Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Flexible and Additive-Free Organic Electrodes for Aqueous Sodium Ion Batteries

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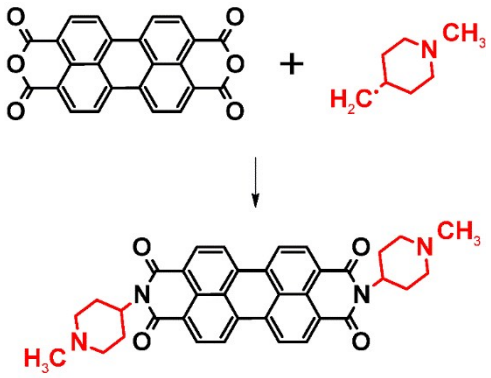


Figure S1. The synthetic route of PTCDI D-A molecule (2,9-bis[1-[(1-methyl-4-piperidyl)methyl]]-3,4,9,10-perylene tetracarboxylic diimide)

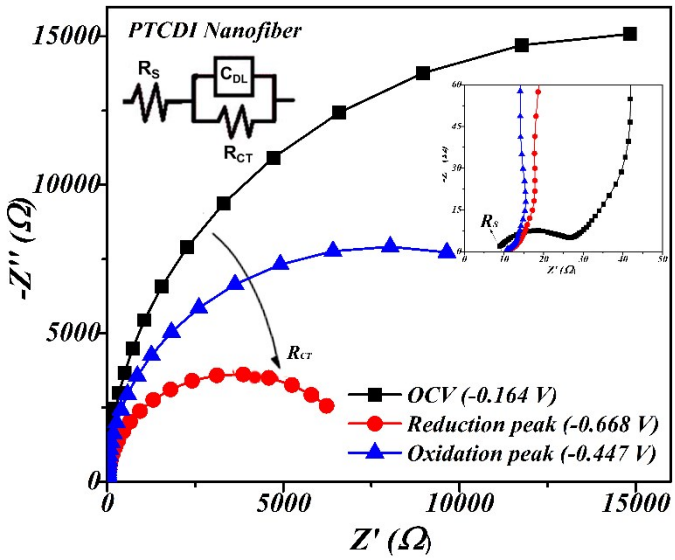


Figure S2. Nyquist plots of the PTCDI electrode at different potentials (insert is an enlarged view of the corresponding color at high frequency range). The electrical equivalent-circuit model (inset) was used to simulate the EIS test, where R_S is the solution resistance, C_{DL} is the constant phase element for the double layer capacitance, and R_{CT} is the charge transfer resistance across the electrode/electrolyte interface.

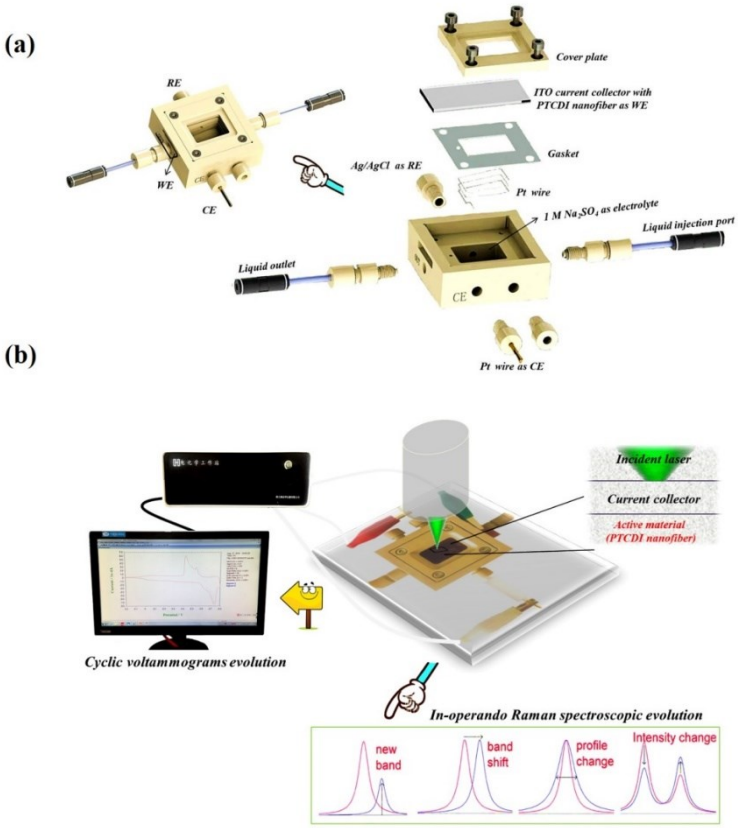


Figure S3. (a) Structure diagram of *in-situ* Raman electrochemical cell; (b) Operation diagram of in-situ Raman test.

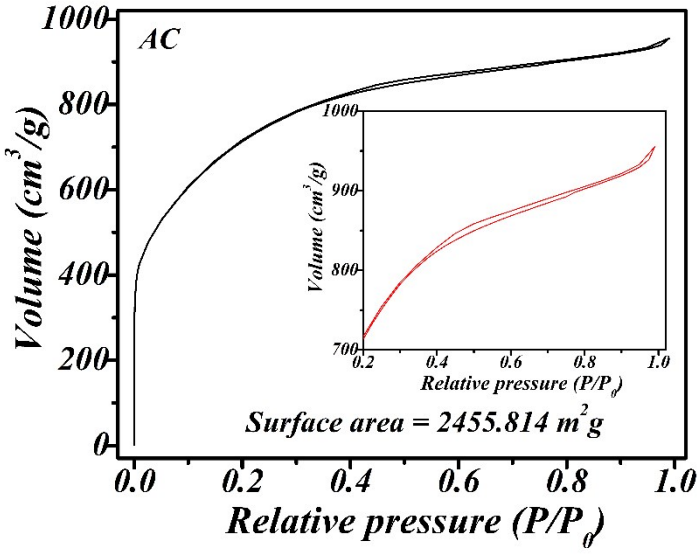


Figure S4. Nitrogen adsorption/desorption isotherms of AC.

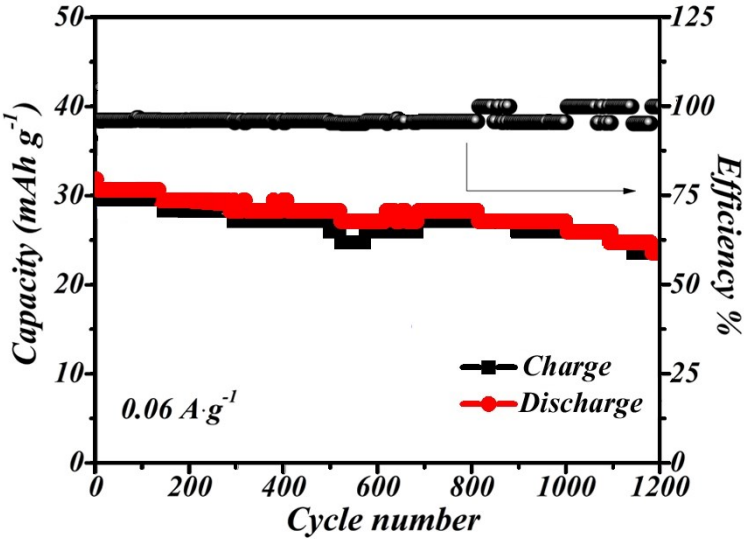


Figure S5. The long cycling performance of FSISD at the current density of 0.06 A g^{-1}.

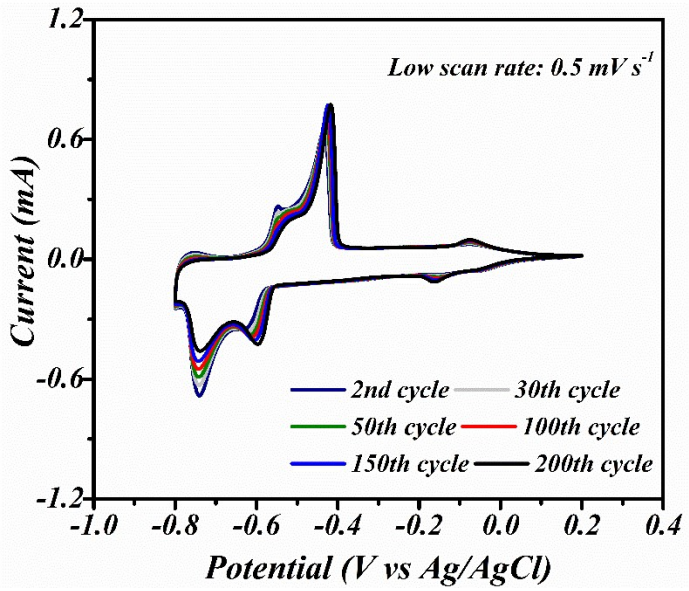


Figure S6. The cyclic CV tests of PTCDI single electrode in 1 M Na_2SO_4 at low san rate.

Table S1-Textural properties of AC

Textural property	S_{BET}[a] [$m^2\ g^{-1}$]	S_{micro}[b] [$m^2\ g^{-1}$]	S_{meso}[c] [$m^2\ g^{-1}$]	V_{total}[d] [$cm^3\ g^{-1}$]	V_{micro}[e] [$cm^3\ g^{-1}$]	V_{meso}[f] [$cm^3\ g^{-1}$]	Average pore diameter (nm)
AC	2455.814	1473.294	982.520	1.478	0.704	0.774	2.407

[a] Specific surface area from multiple BET method (calculated in the linear P/P_0 range from 0.05 to 0.3).

[b] Micropore surface area from t-plot method.

[c] t-method external surface area ($S_{meso} = S_{BET} - S_{micro}$).

[d] Total pore volume at $P/P_0 = 0.99$.

[e] Micropore pore volume from t-plot method micropore analysis.

[f] $V_{meso} = V_{total} - V_{micro}$.

Table S2-Comparison of electrochemical performances in water-in-salt systems for various energy storages

Systems	Electrolyte	Voltage	Capacity	Energy density	Power density	Ref.
Hydrophobic few layer graphene//Prussian blue	3 M $NaNO_3$	1.3 V	83 mAh/g (400 mA/g)	NG	NG	[1]
Perylene polyimide-polyether //PEDOT-Lignin	1 M Na_2SO_4 and 0.1 M $HClO_4$	1.1 V	40 mAh/g (100 C)	NG	NG	[2]
Aromatic polyimide//porous carbon microspheres	17 M $NaClO_4$	2.0 V	70 F/g (20 A/g)	65 Wh/Kg (0.25 A/g)	20000w/kg (20 A/g)	[3]
$K_{1.04}Mn_8O_{16}$//commercial activated carbon	1 M Na_2SO_4	2.4 V	NG	170 Wh/kg (133 W/kg)	3000 W/kg (19 Wh/kg)	[4]
Cobalt hexacyanoferrate //carbon micro-spheres	0.5 M Na_2SO_4	2.0 V	98 F/g (0.8 A/g)	54 Wh/kg (800 W/kg)	5037 W/kg (37 Wh/kg)	[5]
MnO_2//AC	2 M $ZnSO_4$	2.0 V	54 mAh/g (100 mA/g)	34 Wh/kg (100 mA/g)	NG	[6]
MnO_2//AC	2 M Na_2SO_4	2.0 V	NG	Less than 6 Wh/kg	NG	[6]
AC//AC	1 M Na_2SO_4	1.2 V	NG	Less than 7 Wh/kg	NG	[7]
KFeMnHCF-3565/PTCDI	22 M KCF_3SO_3	2.6 V	63 mAh/g (0.5 C)	80 Wh/kg (410 W/kg)	1612 W/kg (67 Wh/kg)	[8]
PTCDI Nanofiber//AC	**1 M Na_2SO_4**	**1.46 V**	**147 F/g (60 mA/g)**	**84 Wh/kg (35 W/kg)**	**86 W/kg (44 Wh/kg)**	**This work**

NG: not given.

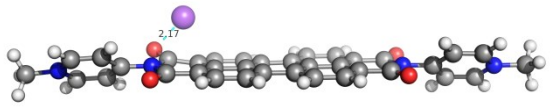
Table S3-Cartesian coordinates of PTCDI molecules

Nomomer, 66 atoms

Atom	X	Y	Z
C	-0.04530600	-2.46260200	0.08473500
C	0.71341700	-1.24797500	0.03784200
C	0.00473200	0.00045000	-0.00132100
C	-1.43942700	-0.00203200	0.00259900
C	-2.13850500	-1.23413000	0.05158400
C	-1.41549300	-2.45634300	0.09276500
H	0.47163500	-3.42052000	0.11296300
C	0.70921100	1.24690200	-0.04299600
C	-2.14922200	1.23247700	-0.03515700
H	-1.98364100	-3.38745700	0.12814600
C	-1.42339900	2.45451700	-0.06588100
C	-0.05387500	2.46063900	-0.07281000
H	-1.99348200	3.38469400	-0.08707600
H	0.46140800	3.41964900	-0.10238300
C	2.14509600	1.24873100	-0.05057100
C	2.85377900	0.00030500	-0.01138700
C	2.90382900	2.46335800	-0.09729200
C	2.14929900	-1.24614900	0.03012200
C	4.29793800	0.00278500	-0.01509500
C	4.27401800	2.45710300	-0.10499100
H	2.38689300	3.42127800	-0.12557900
C	2.91237700	-2.45989700	0.05969000
C	5.00772800	-1.23173200	0.02248900
C	4.99702700	1.23488800	-0.06372200
H	4.84217200	3.38821900	-0.14016000
C	4.28190100	-2.45378100	0.05282500
H	2.39708400	-3.41890900	0.08898400
H	4.85197600	-3.38396600	0.07381300
C	6.43541200	1.28437800	-0.08074500
C	6.44110300	-1.28781100	0.00838700
C	-3.58260000	1.28856200	-0.02087200
C	-3.57688500	-1.28359500	0.06914300
O	-4.25974800	2.32107800	-0.02958900
O	-4.25130900	-2.30925900	0.08178400
O	7.11824800	-2.32034000	0.01669500
O	7.10980100	2.31007300	-0.09284100
N	7.12317200	-0.00898100	-0.05093000
N	-4.26462600	0.00975700	0.03927000
C	-5.65237000	0.00648700	0.03271600
C	-6.40421000	-0.93286500	0.78744700
C	-6.39914300	0.94080300	-0.73668300
C	-7.77820200	-0.91885900	0.75054100
H	-5.90272300	-1.66900600	1.40825300
C	-7.77219700	0.89613100	-0.74369100
H	-5.88937100	1.70033600	-1.32164200
N	-8.46819700	-0.01943400	-0.00989300
H	-8.37845600	-1.61664400	1.33581200
H	-8.36712400	1.58732600	-1.34208800
C	-9.92743700	-0.08874400	-0.09073500
H	10.32832900	0.89711600	-0.35824600
H	10.24153100	-0.82332400	-0.84967900
H	10.33842800	-0.38340400	0.88419800
C	8.51090800	-0.00571900	-0.04347700
C	9.26329600	0.93406100	-0.79712200
C	9.25715400	-0.94047100	0.72593200

C	10.63727000	0.92013300	-0.75911700
H	8.76226900	1.67052800	-1.41790500
C	10.63018800	-0.89572700	0.73403300
H	8.74697700	-1.70038500	1.31004200
N	11.32671900	0.02032000	0.00132000
H	11.23792200	1.61831700	-1.34349800
H	11.22469800	-1.58724100	1.33247700
C	12.78586400	0.08968100	0.08381400
H	13.09906300	0.82058300	0.84674400
H	13.18689500	-0.89744000	0.34669700
H	13.19755100	0.38940700	-0.88930700

Nomomer-1 Na^+, 67 atoms



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C	-1.43721600	-2.47743500	0.09294500
H	0.45725000	-3.42755800	0.12945700
C	0.68317700	1.23493900	-0.07965000
C	-2.19852900	1.20485000	-0.05434000
H	-2.00123800	-3.41006300	0.13500000
C	-1.45912700	2.43356800	-0.21301000
C	-0.08603400	2.43500200	-0.22190000
H	-1.99727900	3.34414300	-0.50354000
H	0.42956500	3.37662000	-0.41217000
C	2.11150600	1.24981500	-0.03859000
C	2.82760000	0.00052500	0.00524200
C	2.86936300	2.46358700	-0.03702000
C	2.13081400	-1.24891400	0.03435200
C	4.26903000	0.00911600	0.01909900
C	4.24160800	2.45900400	-0.02138000
H	2.35439300	3.42362400	-0.04038000
C	2.88786500	-2.45467000	0.06846400
C	4.97512300	-1.22076900	0.05784300
C	4.97051300	1.24414800	-0.00307000
H	4.80562700	3.39338200	-0.02188000
C	4.26442500	-2.43984500	0.07836000
H	2.37974200	-3.41704900	0.08395000
H	4.83574200	-3.36925900	0.10197800
C	6.40816900	1.30385800	0.00511300
C	6.42238400	-1.26689600	0.07184900
C	-3.59509000	1.22916200	0.13986000
C	-3.60649300	-1.30427500	0.06545000
O	-4.26199500	2.28931500	0.39884800
O	-4.26819800	-2.32967600	0.03176700
O	7.08802300	-2.29375500	0.08514700
O	7.07750500	2.33142600	0.01264500
N	7.10103300	0.01799500	0.03459600
N	-4.28897800	-0.01478900	0.12862200
C	-5.68452400	-0.00716100	0.10755500
C	-6.45460700	-1.00108400	0.76220900
C	-6.40360000	0.98767200	-0.60643000
C	-7.82797500	-0.98586200	0.67351100
H	-5.97777800	-1.78753700	1.33920200
C	-7.77614700	0.94125000	-0.66902000

H	-5.88006100	1.79349800	-1.11343000
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H	-8.44560400	-1.73170500	1.17551500
H	-8.35119600	1.67586000	-1.23408000
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H	10.34104300	0.88470000	-0.45183000
H	10.22504800	-0.82779000	-0.96559000
H	10.39876700	-0.41576400	0.77031200
C	8.49137900	0.02649800	0.02087700
C	9.21972100	0.97081300	-0.74695000
C	9.25202900	-0.90835900	0.76544900
C	10.59604000	0.94697700	-0.75094000
H	8.70482400	1.71578800	-1.34588000
C	10.62889600	-0.86937600	0.72838200
H	8.76502900	-1.66352200	1.37469000
N	11.29865200	0.04133200	-0.02203000
H	11.18166100	1.64689900	-1.34875000
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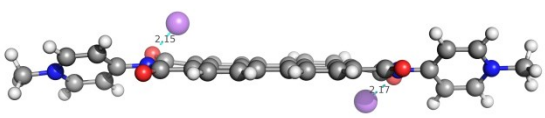
Na	-2.91791300	3.37089000	1.70710800

Nomomer-1, 2 Na^+, 68 atoms



Atom	X	Y	Z
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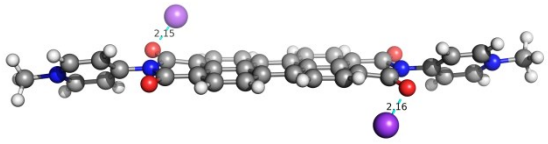
C	-1.42756300	0.00187100	0.20227400
C	-2.11937700	-1.22546800	0.23182700
C	-1.40448500	-2.44534800	0.28604700
H	0.48575900	-3.40179800	0.34935600
C	0.72590000	1.26376300	0.18098500
C	-2.16064700	1.23573400	0.16525000
H	-1.96953600	-3.37831700	0.30305200
C	-1.41817900	2.46197000	0.07378700
C	-0.04942900	2.47380200	0.08538700
H	-1.94750600	3.39320600	-0.16148100
H	0.45971600	3.42848400	-0.04304900
C	2.14539300	1.26607900	0.18251300
C	2.86335900	0.01489500	0.22615600
C	2.91691800	2.47870500	0.08893000
C	2.16446700	-1.22904600	0.27605500
C	4.30293700	0.01128200	0.20806900
C	4.28570500	2.47131600	0.07970300
H	2.40489600	3.43180500	-0.03965900
C	2.91418200	-2.44045000	0.31395100
C	4.99861500	-1.21381000	0.23922000
C	5.03203100	1.24756000	0.17187000
H	4.81230400	3.40449800	-0.15390000
C	4.28759900	-2.43609200	0.29257800
H	2.40035100	-3.39879800	0.35237600
H	4.85574400	-3.36711000	0.31085700
C	6.44277300	1.26836300	0.25740800
C	6.45053500	-1.26559400	0.19659800
C	-3.57151400	1.25193300	0.24977500

C	-3.57107800	-1.28194600	0.18727800
O	-4.26750200	2.29962800	0.43652000
O	-4.22632300	-2.30821300	0.13945500
O	7.10925800	-2.28970200	0.14977200
O	7.13560000	2.31826000	0.44359900
N	7.13083400	0.02217900	0.19444400
N	-4.25567600	0.00365600	0.18524900
C	-5.65032700	-0.00124200	0.05073000
C	-6.45586200	-0.96993000	0.69136800
C	-6.30966300	0.94025700	-0.77288800
C	-7.81975200	-0.98125300	0.48195400
H	-6.02237900	-1.71750100	1.34914900
C	-7.67508400	0.86888600	-0.94979400
H	-5.75337500	1.71988600	-1.28700800
N	-8.42351200	-0.08177800	-0.33509400
H	-8.46926600	-1.71214100	0.96592600
H	-8.20828800	1.56117800	-1.60276300
C	-9.87141200	-0.17744500	-0.59763900
H	-10.26033300	0.81215200	-0.86539500
H	-10.05539100	-0.88026400	-1.42385700
H	-10.38360000	-0.53274900	0.30509000
C	8.52544800	0.02131400	0.05927500
C	9.18157500	0.96247300	-0.76642900
C	9.33400200	-0.94432400	0.70174000
C	10.54731600	0.89344300	-0.94519700
H	8.62302600	1.73976700	-1.28170800
C	10.69723800	-0.95299600	0.49087600
H	8.90261700	-1.69127600	1.36160100
N	11.29806700	-0.05423100	-0.32991800
H	11.07773400	1.58562000	-1.60037600
H	11.34966600	-1.68096500	0.97560900
C	12.74841000	-0.14829600	-0.58062000
H	13.27261200	-0.33175300	0.36630000
H	12.95261500	-0.97251500	-1.28010500
H	13.10544500	0.79426600	-1.01234900
Na	-3.32696500	3.66149300	1.78931500
Na	6.19490500	3.68189900	1.79358500

Nomomer-1, 3 Na^+, 68 atoms



Atom	X	Y	Z
C	-0.02209900	-2.46349700	0.05538500
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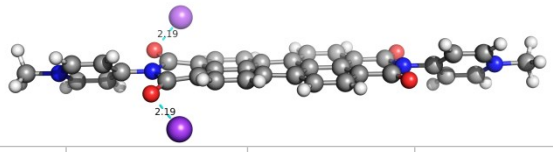
C	0.01694500	0.00117000	-0.00064900
C	-1.42633500	-0.01348200	0.01569600
C	-2.11579600	-1.24118000	0.05195100
C	-1.39123200	-2.46418700	0.06214100
H	0.49574400	-3.42126200	0.05894300
C	0.71680900	1.24889300	-0.04891800
C	-2.15450000	1.22054900	0.01380400
H	-1.95598300	-3.39746600	0.07433600
C	-1.42299500	2.44681300	-0.11831500
C	-0.05359900	2.45869900	-0.14716200
H	-1.96389600	3.37208800	-0.35087500
H	0.45661200	3.40694100	-0.31007800
C	2.14973700	1.26585800	-0.04377900
C	2.86271100	0.02026800	-0.01002500
C	2.90182500	2.48488300	-0.06746100
C	2.16283000	-1.22743300	0.03843100

C	4.30599700	0.03485900	-0.02608600
C	4.27096700	2.48551800	-0.07430700
H	2.38404100	3.44267800	-0.07187800
C	2.93314100	-2.43721800	0.13763800
C	5.03410700	-1.19920800	-0.02316700
C	4.99551600	1.26250700	-0.06307000
H	4.83573200	3.41878000	-0.08733900
C	4.30253800	-2.42537600	0.10943800
H	2.42280700	-3.38531700	0.30101100
H	4.84332200	-3.35048700	0.34291600
C	6.44197400	1.31883100	-0.07177700
C	6.44239400	-1.21649700	-0.18794100
C	-3.56273100	1.23765300	0.17921000
C	-3.56223100	-1.29757000	0.06087500
O	-4.23537200	2.28434700	0.42844800
O	-4.22839600	-2.31864200	0.01013800
O	7.11511700	-2.26341300	-0.43604500
O	7.10820000	2.33990800	-0.02191500
N	7.12640300	0.02809300	-0.14095400
N	-4.24671900	-0.00693300	0.13153400
C	-5.64789100	-0.01206500	0.10249300
C	-6.39977600	-0.99594100	0.78335000
C	-6.36900700	0.94630800	-0.64461400
C	-7.77628400	-1.00167400	0.68597200
H	-5.91461900	-1.75867100	1.38547200
C	-7.74515400	0.87984500	-0.71088300
H	-5.85494600	1.73740100	-1.18460400
N	-8.44226900	-0.08320900	-0.05811200
H	-8.38631700	-1.74259000	1.20488400
H	-8.32814600	1.58758500	-1.30174300
C	-9.90807200	-0.17106800	-0.19705100
H	-10.30949100	0.81501300	-0.45876400
H	-10.16508200	-0.89341500	-0.98603800
H	-10.34644600	-0.49690100	0.75457500
C	8.52756500	0.03305600	-0.11132600
C	9.27994800	1.01600400	-0.79297300
C	9.24813800	-0.92467600	0.63711100
C	10.65643300	1.02130600	-0.69530000
H	8.79518100	1.77828100	-1.39598100
C	10.62428500	-0.85865400	0.70364000
H	8.73365200	-1.71493900	1.17791300
N	11.32190700	0.10336700	0.04989000
H	11.26688600	1.76140700	-1.21489000
H	11.20686400	-1.56593900	1.29544300
C	12.78775500	0.19069400	0.18869900
H	13.04516500	0.91563800	0.97510400
H	13.18839600	-0.79468400	0.45399700
H	13.22654300	0.51277200	-0.76399300
Na	-3.14699400	3.62342900	1.71907900
Na	6.02745800	-3.60354600	-1.72613800

Nomomer-1,4 Na^+, 68 atoms



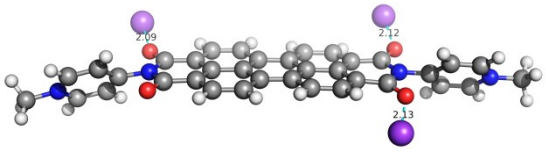
Atom	X	Y	Z
C	-0.10155300	-2.43699400	0.14125500
C	0.65217800	-1.23038400	0.02050900
C	-0.05120600	0.01592400	-0.01068500
C	-1.49368400	0.01548100	-0.01248000
C	-2.20996900	-1.21521300	0.01737900

C	-1.47594600	-2.44970000	0.13606000
H	0.42518100	-3.37693300	0.30642800
C	0.65185300	1.26229700	-0.04009400
C	-2.21114500	1.24585000	-0.04387000
H	-2.00449900	-3.36392600	0.43112900
C	-1.47686500	2.48043000	-0.16046100
C	-0.10239600	2.46830500	-0.16236000
H	-2.00492100	3.39433300	-0.45735800
H	0.42421000	3.40859100	-0.32615700
C	2.09557200	1.26814000	0.00547900
C	2.80031300	0.01630100	-0.00747200
C	2.84934600	2.47066400	0.05707800
C	2.09609100	-1.23573200	-0.02182300
C	4.24025100	0.01647000	-0.00597800
C	4.23014500	2.45837400	0.06541600
H	2.34192800	3.43346300	0.10039400
C	2.85008600	-2.43817500	-0.07154000
C	4.94444200	-1.21451200	-0.03556600
C	4.94421700	1.24751200	0.02522200
H	4.79731700	3.39011500	0.10407100
C	4.23094600	-2.42557200	-0.07699300
H	2.34302800	-3.40111900	-0.11564300
H	4.79849700	-3.35713200	-0.11423000
C	6.39682000	1.29606400	0.02544800
C	6.39734800	-1.26300600	-0.03257100
C	-3.62147900	1.26223600	0.11483600
C	-3.62033400	-1.23178900	-0.14294200
O	-4.29160600	2.29368100	0.41849900
O	-4.28905800	-2.26212600	-0.45037000
O	7.05561600	-2.28957200	-0.07281900
O	7.05550000	2.32241800	0.06797800

N	7.07736800	0.01659300	-0.00343500
N	-4.30666200	0.01530400	-0.01311100
C	-5.71153600	0.01439500	-0.01508200
C	-6.44522700	-1.00574700	0.62834600
C	-6.44487500	1.03185900	-0.65926000
C	-7.82481500	-0.97660300	0.61215400
H	-5.94142100	-1.82148400	1.14073500
C	-7.82620700	0.99878700	-0.64868800
H	-5.94207500	1.84919800	-1.17004400
N	-8.50729700	0.01038500	-0.02091000
H	-8.42448200	-1.73855200	1.11288300
H	-8.42339200	1.76042100	-1.15182200
C	-9.98410300	0.00520000	0.00413500
H	-10.36118700	0.77614500	-0.67716700
H	-10.35354100	-0.97665900	-0.32023100
H	-10.33744600	0.21451700	1.02398700
C	8.47780000	0.01784300	-0.00325900
C	9.21469000	0.96267900	-0.75358100
C	9.21718100	-0.92597500	0.74424900
C	10.59342500	0.93425500	-0.73734400
H	8.71399500	1.71546400	-1.35558500
C	10.59659700	-0.89530100	0.72545300
H	8.71922900	-1.68392400	1.34199000
N	11.27812300	0.01945500	-0.00671400
H	11.19052800	1.63890500	-1.31798300
H	11.19468100	-1.60006200	1.30458400
C	12.75167100	0.05675700	0.02706200
H	13.08989300	0.78715200	0.77705300
H	13.13541300	-0.93744900	0.28474500
H	13.13245100	0.34310100	-0.96131300
Na	-3.06449200	3.59245400	1.67888100

Na	-3.05495400	-3.55600000	-1.71208000

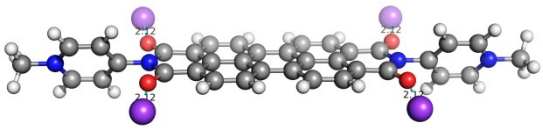
Nomomer-1,2,3 Na^+, 69 atoms



Atom	X	Y	Z
C	-0.02472900	-2.42075200	0.14676800
C	0.73385500	-1.21499800	0.21481400
C	0.03709600	0.03544300	0.30400800
C	-1.40506200	0.04157700	0.31912400
C	-2.10242100	-1.18121500	0.24568000
C	-1.39710400	-2.40495000	0.16289400
H	0.47892300	-3.38248200	0.07023100
C	0.75633200	1.27625700	0.36980500
C	-2.12074800	1.28040500	0.41856700
H	-1.97257600	-3.32990800	0.10405700
C	-1.36995600	2.48846600	0.50843400
C	-0.00295000	2.49133200	0.48373000
H	-1.90258600	3.43964000	0.57240400
H	0.51352700	3.44765400	0.54682100
C	2.18314100	1.26893400	0.31026200
C	2.88620200	0.01840400	0.22167700
C	2.95411800	2.48094500	0.30476200
C	2.17385700	-1.21884200	0.19148100
C	4.32817500	0.01126600	0.15773000
C	4.31845300	2.47187800	0.25241800
H	2.44172900	3.44164500	0.30601800
C	2.92192800	-2.44037200	0.15311600
C	5.02861600	-1.22449700	0.05779700
C	5.05231700	1.23936500	0.19632300
H	4.85126000	3.42151400	0.15072800
C	4.28705500	-2.44756300	0.08669200
H	2.39820900	-3.39314900	0.20581700
H	4.81838700	-3.40128300	0.14550800
C	6.46858200	1.24287800	0.21278000
C	6.44167000	-1.24716200	-0.10278200
C	-3.54104000	1.30622700	0.43104400
C	-3.55166800	-1.22546000	0.23726600
O	-4.24955800	2.34705100	0.58197900
O	-4.22590000	-2.23690300	0.15883500
O	7.12314500	-2.27561100	-0.38217600
O	7.19863200	2.25922700	0.42196900
N	7.12355800	-0.00644900	0.01507400
N	-4.21803300	0.06880900	0.29136300
C	-5.61200500	0.05059400	0.10002300
C	-6.42708400	-0.88081200	0.77665800
C	-6.23404800	0.89863900	-0.83734800
C	-7.77534300	-0.95308100	0.48480800
H	-6.01463700	-1.55432900	1.52346100
C	-7.58634300	0.77052900	-1.09424400
H	-5.65684300	1.63144700	-1.39786400
N	-8.34345100	-0.14837000	-0.44782800
H	-8.43744000	-1.66197400	0.98503400
H	-8.09299100	1.38073800	-1.84323500
C	-9.77452600	-0.31746800	-0.77792900
H	-10.10703200	0.52307000	-1.39719300
H	-9.91486900	-1.25780700	-1.33054500
H	-10.36389400	-0.34288500	0.14798300
C	8.53289100	-0.00511800	-0.09511200
C	9.19187600	0.90256200	-0.94689900

C	9.32318700	-0.91129600	0.63273100
C	10.56938700	0.87124300	-1.05003900
H	8.63191000	1.62326500	-1.53968800
C	10.70056200	-0.88736400	0.49667200
H	8.87117100	-1.63124100	1.31227200
N	11.31159400	-0.01123200	-0.33589200
H	11.11716300	1.54288000	-1.71360900
H	11.34844600	-1.56325200	1.05699700
C	12.78673300	0.01279200	-0.45778200
H	13.18350300	0.90675300	0.04452300
H	13.20434500	-0.88555900	0.01035400
H	13.06440100	0.03150400	-1.51986100
Na	-4.64349500	4.19196200	1.47992000
Na	6.87582200	4.01615200	1.56856400
Na	6.70271600	-4.06298000	-1.46702900

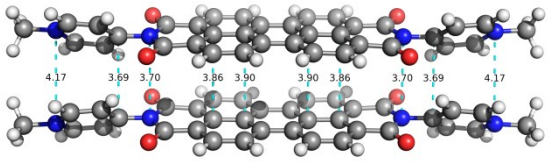
Nomomer-1,2,3,4 Na^+, 70 atoms



Atom	X	Y	Z
C	-0.02819800	-2.41796100	-0.37720200
C	0.73094800	-1.21238800	-0.19636500
C	0.01876200	0.01728400	-0.01001600
C	-1.42659500	0.01598800	-0.01379700
C	-2.13421500	-1.20414100	-0.21527800
C	-1.39259300	-2.41286300	-0.38839900
H	0.48652800	-3.36854900	-0.50245800
C	0.72773500	1.24822800	0.18004700
C	-2.13758900	1.23479700	0.18380800
H	-1.92824900	-3.35610200	-0.50737700
C	-1.39900100	2.44472300	0.36138500
C	-0.03457900	2.45230800	0.35739300
H	-1.93697700	3.38682200	0.47865500
H	0.47771400	3.40375700	0.48603600
C	2.15936100	1.24956100	0.18349400
C	2.87154900	0.01986900	-0.00273000
C	2.91851700	2.45519700	0.36387300
C	2.16257200	-1.21109900	-0.19261200
C	4.31690900	0.02116900	0.00096300
C	4.28291600	2.45014200	0.37472500
H	2.40379400	3.40580900	0.48896400
C	2.92486600	-2.41525400	-0.36951500
C	5.02788100	-1.19772900	-0.19617900
C	5.02454900	1.24139100	0.20185000
H	4.81855000	3.39343800	0.49334400
C	4.28928500	-2.40770500	-0.37334900
H	2.41256200	-3.36673500	-0.49786800
H	4.82725300	-3.34984800	-0.49027500
C	6.44761800	1.25752900	0.24301900
C	6.45131300	-1.21178200	-0.22966000
C	-3.56102200	1.24878800	0.21738000
C	-3.55726700	-1.22021300	-0.25690700
O	-4.28385900	2.25573600	0.46341800
O	-4.27748400	-2.22792600	-0.50829100
O	7.17414600	-2.21891100	-0.47496900
O	7.16793400	2.26544100	0.49334300
N	7.10688900	0.02374000	0.00786100
N	-4.21660000	0.01341800	-0.02098100
C	-5.63913800	0.01052100	-0.02355300
C	-6.36075700	-0.78944200	0.87837900

C	-6.36151700	0.80597000	-0.92495500
C	-7.74461100	-0.76862700	0.85758300
H	-5.84780700	-1.41682500	1.60691100
C	-7.74776100	0.77963400	-0.90671800
H	-5.85107300	1.43567500	-1.65321800
N	-8.42298500	0.00468400	-0.02603800
H	-8.34709600	-1.35985000	1.55037800
H	-8.34813700	1.36954300	-1.60149200
C	-9.90695800	-0.00584800	-0.00813800
H	-10.28390600	0.63398500	-0.81368100
H	-10.26622100	-1.03291900	-0.15842100
H	-10.26228600	0.37362100	0.96011500
C	8.52944000	0.02663800	0.01009300
C	9.25085500	0.82535900	-0.89312500
C	9.25199900	-0.76792500	0.91209300
C	10.63469700	0.80387600	-0.87321800
H	8.73771500	1.45182300	-1.62231900
C	10.63826300	-0.74224600	0.89296600
H	8.74171700	-1.39682100	1.64116900
N	11.31327400	0.03123700	0.01086300
H	11.23705300	1.39395100	-1.56711000
H	11.23878400	-1.33164800	1.58803800
C	12.79724500	0.04575200	-0.00422800
H	13.15421600	1.06554900	0.19469900
H	13.17447900	-0.63074600	0.77062700
H	13.15457100	-0.28713600	-0.98853600
Na	-4.52295500	4.18433100	1.31508000
Na	-4.50266500	-4.15148300	-1.37590800
Na	7.39328800	4.19027900	1.35801400
Na	7.41374500	-4.14846700	-1.32425100

Dimer, 132 atoms



Atom	X	Y	Z
C	-0.02683800	-2.59326600	-0.72216900
C	0.71224400	-1.39209400	-0.59448600
C	0.00378000	-0.15501900	-0.45267200
C	-1.43437600	-0.17135100	-0.43316100
C	-2.12517100	-1.40084700	-0.57989400
C	-1.40848200	-2.59799600	-0.72445000
H	0.49269300	-3.54386400	-0.82916100
C	0.70139600	1.09156400	-0.31981600
C	-2.16020300	1.03750800	-0.25947100
H	-1.97149700	-3.52598900	-0.83482500
C	-1.45342100	2.25049600	-0.14096400
C	-0.07025100	2.27651800	-0.17969600
H	-2.02615800	3.16986200	-0.00812000
H	0.43122500	3.23870400	-0.08166200
C	2.15417100	1.09637000	-0.31833100
C	2.86028500	-0.14556800	-0.44979800
C	2.91767900	2.28639300	-0.17658000
C	2.16030700	-1.38730000	-0.59303700
C	4.29847300	-0.15239000	-0.42734200
C	4.30090800	2.26951600	-0.13504100
H	2.40965800	3.24523500	-0.07949100
C	2.90757300	-2.58355400	-0.71922400
C	4.99767900	-1.37729400	-0.57264400
C	5.01593800	1.06123600	-0.25214700
H	4.86728300	3.19263600	-0.00095900
C	4.28922100	-2.57915300	-0.71867600
H	2.39455600	-3.53756500	-0.82725400

H	4.85859000	-3.50340100	-0.82786300
C	6.47142000	1.07123100	-0.16394200
C	6.45090700	-1.42800900	-0.59071800
C	-3.61590300	1.03788500	-0.17430900
C	-3.57798500	-1.46115100	-0.60111300
O	-4.29719200	2.03925700	0.04181900
O	-4.21831800	-2.47850800	-0.82506200
O	7.09843200	-2.44111000	-0.81327100
O	7.14562700	2.07709700	0.05351200
N	7.13040900	-0.18875100	-0.33599800
N	-4.26620600	-0.22639000	-0.34794700
C	-5.67739000	-0.28131300	-0.33948300
C	-6.36152500	-1.33084900	0.31673500
C	-6.46727100	0.67603200	-1.02861400
C	-7.72871500	-1.43931300	0.21912800
H	-5.81358400	-2.04667400	0.92707900
C	-7.83035700	0.52706200	-1.09946100
H	-6.00360300	1.53400900	-1.50925600
N	-8.46966100	-0.55061100	-0.53805100
H	-8.28516000	-2.24426400	0.69929700
H	-8.46154300	1.23124200	-1.64328700
C	-9.91413600	-0.67353900	-0.58826000
H	-10.30877000	-0.10166400	-1.43824400
H	-10.20067600	-1.72765400	-0.71463000
H	-10.38411100	-0.29279300	0.34028200
C	8.54189700	-0.23443000	-0.32418100
C	9.32716900	0.72798800	-1.01149700
C	9.23127800	-1.27939900	0.33383300
C	10.69136900	0.58791300	-1.07902100
H	8.85907700	1.58287200	-1.49335800
C	10.59937500	-1.37893500	0.23957000

H	8.68653700	-1.99867600	0.94298400
N	11.33632900	-0.48550400	-0.51593700
H	11.31926000	1.29613800	-1.62140700
H	11.15990600	-2.18016100	0.72121500
C	12.78169000	-0.59904500	-0.56267200
H	13.24694300	-0.21531200	0.36701500
H	13.07537800	-1.65126500	-0.68839800
H	13.17464600	-0.02456700	-1.41167300
C	-0.05907800	-2.28563400	3.16558400
C	0.70438700	-1.09559100	3.30738900
C	-0.00177100	0.14632000	3.43887300
C	-1.43995900	0.15309200	3.41641900
C	-2.15738000	-1.06055200	3.24117000
C	-1.44230700	-2.26880300	3.12401900
H	0.44897700	-3.24445500	3.06846200
C	0.69816300	1.38807500	3.58212800
C	-2.13920800	1.37796500	3.56177500
H	-2.00864800	-3.19193700	2.98988800
C	-1.43079300	2.57984300	3.70784700
C	-0.04914600	2.58429700	3.70836800
H	-2.00019600	3.50406600	3.81708300
H	0.46383700	3.53832300	3.81643200
C	2.14622600	1.39292500	3.58353500
C	2.85473300	0.15587200	3.44174300
C	2.88526600	2.59412900	3.71115700
C	2.15716200	-1.09073800	3.30891200
C	4.29288900	0.17225400	3.42223000
C	4.26691000	2.59891100	3.71341200
H	2.36570100	3.54471300	3.81811100
C	2.92885000	-2.27567200	3.16885200
C	5.01875900	-1.03658700	3.24859900

C	4.98364100	1.40178100	3.56890200
H	4.82989200	3.52693000	3.82373300
C	4.31201900	-2.24960500	3.13014400
H	2.42740800	-3.23787900	3.07085600
H	4.88479000	-3.16895800	2.99735200
C	6.43645400	1.46214100	3.59008800
C	6.47445900	-1.03692000	3.16344800
C	-3.59243800	1.42862300	3.57988200
C	-3.61286100	-1.07059400	3.15295200
O	-4.23999700	2.44168600	3.80250700
O	-4.28703200	-2.07646500	2.93541500
O	7.15578200	-2.03828900	2.94740200
O	7.07675400	2.47953600	3.81396200
N	7.12471600	0.22739100	3.33698200
N	-4.27189700	0.18935200	3.32510900
C	-5.68338600	0.23496600	3.31334400
C	-6.46858700	-0.72755100	4.00060900
C	-6.37284300	1.27995100	2.65543700
C	-7.83279100	-0.58755300	4.06818800
H	-6.00043500	-1.58245000	4.48238400
C	-7.74094400	1.37940400	2.74975100
H	-5.82815900	1.99931400	2.04633600
N	-8.47782700	0.48587400	3.50520900
H	-8.46062700	-1.29585900	4.61053200
H	-8.30153200	2.18064100	2.26819000
C	-9.92319600	0.59930200	3.55195200
H	-10.21695800	1.65149700	3.67766900
H	-10.38841600	0.21552700	2.62227100
H	-10.31611200	0.02479800	4.40095700
C	8.53590000	0.28237500	3.32846900
C	9.21996400	1.33189500	2.67214800
C	9.32584700	-0.67488000	4.01764500
C	10.58715000	1.44043300	2.76970300
H	8.67196900	2.04764000	2.06175700
C	10.68892900	-0.52583900	4.08843500
H	8.86223500	-1.53284200	4.49836700
N	11.32816300	0.55182200	3.52692400
H	11.14354200	2.24537100	2.28945000
H	11.32016600	-1.22994600	4.63229700
C	12.77263000	0.67485600	3.57711700
H	13.05909600	1.72898100	3.70354700
H	13.16731900	0.10295800	4.42705600
H	13.24261900	0.29420200	2.64854700

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