

ELECTRONIC SUPPLEMENTARY INFORMATION

**A DFT study of planar vs. corrugated graphene-like carbon nitride
(g-C₃N₄) and their role in the catalytic performance of CO₂
conversion**

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Additional Computational Details

Computational settings:

Settings PBE optimisation	Settings DFT-D3 optimisation	Settings HSE06 single point
ENCUT = 450 PREC = Medium EDIFF = 1E-4 EDIFFG = -0.01/-0.05 ^a ISIF = 2 ISPIN = 1/2 ^b ISMear = 0 SIGMA = 0.02 IBRION = 2 POTIM = 0.5	ENCUT = 450 PREC = Medium EDIFF = 1E-4 EDIFFG = -0.01/-0.05 ^a ISIF = 2 ISPIN = 1/2 ^b IVDW = 11 VDW_RADIUS = 50.2 VDW_CNRRADIUS = 20.0 VDW_S6 = 14.0 VDW_S8 = 16.0 VDW_SR = 1.0 ISMear = 0 SIGMA = 0.02 IBRION = 2 POTIM = 0.5	PREC = Accurate ALGO = Accurate GGS = PE LHFCALC = .TRUE. HFSCREEN = 0.2 AEXX = 0.25 AGGAX = 0.75 AGGAC = 1.0 ALDAC = 1.0
ZPE calculation over Γ points	Settings NVT MD	
NSW = 1 IBRION = 5 POTIM = 0.02 NFREE = 2	ENCUT = 400 PREC = Normal EDIFF = 1E-4 ISYM = 0 ALGO = Fast LREAL = Auto ISMear = 0 SIGMA = 0.1 IBRION = 0 ^c POTIM = 1 ^c NSW = 2000 ^c TEBEG = 298 TEEND = 298 SMASS = 0 LVDW = .TRUE.	

^aForce convergence limits of |0.01| and |0.05| eV/Å for corrugated and planar g-C₃N₄, respectively. Force convergence limit of |0.05| eV/Å for corrugated g-C₃N₄ when interacting with 13 explicit H₂O molecules. Geometrical constraints applied for planar g-C₃N₄, freezing all atoms that do not interact with a chemisorbed solute.

^bFor radical states, spin-polarised calculations have been considered. (ISPIN = 2. For neutral systems, by default ISPIN = 1).

^cNVT canonical ensemble (T = 298 K), 1 fs time-step along 2000 steps = 2 ps of MD simulation.

Pseudo-potentials applied:

Nitrogen: PAW_PBE N 08Apr2002

Carbon: PAW_PBE C 08Apr2002

Oxygen: PAW_PBE O 08Apr2002

Hydrogen: PAW_PBE H 15Jun2001

Table S1. Gibbs free energies at room temperature, in eV, corresponding to the isolated CO₂, H₂, and H₂O species,^a and for the different states along the CO₂ conversion mechanism catalysed by g-C₃N₄.^b ZPE corrections calculated over the Γ points from the optimised super-cell using 3×3×1 *k*-points. Calculations at PBE computational level including dispersion corrections *via* the DFT-D3 Grimme's method^c (see **Computational details** at the main text).

Species		<i>G</i>	
CO ₂ (g)		−23.36	
H ₂ (CHE)		−3.43	
H ₂ O (g)		−14.28	

Planar g-C ₃ N ₄			
Species	<i>G</i>	Species	<i>G</i>
Clean surface	−473.81	HCO•	−491.39
*CO ₂	−496.91	H ₂ CO	−496.18
HOCO•	−498.54	CH ₃ O•	−497.97
CO	−488.72	CH ₃ OH	−504.40

Corrugated g-C ₃ N ₄			
Species	<i>G</i>	Species	<i>G</i>
Clean surface	−469.95	HCO•	−487.89
*CO ₂	−493.01	H ₂ CO	−491.92
HOCO•	−495.29	CH ₃ O•	−494.13
CO	−484.85	CH ₃ OH	−499.51

Corrugated g-C₃N₄ + 13H₂O

Species	<i>G</i>	Species	<i>G</i>
Clean surface	−656.07	HCO•	−673.80
*CO ₂	−678.51	H ₂ CO	−677.63
HOCO•	−680.95	CH ₃ O•	−679.47
CO	−670.93	CH ₃ OH	−685.63

^a $G = E_{elec} - TS + ZPE = H - TS + ZPE$ data obtained by Peterson *et al.* (*Energy Environ. Sci.*, 2010, **3**, 1311-1315) and Lim and co-workers (*Nanoscale*, 2014, **6**, 5087-5092). T = 298 K. Assumed fugacity: 101,325 Pa for the CO₂ (g) and H₂ (CHE) species, and 3,534 Pa for H₂O (g). Since $\int C_p dT$ is almost negligible and $\Delta \int C_p dT \approx 0$ eV, no thermal corrections for the enthalpy have been taken into account for the ΔG calculation.

^bForce convergence limit applied for the CH₃OH step of $|0.025|$ eV/Å.

^cFor neutral systems, no special spin considerations were taken into account, while for radical states, spin-polarised calculations were performed.

Cartesian Coordinates

Γ points at PBE computational level plus explicit DFT-D3 dispersion corrections:

Optimised planar g-C₃N₄

a	14.27487500	0.00000000	0.00000000
b	-7.13743750	12.36240439	0.00000000
c	0.00000000	0.00000000	20.00000000
N	0.46351824	2.41524029	10.00000000
N	7.60095594	2.41524029	10.00000000
N	1.62752984	4.43138079	10.00000000
N	8.76496754	4.43138079	10.00000000
N	1.64735091	0.36477892	10.00000000
N	8.78478861	0.36477892	10.00000000
N	2.81137260	2.40380000	10.00000000
N	9.94881030	2.40380000	10.00000000
N	3.99520525	4.43138079	10.00000000
N	11.13264295	4.43138079	10.00000000
N	3.97538421	0.36477892	10.00000000
N	11.11282191	0.36477892	10.00000000
N	5.15922696	2.41524029	10.00000000
N	12.29666466	2.41524029	10.00000000
N	6.38008640	0.34340000	10.00000000
N	13.51752410	0.34340000	10.00000000
N	-3.10519556	8.59644029	10.00000000
N	4.03224214	8.59644029	10.00000000
N	-1.94118396	10.61258079	10.00000000
N	5.19625374	10.61258079	10.00000000

N	-1.92136289	6.54597892	10.00000000
N	5.21607481	6.54597892	10.00000000
N	-0.75734120	8.58500000	10.00000000
N	6.38009650	8.58500000	10.00000000
N	0.42649145	10.61258079	10.00000000
N	7.56392915	10.61258079	10.00000000
N	0.40667041	6.54597892	10.00000000
N	7.54410811	6.54597892	10.00000000
N	1.59051316	8.59644029	10.00000000
N	8.72795086	8.59644029	10.00000000
N	2.81137260	6.52460000	10.00000000
N	9.94881030	6.52460000	10.00000000
C	0.52154882	1.08176531	10.00000000
C	7.65898652	1.08176531	10.00000000
C	1.60387553	3.10095446	10.00000000
C	8.74131323	3.10095446	10.00000000
C	2.81137259	5.04785928	10.00000000
C	9.94881029	5.04785928	10.00000000
C	2.81137261	1.00951128	10.00000000
C	9.94881031	1.00951128	10.00000000
C	4.01885957	3.10095446	10.00000000
C	11.15629727	3.10095446	10.00000000
C	5.10119638	1.08176531	10.00000000
C	12.23863408	1.08176531	10.00000000
C	-3.04716498	7.26296531	10.00000000
C	4.09027272	7.26296531	10.00000000
C	-1.96483827	9.28215446	10.00000000
C	5.17259943	9.28215446	10.00000000
C	-0.75734121	11.22905928	10.00000000
C	6.38009649	11.22905928	10.00000000
C	-0.75734119	7.19071128	10.00000000
C	6.38009651	7.19071128	10.00000000
C	0.45014577	9.28215446	10.00000000
C	7.58758347	9.28215446	10.00000000
C	1.53248258	7.26296531	10.00000000
C	8.66992028	7.26296531	10.00000000

Optimised corrugated g-C₃N₄ (*a*, *b*, and *c* lattice vectors extensible to the rest of the corrugated structures)

<i>a</i>	13.66800000	0.00000000	0.00000000
<i>b</i>	6.83400000	11.83683522	0.00000000
<i>c</i>	0.00000000	0.00000000	19.99999999
N	1.11104941	0.32524980	8.00912010
N	2.11060985	2.28144032	7.23532329
N	3.49458329	0.47414153	8.00880513
N	3.19514518	4.34229529	6.88555260
N	4.45142017	2.37428659	7.02258609
N	5.81211233	0.54578691	7.56290963
N	5.53628550	4.35187460	6.38822702
N	6.58402212	2.26054057	6.06782219
N	4.46443724	6.26265312	7.26803409
N	5.49822464	8.22338521	7.97837550

N	6.68187558	6.13114888	8.01752878
N	6.66030948	10.22210651	8.32388342
N	7.83992124	8.18231371	8.26111644
N	8.97998135	6.13261886	8.38409128
N	9.02857440	10.18780170	8.63024452
N	10.16567932	8.18705964	8.69425987
N	7.91674079	0.34971625	6.48145515
N	9.09706099	2.39348871	6.71378895
N	10.32486512	0.36300123	6.54867254
N	10.31916141	4.36673979	7.13540909
N	11.31247838	2.28769275	7.48100688
N	12.64622927	0.43745322	6.99622616
N	12.24335076	4.16272090	8.56530930
N	13.39206970	2.11917206	8.55612847
N	11.29980164	6.27076341	8.08012605
N	12.32292319	8.18374880	7.12111708
N	13.62085718	6.54200166	8.31472342
N	13.44084351	10.18689092	6.49482194
N	14.66923872	8.29955067	7.15170090
N	15.95643745	6.58182154	8.09782312
N	15.78429220	10.09248599	6.12673293
N	16.88495257	8.04215890	6.41737133
C	2.31371365	1.05659445	7.74891537
C	3.20608292	3.02046476	7.02724671
C	4.58141662	1.08993443	7.55087045
C	4.40821729	4.92625782	6.83872792
C	5.55292288	3.02659640	6.45846144
C	6.68465257	1.10169616	6.71131943
C	5.62374078	6.90386756	7.76815019
C	6.62894387	8.89615337	8.21262056
C	7.83077867	6.77646488	8.24724099
C	7.88190346	10.78617491	8.34391014
C	9.03125501	8.86372505	8.57043935
C	10.08522348	6.89111872	8.39513598
C	9.17970113	1.06200571	6.58070387
C	10.19839729	3.03640681	7.09716108
C	11.42131230	0.98256267	6.98945512
C	11.30133288	4.84145248	7.91118179
C	12.34095697	2.87296434	8.22927165
C	13.52164914	1.00843263	7.82843465
C	12.48567194	7.05848871	7.83199529
C	13.43070526	8.91818727	6.90691270
C	14.74492070	7.11530573	7.88578235
C	14.65532829	10.76469257	6.37234968
C	15.80732625	8.83264457	6.53109362
C	16.90177265	7.01993257	7.24589354

Optimised corrugated g-C₃N₄:*CO₂

N	1.09337695	0.31411454	8.08367822
N	2.09489701	2.27198930	7.31952547
N	3.48038033	0.45941285	8.07718454
N	3.17825504	4.33364878	6.97861743
N	4.43480111	2.36435518	7.09924696

N	5.79963405	0.53676003	7.62752503
N	5.51901622	4.34602609	6.47965589
N	6.56344757	2.25557679	6.13367782
N	4.44494694	6.25231282	7.36956437
N	5.47943431	8.21288308	8.07591514
N	6.66221805	6.11996858	8.11690901
N	6.64345673	10.21251421	8.40654836
N	7.82175732	8.17161329	8.34731822
N	8.96227029	6.12162384	8.47053008
N	9.01267912	10.17807764	8.70516135
N	10.14974461	8.17756986	8.76421047
N	7.89746382	0.34054969	6.53096839
N	9.07705214	2.38173180	6.78197077
N	10.30698184	0.35500117	6.60626956
N	10.29569298	4.35523966	7.21051992
N	11.29020690	2.27512322	7.55388768
N	12.62623302	0.42482159	7.07014075
N	12.22439223	4.15196652	8.63403406
N	13.37151145	2.10872547	8.62737925
N	11.27966367	6.26031954	8.15034419
N	12.30592177	8.17153508	7.18890235
N	13.59827749	6.53885994	8.40106631
N	13.42440753	10.17520130	6.56218262
N	14.65157080	8.29240893	7.23578007
N	15.93411745	6.57624155	8.19212426
N	15.77023939	10.08178677	6.20862800
N	16.87076394	8.03310621	6.51319482
C	2.29663186	1.04425094	7.82492220
C	3.18981752	3.01103613	7.11188322
C	4.56497406	1.07809330	7.62115574
C	4.39069796	4.91824665	6.93486707
C	5.53524750	3.02052048	6.53701912
C	6.66856364	1.09240752	6.76828585
C	5.60431629	6.89333994	7.86817002
C	6.61118385	8.88622407	8.30218907
C	7.81270360	6.76561815	8.33829549
C	7.86501840	10.77606539	8.42148901
C	9.01477966	8.85397387	8.64731901
C	10.06760895	6.88053459	8.47036275
C	9.16142969	1.05177688	6.64051926
C	10.17642317	3.02414613	7.17011941
C	11.40050996	0.97072370	7.05906353
C	11.28035724	4.83027716	7.98258931
C	12.31945932	2.86122017	8.30030880
C	13.50107602	0.99667597	7.90215277
C	12.46594742	7.04991267	7.90653340
C	13.41384125	8.90814764	6.97993716
C	14.72414848	7.11074649	7.97450367
C	14.63907581	10.75485958	6.44125871
C	15.79264368	8.82454594	6.61952287
C	16.88286788	7.01206665	7.36300388
C	7.41245742	0.97161662	10.10281949
O	6.44166945	1.33014006	10.65793015
O	8.39884370	0.62300715	9.53906627

Optimised corrugated g-C₃N₄:HOCO●

N	1.13054713	0.40569141	7.95111970
N	2.13081165	2.35016359	7.18093677
N	3.52002569	0.57438709	8.02109931
N	3.20912322	4.41956399	6.83337324
N	4.48716573	2.49067079	7.10935712
N	5.92247908	0.81909872	7.80881394
N	5.55798859	4.45549360	6.37266872
N	6.58904198	2.33230095	6.08490885
N	4.47795042	6.36021956	7.24857277
N	5.50429618	8.31732332	7.97829543
N	6.68499065	6.22050585	8.02534685
N	6.67464265	10.31517001	8.29490253
N	7.84805801	8.26913872	8.25095055
N	8.98682304	6.21659894	8.37851942
N	9.04640763	10.27322161	8.58591118
N	10.17066848	8.26951663	8.69978792
N	7.94611265	0.43882055	6.40792094
N	9.12057761	2.48017541	6.66666667
N	10.36019511	0.46173027	6.44837777
N	10.33035543	4.45873962	7.10953198
N	11.33912544	2.37838848	7.41452740
N	12.67570811	0.52823658	6.92070330
N	12.26317496	4.24537092	8.52361183
N	13.41393405	2.20228328	8.49448612
N	11.30918258	6.36099995	8.06780522
N	12.32976446	8.31388236	7.16339049
N	13.63091815	6.62611807	8.28218589
N	13.45303378	10.31776287	6.54037833
N	14.67607423	8.39667427	7.12780539
N	15.95993550	6.66068550	8.04893235
N	15.79554257	10.17795062	6.08215997
N	16.89570097	8.13605789	6.38756356
C	2.31927485	1.14298277	7.71163849
C	3.22382228	3.12275290	7.01859076
C	4.57549920	1.25632628	7.66303037
C	4.43736391	5.02704147	6.80399538
C	5.58779558	3.12795849	6.48099922
C	6.78065249	1.20698439	6.70772900
C	5.62378403	6.99291692	7.76728317
C	6.63562241	8.98447470	8.19948958
C	7.83286267	6.86078959	8.24812568
C	7.89682091	10.86858225	8.30269919
C	9.04038956	8.94722223	8.55417545
C	10.08972600	6.97300464	8.39268340
C	9.21516303	1.15213234	6.51164622
C	10.21967150	3.12731225	7.05096276
C	11.45159457	1.07723933	6.90662753
C	11.31575992	4.93072658	7.88298391
C	12.36392321	2.95920880	8.17181959
C	13.54215213	1.09384426	7.76177954
C	12.49219996	7.15793707	7.83180143
C	13.43972474	9.03537560	6.93161456
C	14.75301057	7.20213179	7.84796398

C	14.67888601	10.86115410	6.34308695
C	15.81710726	8.92550163	6.49916626
C	16.91336748	7.11131129	7.23034280
C	6.42107832	0.21892832	8.97385073
O	14.40977029	11.67132770	9.09454026
O	5.47603875	0.15662669	9.93682482
H	12.72919887	11.55156177	10.68225993

Optimised corrugated g-C₃N₄:CO

N	1.07623184	0.32028262	8.03530157
N	2.07831269	2.27846981	7.27103109
N	3.46164946	0.46092939	8.01994807
N	3.16276867	4.34073654	6.93878811
N	4.41897645	2.37067396	7.05329128
N	5.77962734	0.53644601	7.57157008
N	5.50419140	4.35463876	6.44166608
N	6.55065773	2.26589297	6.09408854
N	4.42852090	6.25885304	7.33378696
N	5.46250972	8.21982764	8.04055500
N	6.64689084	6.12778319	8.07605211
N	6.62626103	10.22012315	8.36734077
N	7.80598987	8.17972699	8.30455229
N	8.94735666	6.13008637	8.42412001
N	8.99570501	10.18617921	8.66261748
N	10.13434161	8.18593778	8.72186141
N	7.88267763	0.34797644	6.48545631
N	9.06456003	2.39183219	6.72193630
N	10.29092480	0.36246311	6.56018398
N	10.28081470	4.36503459	7.15940672
N	11.27518520	2.28399666	7.50238917
N	12.60995348	0.43137421	7.02193967
N	12.20939174	4.16004692	8.58315577
N	13.35537071	2.11600084	8.57822370
N	11.26400001	6.26890529	8.10518699
N	12.29152731	8.17821953	7.14205034
N	13.58148458	6.55032615	8.36400680
N	13.41094193	10.18039790	6.51060201
N	14.63684501	8.30115098	7.19663907
N	15.91779489	6.58558351	8.15743574
N	15.75763320	10.08823630	6.16743584
N	16.85631045	8.03935959	6.47670360
C	2.27966018	1.04891767	7.77297275
C	3.17396488	3.01749791	7.06688359
C	4.54803300	1.08033818	7.56681258
C	4.37533785	4.92527092	6.89627385
C	5.52082841	3.02858198	6.49596601
C	6.65239222	1.09877181	6.72229225
C	5.58795286	6.90039471	7.83060229
C	6.59467332	8.89361530	8.26316279
C	7.79736550	6.77379197	8.29472790
C	7.84801350	10.78357560	8.37802603
C	8.99900775	8.86219693	8.60466636
C	10.05233020	6.88919180	8.42563348

C	9.14642870	1.06092845	6.58947867
C	10.16234708	3.03365759	7.11534740
C	11.38497526	0.97880936	7.00993690
C	11.26462089	4.83911405	7.93317021
C	12.30426336	2.86950315	8.24949527
C	13.48475985	1.00338532	7.85364286
C	12.45050026	7.05907619	7.86383662
C	13.39949031	8.91528037	6.93405378
C	14.70832105	7.12093219	7.93792157
C	14.62537923	10.76153642	6.39462738
C	15.77883807	8.83156822	6.58062244
C	16.86703513	7.01899996	7.32737538
C	8.21338423	0.81663249	9.73160552
O	7.56130375	0.84773781	10.64889409

Optimised corrugated g-C₃N₄:HCO●

N	1.13427742	0.40980869	7.97296974
N	2.13119088	2.34927696	7.19086215
N	3.52352961	0.60684456	8.09667347
N	3.20774048	4.41838530	6.82052191
N	4.48325874	2.49107871	7.10575340
N	5.91358670	0.82877001	7.82567501
N	5.55560543	4.44734738	6.34933048
N	6.59123856	2.32491002	6.08578257
N	4.48307896	6.35865166	7.22195731
N	5.50667876	8.31593769	7.96493506
N	6.68591622	6.21753522	8.00352109
N	6.67938358	10.31160140	8.31350794
N	7.84948904	8.26384626	8.23538510
N	8.98692027	6.20971721	8.36123973
N	9.06044864	10.26554381	8.51830074
N	10.17299171	8.26276658	8.67116844
N	7.94699910	0.43538624	6.48109277
N	9.12470958	2.47880117	6.69439953
N	10.35845565	0.45029609	6.50398766
N	10.34451468	4.45298890	7.11878686
N	11.34386681	2.37455181	7.44346105
N	12.67763984	0.52343156	6.95486453
N	12.26165690	4.24026867	8.55627160
N	13.41981010	2.20296148	8.52128356
N	11.31583554	6.35064692	8.07756317
N	12.33400531	8.30831609	7.19287340
N	13.64001264	6.59678858	8.26727360
N	13.45641591	10.31802674	6.60389759
N	14.67802662	8.38006549	7.12575777
N	15.96887045	6.64200583	8.02809439
N	15.78837715	10.17595280	6.08976041
N	16.89381723	8.13420007	6.37427113
C	2.32261785	1.15646806	7.74934471
C	3.22285087	3.12401613	7.01895210
C	4.57414491	1.27179122	7.69424424
C	4.43777366	5.02268580	6.78308124
C	5.58487257	3.12166851	6.46652065

C	6.76692631	1.20609726	6.72750962
C	5.62654895	6.99176726	7.74607497
C	6.63859494	8.98194712	8.19370382
C	7.83350929	6.85619185	8.23035387
C	7.90362036	10.86491656	8.29249103
C	9.04648977	8.94142604	8.51696844
C	10.08931604	6.96590550	8.38127466
C	9.21891075	1.14949815	6.55705987
C	10.22849040	3.12456868	7.07050211
C	11.45590603	1.07065980	6.94448151
C	11.32347598	4.92332961	7.90258120
C	12.36797439	2.95557563	8.20193533
C	13.54894441	1.09390994	7.78946662
C	12.49681092	7.13925174	7.84086504
C	13.44147176	9.02260519	6.96052960
C	14.75872293	7.17745048	7.83431892
C	14.67659868	10.85447329	6.37749547
C	15.81406168	8.91588704	6.49372398
C	16.91811247	7.10250278	7.21129911
C	6.36632303	0.17657993	8.99243274
O	12.52119031	11.81376328	9.97872829
H	14.27177878	11.73997896	8.88572959

Optimised corrugated g-C₃N₄:H₂CO

N	1.03382037	0.32862308	8.12252874
N	2.03254479	2.28454488	7.34656538
N	3.42199885	0.48142632	8.12115718
N	3.11537642	4.34665928	6.99775200
N	4.37237071	2.37777460	7.12090388
N	5.74257357	0.55851157	7.66948537
N	5.45608518	4.35903652	6.49691507
N	6.50723202	2.27109575	6.16997167
N	4.38474163	6.26822380	7.38007867
N	5.42127905	8.22585799	8.09499936
N	6.60513885	6.13335269	8.11809814
N	6.58608984	10.22337911	8.44153520
N	7.76531000	8.18360702	8.35803409
N	8.90645441	6.13207555	8.46025590
N	8.95615065	10.18814565	8.72979476
N	10.09208928	8.18624082	8.78118202
N	7.84212033	0.35947005	6.56692324
N	9.04387783	2.40613515	6.72164637
N	10.24974899	0.36317279	6.63898431
N	10.26051945	4.37405305	7.18212327
N	11.23211291	2.28898624	7.56379051
N	12.56863806	0.43354014	7.10457920
N	12.15232605	4.16317221	8.65534051
N	13.30065761	2.11988954	8.66359831
N	11.22339222	6.27415860	8.15401978
N	12.24780442	8.19083531	7.20561117
N	13.54060170	6.54965279	8.40645498
N	13.36657284	10.19728135	6.59075399
N	14.59328609	8.30968515	7.25040378

N	15.87666685	6.59374391	8.20485043
N	15.71007314	10.10013101	6.22253630
N	16.81111187	8.04991636	6.52336426
C	2.23566705	1.05981238	7.86031365
C	3.12675639	3.02372004	7.13361719
C	4.50648662	1.09614848	7.65552562
C	4.32743685	4.93228512	6.94990501
C	5.47398372	3.03442449	6.56239680
C	6.61463619	1.11168083	6.80811813
C	5.54623129	6.90759169	7.87790741
C	6.55402025	8.89835171	8.32364566
C	7.75687096	6.77738858	8.33815638
C	7.80743063	10.78852078	8.45405572
C	8.95808224	8.86377037	8.66382336
C	10.01184987	6.89123989	8.47326516
C	9.11258269	1.07124636	6.64533498
C	10.13370731	3.04152332	7.14345196
C	11.34191480	0.98071956	7.08614300
C	11.22510163	4.84168554	7.98144445
C	12.25002629	2.87105915	8.32538388
C	13.43737414	1.00862913	7.93826486
C	12.40733319	7.06340947	7.91504251
C	13.35564848	8.92717338	6.99957490
C	14.66577476	7.12554072	7.98505339
C	14.58171200	10.77596412	6.46690341
C	15.73351996	8.84269445	6.63182612
C	16.82427257	7.02974120	7.37432125
C	8.10549526	0.71253975	10.15895701
O	9.06418109	1.08757133	9.50589806
H	8.06577182	0.85694309	11.26482805
H	7.22566690	0.22001193	9.66123537

Optimised corrugated g-C₃N₄:CH₃O•

N	0.91238915	0.32017942	8.05012140
N	1.99106700	2.33133434	7.58579979
N	3.27651317	0.33763004	7.80199754
N	3.05104474	4.35407461	7.16920374
N	4.33301816	2.40788436	7.35249128
N	5.70808974	0.46981045	7.67153217
N	5.34406833	4.36173951	6.56100032
N	6.39226185	2.28477486	6.24159764
N	4.30805323	6.30525146	7.43088180
N	5.33211012	8.24155923	8.18388060
N	6.53092653	6.16115914	8.13929141
N	6.49326997	10.23661982	8.47718339
N	7.68959353	8.21338866	8.32326001
N	8.83619962	6.16347950	8.43561071
N	8.86889095	10.22667666	8.66160386
N	10.03109568	8.22946913	8.64429133
N	7.73839414	0.33919185	6.48036730
N	8.91914226	2.39008191	6.69593642
N	10.13672299	0.35040828	6.58907621
N	10.12847264	4.37326800	7.11832391

N	11.13290744	2.29483314	7.47087151
N	12.44989821	0.41247060	7.05484881
N	12.07415701	4.18369650	8.52208742
N	13.20424341	2.13377613	8.56291997
N	11.13209541	6.28590623	8.04202975
N	12.17006974	8.16202923	7.04880456
N	13.44487501	6.59222136	8.36090343
N	13.27950848	10.17652492	6.44186387
N	14.50915551	8.31676876	7.16376383
N	15.78625630	6.64922395	8.20540075
N	15.62816991	10.09174062	6.11498768
N	16.75235431	8.06899889	6.51005596
C	2.14702370	1.02167368	7.84274202
C	3.09718250	3.03606116	7.36176670
C	4.49338163	1.10400185	8.05767201
C	4.25111867	4.94407418	7.05040889
C	5.38144216	3.01908794	6.68854508
C	6.48828447	1.06625256	6.81632276
C	5.45557847	6.92762071	7.92583405
C	6.46795300	8.91307529	8.35609517
C	7.68232269	6.80707658	8.32370674
C	7.70180828	10.81688652	8.41066179
C	8.89421014	8.89713873	8.57764386
C	9.94001764	6.91929184	8.37847009
C	8.99068896	1.05256708	6.58960820
C	10.01519229	3.03830574	7.08067428
C	11.23076773	0.97306986	7.01929738
C	11.12039970	4.85453620	7.87670385
C	12.16158215	2.88850836	8.21091065
C	13.32793936	1.00374118	7.86710716
C	12.32682942	7.07107849	7.80671934
C	13.27335877	8.91567857	6.86389300
C	14.57699757	7.16220096	7.94289422
C	14.49307690	10.76602857	6.34583997
C	15.65881935	8.84843483	6.56144786
C	16.75143443	7.07029088	7.38525203
C	5.66312531	1.98956375	9.97326739
O	4.47890901	1.35679591	9.45555888
H	6.53435146	1.32155931	9.90014795
H	5.88284309	2.93927292	9.45473283
H	5.44540564	2.20045901	11.00567101

Optimised corrugated g-C₃N₄:CH₃OH

N	0.94006008	0.22632134	8.23946909
N	1.94212858	2.18239358	7.44923604
N	3.33272594	0.36946203	8.19113274
N	3.01656061	4.25254124	7.13295281
N	4.28503653	2.28511927	7.23138448
N	5.64408597	0.42626477	7.69526798
N	5.35710470	4.28342763	6.63483266
N	6.44363039	2.22215421	6.32171327
N	4.27892675	6.18989570	7.50000000
N	5.32339374	8.12737555	8.25010267

N	6.50364910	6.03300323	8.21757257
N	6.50230802	10.11445908	8.61806792
N	7.67469836	8.07503807	8.42938767
N	8.81748628	6.01514356	8.44907054
N	8.88273661	10.07385667	8.75792929
N	10.01302273	8.07064083	8.76138929
N	7.75107180	0.27093612	6.58791150
N	9.04490408	2.29578937	6.50793788
N	10.12338140	0.21215574	6.86460412
N	10.21775124	4.27279944	7.05385148
N	11.15974111	2.19170346	7.54886544
N	12.45424736	0.27614580	7.27155531
N	12.05526127	4.08840482	8.60681687
N	13.20090739	2.04676994	8.71684798
N	11.12313133	6.17746875	8.08283975
N	12.15402068	8.09328809	7.14379892
N	13.42406180	6.48974992	8.41791938
N	13.27443153	10.10849273	6.55674718
N	14.49530566	8.23447559	7.25856086
N	15.76166081	6.54064092	8.27521709
N	15.61946874	10.01099706	6.21979808
N	16.73434284	7.97444446	6.59486330
C	2.14669245	0.95478557	7.95571389
C	3.03568618	2.92608483	7.24890920
C	4.41898892	0.98337245	7.72193949
C	4.22238702	4.84742132	7.07917199
C	5.39038712	2.95920880	6.70055054
C	6.53356828	1.02118893	6.88055708
C	5.44065064	6.81396471	8.00370893
C	6.46371178	8.79319239	8.46228955
C	7.66465666	6.66987121	8.39085806
C	7.72321271	10.67991659	8.56101958
C	8.87929002	8.75060511	8.68966958
C	9.92314828	6.77906183	8.44054221
C	9.03767477	0.96162790	6.65292426
C	10.10018808	2.93702672	7.01528774
C	11.24107106	0.84420292	7.21312484
C	11.14307098	4.74816534	7.89762734
C	12.16327383	2.78845584	8.31987160
C	13.34075059	0.89700601	8.05198309
C	12.30538916	6.98033506	7.87566789
C	13.26047096	8.83944677	6.96742280
C	14.55638023	7.06635838	8.01701782
C	14.48926403	10.68953508	6.46228911
C	15.64734211	8.76366437	6.65655741
C	16.72704045	6.96592277	7.46021917
C	7.74281605	1.34567383	10.39257594
O	8.39321207	1.99607587	9.29106106
H	7.73849576	1.96824545	11.30265267
H	6.70993385	1.05135666	10.14080830
H	8.31665662	0.43309989	10.59945271
H	7.96120704	2.85140873	9.09484231