10.90	-8.46	8.96	12.76
$^{\bullet}CH_2CF_3$	0.60	-0.27	8.78	-8.17	10.60	11.48
$^{\bullet}CH_2Cl$	5.80	-0.05	14.37	-8.56	10.91	16.76
$^{\bullet}CH_2OCH_3$	9.69	-1.00	16.74	-7.05	10.53	21.23
$^{\bullet}CH_2SCH_3$	10.10	-0.62	16.66	-6.57	11.64	22.36
$^{\bullet}CH_2NHMe$	14.40	-1.50	19.58	-5.18	10.01	25.91
$^{\bullet}CH_2NHCOH$	9.38	-0.70	15.53	-6.15	10.92	21.00
$^{\bullet}CH_2COMe$	1.84	-0.16	7.64	-5.79	12.50	14.50
$^{\bullet}CH_2CONH_2$	3.02	-0.03	10.07	-7.05	13.20	16.25
$^{\bullet}CH_2CF_2H$	2.53	-0.44	11.51	-8.98	12.11	15.09
$^{\bullet}CH_2CFH_2$	4.05	-0.53	12.90	-8.85	12.27	16.85

Table S7 Reaction energies ($\Delta_r E$, kcal mol^{-1}), reaction Gibbs free energies ($\Delta_r G$, kcal mol^{-1}), reaction enthalpies ($\Delta_r H$, kcal mol^{-1}), rate constants (k_H, L mol^{-1} s^{-1}) and activation energies (Ea, kcal mol^{-1}) of the H-atom abstraction reactions of NHC-BH_3 by R$^{\bullet}$ computed at the B3LYP/6-311++G(d,p) in BTF at 376 K.

R$^{\bullet}$	$\Delta_r E$	$\Delta_r G$	$\Delta_r H$	k_H	Ea
$^{\bullet}CH_2NH_2$	-11.98	-12.99	-11.98	9.716×10	14.47
$^{\bullet}CH_2CH=CF_2$	-6.61	-7.04	-6.98	2.283×10^{2}	13.30
$^{\bullet}CH_2CH=CH_2$	-5.02	-5.72	-5.25	3.447×10^{2}	13.83
^{t}Bu	-14.30	-14.03	-14.63	9.821×10^{2}	10.39
$^{\bullet}CH_2N=CH_2$	-7.50	-8.53	-7.39	2.613×10^{3}	11.04
$^{\bullet}CH_2Ph$	-9.59	-11.88	-9.14	3.232×10^{3}	11.44
^{i}Pr	-16.93	-16.79	-17.32	4.319×10^{3}	10.14
$^{\bullet}CH_2SH$	-16.04	-16.26	-16.36	1.292×10^{4}	9.71
^{n}Bu	-21.17	-21.03	-21.48	5.006×10^{4}	8.72
^{n}Pr	-20.97	-21.33	-21.19	1.300×10^{5}	9.04
$^{\bullet}CH(CH_3)CN$	-10.70	-11.02	-10.77	2.455×10^{5}	7.38
$^{\bullet}(CH_2)_4CN$	-21.57	-21.50	-21.84	2.475×10^{5}	7.90
$^{\bullet}(CH_2)_3CN$	-21.89	-21.45	-22.21	3.364×10^{5}	7.35
Et	-20.61	-20.82	-20.92	3.831×10^{5}	8.97
$^{\bullet}(CH_2)_2CN$	-22.92	-23.01	-23.21	3.840×10^{5}	5.26
$^{\bullet}CH_2F$	-22.24	-22.34	-22.33	9.002×10^{6}	6.41
$^{\bullet}CH_2OH$	-20.19	-21.29	-19.96	9.906×10^{6}	6.13
Me	-25.44	-24.66	-25.54	8.676×10^{7}	6.96
$^{\bullet}CH_2CN$	-16.62	-17.70	-16.48	2.597×10^{8}	3.64
$^{\bullet}CH_2CHO$	-13.78	-14.49	-13.97	4.411×10^{8}	2.37
$^{\bullet}CH_2COOH$	-18.21	-18.67	-18.58	7.545×10^{8}	2.18
$^{\bullet}CHF_2$	-22.96	-23.84	-22.84	1.117×10^{9}	3.73
$^{\bullet}CH_2CF_3$	-25.91	-26.11	-26.10	5.428×10^{9}	1.94
$^{\bullet}CH_2Cl$	-20.95	-20.55	-21.31	5.513×10^{6}	6.49
$^{\bullet}CH_2OCH_3$	-16.01	-16.73	-16.07	1.924×10^{4}	10.34
$^{\bullet}CH_2SCH_3$	-14.77	-15.20	-14.99	4.087×10^{3}	10.66
$^{\bullet}CH_2NHMe$	-11.15	-11.90	-11.21	3.976×10	15.16
$^{\bullet}CH_2NHCOH$	-13.83	-14.92	-13.82	2.564×10^{4}	10.03
$^{\bullet}CH_2COMe$	-15.55	-15.49	-15.93	1.005×10^{8}	2.98
$^{\bullet}CH_2CONH_2$	-18.22	-19.23	-18.21	1.029×10^{7}	3.86
$^{\bullet}CH_2CF_2H$	-24.45	-24.36	-24.71	4.698×10^{7}	3.56
$^{\bullet}CH_2CFH_2$	-22.69	-21.80	-23.01	4.987×10^{6}	4.88

Table S8 Activation barrier ($\Delta E^{\neq}$), activation zero-point vibrational energy correction ($\Delta E^{\neq}_{ZPVE}$), intrinsic barrier ($\Delta E^{\neq}_{0}$), thermal contribution ($\Delta E^{\neq}_{therm}$), activation Gibbs free energy correction ($\Delta G^{\neq}_{corr}$), and Gibbs free energy barrier ($\Delta G^{\neq}$) of the H-atom abstraction reactions of NHC-BH_2CN by R$^{\bullet}$ computed at the B3LYP/6-311++G(d,p) in BTF at 376 K. All units are in kcal mol^{-1}.

R$^{\bullet}$	$\Delta E^{\neq}$	$\Delta E^{\neq}_{ZPVE}$	$\Delta E^{\neq}_{0}$	$\Delta E^{\neq}_{therm}$	$\Delta G^{\neq}_{corr}$	$\Delta G^{\neq}$
$^{\bullet}CH_2NH_2$	12.46	-1.30	18.16	-5.70	11.47	25.22
$^{\bullet}CH_2CH=CF_2$	13.18	-1.22	16.54	-3.36	11.94	26.34
$^{\bullet}CH_2CH=CH_2$	13.96	-0.96	16.60	-2.64	12.52	27.44
^{t}Bu	9.30	-0.89	15.83	-6.53	14.18	24.37
$^{\bullet}CH_2N=CH_2$	12.03	-0.50	15.77	-3.74	12.73	25.26
$^{\bullet}CH_2Ph$	11.23	-1.17	15.86	-4.64	12.39	24.78
^{i}Pr	9.08	-0.57	16.65	-7.57	13.31	22.97
$^{\bullet}CH_2SH$	9.44	-0.46	16.68	-7.24	12.30	22.20
^{n}Bu	7.83	-0.71	16.93	-9.10	12.87	21.41
^{n}Pr	8.22	-0.51	17.29	-9.07	12.51	21.25
$^{\bullet}CH(CH_3)CN$	8.57	-0.68	13.59	-5.02	13.73	22.98
$^{\bullet}(CH_2)_4CN$	7.32	-0.67	16.51	-9.19	13.74	21.73
$^{\bullet}(CH_2)_3CN$	6.96	-0.56	16.22	-9.26	13.78	21.29
Et	8.28	-0.42	17.21	-8.93	12.33	21.03
$^{\bullet}(CH_2)_2CN$	6.00	-0.26	15.49	-9.49	13.23	19.49
$^{\bullet}CH_2F$	6.19	-0.60	15.47	-9.28	10.80	17.60
$^{\bullet}CH_2OH$	5.07	0.39	13.42	-8.35	13.05	17.73
Me	6.73	-0.16	17.26	-10.53	10.49	17.38
$^{\bullet}CH_2CN$	5.02	-0.29	12.06	-7.04	12.85	18.17
$^{\bullet}CH_2CHO$	3.73	-0.55	9.53	-5.80	13.45	17.73
$^{\bullet}CH_2COOH$	3.43	-0.53	10.75	-7.32	13.14	17.10
$^{\bullet}CHF_2$	3.62	-1.38	12.62	-9.00	11.46	16.46
$^{\bullet}CH_2CF_3$	2.41	-0.42	11.97	-9.56	13.83	16.67
$^{\bullet}CH_2Cl$	6.67	-0.16	15.54	-8.87	12.66	19.49
$^{\bullet}CH_2OCH_3$	9.22	-1.03	16.43	-7.22	11.63	21.88
$^{\bullet}CH_2SCH_3$	10.04	-0.68	16.81	-6.77	13.32	24.04
$^{\bullet}CH_2NHMe$	13.01	-1.55	18.38	-5.36	11.29	25.85
$^{\bullet}CH_2NHCOH$	9.87	-0.67	16.24	-6.37	13.14	23.68
$^{\bullet}CH_2COMe$	4.21	-0.55	10.73	-6.52	13.96	18.72
$^{\bullet}CH_2CONH_2$	4.53	-0.65	12.07	-7.54	12.67	17.85
$^{\bullet}CH_2CF_2H$	3.89	-0.55	13.48	-9.59	14.02	18.46
$^{\bullet}CH_2CFH_2$	5.29	-0.61	14.58	-9.29	13.67	19.57

Table S9 Reaction energies ($\Delta_r E$, kcal mol^{-1}), reaction Gibbs free energies ($\Delta_r G$, kcal mol^{-1}), reaction enthalpies ($\Delta_r H$, kcal mol^{-1}), rate constants (k_H, L mol^{-1} s^{-1}) and activation energies (Ea, kcal mol^{-1}) of the H-atom abstraction reactions of NHC-BH_2CN by R$^{\bullet}$ computed at the B3LYP/6-311++G(d,p) in BTF at 376 K.

R$^{\bullet}$	$\Delta_r E$	$\Delta_r G$	$\Delta_r H$	k_H	Ea
$^{\bullet}CH_2NH_2$	-12.48	-11.60	-12.81	9.478×10	13.02
$^{\bullet}CH_2CH=CF_2$	-7.11	-5.66	-7.82	2.502×10	13.87
$^{\bullet}CH_2CH=CH_2$	-5.51	-4.33	-6.08	5.752	14.50
^{t}Bu	-14.79	-12.64	-15.47	2.707×10^{2}	9.90
$^{\bullet}CH_2N=CH_2$	-7.99	-7.15	-8.23	9.858×10	12.50
$^{\bullet}CH_2Ph$	-10.08	-10.49	-9.98	1.793×10^{2}	12.05
^{i}Pr	-17.42	-15.40	-18.16	1.719×10^{3}	9.55
$^{\bullet}CH_2SH$	-16.54	-14.88	-17.20	4.892×10^{3}	9.70
^{n}Bu	-21.66	-19.64	-22.32	1.291×10^{4}	8.43
^{n}Pr	-21.46	-19.94	-22.02	1.592×10^{4}	8.85
$^{\bullet}CH(CH_3)CN$	-11.20	-9.63	-11.61	1.789×10^{3}	9.12
$^{\bullet}(CH_2)_4CN$	-22.06	-20.11	-22.68	8.322×10^{3}	7.93
$^{\bullet}(CH_2)_3CN$	-22.39	-20.06	-23.05	1.460×10^{4}	7.53
Et	-21.10	-19.43	-21.75	2.181×10^{4}	8.70
$^{\bullet}(CH_2)_2CN$	-23.41	-21.62	-24.05	1.499×10^{5}	6.70
$^{\bullet}CH_2F$	-22.73	-20.95	-23.17	2.050×10^{6}	6.72
$^{\bullet}CH_2OH$	-20.68	-19.91	-20.80	2.006×10^{6}	5.65
Me	-25.93	-23.27	-26.38	2.541×10^{6}	7.13
$^{\bullet}CH_2CN$	-17.11	-16.31	-17.32	9.200×10^{5}	5.68
$^{\bullet}CH_2CHO$	-14.28	-13.10	-14.81	1.496×10^{6}	4.54
$^{\bullet}CH_2COOH$	-18.70	-17.28	-19.42	3.262×10^{6}	4.41
$^{\bullet}CHF_2$	-23.45	-22.45	-23.68	8.511×10^{6}	4.61
$^{\bullet}CH_2CF_3$	-26.40	-24.73	-26.94	5.506×10^{6}	3.36
$^{\bullet}CH_2Cl$	-21.44	-19.17	-22.15	1.548×10^{5}	7.04
$^{\bullet}CH_2OCH_3$	-16.50	-15.34	-16.91	7.991×10^{3}	9.77
$^{\bullet}CH_2SCH_3$	-15.26	-13.81	-15.82	4.455×10^{2}	10.43
$^{\bullet}CH_2NHMe$	-11.65	-10.52	-12.05	4.168×10	13.77
$^{\bullet}CH_2NHCOH$	-14.32	-13.54	-14.65	7.399×10^{2}	10.31
$^{\bullet}CH_2COMe$	-16.04	-14.10	-16.76	4.189×10^{5}	5.05
$^{\bullet}CH_2CONH_2$	-18.72	-17.84	-19.04	1.314×10^{6}	5.42
$^{\bullet}CH_2CF_2H$	-24.94	-22.97	-25.54	5.462×10^{5}	4.67
$^{\bullet}CH_2CFH_2$	-23.18	-20.41	-23.84	1.386×10^{5}	5.93

Table S10 List of Cartesian coordinates of located stationary points at the B3LYP/6-311++G(d,p) in BTF at 376 K.

NHC-BH_3	C	-0.01195714	0.59840928	0.00036495
	C	0.73707899	-1.53072526	0.00011759
	C	-0.61881869	-1.57624954	0.00042152
	H	1.47209526	-2.32046818	-0.00000226
	H	-1.29830022	-2.41421970	0.00051089
	N	-1.05797167	-0.26736399	0.00054185
	N	1.09067807	-0.19342460	0.00003154
	C	-2.45575981	0.13090918	-0.00001993
	H	-2.84203125	0.14052088	1.02242385
	H	-2.52405257	1.13131172	-0.42381889
	H	-3.04262714	-0.56361400	-0.60659156
	C	2.46988939	0.26781691	-0.00018273
	H	2.98413017	-0.09760485	-0.89279452
	H	2.46515966	1.35601416	-0.00036653
	H	2.98430299	-0.09728658	0.89246058
	H	-0.75242955	2.53027330	0.99719241
	H	0.97620839	2.71293274	0.00121087
	H	-0.75026207	2.52988543	-0.99859987
	B	-0.12474699	2.19536235	0.00003058
NHC-BH_2CN	C	-2.18891000	0.10316100	-0.44796100
	H	-3.16413200	-0.22345100	-0.76400600
	C	-1.64983200	1.34538000	-0.37200500
	H	-2.06288100	2.30928500	-0.61321700
	N	-0.36361400	1.19231200	0.11182200
	C	0.58360200	2.29060000	0.30667900
	H	1.24384900	2.04762000	1.13593900
	H	1.17605500	2.44451000	-0.59611200
	H	0.02694600	3.19718400	0.53710900
	N	-1.21834800	-0.78307000	-0.01512000
	C	-1.40775200	-2.23458200	0.06338800
	H	-2.37653300	-2.47287500	-0.37059800
	H	-0.62577800	-2.74422300	-0.49598200
	H	-1.38470600	-2.56290900	1.10156300
	C	-0.09321800	-0.11569000	0.33054800
	H	1.60289300	-0.11062300	1.89804900
	H	1.11531700	-1.89769200	1.19181000
	B	1.27503600	-0.73559300	0.91207100
	C	2.43621600	-0.61991100	-0.16311600
	N	3.29527000	-0.54104200	-0.93814700
NHC-$^{\bullet}BH_2$	C	0.67933135	-1.50803756	-0.00001675
	H	1.37528748	-2.32932407	-0.00008529

	C	-0.67934825	-1.50804538	0.00016982
	H	-1.37531925	-2.32931900	0.00024863
	N	-1.09459266	-0.19302203	-0.00007515
	C	-2.47794991	0.25000429	-0.00003513
	H	-2.68613661	0.85154082	0.88732044
	H	-2.68600282	0.85210227	-0.88703497
	H	-3.12638188	-0.62469493	-0.00036498
	N	1.09458972	-0.19302400	-0.00017431
	C	2.47795222	0.24998040	0.00004520
	H	3.12636629	-0.62473117	-0.00101163
	H	2.68589571	0.85270947	-0.88654576
	H	2.68628550	0.85088166	0.88780404
	C	-0.00001074	0.66097157	-0.00002694
	B	0.00001983	2.16353766	0.00006256
	H	1.03675603	2.75808017	0.00012678
	H	-1.03667703	2.75814872	0.00015898
NHC-B(•)HCN	C	-2.24247489	0.54701648	-0.00003643
	H	-3.31780369	0.50501618	-0.00006248
	C	-1.40195708	1.61455324	-0.00001640
	H	-1.61311999	2.66980752	-0.00003119
	N	-0.11324127	1.12509943	0.00001660
	C	1.08359139	1.95959081	0.00003099
	H	1.68378147	1.76257506	0.88837966
	H	1.68375510	1.76265221	-0.88835317
	H	0.77420617	3.00281185	0.00008206
	N	-1.46285303	-0.58868237	-0.00001699
	C	-1.98160341	-1.95187208	0.00000390
	H	-3.06877883	-1.90583526	-0.00006615
	H	-1.64301017	-2.48621627	-0.88838518
	H	-1.64311914	-2.48614928	0.88847549
	C	-0.12706772	-0.25168886	0.00002274
	H	0.76938919	-2.41009137	0.00006640
	B	1.01747705	-1.24646575	0.00005393
	C	2.48773786	-0.85242498	0.00002088
	N	3.63008826	-0.61831558	-0.00007520
CH_3NH_2	C	-0.71057100	-0.00000100	0.01716100
	H	-1.12162800	0.88097900	-0.48157700
	H	-1.06828800	-0.00007300	1.05616300
	H	-1.12164600	-0.88089900	-0.48170800
	N	0.75339700	-0.00000100	-0.12456100
	H	1.15060400	0.81209800	0.33804100
	H	1.15060800	-0.81209800	0.33804100
$CH_3CH=CF_2$	C	-2.00947700	0.02868600	0.00000700
	H	-2.82210900	-0.69764300	-0.00005200

	H	-2.12947100	0.66423700	-0.88173700
	H	-2.12952300	0.66415000	0.88180700
	C	-0.68108100	-0.68195900	0.00001200
	H	-0.64341100	-1.76371700	0.00002800
	C	0.48311400	-0.06369800	-0.00000100
	F	1.67857300	-0.65667200	0.00000500
	F	0.65133600	1.26054000	-0.00002200
$CH_3CH=CH_2$	C	1.24070900	-0.15748500	0.00000000
	H	2.01938300	0.60749200	-0.00002800
	H	1.39556600	-0.78804600	-0.88103300
	H	1.39558600	-0.78800000	0.88106300
	C	-0.13860100	0.45854000	0.00000000
	H	-0.18492100	1.54571100	0.00000000
	C	-1.28251800	-0.22498000	0.00000000
	H	-1.29987200	-1.31189900	-0.00000100
	H	-2.24328100	0.27829500	0.00000100
$CH(CH_3)_3$	C	-1.45656600	-0.11922700	0.09590200
	H	-2.06067400	0.71811300	-0.26656700
	H	-1.91546400	-1.04502100	-0.26437600
	H	-1.51344800	-0.12249600	1.19039300
	C	0.83153100	-1.20178400	0.09589800
	H	1.86232300	-1.13693000	-0.26562300
	H	0.86428200	-1.24882000	1.19040300
	H	0.40749800	-2.14362800	-0.26547800
	C	0.62502400	1.32103500	0.09587900
	H	0.64894700	1.37285300	1.19036100
	H	1.65287200	1.42454400	-0.26508400
	H	0.05375700	2.18141100	-0.26590300
	C	-0.00000800	-0.00002300	-0.37232400
	H	0.00002400	-0.00002900	-1.47026000
$CH_3N=CH_2$	C	-1.18290100	0.18280400	-0.00000100
	H	-2.16331800	-0.29172700	0.00009100
	H	-1.15626900	1.28066600	-0.00002000
	N	-0.14182200	-0.53643000	-0.00002900
	C	1.15041000	0.13477700	0.00000700
	H	1.71772900	-0.18567400	-0.87825200
	H	1.07250400	1.23070000	-0.00079400
	H	1.71705100	-0.18444300	0.87914500
CH_3Ph	C	1.20023500	-1.20429900	0.00207700
	C	-0.19455000	-1.20145700	-0.00900600
	C	-0.91413300	0.00000100	-0.01132300
	C	-0.19454900	1.20145700	-0.00900600
	C	1.20023600	1.20429900	0.00207700
	C	1.90405500	0.00000000	0.00849300

	H	1.73672400	-2.14698000	0.00174500
	H	-0.73234000	-2.14435700	-0.01812000
	H	-0.73233900	2.14435800	-0.01812000
	H	1.73672600	2.14697900	0.00174500
	H	2.98825100	-0.00000100	0.01413800
	C	-2.42414600	0.00000000	0.00899800
	H	-2.82932500	-0.88525100	-0.48644700
	H	-2.80125800	-0.00003200	1.03758100
	H	-2.82932500	0.88528200	-0.48639300
$CH_2(CH_3)_2$	C	-1.27709900	-0.25992100	0.00000000
	H	-1.32103700	-0.90522400	0.88338500
	H	-2.17346300	0.36682800	-0.00000400
	H	-1.32103700	-0.90523200	-0.88338000
	C	1.27709900	-0.25992100	0.00000000
	H	2.17346300	0.36682800	-0.00000400
	H	1.32103700	-0.90522400	0.88338500
	H	1.32103700	-0.90523200	-0.88337900
	C	0.00000000	0.58620200	0.00000000
	H	0.00000000	1.24454400	-0.87611300
	H	0.00000000	1.24454900	0.87611000
CH_3SH	C	-1.16695200	0.01961400	0.00000100
	H	-1.53228100	-1.00668100	-0.00005800
	H	-1.52643300	0.52617200	-0.89409800
	H	-1.52644500	0.52608100	0.89414600
	S	0.66684400	-0.08751300	0.00000000
	H	0.91736600	1.23694900	-0.00000100
$CH_3(CH_2)_2CH_3$	C	1.96230300	-0.12104800	-0.00000300
	H	2.10908000	-0.75092900	-0.88356900
	H	2.10912800	-0.75082100	0.88363200
	H	2.74833900	0.63982300	-0.00007300
	C	0.56849100	0.51391100	0.00000300
	H	0.46396900	1.16515300	0.87688700
	H	0.46396400	1.16514400	-0.87688500
	C	-0.56849100	-0.51391100	0.00000400
	H	-0.46396800	-1.16514400	0.87689300
	H	-0.46396500	-1.16515200	-0.87687900
	C	-1.96230300	0.12104800	-0.00000300
	H	-2.10909700	0.75088600	-0.88359700
	H	-2.74833900	-0.63982300	-0.00002000
	H	-2.10911200	0.75086400	0.88360400
$CH_3CH_2CH_3$	C	-1.27709900	-0.25992100	0.00000000
	H	-1.32103700	-0.90522400	0.88338500
	H	-2.17346300	0.36682800	-0.00000400
	H	-1.32103700	-0.90523200	-0.88338000

	C	1.27709900	-0.25992100	0.00000000
	H	2.17346300	0.36682800	-0.00000400
	H	1.32103700	-0.90522400	0.88338500
	H	1.32103700	-0.90523200	-0.88337900
	C	0.00000000	0.58620200	0.00000000
	H	0.00000000	1.24454400	-0.87611300
	H	0.00000000	1.24454900	0.87611000
$CH_2(CH_3)CN$	C	0.00000000	0.80707100	0.00000000
	H	0.29921600	1.38570300	0.87851800
	H	0.29921600	1.38570300	-0.87851800
	C	0.77075500	-0.43407200	0.00000000
	N	1.36961100	-1.42065400	0.00000000
	C	-1.51974500	0.56543900	0.00000000
	H	-2.03617500	1.52659000	0.00000000
	H	-1.82779500	0.00798000	-0.88604300
	H	-1.82779500	0.00798000	0.88604300
$CH_3(CH_2)_3CN$	C	1.65044300	0.48407200	0.00000000
	H	1.69682600	1.13921300	-0.87766700
	H	1.69682600	1.13921300	0.87766700
	C	0.31500700	-0.26621600	0.00000000
	H	0.25290000	-0.91514800	-0.87916200
	H	0.25290000	-0.91514800	0.87916200
	C	-0.88660100	0.70132200	0.00000000
	H	-0.85471600	1.35226500	-0.87928500
	H	-0.85471600	1.35226500	0.87928500
	C	-2.17212700	0.00984100	0.00000000
	N	-3.18081400	-0.55133900	0.00000000
	C	2.85597200	-0.45970800	0.00000000
	H	2.85256800	-1.10501200	-0.88378100
	H	3.79437300	0.10087200	0.00000000
	H	2.85256800	-1.10501200	0.88378100
$CH_3(CH_2)_2CN$	C	-0.88031000	-0.52757400	0.00000000
	H	-0.71884600	-1.15822500	0.87853300
	H	-0.71884600	-1.15822500	-0.87853300
	C	0.16253700	0.61015400	0.00000000
	H	0.03232900	1.24858800	0.87942400
	H	0.03233000	1.24858800	-0.87942400
	C	1.53753700	0.11988600	0.00000000
	N	2.61884000	-0.28392600	0.00000000
	C	-2.30829700	0.01991500	0.00000000
	H	-3.03290900	-0.79761700	0.00000000
	H	-2.49737000	0.63504300	0.88467200
	H	-2.49737000	0.63504300	-0.88467200
CH_3CH_3	C	0.76569900	-0.00003000	0.00000000

	H	1.16238000	0.50966700	-0.88261800
	H	1.16238000	0.50966500	0.88261900
	H	1.16240700	-1.01920200	-0.00000100
	C	-0.76570300	0.00000500	0.00000000
	H	-1.16239900	-0.50960300	0.88264400
	H	-1.16234700	1.01922000	0.00000100
	H	-1.16239900	-0.50960200	-0.88264500
CH_3CH_2CN	C	0.00000000	0.80707100	0.00000000
	H	0.29921600	1.38570300	0.87851800
	H	0.29921600	1.38570300	-0.87851800
	C	0.77075500	-0.43407200	0.00000000
	N	1.36961100	-1.42065400	0.00000000
	C	-1.51974500	0.56543900	0.00000000
	H	-2.03617500	1.52659000	0.00000000
	H	-1.82779500	0.00798000	-0.88604300
	H	-1.82779500	0.00798000	0.88604300
CH_3F	C	0.00000000	0.00000000	-0.64747100
	H	0.00000000	1.03539900	-0.98842700
	H	-0.89668200	-0.51769900	-0.98842700
	H	0.89668200	-0.51769900	-0.98842700
	F	0.00000000	0.00000000	0.76112300
CH_3OH	C	0.67140000	-0.01982600	0.00000200
	H	1.08981700	0.98679100	-0.00119400
	H	1.02440500	-0.54858900	-0.89178300
	H	1.02459200	-0.54656400	0.89292000
	O	-0.75260800	0.12286600	0.00000400
	H	-1.14635000	-0.75560400	0.00001300
CH_4	C	0.00000000	0.00000000	0.00000000
	H	0.62993900	0.62993900	0.62993900
	H	-0.62993900	-0.62993900	0.62993900
	H	-0.62993900	0.62993900	-0.62993900
	H	0.62993900	-0.62993900	-0.62993900
CH_3CN	C	0.00014200	-1.17539600	0.00000000
	H	0.51303100	-1.54879700	0.88806100
	H	0.51303100	-1.54879700	-0.88806100
	C	0.00000000	0.27879300	0.00000000
	N	-0.00023800	1.43232000	0.00000000
	H	-1.02525200	-1.54902600	0.00000000
CH_3CHO	C	-1.16891100	-0.13639100	0.00000300
	H	-1.31116400	-0.76926000	0.88103200
	H	-1.91354900	0.65978300	0.00001800
	H	-1.31119700	-0.76926000	-0.88102200
	C	0.23337500	0.41041900	-0.00002300
	H	0.33646200	1.51344000	0.00004600

	O	1.22658300	-0.28485900	0.00000600
CH_3COOH	C	1.38959900	-0.17233000	0.00000900
	H	1.59792900	-1.24006500	0.00002600
	H	1.83776600	0.29197800	0.88079200
	H	1.83783400	0.29196400	-0.88074600
	C	-0.08581100	0.11622300	-0.00005400
	O	-0.83771600	-1.00584200	0.00000700
	H	-1.77220000	-0.74270900	0.00003500
	O	-0.57779200	1.22277600	0.00001400
CH_2F_2	C	0.00000000	0.51617100	0.00000000
	H	-0.00008400	1.10623400	0.91518000
	H	-0.00008400	1.10623400	-0.91518000
	F	-1.10814400	-0.29492800	0.00000000
	F	1.10816200	-0.29501600	0.00000000
CH_3CF_3	C	1.48437100	-0.00056000	-0.00059300
	H	1.84466100	0.11871100	-1.02202200
	H	1.84468500	-0.94485200	0.40674000
	H	1.84499400	0.82425700	0.61346100
	C	-0.01414000	-0.00002500	-0.00021900
	F	-0.53264000	-1.00789500	-0.74819300
	F	-0.53106700	-0.14418200	1.24715400
	F	-0.53137400	1.15267700	-0.49821800
CH_3Cl	C	0.00000000	0.00000000	-1.14883400
	H	0.00000000	1.03433700	-1.48178400
	H	-0.89576200	-0.51716800	-1.48178400
	H	0.89576200	-0.51716800	-1.48178400
	Cl	0.00000000	0.00000000	0.66696200
CH_3OCH_3	O	0.00000200	0.59143100	0.00000400
	C	-1.17949800	-0.19698100	0.00000100
	H	-1.23180100	-0.83465900	0.89262500
	H	-2.02859100	0.48675200	-0.00090300
	H	-1.23095600	-0.83592700	-0.89176100
	C	1.17949500	-0.19698400	-0.00000200
	H	1.23168500	-0.83481800	-0.89251600
	H	2.02857800	0.48676200	0.00065900
	H	1.23108300	-0.83576900	0.89187300
CH_3SCH_3	C	-1.39902600	-0.51353100	0.00000000
	H	-2.31384200	0.07971800	0.00000000
	H	-1.37977100	-1.13929500	0.89368300
	H	-1.37977100	-1.13929500	-0.89368300
	S	0.00000000	0.66000700	0.00000000
	C	1.39902600	-0.51353100	0.00000000
	H	1.37977100	-1.13929500	-0.89368300
	H	2.31384200	0.07971800	0.00000000

	H	1.37977100	-1.13929500	0.89368300
CH_3NHMe	C	1.21769000	-0.22380700	0.02016200
	H	1.28393700	-0.97021200	-0.77713900
	H	2.09292900	0.42525300	-0.05488500
	H	1.26342400	-0.75877500	0.98373400
	N	0.00000000	0.56627300	-0.15178400
	H	0.00000000	1.32923500	0.51712100
	C	-1.21769100	-0.22380700	0.02016200
	H	-2.09292900	0.42525300	-0.05488500
	H	-1.28393700	-0.97021200	-0.77713900
	H	-1.26342400	-0.75877500	0.98373400
CH_3NHCOH	N	-0.39237300	-0.40735500	-0.00004300
	H	-0.26240400	-1.41117900	0.00000700
	C	0.72354800	0.34508900	-0.00002100
	H	0.51116600	1.42752000	-0.00004100
	O	1.87061000	-0.09158400	0.00002800
	C	-1.75118500	0.11795200	0.00003000
	H	-1.71122900	1.20761200	-0.00088900
	H	-2.29528500	-0.20972800	-0.88859000
	H	-2.29469200	-0.20831400	0.88953200
CH_3COMe	C	-1.28081800	-0.62908300	0.00000000
	H	-1.10840500	-1.70535800	-0.00000700
	H	-1.86902300	-0.35773000	0.88074600
	H	-1.86903100	-0.35771900	-0.88073700
	C	0.00569200	0.17391700	0.00000000
	O	-0.02111500	1.39208700	0.00000000
	C	1.30354800	-0.59506400	0.00000000
	H	1.34401400	-1.24823700	0.87790100
	H	1.34401500	-1.24823600	-0.87790200
	H	2.15682500	0.08197700	0.00000100
CH_3CONH_2	C	1.36082400	-0.34156500	-0.00000100
	H	1.45709400	-1.42766600	-0.00027900
	H	1.86353500	0.06192100	0.88135900
	H	1.86372400	0.06242700	-0.88101300
	C	-0.07661500	0.13741900	-0.00001000
	O	-0.35859900	1.33435400	0.00000200
	N	-1.03042400	-0.82602200	-0.00001800
	H	-2.00327800	-0.55732000	0.00008900
	H	-0.80456700	-1.80716100	0.00002400
CH_3CF_2H	C	0.05062900	0.00072400	0.36315100
	H	0.19087100	0.00030300	1.44438500
	F	0.72074100	-1.10408300	-0.13588200
	F	0.71962700	1.10433800	-0.13609600
	C	-1.37791700	-0.00067500	-0.09442700

	H	-1.88455000	-0.88808100	0.28859400
	H	-1.88612500	0.88625300	0.28781500
	H	-1.41977700	-0.00106400	-1.18533800
CH_3CFH_2	C	0.09449500	0.55421300	-0.00003500
	H	0.20096500	1.17574200	0.89108600
	F	1.19941500	-0.33926200	0.00001500
	C	-1.19631200	-0.22873400	-0.00001700
	H	-1.27234000	-0.85851600	0.88927200
	H	-2.04081700	0.46664400	0.00005600
	H	-1.27291100	-0.85891800	-0.88899000
	H	0.20126900	1.17553000	-0.89124900
$^{\bullet}CH_2NH_2$	C	0.72866700	0.00001100	0.07718200
	H	1.24332700	-0.93220900	-0.11624400
	H	1.24285400	0.93242600	-0.11652100
	N	-0.65439100	-0.00000500	-0.09154600
	H	-1.13861300	-0.83668900	0.20505200
	H	-1.13882800	0.83644000	0.20544200
$^{\bullet}CH_2CH=CF_2$	C	-0.43087500	-0.04969900	-0.00000600
	C	0.80388700	-0.63610900	0.00008400
	H	0.79127500	-1.72014600	0.00018500
	C	2.00790100	0.05066500	0.00005300
	H	2.94214700	-0.49274000	0.00013000
	H	2.04534200	1.13218600	-0.00004900
	F	-0.64941900	1.26007800	-0.00013600
	F	-1.57994100	-0.71657200	0.00002000
$^{\bullet}CH_2CH=CH_2$	C	-1.22867500	-0.19644100	-0.00007800
	H	-2.15537600	0.36337100	-0.00013300
	H	-1.29629500	-1.27933200	0.00012500
	C	0.00003200	0.44303900	0.00018900
	H	0.00007100	1.53126200	-0.00026500
	C	1.22864800	-0.19650900	-0.00001300
	H	2.15527300	0.36354200	-0.00023900
	H	1.29629600	-1.27937400	-0.00007100
^{t}Bu	C	1.47985300	-0.12886800	0.01565300
	H	1.86371300	-1.05302300	-0.42816900
	H	2.01737200	0.71545300	-0.42773500
	H	1.76157600	-0.15364800	1.08424100
	C	0.00014400	-0.00004900	-0.16108100
	C	-0.62829500	1.34575500	0.01564300
	H	-1.62746800	1.38963600	-0.42961700
	H	-0.74979600	1.60125900	1.08418800
	H	-0.01878700	2.14047800	-0.42627300
	C	-0.85157000	-1.21691000	0.01564000
	H	-1.01572400	-1.44737300	1.08417300
	H	-1.84305500	-1.08719300	-0.42989600
	H	-0.38862200	-2.10515500	-0.42604000
$^{\bullet}CH_2N=CH_2$	C	1.14180000	0.15634300	-0.00008600
	H	2.07309100	-0.39842300	0.00020000

	H	1.17809700	1.24931800	-0.00009200
	N	-0.00011800	-0.51110100	0.00005800
	C	-1.14156100	0.15622200	0.00000900
	H	-2.07329200	-0.39794200	-0.00032400
	H	-1.17850300	1.24936000	0.00027700
$^{\bullet}CH_2Ph$	C	-1.13265600	-1.21123300	-0.00000400
	C	0.25193100	-1.21814800	-0.00000200
	C	0.99453800	0.00000000	0.00000100
	C	0.25193100	1.21814800	-0.00000100
	C	-1.13265600	1.21123300	0.00000400
	C	-1.83803900	0.00000000	0.00000100
	H	-1.67507200	-2.15038300	-0.00001500
	H	0.79111900	-2.15951000	-0.00000400
	H	0.79111900	2.15951000	0.00000200
	H	-1.67507200	2.15038300	0.00001600
	H	-2.92176600	0.00000000	0.00000100
	C	2.40026100	0.00000000	0.00000000
	H	2.95890700	0.92791800	-0.00007800
	H	2.95890700	-0.92791800	0.00008100
^{i}Pr	C	0.00000000	0.53528000	-0.04531000
	H	0.00000400	1.61041700	0.10137200
	C	1.29718300	-0.19806800	0.00257000
	H	1.31632600	-1.03096600	-0.71213700
	H	2.14632100	0.45528000	-0.21239200
	H	1.47790900	-0.64695900	0.99434700
	C	-1.29718400	-0.19806600	0.00257200
	H	-2.14633800	0.45532300	-0.21220000
	H	-1.31640300	-1.03084400	-0.71227600
	H	-1.47781300	-0.64713000	0.99428800
$^{\bullet}CH_2SH$	C	1.14623600	0.02202900	-0.00038600
	H	1.64496300	0.97837600	0.00145900
	H	1.69352100	-0.90811200	0.00022900
	S	-0.58460600	-0.08950100	0.00009200
	H	-0.86220500	1.22958300	-0.00084300
^{n}Bu	C	1.88995700	0.11630600	0.00000700
	H	2.03105400	0.74655300	0.88369700
	H	2.03104700	0.74662800	-0.88363300
	H	2.68062100	-0.63922500	-0.00003300
	C	0.50409600	-0.53389300	-0.00001000
	H	0.39638800	-1.18057500	-0.87757800
	H	0.39638100	-1.18059500	0.87754500
	C	-0.64411000	0.50979000	-0.00000500
	H	-0.51796200	1.15105600	-0.88115500
	H	-0.51794900	1.15106400	0.88113800
	C	-2.00540900	-0.09509100	0.00000700
	H	-2.48337600	-0.38879700	0.92758900
	H	-2.48340800	-0.38877800	-0.92756500
^{n}Pr	C	-0.08095800	0.55132500	0.05107600
	H	-0.10807300	1.32014300	-0.73115000
	H	-0.08502900	1.11650600	0.99995900

	C	-1.30514100	-0.29365400	-0.03056800
	H	-2.26185700	0.13531600	-0.30510500
	H	-1.29306400	-1.31992200	0.32085400
	C	1.22919100	-0.24273600	-0.03806300
	H	1.30810200	-0.76306400	-0.99678800
	H	2.09637000	0.41539300	0.06196000
	H	1.28500400	-0.99398100	0.75560000
$^{\bullet}CH(CH_3)CN$	C	-0.44502300	0.56625800	0.00001100
	H	-0.58833800	1.64120000	0.00011100
	C	-1.63110700	-0.33792300	0.00000600
	H	-2.25696900	-0.14104900	0.87828300
	H	-2.25750400	-0.14032100	-0.87772700
	H	-1.34810000	-1.39004200	-0.00050900
	C	0.86100900	0.10713600	-0.00011500
	N	1.96309100	-0.28323100	0.00006200
$^{\bullet}(CH_2)_4CN$	C	-1.43145200	2.56908100	0.00000000
	H	-1.36632500	3.12461200	0.92819200
	H	-1.36632500	3.12461200	-0.92819200
	C	-1.42811600	1.07921600	0.00000000
	H	-1.95860000	0.70137200	0.88188000
	H	-1.95860000	0.70137200	-0.88188000
	C	0.00000000	0.47991200	0.00000000
	H	0.54628200	0.82877200	-0.88009800
	H	0.54628200	0.82877200	0.88009800
	C	-0.04337500	-1.06287700	0.00000000
	H	-0.58048800	-1.43076600	-0.87974000
	H	-0.58048800	-1.43076600	0.87974000
	C	1.28644300	-1.66330700	0.00000000
	N	2.34532200	-2.12287500	0.00000000
$^{\bullet}(CH_2)_3CN$	C	-0.09513800	0.63057200	-0.00000100
	H	0.04158600	1.26346500	0.88055100
	H	0.04158700	1.26346400	-0.88055300
	C	0.95414600	-0.52791700	0.00000100
	H	0.77096000	-1.14726700	0.88255700
	H	0.77096100	-1.14726800	-0.88255400
	C	-1.46646200	0.13223700	-0.00000100
	N	-2.54171000	-0.28731200	-0.00000100
	C	2.35121900	-0.01468000	0.00000100
	H	2.85213900	0.22875700	-0.92915000
	H	2.85214000	0.22875600	0.92915300
Et	C	-0.00982900	-0.69350900	0.00000000
	H	-0.50460200	-1.10064700	0.88717400
	H	-0.50460200	-1.10064700	-0.88717400
	H	1.01369200	-1.10298600	0.00000000
	C	-0.00982900	0.79405900	0.00000000
	H	0.05673200	1.35048900	-0.92723000
	H	0.05673200	1.35048900	0.92723000
$^{\bullet}(CH_2)_2CN$	C	0.55731000	0.59935800	0.03063700
	H	0.66530700	1.20470200	0.94458100
	H	0.68123500	1.30527500	-0.79918600

	C	1.58882900	-0.48309400	-0.02694000
	H	1.35246400	-1.49883000	0.25681900
	H	2.61404300	-0.21133900	-0.23736800
	C	-0.81662100	0.09967500	-0.00178200
	N	-1.89859300	-0.29934900	-0.02519100
$^{\bullet}CH_2F$	C	0.02412900	0.66372700	0.00000000
	H	-0.18096900	1.11091800	0.96223600
	H	-0.18096900	1.11091800	-0.96223600
	F	0.02412900	-0.68935500	0.00000000
$^{\bullet}CH_2OH$	C	0.03555300	0.68895600	0.00000000
	H	0.18257500	1.19251900	-0.94914800
	H	0.18257500	1.19251900	0.94914800
	O	0.03555300	-0.68497000	0.00000000
	H	-0.86289000	-1.03901400	0.00000000
Me	C	0.00000100	0.00001200	0.00000000
	H	-0.92996800	0.55122600	0.00000100
	H	0.94240800	0.52967500	0.00000100
	H	-0.01244500	-1.08097400	0.00000100
$^{\bullet}CH_2CN$	C	-0.00781600	-1.19857400	0.00000000
	H	-0.01166500	-1.75023300	0.93290900
	H	-0.01166500	-1.75023300	-0.93290900
	C	0.00000000	0.18226600	0.00000000
	N	0.01003200	1.37118800	0.00000000
$^{\bullet}CH_2CHO$	C	1.16893600	-0.17254300	-0.00001100
	H	2.05385900	0.45212000	0.00011000
	H	1.27805300	-1.25086400	-0.00004100
	C	-0.12974500	0.40680800	-0.00000800
	H	-0.18726200	1.50770300	-0.00004600
	O	-1.17247400	-0.26431900	0.00001100
$^{\bullet}CH_2COOH$	C	-0.01279000	0.10757700	-0.00000300
	O	-0.85958100	-0.95455200	0.00001000
	H	-1.76691400	-0.61314600	-0.00002000
	O	-0.41635200	1.26186200	-0.00000300
	C	1.37663500	-0.27846900	-0.00000800
	H	2.12549100	0.49998500	0.00007300
	H	1.66581600	-1.31996800	-0.00004000
$^{\bullet}CHF_2$	C	0.02990200	0.51629700	0.00000000
	H	-0.71765600	1.30664000	0.00000000
	F	0.02990200	-0.24469000	-1.09899900
	F	0.02990200	-0.24469000	1.09899900
$^{\bullet}CH_2CF_3$	C	-1.50187300	-0.00024600	-0.02059600
	H	-2.02353000	0.94325700	0.04100400
	H	-2.02325700	-0.94390800	0.04091400
	C	-0.02951700	-0.00003300	-0.01004000
	F	0.48596400	-0.00143700	1.25818600
	F	0.49207300	1.09184300	-0.62212400
	F	0.49253200	-1.09014800	-0.62474000
$^{\bullet}CH_2Cl$	C	1.12953600	0.00001400	-0.00144000
	H	1.62328900	0.95805600	0.00335600
	H	1.62327500	-0.95812800	0.00335500

	Cl	-0.58963400	-0.00000100	0.00011300
$^{\bullet}CH_2OCH_3$	O	-0.09456000	-0.54175400	-0.03332000
	C	1.14645600	0.16876200	0.01088300
	H	1.26595000	0.66739600	0.97715300
	H	1.93622800	-0.56784500	-0.12407600
	H	1.19148700	0.90996000	-0.79335500
	C	-1.20795800	0.22667400	0.06267300
	H	-1.13645100	1.27780800	-0.19814800
	H	-2.13172300	-0.32590100	-0.03634300
$^{\bullet}CH_2SCH_3$	C	-1.36137500	0.57671500	0.02831800
	H	-1.14349700	1.61976300	-0.15461500
	H	-2.37855700	0.21265500	0.04480300
	S	-0.11006500	-0.60674900	-0.01023800
	C	1.39347100	0.42814500	0.01054600
	H	1.43400600	1.01448000	0.92822200
	H	2.24443800	-0.25098300	-0.02712500
	H	1.41207000	1.08291300	-0.86066800
$^{\bullet}CH_2NHMe$	C	1.25874200	-0.25181200	0.08389300
	H	1.25282200	-1.28903700	-0.22986600
	H	2.18816400	0.30203600	0.05054100
	N	0.09524600	0.46832000	-0.12797700
	H	0.11805200	1.42270200	0.20513900
	C	-1.19530600	-0.18650400	0.03120400
	H	-1.98896500	0.48292300	-0.30335000
	H	-1.22264000	-1.08629500	-0.58839500
	H	-1.39477200	-0.48067200	1.07118400
$^{\bullet}CH_2NHCOH$	C	-1.76683900	0.12322000	-0.00010500
	H	-1.91145300	1.19185200	0.00017600
	H	-2.58241000	-0.57941200	0.00045300
	N	-0.48167900	-0.37115600	0.00000200
	H	-0.35231900	-1.37718000	-0.00016600
	C	0.66741800	0.36439800	-0.00000200
	H	0.48669500	1.44955600	-0.00004200
	O	1.79097000	-0.12655400	0.00002600
$^{\bullet}CH_2COMe$	C	1.35575000	-0.35350100	-0.00000300
	H	1.55317400	-0.97282300	-0.87997600
	H	2.02893900	0.50265400	-0.00037100
	H	1.55333000	-0.97215600	0.88040900
	C	-0.08374700	0.11659400	-0.00000900
	O	-0.36863600	1.32405000	0.00000000
	C	-1.12596100	-0.87400300	0.00000000
	H	-0.90308500	-1.93409700	-0.00001500
	H	-2.15951800	-0.55052100	0.00002300
$^{\bullet}CH_2CONH_2$	C	-1.27937200	-0.58997800	-0.00001300
	H	-1.33800500	-1.67127000	0.00000100
	H	-2.18939700	-0.00691000	0.00019600
	C	-0.01107900	0.12154500	-0.00002900
	O	0.04453300	1.35990100	0.00002600
	N	1.11602700	-0.64832200	-0.00019700
	H	2.01792300	-0.19744100	0.00057300

	H	1.08372300	-1.65473600	0.00065500
$^{\bullet}CH_2CF_2H$	C	1.40351900	-0.04037500	-0.10765000
	H	2.21506600	0.16465100	0.57553100
	H	1.59846100	-0.21723700	-1.15741700
	C	0.01107700	0.00144700	0.36413500
	H	-0.11121600	0.02936700	1.44563300
	F	-0.65203800	1.11663700	-0.15281400
	F	-0.70239400	-1.08810500	-0.11414800
$^{\bullet}CH_2CFH_2$	C	1.23845700	-0.20604800	-0.00018200
	H	1.68360400	-0.53130000	-0.93205200
	H	1.67628900	-0.54782700	0.92927200
	C	-0.02726000	0.55063700	0.00167500
	H	-0.15527900	1.15726000	0.89834300
	F	-1.14640700	-0.36761300	-0.00147600
	H	-0.15413600	1.16285200	-0.89123700
TS1	C	-0.48410700	0.00001900	0.62893700
	C	-2.02723100	0.67751800	-0.88769300
	C	-2.02720800	-0.67763800	-0.88764800
	H	-2.61300800	1.37876800	-1.45645400
	H	-2.61295900	-1.37894100	-1.45637100
	N	-1.08717400	-1.08393800	0.04578200
	N	-1.08720900	1.08391500	0.04570400
	C	-0.75181400	-2.47124500	0.33595400
	H	-1.47652300	-3.11608800	-0.15861700
	H	0.24966300	-2.70900100	-0.02847100
	H	-0.78443500	-2.64588800	1.41110200
	C	-0.75191100	2.47125600	0.33578500
	H	-0.78472700	2.64602700	1.41090800
	H	0.24962700	2.70898200	-0.02848700
	H	-1.47653800	3.11603000	-0.15899400
	H	1.83112900	0.00015600	0.88033400
	B	0.69951700	0.00008500	1.64290500
	H	0.77621200	-1.01822000	2.29330500
	H	0.77609100	1.01840000	2.29330300
	C	3.21845500	0.00022100	0.09977700
	H	3.64302200	-0.91503800	0.50264200
	H	3.64265200	0.91587300	0.50213900
	N	2.96501800	-0.00022000	-1.29058000
	H	3.24511100	0.83236500	-1.78916200
	H	3.24555100	-0.83292400	-1.78871700
TS2	C	1.51752500	-0.15632700	0.62784200
	C	2.66593200	0.64394500	-1.14692900
	C	2.04963800	1.69600900	-0.55309000
	H	3.30709400	0.60124300	-2.01015800
	H	2.05060200	2.74287100	-0.80254400
	N	1.35280100	1.19583500	0.53289400
	N	2.33425700	-0.48361800	-0.41640600
	C	0.51390300	1.99629200	1.41897100
	H	-0.54132000	1.78086800	1.24094400

	H	0.75152800	1.77155500	2.45764200
	H	0.70618400	3.04922100	1.22117200
	C	2.78831500	-1.83616000	-0.72485300
	H	3.45814900	-1.78818500	-1.58137100
	H	3.31927900	-2.25810000	0.12815200
	H	1.93901100	-2.47592600	-0.96623600
	H	1.39754300	-2.19256400	1.75669000
	H	0.49164200	-0.60844900	2.67278900
	B	0.83621300	-1.13117700	1.64131200
	H	-0.37163300	-1.45411400	1.05051700
	C	-1.68967500	-1.94355300	0.47541900
	H	-1.84311600	-2.77600100	1.15282800
	H	-1.30764800	-2.22605800	-0.50033300
	C	-2.66478100	-0.88981100	0.53162500
	H	-3.25138700	-0.75226600	1.43291400
	C	-2.86362200	0.03520800	-0.41689500
	F	-3.73938000	1.04636900	-0.33737100
	F	-2.26059900	0.06281500	-1.61235300
TS3	C	0.82486000	0.10604600	0.61225300
	C	1.77813900	-1.47417400	-0.69190100
	C	2.36735000	-0.28991600	-0.99159300
	H	1.94852300	-2.46197700	-1.08342200
	H	3.14919800	-0.05207100	-1.69173100
	N	1.77676600	0.66986200	-0.18880500
	N	0.83817000	-1.22105300	0.29156200
	C	2.11775500	2.08934600	-0.20526300
	H	2.96188300	2.23369400	-0.87711100
	H	1.27155500	2.68022800	-0.55762500
	H	2.38983900	2.42145200	0.79615200
	C	-0.05312700	-2.22484400	0.86448500
	H	0.27651200	-3.20845300	0.53454600
	H	-0.01801800	-2.17574300	1.95191400
	H	-1.07909300	-2.05371700	0.53130700
	H	-0.58777300	0.12934600	2.46708200
	H	0.23232900	1.92536100	1.94598300
	B	-0.14508500	0.83534700	1.59522200
	H	-1.25823600	1.09631400	0.81226200
	C	-2.56912200	1.44750900	0.15847300
	H	-2.30056100	2.45736800	-0.13579700
	H	-3.17212900	1.39162200	1.06121000
	C	-2.83973200	0.49765900	-0.88198900
	H	-2.40172800	0.70936600	-1.85669300
	C	-3.52036300	-0.66979800	-0.73713100
	H	-3.98093600	-0.94402600	0.20750600

	H	-3.64505500	-1.35812000	-1.56500500
TS4	C	-3.64097800	-0.24991600	0.84082500
	H	-3.47766700	-1.21005600	1.34047000
	H	-3.62534400	0.53527700	1.60336900
	H	-4.65980300	-0.27226300	0.41865000
	C	-2.61549000	1.37984400	-0.82845900
	H	-1.74477600	1.54186600	-1.47280000
	H	-3.51130600	1.54441900	-1.45047100
	H	-2.61435800	2.15439800	-0.05459900
	C	-2.38679200	-1.13101100	-1.19680300
	H	-3.25643700	-1.26970000	-1.86083000
	H	-1.51981400	-0.94432300	-1.83933500
	H	-2.22646100	-2.08114600	-0.67648800
	C	-2.61030600	-0.00066200	-0.22778700
	H	-1.23305600	-0.00032600	0.61134000
	B	-0.19243500	-0.00063600	1.46792700
	C	1.10335700	0.00010100	0.59148800
	H	-0.32675400	-1.01836400	2.10917900
	H	-0.32732000	1.01581500	2.11123700
	N	1.76871300	1.08275300	0.08627700
	N	1.77045800	-1.08213700	0.08752200
	C	2.81966600	0.67839900	-0.72071800
	C	1.40791900	2.47127600	0.34596800
	C	2.82059000	-0.67703500	-0.72013000
	C	1.40929300	-2.47092800	0.34507700
	H	3.46972700	1.38089600	-1.21279700
	H	2.14405200	3.11601300	-0.13103100
	H	0.41894400	2.69013800	-0.05983500
	H	1.39832000	2.66256400	1.41893200
	H	3.47140800	-1.37907500	-1.21186200
	H	2.15203700	-3.11511100	-0.12234100
	H	1.38760400	-2.66029200	1.41811600
	H	0.42544000	-2.69227700	-0.07189400
TS5	C	0.78542700	-0.09236900	0.59735900
	C	2.41432900	0.19392900	-0.93843200
	C	1.86592200	1.41052400	-0.69385000
	H	3.21489200	-0.09587200	-1.59650200
	H	2.09678300	2.37969300	-1.10035600
	N	0.87195500	1.22295100	0.24926500
	N	1.74505100	-0.71757400	-0.14287300
	C	0.00398200	2.27960800	0.76046000
	H	0.36645700	3.23516300	0.38613600
	H	-1.02188300	2.12119500	0.42127800
	H	0.02290800	2.28435400	1.84935000

	C	2.01583300	-2.15282600	-0.11640400
	H	2.86687600	-2.35479700	-0.76403100
	H	2.24791500	-2.47240300	0.89897100
	H	1.14942600	-2.70812700	-0.47640100
	H	0.07329800	-1.83394700	1.98083300
	B	-0.25654400	-0.75475700	1.55909600
	H	-1.31773900	-1.04312800	0.72914500
	C	-2.57819500	-1.38588300	0.02528600
	H	-2.28041300	-2.37086200	-0.32149200
	H	-3.21398300	-1.37952200	0.91660000
	C	-3.43029200	0.64484900	-0.65195800
	H	-3.56734600	1.40481100	-1.41566400
	H	-3.86513600	0.82602800	0.33759600
	N	-2.79117400	-0.44937000	-0.94955500
	H	-0.73220900	0.00216300	2.36642900
TS6	C	2.66256800	-0.25055200	-1.75462700
	C	1.94470100	0.82247500	-1.24070800
	C	1.96630500	1.12791600	0.14253500
	C	2.73951000	0.28556300	0.97911900
	C	3.45555900	-0.78635900	0.45997200
	C	3.42558200	-1.06573800	-0.91090400
	H	2.63306000	-0.45394100	-2.82019700
	H	1.36094500	1.44818500	-1.90880500
	H	2.77601700	0.49200600	2.04423400
	H	4.04554200	-1.40874600	1.12501600
	H	3.98772400	-1.90032600	-1.31407500
	C	1.17488700	2.20307200	0.68672000
	H	0.81207400	2.96058100	-0.00104500
	H	1.43708800	2.57606100	1.67158900
	H	-0.19995000	1.63456200	1.08228100
	B	-1.41179300	1.23737200	1.58383700
	C	-1.89014100	0.12207800	0.59607200
	H	-2.08994600	2.23507000	1.56035900
	H	-1.13471200	0.82600700	2.68408100
	N	-1.57000100	-1.20418700	0.62479000
	N	-2.64220000	0.27700300	-0.53255900
	C	-2.10538300	-1.85767400	-0.47069400
	C	-0.74083900	-1.83799000	1.64557700
	C	-2.77808300	-0.92958000	-1.19585100
	C	-3.20704600	1.54301800	-0.99007900
	H	-1.96864200	-2.91243800	-0.63442300
	H	-0.75963600	-2.91458900	1.48637400
	H	0.28724100	-1.47855300	1.57567100
	H	-1.13212000	-1.60987800	2.63618400

	H	-3.34011800	-1.02377100	-2.10873100
	H	-3.84138800	1.34677900	-1.85255800
	H	-3.80164100	1.99528000	-0.19724300
	H	-2.41288900	2.23376700	-1.27630800
TS7	C	-0.82552200	0.01952800	0.60215200
	C	-2.35347700	0.76344300	-0.89276300
	C	-2.43314900	-0.58953600	-0.86987000
	H	-2.90808900	1.48971700	-1.46127000
	H	-3.07035600	-1.26499700	-1.41384800
	N	-1.49747900	-1.03415700	0.04977600
	N	-1.37035100	1.12570600	0.01352500
	H	0.47827100	0.98371300	2.26283500
	H	0.38101800	-1.04679200	2.27407800
	B	0.37014300	-0.03243700	1.61346900
	H	1.49212300	-0.08754900	0.87987500
	C	2.95515300	-0.14805200	0.15886700
	H	3.55444600	-0.30262400	1.05500200
	C	3.09146600	1.20732200	-0.47429300
	H	2.29024200	1.38857600	-1.20111300
	H	3.05652900	2.00768600	0.27088000
	H	4.04229300	1.31278900	-1.02078200
	C	-1.24385400	-2.43572400	0.36322800
	H	-0.24544600	-2.72562400	0.03169200
	H	-1.31950900	-2.59859500	1.43786400
	H	-1.98543900	-3.04525500	-0.15016900
	C	2.84785900	-1.33868700	-0.75095200
	H	2.64594900	-2.25841600	-0.19348300
	H	2.04401700	-1.20636200	-1.48534100
	H	3.77431000	-1.50356800	-1.32397100
	C	-0.94957300	2.49656700	0.27938400
	H	-1.00413800	2.70403700	1.34759700
	H	0.07657600	2.65171200	-0.05806000
	H	-1.61211400	3.17372100	-0.25675900
TS8	C	-0.94320300	-0.08703500	0.58760100
	C	-2.10060600	1.30130100	-0.76833500
	C	-2.56219400	0.04466100	-0.98341600
	H	-2.38755000	2.24048600	-1.20839700
	H	-3.32936400	-0.31873000	-1.64473900
	N	-1.84675100	-0.79581900	-0.14741200
	N	-1.11207400	1.20790000	0.19645000
	C	-2.02555800	-2.24298200	-0.07375000
	H	-2.82506000	-2.52727900	-0.75544300
	H	-1.10635100	-2.75282500	-0.36294600
	H	-2.29063100	-2.53813000	0.94119300

	C	-0.33071200	2.33451500	0.69777700
	H	-0.71592600	3.24869700	0.24996400
	H	-0.41558700	2.39653100	1.78219800
	H	0.71938300	2.21298700	0.42865300
	H	0.48659600	0.16606800	2.40431100
	H	-0.17713000	-1.72413100	2.05329400
	B	0.12875700	-0.65093000	1.58717800
	H	1.21617600	-0.88372800	0.83685300
	C	2.59529100	-1.24602000	0.04391700
	H	3.15882800	-1.75269600	0.82183700
	H	2.20840400	-1.89539800	-0.73541100
	S	3.37700900	0.19107500	-0.66277500
	H	3.69594800	0.81439600	0.49112600
TS9	C	-1.65349700	-0.00014400	0.48118500
	C	-3.47829700	0.67793800	-0.66918000
	C	-3.47839200	-0.67765500	-0.66936500
	H	-4.16927700	1.38129300	-1.10038200
	H	-4.16947600	-1.38079400	-1.10075000
	N	-2.35775100	-1.08087100	0.03792200
	N	-2.35760100	1.08080500	0.03822000
	C	-1.97664200	-2.47103000	0.26756900
	H	-2.74445900	-3.11436500	-0.15829200
	H	-1.01974200	-2.68652100	-0.20880800
	H	-1.89124100	-2.66485700	1.33646500
	C	-1.97624100	2.47084400	0.26816200
	H	-2.74410900	3.11440800	-0.15726000
	H	-1.89048000	2.66433400	1.33709000
	H	-1.01946000	2.68635900	-0.20844900
	H	-0.09146900	1.01534000	1.86953600
	H	-0.09133500	-1.01646100	1.86877000
	B	-0.27766600	-0.00033600	1.23800500
	H	0.65384200	0.00013600	0.28115500
	C	1.94294200	0.00081700	-0.76259200
	C	3.16511100	-0.00012100	0.11105600
	H	1.72524000	-0.91082600	-1.31614200
	H	1.72550300	0.91347100	-1.31457800
	H	3.14737300	-0.87840000	0.76934000
	H	3.14748000	0.87683500	0.77110300
	C	4.50172900	0.00059100	-0.66227700
	H	4.53517300	0.87846700	-1.31812000
	H	4.53486200	-0.87566800	-1.32029900
	C	5.72585800	-0.00077500	0.25981200
	H	6.65795700	-0.00014300	-0.31286600
	H	5.73211100	0.88168800	0.90779300

	H	5.73187400	-0.88494700	0.90545600
TS10	C	-1.11582000	-0.00001900	0.48113400
	C	-2.90158900	0.67790000	-0.72880800
	C	-2.90166600	-0.67770900	-0.72882300
	H	-3.57788400	1.38120400	-1.18278800
	H	-3.57804200	-1.38092900	-1.18281200
	N	-1.80503000	-1.08078300	0.01518300
	N	-1.80490900	1.08083400	0.01520900
	C	-1.43099900	-2.47091700	0.25668200
	H	-2.18648300	-3.11443000	-0.19039500
	H	-0.46095700	-2.68695700	-0.19210400
	H	-1.37615500	-2.66379500	1.32773100
	C	-1.43071500	2.47092300	0.25672300
	H	-2.18625700	3.11452800	-0.19012000
	H	-1.37559900	2.66370400	1.32777300
	H	-0.46076200	2.68692900	-0.19227800
	H	0.39999400	1.01581100	1.91932100
	H	0.39989300	-1.01610800	1.91924200
	B	0.23478800	-0.00011700	1.28243000
	H	1.19585800	-0.00011200	0.35646200
	C	2.51938300	-0.00007100	-0.64593700
	C	3.71048900	0.00009600	0.27024900
	H	2.32201500	-0.91250500	-1.20594400
	H	2.32185600	0.91223700	-1.20609400
	H	3.66796700	-0.87672700	0.92751800
	H	3.66801200	0.87720200	0.92714300
	C	5.06576300	-0.00009800	-0.46562300
	H	5.16672700	0.88340700	-1.10328300
	H	5.89970200	0.00002000	0.24507700
	H	5.16666800	-0.88387400	-1.10291700
TS11	C	0.96058500	0.08495800	-0.62010200
	C	2.53576000	0.23838500	0.98754900
	C	2.28102900	-1.07964700	0.78963900
	H	3.22093200	0.72923000	1.65651300
	H	2.69997100	-1.95409700	1.25637400
	N	1.31870200	-1.15989700	-0.19926100
	N	1.72263300	0.94059000	0.11730600
	H	-0.07066700	1.57883900	-2.08791300
	H	-0.32779800	-0.40143600	-2.50310200
	B	-0.14922000	0.45161800	-1.66905600
	H	-1.31281500	0.42816400	-0.96552400
	C	-2.73537600	0.46445000	-0.31103900
	H	-3.29937200	0.45760000	-1.23964800
	C	-2.72691200	1.76601400	0.46065500

	H	-2.01981000	1.72935100	1.29244500
	H	-2.43900000	2.58709200	-0.19920400
	H	-3.71656700	1.99580200	0.87107300
	C	0.72868900	-2.40810800	-0.67994200
	H	-0.28444100	-2.52182800	-0.29081300
	H	0.69797300	-2.40429500	-1.76787900
	H	1.34552200	-3.23604500	-0.33560800
	C	1.67765300	2.39838200	0.02412600
	H	1.78640000	2.70798200	-1.01379400
	H	0.73095700	2.77582300	0.41259900
	H	2.49710200	2.80573500	0.61311000
	C	-2.81035800	-0.74593800	0.40581800
	N	-2.78829300	-1.75883500	0.98287400
TS12	C	2.53779900	-0.00064700	0.46182900
	C	4.30074500	0.69449900	-0.77018400
	C	4.31426600	-0.66112400	-0.76985400
	H	4.96426700	1.40439400	-1.23264000
	H	4.99182500	-1.35776000	-1.23211500
	N	3.23127600	-1.07452400	-0.01196600
	N	3.20973800	1.08659300	-0.01253800
	C	2.87330600	-2.46860200	0.23309400
	H	2.82388000	-2.65973100	1.30458000
	H	1.90456900	-2.69615200	-0.21280400
	H	3.63466200	-3.10439200	-0.21495700
	C	2.82454000	2.47336600	0.23245200
	H	1.84900900	2.68014600	-0.20864700
	H	2.77686600	2.66528300	1.30390900
	H	3.57028000	3.12390200	-0.22067800
	H	1.04900400	-1.03140700	1.91886200
	H	1.03035200	1.00048400	1.92041600
	B	1.19701700	-0.01356800	1.28130200
	C	-1.10210100	-0.03226300	-0.62858500
	H	-0.91802900	-0.96016800	-1.16574100
	H	-0.90182800	0.86523000	-1.20979200
	C	-2.27997800	0.00017800	0.30229900
	H	-2.23040300	0.89729900	0.93175200
	H	-2.23804700	-0.85892900	0.98331500
	H	0.22663800	-0.02133900	0.36665200
	C	-3.64030100	-0.01553400	-0.42404000
	H	-3.71927300	-0.91307400	-1.04411200
	H	-3.71273300	0.84539600	-1.09475600
	C	-4.81794800	0.01737500	0.57571800
	H	-4.76393700	0.91420400	1.20078300
	H	-4.77151300	-0.84400400	1.24936800

	C	-6.11966800	0.00485600	-0.08269600
	N	-7.14024600	-0.00552100	-0.62265300
TS13	C	3.79282200	-0.67810300	-0.58107500
	H	4.50413500	-1.38149300	-0.97762100
	C	3.79297900	0.67769400	-0.58116000
	H	4.50446700	1.38086800	-0.97777500
	N	2.63976600	1.08037900	0.07105100
	C	2.24778500	2.47142600	0.28044200
	H	1.32300700	2.69016400	-0.25423000
	H	2.09706600	2.66187400	1.34241000
	H	3.04217400	3.11373000	-0.09510000
	N	2.63952900	-1.08044100	0.07120800
	C	2.24715300	-2.47136800	0.28065100
	H	3.04160500	-3.11390000	-0.09436600
	H	2.09584700	-2.66158300	1.34257400
	H	1.32259500	-2.69002500	-0.25444500
	C	1.91604800	0.00007900	0.47872900
	H	0.29469800	-1.01526000	1.79957800
	B	0.50700700	0.00026700	1.17721400
	H	-0.38199600	0.00014800	0.18655700
	C	-1.64754000	-0.00014000	-0.89228000
	H	-1.42538800	0.91379700	-1.43791900
	H	-1.42525800	-0.91422800	-1.43760900
	C	-2.86579300	-0.00006500	-0.01854600
	H	-2.86588300	0.87892300	0.63324000
	H	-2.86599500	-0.87904900	0.63324300
	C	-4.19072600	0.00002400	-0.83688000
	H	-4.23609100	0.88000000	-1.48452100
	H	-4.23621500	-0.87994100	-1.48452600
	C	-5.37719200	0.00010600	0.01508000
	N	-6.29527100	0.00016600	0.71565400
	H	0.29480900	1.01599100	1.79929400
TS14	C	0.53798200	0.00002000	0.45854900
	C	2.41721300	-0.67746100	-0.60130900
	C	2.41697500	0.67807400	-0.60136400
	H	3.12883400	-1.38044100	-0.99809800
	H	3.12834600	1.38127100	-0.99821600
	N	1.26309300	1.08105600	0.05044800
	N	1.26347000	-1.08079200	0.05052800
	C	0.87047300	2.47109400	0.25986100
	H	1.66138000	3.11452100	-0.12135700
	H	-0.05816900	2.68789300	-0.26913400
	H	0.72537600	2.66360000	1.32250200
	C	0.87131900	-2.47094300	0.26006700

	H	1.66219800	-3.11414500	-0.12158800
	H	0.72680000	-2.66355800	1.32277100
	H	-0.05753000	-2.68793800	-0.26847700
	H	-1.08787800	-1.01597100	1.77076400
	H	-1.08849700	1.01556600	1.77039500
	B	-0.87211800	-0.00024700	1.14859400
	H	-1.76005300	-0.00073700	0.15066200
	C	-3.01459600	-0.00137100	-0.93085600
	C	-4.25913000	0.00064700	-0.09005500
	H	-2.78060400	-0.91398400	-1.47440600
	H	-2.77932500	0.90939800	-1.47694200
	H	-4.30510100	0.88489200	0.55377400
	H	-5.17622600	0.00045700	-0.69795700
	H	-4.30631800	-0.88179800	0.55615200
TS15	C	-3.17937500	0.68506200	-0.76219200
	H	-3.84808500	1.39164800	-1.22213900
	C	-3.18478100	-0.67093300	-0.76305400
	H	-3.85908900	-1.37154500	-1.22396400
	N	-2.09778400	-1.07761400	-0.00833900
	C	-1.72994300	-2.47083600	0.23304200
	H	-0.76320300	-2.69166100	-0.22006000
	H	-1.67306100	-2.66220900	1.30379800
	H	-2.49074400	-3.10982800	-0.21104700
	N	-2.08916800	1.08211600	-0.00700300
	C	-1.71061000	2.47207200	0.23658900
	H	-2.46469600	3.11761100	-0.20948600
	H	-1.65553900	2.66230700	1.30765900
	H	-0.74067300	2.68517500	-0.21332200
	C	-1.41150100	-0.00076300	0.46323700
	H	0.08173600	1.00741200	1.93364400
	B	-0.07079500	-0.00660400	1.29182600
	H	0.89609900	-0.00964500	0.39090700
	C	2.27680000	-0.01222100	-0.57801400
	H	2.13907800	-0.93441600	-1.13319700
	H	2.13204800	0.89988600	-1.14788900
	C	3.38013800	0.00030900	0.45352700
	H	3.30588600	0.88384100	1.09565000
	H	3.31302800	-0.87357400	1.10950700
	C	4.71612200	0.00091100	-0.15195500
	N	5.75357000	0.00108000	-0.66158600
	H	0.07376300	-1.02266600	1.93221400
TS16	C	-0.44758000	-0.00004800	0.63025100
	C	-2.00602000	0.67813000	-0.85734400
	C	-2.00618000	-0.67765600	-0.85743600

	H	-2.59893400	1.38099600	-1.41629300
	H	-2.59925900	-1.38030600	-1.41648400
	N	-1.05083900	-1.08029700	0.06008500
	N	-1.05058500	1.08042100	0.06023100
	C	-0.70891200	-2.47160100	0.34335700
	H	-1.45511300	-3.11325600	-0.12164300
	H	0.27601900	-2.71121900	-0.05993100
	H	-0.70288700	-2.63936600	1.41897200
	C	-0.70831600	2.47160600	0.34367600
	H	-1.45432700	3.11350000	-0.12129700
	H	-0.70230200	2.63925400	1.41931000
	H	0.27669800	2.71101500	-0.05953400
	H	0.80796900	1.01544700	2.30443500
	H	0.80772100	-1.01602000	2.30434000
	B	0.75192100	-0.00024900	1.64964700
	H	1.84840300	-0.00035200	0.89947000
	C	3.23441800	-0.00043100	-0.03630800
	H	3.74228200	0.93177800	0.19404800
	H	3.74169200	-0.93314200	0.19331800
	F	2.75754900	0.00022800	-1.33625900
TS17	C	-0.51066400	-0.10313500	0.53802900
	C	-1.78602100	1.34247000	-0.64602400
	C	-2.33441000	0.11056700	-0.78386200
	H	-2.08865900	2.29488100	-1.04544400
	H	-3.20600200	-0.21361400	-1.32547500
	N	-1.54789900	-0.76594500	-0.05389600
	N	-0.67226500	1.20053400	0.16498200
	C	-1.77812800	-2.20343200	0.04188200
	H	-2.74263800	-2.43118000	-0.40872100
	H	-0.99558900	-2.75233700	-0.48452300
	H	-1.78308600	-2.51096100	1.08684200
	C	0.22570300	2.28536800	0.54512000
	H	-0.14239300	3.21010400	0.10430700
	H	0.25653600	2.38754000	1.63014000
	H	1.23322800	2.08393000	0.17850200
	H	1.15694000	0.07270400	2.14650300
	H	0.42097500	-1.79784900	1.83169800
	B	0.67365200	-0.71260100	1.36112700
	H	1.65609100	-0.92746700	0.46241500
	C	2.97614100	-1.07705900	-0.47567400
	H	3.62649300	-1.70423500	0.13409200
	H	2.58844800	-1.53481200	-1.38067100
	O	3.45209900	0.20530400	-0.73788100
	H	3.82002200	0.57306300	0.07333200

TS18	C	0.02908100	-0.00001200	0.46415800
	C	1.89805500	-0.67780100	-0.60841900
	C	1.89798000	0.67797800	-0.60842100
	H	2.60627000	-1.38127200	-1.01030800
	H	2.60612100	1.38152500	-1.01030700
	N	0.74914000	1.08000800	0.05193600
	N	0.74926200	-1.07995500	0.05194700
	C	0.35710400	2.47117200	0.26238300
	H	1.14718000	3.11366200	-0.12179600
	H	-0.57280800	2.68716400	-0.26418700
	H	0.21590200	2.66334700	1.32528100
	C	0.35735300	-2.47116100	0.26234500
	H	1.14763200	-3.11356100	-0.12156600
	H	0.21586000	-2.66329600	1.32520900
	H	-0.57237600	-2.68731600	-0.26448700
	H	-1.57768700	-1.01484800	1.80198800
	H	-1.57776800	1.01462600	1.80204200
	B	-1.37761400	-0.00008600	1.17330900
	H	-2.26918000	-0.00009400	0.19652000
	C	-3.52727200	-0.00010300	-0.94128800
	H	-4.39036600	-0.00130800	-0.28491100
	H	-3.32737300	0.92268100	-1.47509900
	H	-3.32596400	-0.92168200	-1.47665000
TS19	C	-0.73065800	-0.15439100	0.59133000
	C	-2.30139500	0.32114100	-0.95394600
	C	-1.70174800	1.48829000	-0.60812200
	H	-3.09906800	0.11844400	-1.64723600
	H	-1.87418000	2.49507400	-0.94687000
	N	-0.74549100	1.18258400	0.34174700
	N	-1.69775900	-0.67615300	-0.21083200
	C	0.16857500	2.15792600	0.93479300
	H	-0.25939600	3.15146600	0.81494500
	H	0.29515600	1.93972600	1.99285300
	H	1.13943700	2.11571800	0.43830000
	C	-2.04137600	-2.09492600	-0.30030400
	H	-1.22793200	-2.65366500	-0.76397100
	H	-2.22954300	-2.49547800	0.69398300
	H	-2.93869000	-2.19256200	-0.90804400
	H	0.62958700	-0.28275600	2.48418800
	H	-0.13639900	-2.04789200	1.82019600
	B	0.24941600	-0.93923200	1.54535200
	H	1.35391500	-1.12350400	0.82039600
	C	3.08161900	-0.22716800	-0.63862000
	N	3.27518100	0.78501900	-1.18444100

	C	2.76892000	-1.40500500	0.05200800
	H	2.45013000	-2.25240700	-0.54299500
	H	3.36275500	-1.63136300	0.92934700
TS20	C	-0.81804700	-0.15276000	0.54539000
	C	-1.76465000	1.57003800	-0.55325700
	C	-2.49978400	0.46099000	-0.82172100
	H	-1.88318000	2.58844400	-0.87989000
	H	-3.38261200	0.33034700	-1.42290500
	N	-1.90815100	-0.58666100	-0.14118700
	N	-0.74103800	1.17899000	0.28801500
	C	-2.38904800	-1.96822000	-0.17572100
	H	-1.67753500	-2.60462600	-0.70192500
	H	-2.52295600	-2.34153800	0.83773500
	H	-3.34332100	-1.98473600	-0.69836700
	C	0.31519500	2.06701900	0.77577400
	H	-0.00492300	3.09656400	0.62701500
	H	0.48037400	1.88658300	1.83620900
	H	1.24198900	1.88552500	0.22923500
	H	0.65863800	-0.40727200	2.33382600
	B	0.19012200	-1.01697700	1.40246500
	H	1.22782700	-1.21178500	0.61299600
	C	2.47597200	-1.48665600	-0.42223900
	H	2.73803200	-2.44996000	-0.00040700
	H	1.83365500	-1.48357100	-1.29593000
	C	3.36188600	-0.38775900	-0.22485600
	O	3.27794600	0.70787300	-0.80882600
	H	-0.23146500	-2.11330200	1.67152400
	H	4.14647800	-0.53099000	0.54115400
TS21	C	-1.17296200	-0.16370800	0.52775200
	C	-2.29430600	1.50547700	-0.48713400
	C	-2.97700700	0.35541700	-0.71824100
	H	-2.49553900	2.51680900	-0.79470600
	H	-3.88760500	0.17545100	-1.26251600
	N	-2.27744900	-0.65897000	-0.09063200
	N	-1.19356100	1.17159500	0.27869400
	C	-2.67415800	-2.06714300	-0.10293200
	H	-1.91311300	-2.66939000	-0.59812700
	H	-2.80990400	-2.42771600	0.91556400
	H	-3.61264100	-2.15321500	-0.64690500
	C	-0.16638200	2.11845300	0.71485500
	H	-0.51290800	3.12604100	0.49329800
	H	-0.00420800	2.01644900	1.78666400
	H	0.76903000	1.92760300	0.18719700
	H	0.43470600	-0.32263800	2.20524300

	B	-0.05986900	-0.96792000	1.31141600
	H	0.91706900	-1.12820400	0.44943800
	C	2.15828100	-1.33821700	-0.67379200
	H	2.48089100	-2.30200800	-0.30518100
	H	1.50641500	-1.31097400	-1.53516300
	C	2.98636700	-0.18865000	-0.44826400
	O	2.84339600	0.92113200	-0.95866000
	O	3.97333100	-0.40628100	0.47634200
	H	4.44458800	0.43197300	0.59116500
	H	-0.41318700	-2.07752100	1.62560700
TS22	C	-0.80196200	-0.00653600	0.62833500
	C	-2.35939500	0.47387500	-0.93161600
	C	-2.19265700	-0.87210300	-0.92323900
	H	-3.00608300	1.09903900	-1.52218900
	H	-2.66606600	-1.64294100	-1.50593200
	N	-1.23706700	-1.15205700	0.03764600
	N	-1.50235300	0.99083700	0.02431100
	C	-0.74308800	-2.49039700	0.35494500
	H	-1.29335200	-3.21229100	-0.24539900
	H	0.32011500	-2.56314000	0.12535200
	H	-0.89501700	-2.70409400	1.41222200
	C	-1.35493000	2.41414100	0.32213600
	H	-2.08903700	2.96542100	-0.26237000
	H	-1.52493200	2.59321600	1.38273900
	H	-0.35317500	2.75377800	0.05839900
	H	0.26599500	1.17313900	2.32884600
	H	0.42580700	-0.85008300	2.41442600
	B	0.33271800	0.13334800	1.71597800
	H	1.45961800	0.18651700	1.03566300
	C	2.87865400	0.22071900	0.10649600
	H	3.79254100	0.40593100	0.67211800
	F	2.93141600	-0.98375700	-0.52713500
	F	2.68149500	1.18588100	-0.83395400
TS23	C	-1.42418700	0.02365900	0.67521700
	C	-2.61362600	0.37273100	-1.20745700
	C	-2.40329600	-0.96306200	-1.09899800
	H	-3.13694300	0.94403900	-1.95414500
	H	-2.70873400	-1.77702200	-1.73311000
	N	-1.67613500	-1.16156300	0.06070900
	N	-2.00934300	0.96362200	-0.11250600
	C	-1.20603900	-2.46421700	0.53071400
	H	-1.68740500	-3.23892000	-0.06300100
	H	-0.12429200	-2.53704400	0.41625400
	H	-1.46572900	-2.59356200	1.57966700

	C	-1.98176300	2.40347400	0.14161900
	H	-2.59353700	2.89694500	-0.61099300
	H	-2.38077900	2.61515000	1.13227800
	H	-0.96008200	2.77819200	0.07963400
	H	-0.86087000	1.30268000	2.53594600
	H	-0.57236100	-0.69657500	2.71862200
	B	-0.57002600	0.26573400	1.98621800
	H	0.65774900	0.40517900	1.58909300
	C	2.37400200	0.62151500	1.17978200
	H	2.44657300	1.69567000	1.28453100
	H	2.81633400	0.00617100	1.95155900
	C	2.46957600	0.10359500	-0.18620500
	F	2.13472000	-1.21414200	-0.28022700
	F	1.67343200	0.77216100	-1.06638000
	F	3.73968700	0.18307600	-0.73149100
TS24	C	-0.89976600	-0.10293300	0.63528600
	C	-2.00024700	1.21458500	-0.83005000
	C	-2.36049600	-0.06770900	-1.08505700
	H	-2.30050400	2.13557500	-1.29861000
	H	-3.03587300	-0.47597900	-1.81661600
	N	-1.68055400	-0.86380500	-0.17955200
	N	-1.10765400	1.17853700	0.22678300
	C	-1.77324300	-2.32110200	-0.12516000
	H	-2.52937500	-2.64495500	-0.83777600
	H	-0.81527000	-2.77186700	-0.38544800
	H	-2.05656800	-2.64033200	0.87667000
	C	-0.44245600	2.34976500	0.79258000
	H	-0.87846200	3.24290900	0.34907400
	H	-0.58354600	2.37217000	1.87202000
	H	0.62539000	2.31950700	0.57250500
	H	0.27158200	0.22935600	2.61664100
	H	-0.18471900	-1.69885400	2.17129000
	B	0.09554900	-0.59952800	1.75293700
	H	1.26229600	-0.72548000	1.14724200
	C	2.79977200	-0.91996100	0.48597200
	H	3.44569600	-0.65307800	1.31366200
	H	2.79651000	-1.95555700	0.16780200
	Cl	3.00477400	0.18501400	-0.88736400
TS25	C	-0.93597300	-0.04293200	0.51834900
	C	-2.43015600	1.18658400	-0.65519400
	C	-2.84730600	-0.10254600	-0.69222300
	H	-2.85850800	2.07612000	-1.08333700
	H	-3.70827400	-0.54933900	-1.15834400
	N	-1.92725600	-0.84600000	0.02898600

	N	-1.26136200	1.21219900	0.08798900
	C	-1.99729000	-2.28946200	0.22600800
	H	-2.90855900	-2.65893700	-0.24103400
	H	-1.13501600	-2.77758900	-0.22989600
	H	-2.01387000	-2.52431000	1.29032400
	C	-0.47198800	2.40934000	0.35497300
	H	-0.99112300	3.26790400	-0.06747800
	H	-0.35312200	2.54943900	1.42935500
	H	0.51496400	2.32261800	-0.10145900
	H	0.83711800	0.41132700	1.94932700
	H	0.21804800	-1.52623700	1.88628800
	B	0.35124300	-0.48048000	1.29247400
	H	1.27070500	-0.74463600	0.33025800
	C	2.45545400	-1.05881600	-0.73540700
	H	2.93013500	-1.94942500	-0.31592500
	H	1.89179600	-1.20914900	-1.65212800
	O	3.27645800	0.04707000	-0.83965100
	C	4.14818200	0.22263500	0.27371000
	H	4.80479300	-0.64859100	0.39080000
	H	4.75212600	1.10709100	0.07282400
	H	3.57569200	0.36735700	1.19515000
TS26	C	-1.28075600	-0.05931100	0.57481200
	C	-2.43872900	1.39689500	-0.70962300
	C	-3.04244200	0.18803800	-0.82087200
	H	-2.67958200	2.34623900	-1.15551300
	H	-3.90974800	-0.11547100	-1.38108300
	N	-2.32664100	-0.69469800	-0.02935600
	N	-1.36420400	1.23406400	0.14816200
	C	-2.63632300	-2.11340600	0.11844600
	H	-3.58733700	-2.31274900	-0.37221600
	H	-1.85812700	-2.72446600	-0.34102500
	H	-2.71070500	-2.37055700	1.17423000
	C	-0.42462800	2.28934100	0.51422200
	H	-0.77215100	3.22658300	0.08328400
	H	-0.37295500	2.38482500	1.59847900
	H	0.56994600	2.05893800	0.12866900
	H	0.34462100	0.09774400	2.23015600
	H	-0.48524600	-1.74290400	1.97209900
	B	-0.15930900	-0.69411700	1.46719900
	H	0.83233500	-1.00292900	0.60009000
	C	2.03490100	-1.43545400	-0.38610300
	H	2.55209700	-2.18940300	0.20461300
	H	1.45375900	-1.83251400	-1.21399900
	S	3.02719400	-0.06127400	-0.89579300

	C	3.89020500	0.33236300	0.66565600
	H	4.49246200	-0.51733100	0.99064700
	H	4.54386800	1.18176400	0.46698600
	H	3.17075600	0.59684800	1.44041700
TS27	C	-0.96601200	-0.05880800	0.59914900
	C	-2.09091600	1.34886500	-0.77662400
	C	-2.59935200	0.10682200	-0.96467400
	H	-2.34994400	2.28941900	-1.23115000
	H	-3.38617900	-0.23863300	-1.61264700
	N	-1.90877600	-0.74702800	-0.11928200
	N	-1.09751500	1.24030400	0.18329700
	C	-2.13878800	-2.18190300	-0.01762400
	H	-2.97815000	-2.44604200	-0.65891900
	H	-1.25379400	-2.73465800	-0.33724100
	H	-2.36986500	-2.45499200	1.01245900
	C	-0.26635300	2.34233800	0.64728200
	H	-0.29711300	2.40435200	1.73514100
	H	0.76882200	2.19644100	0.33197900
	H	-0.64672600	3.26905600	0.22065400
	H	1.17100600	-0.96172500	0.77548100
	B	0.10206500	-0.64415700	1.57032700
	H	-0.21988300	-1.69965500	2.06799500
	H	0.54466300	0.16737700	2.35114800
	C	2.47160500	-1.38490500	-0.03020400
	H	2.06190700	-2.22356200	-0.58583000
	H	3.11294300	-1.66361900	0.80725100
	N	2.91071900	-0.31414800	-0.82634000
	H	3.00405800	-0.52421700	-1.81034800
	C	3.96819700	0.53783100	-0.30578900
	H	4.16834500	1.34846900	-1.00894500
	H	3.64974300	0.98388000	0.64011200
	H	4.90855700	-0.00643600	-0.12160400
TS28	C	1.20476800	0.21144300	0.60885200
	C	1.90955400	-1.57455100	-0.58495800
	C	2.40122600	-0.46384500	-1.18721800
	H	2.01632300	-2.61554600	-0.83575800
	H	3.02001200	-0.35409600	-2.06077700
	N	1.96615900	0.62260400	-0.44736000
	N	1.18372400	-1.15039400	0.51488700
	C	2.26304800	2.01566000	-0.76542800
	H	2.95444100	2.03880000	-1.60576300
	H	1.35001200	2.54805900	-1.03538800
	H	2.71812500	2.50741300	0.09374700
	C	0.46255900	-2.03676000	1.42263700

	H	0.72355400	-1.80439000	2.45415000
	H	-0.61473800	-1.92078300	1.29316400
	H	0.74331900	-3.06438700	1.19886600
	H	-0.76615500	1.36591900	1.07734600
	B	0.44178300	1.11264000	1.63851400
	H	0.93975100	2.20506100	1.77933800
	H	0.17418700	0.54112300	2.66923600
	C	-2.22147000	1.70642800	0.52217600
	H	-1.95319800	2.30969100	-0.33858500
	H	-2.65897400	2.24438000	1.35469800
	N	-2.88669500	0.50821500	0.20186900
	H	-3.35159900	0.00705200	0.95003300
	C	-2.80799300	-0.15052900	-0.97866300
	H	-2.27016300	0.41737000	-1.75417200
	O	-3.29328600	-1.26236500	-1.19285800
TS29	C	-1.17436300	-0.17813800	0.52109700
	C	-2.32006300	1.50659200	-0.43894300
	C	-3.00902900	0.36030500	-0.67077200
	H	-2.52831200	2.52248000	-0.72621200
	H	-3.93334700	0.18925000	-1.19439600
	N	-2.29460700	-0.66398500	-0.07730300
	N	-1.20071000	1.16124300	0.29371500
	C	-2.69242200	-2.07158100	-0.10197600
	H	-1.94744800	-2.66554900	-0.63060700
	H	-2.79768100	-2.44977600	0.91376900
	H	-3.64707400	-2.14809800	-0.61857100
	C	-0.16048800	2.10075800	0.71489900
	H	-0.51685800	3.11215600	0.52903000
	H	0.03849200	1.97480700	1.77798700
	H	0.75669500	1.92392500	0.15099200
	H	0.47692100	-0.37129000	2.15456400
	B	-0.04155700	-0.99336400	1.25860100
	H	0.92806300	-1.11004500	0.36203400
	C	2.08706700	-1.24901500	-0.77539600
	H	2.37043800	-2.26036300	-0.50990300
	H	1.40066700	-1.13263000	-1.60607900
	C	2.98098400	-0.16040400	-0.49426500
	O	2.81231600	0.97374400	-0.98494500
	H	-0.36826400	-2.11844800	1.54147200
	C	4.09584200	-0.38853400	0.51100400
	H	3.73375700	-0.11414300	1.50880000
	H	4.41947100	-1.43018900	0.54908400
	H	4.94580200	0.25407500	0.27582300
TS30	C	1.16496100	0.17503000	0.52755000

	C	2.27830300	-1.52341200	-0.44960200
	C	2.97864900	-0.38600700	-0.68867000
	H	2.47016800	-2.54155300	-0.74024200
	H	3.89841000	-0.22572700	-1.22366500
	N	2.28499600	0.64681300	-0.08426300
	N	1.17221100	-1.16499700	0.29777900
	C	2.69846900	2.04903800	-0.11531500
	H	1.96437300	2.64857800	-0.65332800
	H	2.79986400	2.43285000	0.89871800
	H	3.65792500	2.11170800	-0.62499400
	C	0.12431300	-2.09143200	0.72725600
	H	0.46611200	-3.10713800	0.53672800
	H	-0.06315800	-1.96483600	1.79246400
	H	-0.79572100	-1.90183300	0.17168100
	H	-0.47722600	0.38574400	2.16675200
	B	0.05033800	1.00496600	1.27298900
	H	-0.91916700	1.15405300	0.37541300
	C	-2.14197700	1.33896500	-0.70002100
	H	-2.47439600	2.31254100	-0.35888900
	H	-1.52353900	1.31680200	-1.58741000
	C	-2.97235200	0.17325900	-0.46411400
	O	-2.78441900	-0.92016900	-1.02856400
	H	0.40423500	2.11959100	1.56909700
	N	-3.98721600	0.31614400	0.45407000
	H	-4.02037800	1.12150800	1.05932800
	H	-4.43596700	-0.52413600	0.78630500
TS31	C	1.22357800	-0.11308500	0.64846500
	C	2.47447700	-0.23425200	-1.22470500
	C	2.21744500	1.07674000	-0.98935900
	H	3.03804500	-0.71138900	-2.00741800
	H	2.51044600	1.95928200	-1.53087000
	N	1.45454400	1.13565000	0.16261500
	N	1.85903600	-0.95150700	-0.21379000
	C	0.91411100	2.36600600	0.73707600
	H	1.42457200	3.21347100	0.28328700
	H	-0.15591400	2.43323600	0.53781200
	H	1.08076600	2.37235400	1.81252900
	C	1.89142200	-2.40846300	-0.09593100
	H	2.48356400	-2.80552700	-0.91809900
	H	2.34325200	-2.69939700	0.85151400
	H	0.88173500	-2.81477000	-0.14923400
	H	0.56643100	-1.62156200	2.29690000
	H	0.36366100	0.34455400	2.76154300
	B	0.34190700	-0.50333200	1.89912900

	H	-0.90491000	-0.51010600	1.46937600
	C	-2.55748800	-0.53350900	1.05818000
	H	-2.79491900	-1.53271800	1.40308800
	H	-2.92697100	0.29099500	1.65800300
	C	-2.54776700	-0.33882700	-0.39348200
	F	-1.97502400	0.87931100	-0.73873900
	F	-3.85495100	-0.26403800	-0.93718900
	H	-2.03924200	-1.11589500	-0.96395600
TS32	C	1.07227900	-0.02934300	0.49058900
	C	2.92225200	-0.37467400	-0.75570500
	C	2.69878900	0.96249300	-0.72019200
	H	3.69908300	-0.94528300	-1.23415900
	H	3.24386500	1.77856300	-1.16173100
	N	1.56435100	1.16025800	0.04742000
	N	1.92058100	-0.96982800	-0.00890400
	C	0.96381600	2.46431400	0.31870100
	H	1.63739300	3.23718300	-0.04651200
	H	0.00272100	2.55300000	-0.18909500
	H	0.81316800	2.58823400	1.38990500
	C	1.78039500	-2.41073700	0.18978400
	H	2.67147800	-2.90049400	-0.19815000
	H	1.67631300	-2.63031700	1.25103000
	H	0.90293700	-2.78434700	-0.33930700
	H	-0.23666000	-1.31959600	1.91961900
	H	-0.55507400	0.68647300	1.99205900
	B	-0.24347300	-0.26972300	1.32164500
	H	-1.21391800	-0.38866800	0.41771600
	C	-2.51992100	-0.54870100	-0.60396100
	H	-2.14428100	0.00645600	-1.45791400
	H	-2.52479100	-1.62843700	-0.71379500
	C	-3.59618300	0.06397000	0.19155800
	F	-4.87393700	0.03886000	-0.52138100
	H	-3.42075200	1.12025800	0.39874300
	H	-3.79177400	-0.47108000	1.12153500
TS33	C	-0.54495900	-0.17975500	0.30435600
	C	-2.60507200	0.57215500	-0.23397700
	C	-2.28301100	-0.40036500	-1.12062600
	H	-3.49069900	1.17678000	-0.14463200
	H	-2.83502700	-0.80720100	-1.94987800
	N	-1.01740500	-0.85105600	-0.78625300
	N	-1.53590600	0.69818900	0.63642800
	C	-0.29500600	-1.88906900	-1.51681900
	H	-0.79867900	-2.05459000	-2.46750000
	H	0.72764500	-1.56421000	-1.70466900
	H	-0.27481900	-2.82008400	-0.94978800

	C	-1.47821200	1.66126900	1.73228900
	H	-1.25601200	1.15146600	2.66895400
	H	-0.70864900	2.41041600	1.54163700
	H	-2.44699100	2.15153300	1.80764200
	H	1.72564300	0.41302600	0.17233700
	B	0.86738300	-0.27516100	0.98153300
	H	0.92115100	0.31478700	2.02842400
	C	2.75282200	1.27855300	-0.65004400
	H	2.95632400	0.57665000	-1.45378400
	H	3.53462900	1.35845700	0.09964000
	N	2.13817800	2.48301700	-1.03057400
	H	2.47595400	3.32405100	-0.58638900
	H	1.97032600	2.61565000	-2.01700300
	C	1.47923400	-1.70462000	1.10993400
	N	1.98763600	-2.74442600	1.22277900
TS34	C	1.29292600	-0.32196500	0.23379500
	C	1.27050400	-2.53450600	-0.18959200
	C	1.37530300	-1.89198900	-1.37908000
	H	1.22816700	-3.58460100	0.04120400
	H	1.44263900	-2.27526100	-2.38215000
	N	1.38345800	-0.53651700	-1.10763700
	N	1.22172600	-1.56200600	0.79184500
	C	1.47152400	0.50430000	-2.13197600
	H	1.31609500	0.04055700	-3.10398600
	H	0.69967800	1.25415600	-1.96639700
	H	2.45002700	0.98324700	-2.10922500
	C	1.10415500	-1.84397500	2.22244600
	H	1.15587300	-2.92178500	2.36136800
	H	1.91960800	-1.36859300	2.76548600
	H	0.15263500	-1.47647500	2.60625200
	H	1.29257700	0.91522200	2.20127600
	B	1.17877800	1.03818900	1.01330900
	H	-0.14391600	1.42557600	0.86974200
	C	-1.55165400	1.95050000	0.76497000
	C	2.00979400	2.23876400	0.47254600
	N	2.60088200	3.16987900	0.10782600
	H	-1.50984600	2.64332500	1.59801000
	H	-1.45136800	2.41670000	-0.20988100
	C	-2.47114600	0.85322500	0.89269500
	H	-2.79367700	0.53421900	1.87709400
	C	-2.92372700	0.10709800	-0.12300200
	F	-3.73869000	-0.94477900	-0.00029800
	F	-2.65696800	0.31750800	-1.41485600
TS35	C	0.89231800	-0.31752200	-0.10604100
	C	2.67839800	0.96566300	0.38157900
	C	1.97998100	0.78357000	1.52966000

	H	3.58675200	1.50955900	0.19009800
	H	2.16373800	1.13940300	2.52833900
	N	0.88582400	-0.00190900	1.21819900
	N	2.00217000	0.28629200	-0.61446500
	C	-0.14735400	-0.38991500	2.17890100
	H	0.09160700	0.06496000	3.13795700
	H	-1.11997500	-0.02872500	1.84219800
	H	-0.17807600	-1.47258300	2.28923500
	C	2.43530400	0.22926800	-2.01066900
	H	3.39015200	0.74459800	-2.09167100
	H	2.55507900	-0.80704000	-2.32355000
	H	1.70609400	0.71839500	-2.65609000
	H	0.17692400	-1.36767400	-2.05418900
	B	-0.18439800	-1.09860700	-0.94261700
	H	-1.20184000	-0.17356000	-1.14991200
	C	-2.36971000	0.68788100	-1.49849100
	C	-0.88480100	-2.30498500	-0.25178600
	N	-1.44400500	-3.20853500	0.21759900
	H	-2.04640300	0.93963000	-2.50392500
	H	-3.12071800	-0.09695400	-1.45271300
	C	-2.46211800	1.75294400	-0.53901100
	H	-1.85882100	2.63806200	-0.73497900
	C	-3.18085900	1.71699400	0.61107300
	H	-3.80290100	0.86352300	0.86391700
	H	-3.17449500	2.54711400	1.30776300
TS36	C	-1.14387000	0.06810100	0.32490800
	C	-2.85000500	0.11249600	-1.14983800
	C	-2.98567700	-1.01097800	-0.40444100
	H	-3.45197000	0.50188700	-1.95226800
	H	-3.72787900	-1.78944200	-0.43404800
	N	-1.93660100	-1.02672600	0.49812500
	N	-1.71607700	0.76409300	-0.69711100
	C	-1.71814300	-2.08336100	1.48395900
	H	-0.79724700	-2.62481700	1.26564400
	H	-1.65340900	-1.65542200	2.48335400
	H	-2.55991600	-2.77149800	1.43827900
	C	-1.21282800	2.01747700	-1.25596900
	H	-1.39025300	2.84473700	-0.56904400
	H	-0.14379300	1.93419600	-1.44717200
	H	-1.73102800	2.20669000	-2.19410700
	H	0.30456300	-0.30781100	2.09079200
	B	0.19955600	0.35946000	1.09536300
	C	0.49725200	1.86169500	1.40499100
	N	0.76374100	2.96383500	1.65961700

	H	1.20809100	-0.06855800	0.31165100
	C	2.49110400	-0.64641900	-0.44613700
	C	3.58837300	-0.38751800	0.55211000
	H	4.56003700	-0.74266900	0.17192200
	H	3.69560700	0.68030900	0.76486900
	H	3.40218800	-0.90633100	1.49746300
	C	2.10422500	-2.08914100	-0.63668900
	H	1.93155800	-2.58906400	0.32164300
	H	1.19758900	-2.18682400	-1.24268500
	H	2.90041300	-2.64806200	-1.15447800
	C	2.53296200	0.19028400	-1.69782100
	H	1.62852200	0.06028400	-2.30076800
	H	2.64452900	1.25450900	-1.46838300
	H	3.38682600	-0.09366000	-2.33433900
TS37	C	-0.75919200	-0.08512500	0.31669100
	C	-2.29066100	-1.00719100	-1.04953300
	C	-1.89943400	-1.96308000	-0.17031000
	H	-3.00177600	-1.04236800	-1.85621000
	H	-2.20391200	-2.98983100	-0.06697900
	N	-0.96120000	-1.38497900	0.66332600
	N	-1.58055000	0.13794200	-0.74428000
	C	-0.26664500	-2.09555900	1.73677200
	H	-0.72914500	-3.07341500	1.85300400
	H	0.78777900	-2.22053200	1.48664400
	H	-0.35352900	-1.54000600	2.66869000
	C	-1.70285400	1.39939100	-1.47617900
	H	-2.24829300	1.20762700	-2.39780300
	H	-2.24063900	2.13703900	-0.88124600
	H	-0.71354000	1.78295300	-1.71955400
	B	0.30037100	0.87928800	0.96640900
	H	1.38019700	0.82987900	0.10446100
	C	2.63868800	0.78930700	-0.66367300
	H	2.37957900	1.54116700	-1.40313900
	H	3.29478500	1.13256100	0.14259500
	C	3.40344600	-1.36761800	-0.41398300
	H	3.48526600	-2.39039500	-0.77063700
	H	3.87338200	-1.11852300	0.54423800
	N	2.78212700	-0.49122100	-1.13923700
	H	0.75683700	0.46492200	1.99410300
	C	-0.06607200	2.39000700	1.05647900
	N	-0.28502000	3.52707000	1.14193500
TS38	C	1.20439900	-2.63757400	0.18999400
	H	0.84976600	-3.61034600	0.48244600
	C	1.87609600	-2.23508100	-0.91699800

	H	2.22158300	-2.79107700	-1.77092700
	N	2.08267300	-0.87374700	-0.79199900
	C	2.75816900	-0.05075300	-1.79513700
	H	2.14456900	0.81546000	-2.03887900
	H	3.72624300	0.28631400	-1.42625200
	H	2.89990000	-0.65187900	-2.69092400
	N	1.01653500	-1.51770000	0.97815200
	C	0.30810800	-1.52343900	2.25798900
	H	0.10637000	-2.55731100	2.53087300
	H	0.92404900	-1.05943500	3.02643600
	H	-0.63390000	-0.98062600	2.17225600
	C	1.55611500	-0.42115100	0.37903500
	H	1.14356500	1.11032800	2.07585300
	B	1.45431500	1.05359500	0.91802500
	C	2.63778900	2.01499400	0.59542500
	N	3.48565300	2.77873800	0.37900500
	H	0.36489200	1.58800100	0.28285200
	C	-0.87357800	2.26519100	-0.30260900
	H	-0.93227100	3.06445500	0.42948100
	C	-1.93455100	1.28642300	-0.31902900
	C	-2.76687400	1.08831200	0.80828600
	C	-2.14006900	0.44348000	-1.43687600
	C	-3.75462000	0.11064400	0.81030200
	H	-2.63202500	1.72020700	1.68039000
	C	-3.12939500	-0.53255300	-1.43025400
	H	-1.51698200	0.57276300	-2.31624600
	C	-3.94532400	-0.70812200	-0.30768500
	H	-4.38409700	-0.01403000	1.68513600
	H	-3.27079900	-1.15932600	-2.30447300
	H	-4.71875900	-1.46761300	-0.30547100
	H	-0.43529800	2.55288100	-1.25342500
TS39	C	-0.91101400	0.09679700	0.27977200
	C	-2.69259300	0.05111100	-1.10034900
	C	-2.84816500	-0.95061400	-0.20055300
	H	-3.31688600	0.36536800	-1.91849100
	H	-3.63383900	-1.67685600	-0.08596400
	N	-1.75082700	-0.91091500	0.64226200
	N	-1.49842700	0.68181500	-0.79943400
	C	-1.53073800	-1.84103600	1.74909400
	H	-0.69496900	-2.50584500	1.52874700
	H	-1.31808400	-1.28869700	2.66270400
	H	-2.43485800	-2.43119800	1.88431700
	C	-0.95125100	1.81225900	-1.54786200
	H	-1.10972100	2.74584100	-1.00767800

	H	0.11622000	1.66507900	-1.70283900
	H	-1.45087100	1.86086300	-2.51358900
	H	0.68154900	-0.18856300	1.94342900
	B	0.49357800	0.42050000	0.92370800
	C	0.80217600	1.94079500	1.12009100
	N	1.07656400	3.05886700	1.27784800
	H	1.42279900	-0.03395500	0.07183600
	C	2.63683300	-0.63524000	-0.80643200
	C	2.18988800	-2.04175400	-1.08674200
	H	2.93609500	-2.59326200	-1.67951700
	H	2.04594200	-2.60512900	-0.15745800
	H	1.25059700	-2.06701800	-1.64722800
	H	2.56204100	0.05231700	-1.64848900
	C	3.83784900	-0.43808800	0.07395600
	H	4.75591600	-0.81159600	-0.40593400
	H	4.00081100	0.61768800	0.30750900
	H	3.73028700	-0.98128000	1.01952900
TS40	C	-0.88148100	0.03133800	0.27972500
	C	-2.12261900	1.82900800	-0.26786900
	C	-2.26167400	0.91897400	-1.26305900
	H	-2.54612700	2.81083200	-0.14809300
	H	-2.83300800	0.95422400	-2.17417400
	N	-1.49134700	-0.17652000	-0.91782600
	N	-1.27553100	1.27184000	0.67319100
	C	-1.35625400	-1.37952700	-1.73865100
	H	-1.70093200	-1.14974800	-2.74496600
	H	-0.31108800	-1.68094200	-1.77789000
	H	-1.95033600	-2.19522400	-1.32667000
	C	-0.85030500	1.94967700	1.89774100
	H	-1.43387600	2.86203400	2.00217500
	H	-1.02381200	1.30711900	2.75898300
	H	0.20893400	2.20221300	1.84337700
	H	0.40041100	-0.50892900	2.13933600
	B	0.15432300	-0.89681900	1.02873300
	H	1.31276700	-0.76998700	0.36236700
	C	2.75848700	-0.63263800	-0.32182600
	H	3.37252600	-1.17927400	0.38696200
	H	2.58719000	-1.13929100	-1.26646700
	S	3.19492300	1.06988600	-0.57727500
	H	3.40970800	1.40029600	0.71292200
	C	-0.17926100	-2.42369400	1.02930900
	N	-0.37942000	-3.56763800	1.04929900
TS41	C	-1.40192700	-0.21668900	0.23167700
	C	-2.50964900	-1.37757200	-1.34916800

	C	-2.21158700	-2.23766000	-0.34458700
	H	-3.03020900	-1.53291900	-2.27802900
	H	-2.42075600	-3.28699400	-0.23171800
	N	-1.53321800	-1.51288300	0.61964700
	N	-2.00136900	-0.14335500	-0.98621400
	C	-1.02206400	-2.08216700	1.86693400
	H	-1.39070100	-3.10246800	1.95201700
	H	0.06797300	-2.09101900	1.86305700
	H	-1.37371700	-1.49746200	2.71505900
	C	-2.10006900	1.06361100	-1.80609100
	H	-2.30445800	0.76726900	-2.83321300
	H	-2.90100000	1.70957700	-1.44571200
	H	-1.15712700	1.60581700	-1.76896200
	H	-0.28397200	0.57641900	2.10539900
	B	-0.61453700	0.91950500	1.00153300
	H	0.52034100	1.11876200	0.33565200
	C	1.99152700	1.37825700	-0.34289300
	C	2.80010000	0.16377200	0.01139100
	H	1.69409200	1.49724300	-1.38291500
	H	2.24170600	2.31197000	0.15577400
	H	2.30895500	-0.73684800	-0.37975900
	H	2.83464700	0.04868500	1.10216600
	C	4.24971100	0.19533300	-0.52109500
	H	4.75311800	1.08818700	-0.13325000
	H	4.22891000	0.30261100	-1.61171900
	C	-1.33543000	2.30811400	1.04315400
	N	-1.82948200	3.35832200	1.08976900
	C	5.05034800	-1.05452700	-0.14077900
	H	6.07196800	-1.00602700	-0.52848800
	H	5.11152300	-1.16797000	0.94633400
	H	4.58411600	-1.95978900	-0.54302800
TS42	C	-1.16366300	-0.06285000	0.21995600
	C	-2.88726500	-0.07485600	-1.22996300
	C	-2.97729600	-1.20014100	-0.47952800
	H	-3.51116400	0.29260400	-2.02599000
	H	-3.69438300	-2.00205700	-0.49766700
	N	-1.91489400	-1.18007200	0.40730000
	N	-1.76738000	0.61057200	-0.79463300
	C	-1.64846100	-2.22795200	1.39358900
	H	-2.48577400	-2.92286100	1.38660500
	H	-0.73279200	-2.76356000	1.14328300
	H	-1.54909000	-1.78965300	2.38510900
	C	-1.30624800	1.87933000	-1.35767200
	H	-1.79671000	2.02803100	-2.31762500

	H	-1.55039500	2.70654900	-0.69124200
	H	-0.22842700	1.84373500	-1.50639800
	H	0.40461000	-0.43817400	1.88989800
	B	0.19181500	0.28905600	0.95653700
	H	1.16333600	0.04114600	0.08186200
	C	2.44366200	-0.30446500	-0.88877000
	C	3.59202300	-0.56822100	0.04337200
	H	2.02800900	-1.15591200	-1.42457800
	H	2.47447500	0.61433700	-1.47113700
	H	3.33719500	-1.39383900	0.71793100
	H	3.75979700	0.30933100	0.67832000
	C	4.90771900	-0.91117200	-0.68471800
	H	5.21835900	-0.09248400	-1.34047600
	H	5.71497400	-1.09419700	0.03234600
	H	4.79383700	-1.80812200	-1.30079200
	C	0.35061800	1.78892300	1.37347100
	N	0.51492200	2.89353900	1.69296700
TS43	C	-0.97357300	0.18166400	0.32678700
	C	-2.70749800	-0.35283200	-1.00075100
	C	-2.72035400	-1.20717800	0.05313500
	H	-3.36202200	-0.27476300	-1.85101200
	H	-3.38752000	-2.01590600	0.29478400
	N	-1.65268200	-0.86705900	0.86055700
	N	-1.62916400	0.49139400	-0.82240900
	C	-1.30731200	-1.56462500	2.10101400
	H	-0.37062000	-2.10875000	1.98185700
	H	-1.21091600	-0.84932800	2.91557200
	H	-2.10595600	-2.26740500	2.32820100
	C	-1.25665500	1.55589500	-1.75622100
	H	-1.46452800	2.53354400	-1.32309600
	H	-0.19722800	1.48421900	-1.99687300
	H	-1.83884000	1.42981100	-2.66663000
	H	0.60182800	0.44058300	2.02188600
	B	0.35377400	0.80801300	0.90806100
	C	0.52804400	2.35029400	0.75539600
	N	0.70823000	3.49281600	0.65882600
	H	1.36338000	0.26414300	0.16928700
	C	2.62967200	-0.27574500	-0.53151200
	H	2.68148200	0.47947400	-1.31165500
	C	3.68430400	-0.19475900	0.54999200
	H	4.67676100	-0.43256400	0.15171900
	H	3.72112800	0.81667700	0.95923200
	H	3.47186400	-0.88969200	1.36479100
	C	2.23777800	-1.54805800	-1.00098000

	N	1.85445600	-2.59115700	-1.34833600
TS44	C	4.18728600	-1.33574800	-0.54007400
	H	4.87180300	-2.16539800	-0.56694400
	C	4.12342100	-0.21476600	-1.29976500
	H	4.74185000	0.12015400	-2.11416900
	N	3.04208900	0.51812800	-0.84530300
	C	2.61970300	1.80018600	-1.40889500
	H	1.53708600	1.81155000	-1.52102200
	H	2.92352000	2.62278400	-0.76153600
	H	3.08340500	1.91549200	-2.38660300
	N	3.14799500	-1.26555800	0.37095700
	C	2.86365000	-2.29334100	1.37369300
	H	3.67192000	-3.02150300	1.35348800
	H	2.80589600	-1.84265900	2.36291300
	H	1.92158500	-2.79358200	1.14988700
	C	2.43727100	-0.12157700	0.18974700
	H	0.90024400	-0.41711100	1.90468200
	B	1.11663000	0.29183700	0.95830600
	C	1.02740000	1.80080400	1.36312700
	N	0.91387800	2.91371000	1.67534700
	H	0.11202500	0.07396400	0.11440300
	C	-1.21716100	-0.22651100	-0.80134400
	H	-1.07471900	0.52170900	-1.57779100
	H	-0.98534300	-1.24283400	-1.11208100
	C	-2.37602800	-0.03785900	0.13459600
	H	-2.36442700	0.98111200	0.53926700
	H	-2.27605500	-0.71587900	0.99070400
	C	-3.74381300	-0.28771100	-0.53297700
	H	-3.78086800	-1.30469200	-0.93358700
	H	-3.87627700	0.39574500	-1.37628400
	C	-4.90350600	-0.09232600	0.46862900
	H	-4.89529400	0.92591400	0.86951800
	H	-4.79174400	-0.77163200	1.31937300
	C	-6.21229000	-0.33119700	-0.13010500
	N	-7.23872600	-0.52514300	-0.62179300
TS45	C	-1.85101200	-2.48881800	0.25694200
	H	-1.84895200	-3.55114100	0.08609000
	C	-2.22556500	-1.76587200	1.34103300
	H	-2.61596800	-2.07688400	2.29430300
	N	-2.01591800	-0.43488600	1.02904700
	C	-2.28773100	0.67699300	1.94038000
	H	-1.48125200	1.40508800	1.87891400
	H	-3.23040700	1.16128200	1.68529200
	H	-2.34148900	0.28548700	2.95446100

	N	-1.42651400	-1.58689700	-0.70228400
	C	-0.92434900	-1.96916500	-2.02300200
	H	-1.07770000	-3.03900700	-2.14818100
	H	-1.46715100	-1.43161000	-2.79828100
	H	0.13907100	-1.74441200	-2.10480900
	C	-1.52774100	-0.31566100	-0.23330000
	H	-0.80882300	0.78802900	-2.14388500
	B	-1.06459500	0.99721100	-0.98824800
	C	-2.02835100	2.22244100	-0.84679000
	N	-2.70835500	3.16001200	-0.76464900
	H	0.08464700	1.37234400	-0.43986800
	C	1.57161400	1.84756200	0.07639700
	H	1.75345100	2.64065800	-0.64393400
	H	1.32339300	2.19434800	1.07627800
	C	2.40068900	0.60397000	-0.03980600
	H	2.38227000	0.22934100	-1.06784000
	H	1.99431600	-0.18687100	0.59819600
	C	3.88542500	0.83958900	0.36427400
	H	4.33467500	1.60651700	-0.27247900
	H	3.94650700	1.19853100	1.39526000
	C	4.68967600	-0.37449400	0.25484400
	N	5.29656700	-1.35208900	0.15872700
TS46	C	-0.70960800	-0.04346800	0.22114200
	C	-2.55681800	0.53754500	-0.92955800
	C	-2.79713800	-0.66516400	-0.35224600
	H	-3.17797600	1.15522800	-1.55442400
	H	-3.66771100	-1.29684400	-0.37921800
	N	-1.65650300	-1.01013600	0.35162500
	N	-1.27076900	0.90435900	-0.57550900
	C	-1.50398100	-2.25099400	1.11214400
	H	-0.76172200	-2.89668600	0.64292500
	H	-1.19334100	-2.02776100	2.13129700
	H	-2.46536800	-2.76039300	1.12924100
	C	-0.61637000	2.13859100	-1.00847700
	H	-0.61809000	2.87710400	-0.20662900
	H	0.41094500	1.92448900	-1.29749500
	H	-1.15658000	2.53206400	-1.86740900
	H	0.92263300	-1.00441800	1.56275300
	B	0.76578700	-0.09752900	0.78901600
	C	1.29493100	1.24508700	1.39340500
	N	1.73387200	2.22200100	1.84323800
	H	1.55575800	-0.37456700	-0.24683200
	C	2.62945100	-0.79513800	-1.41285000
	H	2.02376900	-1.52677500	-1.94252100

	H	2.71698600	0.16143500	-1.92234000
	C	3.83476300	-1.29770400	-0.67315200
	H	4.63290900	-1.61786700	-1.35894900
	H	4.26134800	-0.52353500	-0.02818200
	H	3.58993000	-2.15992400	-0.04522700
TS47	C	3.24169100	-1.19960200	-0.53494100
	H	3.97247000	-1.98892600	-0.55758000
	C	3.11330100	-0.08778100	-1.30057000
	H	3.71049800	0.27809500	-2.11747400
	N	1.99325100	0.58436600	-0.84786200
	C	1.49840100	1.83903000	-1.41616600
	H	0.41848200	1.78409700	-1.54091700
	H	1.74460600	2.67732200	-0.76481200
	H	1.96514100	1.98306700	-2.38838000
	N	2.20126300	-1.18377500	0.37644700
	C	1.97776600	-2.22162500	1.38530500
	H	2.81658400	-2.91364900	1.35161300
	H	1.91739700	-1.77254700	2.37497000
	H	1.05525500	-2.76258900	1.17632700
	C	1.42833800	-0.08353500	0.19008500
	H	-0.08956600	-0.45681300	1.90925200
	B	0.09064200	0.26741000	0.96743000
	C	-0.05353800	1.76991000	1.38612400
	N	-0.20400800	2.87516600	1.70743200
	H	-0.90043300	0.01938300	0.13122400
	C	-2.25031000	-0.33753700	-0.76661200
	H	-2.22547300	0.46139600	-1.50050200
	H	-1.98084500	-1.32078700	-1.13858400
	C	-3.35462800	-0.27873200	0.26329300
	H	-3.17249900	-0.98932300	1.07566900
	H	-3.41590900	0.71545400	0.71665400
	C	-4.66727800	-0.58775100	-0.31285200
	N	-5.68641700	-0.83654200	-0.79696100
TS48	C	-0.62352400	0.30081600	-0.00410700
	C	-2.66221800	-0.64806300	0.07414300
	C	-1.92431700	-1.18038500	1.07968800
	H	-3.67874200	-0.83281400	-0.22597000
	H	-2.17504000	-1.91604200	1.82368200
	N	-0.67554400	-0.59152600	1.01812500
	N	-1.85233600	0.26182300	-0.58146300
	C	0.43675300	-0.91423700	1.91389900
	H	0.14466100	-1.76356600	2.52806900
	H	1.31464200	-1.17896000	1.32582000
	H	0.66782000	-0.06452200	2.55514400

	C	-2.27446800	1.04786200	-1.74233500
	H	-3.35177300	0.94157000	-1.85258300
	H	-2.02787200	2.09651200	-1.58971700
	H	-1.78136700	0.68870500	-2.64580500
	H	0.34283700	1.89991200	-1.38951500
	B	0.62594300	1.13850900	-0.50392300
	H	1.47082100	0.26836500	-1.04188100
	C	2.53697200	-0.81208200	-1.67610900
	H	2.14394800	-1.05175900	-2.65959500
	H	3.50177700	-0.31967400	-1.60385200
	F	2.45862100	-1.89563900	-0.82519100
	C	1.42606800	1.86839100	0.62672500
	N	2.05350700	2.41922700	1.43349800
TS49	C	0.57793400	0.07656900	0.27289700
	C	2.56814600	-0.85083100	-0.23557600
	C	2.42078500	0.24906900	-1.01356200
	H	3.37057000	-1.56477200	-0.17219100
	H	3.07130800	0.67825500	-1.75545100
	N	1.19424600	0.80594400	-0.69716300
	N	1.43272700	-0.94554300	0.55017100
	C	0.64284400	2.00147500	-1.33302200
	H	1.22730700	2.21751300	-2.22528400
	H	-0.39291100	1.82199700	-1.61788400
	H	0.68553500	2.85336600	-0.65454700
	C	1.19354300	-2.01080400	1.52277200
	H	2.10345000	-2.60073200	1.61337600
	H	0.94169000	-1.58155900	2.49118800
	H	0.37780100	-2.65370700	1.19085500
	H	-1.06914900	-0.44461600	1.82185100
	B	-0.86530200	0.27084100	0.87674400
	H	-1.72934900	-0.16087700	-0.06353800
	C	-2.82355200	-0.82632000	-1.03740600
	H	-3.74820500	-0.39613200	-0.65493900
	H	-2.50457900	-0.48429200	-2.01693000
	O	-2.70465500	-2.20333000	-0.92961900
	H	-3.08215600	-2.48997700	-0.09041300
	C	-1.27936500	1.74415300	1.18994300
	N	-1.63976900	2.82218300	1.43140100
TS50	C	0.34508700	-0.10321800	-0.16777000
	C	1.90875400	1.38775400	0.46265800
	C	2.54900800	0.23977400	0.13012400
	H	2.29059600	2.33208700	0.80960300
	H	3.59586400	-0.00878600	0.13389100
	N	1.57740300	-0.66650000	-0.25571600

	N	0.55680200	1.16060900	0.28081900
	C	1.85842100	-2.03860800	-0.68259700
	H	1.46001600	-2.75085900	0.03942200
	H	1.41129500	-2.22507300	-1.65735700
	H	2.93773200	-2.15865300	-0.74943600
	C	-0.48883300	2.15143400	0.53789500
	H	-0.83272400	2.59697400	-0.39563000
	H	-1.32802200	1.67360800	1.03968000
	H	-0.07822900	2.92610900	1.18246000
	H	-0.89511600	-1.91420300	-0.92540300
	B	-1.04104200	-0.82853600	-0.43047000
	C	-2.07893600	0.01552500	-1.24601000
	N	-2.88170600	0.60895200	-1.83878700
	H	-1.58284100	-1.04061800	0.75205600
	C	-2.31526500	-1.42038500	2.21013700
	H	-1.45464000	-1.73508700	2.78997600
	H	-2.76019900	-0.46790000	2.47568700
	H	-2.99543800	-2.19999400	1.88656500
TS51	C	2.52681200	-0.93365200	-0.23587400
	H	3.34630300	-1.60706700	-0.05531900
	C	2.15804400	-0.26618200	-1.35846200
	H	2.59545300	-0.24660000	-2.34126200
	N	1.02532500	0.45698900	-1.04205100
	C	0.30336900	1.31104600	-1.98739500
	H	-0.76745800	1.14548800	-1.88741900
	H	0.52693300	2.36117500	-1.80096900
	H	0.61359000	1.04441100	-2.99551100
	N	1.61605400	-0.60151700	0.74772400
	C	1.65306500	-1.13276800	2.11273100
	H	2.57782800	-1.69281100	2.23258200
	H	1.62813900	-0.31596200	2.83126000
	H	0.80489900	-1.79491600	2.28410900
	C	0.68768500	0.25856200	0.25747300
	H	-0.53304500	0.56773900	2.21665600
	B	-0.56670000	0.81881100	1.04492700
	C	-0.92344900	2.31822300	0.78728300
	N	-1.22892500	3.42498600	0.62094800
	H	-1.62005100	0.12068200	0.59344300
	C	-2.95052200	-0.65573300	0.18744400
	H	-3.40817600	-0.69248900	1.16924000
	H	-3.35924900	0.07548700	-0.50050800
	C	-2.54111800	-1.88038000	-0.36293900
	N	-2.13459300	-2.87672700	-0.80840700
TS52	C	-0.81000800	-0.31204700	0.07114800

	C	-2.62056900	0.98745500	-0.20436700
	C	-1.88618300	1.05806900	-1.34411200
	H	-3.55320600	1.45349600	0.06142500
	H	-2.05442000	1.60220600	-2.25699700
	N	-0.77881500	0.25569100	-1.16057000
	N	-1.94687100	0.14392200	0.65604000
	C	0.30939500	0.11891800	-2.13441000
	H	1.19514400	0.64404600	-1.77322600
	H	0.53701900	-0.93303300	-2.29244900
	H	-0.01856300	0.56070700	-3.07289200
	C	-2.41392700	-0.20064200	2.00197300
	H	-3.39447500	0.24810000	2.14489200
	H	-2.49147200	-1.28128800	2.10542700
	H	-1.72631100	0.18845200	2.75186600
	H	-0.04345400	-1.61714000	1.84607100
	B	0.27450600	-1.24492600	0.75286400
	H	1.33966300	-0.45108500	0.96938400
	C	2.68066600	0.28787400	1.21978200
	H	2.77336600	0.03193100	2.26971800
	H	3.25058400	-0.31279300	0.51840200
	C	2.42374800	1.65539100	0.87817400
	O	2.51077900	2.12393600	-0.26729800
	H	2.08158900	2.30590100	1.70433500
	C	0.81610000	-2.41727700	-0.12611400
	N	1.24718000	-3.29572700	-0.74894700
TS53	C	1.10613500	-0.12273900	0.29786300
	C	2.17195600	-2.07064100	-0.04567600
	C	2.84207900	-1.11062600	-0.73145200
	H	2.35635900	-3.12648200	0.04787900
	H	3.72367100	-1.16952600	-1.34544900
	N	2.17340000	0.07904500	-0.51633900
	N	1.10974800	-1.44992000	0.58112000
	C	2.57668500	1.35908600	-1.10450200
	H	3.33601200	1.16124800	-1.85785000
	H	1.72054200	1.83731800	-1.57655800
	H	2.98499600	2.01896400	-0.34036900
	C	0.10961100	-2.14978700	1.39304700
	H	0.42821900	-3.18406900	1.50369400
	H	0.03830600	-1.68547200	2.37503800
	H	-0.86218100	-2.11682800	0.89984300
	H	-0.57910100	0.51454600	1.76210600
	B	-0.01200600	0.89562700	0.77495000
	H	-0.94810100	0.85082200	-0.15511000
	C	-2.13954000	0.66208400	-1.25871700

	H	-2.41587100	1.70450400	-1.34396400
	H	-1.50732000	0.23721300	-2.02597500
	C	-3.03047600	-0.24478700	-0.57995800
	O	-2.93426300	-1.46788500	-0.56199200
	O	-4.00610500	0.39393900	0.13026700
	H	-4.52341700	-0.28649100	0.58641400
	C	0.40483100	2.39550700	0.91615700
	N	0.65730600	3.52074700	1.03933000
TS54	C	0.85859400	0.17077500	0.25041500
	C	2.72319000	-0.73782400	-0.61717500
	C	2.17633400	0.06001000	-1.56807700
	H	3.61052000	-1.34603200	-0.63393400
	H	2.49732500	0.28167900	-2.57085600
	N	1.03077500	0.60776400	-1.02288600
	N	1.90486000	-0.65823100	0.49455400
	C	0.13135500	1.51981600	-1.73253300
	H	0.39892000	1.51171500	-2.78703100
	H	-0.89746600	1.18124000	-1.62033100
	H	0.22712100	2.53145000	-1.33951800
	C	2.14122400	-1.39118400	1.74038800
	H	3.13843800	-1.82397900	1.69587500
	H	2.07818300	-0.71192000	2.58786300
	H	1.40619000	-2.18732300	1.85825600
	H	-0.18340400	0.00691800	2.32460600
	B	-0.35264200	0.47280900	1.23067900
	H	-1.39911400	-0.16324700	0.73790800
	C	-2.67089800	-1.01653600	0.10335100
	H	-3.58078200	-0.93821200	0.69791500
	F	-2.85012000	-0.52863500	-1.15108000
	F	-2.24113000	-2.29950700	0.01077600
	C	-0.76943700	1.97999200	1.32031400
	N	-1.11472800	3.08427400	1.41097400
TS55	C	1.33575000	-0.02652800	0.22064700
	C	2.28758600	-1.96241000	-0.40657700
	C	2.12991700	-1.20378000	-1.52028600
	H	2.70035200	-2.94785100	-0.27969000
	H	2.38095900	-1.40071800	-2.54783200
	N	1.54024700	-0.02063600	-1.11973600
	N	1.79626400	-1.22587300	0.65469800
	C	1.18736600	1.07344600	-2.02686600
	H	1.18609100	0.68767000	-3.04418200
	H	0.19328900	1.44301500	-1.78376600
	H	1.90893400	1.88577100	-1.94364400
	C	1.76610200	-1.70218400	2.04021800

	H	2.31954200	-2.63741500	2.08926100
	H	2.23282500	-0.96977300	2.69567100
	H	0.73826300	-1.87263600	2.35904200
	H	0.70506500	0.83988100	2.28435400
	B	0.62725800	1.08413200	1.11143400
	H	-0.64764200	1.04096500	0.83364700
	C	-2.34534100	1.04198900	0.64981300
	H	-2.63918000	1.08991300	1.69029100
	H	-2.47708100	1.93411400	0.05120400
	C	1.08743500	2.55445100	0.81813200
	N	1.39800900	3.65604900	0.62962900
	C	-2.62481100	-0.22881200	-0.03109800
	F	-2.20612200	-1.31140900	0.67915700
	F	-2.03161600	-0.31200100	-1.25440900
	F	-3.96485800	-0.44963700	-0.26670000
TS56	C	-0.87577100	0.10830200	0.23938400
	C	-2.10158100	-0.77178100	-1.42895600
	C	-2.34783200	-1.50025400	-0.31178600
	H	-2.48602300	-0.86472100	-2.42970300
	H	-2.98668500	-2.35131000	-0.15285400
	N	-1.58984500	-0.94820000	0.70456200
	N	-1.19241200	0.20819000	-1.07688100
	C	-1.55822600	-1.46059100	2.07595900
	H	-2.31480300	-2.23731000	2.16480800
	H	-0.57898400	-1.88263400	2.30038900
	H	-1.77643200	-0.65893300	2.77895100
	C	-0.65123600	1.20263200	-2.00403800
	H	-0.80373000	0.84460600	-3.02017100
	H	-1.15341100	2.16139900	-1.87472300
	H	0.41491500	1.32618500	-1.82429100
	B	0.17254600	0.96731100	1.06269500
	H	1.36973100	0.59288900	0.64305000
	C	2.90475100	0.14985100	0.24046200
	H	3.17471800	0.87488000	-0.51787700
	H	3.41221700	0.20820000	1.19551200
	Cl	2.87547700	-1.49846700	-0.39582400
	H	0.15058000	0.71163000	2.23626800
	C	0.09343000	2.51311000	0.82528500
	N	0.07523700	3.66356700	0.67207700
TS57	C	0.95735600	-0.06997500	0.27302000
	C	2.56472600	-1.56239800	-0.24854300
	C	2.81745500	-0.43004100	-0.94905400
	H	3.09015000	-2.50082100	-0.21466500
	H	3.60623900	-0.19126600	-1.64087500

	N	1.82241500	0.47566900	-0.62588100
	N	1.42281500	-1.32942400	0.49804000
	C	1.71816700	1.81994200	-1.19103000
	H	2.41127800	1.89511200	-2.02661800
	H	0.70419800	1.99256400	-1.54974400
	H	1.96670900	2.57269400	-0.44324000
	C	0.80720900	-2.31405900	1.38644000
	H	1.46696500	-3.17718800	1.44771600
	H	0.67369300	-1.88869200	2.37990400
	H	-0.16147100	-2.62699700	0.99610400
	H	-0.83067500	-0.11515600	1.74807300
	B	-0.37636100	0.53982100	0.84849300
	H	-1.29310400	0.44401100	-0.14548000
	C	-2.45151900	0.27553800	-1.24740400
	H	-3.05295000	1.17231500	-1.08472000
	H	-1.87379000	0.24474700	-2.16671200
	O	-3.09732100	-0.91856700	-1.02785900
	C	-0.33089100	2.05424500	1.22661400
	N	-0.35562900	3.17993000	1.51425000
	C	-4.00687000	-0.89761000	0.07175500
	H	-4.77981800	-0.13567500	-0.08280500
	H	-4.47035500	-1.88210300	0.12092700
	H	-3.47769100	-0.69118700	1.00688900
TS58	C	1.21393600	-0.11861900	0.30108700
	C	2.41693300	-1.96395600	-0.17271600
	C	2.86365000	-0.96858400	-0.97698600
	H	2.72531200	-2.99122100	-0.08758400
	H	3.63803700	-0.96175200	-1.72401700
	N	2.11461400	0.15635000	-0.68125900
	N	1.40667900	-1.43031600	0.60749000
	C	2.27761800	1.44971100	-1.34426100
	H	2.86048400	1.29961900	-2.25085800
	H	1.30172800	1.85357400	-1.60843400
	H	2.79357600	2.15451900	-0.69233300
	C	0.64556300	-2.19036800	1.59856800
	H	1.10109000	-3.17366000	1.69712800
	H	0.67160100	-1.68026800	2.56003800
	H	-0.39029600	-2.30221700	1.27734300
	H	-0.42761600	0.34177600	1.87479400
	B	0.08606700	0.81000700	0.89435700
	H	-0.90412900	0.81571800	-0.02755500
	C	-2.11772300	0.81931900	-1.06196700
	H	-2.61939200	1.74721500	-0.79563600
	H	-1.56783400	0.85136500	-1.99841900

	S	-3.09202200	-0.64415600	-0.92632700
	C	0.47017800	2.30591200	1.12348900
	N	0.69909500	3.43021500	1.30597100
	C	-3.97323700	-0.32655900	0.64197100
	H	-4.58486200	0.57244000	0.55662600
	H	-4.61761000	-1.18585500	0.82686600
	H	-3.26230000	-0.21965900	1.46095100
TS59	C	0.91478600	-0.11809600	0.30225900
	C	2.01061500	-2.01243200	-0.25759800
	C	2.37214100	-1.05610500	-1.14661300
	H	2.30679700	-3.04372800	-0.17652100
	H	3.04478000	-1.09490100	-1.98564300
	N	1.69217500	0.09910100	-0.79956700
	N	1.12047500	-1.42851700	0.62762500
	C	1.79120400	1.36227000	-1.52522700
	H	2.28782600	1.17595600	-2.47570200
	H	0.79423900	1.75897700	-1.71362500
	H	2.36315700	2.09368200	-0.95385900
	C	0.47836100	-2.13259200	1.73341400
	H	0.62895600	-1.58526500	2.66309800
	H	-0.59187400	-2.23720700	1.55002600
	H	0.92726500	-3.12048400	1.81805700
	H	-1.21897900	0.87057400	0.19205300
	B	-0.10188300	0.85349400	0.99420100
	H	-0.50922100	0.43484300	2.04560300
	C	-2.54763300	0.90908600	-0.63394700
	H	-2.21107000	1.50882600	-1.47480200
	H	-3.16990800	1.43970200	0.08594300
	N	-2.94649700	-0.38932100	-0.95528300
	H	-2.96694300	-0.61533100	-1.93858500
	C	0.32969500	2.34747700	1.11116300
	N	0.59430000	3.47524600	1.21538100
	C	-3.96699600	-1.04437700	-0.15374400
	H	-4.09093800	-2.07564200	-0.48829800
	H	-3.65750000	-1.06555400	0.89446000
	H	-4.94338300	-0.53887200	-0.20855000
TS60	C	1.03572600	-0.29425500	0.28878500
	C	1.23718700	-2.50634200	-0.08769000
	C	1.69199100	-1.86212500	-1.19029100
	H	1.16319000	-3.55686800	0.13269800
	H	2.09375200	-2.24361500	-2.11263700
	N	1.55795000	-0.50656600	-0.95010700
	N	0.84001200	-1.53493200	0.81316300
	C	1.92864300	0.53722400	-1.90511200

	H	2.04631400	0.07940300	-2.88543100
	H	1.14249700	1.28883400	-1.95297700
	H	2.86335400	1.01438900	-1.61080000
	C	0.27111700	-1.82116900	2.13002700
	H	0.80764600	-1.26464300	2.89647100
	H	-0.78388400	-1.54727400	2.15694400
	H	0.37102700	-2.88792600	2.31956400
	H	-0.53722400	1.46046700	0.40071800
	B	0.63222000	1.06995400	0.96810500
	H	0.35580000	0.94391500	2.13054300
	C	-1.93984800	1.94493600	-0.13073000
	H	-1.70354300	2.09894300	-1.17825200
	H	-2.08614000	2.84334100	0.45683400
	N	-2.89192500	0.93946500	0.10644800
	H	-3.31444500	0.88666400	1.02623500
	C	1.61164600	2.26554000	0.74731100
	N	2.30146300	3.18952800	0.60673300
	C	-3.18324200	-0.08559300	-0.73298000
	H	-2.68516000	0.00435200	-1.71132300
	O	-3.93326400	-1.01893900	-0.45733600
TS61	C	-1.06966300	0.10466400	-0.17279400
	C	-2.35183000	-1.63240400	0.44783700
	C	-1.88383000	-1.04242000	1.57723400
	H	-2.99863500	-2.48173400	0.31418000
	H	-2.03925200	-1.28459700	2.61396200
	N	-1.10101100	0.02282800	1.18110300
	N	-1.84381500	-0.91755500	-0.61900000
	C	-0.34130900	0.87308200	2.10334700
	H	0.71586600	0.60467500	2.06389600
	H	-0.47177800	1.91908900	1.83488100
	H	-0.72472900	0.71091400	3.10867500
	C	-2.12025500	-1.23036400	-2.02361700
	H	-2.86744300	-2.02042200	-2.05418200
	H	-2.50450400	-0.34903400	-2.53328200
	H	-1.21329500	-1.57152400	-2.52170400
	H	-0.41289900	0.93584400	-2.25065600
	B	-0.24101200	1.10871200	-1.07731600
	H	1.05204700	0.79957900	-0.87143500
	C	2.59209000	0.62475300	-0.67906000
	H	2.85451500	0.64590300	-1.73125200
	H	2.73887000	1.54520300	-0.12516900
	C	2.72218500	-0.61482800	0.05157600
	O	2.66924800	-0.64938100	1.29249600
	C	-0.35629500	2.61904900	-0.69245800

	N	-0.41009100	3.74851700	-0.43274900
	C	2.87875100	-1.89333600	-0.75088600
	H	2.18123500	-1.91897000	-1.59305500
	H	3.88932600	-1.94791800	-1.16922400
	H	2.71710400	-2.76122200	-0.11158300
TS62	C	1.09997000	-0.12271000	0.30699600
	C	2.11467300	-2.10122200	-0.02157500
	C	2.81800200	-1.16285400	-0.70337500
	H	2.26767700	-3.16171200	0.07587600
	H	3.70337400	-1.24837600	-1.30874600
	N	2.18099900	0.04634100	-0.49781500
	N	1.06421900	-1.44910000	0.59381300
	C	2.62372100	1.31188600	-1.08765500
	H	1.78667100	1.80720900	-1.57625100
	H	3.03564700	1.96776500	-0.32192000
	H	3.38986300	1.09123100	-1.82778600
	C	0.03263600	-2.11882300	1.39160200
	H	0.32210400	-3.16091400	1.51062900
	H	-0.04030500	-1.64946900	2.37127300
	H	-0.92967100	-2.05987100	0.88124300
	H	-0.57224400	0.57068100	1.75935200
	B	0.00386500	0.92448400	0.76649600
	H	-0.93623500	0.88105100	-0.16915600
	C	-2.12760500	0.69907300	-1.25323900
	H	-2.41448100	1.74081300	-1.34249600
	H	-1.50605300	0.29241400	-2.04010000
	C	-3.01328600	-0.24388200	-0.58239500
	O	-2.83157400	-1.47316700	-0.61647400
	N	-4.03986100	0.29387600	0.14297200
	H	-4.19622400	1.28673900	0.20011500
	H	-4.64099400	-0.31926600	0.67076400
	C	0.44551500	2.41867800	0.88516800
	N	0.70927100	3.54370200	0.99008000
TS63	C	-1.37323100	0.00147900	-0.24520900
	C	-3.15993700	-0.60524000	0.97764600
	C	-2.56798600	0.44008300	1.60767900
	H	-4.03260400	-1.17984800	1.23424700
	H	-2.82696000	0.95271000	2.51752400
	N	-1.47047500	0.79844400	0.84848800
	N	-2.41624000	-0.86299600	-0.15856900
	C	-0.54972100	1.88399300	1.19557700
	H	-0.73678700	2.17043200	2.22846300
	H	0.47763600	1.53853000	1.09964000
	H	-0.71113000	2.74260300	0.54451600

	C	-2.71948400	-1.93392900	-1.11081600
	H	-3.67245900	-2.37695100	-0.82950100
	H	-2.79099700	-1.52823000	-2.11808700
	H	-1.94300400	-2.69788900	-1.08200500
	H	-0.54604600	-0.71329900	-2.29402700
	B	-0.24461600	-0.01829000	-1.36177300
	H	0.80606700	-0.60615300	-0.82985800
	C	2.15473100	-1.46681000	-0.32606100
	H	1.71444300	-2.09267200	0.44310000
	H	2.39339400	-1.94606300	-1.26808800
	C	0.23774600	1.38778700	-1.85558800
	N	0.62986900	2.40528900	-2.25195200
	C	3.09762000	-0.43517600	0.12837000
	F	2.57669200	0.28069800	1.19864200
	F	4.28619000	-0.99987600	0.63456300
	H	3.40508500	0.28260700	-0.63125500
TS64	C	-1.12093100	-0.06014700	-0.22001700
	C	-2.93392900	-1.20496100	0.45822800
	C	-2.84993400	-0.08495400	1.21841200
	H	-3.64995800	-2.00795000	0.46598600
	H	-3.47895700	0.27505400	2.01378300
	N	-1.72986200	0.60512100	0.79454500
	N	-1.86703300	-1.17628000	-0.42126300
	C	-1.27778300	1.87472900	1.36564000
	H	-1.77623100	2.01776300	2.32210900
	H	-0.20125100	1.84347200	1.52300000
	H	-1.52175500	2.70187800	0.69937000
	C	-1.59232200	-2.21817700	-1.41351000
	H	-2.43246100	-2.90939600	-1.42184600
	H	-1.47999600	-1.77204400	-2.39980300
	H	-0.68222600	-2.75902400	-1.15507300
	H	0.46747400	-0.42314700	-1.87941900
	B	0.23435000	0.30758200	-0.95544000
	H	1.20334600	0.07798300	-0.07572500
	C	2.45148000	-0.25869700	0.94048200
	H	2.52748300	0.69403000	1.45505100
	H	1.99497700	-1.06313000	1.50901900
	C	0.37813000	1.80844000	-1.37501100
	N	0.52885100	2.91351200	-1.69638100
	C	3.53119800	-0.61454000	-0.00192900
	F	4.74536700	-0.97649200	0.71131500
	H	3.29073200	-1.48894900	-0.60781100
	H	3.81961400	0.21734000	-0.64534900