Supporting Information

Probing Hydrogen Bonding Properties of Negatively Charged MoS_2 Monolayer by PXRD and DFT Calculations

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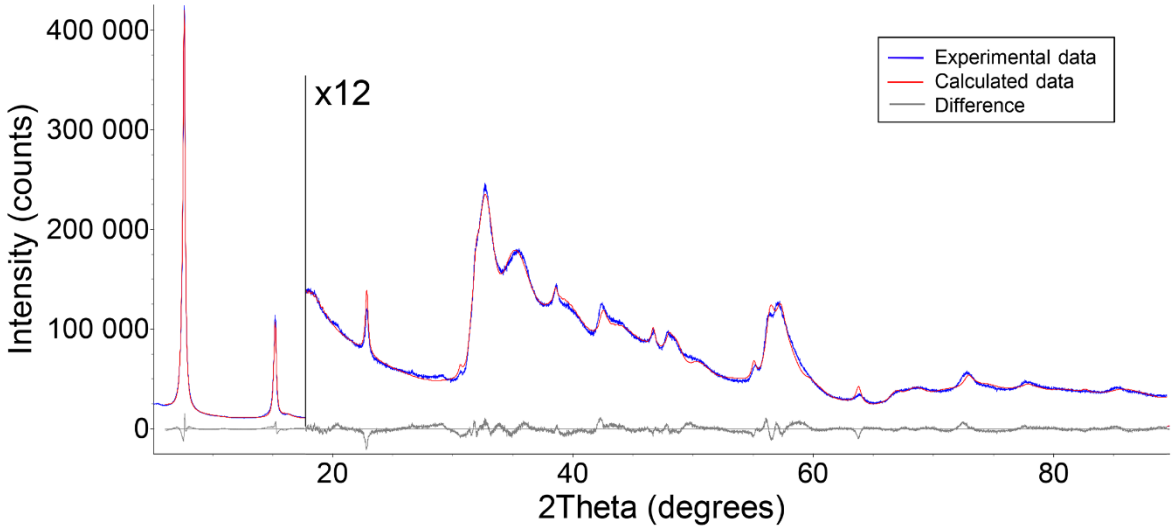

Figure S1. Powder X-ray diffraction pattern of $(HMTA)_{0.24}MoS_2$ and its fit according to **str-H-N**.

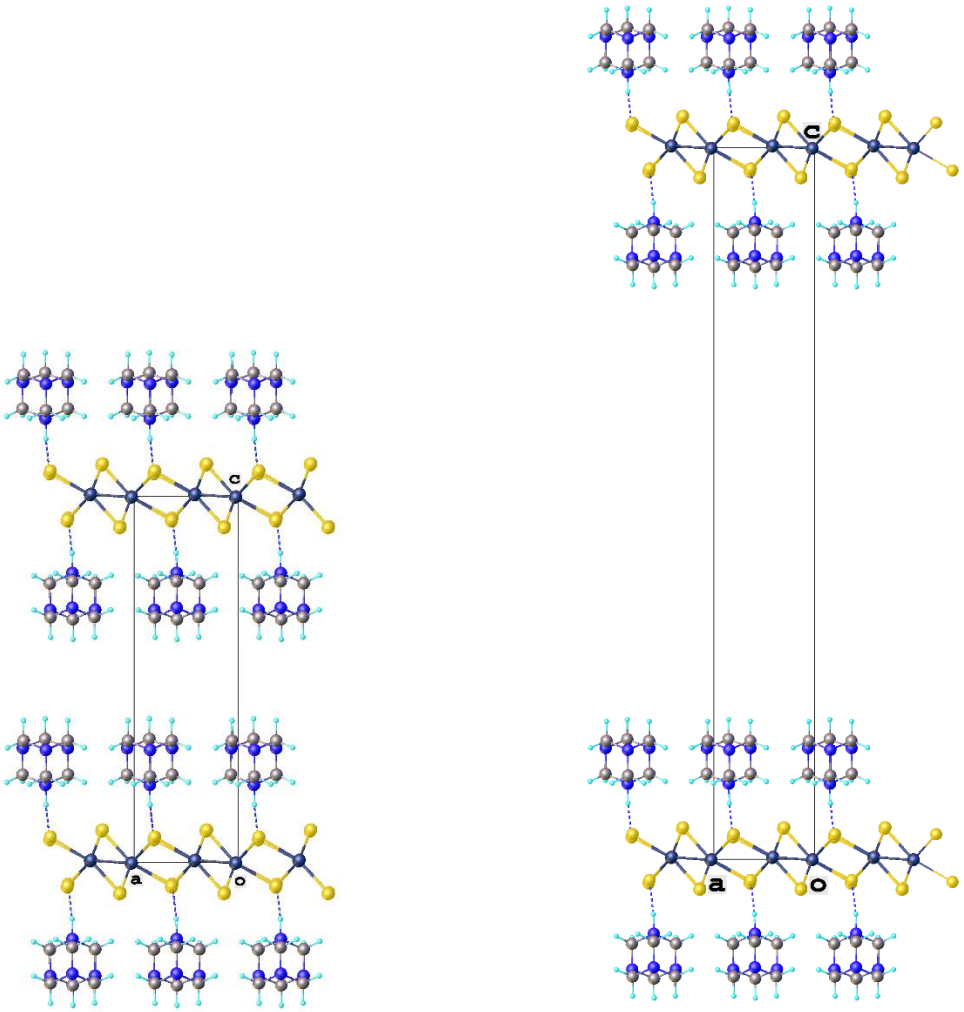

Figure S2. Models of delaminated compound with the interlayer periodicity increased to 20 Å (left) and 40 Å (right).

Table S1. Summary of Average Critical Point Properties (a.u. if not given) for Non-Covalent Interactions in the Hypothetical Ordered Structure with NH…S bond (str-H-S)

Atom1	Atom2	Count	d, Å	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	$g_e(\mathbf{r})$	$v_e(\mathbf{r})$	$h_e(\mathbf{r})$	Energy, kcal/mol
N**H**	S	1	2.033	0.045285	0.038772	0.022981	-0.03627	-0.01329	-11.3655
C**H**	S	14	2.695-3.676	0.005733	0.0156828	0.0031939	-0.0024671	0.0007267	-1.33729
C**H**	N	3	2.634-2.690	0.0080371	0.0184779	0.0040071	-0.0033948	0.0006123	-1.06380
H	H	4	2.806-2.903	0.008732	0.024449	0.00519	-0.00427	0.000922	-1.33729

Table S2. Summary of Average Critical Point Properties (a.u. if not given) for Non-Covalent Interactions in the Hypothetical Ordered Structure with NH…N Bond (str-H-N)

Atom1	Atom2	Count	d, Å	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	$g_e(\mathbf{r})$	$v_e(\mathbf{r})$	$h_e(\mathbf{r})$	Energy, kcal/mol
N**H**	N	4/1	1.896-1.964	0.037682	0.054945	0.02133	-0.02892	1.992406	-9.06374
C**H**	S	37/9	2.483-3.555	0.008313	0.021671	0.004729	-0.00404	0.08177	-1.26578
N	S	8/2	3.296-4.233	0.0080371	0.0184779	0.0040071	-0.0033948	0.0006123	-1.06380
H	H	21/5	2.366-3.456	0.00383	0.013619	0.002594	-0.00178	0.000811	-1.06647

* per unit cell /per 1 cation

Table S3. Summary of Average Critical Point Properties (a.u. if not given) for Non-Covalent Interactions in the Delaminated Ordered Structure with NH…S bond

Atom1	Atom2	Count	d, Å	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	$g_e(\mathbf{r})$	$v_e(\mathbf{r})$	$h_e(\mathbf{r})$	Energy, kcal/mol
N**H**	S	2/1	1.956	0.054563	0.033989	0.028202	-0.047906	-0.019704	-15.01195
C**H**	S	12/6	3.016-3.384	0.005334	0.015347	0.003038	-0.00224	0.000798	-0.70185

Table S4. Fractional Coordinates of str-H-N (a = 11.8130 Å, b = 12.8800 Å, c = 12.0960 Å, α = 79.694º β = 78.188 º, γ = 74.218 º, space gr. P1)

Atom	X	Y	Z
Mo	0.008494	0.030843	0.986456
Mo	0.204501	0.10422	0.997092
Mo	0.507911	0.905966	0.98756
Mo	0.703516	0.980073	0.999221
Mo	0.008137	0.280065	0.986625
Mo	0.204018	0.355168	0.997901
Mo	0.507943	0.156032	0.986021
Mo	0.704129	0.229931	0.997662
Mo	0.00709	0.531768	0.988865
Mo	0.203508	0.604501	0.000215
Mo	0.508516	0.406055	0.985868
Mo	0.703977	0.480254	0.999077
Mo	0.007632	0.779876	0.989134
Mo	0.203853	0.854037	0.998629
Mo	0.50789	0.653777	0.989078
Mo	0.703652	0.728545	0.001367
S	0.335643	0.966265	0.87776
S	0.09022	0.158664	0.84423
S	0.835103	0.84108	0.882899
S	0.590799	0.033239	0.845229
S	0.335219	0.216803	0.879202
S	0.088062	0.410855	0.847067
S	0.835352	0.091454	0.878867
S	0.589803	0.284205	0.844641
S	0.334951	0.467833	0.87882
S	0.089358	0.659037	0.847189
S	0.83537	0.342421	0.880241
S	0.590884	0.534626	0.845283
S	0.335792	0.715433	0.88131
S	0.088768	0.908162	0.846564
S	0.834831	0.592874	0.879722
S	0.59009	0.782175	0.848929
S	0.376284	0.044345	0.104756
S	0.122713	0.9768	0.138981
S	0.876777	0.168069	0.106934
S	0.620383	0.852186	0.141697
S	0.377044	0.293714	0.103943
S	0.122722	0.225892	0.13874
S	0.876774	0.417894	0.105416
S	0.620493	0.102714	0.139648
S	0.376517	0.542178	0.108174
S	0.121998	0.475413	0.141122
S	0.876307	0.667691	0.109846
S	0.62162	0.351066	0.138986
S	0.376904	0.79343	0.105974
S	0.122157	0.726245	0.141699
S	0.876563	0.919759	0.105839
S	0.621077	0.6004	0.142435
N	0.294986	0.831884	0.614399
N	0.456794	0.845198	0.457218
N	0.339759	0.713765	0.466536
N	0.250574	0.908959	0.425819
N	0.213374	0.360032	0.45745
N	0.430988	0.302329	0.441088
N	0.327243	0.491233	0.458695
N	0.309797	0.351653	0.619969
N	0.804397	0.321177	0.614067
N	0.972131	0.330526	0.46251
N	0.849613	0.205259	0.464272
N	0.769101	0.401971	0.423556
N	0.698387	0.868893	0.452012
N	0.91517	0.798195	0.42878
N	0.825347	0.986677	0.460629
N	0.803143	0.840141	0.613319
C	0.411433	0.851052	0.585861
C	0.299478	0.723716	0.590728
C	0.458651	0.733071	0.431998
C	0.367293	0.930215	0.390354
C	0.256159	0.799692	0.40131
C	0.213011	0.913781	0.549177
C	0.325562	0.286975	0.404937
C	0.219998	0.472813	0.420692
C	0.439158	0.413368	0.403284
C	0.417796	0.279706	0.566707
C	0.315866	0.462291	0.589336
C	0.206049	0.336292	0.583865
C	0.922813	0.335984	0.590627
C	0.80504	0.214981	0.588012
C	0.970696	0.219834	0.435489
C	0.887781	0.419096	0.393144
C	0.771765	0.294414	0.396208
C	0.72755	0.406349	0.546582
C	0.804898	0.794227	0.392658
C	0.712537	0.980023	0.423113
C	0.930766	0.90761	0.398036
C	0.905254	0.767113	0.553209
C	0.817204	0.949037	0.589823
C	0.694348	0.836514	0.57737
H	0.473446	0.788989	0.6342

H	0.410187	0.932377	0.602955
H	0.210035	0.708636	0.617176
H	0.360304	0.663214	0.641875
H	0.52232	0.673106	0.480581
H	0.489268	0.730623	0.340012
H	0.399166	0.925826	0.298849
H	0.367619	0.010404	0.409326
H	0.286349	0.795323	0.309431
H	0.167405	0.783066	0.425694
H	0.123556	0.898844	0.576244
H	0.209919	0.994841	0.568719
H	0.543817	0.858495	0.434927
H	0.333163	0.573112	0.438512
H	0.33468	0.302327	0.311303
H	0.319325	0.202457	0.433249
H	0.14008	0.529078	0.459979
H	0.230773	0.491712	0.327289
H	0.443973	0.433598	0.310373
H	0.516188	0.429682	0.428504
H	0.49525	0.291384	0.595854
H	0.412254	0.194966	0.594697
H	0.394035	0.475859	0.615118
H	0.234647	0.516991	0.628579
H	0.126113	0.390433	0.625913
H	0.200049	0.251613	0.611877
H	0.981735	0.271741	0.640253
H	0.923682	0.416037	0.609542
H	0.7136	0.204184	0.609918
H	0.861	0.151553	0.641286
H	0.029876	0.157847	0.486905
H	0.00561	0.216641	0.344093
H	0.921783	0.414014	0.301959
H	0.890448	0.497943	0.41389
H	0.805384	0.290559	0.304896
H	0.681254	0.281504	0.415571
H	0.6365	0.394741	0.569996
H	0.726801	0.486188	0.567751
H	0.836849	0.06732	0.443845
H	0.811699	0.817691	0.300046
H	0.792789	0.710973	0.414071
H	0.637096	0.036617	0.467963
H	0.720199	0.005633	0.330649
H	0.93299	0.933337	0.306005
H	0.011886	0.915964	0.422748
H	0.986728	0.770037	0.582008
H	0.893671	0.683654	0.57558
H	0.899518	0.953904	0.615305
H	0.740477	0.004493	0.634625

H	0.618729	0.89146	0.623836
H	0.682406	0.753213	0.599743
H	0.060101	0.341416	0.44305
S	-0.12344	-0.08024	1.105839
S	-0.16465	0.091454	0.878867
S	-0.12322	0.168069	1.106934
S	0.088768	-0.09184	0.846564
S	0.122713	-0.0232	1.138981
S	0.122722	0.225892	1.13874
S	0.335643	-0.03374	0.87776
S	0.376284	0.044345	1.104756
S	0.376904	0.79343	1.105974
S	0.376284	1.044345	1.104756
S	0.620383	0.852186	1.141697
S	0.590799	1.033239	0.845229
S	0.620493	1.102714	1.139648
S	0.876563	0.919759	1.105839
S	0.835352	1.091454	0.878867
S	-0.16463	0.342421	0.880241
S	-0.12323	0.417894	1.105416
S	0.121998	0.475413	1.141122
S	0.377044	0.293714	1.103943
S	0.620493	0.102714	1.139648
S	0.62162	0.351066	1.138986
S	0.876777	0.168069	1.106934
S	-0.16517	0.592874	0.879722
S	-0.12369	0.667691	1.109846
S	0.089358	0.659037	-0.15281
S	0.334951	0.467833	-0.12118
S	0.335792	0.715433	-0.11869
S	0.376517	0.542178	1.108174
S	0.621077	0.6004	1.142435
S	0.876774	0.417894	1.105416
S	-0.1649	0.84108	0.882899
S	-0.12344	0.919759	1.105839
S	0.122157	0.726245	1.141699
S	0.122713	0.9768	1.138981
S	0.59009	0.782175	-0.15107
S	0.834831	0.592874	-0.12028
S	0.835103	0.84108	-0.1171
H	0.367619	1.010404	0.409326
H	1.029876	0.157847	0.486905
H	1.00561	0.216641	0.344093
H	0.637096	1.036617	0.467963
H	0.720199	1.005633	0.330649
H	1.011886	0.915964	0.422748
H	0.740477	1.004493	0.634625
N	0.825347	-0.01332	0.460629

N	-0.02787	0.330526	0.46251
C	0.712537	-0.01998	0.423113
C	0.817204	-0.05096	0.589823
C	0.930766	-0.09239	0.398036
C	-0.0293	0.219834	0.435489
C	-0.11222	0.419096	0.393144
C	-0.07719	0.335984	0.590627
N	0.698387	-0.13111	0.452012
N	0.803143	-0.15986	0.613319
H	0.899518	-0.0461	0.615305
N	0.91517	-0.20181	0.42878
H	0.93299	-0.06666	0.306005
H	1.011886	-0.08404	0.422748
N	-0.15039	0.205259	0.464272
N	-0.2309	0.401971	0.423556
H	-0.07822	0.414014	0.301959
H	-0.10955	0.497943	0.41389
N	-0.1956	0.321177	0.614067
H	-0.01827	0.271741	0.640253
H	-0.07632	0.416037	0.609542
C	0.804898	-0.20577	0.392658
C	0.694348	-0.16349	0.57737
C	0.905254	-0.23289	0.553209
C	-0.19496	0.214981	0.588012
C	-0.22824	0.294414	0.396208
C	-0.27245	0.406349	0.546582
H	0.792789	-0.28903	0.414071
H	0.811699	-0.18231	0.300046
H	0.618729	-0.10854	0.623836
H	0.682406	-0.24679	0.599743
H	0.893671	-0.31635	0.57558
H	0.986728	-0.22996	0.582008
H	-0.2864	0.204184	0.609918
H	-0.139	0.151553	0.641286
H	-0.31875	0.281504	0.415571
H	-0.19462	0.290559	0.304896
H	-0.3635	0.394741	0.569996
H	-0.2732	0.486188	0.567751
Mo	0.203508	0.604501	1.000215
H	0.836849	1.06732	0.443845
H	1.060101	0.341416	0.44305

Table S5. Fractional Coordinates of str-H-S (a = 6.5290 Å, b = 6.4400 Å, c = 12.0960 Å, α = 79.694° β = 86.972 °, γ = 119.512 °, space gr. P1)

Atom	X	Y	Z
Mo	0.987862	0.043253	0.998912
Mo	0.377522	0.482519	0.010668
Mo	0.987764	0.538752	0.999306
Mo	0.378335	0.981005	0.011466
S	0.72513	0.620745	0.114842
S	0.214346	0.10303	0.152464
S	0.64085	0.402465	0.892624
S	0.151019	0.420817	0.857604
S	0.724335	0.11884	0.119481
S	0.214468	0.601383	0.15273
S	0.641133	0.903794	0.891226
S	0.152166	0.920332	0.858295
N	0.894116	0.520614	0.544287
N	0.676861	0.740386	0.531879
N	0.743209	0.591256	0.370962
N	0.465833	0.2999	0.540766
C	0.872749	0.719197	0.578756
C	0.943572	0.572638	0.422025
C	0.72349	0.794372	0.409368
C	0.452031	0.502421	0.575168
C	0.510201	0.349163	0.418594
C	0.665541	0.286129	0.587162
H	0.768175	0.622638	0.280002
H	0.042459	0.894409	0.549214
H	0.833686	0.676555	0.672085
H	0.955122	0.426372	0.392605
H	0.108652	0.74912	0.3863
H	0.893097	0.965965	0.373422
H	0.579122	0.805057	0.370895
H	0.302226	0.513974	0.543477
H	0.419448	0.463375	0.668436
H	0.369514	0.367747	0.37997
H	0.5295	0.206766	0.389192
H	0.678314	0.135547	0.562949
H	0.629864	0.248218	0.680421
S	0.641133	-0.09621	0.891226
S	0.72513	-0.37926	1.114842
S	0.724335	0.11884	1.119481
S	1.152166	-0.07967	0.858295
S	1.214346	0.10303	1.152464
S	1.151019	0.420817	0.857604
S	0.151019	0.420817	-0.1424
S	0.64085	0.402465	-0.10738

S	0.641133	0.903794	-0.10877
S	0.72513	0.620745	1.114842
S	1.214468	0.601383	1.15273
S	1.152166	0.920332	0.858295
S	0.152166	0.920332	-0.14171
S	0.214346	1.10303	0.152464
S	0.64085	1.402465	-0.10738
S	0.724335	1.11884	0.119481
H	1.042459	0.894409	0.549214
H	1.108652	0.74912	0.3863

Table S6. Fractional Coordinates of dm-H-S-40 (a = 8.5890 Å, b = 12.8800 Å, c = 40.0000 Å, α = 90.000 º β = 90.000 º, γ = 138.572 º, space gr. P1)

Atom	X	Y	Z
Mo	0.421206	0.352529	0.002071
Mo	0.024404	0.277574	0.999837
Mo	0.421821	0.594048	0.002622
Mo	0.024401	0.035042	0.000046
Mo	0.413711	0.861443	0.003711
Mo	0.023225	0.793229	0.999515
Mo	0.420566	0.109388	0.002827
Mo	0.030384	0.523932	0.998948
S	0.810988	0.549304	0.030984
S	0.310762	0.176542	0.04458
S	0.802783	0.796709	0.035561
S	0.310804	0.420356	0.044715
S	0.644213	0.339814	0.966948
S	0.133218	0.210519	0.957651
S	0.641987	0.590737	0.96628
S	0.137232	0.96806	0.957596
S	0.800881	0.04684	0.035534
S	0.312123	0.673168	0.042811
S	0.805419	0.298197	0.034698
S	0.302113	0.926447	0.045121
S	0.634049	0.837952	0.971147
S	0.133202	0.712972	0.959665
S	0.640091	0.089075	0.968376
S	0.141061	0.459209	0.957433
N	0.068013	0.662083	0.156468
N	0.847218	0.714868	0.154062
N	0.850664	0.600071	0.106343
N	0.636711	0.443773	0.156544
N	0.374436	0.691201	0.845506
N	0.592811	0.96412	0.848365
N	0.592278	0.845812	0.895701
N	0.805749	0.905413	0.845246
C	0.059695	0.768134	0.166665
C	0.069885	0.657539	0.120236
C	0.847205	0.711005	0.117806
C	0.638403	0.554932	0.166728
C	0.634999	0.43741	0.120329
C	0.854122	0.503289	0.169105
C	0.381021	0.80501	0.835636
C	0.373493	0.684184	0.881722
C	0.593623	0.959508	0.884612
C	0.802051	0.014175	0.835394
C	0.808511	0.900254	0.881446
C	0.588814	0.747481	0.832635
H	0.846929	0.591621	0.078993
H	0.216531	0.88648	0.156982
H	0.060475	0.772577	0.194123
H	0.070085	0.576952	0.111333
H	0.222948	0.774512	0.109657
H	0.003233	0.827093	0.107221
H	0.689045	0.668336	0.107256
H	0.478957	0.513217	0.157097
H	0.637835	0.55869	0.194187
H	0.479206	0.397908	0.109742
H	0.640492	0.359421	0.111486
H	0.856624	0.422632	0.161332
H	0.854234	0.507256	0.196567
H	0.596489	0.840952	0.923055
H	0.223552	0.76546	0.845425
H	0.380178	0.809374	0.808187
H	0.37458	0.603735	0.890326
H	0.220208	0.647316	0.892515
H	0.437156	0.918464	0.895398
H	0.751425	0.074988	0.895213
H	0.961374	0.132027	0.844986
H	0.801366	0.018602	0.807945
H	0.963942	0.016615	0.892049
H	0.804809	0.8174	0.890052
H	0.587639	0.66475	0.840157
H	0.588083	0.751787	0.805184
S	0.133218	0.210519	-0.04235
S	0.644213	0.339814	-0.03305
S	0.641987	0.590737	-0.03372

S	-0.35991	0.089075	0.968376
S	-0.19912	0.04684	1.035534
S	-0.19458	0.298197	1.034698
S	0.310804	0.420356	1.044715
S	0.141061	0.459209	-0.04257
S	0.634049	0.837952	-0.02885
S	-0.36595	-0.16205	-0.02885
S	-0.19722	-0.20329	0.035561
S	-0.19912	0.04684	0.035534
S	0.137232	-0.03194	-0.0424
S	0.133202	0.712972	-0.04034
S	0.640091	1.089075	-0.03162
S	0.800881	1.04684	0.035534
S	-0.35801	0.590737	0.96628
S	-0.18901	0.549304	1.030984
S	-0.19722	0.796709	1.035561
S	0.302113	0.926447	1.045121
S	0.302113	-0.07355	0.045121
S	0.640091	0.089075	-0.03162
S	-0.35579	0.339814	0.966948
S	0.312123	0.673168	1.042811
C	-0.14588	0.503289	0.169105
C	1.059695	0.768134	0.166665
C	1.069885	0.657539	0.120236
C	0.802051	1.014175	0.835394
N	-0.15278	0.714868	0.154062
N	-0.14934	0.600071	0.106343
H	1.003233	0.827093	0.107221
N	1.068013	0.662083	0.156468
H	0.751425	1.074988	0.895213
N	0.592811	-0.03588	0.848365
N	0.805749	-0.09459	0.845246
H	0.963942	1.016615	0.892049
N	-0.36329	0.443773	0.156544

H	-0.14338	0.422632	0.161332
H	-0.14577	0.507256	0.196567
H	1.216531	0.88648	0.156982
H	1.060475	0.772577	0.194123
H	1.070085	0.576952	0.111333
H	1.222948	0.774512	0.109657
H	0.801366	1.018602	0.807945
H	0.961374	1.132027	0.844986
C	-0.3616	0.554932	0.166728
C	-0.1528	0.711005	0.117806
C	-0.365	0.43741	0.120329
C	0.381021	-0.19499	0.835636
C	0.593623	-0.04049	0.884612
C	0.588814	-0.25252	0.832635
C	0.808511	-0.09975	0.881446
H	-0.52104	0.513217	0.157097
H	-0.36217	0.55869	0.194187
H	-0.31096	0.668336	0.107256
H	-0.52079	0.397908	0.109742
H	-0.35951	0.359421	0.111486
H	0.380178	-0.19063	0.808187
N	0.374436	-0.3088	0.845506
H	0.223552	-0.23454	0.845425
H	0.437156	-0.08154	0.895398
N	0.592277	-0.15419	0.895701
H	0.587639	-0.33525	0.840157
H	0.588083	-0.24821	0.805184
H	0.804809	-0.1826	0.890052
C	0.373493	-0.31582	0.881722
H	0.37458	-0.39627	0.890326
H	0.220208	-0.35268	0.892515
H	-0.15307	0.591621	0.078993
H	0.596489	-0.15905	0.923055