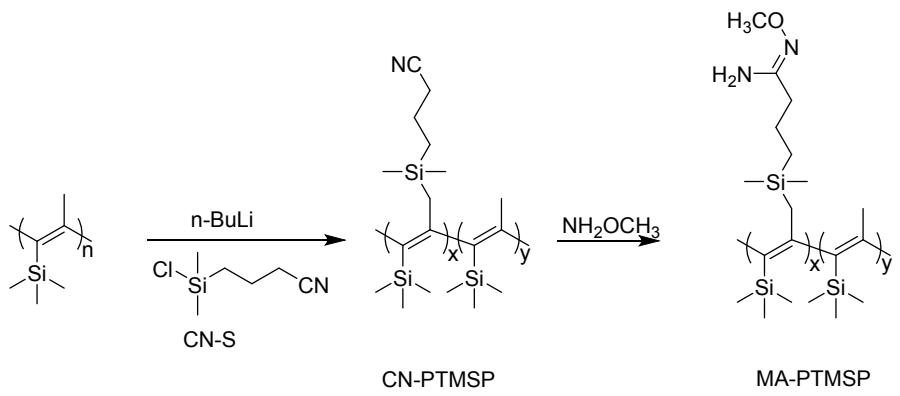
Electronic Supplementary Material (ESI) for Polymer Chemistry.

Gas separation mechanism of CO_2 selective Amidoxime-poly(1-trimethylsilyl-1-propyne) membranes

Hongbo Feng[1], Tao Hong[1], Shannon M. Mahurin[2], Konstantinos D. Vogiatzis[1], Kevin Gmernicki[1], Brian Long[1], Jimmy W. Mays[1,2], Alexei P. Sokolov[1,2], Nam-Goo Kang*[1], Tomonori Saito*[2]

[1]Department of Chemistry, University of Tennessee, Knoxville, Tennessee, United States, 37996

[2]Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States 37831



Scheme R1. The synthetic routine for MA-PTMSP.

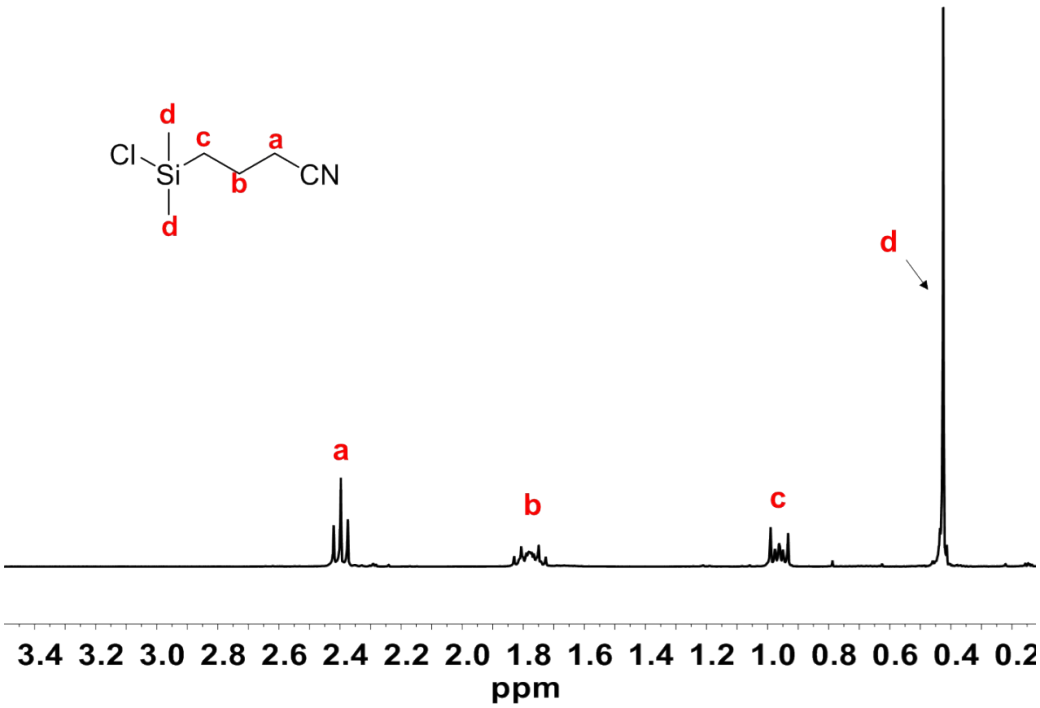


Figure S1. ^{1}H-NMR spectrum of 4-(chlorodimethylsilyl) butanenitrile.

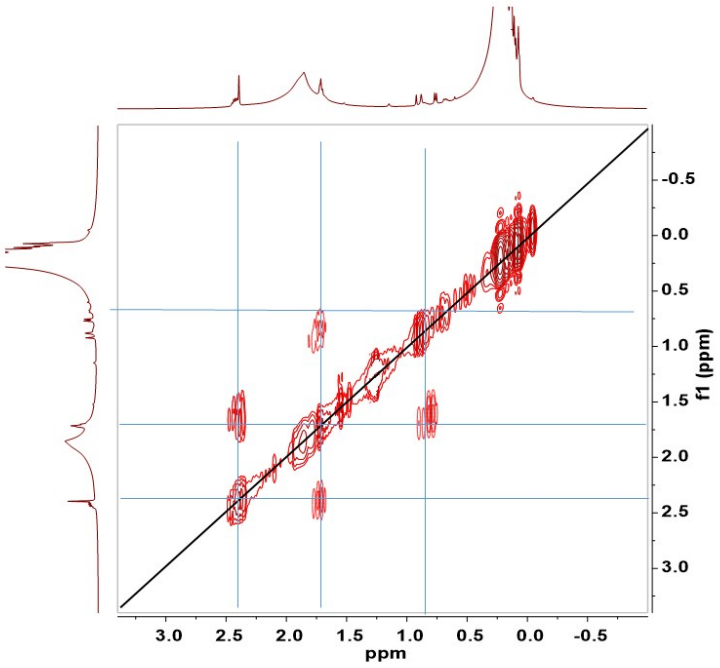


Figure S2. gCOSY of CN-PTMSP. The blue lines are guided to the eyes.

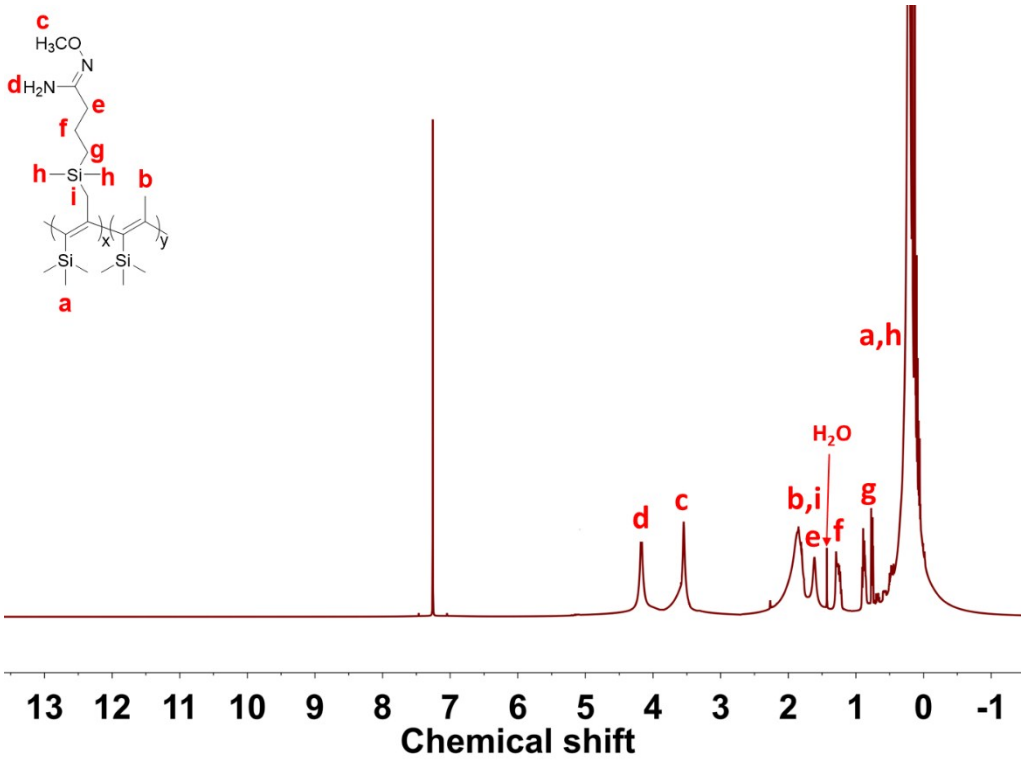


Figure S3. Full spectrum of ^{1}H-NMR of MA-20-PTMSP.

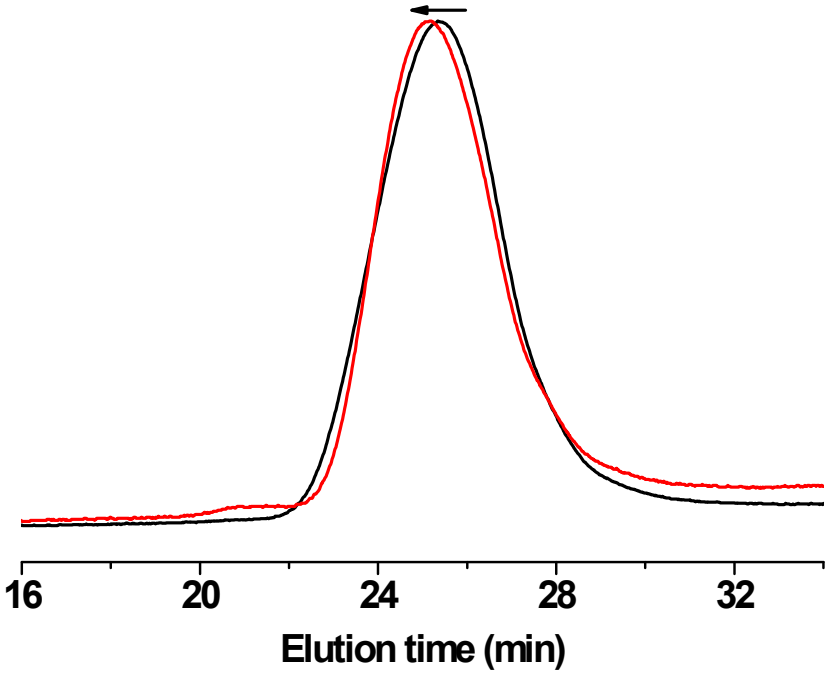


Figure S4. SEC profiles of neat PTMSP (black) and cyano-functionalized PTMSP (CN-PTMSP) (red).

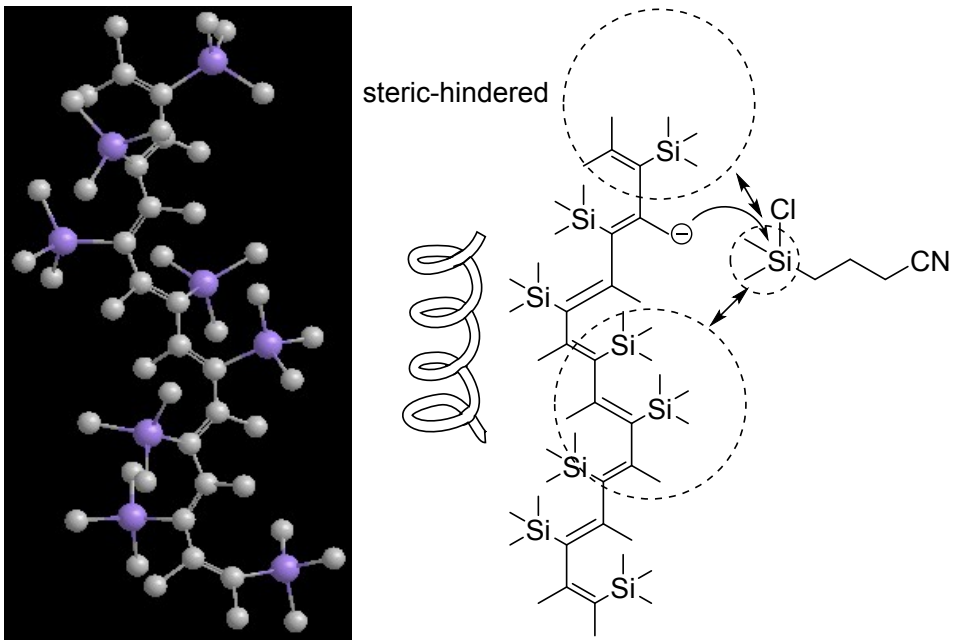


Figure S5. Illustration of nucleophilic reaction on the α-carbon of the "twisted" PTMSP backbone. (The purple spheres represent silicon atoms; gray spheres represent carbon atoms and hydrogen atoms are not shown in order to clarify the "twisted" structure.)

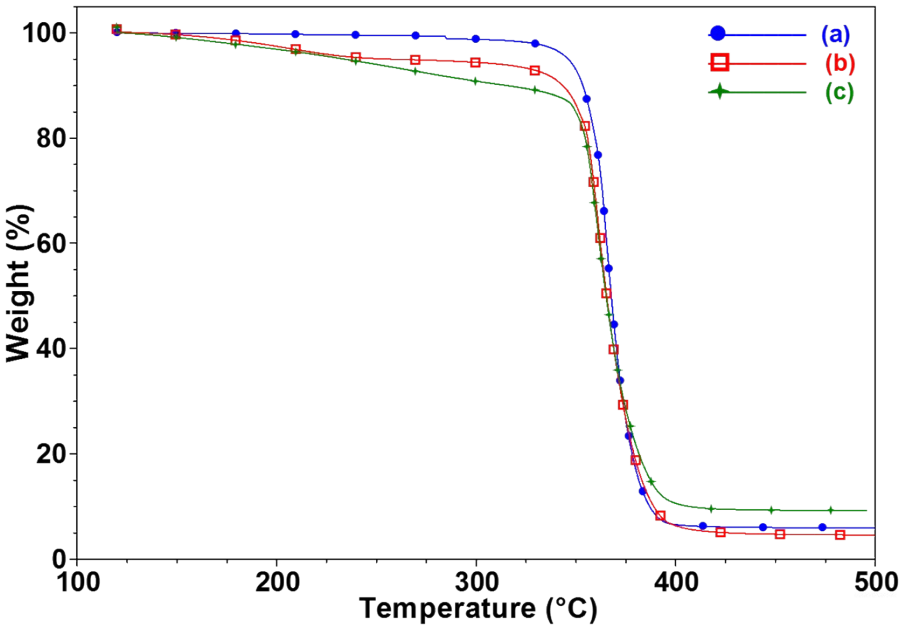


Figure S6. Representative TGA curves of (a) neat PTMSP, (b) CN-8-PTMSP and (c) AO-8-PTMSP.

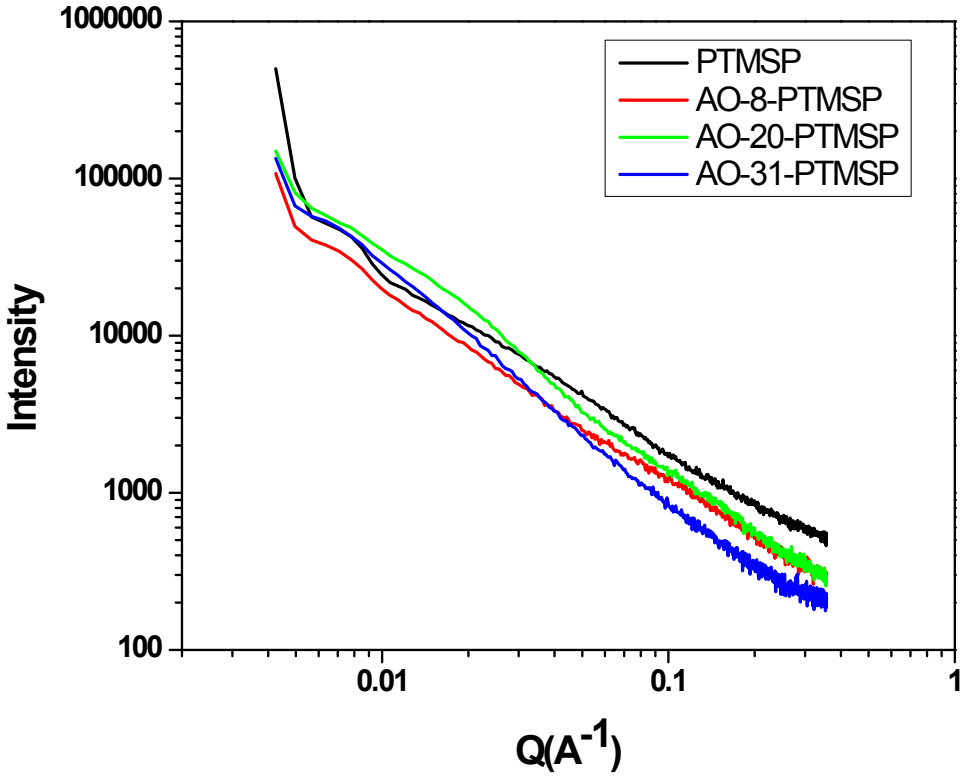


Figure S7. SAXS patterns of neat PTMSP, AO-8-PTMSP, AO-20-PTMSP and AO-31-PTMSP membranes.

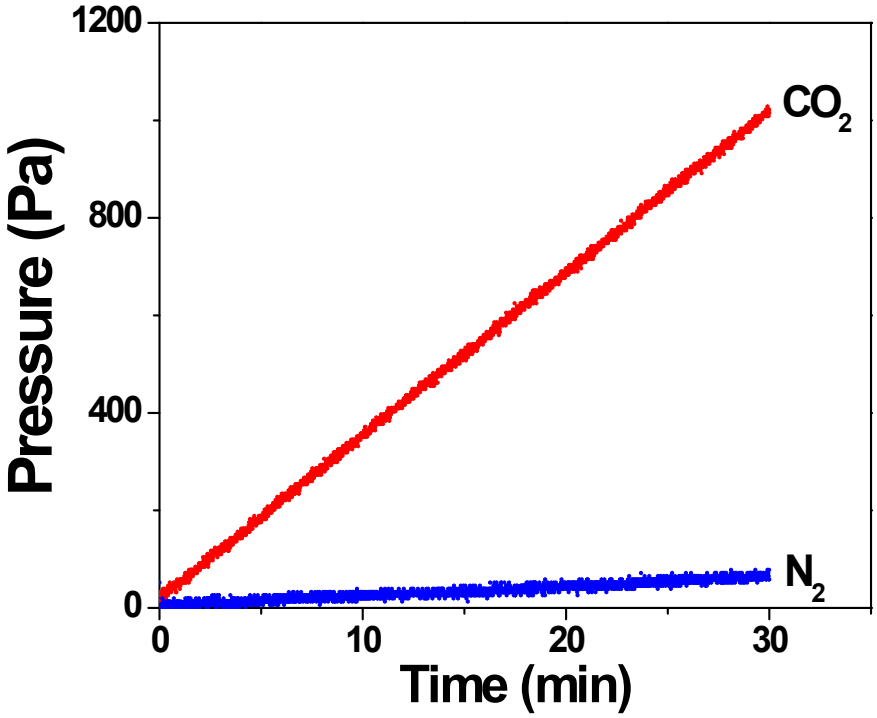


Figure S8. Pressure rise of CO_2 and N_2 in the AO-31-PTMSP membrane.

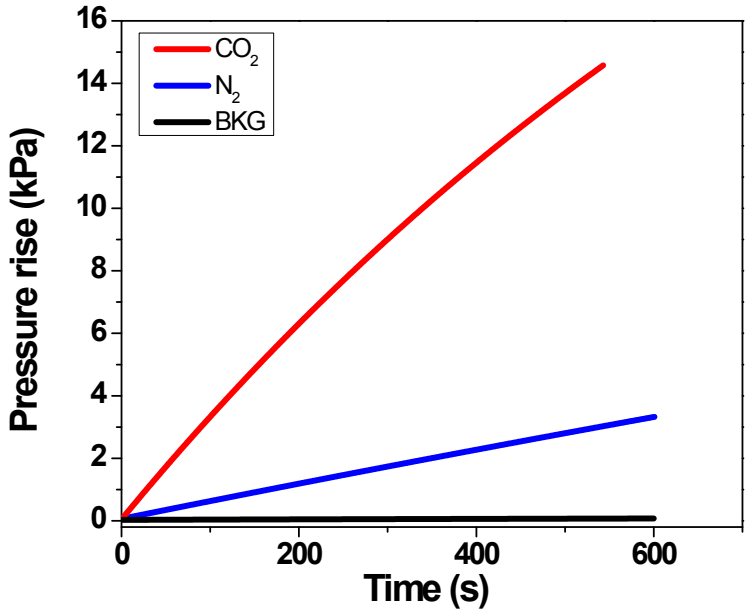


Figure S9. Pressure rise of CO_2 and N_2 in the MA-20-PTMSP membrane.

Table S1. Comparison of gas permeability of CN-20-PTMSP, methoxyamine treated and hydroxylamine treated samples.

Sample	CO_2 permeability [Barrer]	N_2 permeability [Barrer]	CO_2/N_2 selectivity
CN-20-PTMSP	18000	3800	4.7
MA-20-PTMSP	11000	1800	6.0
AO-20-PTMSP	6500	480	13.5

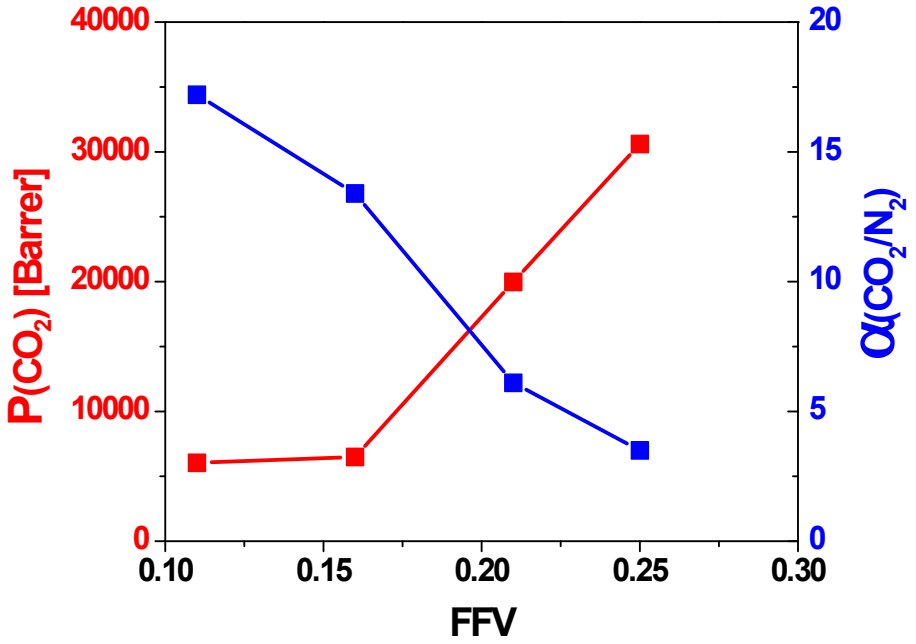


Figure S10. CO_2 permeability and CO_2/N_2 selectivity as a function of FFV.

Quantum Chemical Calculations

1. Examination of the hydrogen bonds

1.1 Figures representing the optimized AO monomer, dimer and trimer geometries

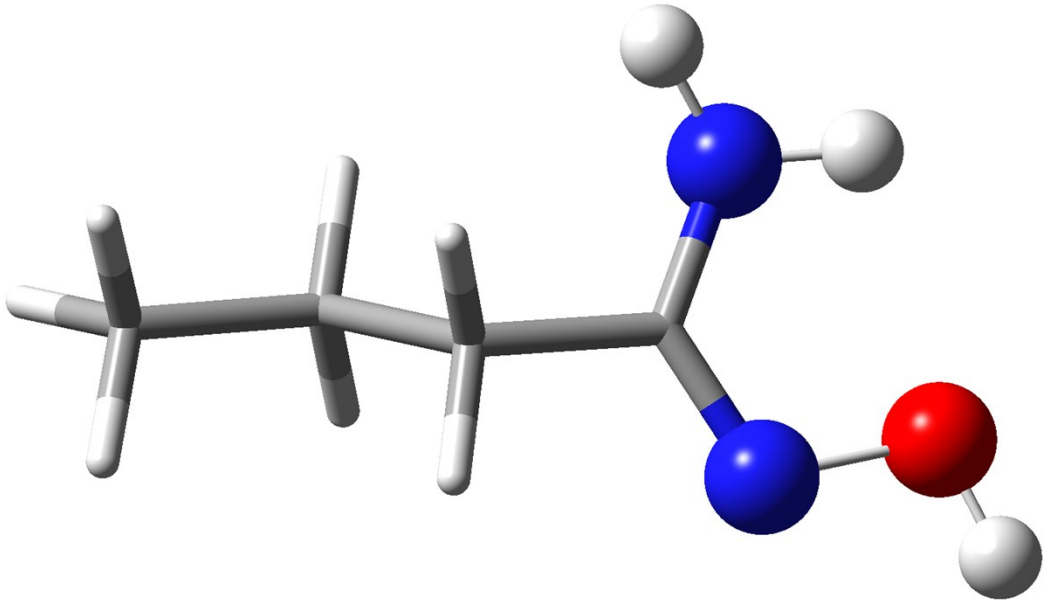


Figure S11. Optimized geometry of the AO monomer.

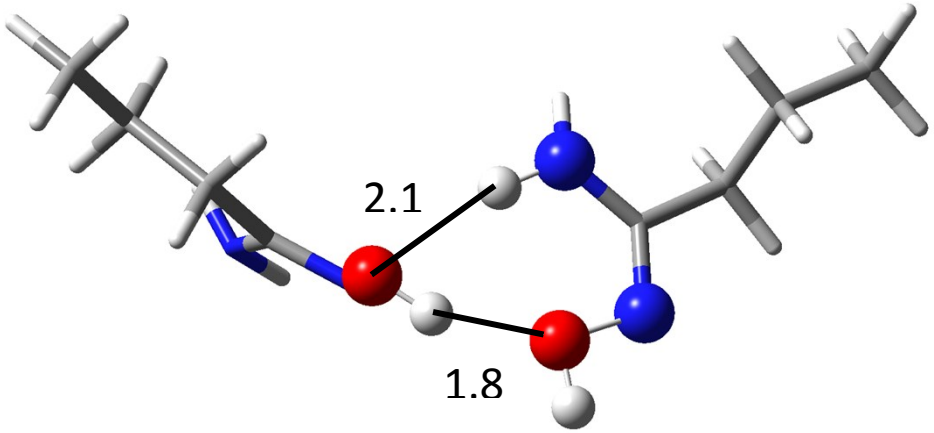


Figure S12. Conformer 1 for the AO dimer with a hydrogen bond via the O-H···O mode (1.845 Å). Key bond distances are shown (in Å). The 1.845 Å atom distance corresponds to the O(1)-H(1) hydrogen bond, the 2.121 Å atom distance corresponds to the O(2)-H(2) hydrogen bond. For the atom labels, see Cartesian coordinates (*vide infra*).

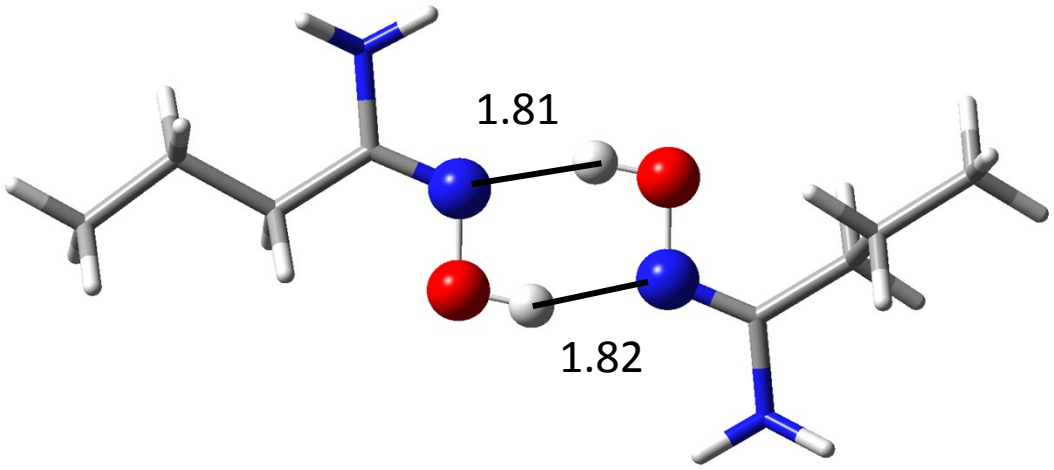


Figure S13. Conformer 2 for the AO dimer with a hydrogen bond via the O-H···N mode (1.826 and 1.817 Å). Key bond distances are shown (in Å). The 1.817 Å atom distance corresponds to the N(1)-H(1) hydrogen bond, the 1.826 Å atom distance corresponds to the N(2)-H(2) hydrogen bond. For the atom labels, see Cartesian coordinates (*vide infra*).

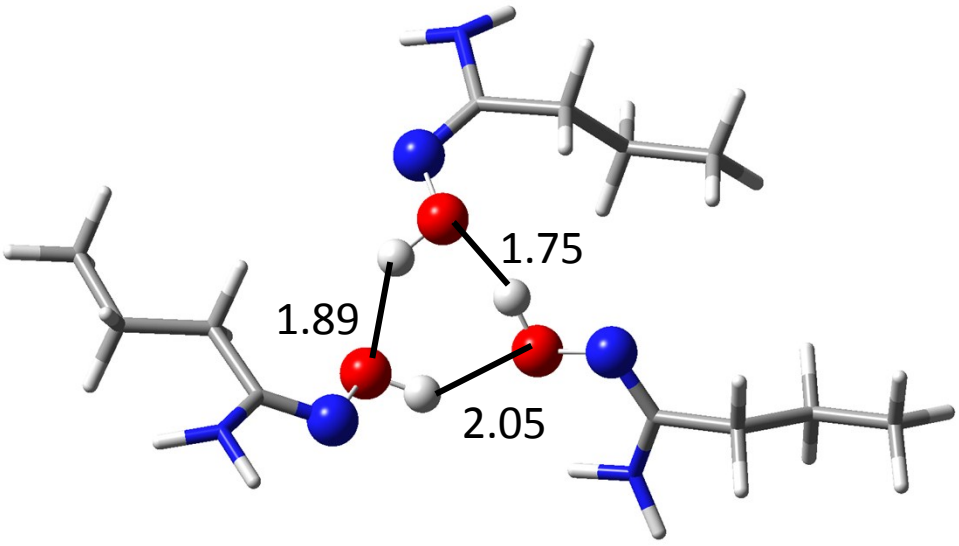


Figure S14. Conformer 1 for the AO trimer with three O-H···O hydrogen bonds. Key bond distances are shown (in Å). The 1.752 Å atom distance corresponds to the O(1)-H(1) hydrogen bond, the 1.899 Å atom distance corresponds to the O(2)-H(2) hydrogen bond, and the 2.053 Å atom distance corresponds to the O(3)-H(3) hydrogen bond. For the atom labels, see Cartesian coordinates (*vide infra*).

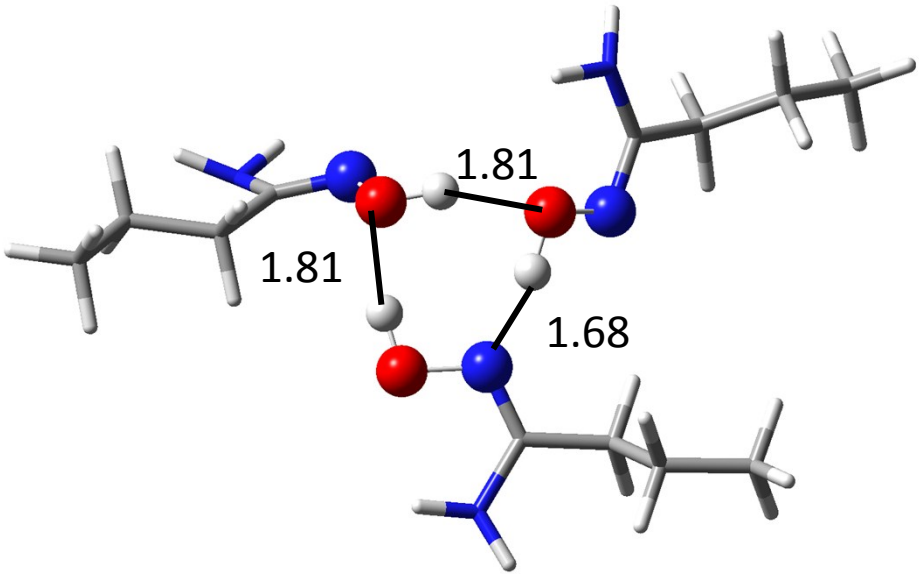


Figure S15. Conformer 2 for the AO trimer with two O-H···O hydrogen bonds and one O-H···N hydrogen bond (1.684 Å). Key bond distances are shown (in Å). The 1.817 Å atom distance corresponds to the O(1)-H(1) hydrogen bond, the 1.811 Å atom distance corresponds to the O(2)-H(2) hydrogen bond, and the 1.684 Å atom distance corresponds to the N(1)-H(3) hydrogen bond. For the atom labels, see Cartesian coordinates (*vide infra*).

1.2 Characteristics of the AO monomer, dimer, and trimer geometries

Table S2: IR peaks of the O-H stretch mode (in cm^{-1}) with a short description, dissociation energies (in kJ/mol), and relative energies between the different dimer and trimer conformers (in kJ/mol).

	Monomer	Dimer (Conformer1)	Dimer (Conformer2)	Trimer (Conformer1)	Trimer (Conformer2)
O-H stretch	3718 (free O-H)	3714 (free O-H)	3273 (O-H···N)	3550 (O-H···O)	3381 (O-H···O)
		3471 (O-H···O)		3484 (O-H···O)	3336 (O-H···O)
				3315 (O-H···O)	2938 (O-H···N)
$\Delta E_{\text{Dissociation}}$	-	-10.3	-25.2	-36.7	-76.9
$\Delta E_{\text{Conformer}}$ [a]	-	14.9	0	40.2	0

[a] Relative energy difference between conformers

1.3 Cartesian coordinates of the AO monomer, dimer, and trimer geometries

AO monomer

C	-3.16073800	-0.25272000	-0.08828000
C	-1.74158200	0.09675700	-0.49811000
C	-0.73188100	-0.22658000	0.59962900
C	0.67657300	0.09630400	0.22571100
N	1.49084700	-0.88060000	0.07997100
O	2.76070900	-0.39439700	-0.28623500
N	1.00133100	1.40390500	-0.00312300
H	-3.46371600	0.30453700	0.80201200
H	-3.25212000	-1.31662700	0.14341700
H	-1.46359200	-0.45450200	-1.40058100
H	-1.67927600	1.15710400	-0.75846800
H	-0.99619700	0.32165800	1.51265600
H	-0.76783000	-1.28958400	0.84174100
H	0.44094000	2.10243000	0.45012300
H	1.98566100	1.60186900	-0.06712700

H	3.28426500	-1.19448200	-0.32327100
H	-3.87329000	-0.02292400	-0.88226100

AO dimer – Conformer 1

C	5.625899	-1.839181	0.339625
C	4.445630	-1.185119	-0.355692
C	3.656833	-0.280058	0.585989
C	2.494165	0.392146	-0.071736
N	1.490433	-0.397692	-0.540147
N	2.571904	1.665753	-0.190852
O(1)	1.430674	2.181403	-0.853550
H	5.297252	-2.456134	1.180010
H	6.315253	-1.088394	0.733268
H	4.791892	-0.588709	-1.204263
H	3.787709	-1.952912	-0.772587
H	3.293648	-0.864474	1.440200
H	4.304340	0.502354	0.983249
H	1.423487	-1.315765	-0.139852

H(2)	0.604162	0.028679	-0.769212
H	1.616163	3.120502	-0.869875
H	6.186275	-2.479655	-0.343539
O(2)	-1.149517	1.213704	-0.624226
H(1)	-0.336144	1.738777	-0.561749
N	-1.501438	1.016680	0.714257
C	-2.606183	0.384472	0.819183
N	-3.136459	0.243172	2.087830
H	-3.592269	-0.635593	2.268753
H	-2.487972	0.507391	2.813727
C	-3.399967	-0.124348	-0.346113
C	-4.515179	-1.103534	-0.018483
H	-3.812008	0.747771	-0.866208
H	-2.699782	-0.568426	-1.057818
C	-5.247310	-1.561340	-1.268012
H	-4.102063	-1.979061	0.495732
H	-5.226624	-0.639732	0.670634
H	-6.046114	-2.265176	-1.028694

H -5.695347 -0.712627 -1.790051

H -4.565517 -2.053281 -1.965691

AO dimer – Conformer 2

C -6.07255800 -0.68456300 0.60492400

C -4.99406000 0.34635200 0.32020700

C -3.65302400 -0.30815900 0.03308300

C -2.51359200 0.62191200 -0.24542700

N -2.79430400 1.92941800 -0.58682200

N(1) -1.29322100 0.24569400 -0.25886100

O -1.14124600 -1.11585300 -0.04197300

H(2) -0.16457900 -1.20924700 -0.06723200

H -3.55647300 2.35044100 -0.08268200

H -1.97874100 2.52030000 -0.63095200

H -3.74272100 -0.98214000 -0.82644400

H -3.35221200 -0.95191800 0.86312600

H -4.90308500 1.01682800 1.18254000

H -5.29795400 0.96375300 -0.53019300

H	-7.03373300	-0.21130100	0.81199200
H	-6.20657600	-1.35409000	-0.24792600
H	-5.80931500	-1.30021000	1.46809300
N(2)	1.56409500	-0.64859800	-0.24058600
O	1.40432700	0.70849000	-0.48264200
H(1)	0.42633600	0.79620200	-0.46122300
C	2.78351200	-1.02499500	-0.26534800
N	3.06011900	-2.37037500	-0.12738400
H	3.92998900	-2.57785200	0.33427300
H	2.28967300	-2.92086900	0.21847900
C	3.94246000	-0.10463000	-0.46822200
H	3.67023200	0.62067500	-1.23730600
C	4.31594700	0.63971200	0.81268600
H	4.79653200	-0.67846400	-0.83819900
C	5.47899400	1.59125700	0.60031000
H	3.43763500	1.18727300	1.16011700
H	4.56532500	-0.08329800	1.59640000
H	5.73700800	2.11664900	1.52151500

H	6.37098800	1.05940000	0.25906800
H	5.23414400	2.34247700	-0.15424000

AO trimer – Conformer 1

C	6.53734600	-1.91325000	0.61416500
C	5.31046100	-1.54805400	-0.20140400
C	4.02189400	-2.05654700	0.43948500
C	2.79783400	-1.69278700	-0.33321100
N	2.01279100	-0.82031400	0.17709800
O(3)	0.92999100	-0.57366100	-0.67990700
N	2.62536200	-2.24983700	-1.56924300
O(2)	-1.86474100	-1.13623700	-0.52374400
N	-2.49069100	-2.17607100	0.17627700
C	-3.71971900	-1.90735200	0.40100900
C	-4.41132900	-0.66113600	-0.06353000
C	-5.93066700	-0.68651100	-0.02065300
C	-6.52669200	0.61314200	-0.53311400
N	-4.42224500	-2.78960900	1.19558200

H	6.63569500	-2.99706900	0.71703900
H	6.47940300	-1.49187100	1.62069300
H	5.23966000	-0.46196100	-0.30809900
H	5.40201200	-1.94847700	-1.21486700
H	4.07215100	-3.14685900	0.55027000
H	3.90998800	-1.63766100	1.44049500
H	3.05030600	-3.14310800	-1.73815500
H	1.72699000	-2.09862100	-1.99516100
H(1)	0.45154300	0.15014200	-0.22983300
H	7.45134600	-1.53959600	0.14933800
H(3)	-0.94036600	-1.41488200	-0.57620200
H	-5.38441500	-2.93080700	0.93775700
H	-3.92586300	-3.65078400	1.36536000
H	-4.04478900	0.17065300	0.54997400
H	-4.06334900	-0.44554700	-1.07612000
H	-6.30438000	-1.51857600	-0.62818500
H	-6.27150500	-0.86286700	1.00364600
H	-7.61715300	0.59330700	-0.49908800

H	-6.18800000	1.46052400	0.06736300
H	-6.22664800	0.80227500	-1.56629500
H(2)	-1.48789100	0.56698800	0.22773600
O(1)	-0.77303500	1.15654000	0.51556800
N	-1.08316300	2.39273100	-0.06684300
C	-0.15145600	3.24859200	0.11255500
N	-0.38715300	4.53868400	-0.32073700
H	0.42871700	5.02810500	-0.64953700
H	-1.17432500	4.61926600	-0.94576600
C	1.16812600	2.99672100	0.77087700
H	1.07968300	2.13412300	1.43035700
C	2.28606800	2.74740200	-0.24359400
H	1.41796500	3.86322500	1.39000700
C	3.60601800	2.43713000	0.43801800
H	2.00435900	1.91313300	-0.89008700
H	2.39828500	3.62119500	-0.89493300
H	4.40071300	2.28045400	-0.29403700
H	3.91467200	3.25187100	1.09837100

H	3.51587800	1.52710000	1.03406300

AO trimer – Conformer 2

C	5.915176	3.133389	-0.732084
C	4.817676	2.605993	0.174316
C	3.488492	2.455280	-0.559866
C	2.388451	1.930742	0.301725
N	1.938952	0.760072	0.047812
O(1)	0.927889	0.407647	0.947104
N	1.970544	2.702267	1.352433
O(2)	-1.774959	0.767500	0.715537
N	-2.188905	1.636870	-0.299435
C	-3.431349	1.503038	-0.563138
C	-4.358370	0.564663	0.148782
C	-5.841327	0.877672	0.023918
C	-6.690643	-0.105616	0.810438
N	-3.925369	2.214080	-1.639906
H	5.657084	4.116780	-1.133815

H	6.078796	2.465193	-1.581174
H	5.102227	1.632120	0.582537
H	4.691756	3.270208	1.033817
H	3.189170	3.425596	-0.976117
H	3.597929	1.767288	-1.399378
H	2.067871	3.696815	1.254465
H	1.127555	2.390723	1.804780
H(3)	0.615767	-0.473858	0.599145
H	6.862194	3.231038	-0.198336
H(1)	-0.808995	0.905432	0.752773
H	-4.850220	2.591494	-1.516992
H	-3.267882	2.892562	-1.993207
H	-4.167389	-0.444710	-0.235453
H	-4.064097	0.540525	1.199923
H	-6.035770	1.893433	0.385987
H	-6.140521	0.852289	-1.027967
H	-7.754024	0.120980	0.717689
H	-6.534264	-1.126880	0.455142

H	-6.434854	-0.084008	1.872246
H(2)	-1.784873	-1.007701	0.355832
O	-1.540896	-1.926434	0.134964
N(1)	-0.161168	-1.838441	-0.009621
C	0.356195	-2.918725	-0.460215
N	-0.382988	-4.004253	-0.813111
H	0.082035	-4.889293	-0.886732
H	-1.337645	-4.014049	-0.497048
C	1.838833	-2.962096	-0.624114
H	2.072771	-3.352123	-1.620829
H	2.207200	-1.934746	-0.584852
C	2.539256	-3.805052	0.438559
C	4.046859	-3.799196	0.261132
H	2.277393	-3.411259	1.424371
H	2.168667	-4.835387	0.410133
H	4.541882	-4.395435	1.029505
H	4.331737	-4.205838	-0.712568
H	4.439280	-2.781612	0.321364

2. Noncovalent interactions of CO_2 and N_2 with the AO functional group

2.1 Figures of the optimized CO_2- and N_2-AO geometries

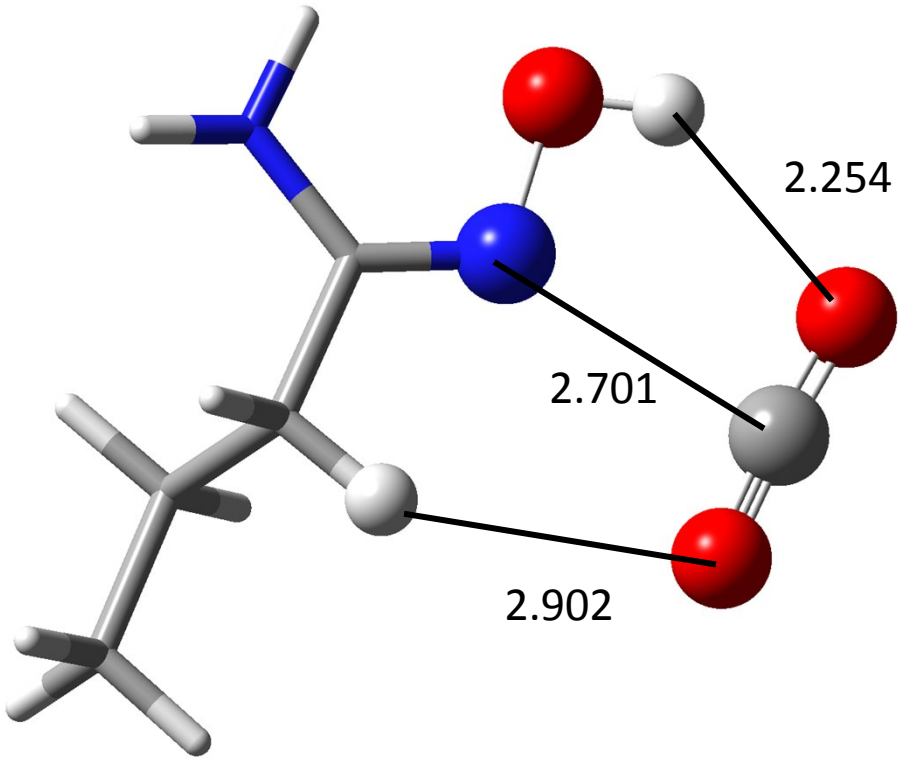


Figure S16. Optimized geometry of the CO_2- 1 AO supersystem. Key bond distances are shown (in Å). The 2.254 Å atom distance corresponds to the O(1)-H(1) hydrogen bond, the 2.701 Å atom distance corresponds to the C(1)-N(1) interaction, and the 2.902 Å atom distance corresponds to the O(2)-H(2) hydrogen bond. For the atom labels, see Cartesian coordinates (*vide infra*).

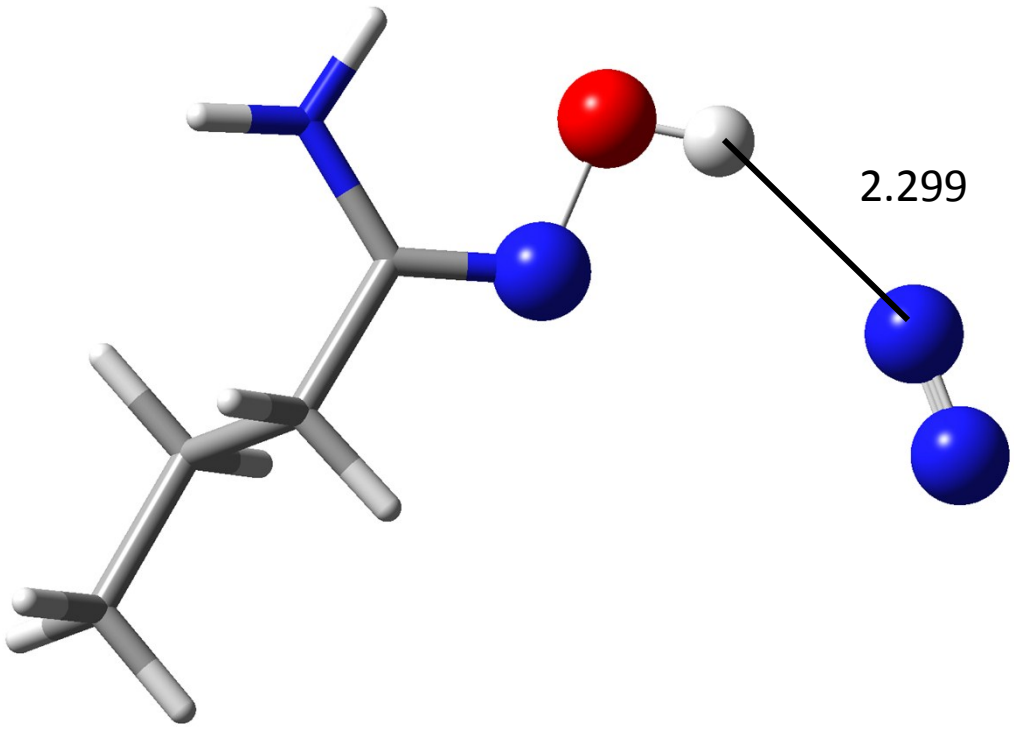


Figure S17. Optimized geometry of the N_2- 1 AO supersystem. Key bond distances are shown (in Å). The 2.299 Å atom distance corresponds to the N(1)-H(1) interaction. For the atom labels, see Cartesian coordinates (*vide infra*).

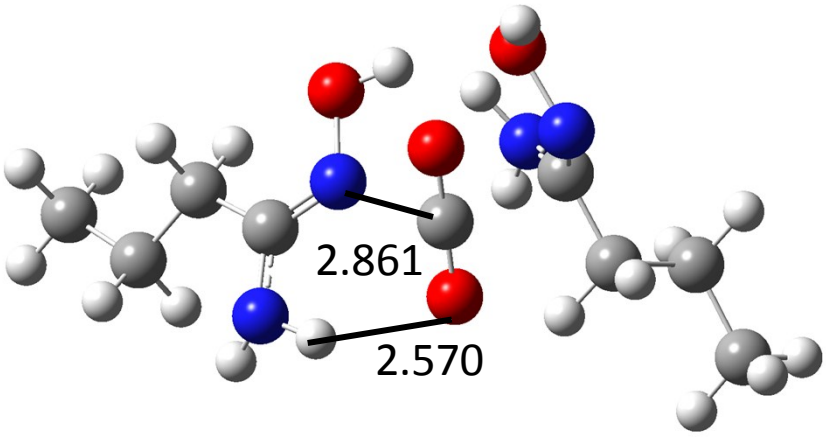


Figure S18. Optimized geometry of the CO_2- 2 AO supersystem. Key bond distances are shown (in Å). The 2.861 Å atom distance corresponds to the C(1)-N(1) interaction, the 2.570 Å atom distance corresponds to the O(1)-H(1) hydrogen bond. For the atom labels, see Cartesian coordinates (*vide infra*).

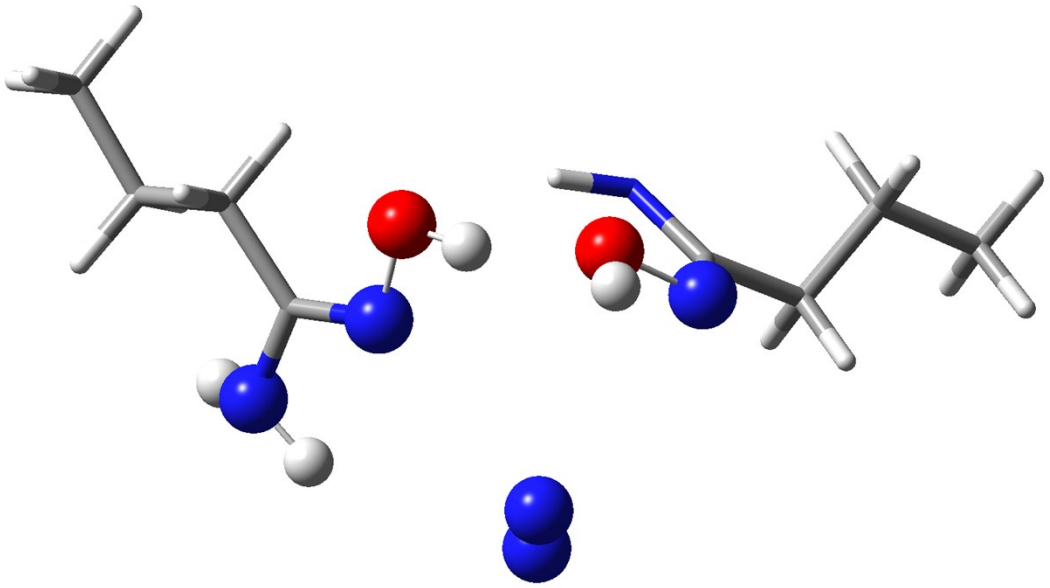


Figure S19. Optimized geometry of the N_2- 2 AO supersystem.

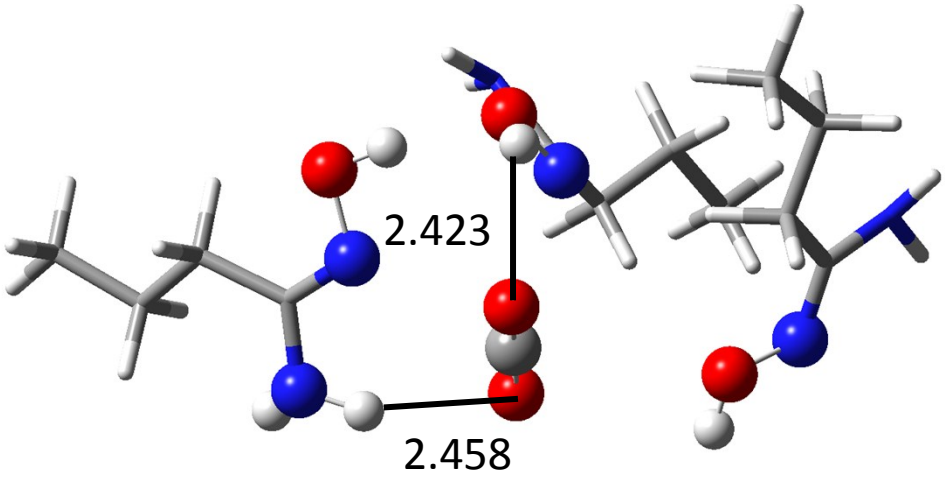


Figure S20. Optimized geometry of the CO_2- 3 AO supersystem. Key bond distances are shown (in Å). The 2.423 Å atom distance corresponds to the O(1)-N(1) hydrogen bond, the 2.458 Å atom distance corresponds to the O(2)-H(2) hydrogen bond. For the atom labels, see Cartesian coordinates (*vide infra*).

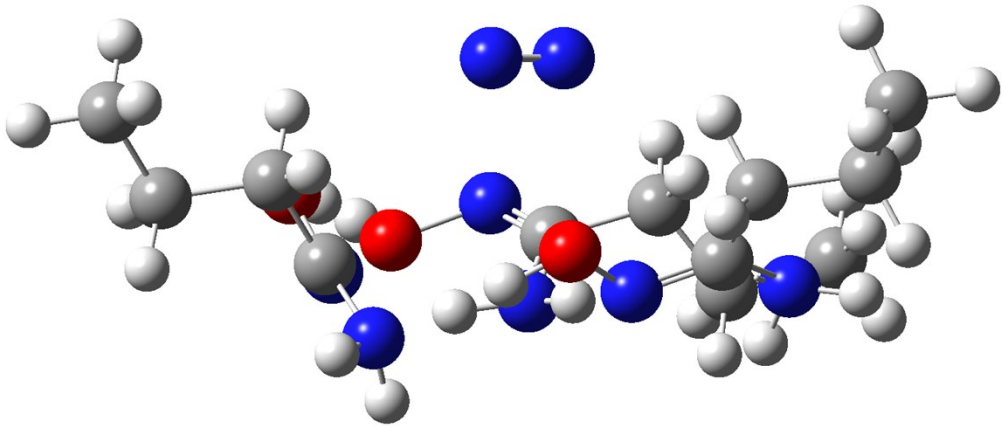


Figure S21. Optimized geometry of the N_2- 3 AO supersystem.

2.2 Cartesian coordinates of the AO monomer, dimer, and trimer geometries

CO_2-1AO

C	-3.35077200	-1.59819900	-0.16620100
C	-2.44234400	-0.43811700	-0.53057500
C	-1.44064600	-0.12666900	0.57817300
C	-0.51999900	0.99967900	0.24476700
N	-1.04661000	2.24739200	0.09037300
N(1)	0.71622800	0.72200200	0.05919700
O	1.44088200	1.87776200	-0.26270400
H	-3.92744800	-1.38047300	0.73651200
H	-2.77162600	-2.50485100	0.02408600
H	-1.88879900	-0.66704500	-1.44534600
H	-3.04101000	0.45023000	-0.75097500
H	-1.97991100	0.11192500	1.50319100
H(2)	-0.82446100	-1.00335700	0.78174300
H	-1.91744200	2.44613800	0.54708700
H	-0.38448800	3.00265400	0.03781600

H(1)	2.33587500	1.54035200	-0.34391600
H	-4.05836200	-1.81700900	-0.96760900
C(1)	2.50914800	-1.29716600	0.00950500
O(1)	3.30802600	-0.49032900	-0.22988400
O(2)	1.78084400	-2.16261800	0.24464000

N_2-1AO

C	-3.45250400	-1.61817900	-0.09617300
C	-2.45636600	-0.54714300	-0.50186700
C	-1.44062500	-0.26142600	0.60077000
C	-0.43877000	0.78122700	0.23100600
N	-0.88368100	2.05282900	-0.00051400
N	0.77892100	0.41283000	0.08995500
O	1.57611700	1.51189900	-0.27228400
H	-4.01646100	-1.31795000	0.79082400
H	-2.94577400	-2.55720100	0.13927000
H	-1.91660500	-0.85599800	-1.40127600
H	-2.98507400	0.37302900	-0.76591300

H	-1.96766800	0.05219000	1.51071000
H	-0.88830900	-1.16940600	0.84681600
H	-1.73540500	2.33061700	0.45214700
H	-0.16727300	2.75673600	-0.06133700
H(1)	2.45259400	1.12563600	-0.30634600
H	-4.17000300	-1.81842500	-0.89370700
N	3.88243500	-1.84494600	0.07760200
N(1)	3.71670100	-0.78375500	-0.10066000

CO_2-2AO

C	-4.58562200	-2.49327300	-1.16415300
C	-3.84933000	-1.91219800	0.02936500
C	-2.78084600	-0.90908300	-0.39339000
C	-2.03846800	-0.30544600	0.75279400
N	-2.17134700	0.95743900	0.92174500
O	-1.40763600	1.39586300	2.03196900
N	-1.31979200	-1.13622100	1.55805800
O	1.29207200	0.79346700	1.47473700

N(1)	1.15565100	0.68945000	0.09115800
C	2.16900600	0.13959300	-0.45817800
C	3.35086700	-0.38546100	0.29797900
C	4.27386300	-1.31709800	-0.47039500
C	5.42195900	-1.81021700	0.39308300
N	2.20193000	0.11281500	-1.83888800
H	-3.89914000	-3.01521800	-1.83579000
H	-5.07701300	-1.70759800	-1.74288800
H	-4.55427600	-1.41211500	0.69921600
H	-3.39523600	-2.71755700	0.61369400
H	-2.05717800	-1.39460200	-1.05945100
H	-3.23136100	-0.09184900	-0.95738000
H	-1.02666200	-2.00317800	1.14380700
H	-0.62274600	-0.70239100	2.14062500
H	-1.54714500	2.34431100	2.00399400
H	-5.35134200	-3.20539300	-0.85211600
H	0.43340600	1.16654500	1.72697300
H	2.61740200	-0.70826200	-2.24510000

H(1)	1.32085500	0.36434300	-2.26225900
H	3.91721500	0.47862700	0.66368400
H	2.97423200	-0.87612900	1.19852900
H	3.70684200	-2.17874000	-0.84116500
H	4.67606800	-0.80248400	-1.34788900
H	6.08206500	-2.47856000	-0.16213300
H	6.02300500	-0.97367300	0.75704100
H	5.05249900	-2.35350700	1.26595300
C(1)	-0.71983200	2.44856500	-1.16255300
O	-0.59813900	3.24381400	-0.33176200
O(1)	-0.85581700	1.71320000	-2.04734100

N_2-2AO

C	-5.43884000	2.07483000	1.06123600
C	-4.30206300	1.76463000	0.10428500
C	-3.48963700	0.55428900	0.55494500
C	-2.36874100	0.21193500	-0.37353100
N	-1.37242700	1.12630500	-0.52590200

N	-2.47348100	-0.90201700	-0.99822100
O	-1.37314500	-1.09977600	-1.86818900
N	-0.79707200	-3.53309800	0.18641200
N	-0.72802500	-3.21989100	1.22701700
N	1.47497000	-0.78486700	0.07768500
C	2.59286900	-0.33441200	0.50002000
N	3.00970800	-0.74958600	1.75052500
O	1.23497700	-0.40915000	-1.24703100
C	3.51191100	0.53091400	-0.30800500
C	4.63091400	1.21570100	0.45933700
C	5.49334300	2.07407900	-0.44966700
H	-5.06274400	2.29362900	2.06400200
H	-6.12394100	1.22781300	1.14498600
H	-4.69565200	1.56768500	-0.89668600
H	-3.64905100	2.63663600	0.00765900
H	-3.07883000	0.73781400	1.55525800
H	-4.13328000	-0.32309000	0.62708400
H	-1.27133300	1.79677600	0.21456000

H	-0.50137900	0.82192600	-0.93527900
H	-1.55223600	-1.97186700	-2.22178600
H	-6.01662500	2.93830200	0.72734700
H	0.39556800	-0.85415900	-1.44660300
H	3.48957200	-0.05481500	2.29789500
H	2.28594200	-1.22710900	2.26584700
H	3.93457700	-0.09421900	-1.10264800
H	2.89950700	1.27004500	-0.83009700
H	4.20781400	1.84486000	1.25099500
H	5.25641500	0.46620900	0.95250900
H	6.29467900	2.56475100	0.10514600
H	5.95263400	1.46981600	-1.23546600
H	4.89946800	2.85067600	-0.93730200

CO_2-3AO

C	2.41249700	3.60114700	0.04866600
C	1.88486000	2.52924300	0.98435300
C	0.79086500	1.69553700	0.32367000

C	0.23312800	0.62837100	1.20608500
N	-0.47420900	1.00244000	2.30653600
N	0.50562600	-0.58095900	0.88441500
O	-0.08448000	-1.49644500	1.79007900
O	-2.85307600	-1.16758900	1.28872600
N	-2.70435100	-0.80200200	-0.04884800
C	-3.77049100	-0.29436300	-0.53491600
N	-3.78092500	-0.02142600	-1.89003700
C	-5.02540200	-0.06661100	0.25118500
C	-6.03638100	0.88414500	-0.36885200
C	-7.25421600	1.06925000	0.51972100
C	-0.39502700	-1.73519400	-1.61534900
O(2)	-0.51766300	-0.80429600	-2.29215100
O(1)	-0.26034600	-2.71003700	-1.00657400
H	1.62151200	4.29955600	-0.23816400
H	2.80983100	3.15038100	-0.86334700
H	2.70280500	1.86652600	1.27890600
H	1.50631400	2.98280700	1.90524200

H	-0.03193900	2.34783100	0.00641600
H	1.18025000	1.21277600	-0.57317400
H	-0.89335500	1.91442300	2.28213500
H	-1.02785200	0.29140500	2.75288400
H(1)	0.09899900	-2.33576900	1.36003000
H	3.21218700	4.17674000	0.51784300
H	-1.94670400	-1.41761500	1.52155100
H	-4.29244700	0.80349300	-2.15486700
H(2)	-2.86196300	-0.06397900	-2.30607700
H	-5.49204600	-1.04393800	0.41959400
H	-4.73154400	0.28081300	1.24430500
H	-5.56832000	1.85929400	-0.54575100
H	-6.35500800	0.50519900	-1.34434700
H	-7.97736200	1.75234900	0.07111400
H	-7.75863800	0.11580000	0.69328400
H	-6.97180300	1.47356200	1.49462100
H	2.23292400	0.25123900	-3.15857700
O	2.59702600	-0.17202400	-2.38079000

N	3.60943300	0.71968900	-1.99477500
C	4.15445700	0.33998400	-0.90197900
N	5.09644200	1.17985600	-0.34327200
H	5.84055100	0.72157500	0.15459500
H	5.41872600	1.89812200	-0.97272100
C	3.77079000	-0.90523900	-0.16551000
C	4.46251800	-1.14172900	1.16626300
H	2.68738200	-0.86877600	-0.01145100
H	3.93119100	-1.75449200	-0.83771900
C	3.89507600	-2.36052400	1.87358200
H	5.54105200	-1.27816500	1.02276100
H	4.34030100	-0.26252100	1.80515800
H	4.40228900	-2.54600300	2.82192300
H	2.83244800	-2.21960000	2.08240100
H	3.99837000	-3.25718400	1.25747400

N_2-3AO

C	-4.37181800	-2.95036900	0.05071200

C	-2.93305300	-3.10051800	-0.40913400
C	-1.94472700	-2.56023700	0.61987500
C	-0.52338500	-2.65921200	0.16279000
N	0.18683200	-3.56636300	0.73475000
O	1.50769900	-3.57458800	0.19229100
N	-0.12720900	-1.84918500	-0.84553400
O	3.14575700	-1.35435600	0.42266100
N	2.63880200	-0.77082800	-0.72053000
C	2.88967300	0.47241400	-0.80932100
C	3.68782900	1.27416100	0.16112000
C	5.18909300	1.18318600	-0.11049200
C	5.99712300	1.99228000	0.88732600
N	2.31437400	1.14890300	-1.89300800
N	-0.29652000	0.23042400	2.10328600
N	0.72036100	0.60993800	2.01325700
O	-0.19616500	2.03254200	-0.78253700
N	-1.14332300	1.08026900	-1.14086800
C	-2.31007400	1.39453700	-0.72096800

C	-2.60728500	2.65401800	0.03262600
C	-4.07567000	2.97631400	0.25206200
C	-4.25605500	4.27227300	1.02336000
N	-3.32769700	0.48059600	-0.90507800
H	-4.61296000	-1.90007800	0.23270400
H	-4.54313400	-3.49358200	0.98327500
H	-2.70384500	-4.15275100	-0.59927000
H	-2.78538300	-2.58600900	-1.36348000
H	-2.17990500	-1.51321100	0.83565500
H	-2.03710700	-3.11842200	1.55241700
H	-0.61428500	-0.96690100	-0.96143100
H	0.86600600	-1.77723300	-1.02797500
H	1.86826400	-4.37532400	0.57383800
H	-5.07327500	-3.33672900	-0.69145900
H	2.64887500	-2.19303100	0.45513900
H	2.89119800	1.89552200	-2.25178400
H	2.04170800	0.51460800	-2.63209300
H	3.35712000	2.31617100	0.12449500

H	3.47747800	0.89475700	1.16196700
H	5.48398600	0.13222100	-0.07115600
H	5.40293200	1.52844600	-1.12773800
H	7.06728300	1.91732600	0.68702600
H	5.72442800	3.05016800	0.85366500
H	5.82266900	1.63895800	1.90615000
H	0.62232500	1.72730900	-1.21444900
H	-4.24146500	0.87558000	-1.04771700
H	-3.10787600	-0.24948900	-1.56471100
H	-2.09293400	2.58429200	0.99759800
H	-2.10661300	3.47301600	-0.48999900
H	-4.58732100	3.06089200	-0.71362200
H	-4.55942600	2.15995600	0.79639200
H	-5.31141500	4.50183500	1.17832000
H	-3.77986100	4.21095100	2.00466000
H	-3.80505600	5.11262300	0.49059400