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

Electronic Supplementary Information

Exploring the non-covalent interactions behind the formation of amine–water complexes: The case of the *N*-allylmethylamine monohydrate

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Appendix 1: Cartesian coordinates for the nine conformers of the AMA–w complex

Table S1. Cartesian coordinates of conformer AMA-I-w-I obtained at the B2PLYP-D3/aug-cc-pVTZ level

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	2.736234	0.127976	-0.199353
H	3.437489	0.881907	-0.526021
H	3.110558	-0.882298	-0.094634
C	1.469845	0.428319	0.074184
H	1.108978	1.443740	-0.037589
C	0.459122	-0.573997	0.533681
H	0.046755	-0.266517	1.497740
H	0.935548	-1.552477	0.677159
N	-0.665728	-0.643986	-0.407485
H	-0.305008	-0.874319	-1.325486
C	-1.669766	-1.626653	-0.006753
H	-2.136687	-1.298793	0.920844
H	-1.252097	-2.627031	0.155695
H	-2.442625	-1.691391	-0.769595
O	-1.591602	2.013252	0.071410
H	-1.371079	1.112558	-0.245668
H	-2.288234	2.329676	-0.507706

Table S2. Cartesian coordinates of conformer AMA-II-w-II obtained at the B2PLYP-D3/aug-cc-pVTZ level

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	2.316888	-0.813598	-0.443586
H	2.645285	-1.624437	-1.077263
H	3.037804	-0.037253	-0.221320
C	1.082824	-0.774024	0.049544
H	0.370809	-1.554604	-0.191499
C	0.581562	0.309001	0.955756
H	1.380114	1.043379	1.124819
H	0.316745	-0.124993	1.921626
N	-0.634720	0.938302	0.419114
H	-1.049454	1.509491	1.144136
C	-0.376982	1.764630	-0.759795
H	0.391104	2.527438	-0.585866
H	-1.297895	2.256959	-1.064332
H	-0.043129	1.130182	-1.577323
O	-2.199595	-1.397620	-0.172822
H	-1.793607	-0.527612	0.023626
H	-3.145272	-1.241232	-0.218604

Table S3. Cartesian coordinates of conformer AMA-III-w-III obtained at the B2PLYP-D3/aug-cc-pVTZ level

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	2.033443	0.694903	-0.558359
H	3.009626	1.148821	-0.642650
H	1.266756	1.044905	-1.234407
C	1.796131	-0.244876	0.352506
H	2.596102	-0.553349	1.015594
C	0.496028	-0.956374	0.566566
H	0.112487	-0.706875	1.560490
H	0.685965	-2.040325	0.583515
N	-0.527614	-0.598500	-0.404836
H	-0.179010	-0.780699	-1.338133
C	-1.777733	-1.325843	-0.194813
H	-1.643636	-2.413519	-0.172072
H	-2.479629	-1.074543	-0.986308
H	-2.215464	-1.014183	0.752115
O	-1.415501	2.061355	0.231868
H	-1.032627	1.207839	-0.055674
H	-0.661731	2.598073	0.487202

Table S4. Cartesian coordinates of conformer AMA-IV-w-IV obtained at the B2PLYP-D3/aug-cc-pVTZ level

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	-2.697842	-0.391993	0.560698
H	-3.742206	-0.194293	0.366803
H	-2.417046	-0.603872	1.584262
C	-1.792558	-0.388324	-0.413283
H	-2.106923	-0.170501	-1.429778
C	-0.327843	-0.650903	-0.216700
H	-0.011754	-1.493054	-0.833835
H	-0.132805	-0.923349	0.821268
N	0.547613	0.484394	-0.550504
H	0.433044	0.721227	-1.528536
C	0.315601	1.667859	0.277989
H	0.569065	1.426296	1.309459
H	-0.716698	2.027290	0.254787
H	0.975028	2.467905	-0.051522
O	2.970521	-0.768232	0.301676
H	3.774494	-0.356741	-0.022475
H	2.234933	-0.256469	-0.094349

Table S5. Cartesian coordinates of conformer AMA-VIII-w-V obtained at the B2PLYP-D3/aug-cc-pVTZ level

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	2.490612	0.374214	0.152766
H	3.400488	0.602070	-0.383169
H	2.307868	0.914080	1.072252
C	1.629631	-0.534078	-0.294458
H	1.840527	-1.055503	-1.223077
C	0.358397	-0.906191	0.400576
H	0.272318	-0.354858	1.337595
H	0.373467	-1.977175	0.650470
N	-0.810359	-0.574233	-0.423017
H	-0.690549	-0.964912	-1.349673
C	-2.060229	-1.059200	0.159193
H	-2.045988	-2.134465	0.372363
H	-2.883435	-0.844274	-0.517983
H	-2.245241	-0.528221	1.091705
O	-1.048516	2.242155	0.028632
H	-0.924389	1.318982	-0.272950
H	-0.300551	2.723288	-0.332352

Table S6. Cartesian coordinates of conformer AMA-VI-w-VI obtained at the B2PLYP-D3/aug-cc-pVTZ level

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	-2.822125	-0.725201	-0.223095
H	-3.846387	-0.382523	-0.249853
H	-2.622631	-1.714086	-0.615865
C	-1.845254	0.025873	0.279005
H	-2.083064	1.008258	0.670478
C	-0.407531	-0.401352	0.325306
H	-0.319538	-1.426133	-0.035470
H	-0.038116	-0.392291	1.352682
N	0.508509	0.439035	-0.463054
H	0.161079	0.497489	-1.412707
C	0.701068	1.784691	0.076971
H	1.159415	1.703828	1.061497
H	-0.220724	2.366385	0.171331
H	1.385843	2.333145	-0.566413
O	2.881782	-1.054561	0.089767
H	3.566449	-0.987215	-0.579182
H	2.134888	-0.514730	-0.242876

Table S7. Cartesian coordinates of conformer AMA-V-w-VII obtained at the B2PLYP-D3/aug-cc-pVTZ level

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	-0.978959	-1.546150	0.619828
H	-1.458635	-2.418120	1.039848
H	0.075683	-1.417845	0.814966
C	-1.674436	-0.680059	-0.110367
H	-2.731295	-0.857195	-0.277266
C	-1.145306	0.562597	-0.767336
H	-1.841343	1.387844	-0.555630
H	-1.169233	0.416888	-1.850098
N	0.222197	0.909839	-0.387360
H	0.602098	1.532982	-1.087733
C	0.312447	1.562727	0.921046
H	-0.306936	2.464596	0.985000
H	1.348159	1.828975	1.118344
H	-0.012682	0.872232	1.694395
O	2.506125	-0.837796	-0.204597
H	1.670485	-0.353997	-0.362281
H	2.472605	-1.600323	-0.786593

Table S8. Cartesian coordinates of conformer AMA-VII-w-VIII obtained at the B2PLYP-D3/aug-cc-pVTZ level

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	-2.586007	0.002584	-0.391273
H	-3.656371	-0.134425	-0.356639
H	-2.220464	0.826244	-0.989270
C	-1.767539	-0.805893	0.274660
H	-2.192145	-1.613707	0.861361
C	-0.263162	-0.747818	0.281343
H	0.119821	-1.662787	-0.177993
H	0.093970	-0.771512	1.313467
N	0.368439	0.393043	-0.373765
H	0.004063	0.497449	-1.312031
C	0.247655	1.650401	0.365772
H	0.677364	2.455478	-0.226668
H	0.824185	1.569149	1.286176
H	-0.780033	1.915806	0.625553
O	3.034745	-0.590168	-0.074753
H	2.181184	-0.170257	-0.308676
H	3.687164	-0.188181	-0.652269

Table S9. Cartesian coordinates of conformer AMA-IX-w-IX obtained at the B2PLYP-D3/aug-cc-pVTZ level

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	-2.358536	0.405092	-0.157709
H	-2.994360	0.765222	-0.953428
H	-2.585319	0.740966	0.845710
C	-1.343645	-0.419587	-0.397694
H	-1.149637	-0.735804	-1.415736
C	-0.442989	-0.967918	0.668042
H	-0.525314	-2.064758	0.678476
H	-0.774872	-0.601807	1.638789
N	0.954378	-0.549648	0.481333
H	1.462035	-0.737745	1.336098
C	1.624804	-1.220897	-0.630725
H	1.531297	-2.312972	-0.589893
H	2.679690	-0.957793	-0.623699
H	1.207728	-0.877027	-1.574701
O	1.053055	2.316110	0.015891
H	1.009331	1.355030	0.190989
H	0.175764	2.539777	-0.303846

Appendix 2: Assigned transitions and residuals for the observed conformers of AMA–w

Table S10. Assigned transitions and residuals for AMA-I-w-I

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs} /MHz	$\nu_{obs - calc}$
3	2	2	4	3	1	3	3	7369.1091	0.0004
2	1	2	2	1	0	1	1	7434.8652	0.0000
2	1	2	3	1	0	1	2	7435.8633	-0.0001
2	1	2	1	1	0	1	0	7436.7354	0.0027
4	3	1	5	4	2	2	5	7685.2387	-0.0056
3	0	3	2	2	1	2	1	8269.3969	0.0015
3	0	3	4	2	1	2	3	8269.6630	0.0012
3	0	3	3	2	1	2	2	8270.0332	0.0012
3	3	0	3	3	2	1	3	8356.5387	0.0028
3	3	0	4	3	2	1	4	8357.5371	-0.0033
4	2	3	5	4	1	4	5	8755.3916	-0.0001
3	3	1	3	3	2	2	2	9076.6059	0.0008
2	1	1	3	1	0	1	2	9321.0598	0.0017
2	1	1	2	1	0	1	1	9321.7486	0.0011
2	1	1	2	1	0	1	2	9322.0809	0.0006
4	3	2	5	4	2	3	5	9461.9694	0.0027
3	1	3	3	2	0	2	2	9853.3297	-0.0018
3	1	3	4	2	0	2	3	9854.0715	0.0004
3	1	3	2	2	0	2	1	9854.3431	0.0010
5	3	3	5	5	2	4	5	10150.7284	0.0001
4	1	3	3	3	2	2	2	10381.7656	0.0000
4	1	3	5	3	2	2	4	10381.9887	-0.0007
4	1	3	4	3	2	2	3	10382.8606	0.0008
5	2	4	6	5	1	5	6	10458.2177	0.0002
4	0	4	3	3	1	3	2	11378.1402	0.0001
4	0	4	5	3	1	3	4	11378.2265	0.0000
4	0	4	4	3	1	3	3	11378.3177	0.0001
2	2	1	2	1	1	0	1	11658.2557	0.0026
2	2	1	3	1	1	0	2	11659.2314	0.0005

2	2	1	1	1	1	0	0	11660.3605	-0.0004
2	2	0	2	1	1	0	1	11819.6899	0.0031
2	2	0	3	1	1	0	2	11820.3676	0.0009
2	2	0	1	1	1	0	0	11821.3296	-0.0016
4	1	4	4	3	0	3	3	12214.6408	-0.0011
4	1	4	5	3	0	3	4	12215.1052	-0.0009
4	1	4	3	3	0	3	2	12215.1959	-0.0020
2	2	1	1	1	1	1	0	12286.2766	-0.0029
2	2	1	2	1	1	1	2	12287.1553	-0.0003
2	2	1	3	1	1	1	2	12287.5135	0.0011
2	2	1	2	1	1	1	1	12288.1078	-0.0019
2	2	1	1	1	1	1	1	12288.6642	-0.0005
2	2	0	1	1	1	1	0	12447.2472	-0.0027
2	2	0	3	1	1	1	2	12448.6490	0.0008
2	2	0	2	1	1	1	1	12449.5409	-0.0023
3	1	2	2	2	0	2	1	13597.3900	0.0039
3	1	2	4	2	0	2	3	13597.7169	0.0032
3	1	2	3	2	0	2	2	13598.6853	0.0009
5	0	5	4	4	1	4	3	14278.8088	-0.0035
5	0	5	5	4	1	4	4	14278.8252	0.0019
5	0	5	6	4	1	4	5	14278.8468	-0.0011
3	2	2	3	2	1	1	2	14320.0846	-0.0015
3	2	2	4	2	1	1	3	14321.1143	0.0060
3	2	2	2	2	1	1	1	14321.6776	0.0013
5	1	4	4	4	2	3	3	14398.4253	-0.0003
5	1	4	6	4	2	3	5	14398.5286	0.0012
5	1	4	5	4	2	3	4	14399.0431	-0.0033
5	1	5	5	4	0	4	4	14660.6980	-0.0008
5	1	5	6	4	0	4	5	14660.9565	-0.0022
5	1	5	4	4	0	4	3	14660.9812	0.0010
3	2	1	4	2	1	1	3	15067.4265	0.0021
3	2	2	2	2	1	2	1	16205.9331	0.0000
3	2	2	4	2	1	2	3	16206.3037	0.0007
3	2	2	3	2	1	2	2	16206.9683	-0.0002

4	2	3	4	3	1	2	3	16657.6889	0.0011
4	2	3	5	3	1	2	4	16658.6426	0.0004
4	2	3	3	3	1	2	2	16658.9841	0.0008
3	2	1	2	2	1	2	1	16952.0128	-0.0033
3	2	1	4	2	1	2	3	16952.6132	-0.0057
3	2	1	3	2	1	2	2	16953.9456	-0.0042
6	0	6	6	5	1	5	5	17050.7841	0.0010
6	0	6	5	5	1	5	4	17050.8184	-0.0045
6	0	6	7	5	1	5	6	17050.8424	0.0000
6	1	6	6	5	0	5	5	17208.7240	0.0005
6	1	6	7	5	0	5	6	17208.8696	-0.0018
3	3	1	3	2	2	0	2	18786.6472	0.0012
3	3	1	4	2	2	0	3	18786.9683	0.0017
7	0	7	7	6	1	6	6	19758.4526	0.0040
7	0	7	6	6	1	6	5	19758.4945	-0.0022
7	0	7	8	6	1	6	7	19758.5138	0.0031
7	1	7	7	6	0	6	6	19819.7108	0.0010
7	1	7	6	6	0	6	5	19819.7916	-0.0026
7	1	7	8	6	0	6	7	19819.8049	0.0017

Table S11. Assigned transitions and residuals for AMA-II-w-II

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs} /MHz	$\nu_{obs - calc}$
2	1	2	2	1	0	1	1	7887.0449	-0.0030
2	1	2	3	1	0	1	2	7887.4713	-0.0036
3	0	3	4	2	1	2	3	9560.0477	0.0017
3	1	3	3	2	0	2	3	10766.2999	-0.0002
3	1	3	3	2	0	2	2	10766.6694	-0.0012
3	1	3	4	2	0	2	3	10767.0326	-0.0011
3	1	3	2	2	0	2	2	10767.6614	0.0003
2	2	1	2	1	1	0	1	11322.8517	0.0001
2	2	1	3	1	1	0	2	11323.2269	0.0024
2	2	1	1	1	1	0	0	11323.9693	-0.0016
2	2	0	3	1	1	1	2	12010.5271	-0.0013
2	2	0	2	1	1	1	1	12011.2846	-0.0005
4	0	4	4	3	1	3	3	12995.6647	0.0024
4	0	4	5	3	1	3	4	12995.6908	-0.0025
4	1	4	4	3	0	3	3	13607.9118	0.0001
4	1	4	5	3	0	3	4	13608.1524	-0.0010
4	1	4	3	3	0	3	2	13608.1636	0.0026
3	2	2	3	2	1	1	2	14407.4495	0.0036
3	2	2	4	2	1	1	3	14407.8630	0.0033
3	2	2	2	2	1	1	1	14408.0910	0.0015
5	0	5	5	4	1	4	4	16259.2743	-0.0009
5	0	5	4	4	1	4	3	16259.3016	0.0045
5	0	5	6	4	1	4	5	16259.3273	-0.0028
5	1	5	5	4	0	4	4	16526.7207	0.0016
5	1	5	4	4	0	4	3	16526.8501	-0.0017
5	1	5	6	4	0	4	5	16526.8640	0.0006
5	1	4	4	4	2	3	3	16557.0170	0.0000
3	2	1	2	2	1	2	1	16703.8948	-0.0001
3	2	1	4	2	1	2	3	16704.3675	-0.0011
3	2	1	3	2	1	2	2	16705.3637	0.0007
4	2	3	4	3	1	2	3	17213.7113	-0.0018

4	2	3	5	3	1	2	4	17214.1505	0.0032
4	2	3	3	3	1	2	2	17214.2827	-0.0046
3	3	1	4	2	2	0	3	18048.2654	-0.0008
6	0	6	6	5	1	5	5	19422.4846	-0.0008
6	0	6	7	5	1	5	6	19422.5418	0.0000

Appendix 3: Full set of calculated spectroscopic parameters for conformers AMA-I-w-I and AMA-II-w-II

Table S12. Calculated rotational, centrifugal distortion and ^{14}N quadrupole coupling constants for conformers AMA-I-w-I and AMA-II-w-II at the B2PLYP-D3 and MP2 levels of theory (aug-cc-pVTZ basis set).

	B2PLYP-D3		MP2	
Parameter	AMA-I-w-I	AMA-II-w-II	AMA-I-w-I	AMA-II-w-II
A/MHz	3441	3255	3504	3260
B/MHz	1984	2134	1998	2167
C/MHz	1345	1567	1365	1594
D_J/kHz	2.0705	3.0152	2.2320	2.9632
D_{JK}/kHz	3.9690	-2.4931	1.7254	-1.1806
D_K/kHz	14.6871	7.6969	21.9565	6.2407
d_1/kHz	-1.0942	-0.8154	-1.1567	-0.7958
d_2/kHz	-0.3035	0.0094	-0.2801	0.0193
1.5 (χ_{aa})/MHz	1.84	-0.80	1.70	-1.16
0.25 (χ_{bb}- χ_{cc})/MHz	-1.40	-0.83	-1.26	-0.73

Appendix 4: QTAIM, NCI and NBO analyses for the conformers of AMA–w

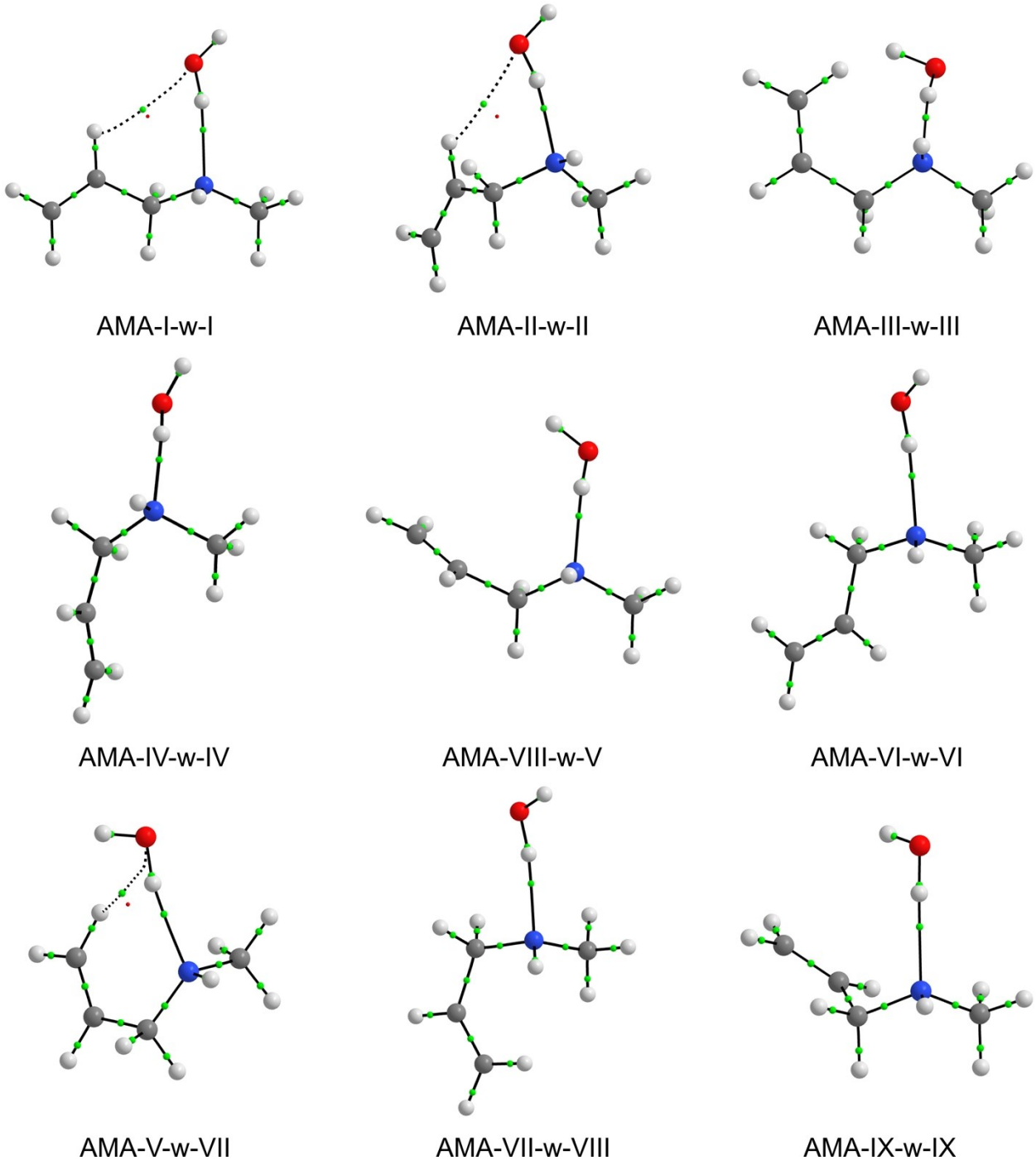

Figure S1. QTAIM molecular graphs for the nine most stable conformers of AMA–w

Table S13. QTAIM parameters at the bond critical point (BCP) associated with each intermolecular interaction observed in the nine conformers of AMA–w.

Conformer	Interaction	ρ (au)[a]	$\nabla^2\rho$ (au)[b]	V (au)[c]	E_{HB} (kJ mol^{-1})[d]
AMA-I-w-I	N···H–O	0.0365	0.0677	-0.0295	-38.7
	C–H···O	0.0055	0.0215	-0.0032	-4.1
AMA-II-w-II	N···H–O	0.0358	0.0664	-0.0286	-37.5
	C–H···O	0.0067	0.0289	-0.0041	-5.3
AMA-III-w-III	N···H–O	0.0358	0.0672	-0.0289	-37.9
AMA-IV-w-IV	N···H–O	0.0364	0.0678	-0.0295	-38.7
AMA-VIII-w-V	N···H–O	0.0360	0.0680	-0.0292	-38.3
AMA-VI-w-VI	N···H–O	0.0365	0.0677	-0.0296	-38.8
AMA-V-w-VII	N···H–O	0.0344	0.0671	-0.0273	-35.9
	C–H···O	0.0073	0.0242	-0.0042	-5.4
AMA-VII-w-VIII	N···H–O	0.0364	0.0679	-0.0295	-38.8
AMA-IX-w-IX	N···H–O	0.0344	0.0657	-0.0272	-35.7

[a]electron density, [b]Laplacian of the electron density, [c]potential energy, [d]HB energy derived as 0.5V.

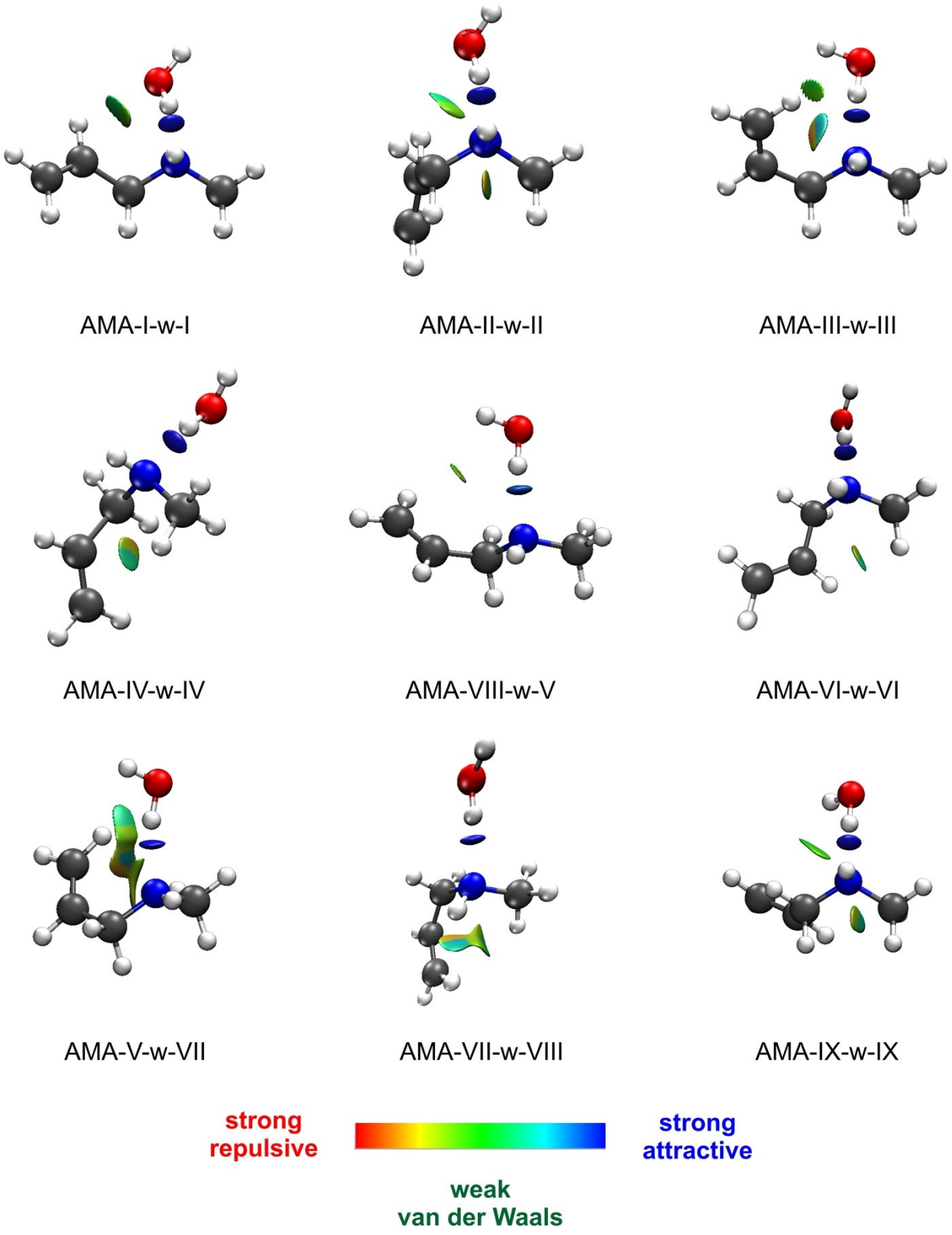

Figure S2. NCI isosurfaces (*s*=0.5 and colour scale BGR: 0.02 < ρ < +0.02) for the nine most stable conformers of AMA–w.

Table S14. Second-order perturbation energies, $E^{(2)}$, for the $n_N \rightarrow \sigma^*_{O-H}$ and $n_O \rightarrow \sigma^*_{C-H}$ charge transfer interactions in the two most stable conformers of AMA–w obtained with the NBO calculations at the B3LYP-D3(BJ)/aug-cc-pVTZ level of theory

Conformer	Charge transfer	$E^{(2)}$ (kJ mol^{-1})
AMA-I-w-I	$n_N \rightarrow \sigma^*_{O-H}$	55.5
	$n_O \rightarrow \sigma^*_{C-H}$	0.8
AMA-II-w-II	$n_N \rightarrow \sigma^*_{O-H}$	55.9
	$n_O \rightarrow \sigma^*_{C-H}$	1.3

Appendix 5: Relative energies and Cartesian coordinates for the 25 energy minima at B3LYP-D3(BJ)/aug-cc-pVTZ

Table S15. Relative energies with ZPE correction (ΔE_0) for the 25 minima obtained at the B3LYP-D3(BJ)/aug-cc-pVTZ. The conformers were labeled in an increasing order of energy from I to XXV.

Conformer	ΔE_0 (kJ mol^{-1})
I	0.0
II	1.5
III	1.9
IV	3.8
V	4.9
VI	5.6
VII	6.2
VIII	6.3
IX	8.8
X	11.4
XI	12.8
XII	13.2
XIII	16.2
XIV	17.2
XV	17.6
XVI	18.4
XVII	18.7
XVIII	19.2
XIX	19.9
XX	20.0
XXI	20.8
XXII	21.3
XXIII	21.6
XXIV	22.7
XXV	27.6

Cartesian coordinates for the 25 minima in B3LYP-D3(BJ)/aug-cc-pVTZ is given below in the format:

Atom	X	Y	Z

I – Equivalent to AMA-I-w-I in B2PLYP-D3/aug-cc-pVTZ

C	-2.744552	-0.150563	-0.202825
H	-3.438126	-0.919102	-0.515512
H	-3.134410	0.857316	-0.121679
C	-1.479077	-0.429173	0.079921
H	-1.105124	-1.443146	-0.009981
C	-0.477150	0.589389	0.525062
H	-0.079706	0.308920	1.504880
H	-0.958264	1.570678	0.638064
N	0.663261	0.639645	-0.398833
H	0.320684	0.840466	-1.330689
C	1.670587	1.623332	-0.010745
H	2.124610	1.317122	0.931910
H	1.261522	2.633644	0.119603
H	2.455003	1.660567	-0.765243
O	1.622921	-2.000125	0.075659
H	1.376545	-1.098479	-0.226606
H	2.284734	-2.315680	-0.544474

II – Equivalent to AMA-II-w-II in B2PLYP-D3/aug-cc-pVTZ

C	-2.342577	-0.795926	0.437951
H	-2.688166	-1.589627	1.086044
H	-3.060284	-0.025564	0.181315
C	-1.101714	-0.770508	-0.028222
H	-0.394544	-1.544627	0.249214
C	-0.573515	0.284586	-0.953112
H	-1.362781	1.020618	-1.160347
H	-0.295053	-0.179232	-1.902467
N	0.639316	0.920203	-0.415457
H	1.080613	1.457221	-1.150803
C	0.382522	1.782840	0.736561
H	-0.368847	2.557161	0.533558
H	1.309468	2.266476	1.041055
H	0.024888	1.178261	1.568115
O	2.221487	-1.396517	0.161562
H	1.789991	-0.529919	-0.004573
H	3.109928	-1.197895	0.467137

III - Equivalent to AMA-III-w-IIII in B2PLYP-D3/aug-cc-pVTZ

C	-2.037618	-0.652717	-0.544137
H	-3.025987	-1.082555	-0.626800
H	-1.275176	-1.052280	-1.198770
C	-1.784160	0.309436	0.333461
H	-2.582945	0.665759	0.975350
C	-0.469692	0.994899	0.545092
H	-0.112526	0.773952	1.556826
H	-0.633821	2.084648	0.522717
N	0.565263	0.580990	-0.391018
H	0.239799	0.725075	-1.339241
C	1.833751	1.276178	-0.187954
H	1.736955	2.369344	-0.214685
H	2.542289	0.967964	-0.954540
H	2.246465	0.993298	0.780388
O	1.308172	-2.120080	0.232429
H	0.986278	-1.232116	-0.031997
H	0.526706	-2.592292	0.530992

IV - Equivalent to AMA-IV-w-IV in B2PLYP-D3/aug-cc-pVTZ

C	2.725776	-0.365344	-0.534524
H	3.765304	-0.173089	-0.305800
H	2.476806	-0.534815	-1.575337
C	1.796492	-0.404323	0.410575
H	2.081078	-0.227542	1.444802
C	0.336804	-0.660683	0.168225
H	0.008007	-1.528702	0.743454
H	0.166244	-0.893429	-0.884236
N	-0.550529	0.458103	0.527104
H	-0.466035	0.654770	1.517180
C	-0.318795	1.676773	-0.248154
H	-0.549070	1.476154	-1.294894
H	0.708879	2.049497	-0.190824
H	-0.995480	2.455644	0.100355
O	-2.998574	-0.758000	-0.285893
H	-3.782684	-0.287990	0.008146
H	-2.234566	-0.259658	0.078244

V - Equivalent to AMA-VIII-w-V in B2PLYP-D3/aug-cc-pVTZ

C	-2.491644	-0.244775	0.174858
H	-3.403510	-0.469041	-0.361533
H	-2.356438	-0.723897	1.136681
C	-1.580541	0.582266	-0.317587
H	-1.747125	1.042402	-1.287988
C	-0.304514	0.949509	0.372894
H	-0.254022	0.459645	1.346794
H	-0.283766	2.035750	0.554359
N	0.864189	0.522470	-0.405681
H	0.777214	0.852245	-1.359404
C	2.129137	0.976871	0.166183
H	2.171331	2.064073	0.313468
H	2.949698	0.677567	-0.483410
H	2.276089	0.496481	1.133639
O	0.867602	-2.308015	0.024785
H	0.844176	-1.362379	-0.235609
H	0.010862	-2.657899	-0.232922

VI - Equivalent to AMA-VI-w-VI in B2PLYP-D3/aug-cc-pVTZ

C	2.824861	0.732465	-0.227034
H	3.849131	0.390033	-0.285328
H	2.625131	1.738827	-0.576189
C	1.856273	-0.034150	0.257695
H	2.095926	-1.034096	0.604067
C	0.418633	0.387919	0.348693
H	0.317862	1.423020	0.020012
H	0.074221	0.350272	1.385191
N	-0.514671	-0.433231	-0.440455
H	-0.193202	-0.466608	-1.400506
C	-0.714543	-1.789794	0.067496
H	-1.153849	-1.731557	1.063458
H	0.201631	-2.387360	0.129294
H	-1.419237	-2.313325	-0.577138
O	-2.883926	1.067289	0.078907
H	-3.564238	0.968174	-0.591595
H	-2.126452	0.520608	-0.224328

VII - Equivalent to AMA-VII-w-VIII in B2PLYP-D3/aug-cc-pVTZ

C	-2.587615	0.007084	-0.412399
H	-3.660229	-0.124099	-0.393806
H	-2.212624	0.824306	-1.015279
C	-1.783704	-0.794409	0.272406
H	-2.218590	-1.595906	0.862289
C	-0.279319	-0.745256	0.305403
H	0.106112	-1.670545	-0.133932
H	0.059199	-0.760794	1.344979
N	0.375447	0.380924	-0.352695
H	0.037955	0.473610	-1.302265
C	0.265293	1.653587	0.361408
H	0.725099	2.439498	-0.236157
H	0.820299	1.579770	1.296899
H	-0.762643	1.946759	0.594315
O	3.040354	-0.597678	-0.089620
H	2.173983	-0.183501	-0.295181
H	3.677752	-0.177006	-0.671806

VIII - Equivalent to AMA-V-w-VII in B2PLYP-D3/aug-cc-pVTZ

C	-0.969561	-1.534428	0.660486
H	-1.450559	-2.404486	1.085690
H	0.072331	-1.380576	0.904423
C	-1.642203	-0.707760	-0.128088
H	-2.686954	-0.911145	-0.341610
C	-1.112081	0.526884	-0.799834
H	-1.838234	1.340928	-0.646006
H	-1.088323	0.347845	-1.878826
N	0.229555	0.923608	-0.378964
H	0.628325	1.526278	-1.086529
C	0.266347	1.613899	0.911872
H	-0.375692	2.503748	0.934702
H	1.290170	1.911261	1.131075
H	-0.064177	0.938579	1.697584
O	2.486731	-0.849904	-0.200834
H	1.656744	-0.343220	-0.327572
H	2.368468	-1.666129	-0.693286

IX - Equivalent to AMA-IX-w-IX in B2PLYP-D3/aug-cc-pVTZ

C	-2.379692	0.203781	-0.157727
H	-3.043593	0.513224	-0.953434
H	-2.646394	0.506567	0.847706
C	-1.293144	-0.516668	-0.398591
H	-1.061370	-0.800158	-1.419451
C	-0.348472	-0.995728	0.663582
H	-0.345144	-2.097267	0.668433
H	-0.707172	-0.664244	1.637941
N	1.012803	-0.468971	0.481826
H	1.530610	-0.605083	1.340223
C	1.746341	-1.072094	-0.628768
H	1.749692	-2.169971	-0.596005
H	2.775149	-0.717458	-0.613228
H	1.308145	-0.760615	-1.575781
O	0.799030	2.378511	0.017139
H	0.879235	1.418313	0.195333
H	-0.104946	2.490731	-0.288943

X

C	-2.109507	1.010854	-0.229834
H	-3.047200	1.123298	0.297772
H	-2.163541	0.870766	-1.302987
C	-0.941819	1.070802	0.402663
H	-0.915402	1.206850	1.478961
C	0.397279	0.961250	-0.258101
H	0.916693	1.920250	-0.150901
H	0.266408	0.795374	-1.339611
N	1.220647	-0.054478	0.383003
H	0.760355	-0.954158	0.303866
C	2.564455	-0.127771	-0.168826
H	2.588410	-0.286368	-1.257909
H	3.108623	-0.943189	0.305968
H	3.100201	0.799607	0.043410
O	-1.100620	-2.167202	-0.081000
H	-1.546361	-1.319404	0.055371
H	-1.493892	-2.771041	0.555513

XI

C	-1.544524	-1.142610	-0.724129
H	-2.538958	-1.555126	-0.826931
H	-1.114950	-0.644702	-1.582597
C	-0.860430	-1.276109	0.407637
H	-1.312568	-1.802000	1.242923
C	0.527500	-0.769868	0.664315
H	1.191963	-1.636677	0.761049
H	0.541483	-0.283018	1.655649
N	1.047204	0.084522	-0.384510
H	0.485603	0.926414	-0.435150
C	2.443127	0.441388	-0.183909
H	2.647076	0.902425	0.794977
H	2.754787	1.139149	-0.959980
H	3.066534	-0.450790	-0.267281
O	-1.456569	1.976512	0.140585
H	-1.800021	1.072305	0.137156
H	-2.089729	2.499386	0.639830

XII

C	1.557063	1.146041	-0.726178
H	2.557264	1.544964	-0.826945
H	1.104271	0.693241	-1.597693
C	0.891017	1.246655	0.419719
H	1.364703	1.729094	1.268936
C	-0.501379	0.753044	0.676079
H	-1.150601	1.625752	0.814402
H	-0.509804	0.228731	1.647734
N	-1.047516	-0.053787	-0.397807
H	-0.496700	-0.900117	-0.485991
C	-2.444731	-0.401092	-0.187725
H	-2.638143	-0.897091	0.775811
H	-2.778291	-1.064308	-0.984805
H	-3.057723	0.501306	-0.226340
O	1.402642	-1.997481	0.192599
H	2.067762	-2.588329	-0.171335
H	1.760830	-1.104489	0.091024

XIII

C	-1.926257	-1.197949	0.160967
H	-2.655566	-1.286721	0.955325
H	-2.301838	-1.236018	-0.855622
C	-0.625020	-1.081283	0.410411
H	-0.287453	-1.056288	1.441528
C	0.439060	-0.950562	-0.646033
H	-0.032242	-0.953258	-1.631270
H	1.095372	-1.825727	-0.607892
N	1.282561	0.235614	-0.533172
H	0.704800	1.067415	-0.510443
C	2.211035	0.225798	0.586809
H	2.904084	-0.610739	0.475770
H	1.742655	0.143680	1.577933
H	2.795692	1.144854	0.573482
O	-1.227003	2.099475	0.012578
H	-1.575166	1.207523	0.150165
H	-1.913862	2.579452	-0.458647

XIV

C	-1.326135	-1.648345	-0.334092
H	-1.981489	-2.390032	0.102430
H	-1.386438	-1.510807	-1.407097
C	-0.480135	-0.941557	0.407922
H	-0.425817	-1.110616	1.478353
C	0.454640	0.099724	-0.123162
H	0.192978	1.069078	0.312271
H	0.322909	0.200454	-1.211641
N	1.828939	-0.197188	0.264138
H	2.094677	-1.102841	-0.101306
C	2.779148	0.817978	-0.167463
H	2.753830	1.018711	-1.248968
H	3.788889	0.510996	0.102080
H	2.565502	1.755206	0.348655
O	-2.788980	1.405790	-0.000216
H	-3.628340	1.392721	0.467988
H	-2.442693	0.506631	0.071988

XV

C	0.783399	1.680512	0.143747
H	1.188531	2.534810	-0.381790
H	0.838793	1.698189	1.225663
C	0.233207	0.659355	-0.503675
H	0.168435	0.674165	-1.586941
C	-0.335578	-0.565763	0.149220
H	-0.256657	-0.463541	1.242790
H	0.272185	-1.426866	-0.138268
N	-1.701498	-0.814668	-0.300301
H	-1.953736	-1.773798	-0.108323
C	-2.684553	0.091033	0.277971
H	-2.492284	1.107784	-0.064562
H	-2.675832	0.103447	1.378451
H	-3.681496	-0.191591	-0.057320
O	3.125398	-0.791270	0.136459
H	2.531989	-0.044444	-0.018964
H	3.954572	-0.548712	-0.284841

XVI

C	0.594103	-1.450343	-0.883379
H	1.104453	-2.311347	-1.292353
H	0.495730	-0.588602	-1.530332
C	0.094555	-1.464596	0.347545
H	0.210128	-2.363821	0.947809
C	-0.627818	-0.335758	1.045057
H	-0.049760	-0.075758	1.938811
H	-1.578327	-0.726109	1.425415
N	-0.900205	0.876290	0.305934
H	-0.046433	1.295100	-0.037585
C	-1.931961	0.781645	-0.713924
H	-2.033133	1.747131	-1.208329
H	-2.888889	0.554330	-0.238694
H	-1.757363	0.019710	-1.484396
O	2.282693	1.144187	-0.056603
H	2.140254	0.188850	-0.034421
H	2.962223	1.324551	0.598964

XVII

C	0.976317	-1.779372	0.212099
H	1.811817	-2.193443	-0.336750
H	1.027992	-1.829816	1.293067
C	-0.077660	-1.261541	-0.409112
H	-0.102986	-1.215156	-1.493185
C	-1.310137	-0.747224	0.274586
H	-1.131791	-0.707475	1.361019
H	-2.112789	-1.471619	0.107690
N	-1.754222	0.526849	-0.276642
H	-2.726686	0.673202	-0.046075
C	-0.960270	1.671636	0.156001
H	-0.874523	1.754066	1.249652
H	-1.411912	2.586589	-0.224768
H	0.048142	1.607794	-0.249160
O	2.573567	1.099379	0.001644
H	2.029134	0.301031	-0.028428
H	3.306202	0.927477	-0.596519

XVIII

C	-0.455446	-1.487021	0.916759
H	-1.261149	-2.156655	1.185725
H	0.031280	-0.935845	1.709578
C	-0.053333	-1.364400	-0.342717
H	-0.548889	-1.934574	-1.122713
C	1.075926	-0.494082	-0.821455
H	0.726850	0.064254	-1.705877
H	1.871963	-1.152750	-1.181888
N	1.625790	0.382829	0.198842
H	2.603125	0.552430	0.014476
C	0.917669	1.650209	0.345594
H	1.428019	2.264463	1.086368
H	-0.097557	1.477561	0.697733
H	0.846309	2.218993	-0.592338
O	-2.548940	0.867219	-0.250771
H	-1.976265	0.123392	-0.016679
H	-3.438915	0.581740	-0.026285

XIX

C	-0.700721	-1.625429	-0.121955
H	-1.155481	-2.417995	0.457144
H	-0.609803	-1.788807	-1.189633
C	-0.263159	-0.504721	0.441742
H	-0.359044	-0.379988	1.517382
C	0.400898	0.631463	-0.289288
H	-0.173283	1.547379	-0.134246
H	0.395172	0.427581	-1.363005
N	1.780526	0.896224	0.115272
H	1.812054	1.205868	1.077861
C	2.702196	-0.211456	-0.100288
H	2.759507	-0.423274	-1.169649
H	2.424897	-1.143583	0.408465
H	3.696933	0.081831	0.232914
O	-3.310963	0.651882	0.010100
H	-2.583301	0.017033	-0.026714
H	-3.870784	0.438032	-0.741479

XX

C	-0.700471	-1.663738	-0.127836
H	-1.086648	-2.522983	0.404536
H	-0.696190	-1.719327	-1.210124
C	-0.243433	-0.590224	0.507812
H	-0.251527	-0.573770	1.594838
C	0.333512	0.630807	-0.158114
H	-0.246627	1.510106	0.129072
H	0.244906	0.531552	-1.242470
N	1.735270	0.894892	0.162188
H	1.838438	1.108130	1.145707
C	2.659893	-0.157896	-0.236956
H	3.672076	0.130067	0.044445
H	2.633915	-0.260291	-1.323458
H	2.445353	-1.144078	0.194613
O	-3.180733	0.717644	-0.117128
H	-4.040992	0.326627	0.058854
H	-2.545678	-0.002833	-0.010899

XXI

C	0.713393	-1.860693	0.726264
H	0.154101	-2.773725	0.884734
H	1.390395	-1.559505	1.516812
C	0.597919	-1.152662	-0.392496
H	-0.087231	-1.492505	-1.164186
C	1.298186	0.150910	-0.669457
H	1.654619	0.164637	-1.701164
H	2.172783	0.251093	-0.023385
N	0.455062	1.334186	-0.465077
H	-0.410861	1.236871	-0.981290
C	0.166512	1.625506	0.930456
H	-0.518200	2.470385	0.983933
H	1.090980	1.908465	1.437634
H	-0.278222	0.791151	1.491749
O	-2.495460	-0.255201	-0.235204
H	-1.756493	-0.645148	0.247365
H	-3.183365	-0.111120	0.420810

XXII

C	0.380935	1.511138	-0.966418
H	1.127333	2.220582	-1.296330
H	-0.122482	0.941189	-1.736321
C	0.088539	1.361966	0.320710
H	0.622173	1.961225	1.053854
C	-0.959784	0.446464	0.903812
H	-1.683811	1.075413	1.433977
H	-0.489799	-0.167045	1.678561
N	-1.678592	-0.438360	0.010374
H	-2.107289	0.075443	-0.746920
C	-0.931112	-1.590287	-0.480270
H	-0.625631	-2.203235	0.368351
H	-0.027006	-1.352164	-1.051677
H	-1.584327	-2.195145	-1.108437
O	2.506486	-0.891157	0.236747
H	3.407859	-0.559759	0.195755
H	1.950801	-0.152713	-0.047013

XXIII

C	-1.136769	-1.744803	-0.117501
H	-1.604372	-2.338327	-0.891941
H	-1.390907	-1.989600	0.907415
C	-0.282302	-0.766268	-0.401199
H	-0.049619	-0.553119	-1.439593
C	0.422702	0.072494	0.629026
H	0.122289	-0.253410	1.626659
H	0.111031	1.115716	0.531264
N	1.882214	0.040488	0.544027
H	2.207857	-0.917301	0.561770
C	2.450306	0.754255	-0.591319
H	3.536531	0.677345	-0.556144
H	2.189332	1.810844	-0.514096
H	2.118749	0.398840	-1.576740
O	-2.810697	1.257061	0.003061
H	-3.693727	1.195199	-0.371489
H	-2.403296	0.395711	-0.157487

XXIV

C	-1.336751	-1.662209	0.315676
H	-2.029372	-2.337924	-0.167885
H	-1.354069	-1.633151	1.398301
C	-0.492452	-0.913000	-0.383145
H	-0.499862	-0.979340	-1.468012
C	0.483883	0.058750	0.202203
H	0.477540	-0.021568	1.291442
H	0.155054	1.083725	-0.040367
N	1.841439	-0.203825	-0.270833
H	1.846378	-0.245392	-1.282483
C	2.800360	0.791458	0.187725
H	2.517376	1.825702	-0.059666
H	3.777116	0.585634	-0.248003
H	2.898965	0.725754	1.272525
O	-2.803706	1.419738	-0.039598
H	-3.756448	1.313647	-0.109457
H	-2.446335	0.521934	-0.034363

XXV

C	0.753177	-2.008199	-0.071975
H	0.522176	-3.027415	-0.348935
H	1.791207	-1.789376	0.145087
C	-0.191504	-1.079765	-0.007679
H	-1.219237	-1.341011	-0.237547
C	0.001340	0.361102	0.394943
H	-0.557118	0.524027	1.323861
H	-0.486377	0.995540	-0.350626
N	1.356399	0.849976	0.580704
H	1.862724	0.261405	1.228307
C	2.113930	1.041085	-0.649813
H	3.123694	1.367409	-0.402178
H	1.645940	1.834532	-1.235548
H	2.183924	0.152062	-1.288287
O	-3.289196	0.477869	-0.185700
H	-4.222150	0.508072	-0.417567
H	-3.163050	1.193009	0.445240