Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Bottom-up design of high-energy-density molecules $(N_2CO)_n$ (n=2-8)

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Table S1 The coordinate of (*cyc*-$N_2CO)_2$

atom	X	Y	Z
O	-0.00001100	-1.03031000	-0.00028700
O	0.00001500	1.03036600	-0.00030000
C	-0.95443900	0.00006100	-0.00035300
C	0.95443300	0.00000800	-0.00029500
N	-2.20262400	-0.00003700	-0.63425100
N	-2.20198900	-0.00002800	0.63488400
N	2.20202000	-0.00002100	0.63486400
N	2.20259300	-0.00003700	-0.63427000

Table S1-1 The critical transition state coordinate of (*cyc*-$N_2CO)_2$

atom	X	Y	Z
O	-0.02262500	1.02311000	-0.33760800
O	-0.02261600	-1.02303700	-0.33780300
C	0.88359600	0.00006100	-0.54838300
C	-0.94769000	0.00000400	-0.05964400
N	2.39750200	0.00001600	-0.19782400
N	2.00372900	-0.00009200	0.91972000
N	-1.97741100	-0.00008500	0.89570500
N	-2.31717800	0.00002200	-0.32453600

Table S2 The coordinate of (*cyc*-$N_2CO)_3$

atom	X	Y	Z
O	-0.94596200	0.55043300	-0.67948300
O	0.94549400	0.55099100	0.67935400
O	0.00046400	-1.46393200	-0.00028200
C	-0.00048100	1.30999800	-0.00005200
C	1.15425500	-0.70213200	0.13135400
C	-1.15385300	-0.70277700	-0.13146900
N	0.33273900	2.57680300	-0.53287100
N	-0.33434300	2.57655200	0.53298400
N	-2.35793200	-1.37690400	-0.42424100
N	-2.24759300	-0.95338000	0.75071500
N	2.24850500	-0.95193600	-0.75047000
N	2.35869700	-1.37548800	0.42449500

Table S2-1 The critical transition state coordinate of (*cyc*-$N_2CO)_3$

atom	X	Y	Z
O	0.02164300	-0.84922000	0.75252800
O	1.13902900	0.63700400	-0.66914900
O	-1.16658700	0.57647200	-0.67409000
C	1.17436100	-0.57431300	0.04456300
C	-0.03202000	1.30155100	-0.67131400
C	-1.14287900	-0.63311200	0.04322000
N	2.41175600	-1.00954900	0.56329400
N	2.00892900	-1.60496900	-0.46536400
N	-2.35752500	-1.12748300	0.56285500
N	-1.92520000	-1.70500100	-0.46407200
N	-0.05880400	2.17645800	0.99314100
N	-0.07193400	2.77357300	-0.01458700

Table S3 The coordinate of (*cyc*-$N_2CO)_4$

atom	X	Y	Z
O	-0.51017900	1.25937600	-0.78702900
O	1.48884600	0.05135800	-0.88875800
O	0.41680200	-1.89824100	-0.13795200
O	-1.03251100	-0.35729200	0.83121700
C	-0.88253700	-1.42256200	-0.04254000
C	-1.32691200	0.87255700	0.25873500
C	0.85700700	1.23406100	-0.55474000
C	1.44252600	-0.98934600	0.02549900
N	-1.90689900	-2.40031700	-0.15423500
N	-1.77864800	-1.63463800	-1.13416100
N	-1.92850500	1.83915800	1.11609800
N	-2.66874600	1.35295700	0.23639900
N	1.45312000	2.15018300	0.38276600
N	1.57505300	2.43763500	-0.82036800
N	2.07975500	-0.86207600	1.30763200
N	2.68284500	-1.54145300	0.45707600

Table S3-1 The critical transition state coordinate of (*cyc*-$N_2CO)_4$

atom	X	Y	Z
O	-0.13777100	1.27372300	-0.82658100
O	1.51032900	-0.40994400	-0.97643700
O	-0.16685400	-1.92944000	-0.28396600
O	-1.08304000	-0.06711300	0.83352100
C	-1.27740900	-1.09132100	-0.06093500
C	-0.97352500	1.19696800	0.27060500
C	1.17555000	0.89531300	-0.61677300
C	1.11219200	-1.54381900	-0.35687400
N	-2.52628900	-1.77052400	-0.10029900
N	-2.27655400	-1.04106200	-1.08110600
N	-1.16370800	2.30454300	1.14460700
N	-2.07505400	2.09894300	0.31614000
N	2.00650900	1.59641800	0.32163100
N	2.18799900	1.86299600	-0.87943900
N	1.60251300	-1.20792800	1.48436500
N	2.07284800	-2.08348000	0.88146600

Table S4 The coordinate of (*cyc*-$N_2CO)_5$

atom	X	Y	Z
O	-1.02470600	-1.39294400	-0.96405500
O	-1.45195500	0.90790200	-0.78321700
O	0.32311100	1.17256600	0.72910600
O	1.11189800	-2.02063700	-0.37669000
O	1.59695900	0.18231300	-0.95702500
C	1.96148600	-0.94163100	-0.23218800
C	1.31565400	1.31906800	-0.22631200
C	-0.96101200	1.53150800	0.34386400
C	-1.92106600	-0.39416800	-0.66568600
C	-0.19251200	-1.88579600	0.03549500
N	3.34393400	-1.26626400	-0.10713200
N	2.79993600	-0.83453700	0.92818900
N	-0.68850700	-2.90318800	0.90919800
N	-0.54027500	-1.77738200	1.42359200
N	-3.09969300	-0.66488600	0.12552600
N	-3.26639600	-0.60817200	-1.10278200
N	-1.82865600	1.97789600	1.38836500
N	-1.42403800	2.86012300	0.60884300
N	1.54360500	2.57004100	-0.87417100
N	2.35184000	2.27958700	0.02666000

Table S4-1 The critical transition state coordinate of (*cyc*-$N_2CO)_5$

atom	X	Y	Z
O	0.55517300	-1.63809400	0.72119700
O	-1.20903200	-0.74000800	-0.49566600
O	-1.55195000	0.87912200	1.10523200
O	1.55955400	-0.04201100	-0.67921100
O	0.62189500	1.56228600	0.77600600
C	1.56860600	1.24999100	-0.17577600
C	-0.69953500	1.71951800	0.38356700
C	-1.97463000	-0.26519700	0.53964200
C	-0.46248000	-1.86714500	-0.18196300
C	1.72395400	-1.08126300	0.21680600
N	2.08801300	2.25573000	-1.05369200
N	2.81268000	1.95513300	-0.08868700
N	2.87070600	-1.92318100	0.05896600
N	2.87188200	-1.17537700	1.05657200
N	-1.05978000	-3.16398600	-0.20067700
N	-0.35729800	-2.87660600	-1.18758500
N	-3.59863900	-0.45618800	0.40073400
N	-3.47437700	0.29897600	-0.47584600
N	-1.07278900	2.24760200	-0.89153600
N	-1.18620000	3.02278500	0.07973600

Table S5 The coordinate of (*cyc*-$N_2CO)_6$

atom	X	Y	Z
O	-1.23545700	-1.06101700	-0.96946600
O	-1.66852100	1.24315100	-0.80855600
O	-0.00816000	1.14677400	0.84181300
O	1.73168700	-1.32842500	-0.86517600
O	1.41967800	0.99143600	-1.00618200
C	2.29698500	-0.07453400	-0.88578200
C	-1.27395000	1.57247000	0.47109000
C	-2.15246100	-0.03698000	-1.03497900
N	3.52424800	0.03538400	-1.61406300
N	3.63568500	0.13745900	-0.38253600
N	-2.21921600	-2.46680700	0.79655700
N	-1.76649800	-1.47739900	1.41601100
N	-3.56857400	-0.28799900	-0.90404600
N	-3.14575500	-0.12144100	-2.05908900
N	-2.23166300	1.72793900	1.52387200
N	-1.80449100	2.78372300	1.02472800
N	1.26242800	3.10295300	0.12284100
N	2.01714000	2.45068000	0.86368500
C	-1.10413400	-1.81664900	0.19449500
O	0.07453100	-2.52088500	0.19661400
C	1.05194900	1.68440200	0.12691700
N	1.67984200	-1.30367900	1.60007500
N	2.18865600	-2.39513600	1.27387000
C	1.26283400	-1.84004400	0.33730800

Table S5-1 The critical transition state coordinate of (*cyc*-$N_2CO)_6$

atom	X	Y	Z
O	-2.15256400	0.04704500	-0.91049700
O	-1.32200200	2.05673400	-0.14015800
O	0.73933300	0.99490500	0.15967500
O	1.68295500	-2.03465600	-0.15150400
O	2.49142600	0.03974300	-0.99040300
C	2.63070400	-1.08713600	-0.27899400
C	-0.05243600	2.09466800	0.40738700
C	-2.09730000	0.94766400	0.14065100
N	3.72801900	-0.98666600	0.95437900
N	2.86700900	-0.47437300	1.54564500
N	-2.64165800	-2.23735900	-1.30220600
N	-2.64605000	-2.20169800	-0.06242100
N	-2.38646200	0.55336800	1.49116800
N	-3.29000600	1.17200800	0.89899500
N	0.17091200	2.79146100	1.63786500
N	0.51838200	3.39030300	0.60407500
N	0.69260000	0.97125300	-2.31651800
N	1.45592300	1.92169500	-2.01774300
C	-1.76641500	-1.26294000	-0.72106600
O	-0.41016900	-1.49745300	-0.83183300
C	1.36601100	0.87211300	-1.06906700
N	0.06150100	-1.50212600	1.61493700
N	-0.09026600	-2.70638200	1.30071700
C	0.36757600	-1.84619400	0.26700900

Table S6 The coordinate of (*cyc*-$N_2CO)_7$

atom	X	Y	Z
O	-1.15725200	-1.43274100	-0.94964400
O	-1.53941100	0.88983300	-1.01812100
O	1.76361900	-2.15723600	-0.34914000
O	1.46874900	-0.00786700	-1.11456400
C	2.37112700	-0.97223500	-0.67390000
C	-1.97739100	-0.39119700	-1.31774100
N	3.65556700	-1.07886300	-1.28625800
N	3.65028800	-0.61011800	-0.12976400
N	-2.58549900	-2.60281500	0.68045200
N	-2.19566100	-1.58376300	1.29582900
N	-3.37775600	-0.61736100	-1.59961200
N	-2.63023200	-0.52324200	-2.58432100
N	-3.05349400	1.41720200	0.82974000
N	-2.60883800	2.50174500	0.41922300
N	1.38331800	2.30330600	-1.71406000
N	2.59380400	2.11866900	-1.50371600
C	-1.32719600	-2.07699000	0.27217600
O	-0.22914800	-2.84010900	0.58473200
C	1.68878500	1.29784500	-0.74263600
N	1.19593700	-1.33951000	1.91020500
N	1.62077800	-2.50274000	2.04545400
C	0.98281900	-2.21948700	0.79658100
O	1.57500300	1.56021700	0.61115000
C	-1.73635100	1.37026400	0.26346800
O	-0.67890300	1.17828300	1.12966200
C	0.38195000	2.07313500	1.07736000
N	0.50147000	3.02253700	2.13727700
N	0.14693100	3.49337400	1.04177400

Table S6-1 The critical transition state coordinate of (*cyc*-$N_2CO)_7$

atom	X	Y	Z
O	-2.66367700	0.36709300	-0.22235800
O	-2.30985000	-1.90831100	-0.23593300
O	1.13723800	2.50884000	0.26291700
O	2.01571700	0.41181600	0.54379600
C	2.24430900	1.72065800	0.07906700
C	-2.60863700	-0.80347000	0.53221700
N	3.50944100	2.34163500	0.19655100
N	3.19413000	1.96721300	-0.95873400
N	-3.14670200	2.24036500	1.25996800
N	-3.04141400	2.70601200	0.11595800
N	-3.50375400	-1.02958200	1.61344600
N	-2.31507800	-0.79567100	1.93010500
N	-1.43965200	-1.66966000	-2.48619200
N	-1.10871100	-2.80600300	-2.09630100
N	3.63304200	-1.26416400	1.51710700
N	4.25681200	-0.82226000	0.63651700
C	-2.24703400	1.53788200	0.38331300
O	-0.90486100	1.64063000	0.65966300
C	2.78420400	-0.55443000	-0.00635600
N	-0.07528800	1.64259400	-1.67719000
N	-0.51138100	2.80053200	-1.48547900
C	-0.04159700	2.10629700	-0.32785400
O	2.14186600	-1.62126100	-0.51503900
C	-1.21658100	-1.80980900	-1.08147900
O	-0.11233000	-1.19456200	-0.53224200
C	0.89826600	-1.96067500	0.02161200
N	0.70069900	-3.30011000	0.45767400
N	0.80351500	-2.44699500	1.36377800

Table S7 The coordinate of (*cyc*-$N_2CO)_8$

atom	X	Y	Z
O	1.58205500	0.76178800	1.26892400
O	2.56268900	-0.06629600	-0.66815500
O	-2.28855600	0.70883900	0.14750200
O	-2.50797800	-1.63498500	0.15560100
C	-3.07759700	-0.39669800	0.39448900
C	2.74619300	0.52270100	0.57247500
N	-4.50016400	-0.31334200	0.23667000
N	-4.07935800	-0.24351000	1.40480300
N	1.16578600	2.92224000	2.28247200
N	0.05650400	2.36949800	2.14615500
N	3.93995500	0.26487200	1.32571300
N	3.89185400	1.36692400	0.75220200
N	4.01378500	-2.00439900	-0.96051600
N	3.26356800	-1.95683300	-1.95166000
N	-1.59089100	-3.29536900	1.63468000
N	-1.70859100	-2.30032100	2.36811200
C	1.03585000	2.02814500	1.16920900
O	1.02106000	2.57750400	-0.10052300
C	-1.46428600	-2.02263600	0.98234300
N	-1.13128800	3.57292100	-0.69200300
N	-0.38624800	3.63132800	-1.69283000
O	-0.22793300	-1.52200800	0.65302500
C	2.71841900	-1.43672900	-0.73306300
O	1.84631000	-2.19875300	0.02209700
C	0.51142100	-2.16518300	-0.33032300
N	-0.03986400	-3.22661400	-1.11487700
N	0.11205700	-2.13371800	-1.70249200
C	-0.15297100	2.53263500	-0.81587000
O	-0.50490100	1.24145600	-1.20228300
C	-1.83273100	0.90153800	-1.15400000
N	-2.74157600	1.35838600	-2.17189200
N	-2.37520600	0.17036300	-2.25325900

Table S7-1 The critical transition state coordinate of (*cyc*-$N_2CO)_8$

atom	X	Y	Z
O	1.13048900	1.48740500	0.50621900
O	2.83639300	0.28894400	-0.48713800
O	-2.96408600	-0.02060300	0.54661800
O	-1.93504200	-2.08228100	0.06691200
C	-2.99200600	-1.40055100	0.63600700
C	2.37732400	0.90782900	0.66650400
N	-4.24596900	-2.09085500	0.66674200
N	-3.68356000	-1.94415900	1.76658500
N	1.88103000	3.85693200	-0.11821500
N	1.02646400	4.04131200	0.66034300
N	2.70956000	0.43754700	1.96816900
N	3.30324200	1.47255700	1.60270200
N	4.66596500	-1.26468700	-0.04007700
N	4.38171100	-1.36267800	-1.24758200
N	-0.18586600	-2.68178300	1.65421900
N	-0.50473700	-1.52026900	1.97608600
C	1.06822500	2.48635700	-0.41328600
O	-0.06327100	2.57075700	-1.11942400
C	-0.67290200	-1.85045800	0.59381500
N	-1.58527300	2.62991500	0.81142200
N	-2.16245600	3.25283000	-0.11381900
O	0.18241400	-1.32063000	-0.35255000
C	3.29970000	-1.00805100	-0.38147300
O	2.38398700	-1.96917000	0.01032500
C	1.24317700	-2.09747600	-0.76634400
N	1.02134900	-3.35243300	-1.42235600
N	1.34321300	-2.40697500	-2.16188900
C	-1.27608000	2.22050100	-0.51710100
O	-1.70661600	1.03467400	-1.09692700
C	-2.92819000	0.53111800	-0.72715800
N	-4.14156400	1.09739500	-1.25402500
N	-3.77019800	0.02843600	-1.76803000

Table S8 Relative energies of the singlet and triplet state for isomers **1-4** at the B3LYP/6-311G(2d,d,p)(CBS-QB3) levels.

	Isomer **1**	Isomer **2**	Isomer **3**	Isomer **4**
Total energies of singlet state (a.u.)	-445.5473301 (-444.891981)	-445.4579601 (-444.802859)	-445.6367501 (-444.97355)	-445.5945446 (-444.887639)
The rate controlling step of barriers (kcal mol^{-1})	31.4 (29.9)	21.1 (19.8)	17.9 (22.2)	2.8 (-1.7)
Total energies of triplet state (a.u.)	-445.45661 (-444.800049)	-445.37207 (-444.705405)	-445.55239 (-444.876969)	-445.5472 (-444.879659)
The rate controlling step of barriers (kcal mol^{-1})	4.16 (9.31)	6.80 (10.20)	3.01 (0.08)	0.17 (-1.15)

Table S9 Calculated heats of formation and related parameters

Species	A ($Å^2$)	*v*	σ_{total}^2(kcal mol^{-1})^2
cyc-N_2CO	77.89	0.23	140.8
(*cyc*-$N_2CO)_2$	122.00	0.17	53.5
(*cyc*-$N_2CO)_3$	163.06	0.19	48.9
(*cyc*-$N_2CO)_4$	198.19	0.18	42.7
(*cyc*-$N_2CO)_5$	233.02	0.16	42.7
(*cyc*-$N_2CO)_6$	265.47	0.16	44.9
(*cyc*-$N_2CO)_7$	297.90	0.15	44.1
(*cyc*-$N_2CO)_8$	345.99	0.16	43.6