Controlling the Strength of Interaction between Carbon Dioxide and Nitrogen-Rich Carbon Materials by Molecular Design

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Electronic Supplementary Information (ESI†)

Supplementary Figures

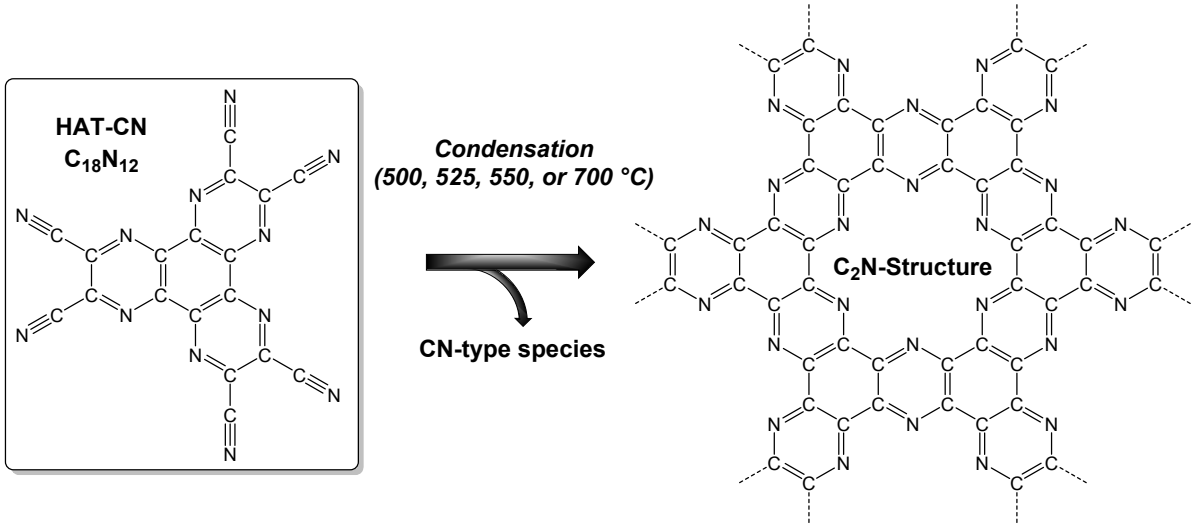

Figure S1. Thermal condensation of HAT-CN to C_2N-type products.

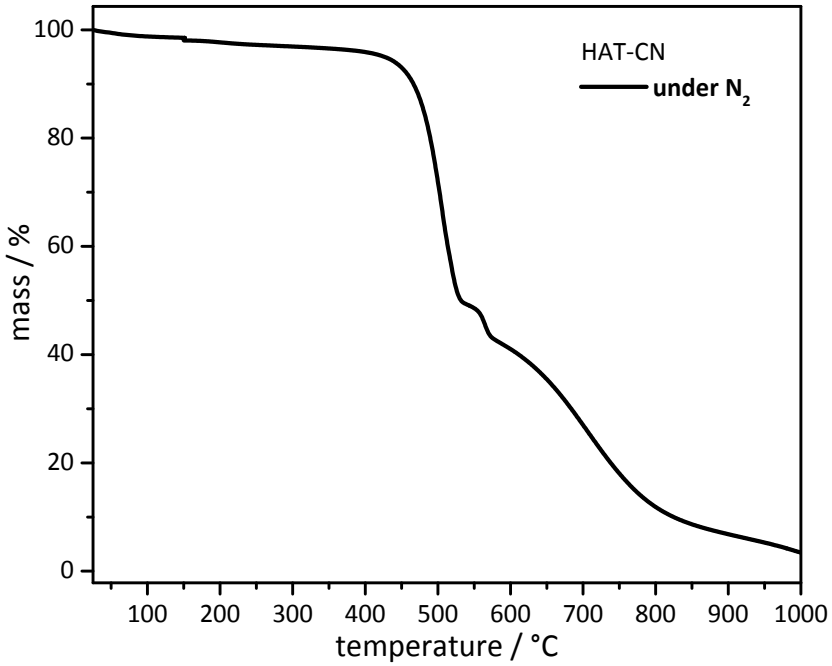

Figure S2. Thermal analysis of HAT-CN under nitrogen with a heating rate of 5 °C min^{-1}.

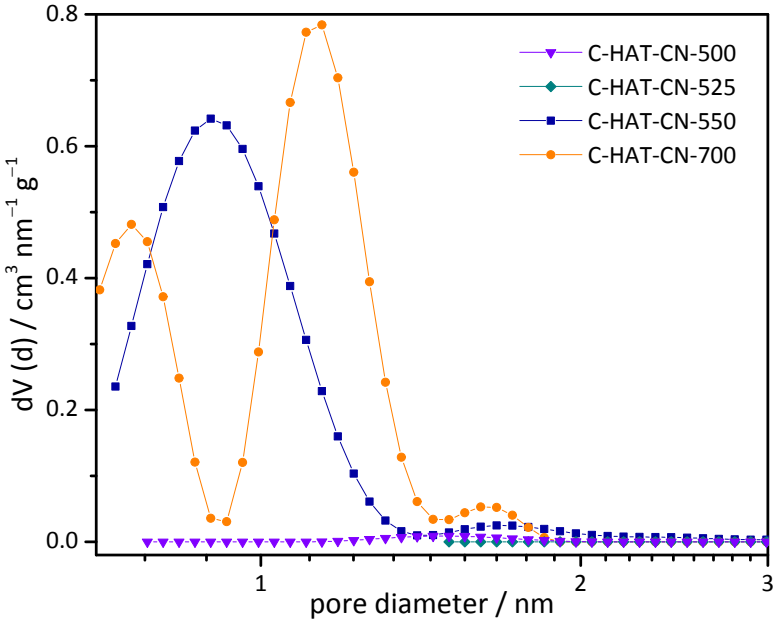

Figure S3. Differential pore size distribution plot calculated with QSDFT (Ar on carbons with cylindrical/sphere pores at -186 °C, adsorption branch kernel) of C-HAT-CN-500, of C-HAT-CN-525, of C-HAT-CN-550, and C-HAT-CN-700.

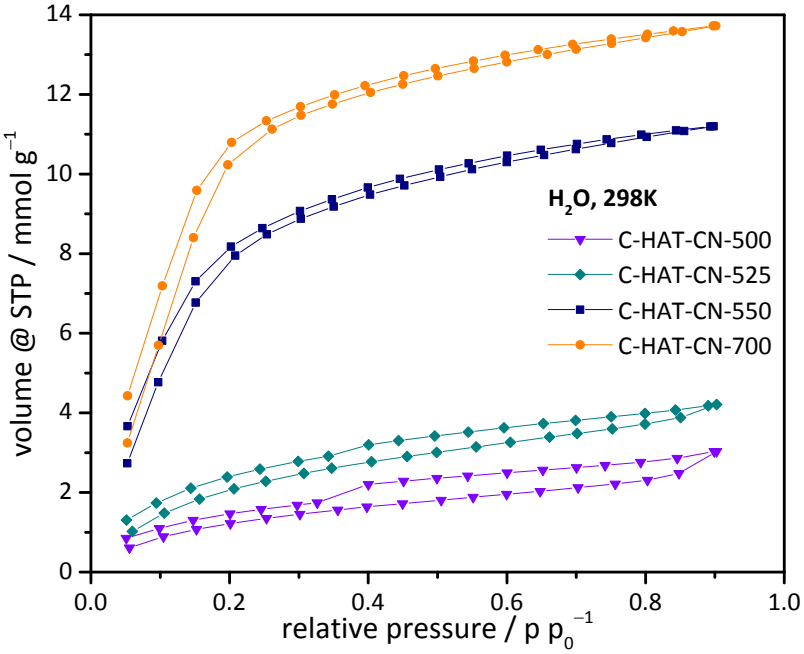

Figure S4. H_2O vapor physisorption isotherms (at 25 °C) of C-HAT-CN-500, C-HAT-CN-525, C-HAT-CN-550, and C-HAT-CN-700.

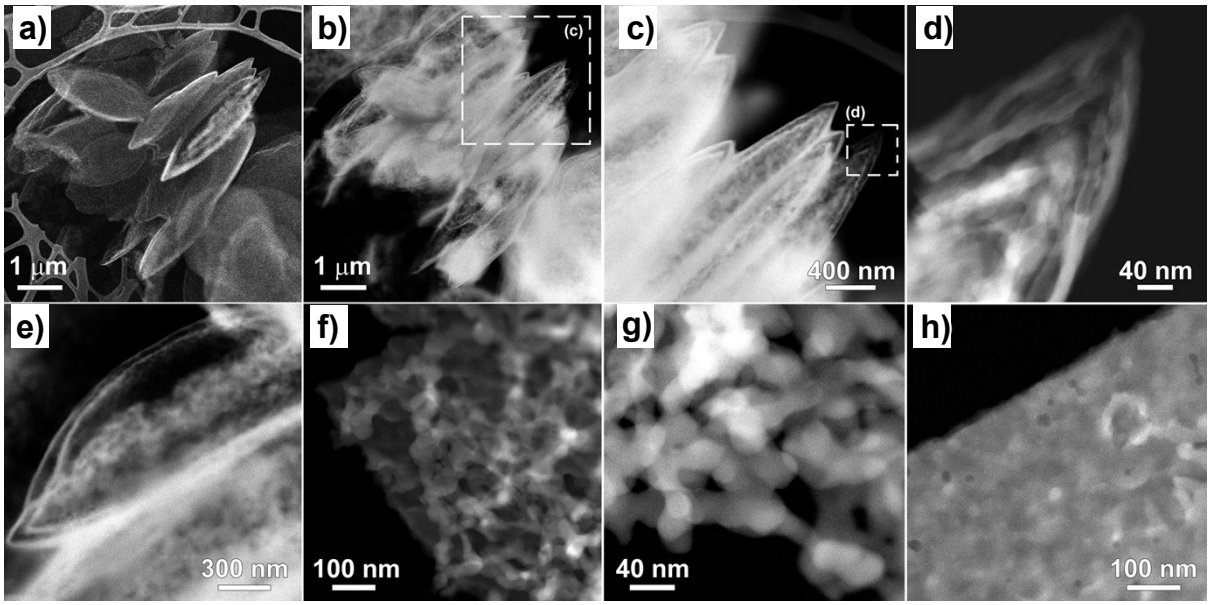

Figure S5. Backscattered electron image (a) and ADF-STEM images (b-h) of HAT-525. (b) shows the same areas as in (a), dotted lines in (b) and (c) indicate areas enlarged in (c) and (d), respectively. Images (f) and (g) show the inner morphology of the particles. (h) shows the morphology of the outer layer of the particles.

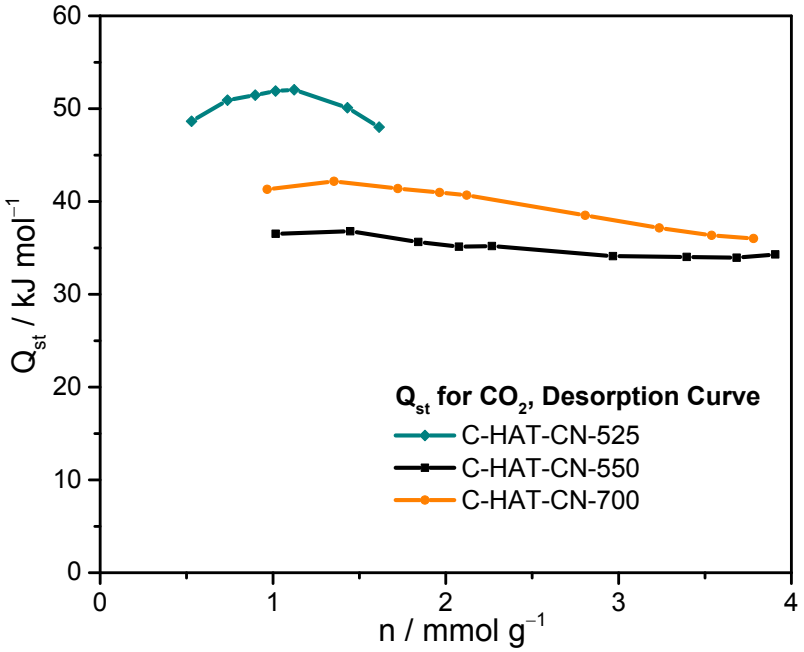

Figure S6. Isosteric heat (Q_{st}) of CO_2 adsorption of C-HAT-CN-525, C-HAT-CN-550, and C-HAT-CN-700.

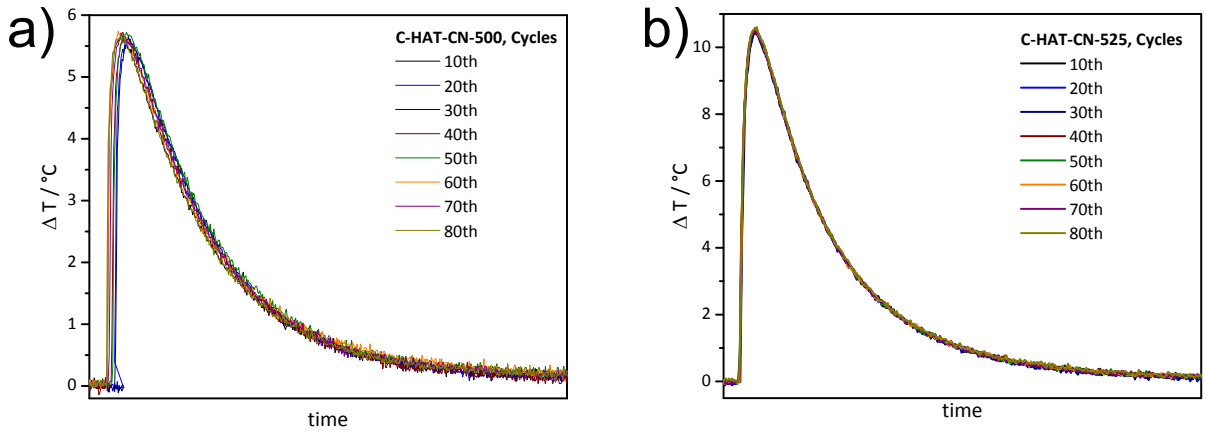

Figure S7. Thermal response curves during cycling experiments on C-HAT-CN-500 (a) and C-HAT-CN-525 (b) using CO_2 as test gas at 1 bar at 25 °C over 80 adsorption/desorption cycles.

Experimental and Computational Details

Electron Microscopy Investigations

For high-resolution transmission electron microscopy HRTEM and scanning transmission electron microscopy (STEM) observations, a suspension of the sample in ethanol was sonicated for 10 minutes and then drop-casted to the Cu grid with a lacey carbon support and dried for 5 minutes. The STEM study was performed using a double Cs corrected JEOL JEM-ARM200F (S)TEM operated at 80kV and equipped with a cold-field emission gun, a high-angle silicon drift Energy Dispersive X-ray (EDX) detector (solid angle up to 0.98 steradians with a detection area of 100 mm^2) and a Gatan Quantum GIF spectroscopy system. Annular Dark Field Scanning Transmission Electron Microscopy (ADF - STEM) images were collected at a probe convergence semi-angle of 24 mrad. HRTEM was performed at the same instrument operating at 200 kV

Computational Details

Periodic density functional theory calculations were carried out using the hybrid Gaussian and plane wave approach,[1] as implemented in the CP2K/Quickstep code.[2] The Kohn-Sham orbitals were described by an accurate molecularly optimized double-zeta basis set with one additional set of polarization function, while the charge density was represented by plane waves with a density cutoff of 500 Ry.[3] Separable norm-conserving pseudopotentials were used to mimic the interactions between the valence electrons and the ionic cores.[4] The B97-D exchange and correlation functional, which is based on Becke's power-series *Ansatz*, plus a damped atom-pairwise dispersion correction to account for long-range van der Waals interactions was employed.[5] The C_2N structure was modeled using a supercell with a=b=16.8, c=12.3 Å and α=β=90.0 and γ=16.0, which consists of 4 C_2N-layers. Optimized structures were obtained by globally minimizing the potential energy, while varying the atomic positions by dynamical simulated annealing[6] based on the second-generation Car-Parrinello approach of Kühne *et al*.[7]

Atomic coordinates CO_2 in C_2N

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O	8.436074	9.699453	1.167809
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O	12.618105	2.456320	11.137695

O	12.618034	2.456198	8.801399
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O	12.618105	2.456320	4.537695
O	12.618034	2.456198	2.201400
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Atomic coordinates CO_2 in C_3H

C	7.685840	6.068870	9.900010
C	11.885950	13.343670	9.900130
C	16.085899	6.068990	9.900110
C	20.285879	13.343590	9.900160
C	7.701030	3.621620	9.899970
C	11.901100	10.896260	9.900000
C	16.101101	3.621650	9.900000
C	20.301050	10.896240	9.900060
C	9.114010	6.068970	9.900010
C	13.314110	13.343640	9.900210
C	17.514040	6.069070	9.900050
C	21.714081	13.343720	9.900260
C	6.987030	-0.008880	9.900180
C	11.186960	7.265800	9.900000

C	15.387120	-0.008830	9.900380
C	19.587021	7.265820	9.900140
C	7.700950	1.228010	9.900050
C	11.901060	8.502650	9.900000
C	16.101160	1.228020	9.900230
C	20.301041	8.502630	9.900150
C	9.098780	3.621610	9.900040
C	13.298900	10.896230	9.899930
C	17.498989	3.621620	9.899600
C	21.698879	10.896210	9.899520
C	9.812930	4.858420	9.900030
C	14.013030	12.133000	9.899950
C	18.213020	4.858480	9.899600
C	22.413090	12.133020	9.899530
C	3.485860	6.055320	9.899770
C	7.685950	13.329990	9.899720
C	11.885880	6.055230	9.899990
C	16.085930	13.329890	9.899970
C	1.413050	-0.008760	9.899870
C	5.612990	7.265800	9.899900
C	9.813000	-0.008810	9.899920
C	14.013030	7.265840	9.900000
C	4.914000	6.055120	9.899900
C	9.114120	13.329920	9.899820
C	13.314070	6.055210	9.900000

C	17.514059	13.329810	9.899960
C	6.986980	4.858420	9.900000
C	11.187040	12.133090	9.900050
C	15.387040	4.858480	9.900090
C	19.587000	12.133050	9.900150
C	0.698950	1.228040	9.899780
C	4.898880	8.502630	9.899780
C	9.098880	1.228020	9.899990
C	13.298930	8.502650	9.899990
C	11.184560	4.876130	9.900000
C	15.384680	12.150740	9.899980
C	19.584629	4.876210	9.899180
C	23.784740	12.150850	9.899180
C	5.615270	-0.026600	9.900610
C	9.815160	7.247990	9.899980
C	14.015340	-0.026520	9.900910
C	18.215219	7.248100	9.900110
C	7.030490	2.424830	9.899850
C	11.230590	9.699440	9.900000
C	15.430650	2.424780	9.899970
C	19.630510	9.699410	9.900140
C	2.784680	-0.026470	9.900160
C	6.984640	7.247980	9.900180
C	11.184640	-0.026550	9.899830
C	15.384690	7.248120	9.900060

C	5.615230	4.876110	9.900210
C	9.815270	12.150900	9.900110
C	14.015270	4.876210	9.900060
C	18.215219	12.150760	9.900010
C	9.769300	2.424840	9.900030
C	13.969430	9.699430	9.899950
C	18.169460	2.424790	9.899120
C	22.369360	9.699410	9.899170
C	7.685860	6.068940	6.600000
C	11.885980	13.343740	6.600010
C	16.085930	6.069060	6.600010
C	20.285910	13.343660	6.600020
C	7.701030	3.621600	6.599990
C	11.901100	10.896240	6.600000
C	16.101110	3.621630	6.600000
C	20.301060	10.896220	6.600000
C	9.114030	6.068880	6.600000
C	13.314120	13.343540	6.600020
C	17.514050	6.068980	6.600000
C	21.714100	13.343630	6.600030
C	6.986960	-0.008840	6.600020
C	11.186890	7.265840	6.600000
C	15.387050	-0.008780	6.600040
C	19.586950	7.265860	6.600010
C	7.700990	1.228020	6.600000

C	11.901100	8.502650	6.600000
C	16.101200	1.228030	6.600020
C	20.301081	8.502640	6.600010
C	9.098820	3.621620	6.600000
C	13.298940	10.896240	6.599990
C	17.499029	3.621630	6.599950
C	21.698931	10.896220	6.599950
C	9.812860	4.858470	6.600000
C	14.012960	12.133050	6.600000
C	18.212950	4.858520	6.599960
C	22.413019	12.133070	6.599950
C	3.485880	6.055230	6.599970
C	7.685970	13.329900	6.599970
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C	16.085951	13.329800	6.600000
C	1.412990	-0.008780	6.599990
C	5.612940	7.265770	6.600000
C	9.812940	-0.008830	6.599990
C	14.012980	7.265820	6.600000
C	4.914030	6.055190	6.600000
C	9.114140	13.329990	6.599990
C	13.314100	6.055280	6.600000
C	17.514080	13.329880	6.599990
C	6.986930	4.858390	6.600000
C	11.186990	12.133070	6.600010

C	15.386990	4.858450	6.600010
C	19.586950	12.133030	6.600020
C	0.698950	1.228020	6.599970
C	4.898880	8.502600	6.599970
C	9.098880	1.227990	6.600000
C	13.298930	8.502630	6.600000
C	11.184630	4.876160	6.600000
C	15.384760	12.150770	6.599990
C	19.584709	4.876240	6.599940
C	23.784821	12.150880	6.599930
C	5.615350	-0.026570	6.600040
C	9.815240	7.248020	6.600000
C	14.015420	-0.026490	6.600070
C	18.215300	7.248130	6.600020
C	7.030520	2.424850	6.599990
C	11.230620	9.699450	6.600000
C	15.430680	2.424800	6.600010
C	19.630550	9.699430	6.600020
C	2.784750	-0.026480	6.600010
C	6.984710	7.247960	6.600010
C	11.184710	-0.026570	6.599990
C	15.384760	7.248110	6.600010
C	5.615300	4.876100	6.600010
C	9.815340	12.150880	6.600000
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C	18.215290	12.150750	6.600000
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C	22.369390	9.699430	6.599940
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C	16.101101	3.621650	3.300000
C	20.301050	10.896240	3.300000
C	9.114010	6.068970	3.300000
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C	17.514040	6.069070	3.300000
C	21.714081	13.343720	3.300000
C	6.987030	-0.008880	3.300000
C	11.186960	7.265800	3.300000
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C	19.587021	7.265820	3.300000
C	7.700950	1.228010	3.300000
C	11.901060	8.502650	3.300000
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C	9.098780	3.621610	3.300000
C	13.298900	10.896230	3.300000
C	17.498989	3.621620	3.300000
C	21.698879	10.896210	3.299990
C	9.812930	4.858420	3.300000
C	14.013030	12.133000	3.300000
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C	1.413050	-0.008760	3.300000
C	5.612990	7.265800	3.300000
C	9.813000	-0.008810	3.300000
C	14.013030	7.265840	3.300000
C	4.914000	6.055120	3.300000
C	9.114120	13.329920	3.300000
C	13.314070	6.055210	3.300000
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C	11.187040	12.133090	3.300000
C	15.387040	4.858480	3.300000
C	19.587000	12.133050	3.300000
C	0.698950	1.228040	3.300000

C	4.898880	8.502630	3.300000
C	9.098880	1.228020	3.300000
C	13.298930	8.502650	3.300000
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C	19.584629	4.876210	3.299990
C	23.784740	12.150850	3.299990
C	5.615270	-0.026600	3.300000
C	9.815160	7.247990	3.300000
C	14.015340	-0.026520	3.300010
C	18.215219	7.248100	3.300000
C	7.030490	2.424830	3.300000
C	11.230590	9.699440	3.300000
C	15.430650	2.424780	3.300000
C	19.630510	9.699410	3.300000
C	2.784680	-0.026470	3.300000
C	6.984640	7.247980	3.300000
C	11.184640	-0.026550	3.300000
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C	9.815270	12.150900	3.300000
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C	16.101101	3.621630	0.000000
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C	9.114030	6.068880	0.000000
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C	15.387050	-0.008780	0.000040
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C	7.700990	1.228020	0.000000
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C	16.101200	1.228030	0.000020
C	20.301069	8.502640	0.000010
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C	13.298940	10.896240	-0.000010
C	17.499020	3.621630	-0.000050

C	21.698919	10.896220	-0.000050
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C	15.386980	4.858460	0.000010
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C	0.698950	1.228020	-0.000030
C	4.898880	8.502600	-0.000030
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C	13.298930	8.502630	0.000000

C	11.184630	4.876160	0.000000
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C	11.230620	9.699460	0.000000
C	15.430670	2.424800	0.000010
C	19.630541	9.699430	0.000020
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C	15.384760	7.248110	0.000010
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C	13.969460	9.699450	-0.000010
C	18.169479	2.424810	-0.000060
C	22.369390	9.699430	-0.000060
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H	17.695791	11.251287	-0.008640
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H	17.695791	8.147600	-0.008405
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H	14.360282	2.424904	0.001293
H	13.480222	3.949252	0.001868
H	11.719739	3.949169	-0.000109
H	10.839813	2.424971	0.001444
H	9.295902	8.147410	-0.023355
H	10.193801	9.699417	-0.069973
H	9.296036	11.251463	-0.023139
H	7.503943	8.147390	0.024146
H	5.080368	3.949121	0.003308
H	5.960238	2.424974	0.001620
H	13.480362	0.900653	0.002759
H	11.719834	0.900601	0.000652
H	5.080392	0.900580	0.001549
H	23.406221	9.699437	0.069461
H	24.304045	11.251432	0.023423
H	20.119968	3.949266	0.000866
H	19.240051	2.424888	0.001078
H	3.319952	0.900671	-0.000650
H	15.039849	9.699442	9.901167
H	15.919790	11.223706	9.901350

H	17.680153	11.223715	9.901296
H	18.560099	9.699394	9.901690
H	17.680136	8.175150	9.901580
H	15.919827	8.175140	9.901342
H	14.393227	2.421453	9.890381
H	13.497146	3.978935	9.893141
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H	10.809258	2.421523	9.893456
H	9.280028	8.175064	9.899898
H	10.160113	9.699377	9.900213
H	9.280204	11.223796	9.900590
H	7.519808	8.175038	9.900450
H	5.094363	3.981937	9.891177
H	5.995728	2.420956	9.886067
H	13.492427	0.872469	9.897902
H	11.705341	0.875003	9.894488
H	5.090700	0.870027	9.897235
H	23.439842	9.699367	9.898725
H	24.319860	11.223771	9.898786
H	20.098999	3.973715	9.892665
H	19.211752	2.422086	9.892245
H	3.303652	0.877485	9.896215
H	15.008019	9.699457	6.580808
H	15.904164	11.251211	6.596007
H	17.695791	11.251287	6.591360

H	18.591827	9.699405	6.604043
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H	15.904204	8.147633	6.596087
H	14.360292	2.424907	6.601294
H	13.480221	3.949252	6.601869
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H	10.839813	2.424971	6.601444
H	9.295902	8.147408	6.576644
H	10.193802	9.699408	6.530026
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H	7.503945	8.147389	6.624147
H	5.080363	3.949125	6.603308
H	5.960238	2.424976	6.601620
H	13.480361	0.900652	6.602761
H	11.719834	0.900600	6.600652
H	5.080394	0.900577	6.601550
H	23.406221	9.699433	6.669457
H	24.304050	11.251432	6.623426
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H	19.240059	2.424882	6.601077
H	3.319954	0.900668	6.599350
H	15.039849	9.699442	3.301255
H	15.919790	11.223705	3.301342
H	17.680153	11.223715	3.301425
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H	17.680136	8.175148	3.301398
H	15.919827	8.175140	3.301256
H	14.393217	2.421454	3.291707
H	13.497147	3.978937	3.292723
H	11.700561	3.976118	3.291643
H	10.809258	2.421524	3.293221
H	9.280028	8.175064	3.300013
H	10.160112	9.699377	3.300226
H	9.280204	11.223795	3.300186
H	7.519808	8.175036	3.299766
H	5.094385	3.981951	3.288222
H	5.995704	2.420946	3.288459
H	13.492440	0.872461	3.293910
H	11.705345	0.875008	3.296102
H	5.090696	0.870020	3.295138
H	23.439842	9.699368	3.300112
H	24.319860	11.223771	3.300013
H	20.099012	3.973714	3.295269
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H	3.303652	0.877480	3.295360
C	16.799982	9.699406	6.671480
O	16.799789	9.699494	7.845218
O	16.800217	9.699481	5.494851
C	16.799982	9.699405	0.071479
O	16.799789	9.699494	1.245218

O	16.800215	9.699481	-1.105150
C	8.399996	9.699311	6.600009
O	8.435630	9.699464	7.774882
O	8.364381	9.699514	5.425118
C	8.399999	9.699309	0.000010
O	8.435629	9.699465	1.174882
O	8.364379	9.699515	-1.174883
C	12.610610	2.443860	9.971267
O	12.616999	2.454438	11.144994
O	12.616683	2.453745	8.794632
C	12.610607	2.443859	3.371273
O	12.617016	2.454414	4.544990
O	12.616665	2.453769	2.194628
C	4.233090	2.444057	9.970882
O	4.250941	2.454313	11.144579
O	4.249745	2.453500	8.794217
C	4.233086	2.444064	3.370876
O	4.250987	2.454287	4.544582
O	4.249690	2.453526	2.194217

Supplementary References

[1] G. Lippert, J. Hutter, M. Parrinello, *Mol. Phys.*, 1997, **92**, 477-488.

[2] J. VandeVondele, M. Krack, F. Mohamed, M. Parrinello, T. Chassaing, J. Hutter, *Comput. Phys. Commun.*, 2005, **167**, 103.

[3] J. VandeVondele, J. Hutter, *J. Chem. Phys.*, 2007, **127**, 114105.

[4] a) S. Goedecker, M. Teter, J. Hutter, *Phys. Rev. B*, 1996, **54**, 1703; b) M. Krack, *Theor. Chem. Acc.*, 2005, **114**, 145-152.

[5] S. Grimme, *J. Comput. Chem.*, 2006, **27**, 1787-1799.

[6] a) S. Kirkpatrick, C. D. Gelatt, M. P. Vecchi, *Science*, 1983, **220**, 671; b) R. Car, R. Parrinello, *Phys. Rev. Lett.*, 1985, **55**, 2471.

[7] a) T. D. Kühne, M. Krack, F. R. Mohamed, M. Parinello, *Phys. Rev. Lett.*, 2007, **98**, 066401; b) T. D. Kühne, *WIREs Comput. Mol. Sci.*, 2014, **4**, 391.