Electronic Supplementary Information

Astro-electrochemistry of NH_3 clusters and ice: e^- trapping, stability and electron transfer.

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Geometry Optimization+Freq

```
! UKS RIJCOSX PBE0 def2-TZVPPD def2/J SmallPrint TightSCF Slowconv
! D4
! TightOpt
! defgrid3
! UNO
! UCO
! DIIS
! MOREad

%moinp "Start.gbw"

%scf Maxiter=350
     end

%geom maxiter=300
end

%geom
Calc_Hess true
NumHess true
Recalc_Hess 5
end

%geom
inhess Read
InHessName "Start.hess"
end

%base "OPT"

* xyzfile -1 2 Start.xyz

$new_job
%MaxCore 3000
! UKS PBE0 RIJCOSX def2-TZVPPD def2/J SmallPrint TightSCF Slowconv
! D4
! NumFreq
! defgrid3
! UNO
! UCO
! DIIS
! MORead

%moinp "OPT.gbw"

%scf Maxiter=150
     end

%base "FREQ"

%freq Temp 100, 200, 300
      CentralDiff true
      Increment 0.0030
      end

* xyzfile -1 2 OPT.xyz
```

TightSCF

Energy Change	TolE	.... 1.000e-08 Eh
1 e- energy change		.... 1.000e-05 Eh
DIIS Error	TolErr	.... 5.000e-07

TightOPT

Convergence Tolerances:

Energy Change	TolE	.... 1.0000e-06 Eh
Max. Gradient	TolMAXG	.... 1.0000e-04 Eh/bohr
RMS Gradient	TolRMSG	.... 3.0000e-05 Eh/bohr
Max. Displacement	TolMAXD	.... 1.0000e-03 bohr
RMS Displacement	TolRMSD	.... 6.0000e-04 bohr

defgrid3

General Integration Accuracy	IntAcc	... 4.871
Radial Grid Type	RadialGrid	... OptM3 with GC (2021)
Angular Grid (max. ang.)	AngularGrid	... 4 (Lebedev-302)
Angular grid pruning method	GridPruning	... 4 (adaptive)
Weight generation scheme	WeightScheme	... Becke
Basis function cutoff	BFCut	... 1.0000e-11
Integration weight cutoff	WCut	... 1.0000e-14

DLPNO-CCSD(T)

```
! UHF RIJCOSX DLPNO-CCSD(T) aug-cc-pVQZ aug-cc-pVQZ/C NormalPNO TightSCF SCFConvForced VerySlowConv
! UNO
! defgrid3
! DIIS
! MORead

%moinp "OPT.gbw"

%base "DLPNO"

%scf sthresh 1e-7
end

%scf Maxiter 1500
    DIISMaxEq 15
    DirectResetFreq 1
end

%scf GuessMode CMatrix
end

%mdci Maxiter 500
end

%mdci MaxDIIS 14
LShift 0.1
end

%mdci
UseFullLMP2Guess false
end

%mdci LocRandom 0
end

%mdci KCOpt KC_MO
end

%mdci TrafoType trafo_full
end

%mdci Triples 2
end

* xyzfile -1 2 OPT.xyz
```

NormalPNO
TCutMKN: 1.000e-03
TCutPAO: 1.000e-03
TCutPNO: 3.330e-07
TCutPNOSingles: 9.990e-09
TCutPAOExt: 1.000e-01
TCutPairs: 1.000e-04
TCutPre: 1.000e-06
TCutDOij: 1.000e-05
PAO overlap thresh 1.000e-08

Number of singly-occupied orbitals: 1
TCutTNO: 1.000e-09
TCutMP2Pairs: 1.000e-05
TCutDOStrong: 2.000e-03
TCutMKNStrong: 1.000e-02
TCutMKNWeak: 1.000e-01
TCutDOWeak: 4.000e-03
NTCutTNO: 1

WF Stability

```
%MaxCore 4000
! UHF RIJCOSX aug-cc-pVQZ aug-cc-pVQZ/C SmallPrint TightSCF
! defgrid3
! DIIS
! MORead

%scf Maxiter 1500
    DIISMaxEq 15
    DirectResetFreq 1
end

%scf
HFTyp UHF
STABPerform true
end

%base "Stab"

%moinp "DLPNO.gbw"

* xyzfile -1 2 OPT.xyz
```

AIMD

```
! r2scan-3c
! defgrid2
! UNO
! UCO
! DIIS
#! MOread

#%moinp "Start.gbw"

%scf Maxiter=350
     end

%base "OPT"

%md
Timestep 0.5_fs
Initvel 210_K
Thermostat NHC 210_K Timecon 10.0_fs
Dump Position Stride 1 Filename "trajectory.xyz"


Restart IfExists

Run 5000
```

Optimized Geometries XYZ Coordinates (Coord.=Å)

Water Clusters

$(H2O)_4^-$
12
Coordinates from ORCA-job OPT

O	-0.12652488318557	-0.30451734839420	3.27262498255166
O	3.25666199988059	-0.89919987238253	4.92784399353940
O	0.99158978555019	0.32410132887491	5.83798908092144
H	2.85323944624223	-1.69574934587316	4.57668777886452
H	-0.58906130292863	0.54902811524744	3.27141209120202
H	0.74248296683656	-0.07007500562759	2.89179514728388
H	2.50604849930829	-0.43361136871538	5.36676906309748
O	2.49201274227555	0.64925074851664	2.57522774417603
H	2.18141394171333	1.51914350984235	2.87888367157232
H	2.91194501345743	0.25780957398309	3.36073145207138
H	1.04558293883385	1.28686661915705	5.70781181301702
H	0.47115885201611	0.04269304537138	5.05926318170259

$(H2O)_4$
12
Coordinates from ORCA-job OPT

O	-0.17899893938445	0.29499360355025	3.42677801525066
O	3.28081779273093	-0.39925414688171	4.83501782008261
O	0.80404507766858	-0.18779004902059	5.90699872745761
H	3.62641858856045	-1.28359398398993	4.95724100002496
H	-0.74397831080144	0.99090057298511	3.09378052961707
H	0.66155803002511	0.34717339006661	2.92376348513832
H	2.43372981780195	-0.36737481502805	5.33140732649175
O	2.32869494395421	0.24863665051846	2.38533409880241
H	2.79119771490412	1.00965447295476	2.03520177489046
H	2.78598866092215	0.01441103403430	3.22299729855103
H	0.63243219792571	0.52493863541436	6.52207869077797
H	0.31464442569266	0.03304463539643	5.08644123291511

I) $(H2O)_5^-$ (VDE=8.3 kcal/mol)
15
Coordinates from ORCA-job OPT

O	3.32839614813928	0.48057800995322	3.19497765724309
O	1.09364850080621	1.99485650478074	2.37260170140345
O	-0.70871538353979	1.64219867211250	4.39803746815947
O	2.27927634783936	-0.57272863194741	5.61997456637642
O	-0.04521316204268	-1.12864915216478	4.27139193049745
H	0.79038365360752	1.32247858438795	1.73956001730777
H	-0.26736194195859	1.95945141140015	5.19131684199987
H	2.02084207162308	0.21300369847437	6.11072580472501
H	-0.40732580636910	-0.22135118136928	4.28821025431535
H	0.23815325397031	-1.25115234387199	3.34852928019291
H	3.05603717215622	0.09806678824753	4.05213901867366
H	3.03563153638361	-0.17959353991653	2.54594682822001
H	1.92256003317015	1.59656400744027	2.71216069414654
H	-0.07641199987969	1.84349873973280	3.66751015545683
H	1.44720957609396	-0.86042156725959	5.17499778128168

I) $(H2O)_5$

15

Coordinates from ORCA-job OPT

O	3.35088746867867	0.74580553128985	3.28742830244762
O	1.24630639337733	2.18560268557277	2.41602029767132
O	-0.91175401059902	1.38400649485199	3.79683697480999
O	2.43823953780600	-1.05730820357184	5.05496040602716
O	-0.23076645337757	-0.81259741929750	5.17895061940901
H	1.19241948557683	2.13579150076410	1.46204538515832
H	-1.21186689831894	2.13924488350275	4.30246889837304
H	2.76335360288026	-0.97035205333305	5.95100574433460
H	-0.51685316928565	-0.00699538464360	4.68985586768562
H	-0.76424069952323	-1.53102840600869	4.83983331492811
H	3.04642121770655	0.07702883194746	3.94338941428287
H	3.94616163616819	0.28336754026109	2.69826701875350
H	2.04177698087859	1.66776795861298	2.67502692964657
H	-0.13985249710553	1.69988897521258	3.27328236213007
H	1.45687740513746	-1.00342293516089	5.11870846434199

II) $(H2O)_5^-$

15

Coordinates from ORCA-job OPT

O	2.76942466871655	2.29971185345803	3.81767075063747
O	2.28794910293484	0.60188634054783	1.48912812835583
O	1.34722116157476	-1.61736495188313	3.17394313799563
O	1.16071430153689	-0.33190383839960	5.58862817299178
H	1.90808050565449	2.48295336309462	4.23104549998967
H	1.85613658402046	-0.12345772230003	1.96162801584898
H	1.18868331660748	-1.17189032459473	4.03310757729609
H	0.60887963194375	-0.69165090891458	6.29018084222541
H	3.12398695588378	1.59338310609938	4.36161383254771
H	0.31265338263661	2.68863604752233	6.14149658063139
O	0.37374032389528	2.28329683744106	5.25775146568010
H	2.42050909658135	1.27328640633324	2.17381715557826
H	-0.54012883657124	2.31639575677470	4.92777720159054
H	2.22879115128590	-1.98086077033550	3.26135149737221
H	0.83411865329884	0.58914880515628	5.49489014125817

II) $(H2O)_5$

15

Coordinates from ORCA-job OPT

O	3.18465909657348	2.60848555524607	3.79640565493457
O	1.10634994471182	1.13882966261350	2.43091413400982
O	1.31677496104384	-1.48552539066652	3.23643136718947
O	1.02447274228616	-0.64098695752580	5.82990555741536
H	2.46650621836325	2.53685611777709	4.44087325139930
H	1.22889637623858	0.17682532422643	2.55092082689163
H	1.23162977213858	-1.31837396922625	4.19643398689231
H	0.30709932425747	-0.99040832812342	6.35862640026270
H	3.97761734047601	2.33405684433159	4.25704866762718
H	-0.10830019827975	2.51000476090751	5.02049443362794
O	0.62772411606197	1.91157580317215	4.89253644605944
H	1.99170547407371	1.52228558902601	2.48381147328132
H	0.63386525331840	1.65349448396397	3.92966644269844
H	2.08979406316172	-2.03900337827243	3.12814970803981
H	0.80196551557460	0.29345388255001	5.65181164967025

I) $(H2O)_6^-$ (VDE=9.3 kcal/mol)

18

Coordinates from ORCA-job OPT

O	3.23827474792069	1.61250311138276	3.56899230736888
O	0.68349702952601	0.41168003674783	3.41736926819815
O	3.78018505565776	-0.70673587660556	5.13107663546416
O	1.19507972839110	-0.87188784276347	5.88634868878994
H	2.70784212544820	2.24280667698358	4.07367539682562
H	0.06572073487895	0.47736787696752	2.67484010288927
H	0.47244957678356	1.99058975859840	4.39221562637137
H	0.82779364623543	-0.55239475979065	5.04529829358060
H	3.50346176155215	0.92438150394280	4.20427632963050
H	0.24960048686476	3.46998920075415	4.77063462690158
H	1.09661169804032	-0.11908762434935	6.49763582730048
H	1.54370961990423	0.74532480821298	3.09878964570768
H	2.85552590710394	-0.83360460818444	5.45699973472372
H	3.85885028680461	-1.31473194962787	4.39463968276584
O	1.17186114539355	1.52457606942626	7.39419509268467
O	0.79822562493320	2.70213956348344	4.98076116642378
H	2.10747905424873	1.68929114382675	7.52352289727031
H	0.94775177031246	2.04973291099468	6.59358867710239

I) $(H2O)_6^-$

18

Coordinates from ORCA-job OPT

O	3.33453316914665	0.88612752414751	2.91442375923612
O	0.75352828726963	0.98074301427634	3.47970958535118
O	3.93850194604348	-0.64380618000837	5.00701949588644
O	1.39521748603367	-0.67548420755331	5.77517285971965
H	3.82762802064983	1.70479164827622	2.96986080453118
H	0.22704089897802	0.74982591775123	2.71449515546480
H	0.36501590031232	2.31959811392542	4.60715087405721
H	0.99635160652970	-0.26735010025285	4.99424354567626
H	3.67096761795259	0.31165065751582	3.64511247153038
H	-0.60246627530098	3.34621311696868	5.24252652165892
H	1.19199115123753	-0.05409755382706	6.50092263153214
H	1.70072593837875	0.98146528712901	3.18510467701317
H	3.02458353115247	-0.71178882902622	5.38381699833647
H	4.24915543978795	-1.54180779075505	4.89334584046678
O	0.75536399928075	1.35963251270909	7.53953918097707
O	0.25774598893868	2.94129118337344	5.35212617097535
H	1.46405468353593	1.74058945601357	8.05836221025634
H	0.55398061007283	2.01434622933641	6.84192721732995

II) $(H2O)_6^-$ (VDE=8.3 kcal/mol)

18

Coordinates from ORCA-job OPT

O	3.40863786405635	1.42232501425841	3.82805429021672
O	1.04695573519539	1.48940308318008	2.34906742141434
O	-0.56366179511168	2.15383145763799	4.52470406318353
O	3.07396174552973	-1.21083472268352	4.67491655457511
O	-0.89814288096366	-0.47915609579097	5.37214357619371
O	1.46278825284573	-0.54875994483903	6.85042561616064
H	0.83548647953702	0.55031047419197	2.26104435415067
H	1.67571168048895	0.39007742208919	6.93730862418870
H	3.13443244870616	1.92428638473588	4.60727654662244
H	-0.02887290016709	1.99169342201435	3.71729143533257
H	3.38003841222859	0.48829689675506	4.13007730938670
H	0.58739807796884	-0.54960478700860	6.40524761727035

H	0.08592169860989	2.45702132472258	5.17316987717035
H	1.92215899125212	1.49065808684500	2.79438100307523
H	-0.62212313691769	-0.98002349244999	4.59282118762398
H	-0.87012343585071	0.45520205008907	5.07117315392410
H	2.42537268557601	-1.51450749093401	4.02568030265929
H	2.53842007701591	-1.05076908281351	5.48235706685110

II) $(H2O)_6$

18

Coordinates from ORCA-job OPT

O	3.48694287342026	1.05498205874063	3.25355118753482
O	1.14482703272173	2.12474418172077	2.52396152630167
O	-0.98843949658128	1.83647807383961	4.11323531933447
O	3.50255125849924	-0.88487308905163	5.09643800342033
O	-0.97881508562346	-0.11638507723174	5.94220544726536
O	1.36157875098444	-1.18913141359583	6.67211163740895
H	1.03326633953407	1.87151034467168	1.60801120538166
H	1.47225898200641	-0.93769296578325	7.58874446180512
H	4.16633749709789	1.66802549185840	3.53340394309402
H	-0.19998462312765	1.92699803265525	3.53004013466481
H	3.47640251181131	0.33843779941007	3.92929892768259
H	0.50619163380780	-0.79337973740268	6.38607362132282
H	-1.17933260474565	2.71754333136631	4.43384370818627
H	2.00116130848353	1.73101246296577	2.80972000343642
H	-1.65412918300962	-0.72959083754406	5.65324855378623
H	-0.96752242430007	0.60636102279176	5.27310451881312
H	3.70215547587541	-1.76501159365586	4.77833454395678
H	2.70890975314561	-0.98057808575520	5.67181325660440

III) $(H2O)_6^-$ (VDE=7.5 kcal/mol)

18

Coordinates from ORCA-job OPT

O	1.41184228529580	-0.27213145959234	1.42798548505304
H	0.56523503993019	-0.72006374781828	1.63355041208227
H	2.09734916982052	-0.66167860015516	1.98702181021947
O	0.75077026993368	1.95930266501937	-0.11067336607511
H	1.08403656625813	1.45870214251340	0.65499699969056
H	1.11325778102453	1.43537282744982	-0.84301489407808
O	1.58203634730829	-0.49896944807445	-1.32257363886498
H	2.37057673217646	-0.83476926121478	-1.76807864284107
H	1.75920662468927	-0.61297096872715	-0.36587256653683
O	-1.82065950577960	1.26434507962125	-0.04651019626025
H	-0.88440988744743	1.59339195382351	-0.07413963092465
H	-2.37434585457180	2.03968681531430	-0.13345957998459
O	-1.10478599820335	-1.27679533307910	-1.39796895915581
H	-0.15216747230857	-1.10782518680462	-1.52321963297292
H	-1.47913327391958	-0.39866211567788	-1.25401702502662
O	-1.21118964445289	-1.19346252402693	1.42787632171733
H	-1.14968573707053	-1.50486288394338	0.50563026716252
H	-1.59469521268312	-0.31573480462762	1.30494044679572

III) $(H2O)_6$ (Prismatic)

18

Coordinates from ORCA-job OPT

O	1.46698224215191	-0.37482780420978	1.38665975663261
H	0.53193600061862	-0.70305423463334	1.50221896093689
H	1.97153281346353	-0.68100407192302	2.13966566967876
O	0.76296621671074	1.97039708551623	-0.06535748824424
H	1.09327804750425	1.42562863629834	0.66421982781905

H	1.12454872280053	1.52193962917076	-0.83876580276800
O	1.65356752920947	-0.50132419005112	-1.33946426092700
H	2.38665216548571	-0.93028115511320	-1.78071566026719
H	1.78293901105915	-0.63038293727176	-0.38037789689548
O	-1.84811403158840	1.24349117126292	-0.06558691920628
H	-0.94696300620570	1.63553763938012	-0.07790573217498
H	-2.46512914393791	1.96988554216507	-0.15098989925795
O	-1.12620176484609	-1.26860439079565	-1.34498892583251
H	-0.19565555509512	-1.08453831132076	-1.53951760296070
H	-1.53048506512491	-0.39607349159159	-1.24628319546720
O	-1.05101696646554	-1.11622626290954	1.40759674344092
H	-1.11014746532766	-1.44362927188955	0.48687375998478
H	-1.53745152041259	-0.28405843208414	1.34519227550851

Ammonia Clusters

Tetramer Neutral

16
Coordinates from ORCA-job OPT

N	-0.44860736017956	0.58994029045208	3.31065939956275
N	3.41390358165641	-0.88869508624130	4.86696275484252
N	0.58046574698600	-0.42966709703999	6.06408366597763
H	-1.13347724793384	0.03893020572840	2.80916155842495
H	4.10767824603059	-0.35315714049141	5.37295257636076
H	0.04625423979966	-1.23207656473068	6.37226662647613
H	-0.73270937266833	1.55673902825288	3.21721048016707
H	0.44573971282125	0.48518331328969	2.82187072386809
H	2.52188162360359	-0.77538539769451	5.35809425872547
H	3.68333526120680	-1.86059820270308	4.95047191061915
N	2.39233600742818	0.15971350070535	2.12108404995263
H	2.92169236689497	0.97102488447268	1.82817509666977
H	2.82956943306168	-0.19845593969937	2.97549455094945
H	2.51787155572667	-0.54039764899870	1.40114449543103
H	0.46559384852696	0.28193906576650	6.77447254583381
H	0.14083235703896	-0.08015721106854	5.20731530613869

Tetramer+e$^-$

16
Coordinates from ORCA-job OPT

N	-0.47819606584141	0.58492466413842	3.30325987473134
N	3.45851033220667	-0.90793756928774	4.86384521324361
N	0.57429430902461	-0.43363504879575	6.13078630740876
H	-1.14155414909633	0.02581432850777	2.77367630693189
H	4.14056581548183	-0.36044196159990	5.38176813740004
H	0.01431947906807	-1.22881108890940	6.42627883728932
H	-0.75015713095209	1.55592343370308	3.17583143833744
H	0.43117495499379	0.47322509391372	2.84270073637235
H	2.55954385498413	-0.78262020476672	5.34106812823981
H	3.71764642116425	-1.88355666898408	4.98259423974817
N	2.42530259680939	0.17535139718259	2.05918334280723
H	2.95999404859175	1.00523319068005	1.81688308265585
H	2.82426360139289	-0.18334077332948	2.93337644043047
H	2.62524685208565	-0.51761920629476	1.34304588178841
H	0.42948841622520	0.29726818382205	6.82204711716920
H	0.16191666386152	-0.09489776997985	5.25507491544588

Pentamer Neutral (Pentagonal)

20

Coordinates from ORCA-job OPT

N	3.67007369602507	1.00728414476839	3.39193241031469
N	1.13066998619011	1.98821890910820	1.90410530551409
N	-0.78561592605230	2.06760520528720	4.34109915511458
N	2.57468971301175	-1.44543331971092	4.96308094117101
N	-0.47440145749705	-0.88344451457634	5.26412142154216
H	3.98054421697723	1.70865573832148	4.05247203678276
H	0.82248704316055	1.28403678132422	1.24554854300626
H	-1.68333526870587	2.42511094902724	4.04131540939006
H	2.96488599173617	-1.58012409823280	5.88727981903321
H	-0.63115000692298	0.08444256326687	4.96504619467999
H	-1.05295961857224	-1.47260025301612	4.67835630515850
H	3.33959120209043	0.20404614053499	3.93621412480315
H	4.49170934454545	0.70754402394798	2.88292428791958
H	1.36010011600440	2.80999762432081	1.36002503381963
H	2.00093345576856	1.64898108502362	2.32630030018313
H	-0.43096960311398	2.71460963247034	5.03383928693615
H	-0.15441811417902	2.11009270688583	3.53473088636896
H	1.56828733417344	-1.28917585301213	5.07947438791670
H	2.68413388695156	-2.32694198631679	4.47735886511069
H	-0.84136599159133	-0.96726547942207	6.20382528523446

Pentamer Neutral (Trigonal Bipyramidal distorted)

20

Coordinates from ORCA-job OPT

N	3.13747052306530	1.95491629872913	4.12959470737517
N	0.63791208984674	0.82387715276531	2.58088306304736
N	2.07794103977831	-1.95711484973782	3.03093691181538
N	1.02634371808192	-0.36113965777177	5.54428365798210
H	2.38349261331416	2.41999674422350	4.63143595922570
H	0.86134238959149	-0.15916983963721	2.43397856275994
H	2.01203934154174	-1.60983537982667	3.98593431229105
H	0.33913168301001	-0.94870892018205	5.99811738120336
H	3.30950261504093	1.07920814912204	4.60818822037974
H	3.97112939828680	2.51868614815555	4.22843855547197
H	0.18377785688088	1.15990422241898	1.74177726422919
H	1.53447476917730	1.30022600727124	2.66267791795785
H	1.97016176016399	-2.96232805834440	3.06071885524237
H	3.01711701645254	-1.77052649261909	2.70387461019630
H	1.23040976911525	0.40140025103111	6.17743010778206
H	0.58693973651352	0.04988253520834	4.72410443175395
N	0.21532661833370	2.93124950220624	4.94860336105644
H	-0.48965775547685	2.77123433825270	5.65629513327807
H	0.03901938467027	3.85159775616648	4.56654375645084
H	0.05924543261177	2.25558409256828	4.20156323050049

Pentamer+e$^-$

20

Coordinates from ORCA-job OPT

N	3.74956805263399	1.58730251962560	3.37875573231814
N	0.68031602836917	0.90282078714299	2.12715891075018
N	0.63045908349877	2.62003246748312	5.04978875534186
N	2.42095362395534	-0.76707077100311	5.31078353847368
N	-0.90927970613656	-1.17579399094018	3.85201105987417
H	2.83146601723253	1.58357093899525	2.93922214882675
H	0.12720437114803	0.23322295148164	2.67528557080600
H	1.44032863621060	2.26643110156659	5.54917409154015
H	1.90349683339988	-0.66998596496646	6.18265020779875

H	-1.87278468577840	-1.31804177319297	3.54930344885261
H	-0.47377528186937	-2.09978287814309	3.85867210154748
H	3.68648490213958	0.88113525311285	4.10945978593748
H	3.82066826779356	2.47815212303723	3.85689497988719
H	0.01950908764914	1.43510628288098	1.57126863871709
H	1.22309516791759	0.34800971044068	1.47329977446954
H	-0.16408442794860	2.14205617702578	5.46573438394884
H	0.71370061845250	2.23042555937912	4.11269997844038
H	1.75272928435395	-0.49699999276507	4.59263969369635
H	2.54139590667377	-1.77010038086931	5.18738343876347
H	-0.96066403010367	-0.89153761377692	4.83283953026209

Hexamer Neutral (Hexagon)

24

Coordinates from ORCA-job OPT

N	3.76040571763479	1.16276656219368	3.48552860492754
N	1.09035576824120	1.68492334014856	1.98572453801074
N	-0.93279595895370	2.25497192968996	4.27283534728319
N	3.30280535348820	-1.58669360827181	4.85419404259277
N	-1.35574630875850	-0.58606200477164	5.44399767998553
N	1.24657725627951	-0.95115880972377	7.08978099711418
H	3.91483533225871	1.85316577028177	4.20951152614666
H	0.85487028899299	0.84998804382035	1.46431273047326
H	-1.70966038509958	2.79268475630255	3.91019848105989
H	4.10998495590207	-2.05069862897636	5.25130971251889
H	-1.28653270925705	0.36180470713866	5.05951961538682
H	-1.36315467836773	-1.22447267161523	4.65855523078518
H	1.09385782797947	-1.61356117876208	7.83959912743632
H	1.46001720831833	-0.06436245779316	7.52874075671220
H	3.64814336731015	0.25623212967492	3.95142607955185
H	4.61531664542109	1.11707351252451	2.94558149814291
H	1.23599622580960	2.41850542482553	1.30375586750970
H	1.99197068647823	1.51238201462291	2.44228046831082
H	-0.46256818807075	2.84676535905194	4.94605159113295
H	-0.27886089985129	2.10174181195876	3.49821653657185
H	2.63886714867118	-1.42531052878071	5.61872399889574
H	2.87237449119123	-2.25029251121116	4.22251125903563
H	-2.26139969132390	-0.66621680355193	5.88854614654595
H	0.35414054570541	-0.83664615877627	6.59806816386845

Hexamer Neutral (Octahedron distorted)

24

Coordinates from ORCA-job OPT

N	3.32260530520537	1.76094221416106	3.81200917114339
N	0.67008678598867	0.67788774066278	2.73293894913672
N	3.65217508046021	-0.87619481607352	5.50769334674299
N	0.57354870823945	-0.72064073408490	5.73232882094888
H	2.84038753577702	2.44788283665573	4.37989407799763
H	0.68237428740102	-0.32943733116605	2.63420661214813
H	4.03772477564682	-1.17691044825060	6.39378887517713
H	-0.18111446161957	-1.30648934058288	6.06272173140782
H	3.58435138041658	0.99126247801328	4.42960503183523
H	4.17346092676092	2.18919982172625	3.47319183490219
H	0.35873926935115	1.05083313097922	1.84522423188757
H	1.63910159243298	0.97930306272265	2.87378727864625
H	2.64227638623936	-1.03919289944536	5.54683557269710
H	4.03253817020446	-1.49674523871800	4.80436781935035
N	1.98220457427866	1.60837487133456	7.24063268902527
H	2.21000783982382	2.14096081973170	8.06914242207911
H	2.85050771606375	1.25360936223753	6.85742463732479

H	1.58912362758978	2.24929584893696	6.55293845341939
H	0.78156793065938	-0.03418835033745	6.45659404489408
H	0.23627076681932	-0.20743780046610	4.92497873235553
N	0.31109689277718	2.98852643429555	4.91389018171490
H	-0.53929832209624	2.96566998479802	5.46254352476274
H	0.29094447089248	3.85190954855612	4.38643622994474
H	0.25298876068698	2.22302880431324	4.24218573045669

Hexamer Neutral (Boat)

24

Coordinates from ORCA-job OPT

N	3.79427563145844	1.08803586428016	3.40058546356535
N	2.22425339299591	2.74289293167888	5.48190517719049
N	-0.72615781765874	2.18556503838058	4.41337705023060
N	3.55342155406286	-1.49601205904029	5.07348675196412
N	-1.46719142121152	-0.78817294691769	5.11076459063670
N	1.22033596064081	-0.26402054546474	6.65501956551373
H	4.76068695235822	1.31237641091429	3.20072737246401
H	2.71739360809955	2.65934955786434	6.36236295150939
H	-1.33740061129241	2.87564439619374	4.83116731970124
H	4.31801088797218	-1.75290040581450	5.68490713374094
H	-1.32902829103060	0.17579174750775	4.79860334224154
H	-1.46996848508878	-1.37969103790483	4.29002667829595
H	1.14401312810834	-0.28589038280933	7.66358856581256
H	1.28901683888046	0.71081355370022	6.38108650242517
H	3.78338272774729	0.18104388326852	3.87951251244969
H	3.33766177835716	0.96076280680427	2.50634757584997
H	2.78349135347395	2.24737562304920	4.77835472149133
H	2.24495608444628	3.72597022131429	5.24044019930364
H	0.20160680803404	2.32260223157966	4.81827079135889
H	-0.65881895662438	2.41770477696621	3.43057052874503
H	2.78242795551333	-1.17040438476322	5.66803975722326
H	3.24633946839870	-2.35010391568853	4.62555779663002
H	-2.39099573227493	-0.84942385436241	5.51847182622839
H	0.33573718463357	-0.60517951073663	6.27648582542709

Hexamer+e$^-$

24

Coordinates from ORCA-job OPT

N	2.99264203158677	1.60406780054337	3.90492411551323
N	0.99858872849592	-0.07978658857556	2.15108320871055
N	3.57896754565906	-0.83208077541708	6.11974001056986
N	0.63858695235077	-0.48758410186477	5.32830732642816
H	2.17562564784726	2.00728933033697	4.36123428695433
H	1.24046638446174	-0.25665764071632	1.18264479261189
H	3.68262146851873	-1.18610294732912	7.06318722820731
H	-0.19115550599408	-0.92346911306905	5.71328907955965
H	3.44859658912460	1.02918280227391	4.60918157063898
H	3.61116088963529	2.38236828615525	3.70792620433732
H	0.20579652912720	0.55681035584250	2.13702971165103
H	1.77098643503424	0.45327066911211	2.56127436964785
H	2.57139059650659	-0.81431949532309	5.91376613931418
H	3.99524716484001	-1.51652222755727	5.50002166007037
N	2.84774093899786	2.00828362246333	7.67859938911492
H	3.32486993466708	2.87882221111454	7.46786340290036
H	3.32134060397214	1.29361133407904	7.13110416057150
H	1.93402618230060	2.10633897705947	7.24335141436010
H	0.48820282037909	0.51895570944951	5.40005047524998
H	0.64515462912323	-0.69364328932882	4.33032775516861
N	0.12686626738327	2.80590532010582	5.29797889150224

H	-0.60428725998024	2.80813285623251	6.01226377551072
H	0.56218560036722	3.72984648246560	5.35144494046170
H	-0.37171350085842	2.79472056792628	4.40391202801597

Octamer Neutral

32

Coordinates from ORCA-job OPT

N	-0.44196323024231	0.14316518630659	3.22119283055870
N	3.15408416727991	-1.25569909107222	4.72846669100902
N	0.53619710348556	0.01335603364763	6.13101211430173
H	-0.84760592516359	-0.77061351983989	3.03606507169799
H	3.98090052615815	-1.22407297199558	5.31024893175632
H	-0.23569314772281	0.03515583054422	6.78530593517340
H	-1.07630362033604	0.83476977859749	2.84392139954954
H	0.42114451553662	0.19887312054543	2.68576013069851
H	2.35424710555139	-1.06439537008297	5.32742590941904
H	3.05692239943485	-2.21149383798070	4.39629588219911
N	2.64176114877645	0.49177758450348	2.26220899731325
H	2.52690279833167	1.46746394854709	2.50655936978870
H	2.92860299651758	-0.00695606735226	3.11250263988912
H	3.41623866073445	0.45045963746764	1.61178776641610
H	1.13040747671722	0.79911124730098	6.36411439986694
H	0.15070475829881	0.18587876451664	5.19549324049611
N	-1.30538961341781	-2.83667324731265	2.21929704420536
N	2.39704277492358	-4.36669812857636	4.03210435365794
N	-0.11560411619661	-3.06430247595538	5.21980523768457
H	-1.55359443940837	-3.81103617689256	2.33715880415317
H	3.00619716163150	-4.73301420318922	4.75264404954094
H	-0.74863560492304	-3.49477959191990	5.88092633342589
H	-1.91338644549934	-2.47355703535386	1.49608881361705
H	-0.34505418940174	-2.80618468977099	1.85715719930679
H	1.52905993442915	-4.06352638813764	4.48857264373441
H	2.16634059334600	-5.14709237613498	3.42993603168308
N	1.65144295394707	-2.51405207266466	1.48579241477658
H	1.84355653203384	-1.52170905661002	1.59578060201240
H	2.13095130643616	-2.99729541855419	2.24177952267771
H	2.07993127065089	-2.80860258318002	0.61826842985144
H	0.20298214016956	-2.19204280198290	5.63340490645740
H	-0.65847799207889	-2.82079402741802	4.39460230308109

Octamer+e$^-$

32

Coordinates from ORCA-job OPT

N	-0.53301877905903	0.10621558611356	3.18704262476033
N	3.21837056857382	-1.34970135337377	4.72094223943469
N	0.62308172170755	0.15817519238853	6.06945450378102
H	-0.89500661615047	-0.82671678147155	2.99952255548288
H	4.04086498030130	-1.36239810375148	5.31258223451735
H	-0.09629885895182	0.31951807573483	6.76715782295188
H	-1.17517655476048	0.76554733480284	2.76320780051995
H	0.34983263645747	0.19088373798081	2.68618127535989
H	2.43014751197941	-1.10278197223390	5.31691487529569
H	3.06522340312800	-2.30445036486538	4.40182039995437
N	2.62354081840736	0.61797832949723	2.39916823280454
H	2.43961421952478	1.53403322705941	2.80024903654882
H	2.92936725597222	0.01548281979826	3.17276881663142
H	3.42028479020850	0.72973684158709	1.78024890957679
H	1.27228483850829	0.93760721982646	6.13905347311543
H	0.16999324366056	0.23565802845554	5.15112478909353
N	-1.25998406253190	-3.01033681877355	2.21781586482154

N	2.27893680885239	-4.46262728217468	3.97451930793443
N	-0.12045002323670	-3.01579940824750	5.30598140165798
H	-1.36457494624460	-4.01036957441833	2.36869808872302
H	2.84234279490954	-4.97246643964125	4.64745604260402
H	-0.77793589456291	-3.39683311487092	5.97622109049753
H	-1.90486621040292	-2.76181435083124	1.47429516545338
H	-0.31207492597946	-2.86628989275750	1.84985577626255
H	1.47256446938324	-4.08468661420430	4.48603656528226
H	1.91217582151313	-5.15245986822586	3.32385963789134
N	1.68964212329950	-2.43937416181638	1.43425448753284
H	1.88185212794879	-1.45243022470096	1.59483029160003
H	2.14019809441351	-2.95783592743277	2.18611905674892
H	2.16066837549334	-2.69859336849184	0.57539118046568
H	0.18651730524985	-2.11480294085746	5.66727788068199
H	-0.64420703761259	-2.83264783010337	4.45162857201254

14mer Neutral

56

Coordinates from ORCA-job OPT

N	0.37581012794404	2.43096251351879	1.11261743101728
H	-0.44664400428120	2.40050207715938	0.52457202274297
H	0.95171093943025	3.21170819633776	0.80007583221888
H	0.89346241464957	1.57974878598932	0.93547908322164
N	1.28859560582907	3.82971211248595	6.98923631770164
N	4.00238201886580	1.56402770784530	3.23421171213126
H	2.20066293148219	3.40530222074925	7.10451143447850
H	4.89329763246588	1.17303647262036	3.52528340034948
H	1.37884549337899	4.82085846248637	7.20858698502093
H	3.32666723348500	0.81068122684645	3.25156758757763
H	0.67281633460028	3.41271296496098	7.67429015817951
H	4.10669509962993	1.85127220178361	2.25871384403302
N	2.14665953944396	5.03974357048591	0.94727154953686
N	1.60403377819183	3.75801653937756	3.82367506909456
H	3.12263078140783	5.28725915541743	0.82000404628063
H	0.88099702873687	3.34791444037957	3.23849140859161
H	1.59191286425300	5.83603491144698	0.66230922410434
H	2.39267364449343	3.11769488967117	3.76689296990722
H	1.99954004660868	4.90386392505620	1.94600311434386
H	1.27989453427075	3.73658391154828	4.79012078630157
N	1.61094614694653	6.96675738534252	7.00792345748569
N	3.25340320671014	6.35955069990975	4.32124531996820
H	2.18546933700817	6.89871092153570	6.16837169683636
H	4.15268537642752	6.04762293307497	3.96646578773269
H	0.68081240969697	7.23739877923774	6.71494485840723
H	2.59346404551889	5.61443590674822	4.07881786624847
H	1.97524739541247	7.72730117899940	7.56660528124200
H	2.99416840065636	7.17817414401383	3.78570040110563
N	7.27733674505571	1.72096769075488	1.72523429555664
N	4.34163685039243	2.77278277023281	0.32272497705300
H	7.92052312113114	2.49972261451856	1.67668207848629
H	3.36634112901578	2.97340073240643	0.13071580379699
H	6.37245124900156	2.04688900119600	1.40600745467159
H	4.78629552899294	3.68617307314830	0.39017161102687
H	7.17970197108478	1.45302277302536	2.70186732678504
H	4.71899057658313	2.30334988775229	-0.49042909503167
N	6.90442758972348	0.86864973563792	4.87842251921646
N	4.54594989319750	2.11573377574542	6.47696786119524
H	7.82166911348635	1.17827837604363	5.17466443040012
H	4.05034545881052	1.64060923564670	7.21909216715353
H	6.22760961171521	1.25085458924774	5.54482733273417

H	4.63193040559056	3.09994895851142	6.72650810234552
H	6.89981131853290	-0.13817455236873	4.98464887067893
H	3.98236587904294	2.06180560035397	5.63487690026938
N	5.48112531360472	5.68525742383354	1.15874082214467
N	5.65790829200867	4.23787883098280	3.93722372461900
H	6.40684139742292	5.68588020660755	0.74880047844424
H	4.91972651320615	3.55337857367631	3.78764358876833
H	5.19337868460781	6.65444148167197	1.20736182861756
H	6.51623212092908	3.73699164774714	3.73797128409067
H	5.57533854108592	5.34662332634441	2.11904612109091
H	5.66038635716636	4.42201484641464	4.93475131420133
N	4.61044771467038	5.30611531769202	7.02008390577412
H	5.42528361249667	5.83542864810719	7.30341402674679
H	4.17793424845281	5.80385238387955	6.24260160274897
H	3.94929599972346	5.36066041615634	7.78551562055063

14mer+e$^-$

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Coordinates from ORCA-job OPT

N	-1.30019251500768	1.31768934879499	3.08586854626167
H	-0.87818903425392	1.33190477093611	2.16524260325494
H	-1.92858405763704	2.11108376700379	3.11892675935981
H	-0.54699585512532	1.51660422444443	3.74985696351872
N	1.05108492035169	1.89951893968506	5.13806624725764
N	3.85392549672407	1.11855536199195	3.85503371970768
H	1.98891100157178	1.64805230858276	4.82009544372977
H	4.78466853943373	1.03740135850405	4.25314680043142
H	1.11681384786323	2.79416655431942	5.62646972676471
H	3.62060888006885	0.20528367292764	3.48504191944334
H	0.77884142597854	1.20713282484565	5.82444760354468
H	3.93870572256957	1.73879860952372	3.04915401864618
N	2.56709536882341	6.22272051871088	0.18621967170385
N	1.22351086319818	4.01328234622257	2.58630230383388
H	3.51370629167000	6.27901644458981	0.55887735030052
H	0.34142669059409	4.41553910038159	2.29585619970188
H	2.07018706743201	7.02605584796779	0.55186117568484
H	0.99618541267666	3.25869540990346	3.22803819643297
H	2.14693582160436	5.40824170237912	0.62153597360656
H	1.71143525114503	4.72458892033206	3.13083574662047
N	1.37974917355691	4.84022173646955	6.32802954702007
N	3.18247793455154	6.15771773430306	3.94340584759245
H	1.81283607800835	5.21566135969744	5.48540904593439
H	3.94610560702852	5.88595772620056	4.55812080579379
H	0.58648309848921	5.43792890689439	6.53089518757089
H	3.58376217242437	6.20513188910697	3.01016504985348
H	2.05109980785400	4.99877510027447	7.07381720627354
H	2.96507705905622	7.11463997816311	4.20673270164357
N	6.85397061344874	1.33324259813452	1.96363544657220
N	4.01775203458953	3.17385630765415	1.40025153843211
H	7.54819439834694	2.04434183892686	1.76926639509831
H	3.04873375511549	3.38482719982650	1.64800797161277
H	5.95040216728948	1.75970917100418	1.77673745736230
H	4.53725426471527	4.03519246954926	1.53471531248904
H	6.88594352816167	1.16218453935783	2.96589076158611
H	4.02808381442447	2.99020084230874	0.40453395418918
N	6.91818026822493	1.25798395960478	5.34662662405008
N	4.71052497147403	3.01635111628203	6.52913221985114
H	7.79496951846846	1.76568275216988	5.35163732359101
H	4.28671732373186	3.01088168510144	7.44966536910987
H	6.25179027427399	1.82329171682408	5.88649865756483

H	4.94177807226709	3.98722040386706	6.33135282160621
H	7.07738686694251	0.40151951442696	5.86303857563522
H	3.98695771873258	2.73693918722227	5.87365481379719
N	5.56967991958619	6.45263078183993	1.55902929602270
N	6.72266424957809	4.55087321287404	3.69493921266582
H	6.15088136394565	6.52645569596089	0.73199465313044
H	6.43189156353964	3.58021159309969	3.64797965588954
H	5.57788440208335	7.36604650583782	2.00178580258833
H	7.72528902023434	4.54824888601064	3.84365602227978
H	6.04469377819927	5.81852444610025	2.21150862128904
H	6.31259564213824	4.95355052271336	4.53680596324958
N	5.63101246313996	6.24162529942331	6.28625231262290
H	5.82210169809597	7.10810266253389	5.77780514079376
H	4.85663260834966	6.46707541236733	6.91601069055803
H	6.44006087756937	6.09129684845556	6.89069522703874

23mer Neutral (amorphous)

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Coordinates from ORCA-job OPT

N	9.83010468028778	2.43660345167386	4.27140298564498
H	9.49575231025002	3.09986645535479	4.96878870530150
H	10.54478669576041	1.87894853377598	4.72188610257427
H	10.29338614131698	2.98252871600148	3.54112318494433
N	4.65729843461374	7.84305152736368	3.01767076922144
N	8.28394784689664	5.39945116024056	0.23171636860375
H	4.50189469917164	8.60998329477221	2.37709542837834
H	8.80877458546948	4.56705202786256	-0.02688135525998
H	5.65537325192165	7.65905574426209	3.04083144405124
H	7.96393226916763	5.82967009246014	-0.62602793597828
H	4.23700009522475	7.01228898945931	2.61136256856514
H	8.93944165990303	6.04208766303080	0.67065272374130
N	5.67930204621845	-0.86557875562330	3.22544549285467
N	9.84198915726336	7.24396220978183	2.42356175303185
H	5.73507173232375	-1.37060756235423	2.34889819720031
H	10.26752269004121	6.97344083417053	3.31302419324163
H	6.31362046249044	-1.33522882453553	3.86053029265997
H	10.17883361288755	8.16811056072603	2.18801608528510
H	4.73102956326166	-1.01762684418978	3.59077279637488
H	8.84692330353370	7.31682920636142	2.61039916061645
N	3.93240030656568	4.88980983875588	1.69678184870242
N	4.23124785959485	4.65272932650379	4.93657683919784
H	4.70383525537375	5.08442725828541	1.06923751044110
H	4.05190569074042	4.90788706036163	3.96769470328856
H	3.89152457381074	3.87273804676129	1.80152963082547
H	4.54051944344486	5.48938156697879	5.42196139981523
H	3.09065086236330	5.16303389851896	1.20464936484643
H	5.00105070650123	3.99188193552495	4.92637061956076
N	10.89042260256585	5.76739319500317	4.95312303833732
N	6.52815763449225	2.21911968459626	4.22896477708059
H	11.27774401592443	5.03634389089567	4.36703431427139
H	6.20364252534464	1.27951874550761	4.00968530295188
H	11.58987638723965	6.00785968306390	5.64276759981114
H	6.29707559926540	2.77347718097991	3.41152145197112
H	10.10508060703846	5.35051521405146	5.44826843603594
H	7.54535386467677	2.17163529035607	4.24063598468796
N	6.48108655484080	2.63928197345659	0.42936261727776
N	2.23302224136736	2.14487349222904	4.87420238657374
H	7.09650701262751	1.99415555252864	0.91204423075039
H	2.49772264354562	1.46662887692021	5.58043931346693

H	6.83522317369154	3.57333328769204	0.60688412041034
H	2.78110942652154	2.98741983348917	5.04064442897272
H	5.56599866582232	2.55820314979437	0.85676238898974
H	1.26356288359054	2.38199534236238	5.03881934049583
N	7.14199668259093	7.14648563341140	6.08991256429317
N	7.17113850663220	5.76080245170093	3.17212645604031
H	7.29018421344315	7.17868445237057	5.08634901988375
H	7.84036235512221	5.26872714338607	3.75218203841792
H	6.14613999630113	7.30787762884264	6.24615165728595
H	6.25658424059470	5.39769569446438	3.41006985637948
H	7.64826275423090	7.92279730707685	6.49462710747237
H	7.36725603849065	5.50593773896313	2.20510625581972
N	8.62898167546600	0.50199916789500	2.07217780117559
H	7.70323697511805	0.19421219123931	2.35138543162503
H	9.20646221683728	-0.32632546390256	2.00501296507633
H	8.99240890379702	1.06918334130320	2.83962308716869
N	11.06388270695688	4.19512387071160	1.94016948483705
H	12.04148434356142	4.23164245121911	1.68059337620748
H	10.58139707688636	3.70880856755156	1.18660479126801
H	10.72629788338913	5.15549044179724	1.93947386436337
N	3.18957827371126	-0.17843948724002	7.29944877009549
H	3.67454963120240	-1.00897304490790	7.61604198021340
H	3.86340319205529	0.59447319438391	7.33154854791829
H	2.47543759204153	0.01416247762991	7.99047237029259
N	9.48951892715723	2.40904600796341	-0.35233762673798
N	8.23861087509582	4.32616809702697	6.33438220934285
H	9.31085708799943	1.72299677207988	0.38272990512787
H	8.47190583837812	4.04474243646308	7.27834716440089
H	8.63668276212455	2.42839056248866	-0.90167926979135
H	7.84212698532254	5.27273782952863	6.38939904643607
H	10.21794787485370	2.03828657415831	-0.94878058254400
H	7.49360971132912	3.71142697131212	6.02334428725377
N	4.03857500695530	7.73177841925139	6.11491050216998
N	3.72209639330868	1.77098944523531	2.14191953213787
H	4.08372263698771	7.93024754279455	5.11441773568779
H	3.15547062304057	1.38671902161617	1.39635826502242
H	3.14555331739111	7.28183592879748	6.30524721017310
H	4.42182119704327	1.07006160367627	2.36447685000016
H	4.03140961178973	8.62071809324342	6.59807762731694
H	3.12631724601778	1.85396327713959	2.96871691721381
N	5.10672417172606	2.22729286133476	7.13351440864976
N	1.55750953276156	5.69389037761382	6.32926854314326
H	5.80956816977728	2.33547847696882	7.85331916606386
H	2.28609082599871	5.11881034954937	5.91167030742620
H	5.59407667104021	2.18787498197144	6.23771247491353
H	1.20049115990148	5.20279458366888	7.13796514238792
H	4.56916742744979	3.08596105445166	7.12208503916417
H	0.80006903699889	5.76365870671212	5.66270476095472
N	2.80725596490221	-1.09314666570815	4.28683347278911
H	2.36008292691088	-0.29724169995922	3.84721707095717
H	2.20582982790325	-1.89419718565395	4.14658068468251
H	2.82511137833898	-0.88639803434114	5.28641065649932

23mer+e$^-$ (amorphous)

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Coordinates from ORCA-job OPT

N	9.52053657312351	2.30018373991091	4.43870355337768
H	9.26808650761360	3.00188905602793	5.12830571322874
H	9.89602332166038	1.50890642238445	4.94898617077740
H	10.25440770445358	2.70145421288250	3.85727801255848

N	4.68584515596661	7.97303247468450	2.55021749245873
N	8.60768512823396	5.34242937487793	0.29577023916036
H	4.61473017579284	8.60807331852652	1.76571285080699
H	9.07734180399993	4.45293101858320	0.13843982091704
H	5.67433738998617	7.79272169229848	2.69974482814559
H	8.42067002772238	5.74986871814685	-0.61091271680333
H	4.29240097668942	7.08192403563514	2.25320967536197
H	9.26158881067814	5.95270432921601	0.78032812897080
N	5.32801778674549	-0.64477720916693	3.17347989369103
N	10.04675397259928	7.17721559914039	2.60818164050369
H	5.54231631118989	-1.35106587736824	2.47681798669754
H	10.36152254131358	6.86050398311475	3.52939713251491
H	5.92767062564986	-0.85355189874595	3.97033471838586
H	10.46096411092852	8.08496329568634	2.44049680715286
H	4.36662856737766	-0.82373237709560	3.48019736181769
H	9.04418336899700	7.31399094954678	2.70063783622005
N	3.81584720937847	5.00854972926839	1.54470086202079
N	4.33361530171288	4.94174999052451	4.87274313403191
H	4.51165666309253	5.07458521996067	0.81070456968803
H	4.08807342292563	5.25594170400549	3.93883094361444
H	3.75838290134303	4.01734219121708	1.80536429427828
H	4.88737955876574	5.66918447038795	5.31274813774787
H	2.92793029536703	5.24078235557696	1.11562287957277
H	4.94167772769612	4.13319794431523	4.75598279925397
N	10.68945148661214	5.61142013986994	5.20402761199753
N	6.33955167359222	2.51898931555054	4.00259721714561
H	11.05462477341117	4.84877835707211	4.64207368690648
H	5.93579648830897	1.59739744415095	3.85476669877699
H	11.30719599980960	5.71536285873598	5.99873427957366
H	6.20810278064671	3.01205417581086	3.12544179999727
H	9.78855244807086	5.29426899905437	5.56769110369363
H	7.34495019950833	2.36919238535155	4.08716174362098
N	6.42791268835587	2.75932600822905	0.24657042266311
N	2.67562509630989	2.22568881026740	5.47376868675474
H	6.95099925785375	2.04296454978320	0.73913541589886
H	3.39521547607182	1.72818165888264	5.99487520747575
H	6.84176828351745	3.64820355643655	0.51000242770595
H	2.98280959523627	3.19536282107990	5.43256363635997
H	5.48592512346986	2.73088187169271	0.61929661691102
H	1.84083632535403	2.20610289805279	6.04671105100913
N	6.57796875616347	7.42969772071783	5.90739144196112
N	7.19109102610767	5.92985295927716	3.06434049047817
H	6.89134734471784	7.39279403157900	4.94238135482644
H	7.78404822416899	5.44306690605556	3.72795443749238
H	5.67769028081168	7.91478525514363	5.92082726264228
H	6.25586208518969	5.57162117658687	3.21824774761818
H	7.24295342053803	7.99996012148651	6.41347200359527
H	7.47954240084865	5.62963651395779	2.13394463345395
N	8.35824006629722	0.46807682241057	2.07930659966239
H	7.37615816261868	0.27390084132693	2.25657679647282
H	8.83064809096025	-0.42591082681209	2.15972476346721
H	8.67165146936424	1.02693693435517	2.87434448485968
N	11.21825287232245	4.02132010548809	2.25746460859797
H	12.18921831070147	4.02305743441485	1.97126519003996
H	10.70383579893291	3.52046119444694	1.53599147917012
H	10.90368735022442	4.98837781189215	2.22440964212144
N	4.04442462602709	-1.51344813478131	7.00737412015944
H	4.84662672747223	-2.05168305397871	6.69000383755185
H	4.37190644535449	-0.54678953720187	7.04649242687077
H	3.87125745569214	-1.79818035871977	7.96512460075971

N	9.57983813498446	2.28227769033642	-0.14998074086955
N	7.80824472387077	4.55082448373548	6.22509436514200
H	9.23648480825850	1.62853651267123	0.56167247671423
H	7.89876561372920	4.16510299532914	7.15827315057271
H	8.82253476924278	2.36230000483783	-0.82070761628539
H	7.31102297361216	5.44005933064613	6.30784357745752
H	10.34665272737302	1.82703978533383	-0.62933655077477
H	7.19164581508387	3.91695144906968	5.72324893602662
N	3.69307602728438	8.55713076191742	5.53999680454167
N	3.49036204162676	2.00444507235842	2.31431686295149
H	3.84141678734601	8.43588431195420	4.53790864105529
H	2.74028483179463	1.62552203039070	1.74802049610521
H	2.99142222204884	7.88394526942991	5.84227459936479
H	4.18579058264002	1.26284600548562	2.37679501312915
H	3.30491878498410	9.48058907645562	5.67863728457349
H	3.11415191972832	2.08922884061009	3.25953598212282
N	5.51409354109057	1.35948441097234	6.96195399873716
N	1.91529597195806	6.01480628152486	6.51258726904487
H	6.32624132479187	0.74990175850870	7.05809848168152
H	2.63434190987248	5.51041340415197	5.98855988737205
H	5.70900234947000	1.93678392627024	6.14556296449226
H	2.04082864611094	5.76733845168529	7.48619179362961
H	5.53050112576525	1.98091196038903	7.76620876053971
H	1.01868440170978	5.64090593763286	6.22892101482946
N	2.44959569647119	-0.87716348814562	4.38223198316147
H	2.30363850085083	0.12184198300463	4.49668578760289
H	1.55042737722944	-1.29954686418556	4.19131883449053
H	2.77668806130425	-1.22828566109126	5.28412518463397

14mer unit cell constrained

56

NH_3 & P 2_1 3-T^4 #198 & cP16 & ND_3 data from Wyckoff Vol II. pp. 117-9

N	1.10474700	1.10474700	1.10474700
H	1.90403400	1.33995120	0.55695540
H	0.55695540	1.90403400	1.33995120
H	1.33995120	0.55695540	1.90403400
N	1.10474700	1.10474700	6.19574700
N	3.65024700	1.44075300	3.98625300
H	1.90403400	1.33995120	5.64795540
H	4.44953400	1.20554880	4.53404460
H	0.55695540	1.90403400	6.43095120
H	3.10245540	0.64146600	3.75104880
H	1.33995120	0.55695540	6.99503400
H	3.88545120	1.98854460	3.18696600
N	1.10474700	6.19574700	1.10474700
N	1.44075300	3.98625300	3.65024700
H	1.90403400	6.43095120	0.55695540
H	0.64146600	3.75104880	3.10245540
H	0.55695540	6.99503400	1.33995120
H	1.98854460	3.18696600	3.88545120
H	1.33995120	5.64795540	1.90403400
H	1.20554880	4.53404460	4.44953400
N	1.10474700	6.19574700	6.19574700
N	3.65024700	6.53175300	3.98625300
H	1.90403400	6.43095120	5.64795540
H	4.44953400	6.29654880	4.53404460
H	0.55695540	6.99503400	6.43095120
H	3.10245540	5.73246600	3.75104880
H	1.33995120	5.64795540	6.99503400
H	3.88545120	7.07954460	3.18696600

N 6.19574700 1.10474700 1.10474700
N 3.98625300 3.65024700 1.44075300
H 6.99503400 1.33995120 0.55695540
H 3.18696600 3.88545120 1.98854460
H 5.64795540 1.90403400 1.33995120
H 4.53404460 4.44953400 1.20554880
H 6.43095120 0.55695540 1.90403400
H 3.75104880 3.10245540 0.64146600
N 6.19574700 1.10474700 6.19574700
N 3.98625300 3.65024700 6.53175300
H 6.99503400 1.33995120 5.64795540
H 3.18696600 3.88545120 7.07954460
H 5.64795540 1.90403400 6.43095120
H 4.53404460 4.44953400 6.29654880
H 6.43095120 0.55695540 6.99503400
H 3.75104880 3.10245540 5.73246600
N 6.19574700 6.19574700 1.10474700
N 6.53175300 3.98625300 3.65024700
H 6.99503400 6.43095120 0.55695540
H 5.73246600 3.75104880 3.10245540
H 5.64795540 6.99503400 1.33995120
H 7.07954460 3.18696600 3.88545120
H 6.43095120 5.64795540 1.90403400
H 6.29654880 4.53404460 4.44953400
N 6.19574700 6.19574700 6.19574700
H 6.99503400 6.43095120 5.64795540
H 5.64795540 6.99503400 6.43095120
H 6.43095120 5.64795540 6.99503400

23mer 2 unit cell constrained

92
NH_3 & P 2_1 3-T^4 #198 & cP16 & ND_3 data from Wyckoff Vol II. pp. 117-9
N 1.10475 1.10475 1.10475
H 1.90403 1.33995 0.55696
H 0.55696 1.90403 1.33995
H 1.33995 0.55696 1.90403
N 1.10475 1.10475 6.19575
N 3.65025 1.44075 3.98625
H 1.90403 1.33995 5.64796
H 4.44953 1.20555 4.53404
H 0.55696 1.90403 6.43095
H 3.10246 0.64147 3.75105
H 1.33995 0.55696 6.99503
H 3.88545 1.98854 3.18697
N 1.10475 6.19575 1.10475
N 1.44075 3.98625 3.65025
H 1.90403 6.43095 0.55696
H 0.64147 3.75105 3.10246
H 0.55696 6.99503 1.33995
H 1.98854 3.18697 3.88545
H 1.33995 5.64796 1.90403
H 1.20555 4.53404 4.44953
N 1.10475 6.19575 6.19575
N 3.65025 6.53175 3.98625
H 1.90403 6.43095 5.64796
H 4.44953 6.29655 4.53404
H 0.55696 6.99503 6.43095
H 3.10246 5.73247 3.75105
H 1.33995 5.64796 6.99503
H 3.88545 7.07954 3.18697

N	6.19575	1.10475	1.10475
N	3.98625	3.65025	1.44075
H	6.99503	1.33995	0.55696
H	3.18697	3.88545	1.98854
H	5.64796	1.90403	1.33995
H	4.53404	4.44953	1.20555
H	6.43095	0.55696	1.90403
H	3.75105	3.10246	0.64147
N	6.19575	1.10475	6.19575
N	3.98625	3.65025	6.53175
H	6.99503	1.33995	5.64796
H	3.18697	3.88545	7.07954
H	5.64796	1.90403	6.43095
H	4.53404	4.44953	6.29655
H	6.43095	0.55696	6.99503
H	3.75105	3.10246	5.73247
N	6.19575	6.19575	1.10475
N	6.53175	3.98625	3.65025
H	6.99503	6.43095	0.55696
H	5.73247	3.75105	3.10246
H	5.64796	6.99503	1.33995
H	7.07954	3.18697	3.88545
H	6.43095	5.64796	1.90403
H	6.29655	4.53404	4.44953
N	6.19575	6.19575	6.19575
H	6.99503	6.43095	5.64796
H	5.64796	6.99503	6.43095
H	6.43095	5.64796	6.99503
N	8.69440	1.26639	3.95734
H	9.49369	1.03119	4.50513
H	8.14661	0.46710	3.72213
H	8.92961	1.81418	3.15805
N	8.69440	6.35739	3.95734
H	9.49369	6.12219	4.50513
H	8.14661	5.55810	3.72213
H	8.92961	6.90518	3.15805
N	11.23990	0.93038	1.07583
N	9.03041	3.47588	1.41184
H	12.03919	1.16559	0.52804
H	8.23112	3.71109	1.95963
H	10.69211	1.72967	1.31104
H	9.57820	4.27517	1.17663
H	11.47511	0.38259	1.87512
H	8.79520	2.92809	0.61255
N	11.23990	0.93038	6.16683
N	9.03041	3.47588	6.50284
H	12.03919	1.16559	5.61904
H	8.23112	3.71109	7.05063
H	10.69211	1.72967	6.40204
H	9.57820	4.27517	6.26763
H	11.47511	0.38259	6.96612
H	8.79520	2.92809	5.70355
N	11.23990	6.02138	1.07583
N	11.57591	3.81189	3.62133
H	12.03919	6.25659	0.52804
H	10.77662	3.57669	3.07354
H	10.69211	6.82067	1.31104
H	12.12370	3.01260	3.85654
H	11.47511	5.47359	1.87512
H	11.34070	4.35968	4.42062

N 11.23990 6.02138 6.16683
H 12.03919 6.25659 5.61904
H 10.69211 6.82067 6.40204
H 11.47511 5.47359 6.96612

38mer 4 unit cell constrained

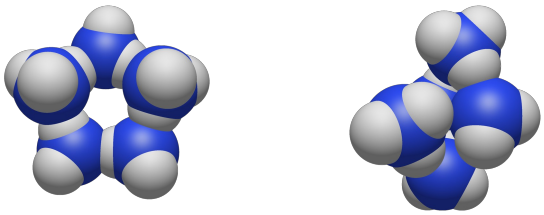
152
NH_3 & P 2_1 3-T^4 #198 & cP16 & ND_3 data from Wyckoff Vol II. pp. 117-9
N 1.10475 1.10475 1.10475
H 1.90403 1.33995 0.55696
H 0.55696 1.90403 1.33995
H 1.33995 0.55696 1.90403
N 1.10475 1.10475 6.19575
N 3.65025 1.44075 3.98625
H 1.90403 1.33995 5.64796
H 4.44953 1.20555 4.53404
H 0.55696 1.90403 6.43095
H 3.10246 0.64147 3.75105
H 1.33995 0.55696 6.99503
H 3.88545 1.98854 3.18697
N 1.10475 6.19575 1.10475
N 1.44075 3.98625 3.65025
H 1.90403 6.43095 0.55696
H 0.64147 3.75105 3.10246
H 0.55696 6.99503 1.33995
H 1.98854 3.18697 3.88545
H 1.33995 5.64796 1.90403
H 1.20555 4.53404 4.44953
N 1.10475 6.19575 6.19575
N 3.65025 6.53175 3.98625
H 1.90403 6.43095 5.64796
H 4.44953 6.29655 4.53404
H 0.55696 6.99503 6.43095
H 3.10246 5.73247 3.75105
H 1.33995 5.64796 6.99503
H 3.88545 7.07954 3.18697
N 6.19575 1.10475 1.10475
N 3.98625 3.65025 1.44075
H 6.99503 1.33995 0.55696
H 3.18697 3.88545 1.98854
H 5.64796 1.90403 1.33995
H 4.53404 4.44953 1.20555
H 6.43095 0.55696 1.90403
H 3.75105 3.10246 0.64147
N 6.19575 1.10475 6.19575
N 3.98625 3.65025 6.53175
H 6.99503 1.33995 5.64796
H 3.18697 3.88545 7.07954
H 5.64796 1.90403 6.43095
H 4.53404 4.44953 6.29655
H 6.43095 0.55696 6.99503
H 3.75105 3.10246 5.73247
N 6.19575 6.19575 1.10475
N 6.53175 3.98625 3.65025
H 6.99503 6.43095 0.55696
H 5.73247 3.75105 3.10246
H 5.64796 6.99503 1.33995
H 7.07954 3.18697 3.88545
H 6.43095 5.64796 1.90403
H 6.29655 4.53404 4.44953

N	6.19575	6.19575	6.19575
H	6.99503	6.43095	5.64796
H	5.64796	6.99503	6.43095
H	6.43095	5.64796	6.99503
N	8.69440	1.26639	3.95734
H	9.49369	1.03119	4.50513
H	8.14661	0.46710	3.72213
H	8.92961	1.81418	3.15805
N	8.69440	6.35739	3.95734
H	9.49369	6.12219	4.50513
H	8.14661	5.55810	3.72213
H	8.92961	6.90518	3.15805
N	11.23990	0.93038	1.07583
N	9.03041	3.47588	1.41184
H	12.03919	1.16559	0.52804
H	8.23112	3.71109	1.95963
H	10.69211	1.72967	1.31104
H	9.57820	4.27517	1.17663
H	11.47511	0.38259	1.87512
H	8.79520	2.92809	0.61255
N	11.23990	0.93038	6.16683
N	9.03041	3.47588	6.50284
H	12.03919	1.16559	5.61904
H	8.23112	3.71109	7.05063
H	10.69211	1.72967	6.40204
H	9.57820	4.27517	6.26763
H	11.47511	0.38259	6.96612
H	8.79520	2.92809	5.70355
N	11.23990	6.02138	1.07583
N	11.57591	3.81189	3.62133
H	12.03919	6.25659	0.52804
H	10.77662	3.57669	3.07354
H	10.69211	6.82067	1.31104
H	12.12370	3.01260	3.85654
H	11.47511	5.47359	1.87512
H	11.34070	4.35968	4.42062
N	11.23990	6.02138	6.16683
H	12.03919	6.25659	5.61904
H	10.69211	6.82067	6.40204
H	11.47511	5.47359	6.96612
N	0.96111	-3.64356	1.07901
H	1.76040	-3.40836	0.53121
H	0.41332	-2.84428	1.31421
H	1.19632	-4.19136	1.87829
N	0.96111	-3.64356	6.17001
N	3.50661	-3.30756	3.96051
H	1.76040	-3.40836	5.62221
H	4.30590	-3.54276	4.50830
H	0.41332	-2.84428	6.40521
H	2.95882	-4.10685	3.72531
H	1.19632	-4.19136	6.96929
H	3.74182	-2.75977	3.16123
N	1.29712	-0.76206	3.62451
H	0.49783	-0.99726	3.07671
H	1.84491	-1.56135	3.85971
H	1.06191	-0.21427	4.42379
N	6.05211	-3.64356	1.07901
N	3.84262	-1.09806	1.41501
H	6.85140	-3.40836	0.53121
H	3.04333	-0.86286	1.96280

H	5.50432	-2.84428	1.31421
H	4.39041	-0.29878	1.17981
H	6.28732	-4.19136	1.87829
H	3.60741	-1.64586	0.61573
N	6.05211	-3.64356	6.17001
N	3.84262	-1.09806	6.50601
H	6.85140	-3.40836	5.62221
H	3.04333	-0.86286	7.05380
H	5.50432	-2.84428	6.40521
H	4.39041	-0.29878	6.27081
H	6.28732	-4.19136	6.96929
H	3.60741	-1.64586	5.70673
N	6.38812	-0.76206	3.62451
H	5.58883	-0.99726	3.07671
H	6.93591	-1.56135	3.85971
H	6.15291	-0.21427	4.42379
N	8.55077	-3.48192	3.93160
H	9.35005	-3.71713	4.47939
H	8.00297	-4.28121	3.69639
H	8.78597	-2.93413	3.13231
N	11.09627	-3.81793	1.05009
N	8.88677	-1.27243	1.38610
H	11.89555	-3.58272	0.50230
H	8.08748	-1.03722	1.93389
H	10.54847	-3.01864	1.28530
H	9.43456	-0.47314	1.15089
H	11.33147	-4.36572	1.84938
H	8.65157	-1.82022	0.58681
N	11.09627	-3.81793	6.14109
N	8.88677	-1.27243	6.47710
H	11.89555	-3.58272	5.59330
H	8.08748	-1.03722	7.02489
H	10.54847	-3.01864	6.37630
H	9.43456	-0.47314	6.24189
H	11.33147	-4.36572	6.94038
H	8.65157	-1.82022	5.67781
N	11.43227	-0.93642	3.59559
H	10.63298	-1.17163	3.04780
H	11.98006	-1.73571	3.83080
H	11.19707	-0.38863	4.39488

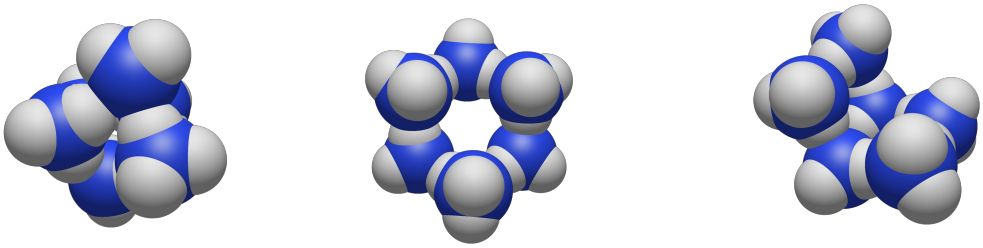
ΔG NH_3 cluster conformers

5 (NH_3)



ΔG=0.0 kcal/mol ΔG=0.4 kcal/mol

6 (NH_3)



ΔG=0.0 kcal/mol ΔG=0.6 kcal/mol ΔG=1.3 kcal/mol

Figure S1. Relative stability of the analyzed NH_3 clusters. The lower in energy were used as starting conformers for the radical-anion forms.

Optimized Geometries Ammonia Clusters+ H_2O, CH_3OH, HCN, CO (Coord.=Å)

4mer+H2O neutral (no e- transfer)

19
Coordinates from ORCA-job OPT

N	3.54001240950509	1.13232557981539	3.66178555192298
N	1.18916747346608	1.95811445771659	1.91946080085890
O	-0.78519459377623	1.71156844815050	3.85892141595487
N	2.46282167458995	-1.61436070832881	4.58953315400352
N	-0.30733542828640	-0.66977346416953	5.63944799222708
H	3.53840142156522	1.75386349942096	4.46087460213474
H	1.07744801937215	1.31683867194037	1.14473472470469
H	-1.58828135375740	2.12717426029491	3.54809430957272
H	2.95255395210741	-2.12261567017921	5.31495585659223
H	-0.52360531445585	0.13434224478528	5.04922456800144
H	-1.08383729349803	-1.31406877058931	5.56192759663729
H	3.25117536785716	0.20768475938985	3.99857171404713
H	4.50117409757545	1.05761809472074	3.35436572113122
H	1.34687507753525	2.87527180071138	1.52225869616524
H	2.04238216522661	1.68838294226706	2.42599853390935
H	-0.11857796775867	1.83543208223276	3.13786971432480
H	1.53762478749262	-1.37224469432267	4.95848100034030
H	2.32047961164171	-2.26596382895274	3.82815023384313
H	-0.30136410640226	-0.34054970490357	6.59646381362784

4mer+H2O e- (no e- transfer)

19
Coordinates from ORCA-job OPT

N	3.08403254598391	1.55142481292962	4.28183450358638
N	1.59611178003225	1.14024743068023	1.51117990178498
O	0.04783936249642	1.41660568114428	3.91613596451872
N	1.95918085994295	-1.47585373124649	3.83526897953427
N	0.06318481258334	-0.51268435300648	6.19092638426008
H	2.11560451652366	1.82780755897627	4.43205937908085
H	1.95126544133588	0.52413718035835	0.78869828903936
H	-0.77691882244573	1.91507532721624	3.85730103451950
H	1.90863125131499	-2.43690512293962	3.52070952706321
H	-0.06170580776369	0.17283093195202	5.44137310581856
H	-0.86587931541402	-0.72808771781072	6.53509351388899
H	3.08763285041834	0.53510835909524	4.33202325926500
H	3.62474467542159	1.89646145258214	5.06449564225475
H	1.23003995431397	1.96858143902624	1.05163053603998
H	2.37872528085758	1.42901828855970	2.09720857088967
H	0.29440994376169	1.20876498271733	2.99682128141868
H	1.36288245888103	-1.39891894418737	4.65995057201962
H	1.51280254389566	-0.91168653112888	3.11843186482789
H	0.53933566785974	-0.02288704491828	6.93997769018804

4mer+H2O neutral (e- transfer)

19
Coordinates from ORCA-job OPT

N	-0.40246782513619	-0.12516546656132	3.31298756498980
N	3.20966898996333	-1.92790501967178	4.49947320338064
N	1.23007870753061	-0.07571425482995	5.99269047587090
H	-0.66124233036804	-1.04380738003829	2.97649718249779
H	4.06410915117923	-2.12148805009970	5.00522414273669
H	0.75812273107258	-0.11106672830232	6.88633475865051
H	-1.08232580445542	0.52300295166245	2.93755264048499
H	0.50677896043389	0.10426764463797	2.90091161272982

H	2.57137773057332	-1.44753188042171	5.14026203387499
H	2.79613000353365	-2.82397254559582	4.27577929409346
N	2.54678701704279	0.50337732184679	2.62712140151024
O	2.83491876467942	2.68137859923957	5.11151445337177
H	2.92808745845397	-0.32819169371221	3.08128343520826
H	3.06420093701892	0.65551734817988	1.77181465194702
H	1.70026973658861	0.82034603494598	5.93274354479422
H	0.51661585802205	-0.07969836453009	5.26189528347848
H	3.70705992938752	2.91775135732605	5.43067965365300
H	2.33725939455042	3.50019139048742	5.09855773406462
H	2.74085058992885	1.28402873543705	3.24404693266184

4mer+H2O e- (e- transfer)

19

Coordinates from ORCA-job OPT

N	-0.53738407410563	0.56824856454919	3.29284975800754
N	3.75383552713024	-1.58707087259686	4.86905830845409
N	0.96720613582939	-0.55890769394143	5.97264589581227
H	-1.14520706865642	0.95376602558172	2.58091382793088
H	4.18870286036919	-0.68254880719682	4.72402642333292
H	0.53034252447921	-0.48873424090231	6.88259251495580
H	-0.34794165981291	1.32187328124476	3.94429267771318
H	0.35543890450792	0.36170124380287	2.84049642185246
H	2.85109823758148	-1.39369970768297	5.30778003858094
H	4.31924666410444	-2.06566635252932	5.55916106018516
N	2.44247693302735	0.04291192548033	2.33790481598074
O	2.50194946844860	1.81951085945023	4.81879886617831
H	2.81284613985227	-0.82874300127077	2.70364130260235
H	3.00762467384828	0.29538691459942	1.53748035221639
H	1.39508096792608	0.34494946252139	5.77689481543271
H	0.22353783183742	-0.66129185152287	5.28893350890828
H	3.26368761260023	2.02195531010792	5.38063452554423
H	2.16316904805277	2.70171711231986	4.60947772620541
H	2.62056927297979	0.73996182798564	3.05978716010571

4mer+CH3OH neutral (no e- transfer)

22

Coordinates from ORCA-job OPT

H	3.84951012436068	0.34712074877784	5.18055188069423
N	3.36071914945277	-1.03713048528787	6.17683208564196
N	0.43135567453691	-1.09120410909615	5.38051136399340
H	1.39595852222462	-2.16885222718726	2.03648725657343
H	3.48914273239943	-0.94293840193803	7.17601132546903
H	-0.28244700246170	-1.72170389051248	5.72216465504283
C	5.32818214303695	1.61922156316721	4.99114257594127
N	0.86496976416343	-1.35813244169965	2.32836320666281
H	2.35239455788901	-1.12874142224530	5.99741885206020
H	3.79845271791249	-1.90838271256918	5.90618201372283
N	2.66599821590692	1.15066115024162	1.96931298397112
O	4.07908446151850	1.11871553043206	4.60569766046677
H	3.33449798464663	1.13656955007858	1.20978540669611
H	2.18112106184994	2.03688467136511	1.91101907569663
H	0.07997674533804	-0.15223335392280	5.52133774250931
H	0.51106285223519	-1.23134051224039	4.36780615027672
H	5.57941927401882	2.45950660331340	4.34078315307713
H	5.32790456644122	1.98561047732543	6.02593374810097
H	6.12670942197774	0.87152630383445	4.89647887356924
H	0.05607145487154	-1.31004731616931	1.72201536915074
H	1.44157844301391	-0.53302806624215	2.13502455872890
H	3.19648713466668	1.15667834057488	2.84210006195392

4mer+CH3OH e- (no e- transfer)

22
Coordinates from ORCA-job OPT

H	3.57128256473166	-0.19543941523306	5.42312182193708
N	4.25301107357938	-1.74193893617096	4.95806302992226
N	0.22947146504063	1.29306233348457	4.82418350459938
H	0.51405918032410	-2.11290900828479	3.16993424499102
H	4.73539177795277	-2.26553538734399	5.68911690796361
H	0.40137059279621	1.12786669206499	3.83763653830558
C	4.29879130168354	1.57444984368066	5.81878296028044
N	0.71185515932415	-1.94254872661945	2.18847691292990
H	3.51126921077486	-2.35406882954831	4.61136766797203
H	4.91570184903848	-1.65548131916667	4.18334796383255
N	2.63986689102856	0.75006243980771	2.41920199265818
O	3.21452942459482	0.72052505608667	5.59123847840789
H	3.31196774448830	0.08282223812389	2.04844646370087
H	2.91911003267737	1.66060960360602	2.07034461937199
H	1.13061057882463	1.13908891605495	5.27214086582361
H	-0.36784358547393	0.53348057862172	5.12904576425877
H	3.92079441643136	2.59642642036232	5.91079072760560
H	4.83667701865958	1.32610992875683	6.74502197897299
H	5.02626652840038	1.55232648689329	4.99492547991721
H	1.49671546803165	-2.55332045888323	1.97672573671009
H	1.09869326043109	-1.00035719073178	2.15544679799488
H	2.79855804665973	0.76352873443863	3.42559954184301

4mer+CH3OH neutral (e- transfer)

22
Coordinates from ORCA-job OPT

N	-0.20433714028521	0.33535883022456	3.38595337896571
N	3.08445045891208	-2.16536670898211	4.43618872908122
N	1.44989852188224	-0.08507649994581	6.05911873592298
H	-0.58490998105181	-0.58800003442992	3.22101995981362
H	3.94670117467787	-2.43121244444095	4.89399789584593
H	0.99101931720874	-0.11554983508962	6.95969258126279
H	-0.80193983186279	0.98403433293457	2.89001486104117
H	0.72102761827506	0.36298031809316	2.94530443792239
H	2.54019936592848	-1.61114528446576	5.10321774186484
H	2.57317568329933	-3.02083371940515	4.26143812035202
N	2.77273175870657	0.38042724850996	2.62973214446482
O	2.89838740361334	2.60443890382889	4.98616056081530
H	3.00861018848937	-0.51502986388385	3.06098999620174
H	3.29313119438294	0.45372214537842	1.76586212968096
H	2.07685352021502	0.71177432547930	6.06495331786748
H	0.73983445705982	0.11261534290082	5.35427017668598
H	3.56873910203812	3.25018534483873	5.20978182351406
C	1.69644856902257	3.28084243676657	4.65903707865116
H	3.11367629512744	1.10358238490213	3.25377177764892
H	0.95046668408382	2.51643349657048	4.44699325517082
H	1.33920456019446	3.89704087394101	5.49009351367051
H	1.81496108008201	3.91072840627434	3.77166778355434

4mer+CH3OH e- (e- transfer)

22
Coordinates from ORCA-job OPT

N	-0.52484816585794	0.31778881048942	3.19999805536685
N	3.41488516617641	-2.05042411745110	4.64461902785279
N	1.27053152780927	-0.18384683753089	5.88531620462715
H	-1.00786077569268	-0.37376476377095	2.64034710968002

H	4.25703813792482	-1.52617654100709	4.85639244494040
H	0.90840824335165	-0.06673887768244	6.82274987774275
H	-0.91670523546016	1.21786489310207	2.95246160526759
H	0.45658007095867	0.32136755844494	2.89386203809740
H	2.65640643267565	-1.57608136518139	5.14501492700509
H	3.52872188089774	-2.96234926658476	5.06916738178660
N	2.48528115075604	0.28535568646505	2.62193349056748
O	2.88554303738351	2.23411908499610	4.92452326118295
H	2.79612298457868	-0.62596142726685	2.95148086581326
H	3.01610223393818	0.49583865535481	1.78614759040722
H	1.89275127920991	0.60456375717814	5.71385591822796
H	0.49299003860679	-0.07599785411357	5.23777506613584
H	3.70677130627159	2.60568689550922	5.27512925973672
C	1.92605739934870	3.24936821081765	4.76226463744862
H	2.78709148569138	0.95576366675019	3.32826654099485
H	1.01036625513606	2.76483031301869	4.41670296226285
H	1.71288571405674	3.76841250594394	5.70304028007021
H	2.23320983223865	3.99233101251869	4.01821145478461

8mer+H2O neutral (no e- transfer)

35

Coordinates from ORCA-job OPT

N	-0.79638621887357	0.06065491429765	3.06754796758503
N	3.27439548732735	-1.70842475165128	5.67401292828136
N	0.70365640603206	0.13447161864912	5.78432047617193
H	-1.07395244282335	-0.89593310042565	2.86502712455854
H	3.80430258865067	-1.93854357698028	6.50408799149194
H	0.22006487585843	0.60341692826429	6.53929558499809
H	-1.54072785513240	0.66625068338052	2.74835865599845
H	0.02523444227122	0.26037652923178	2.50347297152058
H	2.34330529458267	-1.42112682020234	5.97039446545488
H	3.16230699482651	-2.56496396790069	5.13207068330422
N	2.11550122975785	1.09569021318908	1.95980209533028
O	3.71565873430942	0.70030840529574	4.46765467486356
H	2.72283374123562	1.17021246691331	1.15353227938074
H	1.63486486684812	1.98341192907000	2.03642765171999
H	1.53688816953810	0.67763982985637	5.58275149045618
H	0.10786769157137	0.19798659885754	4.95359984435766
N	-1.04790134941782	-3.01937492325013	2.06922211031038
N	2.29282081075684	-4.35449857995842	4.30559888280498
N	-0.27814372690999	-2.94343125656332	5.21082871272524
H	-1.13675608298540	-4.01304843253153	2.24027883899178
H	2.60823298762283	-5.07466782479938	4.94289690814738
H	-0.94898474423500	-3.28218340948171	5.88775794868254
H	-1.55442410855962	-2.82759460607125	1.21442467110118
H	-0.05707232450334	-2.82449005792938	1.89162961013580
H	1.38275588426513	-4.01999524698725	4.64314158749828
H	2.14032678069876	-4.80554260530412	3.41255096523170
N	1.91754716733291	-2.16547699723847	1.87908402315776
H	1.90990861075834	-1.14835922563655	1.91060702880703
H	2.33833751262599	-2.49383661709885	2.74187853949494
H	2.54468732967178	-2.43111775607325	1.13079255735198
H	0.03135505367749	-2.02642326202287	5.52551853840545
H	-0.77678287179787	-2.80001456379544	4.33683951444155
H	2.71449112872474	1.01191005019376	2.78269992937862
H	4.59440857918571	1.03368124729386	4.64471050304197
H	3.68042360221294	-0.21145672941196	4.86769388759597

8mer+H2O neutral (geometry for e- transfer)

35

Coordinates from ORCA-job OPT

N	0.07782963132450	0.61521465623327	3.10602982678924
N	3.51133888331847	-2.00350928066188	4.68220435808423
N	1.17680185018644	-0.28719527550231	6.23782693329606
H	-0.48679728432284	-0.21960032986093	3.23992291799280
H	4.33599840972173	-2.19135088771246	5.23623917313488
H	0.61008816672845	-0.26704892768183	7.07645779760322
H	-0.40577870981654	1.18012393743255	2.41827734252993
H	0.95682565985649	0.31564206215866	2.67883004055239
H	2.79396576085372	-1.64944773575019	5.30966132403879
H	3.18295637328420	-2.89107303470144	4.31226902153914
N	3.11736345444451	0.22249683658527	2.59249548324764
O	1.74290750629479	2.35621964622901	4.58120527705442
H	3.42850496467853	-0.48907990757993	3.26106409257678
H	3.85093063481469	0.33811030486047	1.90548522771462
H	1.85832939238358	0.45744614012391	6.33152356505051
H	0.57815870486585	0.01476252748636	5.47580156444330
N	-1.34513344519508	-2.23500385653081	2.45936593346937
N	2.02689720150955	-4.79783042227887	3.81390100600711
N	-0.10219903573817	-3.12869617632450	5.28740493699552
H	-1.76806055219257	-3.15354496858583	2.51317526748945
H	2.58028713773384	-5.37212834536716	4.43728619445641
H	-0.76470569947994	-3.44934411668385	5.98124913287078
H	-1.90696295422275	-1.70802696919551	1.80240969402573
H	-0.41225430078606	-2.35093739002114	2.04463240311712
H	1.27150530017722	-4.37999488367082	4.36711482941945
H	1.59983875352211	-5.43176128072404	3.15002099417149
N	1.57371274372432	-2.48234423859826	1.56942885700393
H	2.01456619825833	-1.59554900160562	1.80284597881946
H	1.96160256956526	-3.17761655497939	2.20273087170608
H	1.87979819639160	-2.72535997347009	0.63621986577476
H	0.45970893424650	-2.40209457907437	5.72201170698495
H	-0.63169278090965	-2.68460726983565	4.54073972970119
H	3.05142772373584	1.09460978062028	3.10873250813896
H	1.02552383073720	1.83301077500056	4.16333608810980
H	1.46776102541000	3.27101584284596	4.53261169886712

8mer+H2O e- (geometry after e- transfer)

35

Coordinates from ORCA-job OPT

N	-0.53103766686590	0.30681396073430	3.35016967310415
N	3.59694332349922	-1.69500439910778	4.67342266790291
N	0.99881028238531	-0.24604127769706	6.00287675067245
H	-1.10704047841749	-0.43141937171707	2.96169428042548
H	4.40568675846053	-1.50414312705114	5.24951667367132
H	0.59371428847830	-0.08868015951932	6.91757490320856
H	-0.94432916270212	1.19848678397024	3.11251500524952
H	0.37743492817756	0.26266666129314	2.89136379043098
H	2.77538732728716	-1.40908264332393	5.20323956743468
H	3.53240768145788	-2.69534822334418	4.52362369809891
N	2.60352334967625	0.27603739230569	2.48214001348025
O	2.60883175494241	2.03552775407514	4.90894015476799
H	3.16213126702681	-0.37348186238888	3.04018116652688
H	3.18421180242077	0.59619671200613	1.71670462229430
H	1.71668487710998	0.46818289346429	5.88178105950948
H	0.29151534737860	0.00108490143273	5.30715592642833
N	-1.46534781420428	-2.64951016036569	1.97183372991047

N	2.24898896946467	-4.76476406921045	4.12892536940203
N	-0.09850804388159	-3.02671630480597	5.00171254072078
H	-1.81448764697116	-3.59960744170034	1.96961097737185
H	2.71651899312096	-5.16368773302126	4.93322655647250
H	-0.77765924826517	-3.28850848464820	5.70493421472151
H	-1.89802107049305	-2.18033298765797	1.18616005449420
H	-0.45515617825967	-2.69294874970589	1.78262384266091
H	1.41968639121077	-4.26398386444263	4.47478996475209
H	1.91959693709528	-5.54223149469972	3.57063743281579
N	1.56594481708029	-2.59807951374411	1.68134538903364
H	1.77015595284653	-1.62443212303936	1.91400617201255
H	1.99663273892165	-3.16245768420081	2.40882269711770
H	2.06730069225693	-2.79849448603857	0.82535775769471
H	0.37580988166441	-2.19284968226221	5.35406614371470
H	-0.62669395063834	-2.73118906247026	4.18509053398999
H	2.48072249571011	1.07702620969556	3.10139611978141
H	2.09609400949450	2.83483376372883	5.08519540111919
H	3.52459063863645	2.29164497663565	5.07787679178574

8mer+CH3OH neutral (geometry no e- transfer)

38

Coordinates from ORCA-job OPT

N	-0.89913689344135	0.02534198664998	3.07416233046607
N	3.19100448078251	-1.61853303120533	5.78597399265371
N	0.55067514607104	0.13284729540164	5.81692225903390
H	-1.10964697966467	-0.94194215753209	2.84341595472031
H	3.73189996421898	-1.80875035888841	6.61895208573685
H	0.05011808372644	0.59111999595337	6.56732841070131
H	-1.67309385036798	0.59002487681199	2.75045703471106
H	-0.07898130404406	0.29120134956023	2.53575375896458
H	2.24429844093069	-1.38141164166927	6.07579153487979
H	3.13033539283090	-2.48517897919803	5.25050092370770
N	1.97693496072457	1.25679330095033	2.08624530137023
O	3.55725816759985	0.78258180761807	4.56753294324165
H	2.59270390867568	1.40831421503463	1.29744548254893
H	1.45858095857194	2.11713458168767	2.21237846323776
H	1.37538687879700	0.69208702895692	5.62374185443043
H	-0.03731584450744	0.18409667824602	4.97994661420763
N	-0.91016238328648	-3.04490182854909	2.01860442162667
N	2.37796649652291	-4.26303378628784	4.34237867679998
N	-0.27802532306426	-2.97951023666212	5.19167482559108
H	-0.94603727062559	-4.04496746523507	2.17055861300677
H	2.67394176536082	-5.02922280535630	4.93351197226690
H	-0.94951920997698	-3.35437976430698	5.84868316996384
H	-1.39751948583045	-2.86732834102689	1.14966637039361
H	0.07255687175013	-2.78930739406370	1.87848071544634
H	1.44190501723059	-3.97631017798544	4.65124394930206
H	2.28831824713947	-4.63666970694400	3.40612760072864
N	2.00519144821691	-2.00623595692488	1.95843222282622
H	1.90925597374499	-0.99337616770120	1.97520595187270
H	2.39873766905109	-2.28681708217944	2.84999565561118
H	2.69833359198465	-2.22462021517395	1.25445562967406
H	-0.02469181498010	-2.04938670888634	5.51818474855081
H	-0.75902530286264	-2.85705644620334	4.30471217078813
H	2.56478576106779	1.13898724015187	2.91394179955506
C	4.80488033531992	1.35269198650014	4.85553439230882
H	3.51808350572324	-0.12996452743604	4.96487623151020
H	4.83540656858736	2.35589905767190	4.42569545795506
H	5.63386920421720	0.77571045959436	4.42686590900954
H	4.97771682380475	1.44539291862706	5.93518057059877

8mer+CH3OH e- (no e- transfer)

38

Coordinates from ORCA-job OPT

N	-0.73166225455182	0.07315288453784	2.97593477093497
N	3.37203936525904	-1.61886626782300	5.59117209238999
N	-0.00833784104601	0.77459691125128	5.95929781700344
H	-0.88452798123837	-0.93255750302073	2.96403251881314
H	3.86308537291341	-2.13967936823026	6.31065940252443
H	-0.53424777946868	1.47189015157819	6.46865529221063
H	-1.25863929614877	0.45945497937587	2.20295975682137
H	0.25660304119614	0.20690104886616	2.75479678903064
H	2.39888703202555	-1.94143606229929	5.60870807449879
H	3.77007167944719	-1.92637493629541	4.70328572727922
N	2.42063846543149	0.29759639788932	2.62730354413368
O	3.15417202532840	1.09051835567331	5.70459043055233
H	2.55302852920621	0.67862278525714	3.56257374216024
H	2.85696061433736	-0.62523923105059	2.63247414693963
H	0.95717380863740	1.08709596526335	5.91931295437879
H	-0.36831392515360	0.74694471618300	5.00398924432092
N	-0.63384271977129	-3.25810799924411	2.55394606266794
N	1.91852165947196	-4.68830359483375	3.74241796992067
N	0.29839112932626	-2.34194384773645	5.63337032390549
H	0.09231752684240	-3.92242868994346	2.82760376439191
H	2.62176868622257	-4.22273984541811	3.16523147024812
H	-0.16804707314463	-2.95069166064004	6.29343106177425
H	-1.47694228921010	-3.79515343518473	2.38948192908061
H	-0.34790409850568	-2.87890553294747	1.65348883465705
H	1.79184117082330	-4.08226019084948	4.55016508761719
H	2.35929667914562	-5.53632255610556	4.08468355604069
N	1.19412527254130	-1.85852054576477	0.26940546165623
H	1.20939336008831	-1.10847985154443	0.95685330767994
H	1.89162270565430	-2.52165542885471	0.60690016659852
H	1.58763477690688	-1.46318459235992	-0.57848969640451
H	0.07855458500778	-1.37820653323198	5.89081600954753
H	-0.12230181267280	-2.51795356587525	4.72326303829383
H	2.98635506719605	0.85511967544242	1.99584193706391
C	4.39824752446379	1.67664446855265	5.45230446902908
H	3.27359576944029	0.09761092150245	5.72093581586858
H	4.25789237850658	2.75281080938094	5.31755741746721
H	4.86556596155371	1.28195784673361	4.53867659391054
H	5.10397288393731	1.52941332176675	6.28292911499007

8mer+CH3OH neutral (geometry e- transfer)

38

Coordinates from ORCA-job OPT

N	-0.61709267518843	0.06036759454156	3.18260700314665
N	3.37100470616109	-1.48902764960216	4.74174471880195
N	0.81051189329561	0.06360653205568	5.91315816604621
H	-0.97917092863649	-0.86461380051783	2.96848584667674
H	4.12787536140654	-1.62601011912090	5.39895368759489
H	0.23083500098782	0.17969128800309	6.73432416462726
H	-1.26156212406697	0.73680500425304	2.79614284601089
H	0.26799525052748	0.16208409785471	2.69152607238572
H	2.55746054853251	-1.18661828797824	5.27658982443758
H	3.15217616929522	-2.40236640888175	4.35263488965839
N	2.53566904791675	0.47286528917914	2.47704577229323
O	2.88021273886549	2.42893437847149	5.12499224656339
H	2.99644296923286	-0.15435750193530	3.14087914173156
H	3.19790581041507	0.67683793677910	1.73966694060726

H	1.43077785368650	0.86612679296410	5.87332109913292
H	0.20061114755082	0.13685104099535	5.09295440490593
N	-1.35622035962560	-2.95457728625310	2.17865918032464
N	2.29942024255650	-4.48625641612683	3.95824212017472
N	-0.10167263712105	-3.02537167844596	5.17439484306930
H	-1.55810036704652	-3.93632274311507	2.32001211559455
H	2.89416142250592	-4.90714101415100	4.66074188211727
H	-0.70355848367966	-3.34814039951228	5.92039467690161
H	-1.97723265070949	-2.63669623157577	1.44542987878518
H	-0.39664500768224	-2.88484296162562	1.82123876947891
H	1.46467937490405	-4.12742022878282	4.43625279768933
H	2.00089264352175	-5.23812714030421	3.34966208242578
N	1.60126095019389	-2.51318737808449	1.49495955995875
H	1.76026556186160	-1.53078151768260	1.70368408467617
H	2.07609603501106	-3.05188750533180	2.21555220658161
H	2.06395318486565	-2.71032236675173	0.61745264208527
H	0.29052779936463	-2.13575982142268	5.47157329764279
H	-0.69245117888711	-2.83543596750329	4.36869927020908
H	2.38057621466483	1.33942233386942	2.98019086206511
H	2.79116936231539	3.33924019195927	5.40753685063372
C	4.22818122898196	2.02362363115481	5.28727826419500
H	4.28769423964116	0.98980372113666	4.95024675775662
H	4.91013817916562	2.62916802007500	4.68181322953280
H	4.54266147521521	2.07246657141347	6.33484780347970

8mer+CH3OH e- (geometry e- transfer)

38

Coordinates from ORCA-job OPT

N	-0.68704182406367	0.09365278230247	3.26889318012943
N	3.52687382520780	-1.66147621458627	4.72690879833640
N	1.03062929272721	-0.00128068221859	5.86740985657959
H	-1.11586631998637	-0.72729726241508	2.85562694028036
H	4.31106581200632	-1.70913613630921	5.36390118697618
H	0.64596126006808	0.16991638164487	6.78877662786604
H	-1.23121678667001	0.90513715206643	3.00762066773659
H	0.23956931103849	0.20381538129701	2.85963977457728
H	2.74309939978076	-1.25275078541720	5.23798677037832
H	3.27325805190831	-2.61319707533520	4.48246524489386
N	2.48178940584970	0.41135240288939	2.59950293358606
O	2.75914331067185	2.34922933506988	4.92596533411471
H	3.05749884707342	-0.25262657117338	3.11932978577926
H	3.03158420009211	0.73574716603529	1.81326361585503
H	1.61396294337192	0.80921425136355	5.66033436548579
H	0.25830345190683	0.06580919883189	5.20107243990681
N	-1.40012170267055	-2.93684436382869	2.02443548591033
N	2.20550799792307	-4.67432530089042	3.99786605809350
N	-0.04894909245834	-2.94533924646620	5.07654127893750
H	-1.60229081725058	-3.91649422698009	2.17995979487185
H	2.68066739425294	-5.17197464271298	4.74009742050283
H	-0.66958214827358	-3.17191264380743	5.84313098635675
H	-1.92808158021070	-2.65658562910238	1.20761654179625
H	-0.40304578998782	-2.86206833523003	1.78686488367030
H	1.39773867882286	-4.19443735163213	4.41635811661243
H	1.84568899089030	-5.37421644303689	3.36110084530508
N	1.59426909819619	-2.49866580771569	1.61113210639810
H	1.71606195218507	-1.52434682784537	1.88858495365890
H	2.06818041550448	-3.06009616705391	2.31383715694569
H	2.10798123798557	-2.61828403611459	0.74747106879308
H	0.43368062948972	-2.08721663742067	5.34174038184082
H	-0.63971394563939	-2.70292060016830	4.28578905595031

H	2.38694186579695	1.21274588422150	3.22297239556940
H	2.49966784819874	3.27306799407858	5.04656578240114
C	4.10867367683595	2.17824221384867	5.28555464210314
H	4.37126058076692	1.14543585499627	5.04774986317355
H	4.77047028833634	2.84645084972988	4.72430037759555
H	4.27383024032281	2.34630613908527	6.35552328103103

8mer+HCN Neutral

35

Coordinates from ORCA-job OPT

N	-2.89852439879609	1.59855283385812	-0.35024673842149
N	-3.93418945930831	2.94735737165121	3.57152224169655
N	-5.10538848352201	3.44525588093563	0.71123555222493
H	-3.22958339437463	0.63992764396229	-0.28024295895402
H	-4.48035655140204	3.31938933540961	4.33921166779754
H	-5.94198502368020	3.41534349557025	0.14209141579574
H	-2.50171824572406	1.71456544470679	-1.27336358888418
H	-2.14088994032941	1.70086540156441	0.31920219022958
H	-4.52690982822935	2.98371011742372	2.73921655134547
H	-3.78408823293605	1.96418641640392	3.78584430172830
N	-0.94847141497557	2.55225248871772	2.11378414268854
H	-0.14831668757628	2.45912290337851	2.72664726251749
H	-0.79299540231187	3.39056274251309	1.56698727972896
H	-4.79825414001533	4.41084542142414	0.70851156934395
H	-4.38437764676330	2.89838966236908	0.22632202357023
N	-3.53075838139068	-1.54726006782888	0.25282017386987
N	-4.41794886203587	-0.19116176118813	4.32536592678784
N	-5.79015073258881	0.30665241577577	1.62752181623217
H	-4.10594151804356	-2.33292195276027	0.53018089369542
H	-4.95591331886802	0.16655092743144	5.10472659774370
H	-6.73686367583533	0.05945586699811	1.37144372143830
H	-2.98565373120522	-1.86146860340967	-0.54015065271140
H	-2.87645599501370	-1.36076739632712	1.02061337255706
H	-4.99779188943737	-0.09937379022211	3.48337051143487
H	-4.29686483495702	-1.18146996535896	4.49898592728642
N	-1.75982967604703	-0.56169110948682	2.56721384729997
H	-1.35792914619135	0.31091746102584	2.23643030379111
H	-2.45031771445059	-0.32002677752188	3.27480262083379
H	-1.02164114747113	-1.07923906884313	3.02569357191463
H	-5.68741166539224	1.30398459277774	1.46942756580941
H	-5.16456573488210	-0.16556683152897	0.97831631757060
H	-1.75528775214627	2.73410497347860	2.70476420272788
N	-2.25374236007611	6.42098157685131	1.94353525003497
C	-2.62706832361997	5.49344629315631	2.50693794746979
H	-2.98692469040121	4.59010605709160	3.00880717180502

8mer+HCN e-

35

Coordinates from ORCA-job OPT

N	-3.52565849913367	1.40724978954830	-0.72486775136796
N	-4.97602942040773	3.45402212036271	3.76687722757962
N	-3.16857964098806	3.87275710637895	1.15007940084012
H	-4.10679237617463	0.59156017786218	-0.55666691289843
H	-5.90952896510937	3.50564730710962	3.37541169818567
H	-3.54906265586477	4.73795765603240	0.78313062137595
H	-3.53005506759258	1.56265843416947	-1.72766498128584
H	-2.57367136526684	1.11755771510611	-0.50052887259512
H	-4.33421525759678	3.61073060674787	2.98612855328780
H	-4.85094906788650	2.48121786927941	4.06396562330803
N	-0.35818377850467	0.52979219072607	-0.27978628096490

H	0.38556745192668	0.02013305833016	0.20040694198828
H	-0.53778132357737	0.00394683316754	-1.13839058245584
H	-2.15869463865975	3.96274519090267	1.09130669860943
H	-3.42110102882659	3.13098535584331	0.48934412000965
N	-3.26638574613903	-1.59419790190425	1.15804223351983
N	-4.54856435152219	0.40414359262527	4.24358401951419
N	-6.02568930240378	-0.14318219240630	1.49094048479679
H	-3.13082572557895	-2.46701646397473	1.65552892129747
H	-4.51024443480549	-0.23857367297871	5.02358471605883
H	-6.77220787786402	-0.41542671182540	0.86405660746207
H	-2.70801800236612	-1.65649710880610	0.31107374647200
H	-2.82917482645119	-0.86669544937343	1.72397947314026
H	-5.23878238222516	0.05090755739587	3.58360027882303
H	-3.65065818958977	0.35988968995247	3.76447152650100
N	-1.90115328901229	1.03178209698424	2.51752741756216
H	-1.41818550354332	0.89406906459757	1.62768867790482
H	-2.38977087916762	1.91899655820468	2.43932342252530
H	-1.17642775770001	1.16194792260325	3.21443825191926
H	-5.77061128187948	0.80679186917780	1.24423230027441
H	-5.21283579738165	-0.72453501407728	1.27033188095314
H	0.05442142568819	1.41691741684320	-0.57636491030515
N	-4.71338261161781	6.16126354690267	6.81619118314706
C	-4.74931225918376	5.39277597355009	5.96199222771821
H	-4.80256557358925	4.64325781494039	5.12456203709630

8mer+CO Neutral

34

Coordinates from ORCA-job OPT

N	-0.51713267805361	0.12792579897347	3.15290513306194
N	3.08957635326103	-1.12475798839973	4.85905063240923
N	0.36746870759388	0.10734457150261	6.08845756870422
H	-0.87643667374979	-0.80298445239726	2.95844166656753
H	3.88766867639518	-1.11103019390324	5.48037227579406
H	-0.41879244016344	0.06982521699831	6.72489120902309
H	-1.16085402496093	0.79033154700780	2.74086869121885
H	0.36761096129990	0.21573706669723	2.65883070874791
H	2.26198479039496	-0.93130668832719	5.41925755948662
H	2.99965522783474	-2.07437522073826	4.50745239328964
N	2.59545424882429	0.57997657498926	2.34775617185759
O	3.15965823249952	2.45106936310124	5.44380960847910
H	3.38522310733408	0.58005730257050	1.71500290629474
H	2.42691602692121	1.54650095053678	2.59654350557478
H	0.87142383054244	0.95650425461289	6.31156986120775
H	-0.01072473962699	0.22097446576139	5.14070970500045
N	-1.23664652518158	-2.89859505993650	2.16354790535872
N	2.42550191478733	-4.25124308269243	4.14739678773658
N	-0.17250346615593	-3.02171287333798	5.22104532586316
H	-1.44545138977590	-3.88169007785709	2.28530872281521
H	3.03315310860012	-4.57610066174364	4.88881147507569
H	-0.82497011556824	-3.43774948929956	5.87229674210819
H	-1.83888178638170	-2.57020723424196	1.41922788633886
H	-0.26849543880307	-2.83015259834998	1.82899901138037
H	1.53514916882983	-3.97650732052863	4.57753524362398
H	2.24188628321588	-5.05305741509718	3.55729346834024
N	1.73376566621541	-2.46679996304922	1.54291059598732
H	1.88487428367225	-1.46836872764487	1.66065720436832
H	2.18995209557762	-2.93227455178407	2.32430594377653
H	2.21854008927897	-2.74563517492702	0.70015019772458
H	0.11776313187734	-2.13080823120746	5.61402137403065
H	-0.68456627988322	-2.81811552298791	4.36578191310114

H	2.88281505483213	0.08817352694720	3.20094479603417
C	4.05850554204602	1.85604800914261	5.76294614391424

8mer+CO e-

34

Coordinates from ORCA-job OPT

N	-0.68123634847773	0.06773992365099	3.34166558048371
N	3.10583534532547	-2.44491563016639	6.80946832336011
N	0.79248619973511	-0.07717210611898	6.08545984990952
H	-1.07434100514306	-0.83171301391957	3.08041863216564
H	3.96731904451069	-2.02475274218533	6.47468477406587
H	0.35156483456544	0.34845358254486	6.89275583540284
H	-1.24594625149383	0.78492176523635	2.90497494776218
H	0.24803876803252	0.12490598814691	2.92401082028407
H	2.84364230238609	-3.12189618441851	6.10040685417972
H	2.40470856182972	-1.71058149346470	6.73340308937721
N	2.45177785258317	0.25436586945565	2.59386959862491
O	4.52338472327847	3.97794122251224	4.31893944608745
H	2.57521135130074	1.18482131116900	3.00226039730507
H	2.77750273301202	-0.38388561035438	3.31873787540815
H	1.63651349053525	0.46029456595175	5.90279094902338
H	0.17787096095914	0.08523884586728	5.28275119102722
N	-1.60541957709455	-2.94364118366128	2.14870008210389
N	2.65966666950592	-3.97647898715500	3.19070802956207
N	0.20536683587743	-3.09663246837115	4.94165355360855
H	-1.71783484378005	-3.94730316365485	2.22640457922174
H	3.39359536375734	-3.29842854299738	3.37203500243084
H	-0.22912588265515	-3.66743949706165	5.65603209792060
H	-2.37270510516604	-2.60961724388057	1.57852567185477
H	-0.73787935912311	-2.77896168395568	1.62177423175039
H	1.88312776246920	-3.74332686019238	3.81785149298479
H	3.02109341499502	-4.87759803486274	3.48004207391677
N	1.13580168549470	-2.35529891559440	0.95691788960960
H	1.34756268634113	-1.43858238619666	1.34597485379536
H	1.68802133026173	-3.02247315213442	1.49889994293371
H	1.50160116280106	-2.36111367554453	0.01286865868541
H	0.41023640031391	-2.19599105458023	5.37268197581728
H	-0.49605844942197	-2.92935603919113	4.22481366345687
H	3.15274965903555	0.19456284864101	1.85876157267052
C	3.60030285429585	3.67346032288789	3.70382948031454

15mer+H2O Neutral (no e- conformer)

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Coordinates from ORCA-job OPT

N	1.38298289200424	2.68373025236369	0.04618188200836
H	2.23721832450191	2.13264408194299	0.07106427173126
H	0.82563806724137	2.39394446967059	0.84021405250057
H	0.87346184885756	2.41498018481307	-0.78532881535098
N	1.77354707713967	2.06065546723728	6.21903081516298
N	2.37435462488944	0.62836312979409	3.12157173089063
H	1.67871910642082	1.66105698460979	5.29105240831294
H	1.72299513709779	-0.14090788616790	3.21450504577937
H	2.76600010330331	2.07164885680700	6.42325415007264
H	2.67453679705884	0.63677388042881	2.14988881105899
H	1.33120351716719	1.42951584240944	6.87366818720667
H	3.20028115702567	0.38066933926786	3.66087016074987
N	1.67044081100422	5.67197590761578	1.06555972226513
N	2.12575838943609	3.86193669460057	3.56888254740850
H	2.58841951895010	6.08019906559615	0.91709936110688
H	1.73077201565629	4.44747950536041	2.83195581792293

H	1.62795747145310	4.80154091422391	0.53496282771280
H	2.06588020827186	2.88623735565742	3.28544601207734
H	0.98979700470599	6.30436699091179	0.66606329818075
H	1.54768565642602	3.94643543303359	4.39590413087195
N	2.86282147159951	5.01161550953076	7.24525244987723
N	3.52000633913336	6.64504344134738	4.43361409166870
H	2.92467584034787	5.69126685673621	6.49180680821340
H	4.37621844023441	6.83575290411669	3.92251255725815
H	2.18340777023007	4.30753165893403	6.97195521440024
H	3.18908490312032	5.74547423293411	4.08987978285422
H	2.49972662427377	5.48772058132901	8.05986899988984
H	2.83969613739628	7.33062208238195	4.13125534337907
N	5.86861904702392	1.20958805333523	2.29468952385731
N	4.73858094136067	4.02688112705324	1.66711054162408
H	6.82827192124537	0.92900472259766	2.14613004332826
H	3.97178739624013	3.98624309980843	2.33452383906535
H	5.84321812143530	2.22628748448897	2.34956662760781
H	4.69420608948975	4.95823764807701	1.26240650691839
H	5.56438618472300	0.82912933724239	3.18946232172494
H	4.49750100480993	3.37936815087319	0.92515797527368
N	4.94546209797158	0.25793604885143	5.20722076737003
N	4.75390695566563	3.28246829798107	5.46733967006246
H	5.83963217544052	-0.10134376244815	5.51749525295701
H	4.42179752666296	3.82171346712086	6.26477393502855
H	4.91544681126251	1.25805509607829	5.44319007131059
H	5.64849833458913	3.67981304085752	5.20843238174720
H	4.24449785391487	-0.20810977210982	5.76984248159591
H	4.10723524717889	3.50169395502475	4.71205307333914
N	4.75060871993053	7.23583105045081	0.98670185837181
N	6.59402374437696	6.09313044302496	3.28200695459874
H	4.15559002405187	0.27422162856023	-0.25687142332003
H	6.28059793265177	5.19243878850134	2.92883657508693
H	4.20458156604174	8.05996510526651	1.20292589651301
H	7.55782477526653	6.20733065849511	2.99649441233038
H	5.39640252570231	7.08677670506081	1.76423193223340
H	6.58483223775362	6.06196389249056	4.30152348000088
N	6.02470817183756	6.40339383160006	6.39122133655224
H	6.39912731954710	7.26910662940076	6.75766865460075
H	5.09138796094753	6.60019393810860	6.03554407513637
H	5.90149323203060	5.77970917498100	7.17875557725174
H	5.30445740082812	7.46181917285606	0.17037667811398
O	3.94224503349237	0.94367901881786	0.39239055239574
H	4.70256697512953	0.95224820339918	1.04062373342284

15mer+H2O e- (no e- conformer)

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Coordinates from ORCA-job OPT

N	1.10424033372230	0.70088926003660	0.19446214398550
H	2.07114763582563	0.44130026278686	0.00816825541912
H	0.84704704264392	1.38764203406824	-0.50307635933584
H	1.11775013516530	1.18710213765390	1.08408513844277
N	0.35828668819385	2.03323470059583	5.75168110597371
N	2.72185857326387	1.35369108553782	3.06615063506738
H	0.67867086756374	1.78999623031471	4.82093887818504
H	3.29294784909223	1.72343484063085	3.82573607638221
H	0.68614939911362	2.98217525748809	5.91984736047297
H	2.49797035455972	0.39405206733099	3.29683329294331
H	0.86794246253064	1.43613602449986	6.39164664080225
H	3.30543889618496	1.31790713031851	2.23784650432976
N	1.88308641741269	7.37101239158035	1.95943308453013

N	1.34603646720302	4.19463319071937	3.03317076384124
H	2.87280688621211	7.45646441843509	1.74320624899649
H	0.36461810833204	4.21551638471336	2.78543567220472
H	1.73179883236455	7.87657995628131	2.82360944761548
H	1.64131652998748	3.21816814233738	2.98721599721045
H	1.72264048402600	6.39003360080954	2.17386081131728
H	1.40357495211989	4.46394312919258	4.01099702857989
N	1.58112244331037	5.06502436415754	6.36917822128488
N	3.78713516625906	6.69095694630694	4.98426239688844
H	2.25619911110622	5.70251281750940	5.93032409395178
H	4.62585488987101	6.22124141690206	5.32315678533718
H	0.73695531977159	5.59573537163301	6.55055031567892
H	3.75032905716636	6.56211829860552	3.97891526657488
H	1.97214591326025	4.82649404976805	7.27489650040746
H	3.92968938977284	7.68093548300267	5.14609791072479
N	5.67429594516554	2.04585187454236	1.00390822642243
N	3.83398490650362	4.56266332063089	1.02176517707527
H	6.47165819429707	2.24857430225526	0.41461430590987
H	3.04583726936480	4.48244914716323	1.66410843775831
H	5.10649900212641	2.89802298362910	1.04506160246059
H	4.20468736529955	5.50140738387022	1.13885628938832
H	6.03271180796855	1.85245046801925	1.94265769414991
H	3.43897002297807	4.52347938070782	0.09001839358639
N	6.52829751901477	1.49121660423804	3.96743702644486
N	4.05046344547069	2.85887196026467	5.56933328677867
H	7.25405418463175	2.08103149892302	4.36609957363230
H	4.27215965148024	2.39675585363388	6.44692954353224
H	5.65962792227828	1.78999851970043	4.40929150736004
H	4.66225700008285	3.67083625377585	5.54153700829710
H	6.71195059465384	0.55227922256686	4.30338996569794
H	3.10838659308459	3.22711267213382	5.67314143459852
N	5.28567302067531	7.51638862594305	1.71625474039748
N	6.63269066764987	5.15354869879057	3.11993657693008
H	4.41999422088609	-0.79631076022123	0.48910933020991
H	6.03588036713357	4.42905757023922	2.73340085794439
H	5.27884796643453	8.33254588619059	2.31601928154878
H	7.58473684535128	4.81705094635976	3.02867118022205
H	5.86400098716166	6.80901692257485	2.18554963948462
H	6.44515543492631	5.18877205904543	4.11974047651022
N	6.33130289897162	5.24273857531379	6.46284626400467
H	6.93234684425788	6.05620268433828	6.60043338425216
H	5.77620384968099	5.15795488600741	7.31713852538268
H	6.95872046065810	4.43438726878186	6.47072320118872
H	5.76749951180086	7.78631963420521	0.86745109744915
O	4.15683260891604	-0.01571371432619	0.00234023010407
H	4.73604975532881	0.71665592916086	0.35389557706981

15mer+H2O Neutral (e- conformer)

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Coordinates from ORCA-job OPT

N	0.47027281886211	1.85399580660245	2.19858089010570
H	0.19159805038205	0.97647228399872	1.77970936218496
H	0.46017732775028	2.54921178747766	1.46291567935927
H	1.44126408003866	1.76147400755407	2.50087559516566
N	-0.65723222897658	3.21440676032312	4.76177819957956
N	3.50162589386293	1.65966913114515	3.21370679143858
H	-0.40984310236092	2.67548181907428	3.92756761428826
H	3.78859470724880	1.91639871832957	4.15975864087762
H	-0.81450628455000	2.54926729064394	5.50863244305177
H	3.50944657338677	0.64765216123175	3.17820646840524

H	-1.54774829849598	3.66028264953196	4.58195967766673
H	4.23822984124146	1.97126825508514	2.58899435650628
N	1.51098923196451	7.23562732583424	1.68198521950318
N	2.00877024543873	4.61816428862163	3.18134622543329
H	1.96584018665561	7.24520667710526	0.77791836094878
H	1.12808647564882	4.45089019112085	3.65866474468973
H	1.60733048578857	6.28708268404208	2.06168551124673
H	2.42565242614743	3.69657580649708	3.08170305522718
H	0.52726882498474	7.41087673954455	1.52530549320514
H	2.59990278040532	5.11646528563575	3.84647465555179
N	1.92446204708087	4.20011411949745	6.53927413042389
N	4.03692895736833	6.26585403720542	5.00566235086787
H	2.43677035066187	4.94060045067631	6.06710896327426
H	4.34034515269436	6.44702383484397	5.95326150923155
H	1.09503531356434	4.00477283870160	5.98320040334252
H	4.83756713384575	5.88523847715555	4.50746330581023
H	1.61385108030420	4.56525645510221	7.42994170284287
H	3.79521898317633	7.16046426227367	4.58710796826156
N	6.19203645893379	2.32581314688979	0.82660931486833
N	4.31342847777953	5.05293336387367	0.92232130000871
H	5.62818230945256	1.54514053436349	0.51918041704345
H	3.41858415061976	4.94758306076374	1.39019251318636
H	5.60347584213515	3.15443162934175	0.85872602071394
H	4.63342993684419	6.01206777485290	1.07085475391628
H	6.51034324545772	2.13612825212341	1.76998492849100
H	4.16145083487593	4.92861793412680	-0.06985064963982
N	6.82157455648595	1.68456524867506	4.20364843904395
N	4.49188356269194	2.44627912025871	6.20829175373091
H	7.63780438361801	1.71060862455135	4.80160155222861
H	4.54941526474442	1.72716696380767	6.91904091242325
H	6.00560211030299	1.82263737188473	4.80168772743838
H	5.20771394224065	3.13702286470731	6.43498058039074
H	6.76665343527406	0.74397647215412	3.83436223560267
H	3.59007891609432	2.91195036047422	6.34314009753471
N	5.51506615483135	7.77305991188976	1.90759622643442
N	6.52089413728177	4.75819438218577	3.27367576872772
H	2.41547317507988	8.27770459827309	2.78316081645703
H	5.83719537615225	4.78857642834806	2.51861311593190
H	4.79751184107838	8.32649821557107	2.36975261400711
H	7.39201695337736	5.07059618432027	2.86111003516555
H	6.07412279970814	7.34847773173912	2.63772016157344
H	6.65474170644392	3.76971865283411	3.48590191131507
N	6.86684600295498	4.64116401852142	6.43317899816081
H	6.75015444904489	4.88663787367366	5.45054903740364
H	6.74527355959369	5.48695564683032	6.97504735610558
H	7.83035628345811	4.35858652210742	6.55929623082473
H	6.11764056403841	8.40810745545114	1.40138270513090
O	3.04521450622176	8.75732309334980	3.38436366215893
H	2.59080391565776	9.54614286342530	3.67726408315727

15mer+H2O e- (e- conformer)

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Coordinates from ORCA-job OPT

N	1.37989734582129	1.77345426790521	0.44901608904192
H	2.12373262399559	1.67523907706575	-0.23107665598395
H	1.23907480496456	2.76985980483162	0.57922755830871
H	1.75581040313419	1.45317077858325	1.33569996994308
N	0.34823974792913	2.02495941418690	5.65571715008041
N	2.98518060503743	1.49668527096612	3.51297491983792
H	0.85449487416819	1.80885179206854	4.80395766295894

H	3.33742506382659	1.93146103081581	4.36652259320425
H	0.84584365873241	2.79727423316263	6.09301415000414
H	2.97124181378266	0.49947831228360	3.68966086698562
H	0.44956636074789	1.22405659147069	6.26594759578068
H	3.70742828349699	1.64824329394659	2.81523723403768
N	1.85620226626086	7.75525909280040	1.64704872190695
N	1.31390278234287	4.17327069265655	2.72086132768325
H	2.87045817720017	7.69795905959291	1.58971865756419
H	0.31342135073430	4.16147142263683	2.87292706824530
H	1.65548715497231	8.12466213699161	2.56888882135937
H	1.65874296660085	3.25017746288821	2.97579485257298
H	1.51808520535430	6.79946040201461	1.64666327030983
H	1.71766244373107	4.81459918865622	3.40032037425230
N	1.61932633903920	4.86727355715971	6.59742564631789
N	3.42008028638963	5.92826486273480	4.31160561464229
H	2.04640602882618	5.26406485909459	5.75636922464229
H	4.20999187360363	5.43083260335562	4.70968614497709
H	0.62993561687153	5.08084603014035	6.55442086875741
H	3.59822147823583	5.97240197538077	3.31466962961666
H	1.99307311775851	5.39635907190639	7.37752951118817
H	3.52629592106570	6.89031009726219	4.62942554953659
N	5.62075918911965	1.81352912681731	1.04090612881109
N	3.90682659828859	4.68360553254425	0.88656972120208
H	5.00861159796340	1.06348195958905	0.74878850201683
H	2.98681710822797	4.53875348252976	1.30063605421808
H	5.08574239083132	2.67831041753137	1.02231447792709
H	4.14785611577588	5.66437934858260	1.02020123288426
H	5.89821585615055	1.63290480365479	2.00339783220444
H	3.80545329576848	4.54637156129036	-0.11105617100437
N	6.46388277776522	1.54695493857420	4.19814051386715
N	4.22626063082036	2.94029463301472	6.15156462371492
H	7.17604949194006	2.26617686804065	4.22999045008334
H	4.43962792394962	2.41952820103968	6.99391000237376
H	5.66830893007791	1.90537021141660	4.72291722066592
H	4.90219974171742	3.70233049318277	6.10606581085547
H	6.82575812337714	0.75242675823885	4.71011020912314
H	3.31730291262084	3.37338296823958	6.30809828951115
N	5.15595804217512	7.57620716656923	1.89889769535963
N	6.60766222953096	4.87509130836440	2.66497085088122
H	4.08473085652293	9.60749836864350	5.00765307825345
H	5.76998840985118	4.55194065934081	2.18638691960369
H	4.99286561267496	8.09793099692026	2.75762868119007
H	7.35668429769542	4.25462000203496	2.38667617753111
H	5.87757091163528	6.88815935269684	2.11290960923405
H	6.45783428914528	4.75080815376899	3.65981662758901
N	6.30368235871489	5.52769056379706	6.06432920443975
H	6.65252043201806	6.23421537807379	5.41858349866607
H	5.75808984737345	6.06049006349162	6.74324722465146
H	7.11951428340180	5.19705916637212	6.57335012255038
H	5.55025660865829	8.22619806278863	1.23069571984729
O	4.45963433185201	8.74467854228073	4.78713694231646
H	5.13897411632848	8.62012497424041	5.47008226968920

15mer+CH3OH neutral (no e- conformer)

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Coordinates from ORCA-job OPT

N	1.58730827662416	2.93720465528541	-0.48208094598200
H	2.31818356038533	2.31192793910681	-0.14759974436809
H	0.70110418613281	2.54213603585232	-0.19479242351780
H	1.60609344926665	2.91160913611634	-1.49316539099242

N	1.85307277465668	2.01690488111596	6.25558696391445
N	2.38358021897445	0.55679985566427	3.28982393592352
H	1.83000344424355	1.62339343835675	5.31830081452180
H	1.75262223765219	-0.23088123028693	3.36494508537554
H	2.82093635942722	1.98801283603797	6.55265758968090
H	2.60515766943114	0.66378687106811	2.30246180260325
H	1.32958892916248	1.39949159174387	6.86186983585839
H	3.25327341050780	0.28676477472407	3.74185766470571
N	1.64798386012978	5.69624743030980	1.10588735701252
N	2.12666109688104	3.83522387467868	3.56945650676468
H	2.54079168822173	6.17145130701924	1.01254918985916
H	1.71952135448459	4.41249308361654	2.83204069066102
H	1.66350398496071	4.89128994680564	0.47837500357183
H	2.05425947682466	2.85720747283809	3.30157351853141
H	0.93371850221102	6.32810897050883	0.76869593637542
H	1.56229583664259	3.92944109219993	4.40500303525862
N	2.93345162163196	4.94157158920125	7.26018457030347
N	3.47810996235589	6.63162064164932	4.46290039255436
H	2.96260072063857	5.63731025388080	6.51967341956280
H	4.32299025550003	6.84843410240506	3.94397916987359
H	2.27070611788318	4.22277998633497	6.98235928064892
H	3.16990730249103	5.72394690468001	4.11944484476381
H	2.56898086368232	5.39088603735685	8.08932195445474
H	2.77532886604220	7.29805305964048	4.16936718124131
N	5.77673471928626	1.25923471244093	2.22847856391427
N	4.71868064473472	4.11770656948382	1.66459324069242
H	6.70788701626600	0.95641905044621	1.97769997354121
H	3.95206912995788	4.04567628780971	2.33040013410293
H	5.78683350967927	2.27458250868223	2.30512792793437
H	4.67282395554684	5.06711254170854	1.30430858285440
H	5.55285370273953	0.86568607340202	3.14136162852328
H	4.47034026971799	3.50901346242844	0.89310200892185
N	5.08559936416865	0.26171885357256	5.18279589011895
N	4.82276516968822	3.27553748657736	5.39756086089053
H	6.00262869396394	-0.06326086755601	5.46251165933441
H	4.49284980431292	3.78602711433565	6.21414451791260
H	5.03350031772162	1.26591572595447	5.40002050120335
H	5.68490444554428	3.72353730816709	5.11274393146503
H	4.42314286861862	-0.21412029736993	5.78266889573698
H	4.13775714868615	3.46986192214033	4.66992945133921
N	4.71137211697604	7.35975465640337	1.08622641937323
N	6.58396999610652	6.15968083803354	3.31702669108669
C	3.85420925338734	-0.15085584337873	-0.33014442492439
H	6.27729785534249	5.26095806740199	2.95385928501702
H	4.18159044676172	8.18521182135320	1.33547378041717
H	7.55132196638342	6.27750507948013	3.04535372727085
H	5.37973781436954	7.18852362182187	1.84023098137937
H	6.56095318215409	6.12274153909668	4.33641863885206
N	5.98726072032390	6.43236615276977	6.41949468355151
H	6.35730306856557	7.28138894115521	6.82692973278004
H	5.05989316253934	6.64380920823900	6.05722047922136
H	5.84710500611542	5.77730536198990	7.17840443115252
H	5.24184756275049	7.59733087355063	0.25770714768742
O	3.71959116037907	0.97960861342635	0.49031018277434
H	3.89693709288631	-1.07979180225099	0.25186281254274
H	4.75136594587141	-0.09992604414806	-0.95881414674237
H	2.98531922091657	-0.20648060064281	-0.98901143378421
H	4.51228710494136	1.03280684749197	1.09688149763287

15mer+CH3OH + e- (no e- conformer)

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Coordinates from ORCA-job OPT

N	0.90085090286907	0.34504010574439	0.28130408042800
H	1.90253340747916	0.32479570956949	0.10180752642786
H	0.48883877521304	0.94674418914487	-0.42040989965513
H	0.79790754492301	0.82596715239554	1.16778364502851
N	0.33459198574848	2.01086799714973	5.62097018666276
N	2.59058847607376	1.15613311333746	3.08881255761420
H	0.71693603750910	1.73797811529023	4.72157675735354
H	3.25013634903895	1.58374015385255	3.73699191406381
H	0.66659436033120	2.95827887006645	5.78730250345307
H	2.36711474540042	0.24075324392803	3.45867420765955
H	0.78675627843258	1.42422518030172	6.31182037331438
H	3.07329407974013	0.99707543783528	2.20852163907977
N	1.93099703484729	7.40298579324758	1.96253286817131
N	1.43967930970096	4.13172439922511	2.93906631012671
H	2.92542221700884	7.54202107452509	1.80080858825942
H	0.47197086327760	4.21835179277905	2.65406874475097
H	1.71636608997205	7.85932740378415	2.84069115378109
H	1.66281821439344	3.13627296297441	2.91296695584282
H	1.80860405011461	6.40755894166861	2.12626238898227
H	1.47764288039080	4.40672496589713	3.91680395380650
N	1.60505975254594	5.02655147418150	6.24854106611299
N	3.81567503863069	6.76320424678594	5.00514418346210
H	2.27449395290614	5.69271046048238	5.84537099224151
H	4.64097577682583	6.26535209537326	5.33681807876563
H	0.75762486279439	5.54066313674552	6.46020293271572
H	3.82221118301919	6.72069231085931	3.99180221121395
H	2.00029419776794	4.74313154716513	7.13962810927413
H	3.94846822881235	7.73530713730314	5.25826589502461
N	5.77235675731735	2.13281280440717	0.93986458010721
N	3.96569815315015	4.65884627921061	1.04844557074952
H	6.56283943359176	2.30779402703965	0.33361214604433
H	3.17038626738861	4.50676488606802	1.67082956478759
H	5.23431302001289	3.00259878076940	1.00378886529730
H	4.29254704387910	5.60438201383297	1.22310523796244
H	6.13848202133905	1.91511505145098	1.87084167473416
H	3.58711757234573	4.65750414291976	0.10901352521819
N	6.56403827646390	1.47000361671845	3.87598105893646
N	4.07181165892094	2.82073511382728	5.42742734491045
H	7.27384345193447	2.03786418560122	4.33103202505129
H	4.28814886566567	2.37112619208364	6.31298720942187
H	5.67727483024524	1.75942919069182	4.28800615212075
H	4.67165368750557	3.64129069727972	5.40073051639954
H	6.72566136473506	0.51708491044910	4.18239680079250
H	3.12372012822126	3.17691450489144	5.51627532282581
N	5.32213266209286	7.67103345111268	1.85463744553354
N	6.66325338923601	5.23936227255987	3.13236662384006
C	4.52860968513910	-1.01984768480756	0.75902246246718
H	6.05019074254984	4.55084771962691	2.70697399774482
H	5.33999621296081	8.46447693090536	2.48401787896278
H	7.60663172410960	4.88145366009772	3.03420911391708
H	5.91124294013981	6.94410899394694	2.27879542955677
H	6.46664399762096	5.23592181547745	4.13129195511842
N	6.31522529715378	5.21210575065376	6.45793250318903
H	6.91116828954754	6.01612602305614	6.65856335333942
H	5.72625361237700	5.08835185909943	7.28441228882009
H	6.94066333989033	4.40219463555370	6.45317935592253

H	5.77660148410375	7.96960777126711	1.00030231098237
O	3.99568046075181	0.19804449423079	0.32449976523195
H	4.94821854059017	-0.95136356286956	1.77185138620574
H	5.32034370841554	-1.39003285892412	0.09223203511781
H	3.72922223618648	-1.76487552807714	0.77537687385365
H	4.67995197595415	0.91461560363669	0.47817608122310

15mer+CH3OH neutral (e- conformer)

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Coordinates from ORCA-job OPT

N	1.52438689108474	1.40278359431778	1.39394219956180
H	0.99311621606701	0.74683021534030	0.83726749222084
H	2.47050552148878	1.43916811957998	1.01080767060017
H	1.61053009822501	1.01192249273780	2.32441161273064
N	0.33400312933890	2.32353380429711	4.86627958120180
N	3.30247450405167	2.11621475634107	3.99726910457372
H	1.28828704083748	2.08499172667246	4.58580987704805
H	3.74706195542165	2.48477321508512	4.83832952891798
H	0.11230369104749	1.77176773968593	5.68461125003280
H	3.90663880309058	1.39565344710039	3.62467588379779
H	-0.28782435086975	2.01660945418931	4.12974597781629
H	3.29715155361108	2.86098904869444	3.31056012837316
N	2.10720687037931	7.81431606303799	1.41349957445490
N	0.92984444422570	4.30626677557291	2.29656034058877
H	3.08702342278111	7.80161390977329	1.67970668408947
H	1.01898786670020	3.37357196699793	1.88204205044159
H	1.66028136660870	8.53496728343077	1.96556736373821
H	0.55599062744311	4.16150299193767	3.22905191737246
H	1.72121498977648	6.93070125034019	1.72442423623846
H	0.21849247249528	4.79888632710526	1.77117733069130
N	1.59162887065627	4.72480071726339	6.62024278398161
N	3.21576884812465	5.78284906449799	4.17131679337926
H	1.92709682666586	5.44248216739856	5.98224817676580
H	3.85208528521414	5.09779867881294	4.55995345185902
H	0.99138532832124	4.10619910483904	6.07895363710957
H	2.54085119314977	5.28639176254793	3.59639390372689
H	1.01905243710765	5.17405870225859	7.32244426975600
H	3.76125381765830	6.35616568947772	3.53751610301588
N	4.47669419207966	1.87672363012451	0.37453501788012
N	3.79535205135646	4.89624594229250	0.83019236347309
H	5.32786305814454	1.58308445868432	0.83658784630569
H	2.91589945568156	4.73203979087779	1.31768968289156
H	4.39860010509033	2.88786212011054	0.50100615639998
H	4.19631847764696	5.73178360832968	1.24814389105984
H	4.61076613822415	1.70536989229028	-0.61372124594834
H	3.54556161204959	5.15440690818831	-0.11677780076291
N	6.80916175739153	2.25827690442553	4.86190000589245
N	4.49288167058854	3.53530375470218	6.64386364914126
H	7.61739184575667	2.49603346431419	5.42337728338876
H	4.77854894800700	3.09417566329383	7.50940575258328
H	5.98711430602141	2.56700335976904	5.38179736282941
H	5.10002539512942	4.34482553771899	6.50174555862588
H	6.77645484858461	1.24780271440656	4.81560310456935
H	3.54167742614885	3.88407338238606	6.79311427760077
N	5.43728108382803	7.37302766238906	2.32324803110982
N	6.61027001357305	4.38312791134529	2.55869592895261
C	3.88663079080971	8.84392368676028	5.67985374470562
H	5.78175269674380	4.25562602639741	1.98513568103134
H	5.47855843049289	7.95632694626859	3.15374931566563
H	7.40790502769639	4.31456794434435	1.93964988217634

H	6.02083232162599	6.55533239945700	2.49672249946983
H	6.66762136511780	3.59467310807440	3.20674639925540
N	6.45698518853673	5.79026519147234	5.54393838140099
H	6.57750024220050	5.46907783075990	4.58576959936306
H	6.09491781257044	6.73723586916203	5.50298570281158
H	7.38029412016890	5.84892923808087	5.95331416217676
H	5.86142593320667	7.89463365804249	1.56704157803449
O	5.21124877112976	8.76636883632171	5.16970598912764
H	5.69395057150703	9.55270997923418	5.42500688537061
H	3.38941620867774	7.91498521035644	5.40462503351817
H	3.88302893295700	8.94074402009211	6.76896852696035
H	3.33881690567526	9.68443664553116	5.24384025960562

15mer+CH3OH + e- (e- conformer)

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Coordinates from ORCA-job OPT

N	1.39467227586538	1.82604453200004	0.39851026723835
H	2.16134751171085	1.74485651861354	-0.25785253837659
H	1.26231728861682	2.81835806981604	0.56291317232076
H	1.73594735441727	1.46765827225335	1.28443341795620
N	0.34534236838738	2.10289238823073	5.72900570583964
N	2.92801049460220	1.43140054149237	3.49951637670407
H	0.83569446833542	1.87523614074910	4.87106091743477
H	3.28582294107911	1.82877236177402	4.36954207336555
H	0.83263892380939	2.90199339822420	6.12978819131528
H	2.85774116595932	0.43245747123187	3.65035638814054
H	0.49201091217671	1.32491023632222	6.35974536992785
H	3.66999872131280	1.56244751859483	2.81863123743475
N	1.91195904577122	7.78876877355154	1.85667842853982
N	1.37435064783746	4.18058989792764	2.74988967349648
H	2.92276174257863	7.73985000927207	1.74540602878366
H	0.37857202714394	4.21138495380441	2.92796149337568
H	1.75339250245858	7.95220043693319	2.84395768355630
H	1.68491085335796	3.24043034329962	2.98754799082926
H	1.56453616732957	6.85376846739780	1.67501259707437
H	1.82124488076282	4.79754247046296	3.42520601724005
N	1.70952736027027	4.91964685421726	6.63965686091135
N	3.55391613221254	5.88132224474520	4.33351855553463
H	2.13898369404107	5.28804678431416	5.78770868333127
H	4.32691123909340	5.42647612532520	4.81014804070774
H	0.75016200845990	5.24528972770694	6.65334334444706
H	3.77589127577525	5.84016433495618	3.34578375875200
H	2.18106057670098	5.38370099572872	7.40945838909383
H	3.63521344654044	6.86594894069103	4.57789511179880
N	5.54793819024446	1.79968115680176	1.01133616584961
N	3.93028703882608	4.72087302941600	0.90612813009399
H	4.90330001435933	1.07469468722400	0.72558499818159
H	3.00886137362819	4.57593170191105	1.31787574843117
H	5.03925027264439	2.68015698617253	1.02758055517008
H	4.17186143949495	5.70171371740037	1.03195349263318
H	5.84968831981954	1.59297556560104	1.96148415627949
H	3.83851504513115	4.57118184480319	-0.09056674230107
N	6.42688610290075	1.55528597455197	4.13544070038194
N	4.16347731799386	2.81468389057991	6.14523225082163
H	7.01033144715831	2.38337057133789	4.11425253654613
H	4.37180154314591	2.29996862877376	6.99268033704370
H	5.61405554163830	1.80057731235789	4.69673207351359
H	4.86055041725527	3.55580823944038	6.08530392058425
H	6.94049836593720	0.84830265683716	4.64598789576195
H	3.27235683457391	3.28051944382281	6.30909607731423

N	5.21671512013903	7.64275779150431	1.93461317302994
N	6.67268314764268	4.94343496512065	2.64926128098856
C	3.66866839542789	10.00794826730286	4.80263571041967
H	5.85219050683529	4.55753610718237	2.18900485498671
H	5.08547384159263	8.12084960567413	2.82318157808347
H	7.45935839849867	4.36241410294494	2.39164787047986
H	5.92583047334460	6.92773941344806	2.09895634238480
H	6.53664506196218	4.85957559964973	3.65075890748007
N	6.31860062473279	5.35708826533392	6.13820227563066
H	6.66742532121380	6.17604334308562	5.64001440515485
H	5.77365820535172	5.76052069963724	6.90317770896937
H	7.13558949815588	4.94036317548413	6.57948533944792
H	5.61169779242724	8.31764867978471	1.29232379483828
O	4.40383880856336	8.80723865585981	4.75258957992130
H	4.91390688386018	8.70443437639247	5.57302094593365
H	3.16437551175529	10.11869059348320	3.84143928418240
H	2.91091109438431	9.99112184921598	5.59421231881992
H	4.31756764256641	10.87637533598065	4.96085910675329

VDE Determination of the Solid Bulk Crystal Ammonia

	$(NH_3)_{n=14}$	$(NH_3)_{n=23}$	$(NH_3)_{n=38}$
	14	**23**	**38**
	$n^{-1/3}$	**$n^{-1/3}$**	**$n^{-1/3}$**
	0.41	**0.35**	**0.30**
VDE (aug-cc-pVDZ)	**-1.5**	**1.0**	**3.3**
VDE (aug-cc-pVTZ)	**5.8**	**8.0**	**10.1**
VDE (aug-cc-pVQZ)	**9.2**	**11.4**	**-----**
VDE (CBS-2/3)	**7.8**	**10.2**	**12.4**
VDE (CBS-3/4)	**10.0**	**12.2**	**-----**

Table S1. $n^{-1/3}$ and calculated VDE (kcal/mol) values as obtained by different basis sets and CBS at the DLPNO-CCSD(T) level of theory for the three crystalline clusters. Unfortunately the aug-cc-pVQZ value of the $(NH_3)_{38}$ cluster was computationally to heavy.

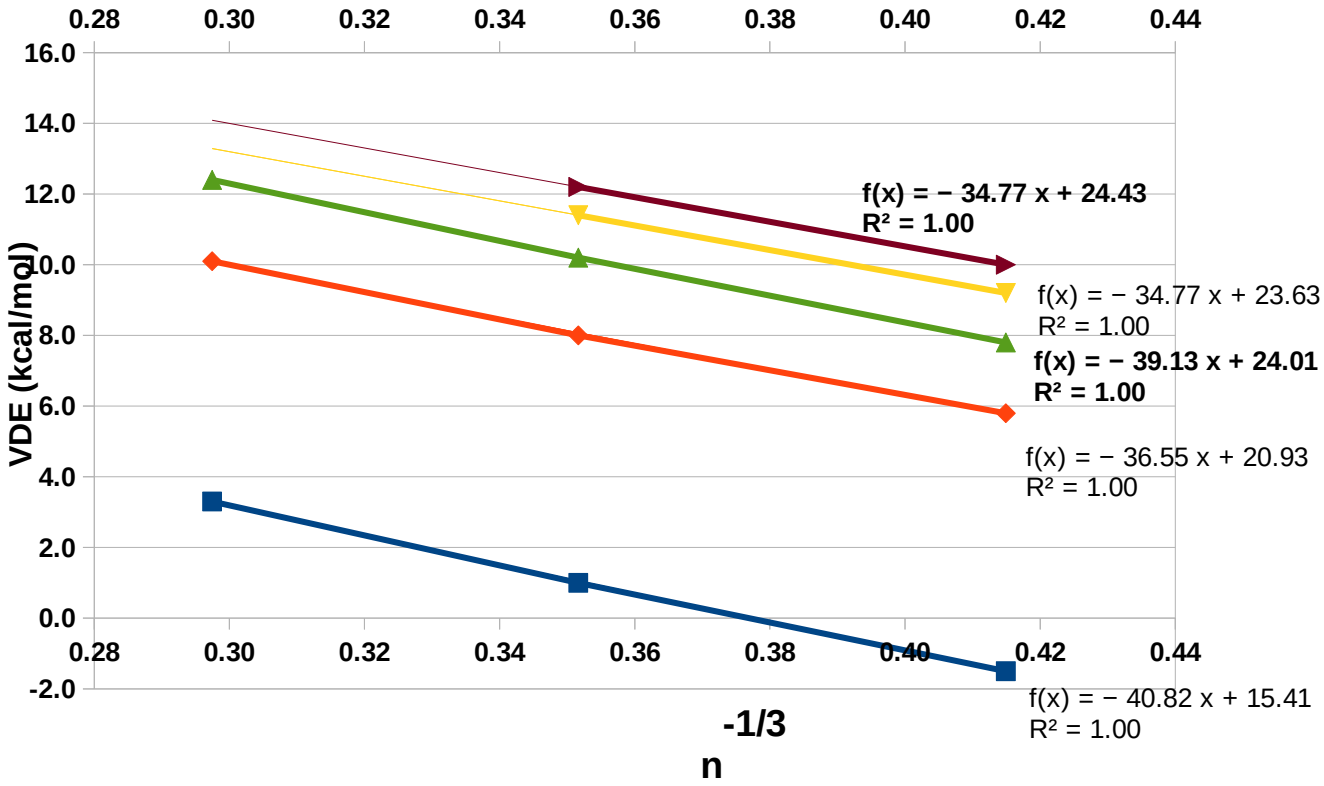

Figure S2. VDE Estimation in solid crystalline bulk by linear fitting of the data reported in Tab. S1. Blue line: aug-cc-pVDZ, orange line: aug-cc-pVTZ; green line: CBS aug-cc-pVDZ/aug-cc-pVTZ; yellow line: aug-cc-pVQZ; maroon: CBS aug-cc-pVTZ/aug-cc-pVQZ.
The intercept determines the VDE in bulk.

		14mer neutral	14mer 1e-	23mer neutral	23mer 1e-	38mer neutral	38mer 1e-
HF	n						
aug-cc-pVQZ	4	-787.15443839	-787.16810917	-1293.18693608	-1293.20417052		
aug-cc-pVTZ	3	-787.10347721	-787.11132559	-1293.10363506	-1293.11506888	-2136.42275409	-2136.43783999
aug-cc-pVDZ	2	-786.89671989	-786.88989513	-1292.76672672	-1292.76547058	-2135.87315590	-2135.87562281
DLPNO-CCSD(T) (correlation correction)	n						
aug-cc-pVQZ	4	-3.84468785	-3.84565862	-6.33208117	-6.33300258		
aug-cc-pVTZ	3	-3.68422854	-3.68560625	-6.06953765	-6.07091153	-10.07352512	-10.07481413
aug-cc-pVDZ	2	-3.11725913	-3.12176600	-5.13860898	-5.14148463	-8.53641350	-8.53925865
DLPNO-CCSD(T)=HF+correlation	n						
aug-cc-pVQZ	4	-790.99912624	-791.01376779	-1299.51901725	-1299.53717310		
aug-cc-pVTZ	3	-790.78770575	-790.79693184	-1299.17317271	-1299.18598041	-2146.49627921	-2146.51265412
aug-cc-pVDZ	2	-790.01397902	-790.01166113	-1297.90533570	-1297.90695521	-2144.40956940	-2144.41488146
	m,n						
CBS E_{HF}(34)	34	-787.16814429	-787.18338099	-1293.20933971	-1293.22813422		
CBS E_{HF}(23)	23	-787.17422670	-787.18709602	-1293.21892042	-1293.23469657	-2136.61081897	-2136.63022292
	m,n						
CBS E_{corr}(34)	34	-3.95891715	-3.95959822	-6.51898314	-6.51958245		
CBS E_{corr}(23)	23	-4.00511734	-4.00472403	-6.59641718	-6.59694110	-10.94348721	-10.94389549
Estimated CBS total energy (3/4)		-791.12706144	-791.14297922	-1299.72832285	-1299.74771666		
Estimated CBS total energy (2/3)		-791.17934404	-791.19182006	-1299.81533761	-1299.83163767	-2147.55430619	-2147.57411841

$$E_{SCF}(n) = E_{SCF}(CBS) + A\exp(-z\sqrt{n}) \qquad (1)$$

$$E_{SCF}(CBS) = \frac{E_{SCF}(n)\exp(-z\sqrt{m}) - E_{SCF}(m)\exp(-z\sqrt{n})}{\exp(-z\sqrt{m}) - \exp(-z\sqrt{n})} \qquad (2)$$

Z_{23}	Z_{34}
4.30	5.79

γ_{23}	γ_{34}
2.51	3.05

$$E_{corr}(n) = E_{corr}(CBS) + An^{-\gamma} \qquad (3)$$

$$E_{corr}(CBS) = \frac{n^{\gamma}E_{corr}(n) - m^{\gamma}E_{corr}(m)}{n^{\gamma} - m^{\gamma}} \qquad (4)$$

Level of Theory and $(NH_3)_n$ Electron Distribution

In Section values``Computational Methods'' the validation of the adopted computational procedure by the available experimental data on single molecules as well as on water clusters, was reported.
Further analysis considered the spin densities visualization, an important parameter to understand electron localization (internal *vs.* external states) and cluster reactivity based on the DLPNO-CCSD(T)/aug-cc-pVQZ level of theory.
As such, the knowledge of the spin densities dependency *vs.* level of theory by comparing DFT and DLPNO-CCSD(T) results will give important clues to better understand/interpret the calculated data.
For such a scope, spin densities derived by two functionals (PBE0, BHandHLYP) and DLPNO-CCSD(T) by using, in each method, four different basis sets; def2-T(Q)ZVPPD, aug-cc-pVT(Q)Z; are performed and results are reported in Figure S3 and Figure S4.

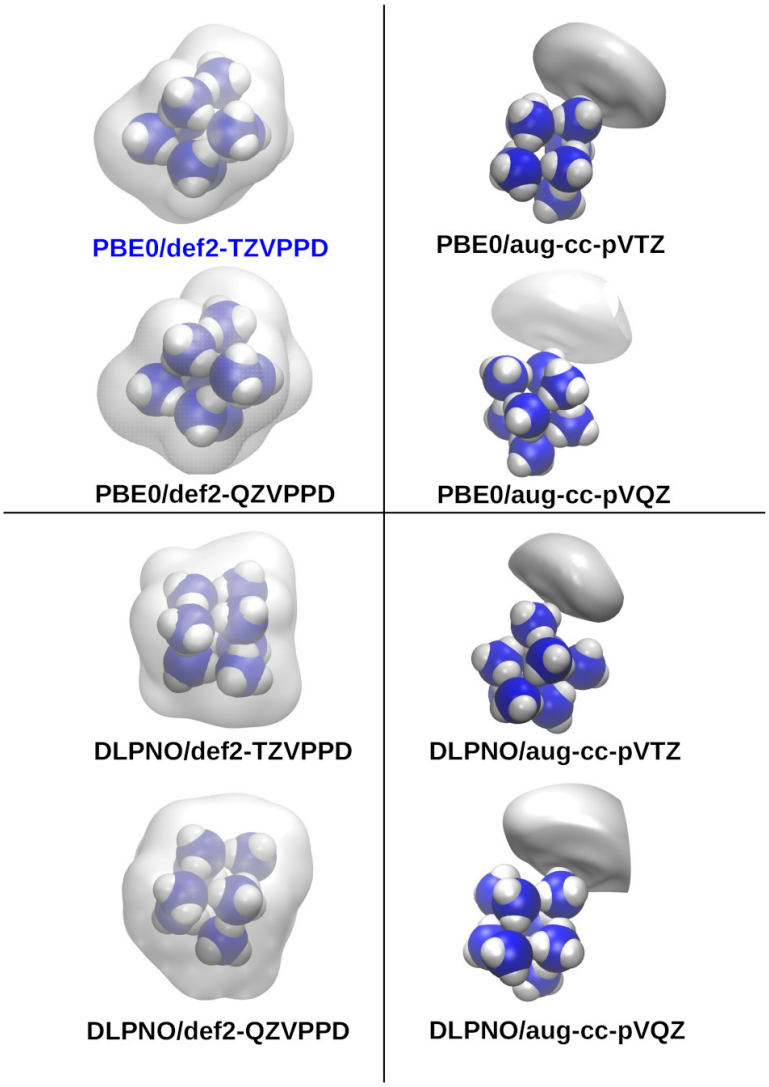

Figure S3. Spin densities calculated at different levels of theory based on the PBE0/def2-TZVPPD $(NH_3)_8^{-\bullet}$ optimized structures. Isosurface value: 0.0001 a.u.

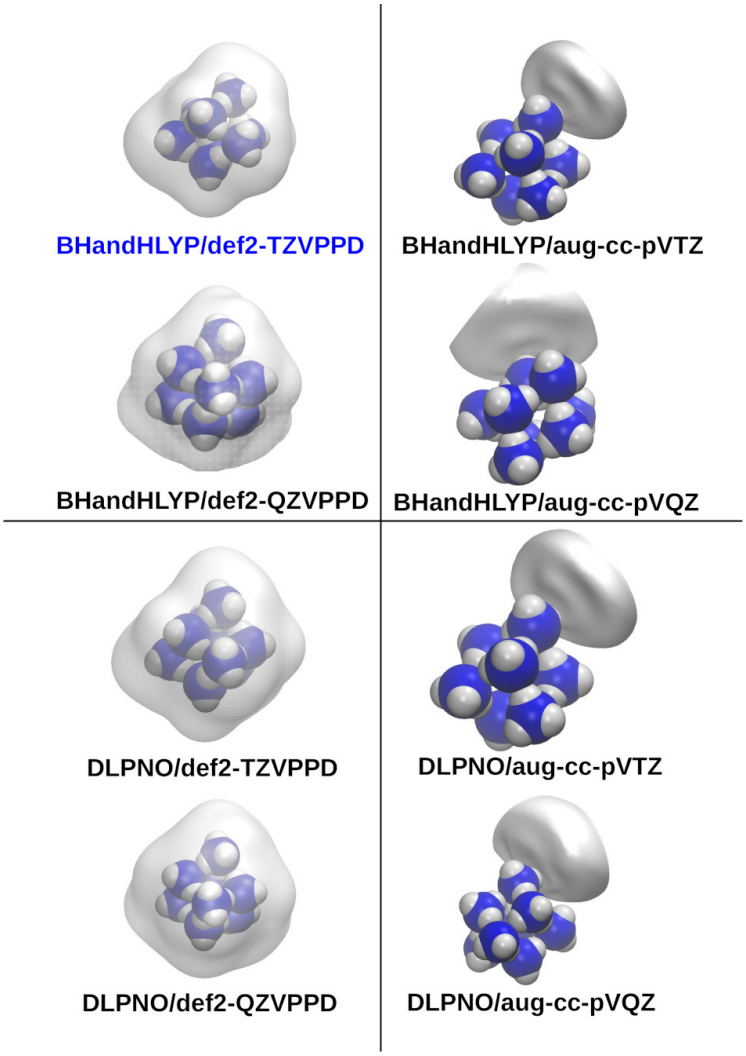

Figure S4. Spin densities calculated at different levels of theory based on the BHandHLYP/def2-TZVPPD $(NH_3)_8^{-\bullet}$ optimized structure. Isosurface value: 0.0001 a.u.

The BHandHLYP functional (Becke1993) was included being reported as a good descriptor of the ammoniated electron in clusters (Baranyi2019, Baranyi2020).
By observing Figure S3 and Figure S4, the spin distribution shows a basis set dependency independent by the applied computational method.
In fact, while both def2-T(Q)ZVPPD basis sets report a spin density enveloping the entire cluster, the electron in both the aug-cc-pVT(Q)Z basis sets is always externally well localized.
However due to the nature of the study, the correlation consistent basis sets should be the preferred one.
A further analysis was performed by comparing the EA estimated by the same computational methods applied to the spin density study.

Method	def2-T	def2-Q	aug-T	aug-Q	Δ[aug-(Q-T)]
PBE0	-21.7	-30.2	1.6	7.0	5.4
BHandHLYP	-26.8	-23.1	-2.1	3.2	5.3
$DLPNO_{PBE0}$	-28.2	-24.5	-2.5	1.2	3.7
$DLPNO_{BHandLYP}$	-28.4	-24.7	-2.4	1.3	3.7

Table S2. Calculated EA (kcal/mol) at different levels of theory based on the optimized geometries (PBE0/def2-TZVPPD; BHandLYP/def2-TZVPPD) of the neutral and radical-anion $(NH_3)_8$

model clusters. Abbreviations: def2-T(Q)ZVPPD=def2-T(Q); aug-cc-pVT(Q)Z=aug-T(Q); DLPNO-CCSD(T) with optimized DFT/def2-TZVPPD input geometry=$DLPNO_{DFT}$.

Assuming the DLPNO-CCSD(T)/aug-cc-pVQZ values as reference, both DFT functionals are in very good agreement reporting only a $\Delta EA_{PBE0\text{-}BHandLYP}$=-0.1 kcal/mol.
However, the general trend shows the correlation consistent basis sets to be the main ``driving force'' determining a good EA estimation also when coupled to DFT methods.
Furthermore though based only on eight data points and a cluster type and conformer, the Δ[aug-(Q-T)] of the EA values as reported in Table S2 show a consistent ~5.3 kcal/mol for both DFT functionals and 3.7 kcal/mol in case of the DLPNO-CCSD(T).
A similar trend was found on the calculated VAE based on the difference Δ[aug-(T-D)] as reported in the Appendix A.
If confirmed on a larger data set based on different cluster dimensions and conformations, such trends can be used to extrapolate values when lower levels of theory are used.

REFERENCES

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VAE dependency on the $(NH_3)_{23}$ cluster geometry during a NVT AIMD simulation

As reported in Section 2, the amorphous $(NH_3)_{23}$ cluster was obtained by ``melting" two ammonia crystal cells (1×1×2) in an AIMD simulation.
In a later Section~\ref{sec:metval} while validating the adopted computational procedure on water clusters, the limitations in comparing experimental to computational data were listed: **I)** experimental data are measured on a finite T PES, while calculated geometries are based on a 0 K PES; **II)** experimental data are measured on a conformational ensemble to be compared to a singly or few computationally optimized cluster conformers.
As such, it was interesting to correlate changes in cluster conformational geometry to VAE during an AIMD simulation.
The VAE is computationally simple to obtain, measuring the neutral cluster ability to stabilize/accept an electron to become a radical-anion at the fixed neutral cluster geometry *i.e.* vertical excitation.
Specifically, eight geometries were extracted by the AIMD trajectory and on each single geometry a DLPNO-CCSD(T)/aug-cc-pVD(T)Z analysis, was conducted.
Results are reported in Table S3.

t (ps)	VAE (DZ)	VAE (TZ)	$\Delta(VAE)_{(TZ-DZ)}$
0.0	3.6	-2.9	-6.6
2.0	3.5	-3.2	-6.8
2.5	2.1	-5.1	-7.2
3.0	5.3	-1.6	-6.9
3.5	4.5	-2.4	-6.9
4.0	1.2	-5.6	-6.8
4.5	6.4	1.0	-5.4
5.0	3.7	-2.1	-5.8

Table S3. Calculated VAE (kcal/mol) on single AIMD snapshots (T=210 K) of the $(NH_3)_{23}$ cluster. Single points evaluated at the DLPNO-CCSD(T)/aug-cc-pVD(T)Z level of theory.

Though based on a simple evaluation by not considering, for example, Boltzmann weights or any population analysis, the results show considerable VAE fluctuations during cluster dynamics.
Notably, as reported in the ESI, by comparing the composite method r2-SCAN-3c (Gasevic2022) (potential energies) and the aug-cc-pVD(T)Z (electronic energies), do show the same trend reporting a MAD=0.6 kcal/mol (compared to aug-cc-pVTZ) proposing the composite electronic-structure method r2-SCAN-3c as a valid tool in cluster AIMD studies (at least in the neutral form).
As such, conformational changes at finite T are important for a better understanding of the cluster behavior and sophisticated AIMD enhanced sampling techniques to expand the conformational space exploration should be applied.
However, single point calculations at high level of theory (correlation consistent) can be properly used to estimate, on the selected AIMD geometric ensemble, electronic related parameters such as EA, VAE and VDE.
To be noticed, a quite constant $\Delta(VAE)_{(TZ-DZ)} \approx 6.5$ kcal/mol between the double-ζ and triple-ζ basis sets, denoting a possible ``correction parameter" characteristic of the theoretical level and cluster (number of NH_3), as similarly found in the spin density distribution (see ESI “Level of Theory and (NH3)n Electron Distribution”).

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Thomas Gasevic, Julius B. Stückrath, Stefan Grimme, and Markus Bursch
J. Phys. Chem. A **2022** *126* (23), 3826-3838 DOI: 10.1021/acs.jpca.2c02951

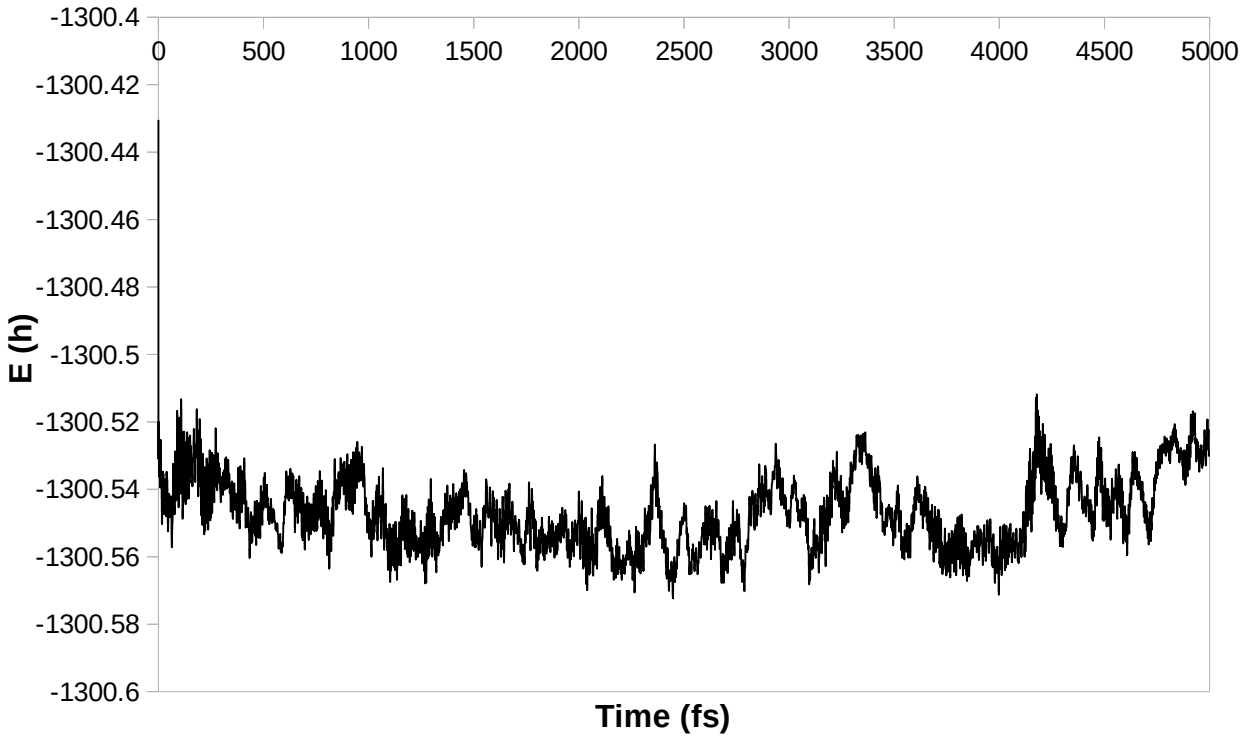

Figure S5. Potential energy time evolution of 23 NH_3 molecules, NVE, T=210 K. Only the last 5ps of a 10 ps simulation are reported.

AIMD : correlation r2-SCAN-3c with aug-cc-pVD(T)Z

Simulation time (fs)	0	2000	2500	3000	3500	4000	4500	5000
$HOME/Neutral/(TZ)	0fs	2000fs	2500fs	3000fs	3500fs	4000fs	4500fs	5000fs
E_pot (AIMD, r2SCAN-3c)	-1300.52876973	-1300.54064459	-1300.54493584	-1300.54825785	-1300.55002641	-1300.55987042	-1300.54514401	-1300.52737086
DLPNO-CCSD(T)/aug-cc-pVDZ	-1297.86635452	-1297.87541010	-1297.88493661	-1297.88336004	-1297.88889504	-1297.89510379	-1297.88819251	-1297.86152378
DLPNO-CCSD(T)/aug-cc-pVTZ	-1299.12059553	-1299.13024475	-1299.13726464	-1299.13859682	-1299.14334703	-1299.15203753	-1299.140473545	-1299.12015285

-0.88	-8.33	-11.02	-13.11	-14.22	-20.39	-11.15	0.00	E_pot (AIMD, r2SCAN-3c)
-3.03	-8.71	-14.69	-13.70	-17.18	-21.07	-16.73	0.00	DLPNO-CCSD(T)/aug-cc-pVDZ
-0.28	-6.33	-10.74	-11.57	-14.55	-20.01	-12.75	0.00	DLPNO-CCSD(T)/aug-cc-pVTZ

									median
2.2	0.4	3.7	0.6	3.0	0.7	5.6	0.0	Δ (r2SCAN-3c – aug-cc-pVDZ)	2.2
-0.6	-2.0	-0.3	-1.5	0.3	-0.4	1.6	0.0	Δ (r2SCAN-3c – aug-cc-pVTZ)	-0.4

0.0	1.8	1.5	1.6	0.8	1.5	3.4	2.2	abs dev
0.2	1.6	0.1	1.1	0.7	0.0	2.0	0.4	abs dev

1.3	MAD
0.6	MAD

Figure S6.
1st Table: list of AIMD r2-SCAN-3c and aug-cc-pVD(T)Z potential energies (hartree) calculated on the selected time-shots;
2nd Table: potential energies differences subtracting the highest value in energy within the same set of data (kcal/mol);
3rd Table: differences between the r2-SCAN-3c and the aug-cc-pVD(T)Z calculated by the 2nd Table and median of the differences (kcal/mol);
4th Table: absolute deviations by Table 3 (kcal/mol);
5th Table: MAD (Median Absolute Deviation) by Table 4th (kcal/mol).

AIMD snapshots: XYZ Coordinates (Coord.=Å)

Neutral+Radical Anion input

0fs
92
ORCA AIMD Position Step 0, t=0.00 fs, E_Pot=-1300.52876973 Hartree, Unit is Angstrom

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N	5.8740071573	-1.2944030425	3.8943812146
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H	1.4469768315	0.9275080412	3.8827062439
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H	1.1571850075	2.3753771564	4.4576790402
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H 4.9091484806 -0.5665860253 7.0439512661
H 4.6865497999 3.3670994435 8.5561868115
H 5.2218890005 -1.9672500643 6.4514645760
N 6.7047960610 2.0684056340 6.0800243251
H 6.4897413623 2.9994267594 5.5940246153
H 7.6654377127 2.0851041859 6.3134853717
H 6.5142136290 1.3916819676 5.3407686495

2500fs

92

ORCA AIMD Position Step 5000, t=2500.00 fs, E_Pot=-1300.54493584 Hartree, Unit is Angstrom

N 9.2627555839 7.3013855881 3.7433859221
H 9.4141699412 8.3350659986 3.9064659718
H 8.3261608091 6.8855907310 3.7987942336
H 9.9419825387 6.7924069782 4.2581270190
N 2.8803426801 6.5089175444 3.1786753250
N 5.8341822650 4.1648200301 0.5670444749
H 3.7841400252 6.8633618258 3.5693334128
H 6.7113593222 3.6746243897 0.8036745526
H 2.9539098761 5.5107615730 3.3174221977
H 6.1777068967 5.0163952061 0.2468096745
H 3.1089418874 6.5889109561 2.1482119601
H 5.3584826596 4.2197831172 1.4855567666
N 12.5400380860 4.7074571257 4.4923304825
N 6.3290235590 7.8056542331 2.7581475493
H 11.8697900065 5.3692644257 4.8347632624
H 6.4115885210 8.2909157889 3.6978211846
H 12.0937368495 4.0274428533 3.8532630527
H 7.2206089388 7.7620094920 2.2216156426
H 12.9062625458 4.2040962398 5.3130464183
H 5.7676387680 8.4698275088 2.2394831189
N 3.6206424886 2.8946621017 2.4399194277
N 3.2683259848 6.0279479358 6.1979775449
H 3.4178074130 3.4595291059 1.5902571796
H 3.4172663512 5.0731887742 5.9209899067
H 2.7950645481 2.4950089180 2.8333979255
H 2.4841861336 6.1108200898 6.8332130751
H 4.0604964138 3.5585086555 3.1008886391
H 2.9755993598 6.5174648926 5.3787767078
N 8.7409596031 7.2590203336 -0.1699320353
N 6.2653620659 3.6718121055 7.6842542816
H 9.0432921022 6.2692805512 -0.4237523600
H 5.3785531212 3.5869442446 7.2483430219
H 9.1398578288 7.8937172401 -0.8622614861
H 6.0303120913 3.8325563256 8.6943341312
H 9.2418237867 7.4215431262 0.6793692288
H 6.7139294374 4.5052841783 7.3800210210
N 7.4166447721 1.2378514685 -0.8559422969

N	3.9816257589	1.6021594668	5.9724754155
H	6.4147169602	1.4063026532	-0.8465087875
H	4.8160592153	1.1992990936	6.4195052397
H	7.7915355129	2.1560452135	-0.6242349302
H	3.2087374559	1.5164985908	6.5671609412
H	7.7560922033	0.9372797097	-1.7595053043
H	3.7719307349	1.1547256776	5.0915329281
N	6.4068068615	8.3732078639	5.6885476801
N	6.7706927361	5.0081130140	4.1820087156
H	5.8330940479	7.6383543788	6.0972440408
H	6.0592978131	4.5245490191	4.6940099178
H	7.4026660825	8.0681496970	5.6439597194
H	6.4103290686	5.5422338883	3.4093566198
H	6.3545421048	9.1828078877	6.3246390479
H	7.2629196689	4.2671731080	3.6954110449
N	7.0524255126	1.2138531468	3.5607596967
H	6.8557269213	0.9368359178	4.5397228083
H	6.1499904009	1.5756878811	3.2051680400
H	7.1120221355	0.3652412286	3.0054579187
N	9.1415647242	2.9591157348	1.3684583724
H	9.1937331332	3.1438133585	2.3675279486
H	9.1190484597	1.9600205766	1.2640088249
H	9.9048236879	3.3990680480	0.9062678740
N	9.2892782696	5.3280156303	6.3295987552
H	8.5388848195	5.3202237133	5.6374260906
H	9.1280276889	4.6383729779	7.0465639416
H	9.4379875742	6.2431622745	6.7087050744
N	7.7460850959	-1.1433944439	1.1279463582
N	11.0528396258	5.4981263179	1.1215050950
H	7.7624885663	-0.3631109958	0.4486295207
H	11.8475577854	5.1864797590	1.6379436012
H	8.7230024277	-1.4209060059	1.2490677403
H	11.3749039002	5.7245463407	0.1912034812
H	7.3378291240	-1.9218608128	0.5945954449
H	10.7623666166	6.3811789554	1.5743463975
N	0.8232917896	1.7548021078	3.7918853738
N	4.1610418940	-0.3310510890	1.6700186893
H	1.1678524706	0.7794545575	3.9849438809
H	5.0930796892	-0.7529253073	1.4590724514
H	1.0167922874	2.1968872579	4.6937970483
H	3.6798092774	-0.5250180368	0.7570889296
H	-0.1719772337	1.6232664694	3.6095498860
H	4.2397971620	0.7202692395	1.7395284751
N	2.8059651551	3.9827369892	9.5865975916
N	2.4262837658	-1.0775232685	4.5936124943
H	1.8596679489	4.1833544951	9.8303773270
H	2.9977290056	-1.3199544573	3.7393989232
H	3.2892270360	4.8133131351	9.3214970026
H	3.0717537967	-1.0907174803	5.3732099416
H	2.8545067024	3.2741323348	8.8789408898
H	1.7795354061	-1.8149411637	4.8325095805
N	6.7928720955	0.2801254169	7.5043584694
H	7.2416396803	1.0906975237	7.2299455257
H	6.5575977771	0.3868187864	8.4664560388
H	7.4748517705	-0.4863199067	7.3979231771

3000fs
92
ORCA AIMD Position Step 6000, t=3000.00 fs, E_Pot=-1300.54825785 Hartree, Unit is Angstrom
N 10.0588547546 6.0813163950 4.2397093886
H 9.3423365361 6.5526576775 3.6909876181
H 9.6659234343 5.1918143687 4.5833938192
H 10.3027493424 6.6378624563 5.0062461529
N 3.8119671695 6.8815935758 3.5861959899
N 6.0145183374 4.7906424916 -0.2309497631
H 3.5113941237 7.6217028207 4.1832106092
H 6.9622449228 4.6003656639 0.0814948503
H 4.1372239561 7.3909032791 2.7907960293
H 5.8667431522 4.0231044335 -0.9507019485
H 2.9673425997 6.4570320907 3.1866445894
H 6.1198334994 5.6894451518 -0.6778158997
N 10.7051711179 2.8135475433 6.1818621593
N 6.7511028574 8.0584021640 2.5937285031
H 10.4244572166 3.4204965816 6.9550356615
H 6.4089827521 7.3454789470 3.2139551588
H 11.7003454301 2.8783554484 5.9621814934
H 7.0884558567 7.7304842011 1.7314282325
H 10.1525714656 2.9703392095 5.3455723757
H 7.5299452321 8.3856216369 3.1110475634
N 3.4297116658 2.9133673674 1.4963133478
N 3.4997198697 4.6828789725 5.9916277517
H 3.8830210530 3.6659084284 0.9676401075
H 3.5881441220 3.7954548424 5.5236682752
H 2.4632790707 2.8631848982 1.2955436802
H 4.2336847571 5.2375972916 5.5607469651
H 3.6355607292 3.0856089241 2.4973439122
H 3.8642556685 4.5645218415 6.9298468592
N 8.5469981807 7.1306416301 -0.3980053559
N 7.0465330532 3.7975968316 7.6627213024
H 9.3330872128 6.5314737513 -0.1170977698
H 6.6681660125 3.0822167391 6.9762409524
H 8.4148187313 7.0274134898 -1.4115516437
H 6.3790044597 3.8144745180 8.4012961606
H 8.9184804416 8.1258544601 -0.2922139287
H 6.8011285294 4.6799338486 7.2330794774
N 6.3414157731 1.3174779191 -0.2197931873
N 3.8259666289 1.6895230699 4.6317660893
H 5.6710328596 1.1787881577 -0.9595161260
H 3.9953478129 0.9762522840 5.2975930261
H 5.8898611872 1.9683043282 0.4228934978
H 2.8074396210 1.6278715143 4.3408907124
H 7.1523717881 1.7599507365 -0.6281933675
H 4.3252351048 1.2675635700 3.8530032918
N 7.4741968200 6.9699615742 6.7386848546
N 6.6932118793 4.3995868585 4.1627068451
H 8.3084393927 7.3582254479 7.1492803194
H 5.9590021192 4.1992110669 4.8358108787
H 7.7986589245 6.3565304685 5.9903846936
H 6.3146710006 4.9427655957 3.4116025750
H 6.9930997071 7.7810469448 6.3468419386
H 6.9629768335 3.4973970582 3.7449612673
N 7.5443871473 1.4273853671 3.1645943437
H 7.3874596158 1.3794403176 4.1699039296
H 6.7281832339 0.9838152180 2.7745434543
H 8.2903651441 0.7939288343 2.8511751538

N 8.7118703940 3.7946645516 1.0640693297
H 9.5609185437 3.6780215277 0.5195603475
H 8.7658243985 4.5563669108 1.7136418294
H 8.5510280840 2.9528706179 1.6313120565
N 10.0287803578 3.6504289289 9.3400788206
H 9.0803091266 3.7486364493 8.9495401003
H 10.2160880087 2.6641301148 9.4267280932
H 10.1508818476 4.1552962468 10.2295418061
N 8.2773788599 -1.2390024448 1.3955046841
N 11.5022790533 5.7955544702 0.9936094136
H 7.6219610227 -0.9328279403 0.6987697598
H 11.6040028521 4.9680872408 1.5808328219
H 9.1099119228 -1.6876595947 1.0132657472
H 12.3487876704 5.8611334182 0.3902601610
H 7.7702676768 -1.8985686290 1.9623435417
H 11.5342785391 6.5597904952 1.6418706523
N -1.1491216020 5.1459954509 4.9978857517
N 3.8916825777 -0.3990668032 1.1495146641
H -0.3361317518 5.1840878058 5.6410175557
H 4.6720505386 -0.7479967644 0.6432028248
H -1.9784364681 4.8913679640 5.5519940784
H 4.0192866227 0.5742390334 1.1287048125
H -0.8575362633 4.3369719922 4.4272525172
H 4.0781290053 -0.6698542565 2.1273990919
N 3.6604559608 4.9236928335 9.1636165394
N 0.9935225986 0.6854277624 2.1462317501
H 2.9918910064 4.2567387927 9.5216895552
H 1.7006889512 0.2728747053 1.5535513684
H 4.0214114848 5.2772716794 10.0153418946
H 0.3003592940 -0.0457068043 2.3488679564
H 2.9691458580 5.6048996521 8.8234655306
H 0.4592526462 1.2765239078 1.5120471512
N 6.9481006288 -0.1981501842 6.7514070142
H 7.3451765242 0.6148420653 7.1563126404
H 6.7667614929 -0.8487715878 7.5301009758
H 7.8180606161 -0.6585403617 6.3886008274

3500fs

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ORCA AIMD Position Step 7000, t=3500.00 fs, E_Pot=-1300.55002641 Hartree, Unit is Angstrom

N 10.2935918830 3.4874289691 4.7589770280
H 10.2925602519 4.3017367634 5.3454697795
H 9.3079828299 3.3820449357 4.6601561196
H 10.4663924718 2.6772032884 5.3882340476
N 3.5777039704 6.2556619705 3.8103102268
N 6.3531757228 5.9491960571 0.2630925545
H 2.6290023334 6.0334992983 3.9628058487
H 7.0119902117 5.2098805034 0.1960441950
H 3.7128340282 7.1511187537 4.1752397944
H 6.1060795138 6.2545785535 -0.7013905398
H 3.8094878751 6.3350348936 2.8233561504
H 6.9139689338 6.7039266024 0.7195960126
N 9.1636332284 -0.3702107600 5.6677232320
N 7.6054132357 8.3694772259 1.9789772961
H 9.8072773165 -0.7174209045 4.9431504000
H 8.4170219414 8.7162806719 2.4203510068
H 8.9498174614 0.6149146985 5.4335424012

H	6.9124241574	9.1433687187	1.9758016922
H	9.6862590019	-0.3556147872	6.5315108719
H	7.3031401803	7.6816771546	2.6924486625
N	4.3888382053	3.2372894632	2.3595254286
N	2.3375625822	4.4643747559	6.8264715898
H	4.9866588150	3.9010066581	1.8321442812
H	2.4326363943	3.4925123801	7.0622205707
H	3.6057440589	3.1215628932	1.7285891066
H	2.9720783864	4.5704787720	6.0305966635
H	4.0678972624	3.7326456054	3.1574352373
H	2.7565429357	5.0672651966	7.5201424620
N	10.2810517801	8.2191826393	-0.8244132055
N	5.2348627310	2.5340700533	7.4435922087
H	10.6595720162	7.3421778744	-1.0940897783
H	5.5094167548	1.5640629028	7.4464034760
H	9.3460657728	7.9966160736	-0.5295786215
H	4.4730999730	2.4666256148	6.7258616732
H	10.1592992704	8.7372148640	-1.7313060732
H	5.9708687327	2.9697301341	6.8289880174
N	6.4778350915	2.0901984869	-0.1937591750
N	2.9177950032	0.9392318459	5.4547192524
H	5.5466364021	1.7067382377	-0.1154454980
H	3.4602056930	1.4723834180	4.7739400477
H	6.5314695535	2.6829616429	0.6273910399
H	3.3561675586	0.0080698645	5.6446819303
H	6.3650885850	2.7238925862	-0.9807425679
H	2.0376361504	0.8522067752	4.9800361574
N	6.1922324408	5.7183110121	5.8468530364
N	7.3779768812	5.2706449528	2.9797593829
H	6.0598912815	6.4302332722	6.5710851702
H	7.4164101108	4.5589115184	3.7239064394
H	6.7921964772	6.1518527609	5.1502612394
H	6.5071352841	5.2642954078	2.4685478381
H	5.2914877500	5.6995634483	5.3910080516
H	8.0501817482	4.9259733858	2.3258653672
N	7.2719468823	2.0335958830	3.9066889716
H	7.0193968539	1.6534271943	4.7991435428
H	6.3770843489	2.1034975843	3.4320585309
H	7.8747551074	1.4096619694	3.3975535316
N	9.3523032716	3.9840085520	0.8052188825
H	9.9134739500	4.4093195596	1.5569355924
H	9.3313464351	2.9774439511	0.9886643476
H	9.9154103927	4.2126996690	-0.0135061056
N	9.0360379451	1.9635335637	8.3518804486
H	8.0677263014	2.1825028956	8.2411995848
H	9.3761798344	2.3861871542	9.2143880957
H	9.4914096285	2.3501961862	7.4928191922
N	8.5921710338	0.1574716345	1.1195963717
N	11.6230916876	5.7750573579	1.6603312373
H	9.2092362993	-0.3144403512	0.4511806646
H	11.1724562255	6.6779399487	1.6921193290
H	8.0211062811	-0.5633192229	1.5949715355
H	11.6675163812	5.4491408061	2.6226619494
H	7.9701078120	0.6227519703	0.4664931185
H	12.5791808241	5.9883239274	1.4059000446
N	0.6118558171	6.5449090060	4.7377548060
N	3.2288090422	0.3119599265	1.7195916850
H	-0.3884171772	6.6202477386	4.8913514741
H	2.9158151355	0.3988600624	0.7548369949
H	1.0704814290	5.9293016933	5.4421867868

H	3.9856114765	1.0106014185	1.9720796903
H	0.9273248584	7.4822367200	5.0228017045
H	3.6522614001	-0.6295493154	1.8999679771
N	4.6915711024	5.4676011215	9.3837989098
N	1.3719040010	3.0728167788	1.3325751386
H	5.4891825098	6.0675471486	9.1281287958
H	1.3628177501	2.1958373921	1.7822232800
H	5.0834366359	5.1676812735	10.2213459067
H	1.1561391408	3.7956390396	1.9958417353
H	4.7838156396	4.6986291900	8.7211783710
H	0.6094396293	3.0667436127	0.6871750753
N	6.6565814439	-0.5149914389	7.3057419150
H	5.9618882959	-1.2432800120	7.5098585004
H	7.3230036475	-0.7419781993	6.6179197517
H	7.2256000797	-0.4292500909	8.1352981261

4000fs

92

ORCA AIMD Position Step 8000, t=4000.00 fs, E_Pot=-1300.55987042 Hartree, Unit is Angstrom

N	10.0721911885	1.9514400814	4.2647907689
H	9.0933664712	2.0133914728	4.3401863455
H	10.4801291905	1.3097161299	4.9914361432
H	10.5886882837	2.8517357321	4.3841072446
N	4.0099509520	9.2617219515	1.6697316695
N	7.1171852616	5.3689349844	0.7705558594
H	3.7186628114	8.6885415089	0.8998651830
H	7.8373032388	5.2855293164	0.0813355946
H	3.5071086442	8.8334275998	2.5119999623
H	6.2621615410	5.3542817738	0.3002337706
H	3.6335905104	10.2000966494	1.6166920284
H	7.1985802757	6.3055955251	1.2299964199
N	8.8411722808	-2.3819318085	4.4932495192
N	6.9552367860	8.1978615164	2.3778754463
H	9.4827198914	-1.8252460013	5.0079915343
H	7.6430898915	8.8392552358	2.8326822899
H	9.3750343893	-3.2446718964	4.3914350483
H	6.1539368652	8.7489782565	2.1343446256
H	8.8657945832	-1.9393144704	3.5838358646
H	6.6814323763	7.5113581468	3.1338072215
N	4.7406170032	4.7162324690	2.9629227012
N	2.1510422447	5.2305227979	6.7310674666
H	5.5965895096	4.5053439081	2.4884561901
H	2.4373107587	4.2390622087	6.7027877630
H	4.2746390902	5.4579200202	2.4490988187
H	2.4692596498	5.5315843554	7.6554436556
H	4.9800081321	5.1107128374	3.9040289172
H	1.1354494741	5.2939996699	6.7969158367
N	9.5809774801	7.7959635778	-0.2745365224
N	4.7471038629	1.8961611316	7.3228623723
H	9.1775223501	7.3753657417	-1.0775331705
H	4.9602155520	0.9388603617	7.1158213689
H	9.9562103183	7.0627588678	0.2677643784
H	3.8034070927	2.0462699129	6.9694607275
H	8.7951291051	8.1109755798	0.2627125124
H	5.3524481563	2.5030510552	6.8789710080
N	7.7719395252	2.0517202311	-0.2067550562
N	1.5520695456	1.7945266881	6.2344720479
H	7.1245275998	2.0248996201	-0.9656424252

H 1.6424324178 2.1247002650 5.2434795333
H 7.3754626244 2.4573569812 0.6193628416
H 1.5093038529 0.7653680271 6.2542148949
H 8.5149158244 2.6662981914 -0.5038252330
H 0.6393226618 2.1069702492 6.4579207651
N 5.7570053912 6.6238906613 5.8522018506
N 8.5521332176 4.9242362489 3.6421320822
H 5.5051960041 5.9459376389 6.5578290739
H 7.9772211662 5.3341351476 4.3953803669
H 6.2829817574 7.3442404866 6.4024040374
H 8.0245349166 5.0794331531 2.7944088945
H 4.8710996971 7.0681865628 5.5908148753
H 8.5233464904 3.9316482419 3.8446933367
N 6.7972595833 1.5405022756 4.0352265882
H 6.9465329335 0.9846332053 3.1871783480
H 6.3680538869 0.8581704299 4.6810867832
H 6.1117477086 2.2831193351 3.8326104912
N 10.5617831836 3.9906741127 -0.2020283271
H 10.6910692654 3.0768859723 0.2426874335
H 11.3769127868 4.1100785223 -0.7978753510
H 10.6989148078 4.6488126068 0.5779207177
N 8.7577419920 0.1800187550 6.6841613798
H 8.0773206701 0.6082456899 6.0715595012
H 8.2012361075 -0.1592343286 7.4800780071
H 9.2816577757 1.0056164140 6.9347707814
N 8.8846711723 -0.2132263133 1.6626054062
N 11.5536174453 4.8920432750 4.1169428378
H 9.1153505736 0.3879432080 2.4257345211
H 12.3852490207 4.9080898470 3.5354277118
H 9.6951489861 -0.7007777355 1.3090196223
H 10.7967119942 5.2716289139 3.5883831614
H 8.5756613895 0.4519146929 0.9700884144
H 11.7314589403 5.5460580076 4.8936866221
N 2.0595549488 8.0861414791 4.2307560446
N 3.7361025399 1.3989508502 2.1870489377
H 1.1556527136 8.4717207299 3.9327357230
H 3.9733111980 2.1487781980 2.8091459771
H 1.8651708867 7.2102149370 4.6853628571
H 3.6830631824 0.5189399822 2.6401128092
H 2.3621947823 8.7901826633 4.9186036032
H 4.5398008229 1.2549232938 1.5481922683
N 4.2118907231 4.5871372268 9.1421894541
N 0.8748138981 4.7789151523 3.3586061310
H 4.9172356780 4.7288105301 9.9148519020
H 0.9363854121 3.9080016082 2.8934652612
H 3.3775994556 4.8101915480 9.6735639547
H 0.7626244073 5.4894011973 2.6631639114
H 4.2141259870 3.5740192047 9.1178623984
H 1.7504654544 4.9491501002 3.7890960673
N 5.5589298413 -1.7937823372 5.3687629391
H 5.0531338475 -2.1618658366 4.5967057634
H 6.5814863002 -1.9500052722 5.1927086198
H 5.2729865906 -2.3338235638 6.1303954694

4500fs

92

ORCA AIMD Position Step 9000, t=4500.00 fs, E_Pot=-1300.54514401 Hartree, Unit is Angstrom

N 12.4046104330 -0.0494194433 4.7610730595

H	11.8644043554	-0.8637912623	5.0665268339
H	13.1952874996	0.0349519273	5.4293118903
H	11.8411619733	0.7078319237	5.1160814130
N	4.0448307992	8.8074111950	1.4085041018
N	6.9530736845	5.1627394032	-1.2377177603
H	3.4942067557	9.0211647371	0.6165914101
H	7.8083550832	5.3461830611	-1.8400230009
H	3.4382824538	9.0268653224	2.1515254215
H	6.1811168451	5.2081356907	-1.8785933634
H	4.7888812925	9.4948503293	1.4954891238
H	6.8766967354	5.9880503608	-0.6447786217
N	6.8208831397	-2.5533497659	2.8569982034
N	7.1717153180	7.1902413740	1.2868316345
H	6.2836229113	-2.8621607943	3.6609097392
H	7.7167606398	8.0539979540	1.3238844769
H	6.3978303411	-3.1369119762	2.1386375091
H	6.2070418979	7.4402965721	1.5398256084
H	7.7006838029	-3.0238775927	2.9499502959
H	7.6152919284	6.6436799073	2.0474319466
N	4.5369754745	5.1291266428	2.6294557406
N	4.2325408935	6.7050964583	6.6076312560
H	5.2721527919	4.8612763904	1.9456893223
H	3.4378841785	6.1954599766	7.0004078224
H	3.9548976854	4.3007755917	2.7041188021
H	3.9977218596	6.7612414821	5.5973363719
H	4.0004976824	5.8683710513	2.2497495475
H	5.0249371094	6.0847280493	6.6642665324
N	10.2059848019	8.3031533151	1.2011463762
N	4.9785252616	2.9186446111	5.2630768281
H	10.0236227183	7.4470481165	1.7007081759
H	5.6347308524	2.1556359217	5.0597655675
H	10.1623537533	8.1255128962	0.1770974115
H	5.2100283798	3.6148105273	4.5411073389
H	11.1581070543	8.5761559110	1.4824826055
H	5.3969071422	3.4117287463	6.1015237552
N	6.2163011547	2.6273772796	1.1659909778
N	2.1021237130	1.9689843930	5.8258407641
H	5.2779555643	2.3405850466	1.3966277818
H	2.9718531059	2.4657277085	5.6395304952
H	6.2399348859	3.5174690892	0.6517470985
H	1.3115427063	2.5780234264	5.6147089583
H	6.5218514615	1.9395660911	0.4786658799
H	2.0967997463	1.9494752780	6.8213896580
N	7.2779559139	7.0689825786	6.6180137757
N	7.9413297093	4.2449396253	3.8001301459
H	6.7092903268	7.6025569669	7.2731124254
H	7.3946585250	3.4146088134	3.7487307633
H	8.1378244726	7.6545570514	6.4689175463
H	7.6891852168	4.7546947510	4.6401578138
H	6.7906056523	7.1358935441	5.7100758736
H	7.6407758367	4.8096343609	2.9704214246
N	7.5435283194	0.6448077015	3.9435236859
H	8.2488238438	0.8487955988	3.2413917531
H	7.3535213500	-0.3371536861	3.8240876858
H	6.7165000979	1.1320198580	3.6712227174
N	10.4296211766	5.1234556716	2.1325940693
H	10.2130301797	4.8589415426	1.1807046883
H	11.3921770070	4.8974617239	2.3535238053
H	9.8195842792	4.6098225077	2.7857796410
N	6.9512468189	-1.2806232185	6.2526618658

H 7.7300156638 -0.9410172087 5.7629527303
H 6.4172823927 -0.5094907288 6.6087082649
H 7.2895020826 -1.7944111190 7.0378568254
N 10.2728308386 0.6605884010 2.0351947590
N 10.7194190632 2.6095974802 6.0377608270
H 11.0521975709 0.1617493405 2.4775191130
H 11.0282937437 3.4837817794 5.6552742823
H 10.3097099524 0.4945113929 1.0200466730
H 9.7547763119 2.4986168804 5.6679715341
H 10.5030900143 1.6952888526 2.1573108928
H 10.6251043753 2.7048277724 7.0603500435
N 2.0128210214 9.0250011690 4.7020194338
N 2.4677321055 2.6548061737 2.5542663623
H 1.7504188187 8.0978801865 4.3443159115
H 1.5577196114 2.8234447914 2.0634856549
H 2.3250874814 8.9067949108 5.6549715297
H 2.7961980507 1.7758901706 2.1275506273
H 1.0754362193 9.4525558828 4.7430148420
H 2.1646805144 2.3213018357 3.4282900001
N 4.0962864538 3.0213781409 9.1241217818
N 1.4940341543 5.5212660016 3.8343271986
H 4.5679302180 3.8796736349 8.8941228259
H 0.9613885150 5.3254650528 4.6983468455
H 3.9028839116 2.8630796698 10.1132783174
H 1.4014010781 4.7193347427 3.2315410396
H 4.7095957460 2.3248839739 8.7122809685
H 2.4738301660 5.6088282496 4.0652584125
N 3.8656080790 -0.4917772211 3.7246430373
H 4.7128464640 -0.0267779670 4.1316794884
H 3.0306651034 -0.2646948556 4.2476102932
H 4.0582464683 -1.4674815458 3.7770233561

5000fs

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ORCA AIMD Position Step 10000, t=5000.00 fs, E_Pot=-1300.52737086 Hartree, Unit is Angstrom

N 10.4699334388 -0.3191463689 4.2162850089
H 9.8707032493 0.1853357085 4.8307881429
H 10.6642556207 -1.2393713879 4.4515781355
H 11.3606863167 0.2465122196 4.1194763779
N 4.7523113994 8.1433374448 2.6724958754
N 6.6835327110 6.0559022967 0.6548325427
H 5.2697248295 8.2764971678 1.8174739494
H 7.1969121321 5.5093882546 -0.1272341003
H 4.9604360336 8.9461954139 3.2074786615
H 5.8083595438 6.3362391990 0.1882636625
H 5.1190401074 7.3159001484 3.1645601221
H 7.2877719500 6.8400536265 0.7799921116
N 5.3982197805 -2.8793437080 3.1317943662
N 8.5523149438 8.4319435699 1.7996663398
H 5.7311839243 -3.8430248689 3.0491351337
H 9.5462453113 8.1817358608 1.7756350564
H 5.7322368233 -2.5852049625 4.0238530683
H 8.5123553956 9.4376520176 1.9751897464
H 4.3810320664 -2.7621603472 3.1464268906
H 8.2817855972 7.9571357346 2.7195936036
N 4.2918300829 5.1500544728 2.5868349810
N 4.1814145466 5.0237545743 5.6534237690
H 5.1842962959 5.1931882941 2.1845089283

H	4.2077676314	4.6898398861	4.7010465101
H	3.9318086151	4.2607558543	2.2017782569
H	4.6691035345	5.9188192446	5.5852162778
H	3.7363486187	5.8498329915	2.0769737140
H	4.7712162505	4.4142660133	6.1816825975
N	12.4898069319	9.1021311259	1.6380100579
N	5.2533196826	1.3840797006	4.1367037893
H	12.2301781963	8.1321685063	1.9211634477
H	5.1082305570	0.4571544804	3.8220054840
H	13.4640899027	9.1346180450	1.4484818470
H	4.4587696250	1.6990378279	4.6724394679
H	12.3134650762	9.6582916002	2.4309845792
H	5.2606798113	1.9845485115	3.3635957047
N	6.6852095532	2.5499978962	0.9099412419
N	1.9397276434	2.4645347375	5.5826172566
H	7.3749780230	2.0714058749	1.4773411882
H	2.4432737511	2.2807535044	6.4745440703
H	6.5107776590	3.5216615132	1.1154778757
H	1.6994530687	3.4664537908	5.4966763402
H	5.8766017541	1.9593729078	0.9851314612
H	1.1087461875	1.9014396748	5.6253873587
N	11.1705197918	8.5921902155	5.5918909468
N	7.5474745813	5.3802908849	3.5448714375
H	10.4346064007	7.9941476151	5.2073100334
H	7.5007189934	4.3848902483	3.8023083553
H	11.1973777092	9.3890622703	4.9122854442
H	6.7658826025	5.7493054780	4.0818388304
H	12.0781146963	8.1166712032	5.4973519732
H	7.2441382118	5.4319814222	2.5768407014
N	7.5825772023	-0.2467058464	2.1057253404
H	7.0187728179	-0.9690044157	2.5260022093
H	7.8221014643	-0.6653808995	1.2462953635
H	8.3815648617	-0.0249296667	2.6638602383
N	11.1002986056	6.2013707408	2.1928374215
H	10.4590247426	5.8585075689	1.4777094309
H	11.9826435165	5.7150424416	2.0107808851
H	10.7803682921	5.7627156239	3.0436813439
N	2.9404102666	-3.2625532528	6.2058905398
H	3.6296382860	-3.9532257443	6.0750280005
H	3.3625230479	-2.4786988426	6.6588256551
H	2.3159711906	-3.6634979857	6.8846637631
N	12.8040976717	2.2151548786	3.3745172455
N	8.2448656956	1.4403965252	5.7763893889
H	12.0941395101	2.4458205973	2.6601294039
H	8.0421252556	0.5689740210	6.1686592215
H	13.5805846551	2.7595362529	3.0810920291
H	8.8897889831	1.9445628293	6.3851307756
H	13.1458852556	1.2835797233	3.1128713345
H	7.3780679098	1.9461454054	5.6366684518
N	3.2705949493	8.7077534650	5.4344706465
N	2.2115080394	2.3253163584	2.0482950639
H	3.3682894622	8.6050251039	4.4297390226
H	1.2256277174	2.2439885473	1.7061216558
H	2.4134728460	8.3029024029	5.7088567960
H	2.5874969226	1.4388128573	1.9243896803
H	3.2127383610	9.7185445374	5.5701730492
H	2.1986350508	2.6247799543	3.0532820622
N	3.7098880390	3.3630659540	8.4879086234
N	0.9184278075	6.3266888406	4.9557316806
H	3.4113024063	3.5047343904	9.4430176866

H	1.7193591441	5.8733260723	5.4553098986
H	4.7176558545	3.1451960888	8.6175884617
H	0.1016978794	5.7469742469	5.1064407468
H	3.5908912631	4.3307444396	8.2006267560
H	1.1090486903	6.2675569721	3.9752505646
N	2.4757644216	-0.9642103503	3.7631036375
H	2.5665365006	-0.0049216198	4.2230233630
H	1.9010422070	-0.8409301856	2.9794892167
H	2.0235602688	-1.5726514627	4.4465942599

Spin densities of (CO,H_2O,HCN,CH_3OH)-$(NH_3)_{n=8}$ (no apparent electron transfer)

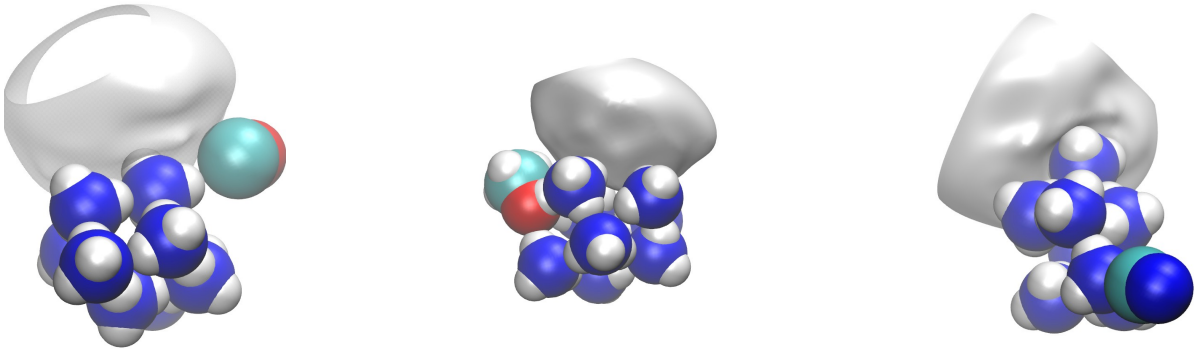

Figure S7. Interaction of the $(NH_3)_8^{\cdot -}$ with CO (left panel), CH_3OH (central panel) and HCN (right panel). No apparent electron transfer was found.

Geometry Optimization+Freq, d-aug-cc-pVDZ

```
%MaxCore 1000
! UKS RIJCOSX PBE0 SmallPrint TightSCF Slowconv
! D4
! TightOpt
! defgrid3
! UNO
! UCO
! DIIS

%basis
GTOName "NH.bas"
end

%basis AuxC "AutoAux"
end

%basis AuxJ "AutoAux"
end

%basis
PCDTrimAuxC Coulomb
PCDThresh -1
end

%basis
PCDTrimAuxJ Coulomb
PCDThresh -1
end

%scf Maxiter=350
    end

%geom Maxiter=300
end

%base "OPT"

* xyzfile -1 2 Start.xyz

$new_job
%MaxCore 2000
! UKS PBE0 RIJCOSX SmallPrint TightSCF Slowconv
! D4
! NumFreq
! defgrid3
! UNO
! UCO
! DIIS
! MORead

%moinp "OPT.gbw"

%basis
GTOName "NH.bas"
end
```

```
%basis AuxC "AutoAux"
end

%basis AuxJ "AutoAux"
end

%basis
PCDTrimAuxC Coulomb
PCDThresh -1
end

%basis
PCDTrimAuxJ Coulomb
PCDThresh -1
end

%scf Maxiter=150
    end

%base "FREQ"

%freq Temp 100, 200, 300
      CentralDiff true
      Increment 0.0030
      end

* xyzfile -1 2 OPT.xyz
```

DLPNO-CCSD(T), d-aug-cc-pV(D.T,Q)Z

```
%MaxCore 5000
! UHF RIJCOSX DLPNO-CCSD(T) NormalPNO VeryTightSCF SCFConvForced VerySlowConv
! UNO
! defgrid3
! DIIS
! MORead
! NoTRAH

%basis
GTOName "NH.bas"
end

%basis AuxC "AutoAux"
end

%basis AuxJ "AutoAux"
end

%basis
PCDTrimAuxC Coulomb
PCDThresh -1
end

%basis
PCDTrimAuxJ Coulomb
PCDThresh -1
end

%moinp "OPT.gbw"

%base "DLPNO"

%scf sthresh 1e-7
end

%scf Maxiter 1500
    DIISMaxEq 15
    DirectResetFreq 1
end


%scf GuessMode CMatrix
end

%mdci Maxiter 500
end

%mdci MaxDIIS 14
LShift 0.1
end

%mdci
UseFullLMP2Guess false
end

%mdci LocRandom 0
end
```

```
%mdci KCOpt KC_MO
end

%mdci TrafoType trafo_full
end

%mdci Triples 2
end

* xyzfile -1 2 OPT.xyz
```

WF Stability, d-aug-cc-pV(D.T,Q)Z

```
%MaxCore 5000
! UHF RIJCOSX SmallPrint VeryTightSCF VerySlowConv
! defgrid3
! DIIS
#! MORead
! NoTRAH

%basis
GTOName "NH.bas"
end

%basis AuxC "AutoAux"
end

%basis AuxJ "AutoAux"
end

%basis
PCDTrimAuxC Coulomb
PCDThresh -1
end

%basis
PCDTrimAuxJ Coulomb
PCDThresh -1
end

%scf Maxiter 1500
DIISMaxEq 15
DirectResetFreq 1
end

%scf
soscfmaxit 12
directresetfreq 1
end

%scf sthresh 1e-7
end

%scf
HFTyp UHF
STABPerform true
end

%base "Stab"

#%moinp "DLPNO.gbw"

* xyzfile -1 2 OPT.xyz
```

Opt. Geom. XYZ (Å) $(NH_3)_4$, d-aug-cc-pVDZ

Tetramer neutral

16
Coordinates from ORCA-job OPT

N	-0.44577929983220	0.58586881379384	3.32248357719557
N	3.41088309239111	-0.88450249798530	4.85496060866407
N	0.59028888308298	-0.43222195896487	6.06403659519922
H	-1.12966998732762	0.03815808050153	2.80682227840843
H	4.10377789193431	-0.35220824970322	5.37472153421829
H	0.04179705884671	-1.23110696424516	6.37151048376919
H	-0.72860035080168	1.55652440737669	3.21557716494886
H	0.45103032437580	0.48193507763104	2.82836536076966
H	2.51647923408829	-0.77199930994575	5.35154812585725
H	3.67916364105919	-1.86031617613108	4.95200488297889
N	2.38266483006994	0.16210417741626	2.12136925945514
H	2.92635514443732	0.96996195921659	1.82916247921745
H	2.82387194861028	-0.19790568978866	2.97859201396395
H	2.52251380423719	-0.54225951905839	1.40170152753571
H	0.46091917129193	0.28378536359898	6.77411695443260
H	0.14666461353643	-0.08093751371250	5.20444715338557

Tetramer+e^-

16
Coordinates from ORCA-job OPT

N	-0.43196082550541	0.56813672731486	3.31643956687137
N	3.41910893121013	-0.88250628302170	4.85636764032646
N	0.59424345412979	-0.43276718171875	6.07787573516974
H	-1.11861484834381	0.02044932065155	2.80239659433355
H	4.11291866426106	-0.34820474503654	5.37477694179683
H	0.04271944350465	-1.22925705248050	6.38945844256083
H	-0.71994330051415	1.53913037317914	3.21656367613207
H	0.46112236562192	0.47126730593551	2.81364814386665
H	2.52539859805183	-0.77046093290831	5.35489619145187
H	3.68860054356282	-1.85885332107733	4.95512517566427
N	2.40855889124712	0.17165560770264	2.11106413531741
H	2.94573732071174	0.99047172139554	1.83449850507289
H	2.84457215351178	-0.19297788455353	2.96941544198226
H	2.56518525004177	-0.52316386069313	1.38426972048937
H	0.46022999855357	0.29016404061202	6.78153636988399
H	0.15448335995508	-0.08820383530145	5.21308771908007

$(NH_3)_4$ EA estimated by CBS

Fitting functions based on 2 sets of basis sets:

$$n^3 = E_{CBS} + (A/n^3)$$

$$n^4 = E_{CBS} + [A/(n+1/2)^4]$$

Fitting functions based on 3 sets of basis sets:

$$\exp(\alpha X) = E_{CBS} + Be^{-\alpha X}$$

$$n^{46} = E_{CBS} + [A/(n+1/2)^4] + [A/(n+1/2)^6]$$

	Neutral Cluster	EA (kcal/mol)	Radical-Anion cluster	
aug-cc-pVDZ	-225.72980995	-11.7	-225.71116307	aug-cc-pVDZ
aug-cc-pVTZ	-225.94926789	-5.0	-225.94125697	aug-cc-pVTZ
aug-cc-pVQZ	-226.00969775	-1.5	-226.00723332	aug-cc-pVQZ

	Neutral Cluster	EA (kcal/mol)	Radical-Anion cluster	
$1/n^3$ CBS_TZ/QZ	-226.05379522	1.0	-226.05537822	$1/n^3$ CBS_TZ/QZ
$1/n^4$ CBS_TZ/QZ	-226.04457566	0.5	-226.04531246	$1/n^4$ CBS_TZ/QZ
n^{46} CBS_DZ/TZ/QZ	-226.04842855	1.1	-226.05023204	n^{46} CBS_DZ/TZ/QZ
exp(-αX) CBS_DZ/TZ/QZ	-226.03266079	0.7	-226.03375625	exp(-αX) CBS_DZ/TZ/QZ

	Neutral Cluster	EA (kcal/mol)	Radical-Anion cluster	
d-aug-cc-pVDZ	-225.73270019	-3.3	-225.72751155	d-aug-cc-pVDZ
d-aug-cc-pVTZ	-225.95008653	-2.9	-225.94541119	d-aug-cc-pVTZ

	Neutral Cluster	EA (kcal/mol)	Radical-Anion cluster	
$1/n^3$ CBS_DZ/TZ	-226.04161762	-2.8	-226.03715841	$1/n^3$ CBS_DZ/TZ
$1/n^4$ CBS_DZ/TZ	-226.02658792	-2.8	-226.02209321	$1/n^4$ CBS_DZ/TZ

Figure S8. Calculated EA values using different CBS fitting functions and basis sets.

Because of the diffuse nature of the radical-anion if reliable results are to be obtained, very fine grids of integration, tight conditions in the SCF and optimization procedures must be set in conjunction with wavefunction stability, T1 and S^2 analysis when the DLPNO-CCSD(T) method, is applied.
CBS extrapolation fitting procedures, though increasing the computational efforts, when possible should be preferred for a better estimation of the considered electronic parameters.