‘

Supporting Information

Nitro ⇌ *aci*-nitro tautomerism and *E/Z* isomeric preferences of Nitroethenediamine Derivatives: A quantum chemical study

Devendra K. Dhaked and Prasad V. Bharatam*

Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research (NIPER), Sector-67, S. A. S. Nagar - 160 062, Punjab, India.

pvbharatam@niper.ac.in

Table of Contents

Table S1. Relative energy of **N-1** and **N-10** at different levels of theory.

Level of theory	**Absolute Energy (a.u.)**		**Relative energy[a] (kcal/mol)**
	N-10	**N-1**	ΔE=(**N-10**) − (**N-1**)
G2MP2	-510.80586197	-510.80921788	2.10
CBS-QB3	-510.78011924	-510.78477869	2.93
B2-PLYP/6-311+(d,p)	-510.85067358	-510.86072385	6.30
MP2-FC/6-31/+G(d,p)	-510.31492	-510.3131403	-1.12
MP2-FC/6-311+G(d,p)	-510.50467	-510.5021036	-1.61
B3PW91/6-31/+G(d,p)	-511.59279	-511.6057988	8.16
B3LYP/6-311+G(d,p)	-511.90522	-511.9165911	7.13

[a] Relative energies are relative to **N-1**, positive sign indicates that **N-1** is preferred while negative sign indicates that **N-10** is preferred.

Table S2. Relative energy of various microsolvated water clusters of **N-1**, **N-10** and **N-13** in the presence of 1-4 water molecules.[a]

Number of water molecules	**Entry**	**B3LYP/6-31+G(d,p)**	**M06-2X/6-31+G(d,p)**
1w	**N-1-1w**	0.00	0.00
	N-1-1w-a	-0.36	1.05
	N-1-1w-b	1.61	2.13
	N-10-1w	8.05	6.03
	N-10-1w-a	8.42	7.29
	N-10-1w-b	10.03	10.17
	N-13-1w	10.89	10.40
	N-13-1w-a	14.77	13.52

	N-13-1w-b	16.32	15.84
2w	**N-1-2w**	0.00	0.00
	N-1-2w-a	3.02	3.42
	N-1-2w-b	4.54	5.03
	N-10-2w	10.06	8.82
	N-10-2w-a	11.47	9.26
	N-10-2w-b	13.34	11.73
	N-13-2w	11.32	10.66
	N-13-2w-a	15.54	13.72
	N-13-2w-b	Converged to **N-13-2w**	17.12
	N-13-2w-c	19.98	19.28
3w	**N-1-3w**	0.00	0.00
	N-1-3w-a	0.47	1.45
	N-1-3w-b	1.64	5.92
	N-10-3w	11.13	9.49
	N-10-3w-a	10.51	9.58
	N-10-3w-b	12.28	10.39
	N-13-3w	7.95	8.77
	N-13-3w-a	12.03	10.84
	N-13-3w-b	14.00	13.17
	N-13-3w-c	17.06	16.25
4w	**N-1-4w**	0.00	0.00
	N-1-4w-a	-0.28	1.78
	N-1-4w-b	3.78	2.60
	N-1-4w-c	Structure distorted	4.16
	N-10-4w	10.70	8.96
	N-10-4w-a	11.69	10.23

	N-10-4w-b	14.70	12.93
	N-13-4w	10.39	8.34
	N-13-4w-a	11.10	8.59
	N-13-4w-b	14.49	10.99
	N-13-4w-c	14.13	13.37

[a] All energies are corrected for zero-point vibrational energy.

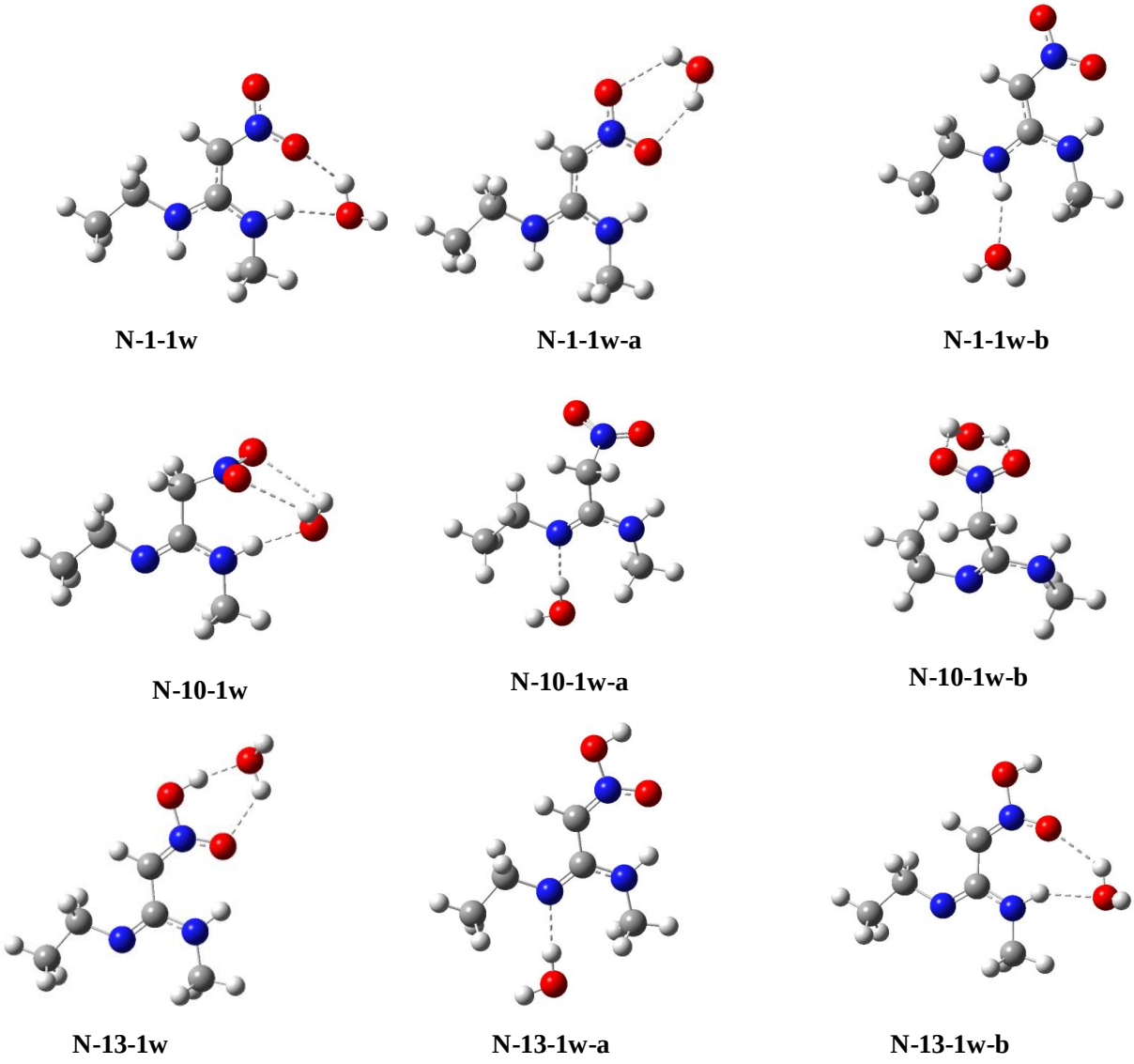

Figure S 1. Optimized geometries (M06-2X/6-31+(d,p)) of microsolvated water clusters of **N-1**, **N-10** and **N-13** in the presence of one water molecules.

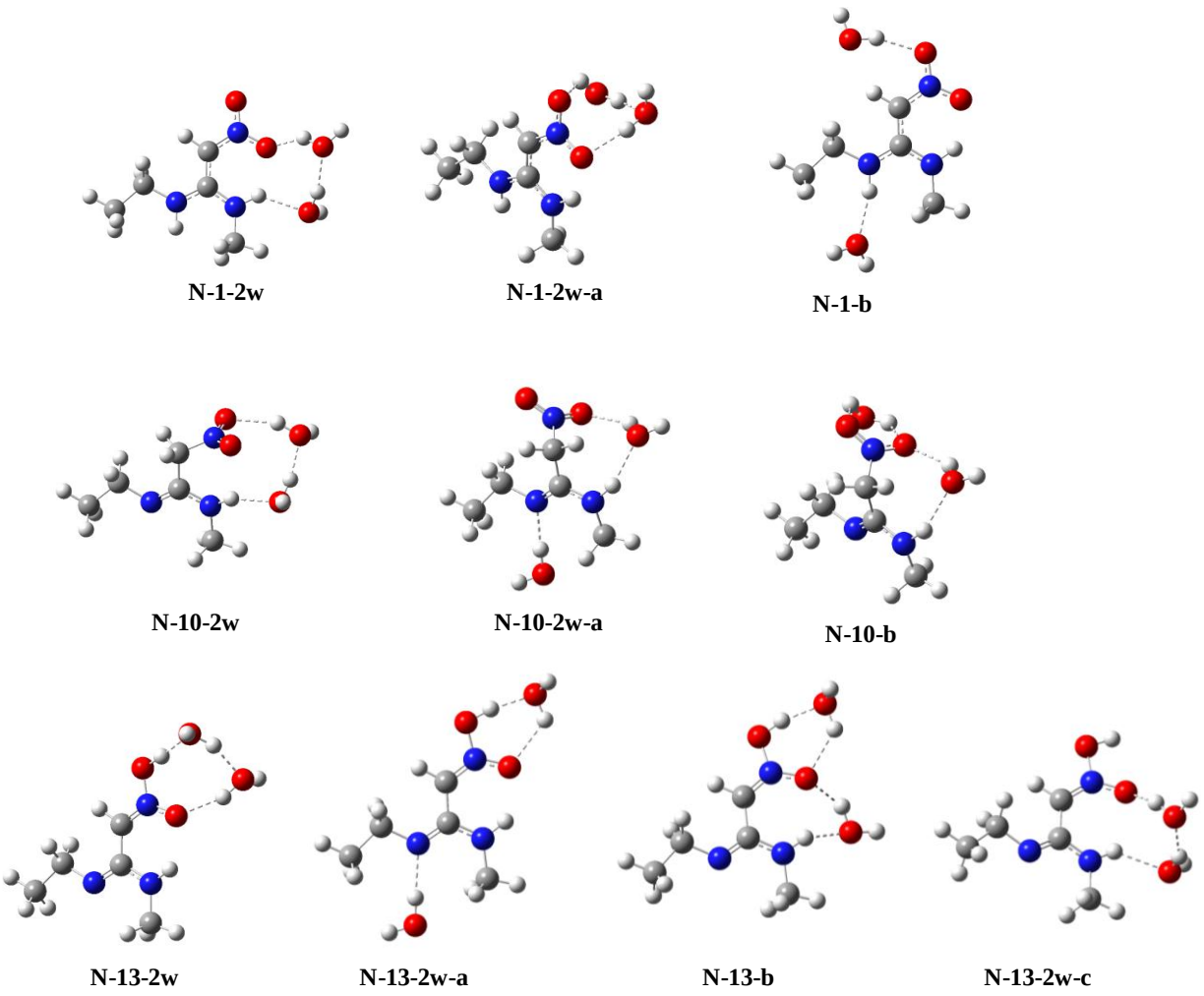

Figure S 2. Optimized geometries (M06-2X/6-31+(d,p)) of microsolvated water clusters of **N-1**, **N-10** and **N-13** in the presence of two water molecules.

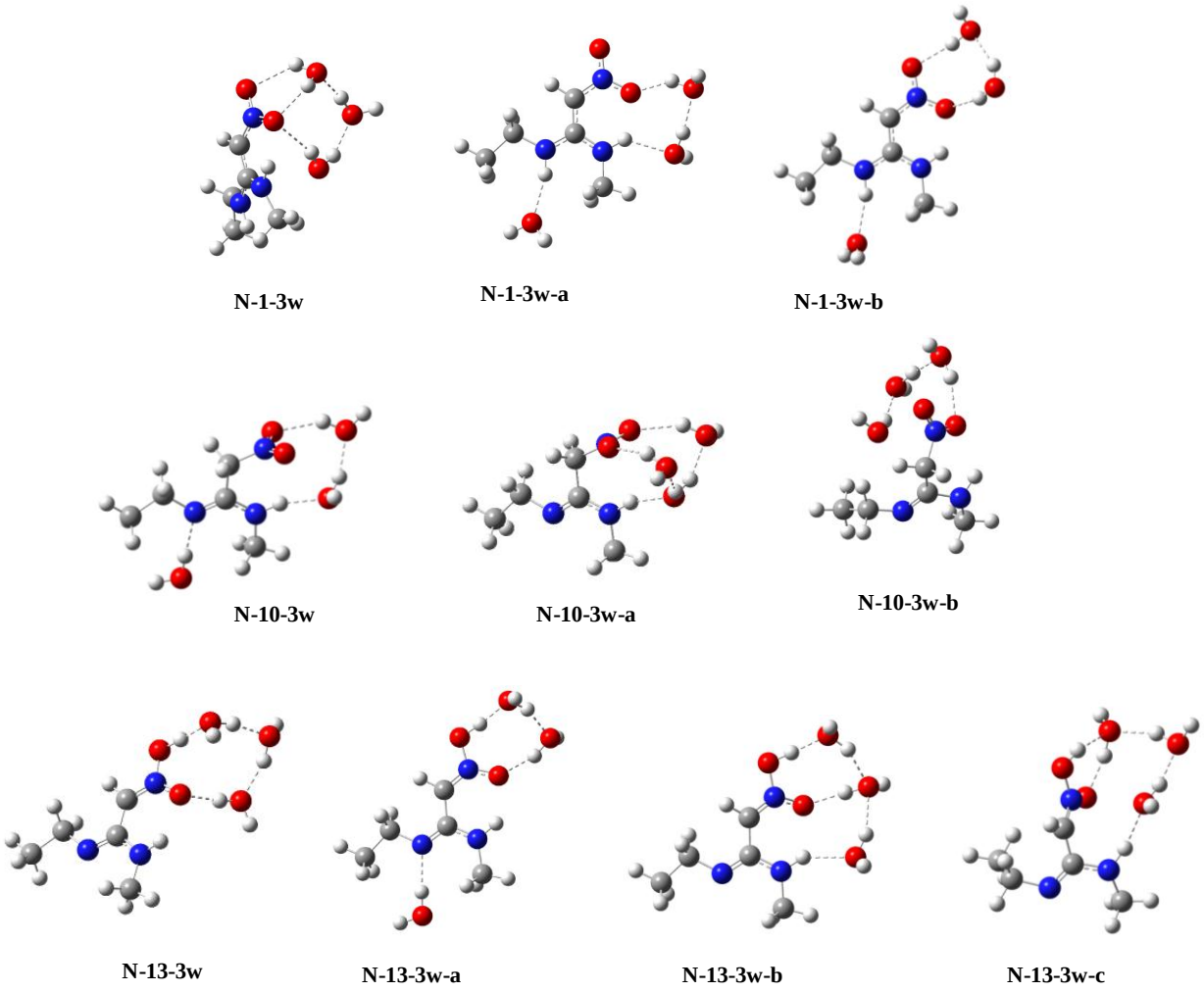

Figure S 3. Optimized geometries (M06-2X/6-31+(d,p)) of microsolvated water clusters of **N-1**, **N-10** and **N-13** in the presence of three water molecules.

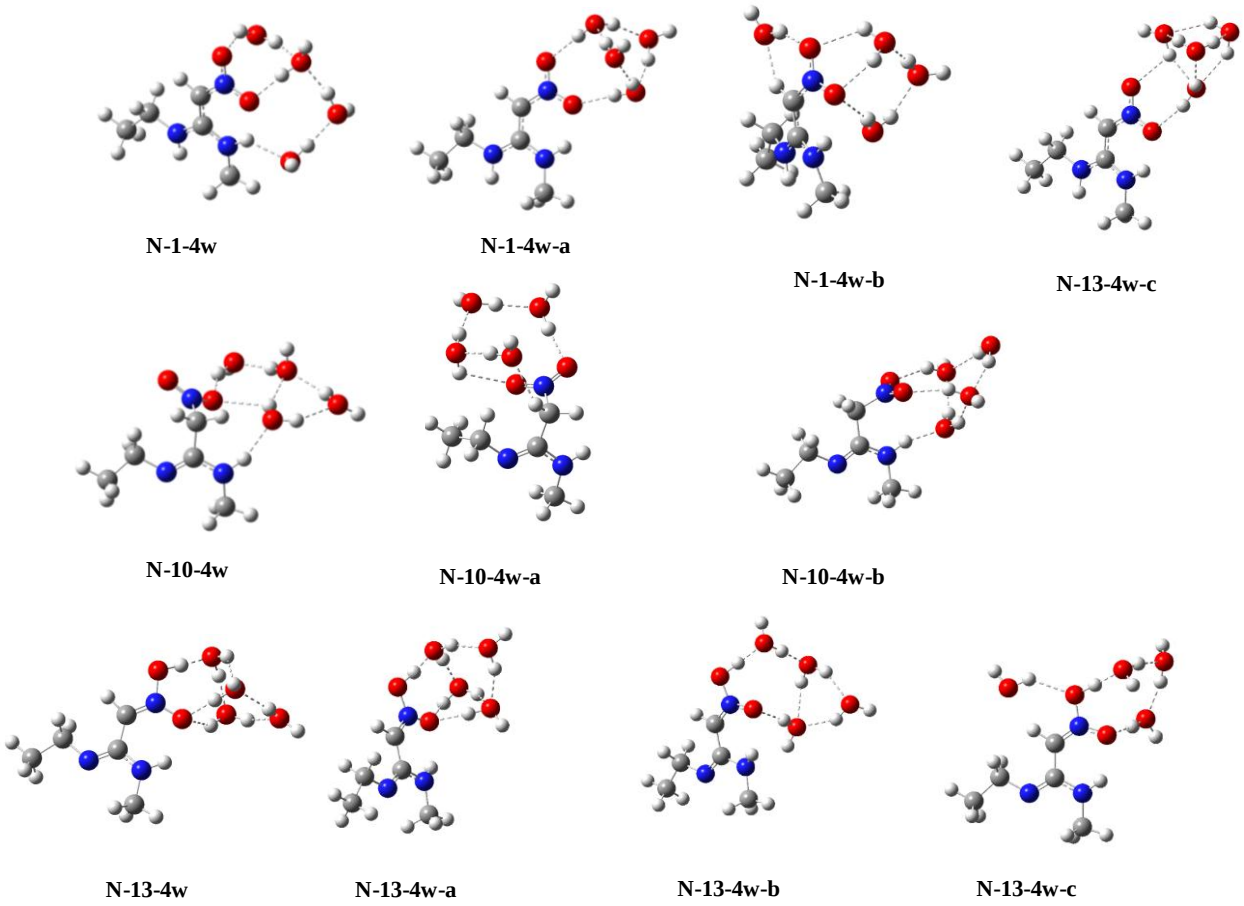

Figure S 4. Optimized geometries (M06-2X/6-31+(d,p)) of microsolvated water clusters of **N-1**, **N-10** and **N-13** in the presence of four water molecules.

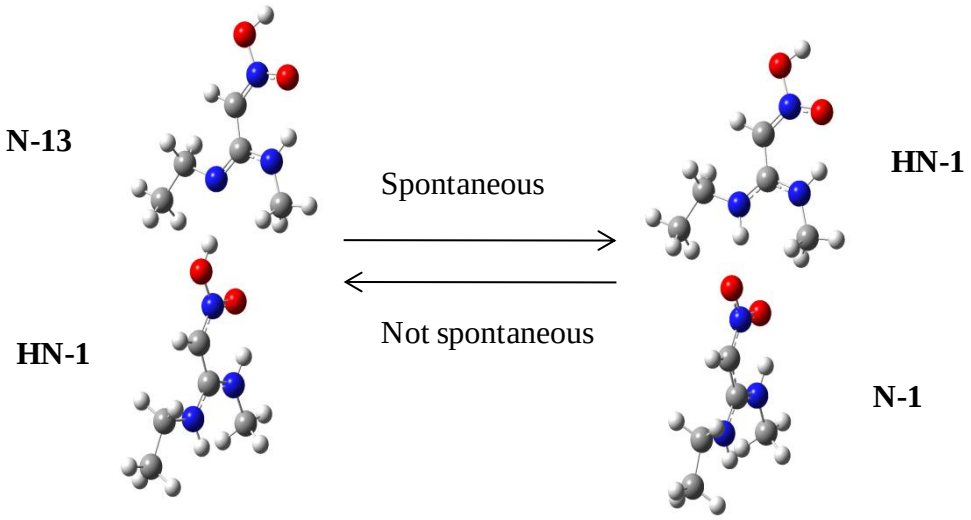

Figure S5. Protonated nitronic acid dependant conversion of nitronic acid to enamine.

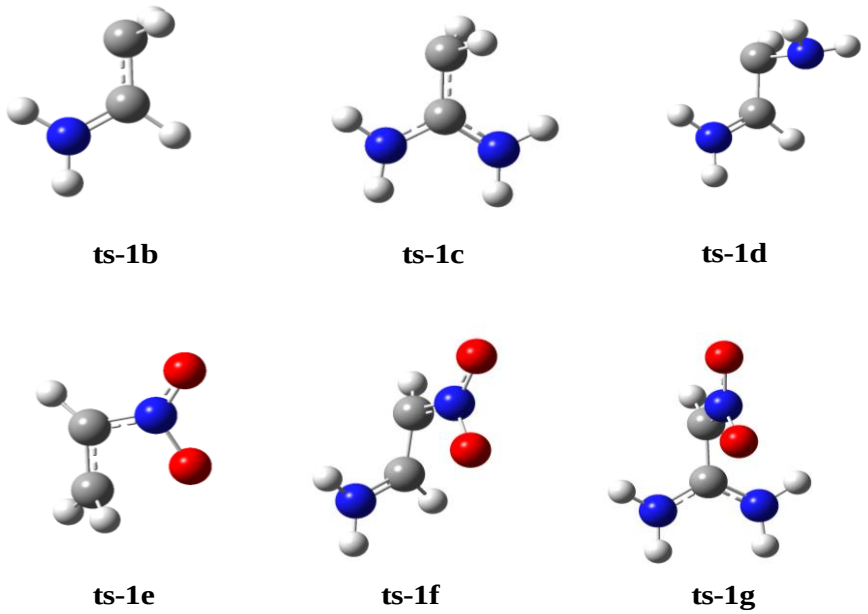

Figure S6. Optimized transition states of amine and nitro substituted molecules (**1b-1g**) for C1-C2 double bond rotational barrier at B3LYP/6-31+g(d,p) level.

Table S3. Absolute energies of given molecules at B3LYP, MP2(Full), M06-2X and BHandHLYP levels of theory. [a]

Entry	**B3LYP** [b]	**MP2 (Full)** [b]	**M06-2X** [b]	**B3LYP** [c]	**BHandHLYP** [c]	**MP2 (Full)** [c]
N-1	-511.6290473	-510.1859021	-511.38816	-511.7449515	-511.413370	-510.5226036
N-2	-511.6287526	-510.1858681	-511.38796	-511.7447485	-511.413337	-510.5226214
N-3	-511.6233806	-510.1825521	-511.38263	-511.73927	-511.406842	-510.5192946
N-4	-511.6230872	-510.182545	-511.38266	-511.7389961	-511.406610	-510.5194178
N-5	-511.6149252	-510.1761088	-511.37614	-511.7312606	-511.399351	-510.5136629
N-6	-511.6148868	-510.1758015	-511.37591	-511.7312212	-511.399306	-510.5131146
N-7	-511.6138766	-510.1739729	-511.37494	-511.7301583	-511.398155	-510.511241
N-8	-511.6141377	-510.1746645	-511.37528	-511.7303922	-511.398409	-510.5121535
N-9	-511.6171092	-510.1861486	-511.37815	-511.7334897	-511.401266	-510.5249029
N-10	-511.6173462	-510.1869951	-511.37843	-511.7338294	-511.401733	-510.5246717
N-11	-511.6152883	-510.1861506	-511.37844	-511.7318501	-511.400549	-510.5240766
N-12	-511.6155688	-510.1862075	-511.3785	-511.7320999	-511.400714	-510.5240027
N-13	-511.607407	-510.1680868	-511.36783	-511.7235269	-511.389913	-510.5054716
N-14	-511.600434	-510.1614227	-511.3606	-511.7165764	-511.382343	-510.4986307
N-15	--	--	-511.38814	--	-511.396750	-510.5136655
N-16	-511.5678635	-510.1204614	-511.32993	-511.6842085	-511.350731	-510.4605897

[a] All energies are corrected for zero-point vibrational energy. [b] Basis set 6-31+G(d,p) is used for optimizations. [c] Basis set 6-311+G(d,p) is used for optimizations.

Table S4. Absolute energies and proton affinities of protonated isomers (**HN-1**, **HN-2** and **HN-3**) of **N-1**.[a]

Entry	Absolute energies		Absolute proton affinities	
	B3LYP [b]	**B3LYP** [c]	**B3LYP** [b]	**B3LYP** [c]
N-1	--	--	-511.4423	-511.5588
HN-1	-511.991347	-512.1066706	-511.7911	-511.9072
HN-2	-511.985548	-512.1013905	-511.7849	-511.9014
HN-3	-511.983102	-512.0990597	-511.7830	-511.8997

[a] All energies are corrected for zero-point vibrational energy. [b] Basis set 6-31+G(d,p) is used for optimizations. [c] Basis set 6-311+G(d,p) is used for optimizations.

Table S5. Absolute energies of amine and nitro substituted molecules at B3LYP and MP2(Full) levels of theory.[a]

Entry	**B3LYP**[b]	**MP2 Full**[b]	**B3LYP**[c]	**MP2 Full**[c]
1b	-133.8975608	-133.4806774	-133.9273744	-133.568993
1c	-189.2475007	-188.6833846	-189.2910774	-188.8086711
1d	-189.2333137	-188.6679405	-189.2771586	-188.7931602
1e	-283.0551652	-282.3040549	-283.1250919	-282.4924377
1f	-338.413552	-337.5083660	-338.4969125	-337.7319321
1g	-393.7730238	-392.7186675	-393.8696525	-392.9790211
ts-1b	-133.810837	-133.3861273	-133.840570	-133.4761303
ts-1c	-189.1837914	-188.6131796	-189.227325	-188.7389799
ts-1d	-189.1370128	-188.5654540	-189.180066	-188.6903594
ts-1e	-282.9784919	-282.2212373	-283.046488	-282.4065702
ts-1f	-338.35199	-337.4412458	-338.434291	-337.6630109
ts-1g	-393.7294312	-392.6736155	-393.825759	-392.9318551
ts-N-1	-511.592275	-510.1516067	-511.708012	-510.4862052
ts-N-3	-511.5848149	-510.1423536	-511.700360	-510.4772502
ts-N-6	-511.5893295	-510.1492786	-511.705074	-510.4838322
ts-N-13	-511.5986697	-510.1624224	-511.715169	-510.4995108
ts-N-14	-511.5973325	--	--	--

[a] All energies are corrected for zero-point vibrational energy. [b] Basis set 6-31+G(d,p) is used for optimizations. [c] Basis set 6-311+G(d,p) is used for optimizations.

S1. Cartesian coordinates of various geometrical isomers and tautomers of model nitroethylenediamine moiety (**N-1** to **N-14** and **N-16**) at B3LYP/6-311+G(d,p) level.

N-1

N	-1.453894	0.114886	0.012712
N	0.345426	1.578720	-0.065558
C	-0.101938	0.306089	-0.029782
H	-2.029579	0.903934	-0.235036
H	1.363463	1.640046	-0.049271
C	0.755992	-0.796878	-0.020942
H	0.392911	-1.807489	-0.029296
N	2.143921	-0.705538	0.009890
O	2.706405	0.424069	0.009857
O	2.796496	-1.757116	0.032892
C	-2.105104	-1.192048	-0.045007
H	-1.742902	-1.800990	0.787985
H	-1.838251	-1.713976	-0.972473
C	-3.618027	-1.032959	0.050912
H	-4.099890	-2.011756	0.012723
H	-3.905819	-0.549797	0.988193
H	-4.010093	-0.439877	-0.781340
C	-0.485391	2.759402	0.046800
H	-1.090876	2.751273	0.960502
H	0.167079	3.630624	0.081888
H	-1.150632	2.884269	-0.817065

N-2

N	-0.987491	-0.360103	-0.080128
N	-0.437198	1.891423	0.037194
C	-0.030294	0.588255	-0.022239
H	-0.606345	-1.307231	-0.075526
H	-1.398789	2.074789	-0.193827
C	1.335010	0.290490	-0.008310
H	2.089489	1.054859	0.004278
N	1.851682	-1.001036	0.004139
O	1.074948	-1.995158	-0.018452
O	3.081810	-1.136640	0.034160
C	-2.419491	-0.126955	0.026942
H	-2.769803	0.483534	-0.817473
H	-2.643896	0.428018	0.947406
C	-3.171290	-1.454078	0.028205
H	-4.246081	-1.277054	0.102575
H	-2.980514	-2.012445	-0.891466
H	-2.868738	-2.073146	0.876301
C	0.468973	3.029170	0.004943
H	1.059382	3.066034	-0.917091
H	-0.125471	3.939640	0.075163
H	1.150298	3.004113	0.858318

N-3

N	1.281224	-0.550720	-0.391500
N	-0.036545	1.311053	0.170385
C	0.041709	-0.009291	-0.084879
H	1.193550	-1.505270	-0.716111
H	-0.995836	1.602818	0.355850
C	-1.060021	-0.857426	-0.078238
H	-0.952746	-1.924103	-0.184367
N	-2.388162	-0.434411	0.024484
O	-2.643745	0.779784	0.233476
O	-3.278611	-1.284812	-0.080564
C	2.427524	-0.392549	0.524917
H	2.183670	-0.800588	1.514975
H	2.635837	0.668672	0.657789
C	3.655045	-1.091600	-0.046899
H	4.503116	-0.979882	0.632247
H	3.476863	-2.163626	-0.177504
H	3.930318	-0.670288	-1.016565
C	0.922676	2.314013	-0.270849
H	0.373657	3.189325	-0.621486
H	1.587022	2.632867	0.538667
H	1.526190	1.929967	-1.094672

N-4

N	0.688432	0.487682	0.349532
N	0.940994	-1.688929	-0.495107
C	0.116802	-0.651392	-0.085866
H	-0.011409	1.184849	0.606894
H	0.410159	-2.429513	-0.931736

C	-1.258558	-0.842005	-0.163931
H	-1.683647	-1.799338	-0.416213
N	-2.212160	0.160782	0.031569
O	-1.849268	1.303425	0.413530
O	-3.399527	-0.120261	-0.165935
C	2.031121	0.957520	0.003933
H	2.388547	0.387722	-0.856976
H	2.721740	0.770282	0.834801
C	2.011732	2.450335	-0.317116
H	3.022643	2.796697	-0.545183
H	1.371946	2.659248	-1.177453
H	1.642999	3.031752	0.532424
C	1.994881	-2.204671	0.388975
H	2.464407	-3.054723	-0.106714
H	2.765362	-1.455647	0.563009
H	1.600877	-2.532111	1.358465

N-5

N	0.957237	-0.847736	0.323098
N	-1.054013	-1.912906	0.078732
C	-0.364521	-0.721263	0.033497
H	1.205242	-1.623168	0.920358
H	-0.536653	-2.724769	-0.224948
C	-1.031524	0.435789	-0.322465
H	-1.961565	0.400502	-0.862916
N	-0.656639	1.749339	0.029401
O	0.230574	1.942447	0.876458
O	-1.283038	2.671849	-0.512861
C	2.043047	0.035526	-0.097824
H	2.207393	0.816670	0.647003
H	1.724045	0.536818	-1.014106
C	3.317199	-0.768185	-0.345504
H	4.128587	-0.095844	-0.633755
H	3.637318	-1.294669	0.559842
H	3.182540	-1.504116	-1.142755
C	-2.504259	-2.014693	0.024028
H	-2.911717	-1.829317	-0.977228
H	-2.792384	-3.020478	0.333033
H	-2.948846	-1.299928	0.717695

N-6

N	1.601848	0.487794	-0.123022
N	-0.326968	1.700351	0.092864
C	0.225047	0.475096	-0.113628
H	2.025796	1.313330	-0.523474
H	0.236552	2.352802	0.615821
C	-0.448460	-0.709864	-0.344231
H	0.030240	-1.537271	-0.838771
N	-1.754893	-1.015818	0.089778
O	-2.332325	-0.278754	0.905982
O	-2.257968	-2.061255	-0.347619
C	2.438975	-0.708757	-0.100059
H	2.431932	-1.217175	-1.073805
H	2.010171	-1.400889	0.627764
C	3.871639	-0.351729	0.284671
H	4.492129	-1.250476	0.296989
H	4.316336	0.344293	-0.433894
H	3.909019	0.106004	1.276002
C	-1.654806	2.136964	-0.314019
H	-2.405364	1.947882	0.454220
H	-1.608082	3.203648	-0.544291
H	-1.950651	1.601379	-1.217201

N-7

N	-1.482669	-0.483740	-0.317774
N	-0.131363	1.374984	-0.131841
C	-0.230887	0.025985	-0.090220
H	-1.523277	-1.464923	-0.542836
H	-0.826489	1.861951	-0.675123
C	0.782696	-0.872717	0.223855
H	0.547371	-1.850277	0.611682
N	2.148816	-0.693501	-0.045846
O	2.531386	0.278198	-0.724209
O	2.927186	-1.557679	0.387378
C	-2.748752	0.209388	-0.086630
H	-3.015206	0.834439	-0.949515
H	-2.630351	0.875641	0.773441
C	-3.871199	-0.791517	0.172015
H	-4.816747	-0.266477	0.323127
H	-4.001076	-1.467412	-0.678465

H	-3.665989	-1.390314	1.062842
C	0.906760	2.186960	0.489039
H	1.752436	2.351886	-0.178616
H	0.462299	3.139424	0.786223
H	1.273273	1.679120	1.381773

N-8

N	-0.922575	0.467792	0.332865
N	-1.208593	-1.811827	0.136236
C	-0.363864	-0.733675	0.061762
H	-1.754254	0.462770	0.904352
H	-0.764714	-2.713918	0.172980
C	0.944433	-0.972943	-0.343319
H	1.191534	-1.864760	-0.895754
N	2.068190	-0.213463	0.020256
O	1.963981	0.697547	0.862271
O	3.149514	-0.521179	-0.505497
C	-0.436660	1.780831	-0.092000
H	0.149292	1.634020	-1.001428
H	0.243301	2.190498	0.656798
C	-1.609906	2.721231	-0.353195
H	-1.236242	3.706125	-0.642318
H	-2.254754	2.351512	-1.155029
H	-2.219885	2.856521	0.546311
C	-2.652807	-1.766107	-0.038261
H	-2.926273	-1.070765	-0.836373
H	-3.001198	-2.761112	-0.316471
H	-3.181093	-1.475373	0.877321

N-9

N	1.161086	-0.222416	0.338886
N	0.160218	1.802459	-0.133179
C	0.063008	0.606052	0.294067
H	0.954796	-1.212562	0.360165
C	-1.196912	-0.043583	0.881830
H	-2.004341	0.665858	1.015008
N	-1.729015	-1.126748	-0.030127
O	-2.752637	-0.897573	-0.650331
O	-1.078573	-2.164466	-0.093302
C	2.409240	0.160435	-0.316964
H	2.725044	1.120226	0.096659
H	2.241176	0.326282	-1.388997
C	3.476975	-0.904722	-0.095658
H	4.408600	-0.610425	-0.584259
H	3.680459	-1.044607	0.969269
H	3.174432	-1.868937	-0.516638
C	-0.932825	2.746641	-0.172426
H	-1.930913	2.338914	0.033987
H	-0.740333	3.559840	0.536117
H	-0.966993	3.199811	-1.167197
H	-0.955171	-0.540092	1.820806

N-10

N	1.401985	0.287481	0.161105
N	-0.392083	1.735475	0.222198
C	0.161636	0.488391	0.375563
H	-1.396270	1.762528	0.118414
C	-0.827489	-0.554638	0.913998
H	-1.331626	-0.165853	1.798590
N	-1.924391	-0.853618	-0.083474
O	-2.751000	0.030886	-0.280161
O	-1.911267	-1.940169	-0.634244
C	2.053278	-0.998991	0.354132
H	1.402140	-1.848647	0.106296
H	2.335275	-1.106470	1.411009
C	3.315452	-1.081628	-0.503397
H	3.829134	-2.033890	-0.342988
H	3.065431	-0.999162	-1.564007
H	4.000612	-0.268427	-0.253994
C	0.370126	2.809394	-0.396569
H	0.681919	2.558612	-1.416636
H	-0.250539	3.705670	-0.416106
H	1.269989	3.009679	0.186296
H	-0.344532	-1.500313	1.127199

N-11

N	1.135506	0.438114	-0.083931
N	0.960038	-1.925410	-0.206686
C	0.471383	-0.746164	-0.321332
C	-0.928850	-0.668063	-0.873673

H	-1.238752	-1.672798	-1.154036
N	-1.969635	-0.196565	0.136484
O	-3.046603	0.145359	-0.325899
O	-1.679662	-0.212726	1.320427
C	0.522650	1.760696	0.063039
H	0.010025	1.849092	1.028107
H	-0.232182	1.888315	-0.716564
C	1.576623	2.855209	-0.072944
H	1.116132	3.838582	0.046233
H	2.347302	2.758170	0.698270
H	2.062849	2.815447	-1.050509
C	2.323818	-2.060848	0.271081
H	2.462939	-1.624971	1.273039
H	2.576040	-3.119400	0.337650
H	3.049904	-1.585751	-0.405829
H	-1.036604	-0.000910	-1.728025
H	2.017365	0.335205	0.397346

N-12

N	-1.389317	-0.526694	-0.307352
N	-0.202382	1.519349	-0.128127
C	-0.316044	0.168995	-0.380862
H	-1.002122	1.929080	0.329360
C	0.903172	-0.551864	-0.896671
H	1.408862	-0.046449	-1.718839
N	1.983047	-0.777367	0.157032
O	1.699119	-0.599994	1.329326
O	3.067579	-1.147936	-0.262746
C	-2.613923	0.119983	0.138103
H	-2.875349	0.952409	-0.535808
H	-2.475828	0.560154	1.140411
C	-3.767470	-0.877781	0.183341
H	-4.689114	-0.393823	0.518952
H	-3.940847	-1.305166	-0.807036
H	-3.536611	-1.697301	0.867743
C	1.047741	2.249619	0.052626
H	1.752694	2.012365	-0.745935
H	0.836546	3.317745	-0.013579
H	1.526281	2.041866	1.015196
H	0.601608	-1.548157	-1.213193

N-13

N	-1.541003	0.127140	-0.000048
N	0.177609	1.658821	-0.001042
C	-0.275212	0.369358	-0.000441
H	1.173634	1.812733	0.000300
C	0.737349	-0.702782	-0.000607
H	0.431498	-1.735149	-0.001262
N	2.028817	-0.521493	0.000176
O	2.709215	0.523884	0.001264
O	2.775782	-1.724616	-0.000161
C	-2.059582	-1.232215	0.000115
H	-1.715966	-1.792337	0.883584
H	-1.716045	-1.792578	-0.883239
C	-3.586586	-1.209099	0.000159
H	-3.991921	-2.225368	0.000312
H	-3.960376	-0.685525	0.883330
H	-3.960434	-0.685769	-0.883132
C	-0.740777	2.779014	0.000075
H	-1.387417	2.758989	0.882379
H	-0.159405	3.701451	-0.000350
H	-1.388961	2.759225	-0.881065
H	3.686314	-1.386760	0.000915

N-14

N	-1.514297	0.137503	-0.032370
N	0.204631	1.652558	-0.185111
C	-0.248706	0.358856	-0.110583
H	1.182731	1.815456	-0.020737
C	0.725409	-0.747937	-0.205309
H	0.360928	-1.730751	-0.458956
N	2.018429	-0.755152	-0.012997
O	2.812093	-1.703104	-0.113517
O	2.615806	0.474161	0.380996
C	-2.063082	-1.209899	-0.005709
H	-1.624208	-1.807880	0.806515
H	-1.845589	-1.743621	-0.944360
C	-3.577274	-1.154210	0.183502
H	-4.004535	-2.161283	0.200013
H	-3.826801	-0.655961	1.123472

H	-4.043695	-0.591710	-0.628858
C	-0.715971	2.764398	-0.030190
H	-1.222628	2.745718	0.941178
H	-0.151782	3.692782	-0.128037
H	-1.486612	2.729777	-0.802502
H	3.555396	0.227410	0.395519

N-16

N	1.595346	0.294554	-0.302428
N	-0.251639	1.644409	0.034012
C	0.257564	0.420003	-0.167379
H	-1.252470	1.620139	0.254264
C	-0.539533	-0.773188	-0.324719
N	-1.789279	-0.627417	-0.008460
O	-2.603934	-1.763261	-0.230554
O	-2.477885	0.347266	0.479748
C	2.297841	-0.971739	-0.539611
H	3.188396	-0.734294	-1.128629
H	1.633890	-1.593213	-1.138745
C	2.676902	-1.699158	0.749394
H	3.229864	-2.612689	0.512953
H	3.307559	-1.079035	1.393647
H	1.776611	-1.977022	1.301055
C	0.497746	2.885678	0.057431
H	1.051033	3.035353	-0.876235
H	-0.202534	3.712102	0.170721
H	1.202864	2.925144	0.897337
H	2.167806	1.107850	-0.136048
H	-3.472582	-1.426772	0.043572

S2. Cartesian coordinates of various microsolvated water clusters of **N-1**, **N-10** and **N-13** in the presence of 1-4 water molecules at M06-2X/6-31+G(d,p) level

N-1-1w

N	1.726262	-0.434721	-0.022430
N	-0.450260	-1.150196	-0.249299
C	0.402451	-0.123851	-0.122731
H	-1.437044	-0.917391	-0.292525
C	0.022367	1.223057	-0.066768
H	0.738167	2.023230	-0.014748
N	-1.289851	1.656182	-0.037153
O	-2.227402	0.825419	-0.116510
O	-1.507285	2.863173	0.059121
C	2.787746	0.558092	0.052289
H	2.608319	1.192275	0.926683
H	2.775744	1.203365	-0.836420
C	4.133755	-0.137948	0.181137
H	4.933698	0.601514	0.254307
H	4.162258	-0.764324	1.077012
H	4.338540	-0.765201	-0.692639
C	-0.085745	-2.541190	-0.098803
H	0.491587	-2.705011	0.818578
H	-1.014620	-3.106884	-0.029643
H	0.487168	-2.915778	-0.957210
O	-3.278223	-1.705794	0.330670
H	-3.349445	-0.751593	0.483019
H	-4.096220	-1.967132	-0.102086
H	1.998623	-1.357267	-0.329149

N-1-1w-a

N	-2.057018	0.052241	-0.001967
N	-0.368882	1.625862	0.010417
C	-0.728744	0.331570	-0.007276
H	-2.694595	0.809861	0.190542
H	0.635467	1.778509	-0.020147
C	0.186840	-0.728613	-0.042495
H	-0.116236	-1.759850	-0.028299
N	1.553190	-0.553700	-0.093214
O	2.045420	0.602550	-0.112569
O	2.272535	-1.555934	-0.116275

C	-2.608023	-1.295321	0.051306
H	-2.248419	-1.813357	0.949489
H	-2.257154	-1.855212	-0.822296
C	-4.127143	-1.227286	0.052356
H	-4.547619	-2.234102	0.085979
H	-4.495360	-0.682177	0.927365
H	-4.496133	-0.734087	-0.851446
C	-1.300951	2.730513	-0.008115
H	-1.914846	2.763307	0.900751
H	-0.728402	3.655804	-0.053602
H	-1.956056	2.691219	-0.886457
O	4.901469	-0.140790	0.193908
H	4.123618	0.420476	0.077395
H	4.517435	-1.023001	0.128905

N-1-1w-b

N	0.949564	-0.390876	0.019683
N	-0.395660	1.487613	0.024764
C	-0.295850	0.145399	0.005166
H	1.756617	0.219191	-0.053227
H	-1.353149	1.829159	0.016395
C	-1.408576	-0.704086	-0.020616
H	-1.323152	-1.774824	-0.050633
N	-2.719492	-0.255224	-0.014682
O	-2.969591	0.971990	0.009400
O	-3.620048	-1.096035	-0.035666
C	1.198887	-1.822125	-0.016505
H	0.786203	-2.252503	-0.938488
H	0.687218	-2.299606	0.827520
C	2.693233	-2.093853	0.062385
H	2.879878	-3.169442	0.037161
H	3.217354	-1.633208	-0.780046
H	3.107115	-1.697948	0.995448
C	0.734881	2.383845	0.068532
H	1.336678	2.323833	-0.847924
H	0.355984	3.401178	0.161745
H	1.385963	2.174076	0.924587
O	3.639334	1.022263	-0.079807
H	4.395392	0.562124	0.299912
H	3.993995	1.786573	-0.545997

N-1-2w

N	2.150306	0.419869	0.063032
N	-0.022380	1.133319	-0.200127
C	0.837424	0.113901	-0.108923
H	2.418447	1.389520	-0.004357
H	-1.011296	0.913026	-0.313046
C	0.477667	-1.246140	-0.160780
H	1.200768	-2.036278	-0.069647
N	-0.816064	-1.692227	-0.260427
O	-1.753168	-0.859841	-0.405732
O	-1.040630	-2.902742	-0.212459
C	3.223412	-0.558730	0.149991
H	3.244445	-1.173525	-0.758580
H	3.034121	-1.224642	0.999607
C	4.554075	0.154329	0.333428
H	5.362969	-0.574721	0.410571
H	4.770369	0.807204	-0.518025
H	4.551256	0.756301	1.246841
C	0.342951	2.523835	-0.043554
H	0.995165	2.870869	-0.855795
H	-0.584276	3.095078	-0.071562
H	0.837260	2.704970	0.918962
O	-2.761844	2.044396	-0.327517
H	-3.299349	1.435317	0.214644
H	-3.157427	2.009556	-1.203944
O	-3.951875	-0.113396	0.975586
H	-3.297761	-0.706884	0.561649
H	-4.800756	-0.563024	0.965343

N-1-2w-a

N	-2.170147	0.111148	-0.006991
N	-0.538610	1.742782	-0.045544
C	-0.892515	0.470673	-0.274400
H	-2.757868	0.780579	0.466140
H	0.437920	1.943758	-0.245488
C	-0.010616	-0.498492	-0.784309
H	-0.297408	-1.527187	-0.906465
N	1.322362	-0.270436	-0.980260
O	1.801498	0.892487	-0.868797

O	2.061128	-1.227377	-1.249417
C	-2.668936	-1.256845	-0.085373
H	-2.069233	-1.906195	0.563784
H	-2.563426	-1.615339	-1.115177
C	-4.130802	-1.291768	0.330614
H	-4.514426	-2.311570	0.264819
H	-4.252523	-0.955065	1.364943
H	-4.738381	-0.657347	-0.321257
C	-1.408215	2.735712	0.543705
H	-1.721619	2.453961	1.556678
H	-0.856278	3.671986	0.611895
H	-2.294978	2.912045	-0.076647
O	1.844137	-1.438175	1.764084
H	2.592390	-0.819715	1.711037
H	1.913254	-1.937263	0.941236
O	3.982030	0.237623	0.801316
H	4.581650	-0.369591	0.355973
H	3.401833	0.580333	0.099180

N-1-2w-b

N	-1.144046	0.374762	-0.020842
N	-0.442694	-1.827912	0.015713
C	-0.132124	-0.520901	-0.019670
H	-2.104144	0.048268	-0.052498
H	0.363513	-2.446313	0.016499
C	1.188620	-0.042869	-0.050567
H	1.410637	1.008893	-0.087770
N	2.292699	-0.858306	-0.023331
O	2.179275	-2.102782	0.005472
O	3.419799	-0.325093	-0.029682
C	-0.926437	1.815713	-0.051604
H	-0.391201	2.092148	-0.968348
H	-0.291368	2.105979	0.792962
C	-2.258695	2.544665	0.018426
H	-2.092716	3.623465	-0.008871
H	-2.898003	2.273322	-0.826922
H	-2.781733	2.305977	0.950460
C	-1.794302	-2.334342	0.068669
H	-2.354577	-2.083644	-0.841276
H	-1.746865	-3.419448	0.154054
H	-2.341575	-1.938378	0.931533
O	3.043179	2.476068	0.085501
H	3.391806	1.566157	0.060287
H	3.786092	3.061758	-0.081769
O	-4.135257	-0.132606	-0.000578
H	-4.663047	0.587591	0.360473
H	-4.746879	-0.703879	-0.476817

N-1-3w

N	2.301392	-0.122214	-0.197516
N	0.954951	-1.415963	1.154878
C	1.148783	-0.795207	-0.016618
H	2.935321	-0.072013	0.586101
H	0.035289	-1.834061	1.245108
C	0.227337	-0.845381	-1.086566
H	0.484054	-0.517301	-2.078248
N	-1.084721	-1.167985	-0.929162
O	-1.540392	-1.497676	0.211445
O	-1.845306	-1.102120	-1.905959
C	2.514567	0.845396	-1.270292
H	1.630438	1.488223	-1.343209
H	2.635942	0.318485	-2.223562
C	3.755992	1.671258	-0.972175
H	3.924168	2.395340	-1.771622
H	3.638100	2.224046	-0.035407
H	4.643903	1.035529	-0.900311
C	1.690097	-1.070855	2.358234
H	1.651336	0.011288	2.529504
H	1.213393	-1.571162	3.200122
H	2.727136	-1.421167	2.308937
O	-3.744551	0.271544	-0.260652
H	-3.562403	0.114328	-1.197444
H	-3.292036	-0.478461	0.159152
O	-0.420011	1.108659	1.464738
H	-1.027357	1.849114	1.289251
H	-0.968275	0.327632	1.304965
O	-2.636934	2.625258	0.642936
H	-3.272028	3.150583	1.136972
H	-3.121452	1.846155	0.296735

N-1-3w-a

N	1.836367	-0.303979	0.016907
N	-0.124175	0.896420	-0.122260
C	0.484232	-0.293005	-0.067708
H	2.340071	0.576469	0.039152
H	-1.140385	0.910987	-0.194685
C	-0.193095	-1.531285	-0.080301
H	0.323592	-2.469836	0.004593
N	-1.556056	-1.659878	-0.130446
O	-2.274982	-0.630316	-0.255663
O	-2.060305	-2.783742	-0.053757
C	2.632936	-1.519029	0.070794
H	2.412608	-2.141610	-0.804935
H	2.368385	-2.098976	0.963909
C	4.112962	-1.169768	0.099480
H	4.711352	-2.082312	0.138619
H	4.394319	-0.615357	-0.801481
H	4.351623	-0.562038	0.977047
C	0.566205	2.162949	-0.039091
H	1.260290	2.304119	-0.876806
H	-0.199441	2.937942	-0.064150
H	1.127520	2.249850	0.900604
O	3.769343	2.033002	0.128840
H	3.662782	2.953997	0.389369
H	4.700040	1.917160	-0.089359
O	-4.569755	0.580405	0.471756
H	-4.998110	0.347203	1.299613
H	-3.964945	-0.152257	0.246816
O	-2.592898	2.419713	-0.222422
H	-3.317451	1.895855	0.172525
H	-2.915870	2.649190	-1.099319

N-1-3w-b

N	2.027055	-0.372551	0.028171
N	0.507946	1.318857	-0.380742
C	0.749597	0.017765	-0.172427
H	2.767288	0.322389	0.047313
H	-0.473541	1.544640	-0.519083
C	-0.271082	-0.957200	-0.154721
H	-0.075018	-1.998354	0.024283
N	-1.595242	-0.669047	-0.332877
O	-1.980208	0.507023	-0.554532
O	-2.416983	-1.600368	-0.275551
C	2.412293	-1.757395	0.266265
H	2.071532	-2.377632	-0.571158
H	1.920162	-2.125588	1.174957
C	3.921686	-1.867362	0.410965
H	4.199699	-2.906491	0.598724
H	4.425167	-1.538047	-0.502768
H	4.281631	-1.255948	1.242679
C	1.524212	2.346966	-0.363896
H	2.294717	2.169209	-1.121175
H	1.041703	3.300625	-0.573551
H	2.012524	2.413569	0.615561
O	-5.149982	-0.687496	-0.091156
H	-5.507759	-1.406827	0.437188
H	-4.232716	-0.945584	-0.289328
O	4.522070	1.353562	0.145897
H	4.855927	1.850790	0.900217
H	5.279855	1.191003	-0.425818
O	-4.140103	1.747708	1.081108
H	-3.352709	1.483541	0.588676
H	-4.785370	1.077816	0.808170

N-1-4w

N	-2.684163	0.432462	0.104512
N	-0.622133	1.409077	-0.195712
C	-1.379385	0.314108	-0.244088
H	-2.990118	1.318545	0.476650
H	0.364452	1.335492	-0.451217
C	-0.918401	-0.964624	-0.635935
H	-1.549183	-1.834522	-0.604430
N	0.370308	-1.233992	-0.965842
O	1.217955	-0.299010	-1.054850
O	0.718136	-2.411013	-1.166673
C	-3.627339	-0.675297	0.186642
H	-3.257304	-1.427687	0.893533
H	-3.712022	-1.148878	-0.797720
C	-4.985579	-0.156777	0.632688
H	-5.699965	-0.980140	0.690251

H	-4.923225	0.303069	1.623924
H	-5.373819	0.581348	-0.075157
C	-1.100977	2.704501	0.236606
H	-1.453767	2.680320	1.275656
H	-0.255207	3.387787	0.172530
H	-1.906430	3.072097	-0.411367
O	1.917803	2.632475	-0.497690
H	2.280201	2.661439	-1.388556
H	2.634563	2.259826	0.056412
O	3.443629	-1.157763	0.161766
H	3.995582	-1.799304	-0.296230
H	2.700112	-0.930894	-0.445657
O	3.973736	1.428341	0.909314
H	4.084758	1.518097	1.860005
H	3.923920	0.470174	0.716275
O	1.309169	-2.458215	1.732119
H	0.988104	-2.899102	0.935253
H	2.127931	-2.030467	1.441768

N-1-4w-a

N	3.447663	0.092878	0.005239
N	1.687879	1.584274	-0.029960
C	2.111838	0.311641	-0.035700
H	4.055097	0.887111	0.136088
H	0.678314	1.690555	-0.074721
C	1.248953	-0.796552	-0.087681
H	1.605407	-1.810384	-0.069552
N	-0.117467	-0.691106	-0.154158
O	-0.667500	0.438021	-0.179275
O	-0.784883	-1.732445	-0.188303
C	4.065782	-1.226217	0.043172
H	3.761494	-1.789277	-0.845990
H	3.715133	-1.774866	0.925865
C	5.579178	-1.082358	0.078429
H	6.047670	-2.067968	0.103633
H	5.942675	-0.556697	-0.809398
H	5.901162	-0.535298	0.970005
C	2.563961	2.734255	-0.000057
H	3.233033	2.754052	-0.868530
H	1.946484	3.630625	-0.028270
H	3.160432	2.767021	0.920019
O	-3.308381	1.639558	-0.146378
H	-3.666035	1.386628	0.725858
H	-2.447866	1.193995	-0.187616
O	-3.663337	-1.697336	0.241412
H	-2.712333	-1.749737	0.055146
H	-4.075897	-1.323964	-0.559591
O	-4.090016	0.201565	2.098241
H	-3.967972	-0.591914	1.522477
H	-4.897994	0.068380	2.600067
O	-4.621004	-0.052761	-1.808425
H	-5.505983	0.199589	-2.083188
H	-4.236658	0.702400	-1.307296

N-1-4w-b

N	2.347210	-0.206817	-0.065299
N	0.963893	-1.487922	-1.394232
C	1.204754	-0.336720	-0.758690
H	2.960652	-1.006840	-0.015608
H	0.044362	-1.533314	-1.820362
C	0.329830	0.780413	-0.800246
H	0.638641	1.749195	-0.444202
N	-0.974179	0.683819	-1.131492
O	-1.478902	-0.412494	-1.528463
O	-1.714974	1.690093	-1.014916
C	2.630015	0.903059	0.845905
H	1.765574	1.050308	1.501825
H	2.773513	1.824109	0.270607
C	3.876692	0.587539	1.656385
H	4.096054	1.413401	2.335581
H	3.733167	-0.315313	2.257700
H	4.745486	0.446403	1.005695
C	1.652999	-2.722945	-1.068406
H	1.591230	-2.916671	0.008686
H	1.155884	-3.536807	-1.594094
H	2.696191	-2.698011	-1.402422
O	-3.736771	0.012220	0.170883
H	-3.484072	0.944426	0.125838
H	-3.264358	-0.357725	-0.592759
O	-0.561678	-1.863267	1.012054

H	-1.196320	-1.786330	1.745585
H	-1.077291	-1.583694	0.242781
O	-2.883029	-1.242999	2.478090
H	-3.574595	-1.785221	2.866512
H	-3.284682	-0.770938	1.719388
O	-0.090518	3.673737	0.221662
H	-0.835067	3.200349	-0.187686
H	-0.281605	4.612717	0.149932

N-1-4w-c

N	3.667811	-0.106874	-0.024668
N	2.224684	1.693129	0.010888
C	2.399008	0.363042	0.018782
H	4.423414	0.558525	0.032906
H	1.251746	1.986484	0.029709
C	1.339234	-0.559310	0.060911
H	1.498156	-1.622190	0.076364
N	0.015731	-0.197184	0.075697
O	-0.312369	1.021120	0.069280
O	-0.843507	-1.083333	0.097464
C	4.025307	-1.519490	0.011225
H	3.551158	-2.029014	-0.834850
H	3.645144	-1.973305	0.934579
C	5.536267	-1.669086	-0.067708
H	5.808392	-2.725816	-0.042507
H	5.923681	-1.241917	-0.997200
H	6.025236	-1.177007	0.778732
C	3.301158	2.654725	-0.077995
H	3.895752	2.510763	-0.988067
H	2.863071	3.650996	-0.116064
H	3.959881	2.611168	0.798078
O	-5.225026	0.330550	1.481192
H	-5.739904	0.362947	0.657323
H	-4.857055	-0.565651	1.470710
O	-3.156354	0.979512	-0.289343
H	-3.660850	1.106142	0.533547
H	-2.218784	1.158922	-0.115299
O	-5.602915	-0.052357	-1.363579
H	-5.235241	-0.931494	-1.188565
H	-4.814880	0.503917	-1.456268
O	-3.732969	-1.718180	0.045654
H	-3.092131	-2.431650	0.123200
H	-3.205081	-0.913102	-0.126388

N-10-1w

N	1.834905	0.410584	0.005641
N	-0.313100	1.222220	-0.087385
C	0.573707	0.199839	-0.039874
H	-1.316583	1.080683	-0.021796
C	0.017405	-1.226083	-0.089952
H	0.391648	-1.801279	0.757499
N	-1.467575	-1.268554	0.003916
O	-1.958130	-1.207570	1.119213
O	-2.103651	-1.316684	-1.033394
C	2.755954	-0.712338	0.026606
H	2.613796	-1.367881	-0.849048
H	2.596277	-1.339768	0.919520
C	4.190416	-0.203117	0.033507
H	4.902288	-1.033316	0.057011
H	4.379471	0.398440	-0.859356
H	4.357836	0.430472	0.908384
C	0.169191	2.586804	-0.025883
H	0.834021	2.794152	-0.869358
H	-0.693595	3.252413	-0.061406
H	0.735598	2.760319	0.895152
H	0.281564	-1.700783	-1.035493
O	-3.269736	1.135635	0.067677
H	-3.590795	0.702468	-0.732029
H	-3.459039	0.512643	0.781322

N-10-1w-a

N	0.905328	-0.281961	0.272449
N	-0.246355	1.717793	0.442703
C	-0.176673	0.359862	0.508453
H	-1.172702	2.108610	0.336547
C	-1.490641	-0.291773	0.936514
H	-1.979826	0.302421	1.708787
N	-2.427589	-0.308276	-0.234942
O	-2.943801	0.754803	-0.533936
O	-2.586768	-1.361565	-0.815886

C	0.936526	-1.739280	0.381611
H	0.125355	-2.196585	-0.201029
H	0.803625	-2.045184	1.429989
C	2.272553	-2.269575	-0.119556
H	2.304249	-3.360119	-0.051222
H	2.425625	-1.985528	-1.165087
H	3.093339	-1.862577	0.478583
C	0.874164	2.487620	-0.072529
H	1.157091	2.169318	-1.081756
H	0.590744	3.540010	-0.082857
H	1.745614	2.358323	0.572852
H	-1.360431	-1.323283	1.249562
O	3.461890	0.911205	-0.556737
H	2.630689	0.470810	-0.294493
H	4.070796	0.214227	-0.815829

N-10-1w-b

N	1.236948	1.142569	-0.160696
N	2.092809	-0.982356	0.141072
C	1.200732	-0.098111	-0.430230
H	1.738597	-1.923859	0.248098
C	0.248586	-0.777522	-1.414676
H	0.651302	-1.735975	-1.743148
N	-1.030569	-1.087978	-0.702551
O	-0.976701	-1.940703	0.168630
O	-2.027075	-0.463972	-1.010228
C	0.300120	2.092862	-0.729832
H	-0.279650	1.694182	-1.575014
H	0.880932	2.941895	-1.106067
C	-0.665029	2.573218	0.353134
H	-1.354583	3.317760	-0.055274
H	-1.246295	1.737763	0.756536
H	-0.108393	3.025192	1.177899
C	2.928289	-0.499330	1.227963
H	2.331067	-0.097536	2.055093
H	3.549841	-1.323684	1.579497
H	3.568595	0.303015	0.857980
H	-0.006778	-0.150421	-2.263729
O	-2.586416	-0.094450	1.863508
H	-3.024270	-0.095211	1.004290
H	-2.149340	-0.952469	1.905619

N-10-2w

N	2.229912	0.418611	-0.129733
N	0.058398	1.170358	0.001853
C	0.990232	0.192912	0.090785
H	-0.886394	1.068344	0.367262
C	0.491704	-1.206247	0.470850
H	0.692797	-1.413997	1.522941
N	-0.978282	-1.346644	0.285876
O	-1.701843	-1.052251	1.216157
O	-1.375454	-1.721338	-0.809539
C	3.191646	-0.668673	-0.069100
H	3.004414	-1.403773	-0.869218
H	3.129763	-1.216236	0.886209
C	4.601379	-0.116306	-0.228502
H	5.344565	-0.918213	-0.192500
H	4.691050	0.406660	-1.184074
H	4.815755	0.600116	0.568775
C	0.470497	2.522709	-0.314834
H	0.966189	2.547465	-1.289289
H	-0.424488	3.144864	-0.333867
H	1.179107	2.905195	0.428057
H	0.948365	-1.954590	-0.175531
O	-2.699530	1.665197	0.616522
H	-3.231204	1.054185	0.070608
H	-3.020218	1.553327	1.516852
O	-3.907383	-0.301269	-0.937900
H	-4.150328	-0.144741	-1.855544
H	-3.228647	-0.993962	-0.943763

N-10-2w-a

N	-1.149599	-0.155421	-0.114549
N	0.204523	1.683778	-0.471915
C	-0.020430	0.346203	-0.462492
H	1.169872	1.990304	-0.488835
C	1.169816	-0.474664	-0.944206
H	1.982542	0.166958	-1.290063
N	1.746142	-1.263890	0.198164
O	2.131134	-0.628740	1.169556

O	1.803099	-2.468641	0.090505
C	-1.344379	-1.600143	-0.120884
H	-0.871468	-2.042801	0.767232
H	-0.878804	-2.080566	-0.994455
C	-2.830923	-1.930571	-0.105215
H	-2.986086	-3.012441	-0.132321
H	-3.296573	-1.540600	0.804603
H	-3.329562	-1.486277	-0.972309
C	-0.798593	2.602579	0.033601
H	-1.093115	2.348976	1.058289
H	-0.382440	3.609991	0.010356
H	-1.698131	2.570465	-0.585357
H	0.891749	-1.200926	-1.705402
O	-3.571156	1.353171	0.543986
H	-2.775359	0.819397	0.349094
H	-4.325269	0.769988	0.422353
O	3.132665	1.757219	-0.025988
H	3.054571	1.166647	0.737631
H	3.911732	2.305114	0.107984

N-10-2w-b

N	-0.462771	1.525805	0.085067
N	1.836429	1.332560	-0.043696
C	0.566224	0.901655	-0.331493
H	2.557813	0.620581	-0.035063
C	0.541512	-0.323083	-1.241565
H	1.551363	-0.661805	-1.483604
N	-0.100728	-1.479736	-0.534635
O	0.364553	-1.801954	0.551967
O	-1.032828	-2.040009	-1.069977
C	-1.802475	1.088632	-0.276743
H	-2.132615	0.316183	0.432579
H	-1.844340	0.635284	-1.280771
C	-2.763307	2.269094	-0.221246
H	-3.782537	1.950918	-0.457854
H	-2.756769	2.708160	0.779465
H	-2.462542	3.042968	-0.933480
C	1.993052	2.445782	0.871786
H	1.530138	2.241106	1.844705
H	3.058140	2.643216	0.999864
H	1.507386	3.331452	0.456094
H	-0.043772	-0.159880	-2.144815
O	-2.442095	-1.892658	1.544024
H	-1.530741	-2.002773	1.838267
H	-2.479503	-2.361671	0.702360
O	3.149256	-1.351543	0.097456
H	2.440624	-1.722501	0.642116
H	3.955723	-1.834818	0.300799

N-10-3w

N	1.949129	-0.211774	-0.038026
N	-0.007676	0.989620	0.188466
C	0.672161	-0.166265	0.120879
H	-1.017162	1.029952	0.325378
C	-0.124646	-1.461316	0.289650
H	0.060303	-1.899938	1.270737
N	-1.599148	-1.263283	0.190031
O	-2.246057	-1.227782	1.217120
O	-2.063099	-1.140873	-0.934100
C	2.620923	-1.502024	-0.099172
H	2.294742	-2.074485	-0.982436
H	2.392263	-2.119753	0.784407
C	4.128550	-1.305262	-0.178681
H	4.644865	-2.268160	-0.220173
H	4.387390	-0.735774	-1.076189
H	4.485042	-0.757317	0.698665
C	0.676189	2.263743	0.057726
H	1.190339	2.335140	-0.905530
H	-0.075384	3.049390	0.134332
H	1.426532	2.391205	0.843478
H	0.131181	-2.160671	-0.506659
O	-2.736798	1.638411	0.711787
H	-3.022075	1.267597	1.553715
H	-3.432836	1.393519	0.074011
O	-4.463385	0.407258	-1.082228
H	-5.367765	0.092382	-0.998864
H	-3.886297	-0.368049	-1.147840
O	3.729849	2.094761	-0.269439
H	3.156654	1.305385	-0.196835

H	4.632922	1.770186	-0.321021

N-10-3w-a

N	-2.620713	0.426432	0.000077
N	-0.452193	1.195506	-0.000937
C	-1.359702	0.198642	-0.000556
H	0.559554	1.050254	-0.000678
C	-0.835680	-1.241369	-0.001308
H	-1.169773	-1.759084	-0.900996
N	0.650277	-1.334752	-0.000373
O	1.212820	-1.366020	-1.080495
O	1.211359	-1.366693	1.080503
C	-3.558018	-0.681763	0.000325
H	-3.419570	-1.326903	0.884927
H	-3.419567	-1.327475	-0.883861
C	-4.984630	-0.150432	0.000145
H	-5.709985	-0.969355	0.000520
H	-5.152383	0.470673	0.883864
H	-5.152457	0.469918	-0.884092
C	-0.902275	2.571861	-0.000192
H	-1.514203	2.778954	0.883651
H	-0.017610	3.208906	-0.000360
H	-1.514991	2.779593	-0.883329
H	-1.170941	-1.760445	0.897152
O	2.345349	1.411367	0.000250
H	2.869008	1.148618	0.775480
H	2.870064	1.148641	-0.774268
O	3.592826	-0.016883	2.073139
H	3.555056	0.102408	3.026616
H	2.982375	-0.734175	1.854552
O	3.595526	-0.016868	-2.071341
H	2.985167	-0.734212	-1.852690
H	3.557436	0.102528	-3.024794

N-10-3w-b

N	2.279855	0.093691	0.036765
N	1.351637	-1.903984	0.697734
C	1.400075	-0.805994	-0.143774
H	0.422623	-2.282550	0.824075
C	0.475031	-0.912887	-1.348266
H	0.648234	-1.865985	-1.858828
N	-0.995945	-0.934682	-1.044489
O	-1.371256	-1.369148	0.037226
O	-1.745787	-0.574284	-1.923742
C	2.477973	1.234942	-0.831639
H	1.662816	1.399863	-1.547405
H	3.399148	1.062249	-1.404250
C	2.639923	2.491929	0.015946
H	2.860853	3.357414	-0.616364
H	1.714020	2.682474	0.563656
H	3.454640	2.361652	0.732980
C	2.171406	-1.871436	1.896724
H	1.953290	-0.997567	2.522749
H	1.991816	-2.788247	2.460502
H	3.224329	-1.821052	1.614250
H	0.591351	-0.093846	-2.048730
O	-2.455839	1.839230	1.706978
H	-2.453581	1.798059	2.666995
H	-3.102679	1.180712	1.382758
O	-3.920167	-0.116460	0.443654
H	-3.191221	-0.729991	0.257349
H	-4.259409	0.145695	-0.418638
O	-0.551885	1.600031	-0.286549
H	-0.932525	2.272890	-0.860304
H	-1.059509	1.678790	0.544649

N-10-4w

N	-2.656254	0.573344	0.388316
N	-0.781138	1.900142	0.181617
C	-1.527094	0.814929	-0.160901
H	0.202413	1.888318	-0.079010
C	-0.874212	-0.033260	-1.251916
H	-0.001287	0.472681	-1.670674
N	-0.348646	-1.288963	-0.626082
O	-0.822936	-2.353578	-0.954556
O	0.544632	-1.151785	0.203065
C	-3.455601	-0.576010	0.007752
H	-3.209082	-1.416931	0.672021
H	-3.258902	-0.928610	-1.016524
C	-4.936780	-0.246884	0.150620

H	-5.555139	-1.115701	-0.093581
H	-5.153426	0.064805	1.175534
H	-5.209614	0.575760	-0.516514
C	-1.208410	2.733997	1.283313
H	-1.297749	2.158090	2.212534
H	-0.480438	3.535416	1.414490
H	-2.189828	3.164639	1.067864
H	-1.574796	-0.347035	-2.021850
O	3.780741	-0.721430	0.113444
H	3.454279	-1.397635	0.741294
H	4.074160	-1.208943	-0.663962
O	2.487651	-2.716960	1.457572
H	2.401938	-3.006987	2.370047
H	1.602169	-2.476119	1.140814
O	4.616177	1.872132	-0.396973
H	4.575805	1.010770	0.050803
H	5.213193	2.435849	0.101856
O	1.894656	1.296717	-0.840720
H	2.689554	1.848101	-0.917085
H	2.224234	0.494462	-0.402876

N-10-4w-a

N	-2.384496	0.939965	-0.031791
N	-3.114990	-1.237899	-0.139382
C	-2.203729	-0.284001	0.260356
H	-2.795308	-2.194488	-0.162428
C	-1.065518	-0.868514	1.085113
H	-1.331733	-1.815787	1.550372
N	0.122331	-1.157532	0.219763
O	0.655729	-2.251700	0.344577
O	0.502043	-0.295639	-0.543547
C	-1.457631	1.978193	0.377007
H	-0.595743	1.608517	0.950695
H	-2.002788	2.677808	1.021946
C	-0.961267	2.727372	-0.857382
H	-0.282972	3.537838	-0.573015
H	-0.441143	2.038649	-1.532632
H	-1.805527	3.151458	-1.406904
C	-4.168087	-0.865978	-1.064643
H	-3.761121	-0.437934	-1.988222
H	-4.761247	-1.752141	-1.293545
H	-4.808631	-0.111847	-0.602926
H	-0.676541	-0.177413	1.835205
O	4.132585	0.546260	-1.061861
H	4.445831	0.690409	-1.958901
H	3.865227	-0.394104	-0.997854
O	3.337003	-2.069097	-0.776296
H	2.403445	-2.133065	-0.515140
H	3.829846	-2.570998	-0.119511
O	2.185093	2.024763	0.182621
H	1.434429	1.918453	-0.414253
H	2.934967	1.587578	-0.273668
O	1.376058	0.404701	2.201834
H	1.866214	0.537268	3.017752
H	1.752189	1.031332	1.541568

N-10-4w-b

N	3.140610	0.319427	0.017926
N	1.039145	1.230470	-0.199151
C	1.871712	0.175647	-0.072653
H	0.023379	1.149317	-0.232971
C	1.246898	-1.223710	-0.080507
H	1.580428	-1.784491	0.793126
N	-0.239854	-1.203469	-0.006490
O	-0.741658	-1.084068	1.097157
O	-0.860627	-1.294839	-1.050974
C	3.996989	-0.846293	0.146451
H	3.837215	-1.563295	-0.676729
H	3.787158	-1.389541	1.083342
C	5.457312	-0.416333	0.145796
H	6.121407	-1.279043	0.251875
H	5.695889	0.099772	-0.787684
H	5.642737	0.276369	0.970646
C	1.582038	2.573381	-0.204656
H	2.282718	2.702395	-1.035230
H	0.748820	3.268729	-0.308083
H	2.125999	2.776728	0.723549
H	1.500073	-1.746240	-1.003358
O	-1.771370	1.602578	-0.258800
H	-2.359589	1.293567	-0.965138

H	-2.276602	1.502895	0.563197
O	-3.343671	-0.095783	-1.887529
H	-3.572255	-0.200897	-2.816462
H	-2.676597	-0.766001	-1.675082
O	-3.041600	0.435201	1.983759
H	-2.410231	-0.286364	1.842656
H	-3.074063	0.607206	2.930127
O	-5.241472	-0.577708	0.312126
H	-4.695295	-0.173809	0.998984
H	-4.787023	-0.371492	-0.515254

N-13-1w

N	-2.130024	0.067396	-0.002448
N	-0.516737	1.696273	-0.122769
C	-0.885649	0.384099	-0.071387
H	0.460940	1.915508	-0.006310
C	0.186059	-0.633589	-0.143212
H	-0.057196	-1.678139	-0.260825
N	1.458771	-0.388862	-0.076001
O	2.041352	0.719778	0.075117
O	2.262556	-1.488638	-0.191396
C	-2.540408	-1.326498	0.015253
H	-2.066829	-1.874196	0.845206
H	-2.248019	-1.838661	-0.915701
C	-4.052944	-1.409914	0.168320
H	-4.389318	-2.450878	0.185185
H	-4.363037	-0.924319	1.097427
H	-4.543740	-0.893950	-0.661053
C	-1.524220	2.724047	0.009854
H	-2.053482	2.643925	0.966664
H	-1.037855	3.697576	-0.062741
H	-2.268609	2.626623	-0.785055
H	3.188194	-1.149742	-0.038324
O	4.591599	-0.289869	0.271395
H	5.328475	-0.206219	-0.341917
H	4.105320	0.549776	0.272083

N-13-1w-a

N	1.077942	-0.336209	0.000157
N	-0.272672	1.531231	-0.000072
C	-0.103788	0.188158	-0.000017
H	-1.213817	1.894482	0.000179
C	-1.321585	-0.652253	-0.000173
H	-1.252840	-1.728307	-0.000396
N	-2.535243	-0.190865	-0.000014
O	-2.962826	0.981172	0.000260
O	-3.515820	-1.166209	-0.000139
C	1.236914	-1.784278	0.000107
H	0.764813	-2.235948	-0.886088
H	0.764908	-2.235953	0.886351
C	2.716256	-2.145547	0.000015
H	2.850719	-3.230682	0.000097
H	3.205563	-1.736945	-0.889358
H	3.205688	-1.736799	0.889253
C	0.866064	2.426376	-0.000059
H	1.493553	2.265517	-0.882178
H	0.494904	3.451175	-0.000311
H	1.493354	2.265858	0.882275
H	-4.330416	-0.633986	-0.000024
O	3.622965	1.107442	-0.000064
H	2.785357	0.601531	0.000082
H	4.330311	0.456976	-0.000079

N-13-1w-b

N	1.790437	-0.511942	-0.021063
N	-0.381415	-1.246953	-0.105661
C	0.530854	-0.245223	-0.051311
H	-1.372946	-1.057149	-0.112358
C	0.033661	1.151093	-0.023543
H	0.731429	1.973891	0.011857
N	-1.209515	1.512507	-0.028678
O	-2.263551	0.835713	-0.070087
O	-1.409693	2.883009	0.011619
C	2.780801	0.547999	0.043464
H	2.645930	1.171442	0.942361
H	2.709632	1.219618	-0.827632
C	4.175147	-0.063118	0.077234
H	4.944151	0.713459	0.129540
H	4.275075	-0.718549	0.946430
H	4.341919	-0.665938	-0.819360

C	0.054551	-2.623457	-0.078677
H	0.662629	-2.819192	0.810914
H	-0.835482	-3.252889	-0.065973
H	0.669722	-2.856329	-0.954404
H	-2.379882	2.944650	-0.008165
O	-3.309406	-1.798366	0.222145
H	-3.434900	-0.854164	0.382108
H	-3.942695	-2.040752	-0.459925

N-13-2w

N	-2.589638	0.117452	0.012725
N	-0.896356	1.655847	-0.157544
C	-1.329345	0.367606	-0.047018
H	0.081789	1.812075	-0.345822
C	-0.308747	-0.701213	0.024011
H	-0.606773	-1.729114	0.161096
N	0.974917	-0.531286	-0.064416
O	1.604506	0.551170	-0.257680
O	1.722756	-1.652722	0.074042
C	-3.071604	-1.244186	0.170146
H	-2.688555	-1.699019	1.097601
H	-2.740755	-1.884723	-0.662829
C	-4.593652	-1.242117	0.215444
H	-4.985059	-2.256663	0.335413
H	-4.942843	-0.628389	1.050059
H	-4.996076	-0.816114	-0.707403
C	-1.860860	2.722637	-0.298552
H	-2.524063	2.750208	0.570667
H	-1.323018	3.668149	-0.377962
H	-2.488621	2.577544	-1.185434
H	2.674220	-1.420986	-0.215375
O	4.174083	-1.212548	-0.518448
H	4.423069	-1.107764	-1.442369
H	4.410096	-0.379139	-0.053484
O	4.107904	1.133878	0.770463
H	4.248644	1.328735	1.701338
H	3.146740	1.116522	0.607948

N-13-2w-a

N	1.667170	-0.315730	-0.020575
N	0.244020	1.495607	-0.040011
C	0.464126	0.159939	-0.026200
H	-0.712293	1.816248	-0.036401
C	-0.717428	-0.729908	-0.023251
H	-0.598020	-1.801377	-0.035892
N	-1.954848	-0.334705	-0.006369
O	-2.405583	0.841446	0.010081
O	-2.877705	-1.339812	-0.003912
C	1.883814	-1.756147	-0.007065
H	1.431982	-2.234523	-0.889788
H	1.427676	-2.218075	0.882099
C	3.376282	-2.058955	-0.000911
H	3.553152	-3.137977	0.010886
H	3.850701	-1.641828	-0.894615
H	3.848624	-1.621009	0.883597
C	1.344522	2.436299	-0.048342
H	1.990303	2.278483	-0.917617
H	0.931404	3.444645	-0.082000
H	1.967269	2.327558	0.845346
H	-3.764682	-0.878274	-0.006038
O	-5.069064	0.144079	-0.032704
H	-5.736424	0.194317	0.659166
H	-4.512701	0.936145	0.027726
O	4.141591	1.229500	0.103005
H	3.327802	0.687701	0.049151
H	4.878996	0.622687	-0.004077

N-13-2w-b

N	2.314792	0.058291	0.101285
N	0.514029	1.468405	0.272184
C	1.040027	0.237520	0.052178
H	-0.476975	1.631376	0.177413
C	0.114578	-0.875404	-0.270224
H	0.509479	-1.826556	-0.593868
N	-1.178596	-0.836023	-0.219492
O	-1.928324	0.118728	0.141764
O	-1.811410	-1.981504	-0.623616
C	2.895707	-1.254303	-0.119872
H	2.682422	-1.621097	-1.137298
H	2.489768	-2.000050	0.582099

C	4.405442	-1.176676	0.064174
H	4.872854	-2.152711	-0.097166
H	4.831760	-0.459085	-0.641664
H	4.641857	-0.834630	1.075246
C	1.388880	2.601761	0.460435
H	2.086815	2.698528	-0.378444
H	0.768524	3.495573	0.530524
H	1.984730	2.486174	1.371804
H	-2.719913	-1.919874	-0.223331
O	-4.102904	-1.469675	0.663507
H	-4.409427	-1.889370	1.473444
H	-3.704765	-0.616447	0.897752
O	-2.032469	2.789609	-0.664381
H	-2.415231	1.901908	-0.692389
H	-2.760427	3.416892	-0.680296

N-13-2w-c

N	-2.018071	-0.652906	-0.034846
N	0.187692	-1.089028	-0.511207
C	-0.826817	-0.225314	-0.271731
H	1.140282	-0.775091	-0.652961
C	-0.531754	1.228151	-0.349215
H	-1.331075	1.941989	-0.485308
N	0.643989	1.755348	-0.259802
O	1.773225	1.220792	-0.101208
O	0.674687	3.135825	-0.360005
C	-3.104693	0.275664	0.223365
H	-3.329710	0.882436	-0.669746
H	-2.857647	0.978288	1.035111
C	-4.355974	-0.502510	0.608484
H	-5.195263	0.172417	0.801325
H	-4.631485	-1.189059	-0.196186
H	-4.165914	-1.095822	1.506756
C	-0.053806	-2.513979	-0.459964
H	-0.801671	-2.804851	-1.205246
H	0.893968	-3.013897	-0.656650
H	-0.439812	-2.804237	0.523314
O	3.023696	-1.703748	-0.723207
H	3.252796	-1.462571	0.190681
H	3.681650	-1.282564	-1.283456
O	2.995739	-0.482846	1.767050
H	2.486791	0.243982	1.373268
H	3.471804	-0.134993	2.525490
H	1.629509	3.317819	-0.332082

N-13-3w

N	-2.991172	0.068559	0.098176
N	-1.363834	1.609538	-0.393136
C	-1.753269	0.327031	-0.132658
H	-0.428335	1.751779	-0.742003
C	-0.710247	-0.722408	-0.108982
H	-0.972791	-1.743792	0.120413
N	0.552142	-0.545693	-0.348066
O	1.138336	0.540205	-0.668144
O	1.337814	-1.636084	-0.237750
C	-3.424522	-1.281073	0.418775
H	-2.923984	-1.656596	1.325266
H	-3.183008	-1.981924	-0.395963
C	-4.930033	-1.290821	0.646380
H	-5.284463	-2.297587	0.886683
H	-5.189979	-0.619847	1.469328
H	-5.447214	-0.939896	-0.250562
C	-2.367313	2.642013	-0.524008
H	-2.927597	2.743225	0.409597
H	-1.867484	3.584058	-0.753308
H	-3.088261	2.401728	-1.314177
H	2.260361	-1.375209	-0.634838
O	3.584505	-1.052749	-1.219379
H	3.457258	-0.287276	-1.792877
H	4.249585	-0.783824	-0.537168
O	2.857388	1.249998	1.386567
H	2.221582	1.063006	0.666176
H	2.661144	2.129841	1.720134
O	5.115967	-0.078870	0.733503
H	5.505652	-0.618598	1.427306
H	4.417807	0.475639	1.141756

N-13-3w-a

N	-2.134994	-0.295839	-0.001054
N	-0.617155	1.407240	-0.315147

C	-0.909907	0.097551	-0.134158
H	0.354444	1.665675	-0.395639
C	0.216219	-0.862345	-0.118314
H	0.031276	-1.924186	-0.087115
N	1.476474	-0.548071	-0.140824
O	1.986400	0.608675	-0.198839
O	2.336794	-1.590383	-0.092632
C	-2.431546	-1.709043	0.192990
H	-1.912010	-2.107667	1.077551
H	-2.103104	-2.304820	-0.672686
C	-3.930024	-1.908486	0.377653
H	-4.164522	-2.966206	0.525908
H	-4.281869	-1.351248	1.251192
H	-4.471682	-1.555736	-0.505316
C	-1.661964	2.408506	-0.360607
H	-2.230699	2.431204	0.574268
H	-1.197018	3.380557	-0.526074
H	-2.370531	2.201639	-1.168559
H	3.274516	-1.225447	-0.287337
O	4.739486	-0.833160	-0.474880
H	5.028421	-0.635712	-1.371734
H	4.866411	-0.019278	0.062466
O	4.383147	1.389273	0.967564
H	4.490630	1.565417	1.906562
H	3.431832	1.292519	0.783518
O	-4.509346	1.401609	0.057479
H	-3.729521	0.809800	0.035370
H	-5.275362	0.834983	0.181890

N-13-3w-b

N	-2.714921	0.207595	-0.073949
N	-0.774947	1.439849	-0.120388
C	-1.428692	0.251230	-0.102940
H	0.234231	1.479982	-0.039122
C	-0.605533	-0.980020	-0.217895
H	-1.015676	-1.880922	-0.649871
N	0.625045	-1.079528	0.170860
O	1.327485	-0.185271	0.718531
O	1.205670	-2.303702	0.007492
C	-3.403202	-1.072051	-0.079189
H	-2.996261	-1.761754	0.676569
H	-3.295335	-1.569642	-1.057500
C	-4.885120	-0.854055	0.195692
H	-5.432321	-1.801411	0.178292
H	-5.020348	-0.387243	1.175031
H	-5.310833	-0.185156	-0.556899
C	-1.522096	2.672314	-0.034777
H	-2.128718	2.703114	0.877558
H	-0.808310	3.497115	-0.031239
H	-2.205603	2.771905	-0.884456
H	2.181642	-2.118927	-0.125302
O	3.761389	-1.860024	-0.507617
H	4.070337	-2.053076	-1.397930
H	4.076126	-0.968394	-0.263257
O	3.845443	0.671091	0.536977
H	4.308778	0.884653	1.353736
H	2.958569	0.327890	0.783038
O	1.944332	2.642399	-0.381918
H	2.761839	2.147178	-0.219610
H	2.068949	3.118822	-1.207760

N-13-3w-c

N	2.807162	0.494843	0.040388
N	0.905570	1.812204	0.017574
C	1.564281	0.655111	0.301513
H	-0.108963	1.785715	0.063615
C	0.706242	-0.357151	0.993811
N	-0.279632	-0.891793	0.361326
O	-0.613979	-0.699612	-0.840812
O	-1.031717	-1.793364	1.081920
C	3.423404	-0.785456	0.346898
H	3.022209	-1.242638	1.265579
H	4.488347	-0.605930	0.523855
C	3.256585	-1.764707	-0.814887
H	3.774319	-2.707401	-0.612087
H	2.195771	-1.976828	-0.986713
H	3.663332	-1.329269	-1.731586
C	1.552584	2.810864	-0.805413
H	1.861068	2.392903	-1.771518
H	0.854672	3.633668	-0.965129

H	2.449717	3.186489	-0.306037
H	0.833930	-0.656487	2.024410
O	-4.374960	0.838983	-0.308120
H	-5.248095	0.844942	0.093122
H	-4.165243	-0.082271	-0.545167
O	-3.107105	-1.568110	-0.852119
H	-2.249490	-1.185711	-1.157095
H	-3.332659	-2.287952	-1.450452
O	-1.916537	1.425283	0.878102
H	-2.047734	1.821378	1.744695
H	-2.800765	1.363272	0.470345
H	-1.886313	-1.838064	0.601855

N-13-4w

N	-3.266078	0.332645	0.047852
N	-1.412570	1.626779	-0.355608
C	-2.003108	0.409090	-0.174325
H	-0.405687	1.663466	-0.313040
C	-1.151977	-0.796889	-0.304849
H	-1.604580	-1.774982	-0.369098
N	0.141923	-0.815300	-0.365076
O	0.927038	0.194702	-0.269949
O	0.719734	-2.010929	-0.571145
C	-3.922196	-0.956060	0.198682
H	-3.451883	-1.555606	0.993141
H	-3.856617	-1.543470	-0.730966
C	-5.389620	-0.741853	0.543550
H	-5.907264	-1.697947	0.664682
H	-5.476959	-0.173912	1.473517
H	-5.882545	-0.171244	-0.247837
C	-2.197252	2.828291	-0.175718
H	-2.627966	2.879733	0.831171
H	-1.552559	3.691351	-0.346742
H	-3.026445	2.845585	-0.887919
H	1.702572	-1.974118	-0.172400
O	3.035456	-1.968765	0.327967
H	3.052254	-1.309166	1.071306
H	3.583879	-1.573024	-0.367847
O	3.350674	0.134471	-1.550531
H	2.423170	0.185604	-1.230191
H	3.327118	0.184024	-2.511215
O	2.797737	0.110618	1.969823
H	3.517289	0.717929	1.719207
H	2.012874	0.431732	1.501151
O	4.707004	1.452323	0.485131
H	4.399785	1.151112	-0.387908
H	5.214412	2.259220	0.366407

N-13-4w-a

N	3.218873	0.121074	0.151237
N	1.480865	1.601197	-0.089198
C	1.972213	0.323375	-0.082621
H	0.567013	1.735949	-0.493916
C	1.025958	-0.787946	-0.328708
H	1.378731	-1.807959	-0.324565
N	-0.242529	-0.676445	-0.576267
O	-0.915175	0.412535	-0.636195
O	-0.912477	-1.810074	-0.812106
C	3.758568	-1.227110	0.220062
H	3.620974	-1.758285	-0.734699
H	3.250386	-1.820793	0.995873
C	5.245822	-1.163900	0.539668
H	5.677658	-2.167459	0.595709
H	5.772118	-0.596542	-0.232357
H	5.403791	-0.659001	1.496300
C	2.408423	2.709280	-0.008446
H	3.145940	2.677946	-0.819260
H	1.841594	3.639969	-0.059570
H	2.958071	2.668227	0.935180
H	-1.957984	-1.609176	-0.735816
O	-3.349164	-1.463802	-0.641629
H	-3.682480	-1.460627	0.279922
H	-3.616801	-0.601722	-1.027099
O	-2.599070	1.386200	1.266168
H	-1.890780	0.967623	0.729430
H	-2.165361	2.006744	1.861070
O	-3.573229	1.158824	-1.464872
H	-3.587827	1.599612	-0.602342
H	-2.632893	1.122720	-1.694651
O	-4.047923	-0.880980	1.932439

H	-4.925717	-0.809370	2.317733
H	-3.646503	0.007545	1.922478

N-13-4w-b

N	-2.954587	0.339133	0.130449
N	-1.128067	1.320037	-0.870110
C	-1.759460	0.219153	-0.317213
H	-0.387879	1.097852	-1.524621
C	-1.001187	-1.044724	-0.227123
H	-1.454374	-1.918961	0.212890
N	0.213828	-1.235563	-0.654774
O	0.987934	-0.393615	-1.194646
O	0.698498	-2.484315	-0.514283
C	-3.619255	-0.775046	0.787868
H	-3.043800	-1.118058	1.661396
H	-3.713010	-1.633819	0.105507
C	-5.007815	-0.346178	1.241182
H	-5.530034	-1.170502	1.735353
H	-4.934337	0.492071	1.939039
H	-5.599479	-0.019393	0.382082
C	-1.948007	2.481842	-1.172986
H	-2.371090	2.883078	-0.250288
H	-1.313909	3.235680	-1.642112
H	-2.785012	2.231205	-1.835496
H	1.734224	-2.391251	-0.510494
O	3.196712	-2.280536	-0.331865
H	3.652167	-3.038479	0.048754
H	3.423749	-1.487848	0.228572
O	3.657249	-0.243642	1.273611
H	2.823545	0.135975	1.589592
H	4.135881	0.533009	0.928859
O	1.474661	1.516080	0.737398
H	0.576281	1.870680	0.780378
H	1.429865	0.896106	-0.019247
O	4.088403	2.344779	0.381235
H	3.125250	2.427799	0.496236
H	4.500428	3.129317	0.752684

N-13-4w-c

N	2.929415	-0.481576	0.092695
N	1.242115	-1.983799	-0.330105
C	1.682707	-0.705812	-0.117035
H	0.316711	-2.089834	-0.717771
C	0.680513	0.384701	-0.103548
H	0.984935	1.396933	0.129571
N	-0.579874	0.249181	-0.365731
O	-1.207470	-0.812350	-0.697414
O	-1.342359	1.369589	-0.274188
C	3.406448	0.866043	0.369153
H	2.945757	1.269477	1.283782
H	3.146016	1.557744	-0.445719
C	4.918840	0.842042	0.541429
H	5.304957	1.844860	0.746970
H	5.194633	0.182148	1.368409
H	5.395014	0.461408	-0.366284
C	2.214585	-3.045447	-0.469169
H	2.795698	-3.142778	0.451600
H	1.684445	-3.978503	-0.665373
H	2.921715	-2.840887	-1.282102
H	-2.275819	1.123085	-0.665225
O	-3.604160	0.841840	-1.227989
H	-3.489519	0.089616	-1.821834
H	-4.256416	0.555481	-0.538614
O	-2.873239	-1.507067	1.384760
H	-2.246627	-1.332262	0.651683
H	-2.671751	-2.380187	1.732501
O	-5.110806	-0.168893	0.715956
H	-5.513472	0.353320	1.415660
H	-4.418168	-0.732999	1.122989
O	0.567889	3.473766	0.111749
H	-0.338983	3.170785	-0.030055
H	0.521880	4.381709	0.423838

S3. Cartesian coordinates of various amino and nitro substituted ethylenes (**1b-1g**).

1b

C	0.069424	0.428139	-0.000529
C	1.252360	-0.196513	0.014553
H	1.333834	-1.278464	0.018907
H	2.170399	0.374017	0.004148
H	0.029117	1.513706	-0.010853
N	-1.184622	-0.169499	-0.079439
H	-1.222011	-1.157103	0.129920
H	-1.949692	0.344582	0.329802

1c

C	0.088991	-0.000092	-0.000018
C	1.433753	-0.000915	0.000013
H	1.992995	0.920256	0.092924
H	1.991890	-0.922763	-0.092869
N	-0.703019	1.153978	-0.078752
H	-1.458162	1.173157	0.596180
H	-0.173987	2.014348	-0.073769
N	-0.704463	-1.153074	0.078708
H	-1.460084	-1.171044	-0.595692
H	-0.176738	-2.014232	0.073562

1d

C	0.543086	-0.390343	0.038462
C	-0.543087	0.390348	0.038485
H	-0.440197	1.473027	0.039861
H	0.440190	-1.473020	0.039764
N	1.877518	0.056845	-0.107262
H	1.970573	1.064895	-0.073167
H	2.517490	-0.367529	0.553477
N	-1.877521	-0.056834	-0.107284
H	-2.517477	0.367407	0.553559
H	-1.970555	-1.064891	-0.073355

1e

C	1.872540	0.052901	0.000069
C	0.746992	-0.642909	0.000004
H	0.644199	-1.717870	-0.000046
N	-0.561819	0.031495	-0.000009
O	-0.599755	1.253634	0.000025
O	-1.539291	-0.708376	-0.000090
H	2.825833	-0.460066	0.000076
H	1.857873	1.135452	0.000115

1f

N	2.570230	-0.116479	-0.000439
C	1.274635	0.268499	0.000216
C	0.203815	-0.553822	0.000027
H	0.223198	-1.632445	-0.000094
H	2.836297	-1.087580	0.001807
H	3.306936	0.566375	0.003271
N	-1.116677	-0.000358	-0.000124
O	-1.264752	1.225097	-0.000109
O	-2.048613	-0.806870	-0.000242
H	1.094923	1.337635	0.000312

1g

N	-2.291667	-0.815929	-0.096960
N	-1.283189	1.261707	0.063495
C	-1.131764	-0.081328	0.011455
H	-3.110587	-0.442733	0.360993
H	-0.414147	1.787971	0.011925
C	0.084180	-0.735408	0.055495
H	0.153503	-1.809574	0.097618
N	1.325702	-0.087079	0.000755
O	1.376049	1.166098	-0.018074
O	2.339503	-0.790350	-0.019339
H	-2.201717	-1.817277	-0.020264
H	-2.121880	1.665145	-0.323694