

Electronic Supplementary Information for:

Hydrazine Bisalane Is a Potential Compound for Chemical Hydrogen Storage. A Theoretical Study

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Table S-1. Total and zero-point energy of equilibrium structures for the formation of hydrazine bisalane calculated with CCSD(T)^a

Structures	Basis set		
	aVDZ	aVTZ	ZPE ^{b)}
dalhyz-C	-599.1724904	-599.3336256	63.57254
dalhyz-T	-599.1719083	-599.3329035	63.55218
alalhyz-C	-599.1692140	-599.3282289	62.76711
alalhyz-T	-599.1722220	-599.3317652	63.12794
alhyzal-C	-599.1713484	-599.3302177	62.84847
alhyzal-T	-599.1750607	-599.3342943	62.81733
TS-dalhyz-C-T	-599.1522476	-599.3114301	62.79258
TS-dalhyz-alalhyz-C	-599.1633615	-599.3241562	62.92873
TS-dalhyz-alalhyz-T	-599.1655406	-599.3267311	63.03292
TS-alalhyz-T-C	-599.1486009	-599.3078810	62.02438
TS-alalhyz-alhyzal-C	-599.1557346	-599.3147632	62.80286

- a) All energy values are given in hartrees.
- b) The harmonic vibrational frequencies were calculated using the MP2/aVDZ method.

Table S-2. Total and zero-point energy of transition states and products for H₂-release from **alhyzal-C** and **alhyzal-T** calculated using CCSD(T) method ^{a)}

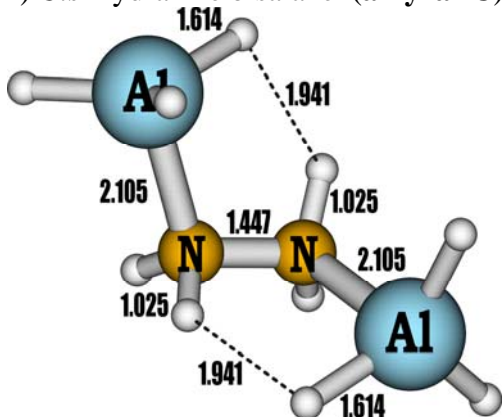
TS's and Prod's	Basis set		
	aVDZ	aVTZ	ZPE ^{b)}
TS12-alhyzal-C	-599.1254621	-599.2869107	59.70718
TS13-alhyzal-C	-599.1294626	-599.2916108	60.02457
TS12-alhyzal-T	-599.1215966	-599.2828317	59.35337
TS13-alhyzal-T	-599.1288088	-599.2915843	59.75846
p-TS12-alhyzal-C	-598.0092773	-598.1658655	51.22086
p-TS12-alhyzal-T	-597.9899651	-598.1462259	50.28833
p-TS13-alhyzal	-597.9990971	-598.1560254	50.15743

^{a)} All energy values are given in hartrees.

^{b)} The harmonic vibrational frequencies were calculated using the MP2/aVDZ method.

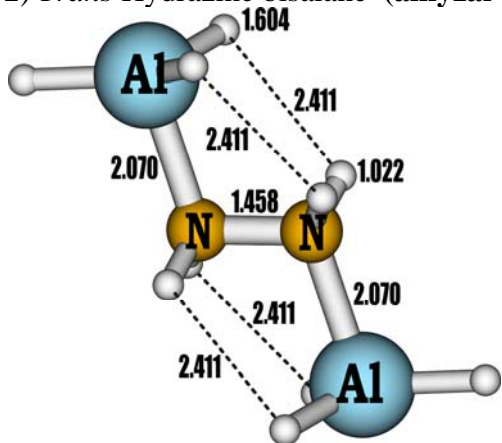
Figure S1. Geometries of the Structures Considered Optimized at the MP2/aug-cc-pVTZ Level of Theory, Given in Cartesian Coordinates (Å). Bond lengths are given in angstrom (Å) and Bond angles in degrees (°).

1) *Cis* Hydrazine bisalane (**alhyzal-C**)



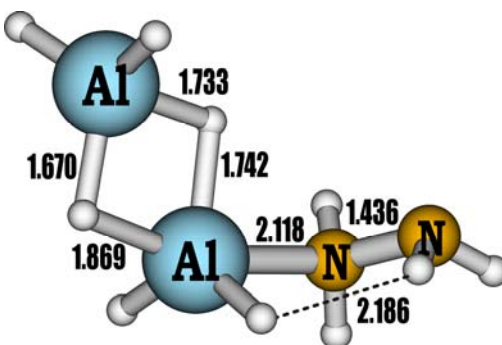
N	-0.516479	0.758554	-0.506340
N	0.516479	0.758553	0.506340
Al	2.137321	-0.448818	-0.081797
Al	-2.137321	-0.448818	0.081796
H	-3.319730	0.477378	-0.452798
H	-0.881214	1.698532	-0.637492
H	-1.725761	-0.276844	1.632935
H	-1.840713	-1.841681	-0.613527
H	3.319730	0.477379	0.452798
H	-0.048127	0.467374	-1.369813
H	1.840715	-1.841681	0.613526
H	1.725760	-0.276843	-1.632935
H	0.881214	1.698531	0.637493
H	0.048127	0.467374	1.369813

2) *Trans* Hydrazine bisalane (**alhyzal-T**)



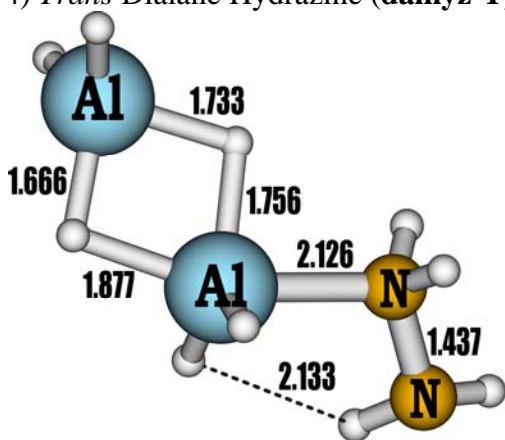
N	0.429046	0.589526	0.000000
N	-0.429058	-0.589526	0.000001
Al	-2.393197	0.067742	0.000000
Al	2.393205	-0.067744	0.000000
H	3.263833	1.258624	0.000002
H	0.130397	1.135445	0.810286
H	2.211551	-0.919499	-1.347229
H	2.211550	-0.919502	1.347227
H	-3.263846	-1.258613	-0.000014
H	0.130395	1.135445	-0.810285
H	-2.211545	0.919491	1.347231
H	-2.211534	0.919509	-1.347219
H	-0.130409	-1.135447	-0.810283
H	-0.130409	-1.135445	0.810287

3) *Cis* Dialane Hydrazine (**dalhyz-C**)



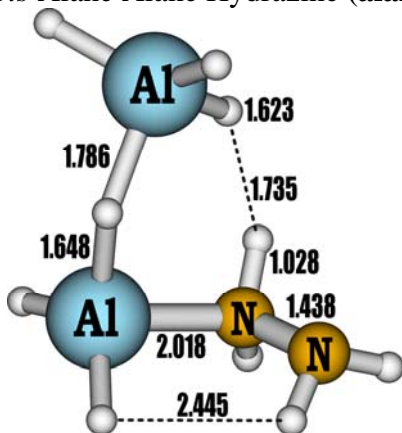
N	-1.821237	0.190928	-0.515507
N	-2.325266	-0.978392	0.147957
Al	0.030694	0.823811	0.293121
Al	2.335509	-0.432651	-0.106998
H	-2.454391	0.985414	-0.444826
H	0.670497	-0.545337	-0.574065
H	0.006687	2.195718	-0.508418
H	-1.723593	-0.032214	-1.500973
H	-0.493102	0.503425	1.765975
H	3.156787	-0.031790	-1.395533
H	1.837654	0.902319	0.764156
H	2.654820	-1.667329	0.824355
H	-3.337235	-0.997496	0.100417
H	-2.053245	-0.885541	1.122158

4) *Trans* Dialane Hydrazine (**dalhyz-T**)



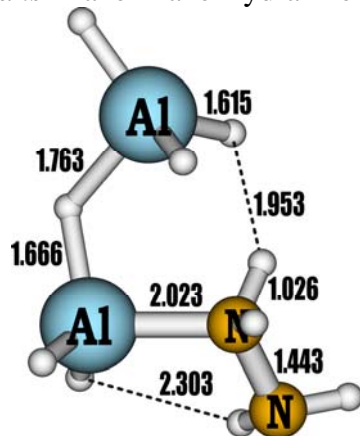
N	-1.659347	-0.647208	0.265720
N	-2.836292	0.022953	-0.213725
Al	0.007576	0.664434	0.125724
Al	2.498063	-0.261772	-0.107152
H	3.304451	-0.520247	1.225882
H	-1.469458	-1.509383	-0.240080
H	0.888452	-0.854986	0.142320
H	2.948482	-0.744649	-1.543135
H	1.774430	1.238119	-0.140025
H	-1.819974	-0.885670	1.239178
H	-0.506292	1.166573	-1.298690
H	-0.171053	1.322459	1.553771
H	-2.536535	0.578797	-1.009520
H	-3.516335	-0.655835	-0.535107

5) *Cis* Alane Alane Hydrazine (**alalhyz-C**)



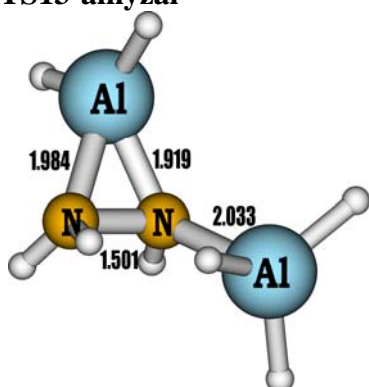
N	1.279909	-0.351533	0.626088
N	1.801345	-1.181029	-0.425856
Al	0.442701	1.317788	-0.137738
Al	-2.173966	-0.431759	-0.027028
H	0.208279	2.252632	1.114621
H	1.961135	-0.157174	1.357719
H	-0.954334	0.669906	-0.725651
H	1.434433	1.647458	-1.332092
H	-3.270935	0.589516	0.493117
H	0.482739	-0.849768	1.041578
H	-2.442733	-1.366667	-1.280216
H	-1.235252	-1.075224	1.130186
H	2.368138	-0.591585	-1.024994
H	2.386193	-1.909540	-0.033921

6) *Trans* Alane Alane Hydrazine (**alalhyz-T**, $\text{AlH}_3\text{AlH}_3\text{N}_2\text{H}_4$)



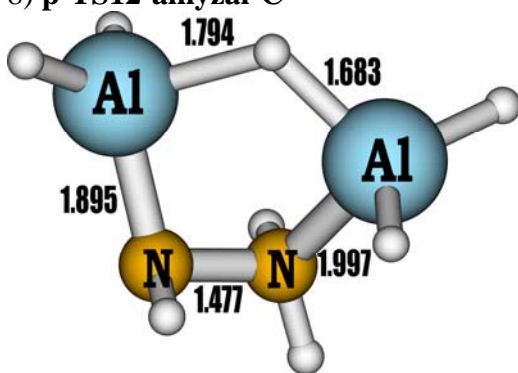
N	-0.979524	-0.604533	0.302966
Al	-0.347349	1.291059	-0.014665
N	-2.357460	-0.762616	-0.093828
Al	2.147025	-0.443114	-0.056280
H	-1.175896	1.626105	-1.327644
H	-0.910539	-0.830141	1.291330
H	1.233145	1.010312	-0.458814
H	-0.447356	2.089037	1.340043
H	1.391948	-1.458185	-1.060059
H	-0.344754	-1.239181	-0.193025
H	3.646145	-0.016265	-0.313785
H	1.574602	-0.653395	1.431960
H	-2.471839	-0.240675	-0.956743
H	-2.532351	-1.740854	-0.294945

7) p-TS13-alhyzal



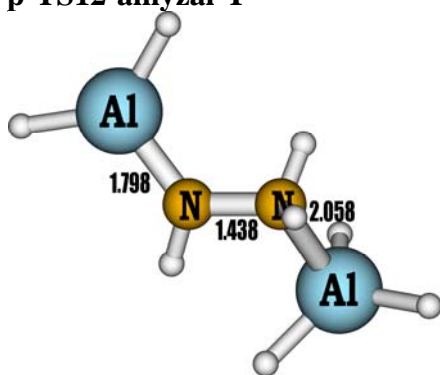
N	-0.018246	0.151192	-0.592718
N	0.636545	1.148026	0.319176
Al	1.658117	-0.530731	0.046905
Al	-1.894464	-0.264916	0.071702
H	-2.809772	0.624027	-0.894931
H	-0.038274	0.556906	-1.523393
H	-1.612146	0.392914	1.530878
H	-2.027438	-1.850805	-0.000042
H	2.858581	-0.271025	-0.937860
H	1.572848	-1.517577	1.260249
H	0.821968	2.025220	-0.153250
H	-0.021356	1.289227	1.091255

8) p-TS12-alhyzal-C



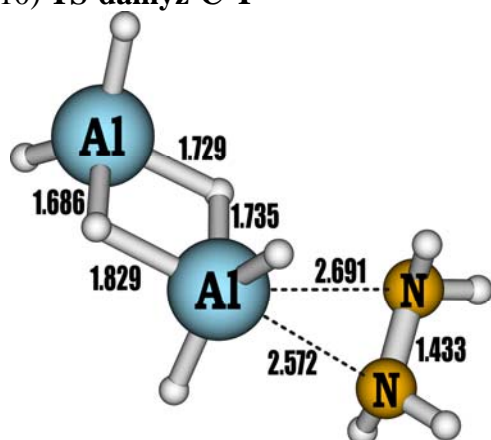
N	0.613440	1.108497	0.358618
N	-0.649193	1.091161	-0.407446
Al	-1.522144	-0.514179	0.095024
Al	1.456243	-0.645530	-0.090275
H	2.497420	-1.091527	1.015699
H	1.115774	1.966694	0.142913
H	1.792912	-0.491951	-1.629911
H	-0.001225	-1.465745	0.095770
H	0.334041	1.203967	1.334006
H	-2.501391	-1.156127	-0.963136
H	-1.763623	-0.446944	1.665503
H	-0.366937	1.160244	-1.380786

9) p-TS12-alhyzal-T



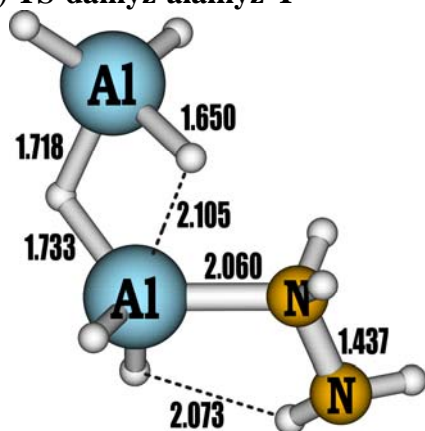
N	-0.453615	0.723942	-0.263149
N	0.607820	-0.230209	-0.437444
Al	2.290785	-0.077550	0.176085
Al	-2.221285	-0.227569	0.190775
H	-3.282731	0.893633	-0.223950
H	-0.532908	1.301119	-1.097728
H	-1.995293	-0.511787	1.746715
H	-1.996643	-1.460840	-0.813776
H	-0.203560	1.351112	0.497416
H	3.256376	-1.295127	-0.041336
H	2.585778	1.314498	0.856031
H	0.186041	-1.082198	-0.788413

10) TS-dalhyz-C-T



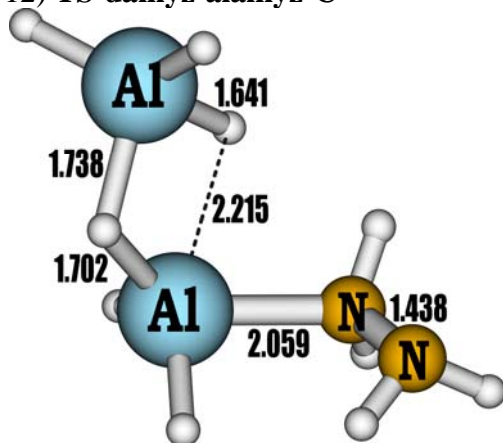
N	1.981410	1.017325	-0.031599
N	2.451450	-0.330175	-0.165718
Al	-0.064606	-0.714554	0.207003
Al	-2.477220	0.303571	-0.104218
H	0.363060	-0.519355	1.713839
H	2.652354	1.700781	-0.367208
H	-1.822079	-1.125514	0.504684
H	0.181900	-1.705659	-0.993930
H	-0.825464	0.722039	-0.398604
H	1.827207	1.179928	0.957031
H	-3.192929	0.071183	-1.492417
H	-3.026998	1.228649	1.052488
H	3.380149	-0.465384	0.221354
H	2.476516	-0.553928	-1.152213

11) TS-dalhyz-alalhyz-T



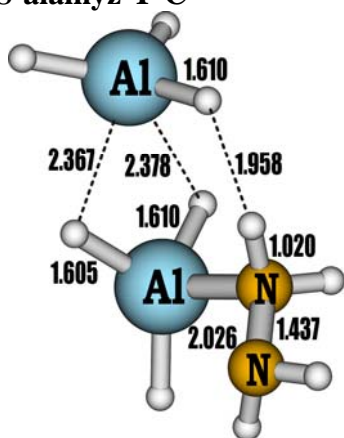
N	1.499917	-0.195870	0.628706
N	2.224040	-0.877747	-0.410016
Al	0.082439	1.078382	-0.148920
Al	-2.200580	-0.518568	-0.005723
H	-1.307041	0.589783	-1.001922
H	1.032754	1.418834	-1.397400
H	-0.185873	2.160614	0.971278
H	1.039496	-0.895877	1.202308
H	2.108772	0.354919	1.232998
H	-3.509426	0.250887	0.434204
H	-2.199596	-1.882707	-0.811193
H	-0.982865	-0.417345	1.089446
H	3.144776	-1.135596	-0.075014
H	2.327138	-0.205777	-1.165168

12) TS-dalhyz-alalhyz-C



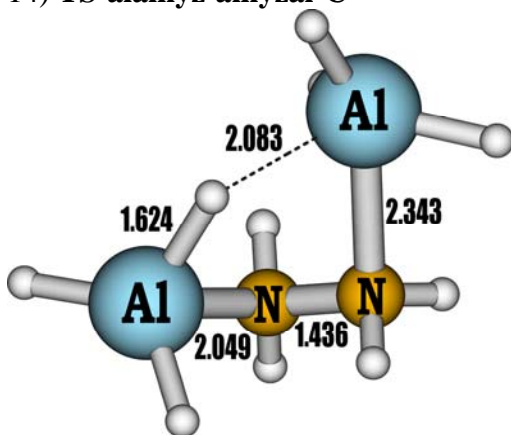
N	1.499917	-0.195870	0.628706
N	2.224040	-0.877747	-0.410016
Al	0.082439	1.078382	-0.148920
Al	-2.200580	-0.518568	-0.005723
H	-1.307041	0.589783	-1.001922
H	1.032754	1.418834	-1.397400
H	-0.185873	2.160614	0.971278
H	1.039496	-0.895877	1.202308
H	2.108772	0.354919	1.232998
H	-3.509426	0.250887	0.434204
H	-2.199596	-1.882707	-0.811193
H	-0.982865	-0.417345	1.089446
H	3.144776	-1.135596	-0.075014
H	2.327138	-0.205777	-1.165168

13) TS-alalhyz-T-C



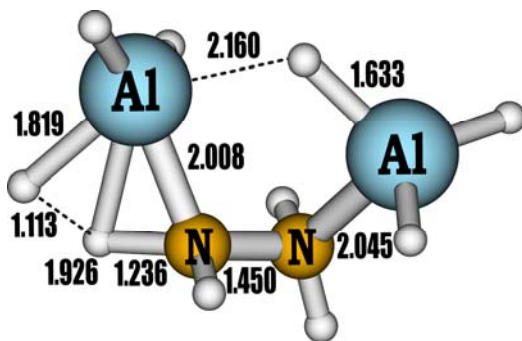
N	1.319468	-0.562139	0.363990
Al	0.209413	1.096439	0.014877
N	2.544266	-0.566527	-0.388202
Al	-2.343328	-0.418578	-0.067795
H	-0.882755	0.973010	1.191576
H	1.467139	-0.699955	1.362338
H	-1.213474	-1.548454	0.131676
H	1.325537	2.223760	0.002408
H	-0.643276	0.691761	-1.283306
H	0.729874	-1.329944	0.041944
H	-3.005383	-0.268767	-1.498635
H	-3.227072	-0.050221	1.195182
H	3.181769	-1.253903	-0.003524
H	2.962397	0.351189	-0.282232

14) TS-alalhyz-alhyzal-C



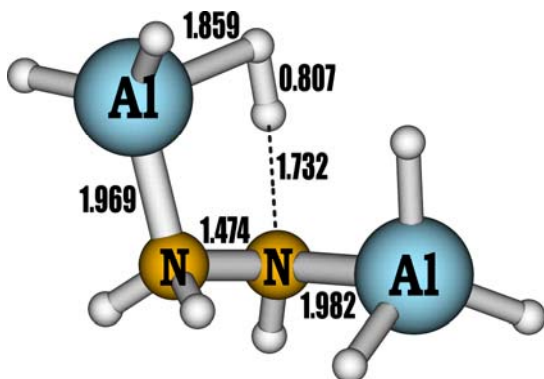
N	0.791030	1.002375	0.518277
Al	1.568002	-0.778678	-0.131515
N	-0.260886	1.183518	-0.441892
Al	-1.806432	-0.503292	0.070894
H	2.094205	-0.260944	-1.547149
H	0.297153	0.830716	1.400898
H	0.061113	-1.375278	-0.237050
H	2.533119	-1.332432	0.992175
H	-2.730579	0.423486	-0.864026
H	1.390983	1.818514	0.606330
H	-2.216478	-2.039094	0.002566
H	-1.422595	0.051114	1.551415
H	0.157136	1.203349	-1.369355
H	-0.775477	2.044929	-0.282429

15) TS12-alhyzal-C



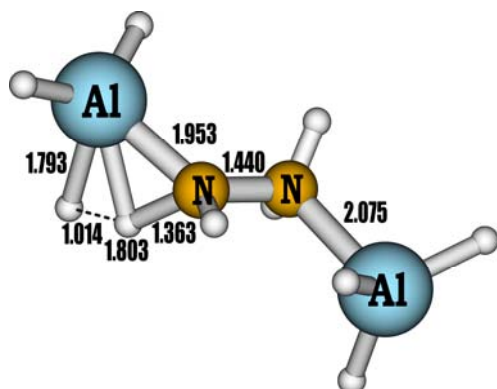
N	0.659269	1.095940	0.401839
Al	1.661616	-0.617385	-0.091695
N	-0.503734	0.970561	-0.454959
Al	-1.615455	-0.604702	0.105718
H	2.772236	-0.865807	1.012302
H	1.086274	2.012801	0.293331
H	2.027867	-0.246006	-1.597621
H	0.294166	-1.500111	0.034690
H	-2.689094	0.845608	-0.121748
H	0.300093	1.038930	1.355134
H	-2.186582	-1.742979	-0.817772
H	-1.404523	-0.500971	1.679976
H	-1.674969	1.291958	-0.226483
H	-0.214304	1.088191	-1.422258

16) TS13-alhyzal-C



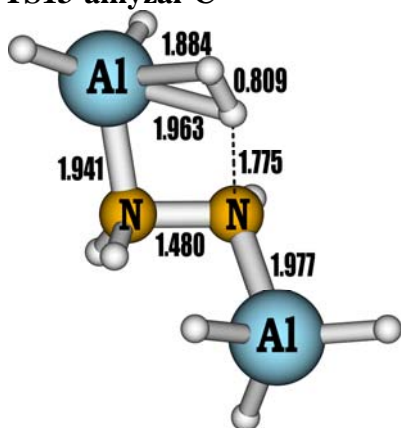
N	0.495508	0.763167	0.630383
Al	1.889830	-0.436952	-0.106578
N	-0.470864	0.887949	-0.476242
Al	-1.868728	-0.424787	-0.028923
H	3.219754	-0.302466	0.758926
H	0.825852	1.699030	0.848459
H	1.848217	0.187000	-1.617877
H	1.049773	-1.815383	-0.069220
H	-3.063136	0.393646	0.594257
H	-0.510232	-0.403232	1.422039
H	-1.967260	-1.693817	-0.938899
H	-1.030679	-1.011474	1.523479
H	-0.870881	1.823993	-0.479368
H	0.051749	0.767490	-1.359266

17) TS12-alhyzal-C



N	-0.496924	0.635894	0.022936
Al	-2.420685	-0.140444	-0.026141
N	0.485425	-0.414967	-0.045786
Al	2.389260	0.017062	-0.081630
H	-3.217296	1.060871	-0.709234
H	-0.325283	1.311391	-0.719673
H	-2.633388	-0.414456	1.531839
H	-2.024213	-1.408556	-0.929847
H	2.023205	-0.327837	1.639369
H	-0.367355	1.139259	0.900156
H	3.309365	-1.129830	-0.635499
H	2.537069	1.581510	-0.240035
H	1.164877	-0.510506	1.132288
H	0.022041	-1.244382	-0.408391

18) TS13-alhyzal-C



N	0.376981	0.369575	-0.534313
Al	2.200492	0.068166	0.167681
N	-0.426219	-0.788694	-0.082675
Al	-2.146113	0.093609	0.093157
H	1.595525	-0.464168	1.597840
H	-0.717379	1.401950	0.408414
H	2.992424	1.451605	0.159573
H	2.776435	-1.165339	-0.693058
H	-2.619696	0.579610	-1.321119
H	0.234861	0.430030	-1.539449
H	-3.028242	-0.358210	1.313560
H	-1.335490	1.593034	0.894829
H	0.031259	-1.047846	0.806698
H	-0.291959	-1.589908	-0.699267