Supporting Information

SERS and DFT studies of highly sensitive detection of trace nitro-explosives assisted by alkali ions

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1. The SERS spectra of CL-20 adjusted by different Na^+ sources

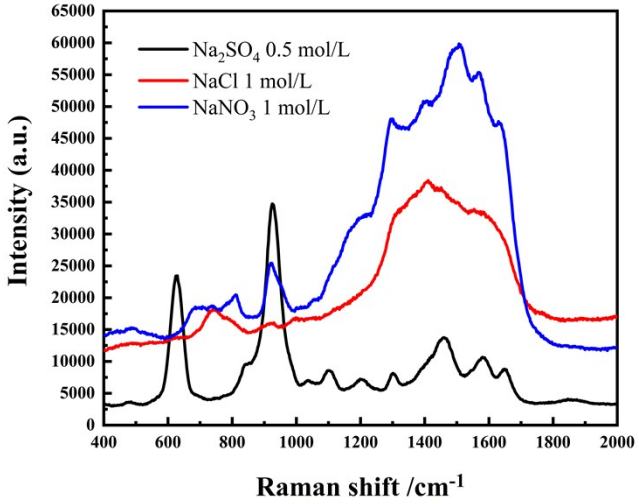

Figure S1. SERS spectra of CL-20 (1000 μM) adjusted by the different Na^+ sources from Na_2SO_4, NaCl and $NaNO_3$, respectively.

To better compare the effect of different Na^+ sources on the SERS detection of CL-20, the SERS spectra of CL-20 (1000 μM) adjusted by Na^+ from Na_2SO_4, NaCl and $NaNO_3$ are displayed in Figure S1. It can be observed that different Na^+ sources show difference Raman spectra. Different anions affect the shape and position of the peak in the Raman spectra. Thus, nitrate salts were selected in this work in order to avoid the influence of anions which may occur interaction with silver colloid (shown in Figure S1).

2. Adding nitrate and selecting the appropriate concentration

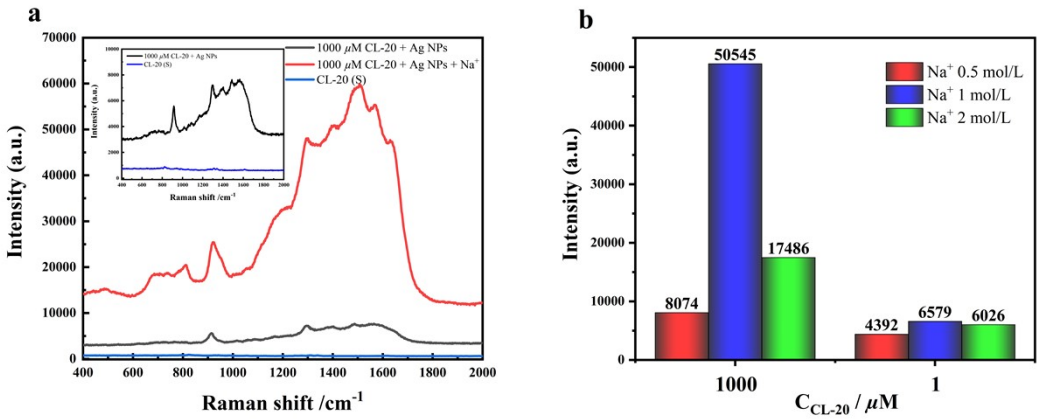

Figure S2. (a) SERS spectra of CL-20 (1000 μM) with and without Na^+ adjustment ; (b) Column chart depicting the SERS intensity at 1400 cm^{-1} for CL-20 (1000 μM and 1 μM) adjusted by Na^+ with the concentrations of 0.5 mol/L, 1 mol/L and 2 mol/L, respectively.

To investigate the impact of Na^+ adjustment on the SERS intensity of CL-20, the SERS spectra of CL-20 (1000 μM) with and without Na^+ adjustment are presented in Figure S2(a). The SERS intensity of CL-20 with Na^+ adjustment is significantly higher than the case without Na^+.

To explore the effect of different Na^+ concentrations on the SERS intensity of CL-20, a column chart depicting the SERS intensity at 1400 cm^{-1} for CL-20 (1000 μM and 1 μM) adjusted with Na^+ concentrations of 0.5 mol/L, 1 mol/L and 2 mol/L, was shown in Figure S2(b). As shown in Figure S2(b), 1 mol/L Na^+ displays the best SERS performance. Thus, 1 mol/L was chosen as the concentration of Na^+ in subsequent experiments.

3. The calculated Raman spectrum of TNCB

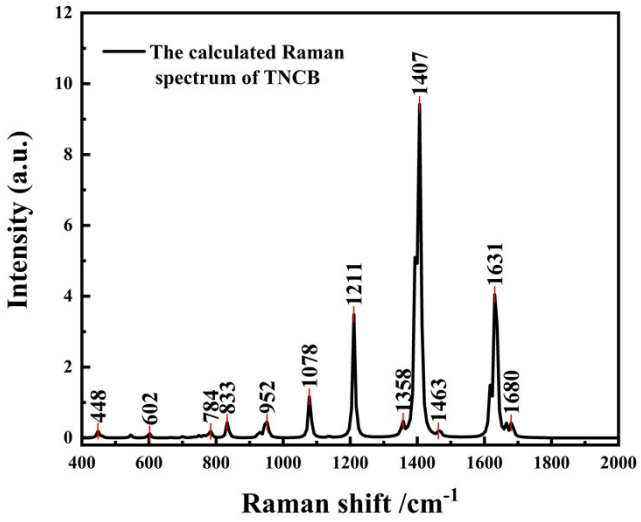

Figure S3. The calculated Raman spectrum of TNCB

The calculated Raman spectrum of TNCB was shown in Figure S3. The peaks at 448 cm^{-1}, 784 cm^{-1}, and 1680 cm^{-1} are associated with NO_2 scissoring. The peak at 602 cm^{-1} arises from asymmetric NO_2 stretching. The peaks at 833 cm^{-1} and 1407 cm^{-1} are due to symmetric NO_2 stretching. The peak characteristic of C-C (ring) stretching is at 952 cm^{-1}. The peak at 1078 cm^{-1} results from CH (ring) bending modes. The peak at 1211 cm^{-1} is attributed to benzene ring breathing vibrations. The peaks at 1358 cm^{-1}, 1463 cm^{-1}, and 1631 cm^{-1} correspond to asymmetric stretching vibrations of the benzene ring.

4. The SERS spectra of TNT at different concentrations adjusted by Na^+.

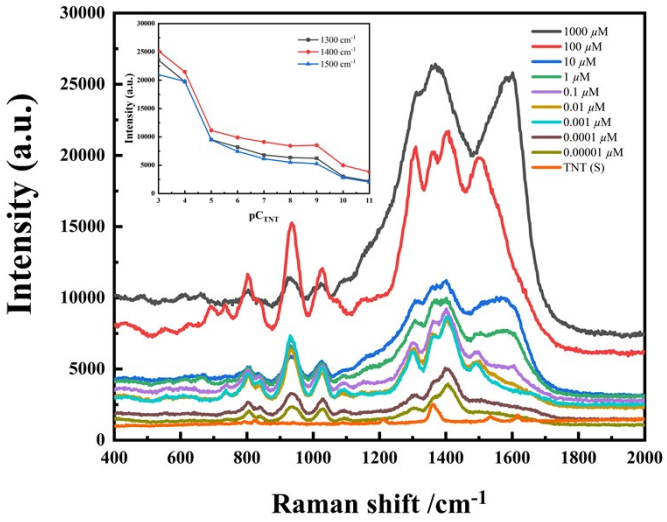

Figure S4. SERS spectra of TNT with concentration from 1000μM to 0.00001μM; (inset) plot of SERS intensity at 1300 cm^{-1}, 1400 cm^{-1} and 1500 cm^{-1} against pC_{TNT} adjusted by Na^+.

The varying concentrations of TNT solution adjusted by Na^+ were detected from 1 mM to 0.01 nM (1000 μM to 0.00001 μM) and shown in Figure S4. It is confirmed that the SERS detection of TNT adjusted with Na^+ also has a good effect, which is slightly inferior to the performance of K^+.

5. Cartesian coordinates for all of the species calculated in this study

Li

E = -7.28454440

Li	0.00000000	0.00000000	0.00000000

Na

E = -162.08122995

Na	0.00000000	0.00000000	0.00000000

K

E = -599.72498925

K	0.00000000	0.00000000	0.00000000

CL-20

E = -1791.18313992

C	0.44585700	0.77941200	1.40051200
C	-1.08485400	0.75022900	0.98157500
H	0.63543800	1.35765700	2.30076800
H	-1.73432100	1.26625100	1.68369300
C	1.08505300	0.74949100	-0.98198300
H	1.73460000	1.26502400	-1.68439200
C	-0.44563100	0.77841900	-1.40088900
H	-0.63523000	1.35598100	-2.30158800
N	-1.44512200	-0.68643900	0.93095200
N	-0.68915600	-0.65579000	-1.61528800
N	1.44530200	-0.68722600	-0.93037400
N	0.68924600	-0.65466700	1.61621300
C	0.21193900	-1.44614800	-0.76848300
H	0.32207200	-2.45889800	-1.14193700
C	-0.21185000	-1.44554300	0.76983500
H	-0.32218800	-2.45798800	1.14404900
N	-1.21255500	1.35152300	-0.31824400
N	1.21296000	1.35144500	0.31749000
N	2.28327600	2.24098700	0.58810900
O	3.00241500	2.51434100	-0.35858000
O	2.34247200	2.67760500	1.72349100
N	-2.28364900	2.23997300	-0.58973700
O	-3.00330200	2.51325100	0.35657800
O	-2.34284700	2.67584400	-1.72539900
N	-2.32066400	-1.14917300	1.98370400
O	-3.05230400	-0.30829900	2.47378800
O	-2.28365500	-2.34146700	2.22275500
N	1.98766200	-1.11779300	1.84276700
O	2.17506100	-2.30572200	1.61450300
O	2.78182600	-0.29864400	2.27979000
N	2.32061000	-1.15071400	-1.98298500
O	3.05220300	-0.31016600	-2.47372600
O	2.28356600	-2.34315300	-2.22121500
N	-1.98743600	-1.11895000	-1.84194600
O	-2.17488000	-2.30678400	-1.61330100
O	-2.78140000	-0.29998200	-2.27976200

CL-20-A_{Li}

E = -1798.53199652

C	0.45305200	0.53568900	-1.45889600
C	-1.10745900	0.42228700	-1.17096700
H	0.69208500	0.94831600	-2.43642100
H	-1.71713100	0.77942100	-1.99935800
C	0.84567200	-1.43905300	-0.05301600
H	1.37998400	-2.38614800	-0.06782200
C	-0.71745500	-1.60136200	0.16835600
H	-1.03939200	-2.63928500	0.21388000
N	-1.35274700	1.27016400	0.02053600
N	-0.86641800	-0.93071700	1.47052500
N	1.32427200	-0.60671700	1.08030900
N	0.84877600	1.49179500	-0.36671000
C	0.16312700	0.08724000	1.62854900
H	0.31281300	0.35362000	2.67076400
C	-0.11838200	1.40186100	0.75665700
H	-0.11107700	2.30391100	1.36268000
N	-1.40948100	-0.95088000	-0.91585900
N	1.06448000	-0.74434400	-1.30140700
N	2.18960400	-1.09458800	-2.12721200
O	2.81056500	-2.07666700	-1.77509300
O	2.36313600	-0.39024000	-3.10282300
N	-2.60178600	-1.53244700	-1.47260600
O	-3.23059100	-0.81057900	-2.22192100
O	-2.81128900	-2.68615200	-1.16593500
N	-2.04801300	2.53987800	-0.24177000
O	-2.79018100	2.53374000	-1.19858700
O	-1.84055400	3.42441500	0.56329400
N	2.08236100	1.91397400	-0.19487600
O	2.91695100	1.79457600	-1.12231700
N	2.14364700	-1.30234700	2.07294200
O	2.72938100	-2.28697900	1.67357300

O	2.20877700	-0.76514100	3.16026700
N	-2.15291600	-0.66703200	1.98625300
O	-2.20832400	0.23940600	2.80415700
O	-3.04395400	-1.38979900	1.58188900
O	2.40371800	2.45740400	0.88977600
Li	4.25262400	2.71371500	0.09035500

CL-20-B'$_{Li}$

E = -1798.54228817

C	-0.83743900	1.08015800	-1.22693500
C	0.73210300	1.23017600	-1.01839800
H	-1.24285000	1.81011600	-1.92423000
H	1.17294900	2.03130900	-1.60819700
C	-1.08755200	0.36774500	1.10755900
H	-1.67871000	0.58271300	1.99618200
C	0.47252100	0.53971300	1.34474400
H	0.72319100	0.89591600	2.34200000
N	1.21314700	-0.09722300	-1.45658300
N	0.92686500	-0.85313500	1.13379400
N	-1.27194300	-1.05465500	0.72608300
N	-0.92637900	-0.28775200	-1.78090500
C	-0.00743300	-1.56225300	0.23737400
H	0.05746300	-2.64043400	0.35235300
C	0.17399200	-1.10984700	-1.30657700
H	0.34273200	-1.96951800	-1.94923300
N	1.04995200	1.42687600	0.36975500
N	-1.46868900	1.26097100	0.05298300
N	-2.74637100	1.93956200	0.12687400
O	-3.34426600	1.80173500	1.17370200
O	-3.03522400	2.60646800	-0.84237500
N	1.78844700	2.58921500	0.78886600
O	2.16207400	3.31798300	-0.10684200
O	1.94635800	2.70121800	1.98659200
N	2.52194000	-0.35462200	-1.65368300
O	3.30466100	0.57308300	-1.61683600
N	-2.18118200	-0.91150600	-1.95119300
O	-3.13220700	-0.16106000	-2.04673800
N	-1.91937400	-1.90256700	1.74110200
O	-2.67685400	-1.32462400	2.48787600
O	-1.66369900	-3.08649200	1.66881100
N	2.22459900	-1.19606500	1.28624300
O	2.54628800	-2.32802900	0.82857000
O	2.97426800	-0.42442000	1.84973300
O	-2.14808900	-2.13088100	-2.01559400
O	2.82366200	-1.56179800	-1.86376000
Li	3.80507100	-2.58780000	-0.58130700

CL-20-C$_{Li}$

E = -1798.53237545

C	0.47276100	0.99483000	1.19697100
C	-1.05495500	1.02175600	0.78244900
H	0.74563900	1.74447000	1.93416300
H	-1.63921500	1.73952100	1.35572700
C	1.04352800	0.34265900	-1.17790800
H	1.70864100	0.61590600	-1.99290300
C	-0.49194000	0.44822300	-1.54740700
H	-0.66193000	0.82268800	-2.55466400
N	-1.54350000	-0.34471700	1.05951900
N	-0.86819600	-0.96633500	-1.42835800
N	1.27469100	-1.04149900	-0.76953900
N	0.61356600	-0.35853600	1.69209700
C	-0.02114600	-1.62816800	-0.43547000
H	-0.01090300	-2.70620400	-0.56841700
C	-0.39814400	-1.23627200	1.06675100
H	-0.58421900	-2.11742200	1.67419500
N	-1.12974500	1.35145900	-0.61490200
N	1.28878800	1.22899700	-0.02531400
N	2.41314800	1.93564700	0.04866400
O	3.24193800	1.88569200	-0.88837100
N	-2.20296800	2.20179800	-1.07794200
O	-2.88857700	2.69585100	-0.20594100
O	-2.24900800	2.37232900	-2.27741600
N	-2.42529400	-0.46484700	2.22971100
O	-3.03950500	0.53989200	2.52143000
O	-2.48288200	-1.56895600	2.72468500
N	1.88886400	-0.86391300	1.98553000
O	2.77409500	-0.02409700	2.11964400
N	2.12638700	-1.82202700	-1.66821000
O	2.93675500	-1.17350100	-2.30240300
O	1.97203600	-3.02040700	-1.62360100
N	-2.22551500	-1.33895400	-1.51743700
O	-2.50211900	-2.41874500	-1.02238000
O	-2.94949800	-0.55601500	-2.10670800
O	1.97019400	-2.07120400	2.09637400
O	2.62466400	2.66633500	1.04009600
Li	4.46835100	3.00199400	0.27985900

CL-20-C'$_{Li}$

E = -1798.54225414

C	0.54331700	-1.23488400	0.85652100

C	-1.02482100	-0.96065900	0.83668300
H	0.80785800	-2.08030900	1.48361700
H	-1.58609300	-1.69583500	1.41139400
C	0.91724100	1.22237000	0.65679600
H	1.49063100	2.02749100	1.10947100
C	-0.64550100	1.46251800	0.70483200
H	-0.92311400	2.37475200	1.22868900
N	-1.41184100	-1.05370000	-0.58804600
N	-0.92703800	1.55881200	-0.73491100
N	1.26790600	1.07936700	-0.76562800
N	0.78984600	-1.49466700	-0.56711300
C	0.03943600	0.76537700	-1.48888300
H	0.09914200	1.08105200	-2.52667400
C	-0.23363000	-0.80675400	-1.39181100
H	-0.31898300	-1.26405300	-2.37405800
N	-1.25838200	0.34275700	1.37821600
N	1.22030900	-0.03569500	1.34324400
N	2.37984800	-0.12452400	2.08199900
O	2.95787900	0.89389300	2.37723300
N	-2.40174300	0.55598700	2.23563400
O	-3.01268800	-0.44788100	2.54339800
O	-2.57826600	1.70084200	2.58932600
N	-2.15371700	-2.27431000	-0.95182400
O	-2.79252500	-2.77808400	-0.05329600
O	-2.08490900	-2.59501400	-2.11841000
N	2.02044600	-1.77551800	-1.07567300
O	2.86399800	-2.24522000	-0.27622000
N	2.06314800	2.18305700	-1.32228600
O	2.78169700	2.74989100	-0.52403300
O	1.96474000	2.34589700	-2.51709100
N	-2.26279100	1.60563500	-1.18880400
O	-2.42799100	1.27135200	-2.35085900
O	-3.08122400	2.00169100	-0.37939500
O	2.20479000	-1.60526500	-2.25895700
O	2.73023000	-1.27986600	2.43531900
Li	3.78884500	-2.39973500	1.32432000

CL-20-A$_{Na}$

E = -1953.31085829

C	0.32685800	0.27337500	-1.50427300
C	-1.22360200	0.45368900	-1.20153400
H	0.60847100	0.54723600	-2.51808600
H	-1.78051700	0.83787900	-2.05424500
C	0.40186000	-1.61674200	0.06543500
H	0.76415200	-2.63966200	0.13257500
C	-1.16058000	-1.48477300	0.31044800
H	-1.65585800	-2.44294100	0.44939500
N	-1.29598600	1.42820400	-0.08629600
N	-1.16417700	-0.68970500	1.54949300
N	1.03868200	-0.78493200	1.11875400
N	0.90129600	1.23698400	-0.51093300
C	0.02825000	0.14710000	1.60877400
H	0.24309700	0.47116100	2.62259800
C	-0.03770900	1.40620500	0.62391800
H	0.13571900	2.34124600	1.14886700
N	-1.75322100	-0.81969200	-0.82252400
N	0.70839300	-1.08138700	-1.24125900
N	1.74043100	-1.68699500	-2.03233000
O	2.20953800	-2.71607900	-1.58606600
O	2.00031400	-1.12497500	-3.07902900
N	-3.03276100	-1.23643600	-1.32401700
O	-3.54324300	-0.48771800	-2.13501600
O	-3.43095400	-2.30689400	-0.91625900
N	-1.76821700	2.76829700	-0.45290700
O	-2.51799900	2.81129000	-1.40395500
O	-1.40060400	3.66989700	0.27277400
N	2.21389900	1.38930700	-0.34804900
O	2.97794000	1.01036600	-1.25619800
N	1.75867600	-1.51170800	2.15432600
O	2.16885700	-2.61090600	1.84025500
O	1.94367600	-0.90009200	3.18870000
N	-2.37411400	-0.16496600	2.04697600
O	-2.25685900	0.80227100	2.78516000
O	-3.38514100	-0.75365000	1.71195700
O	2.62302600	1.93421800	0.69676200
Na	4.88688700	1.75103100	-0.04627600

CL-20-B'$_{Na}$

E = -1953.31646267

C	-1.10230200	1.01276000	-1.25401700
C	0.45534400	1.27458800	-1.04433800
H	-1.55223700	1.69877600	-1.96825800
H	0.84254200	2.08702100	-1.65545300
C	-1.30951300	0.34612500	1.09992700
H	-1.91971100	0.54246300	1.97989200
C	0.23226600	0.64058600	1.33552900
H	0.45355900	1.03925300	2.32304300
N	1.02278200	-0.02873800	-1.46643300
N	0.79174900	-0.72209300	1.16346100
N	-1.38584500	-1.09574500	0.75990700

N	-1.10099400	-0.37027800	-1.77369300
C	-0.08807200	-1.52105200	0.28216800
H	0.06023700	-2.58832100	0.42128900
C	0.05244200	-1.10233700	-1.28326400
H	0.27709200	-1.97070700	-1.89659100
N	0.72517000	1.54949700	0.33757600
N	-1.75320500	1.17502000	0.01792200
N	-3.05682600	1.79354500	0.08183300
O	-3.64369000	1.65615100	1.13555700
O	-3.38400300	2.41880600	-0.90360400
N	1.52601300	2.68169300	0.71047700
O	1.91309500	3.37359900	-0.20981100
O	1.70388100	2.82641200	1.90243300
N	2.34945500	-0.25591500	-1.56940100
O	3.11306000	0.68684700	-1.31447400
N	-2.31411800	-1.07656600	-1.91879800
O	-3.31108400	-0.38943400	-2.02909900
N	-1.96865600	-1.95925800	1.79968700
O	-2.76454800	-1.41686700	2.53406500
O	-1.62944900	-3.12314400	1.75897800
N	2.12668000	-0.93413900	1.23756500
O	2.55361600	-2.01363200	0.78746200
O	2.83377700	-0.04617300	1.71620700
O	-2.20573700	-2.29235000	-1.95048200
O	2.71969500	-1.39804500	-1.86822900
Na	4.58847200	-1.11536700	-0.19570000

CL-20-C'$_{Na}$

E = -1953.31548718

C	0.46627300	1.42611500	-0.22715300
C	-1.10764500	1.30723100	-0.35154000
H	0.83900500	2.42940200	-0.41149000
H	-1.59112400	2.26025100	-0.55979200
C	0.67949700	-0.90088800	-1.09995800
H	1.21750700	-1.48390700	-1.84319900
C	-0.89303800	-0.96041200	-1.28090200
H	-1.19994400	-1.52738700	-2.15704200
N	-1.55741100	0.80348900	0.96505800
N	-1.26038100	-1.64978000	-0.03526800
N	0.95694800	-1.42736700	0.24810400
N	0.67268000	1.01052900	1.16925500
C	-0.28782900	-1.34455300	1.01092300
H	-0.31136700	-2.08050500	1.80922800
C	-0.44218400	0.13379100	1.59962900
H	-0.54687800	0.12791900	2.68102500
N	-1.40232700	0.38351700	-1.40584300
N	1.08454300	0.50449200	-1.19021300
N	2.38273400	0.78236900	-1.55804900
O	3.14453400	-0.16163000	-1.77500700
N	-2.48537600	0.66289600	-2.31307500
O	-3.00905800	1.75105900	-2.17781300
O	-2.70942000	-0.19742800	-3.13737800
N	-2.24344300	1.79132000	1.81114900
O	-2.80457800	2.68445800	1.21317500
O	-2.21921100	1.56284300	3.00133800
N	1.92739300	0.81490300	1.68917800
O	2.86707200	1.35088400	1.06800600
N	1.61429100	-2.73913600	0.28169800
O	2.29814800	-3.00407900	-0.68695600
O	1.45998000	-3.37206000	1.30232800
N	-2.61932900	-1.77218100	0.32243300
O	-2.82943400	-1.96011700	1.51009900
O	-3.41502700	-1.70941000	-0.59706500
O	2.02029000	0.17754900	2.71599600
O	2.70867800	1.97236600	-1.63324700
Na	4.68311800	1.39960800	-0.34031900

CL-20-D$_{Na}$

E = -2115.37202376

C	-0.97810700	-1.08827200	-1.01530700
C	0.59192200	-1.33189600	-0.96482200
H	-1.51856300	-1.84954000	-1.57429200
H	0.89568100	-2.24319700	-1.47781800
C	-0.59248800	1.33184300	-0.96479000
H	-0.89655000	2.24306500	-1.47772700
C	0.97753700	1.08814700	-1.01602900
H	1.51767100	1.84940900	-1.57533700
N	0.93780200	-1.43737300	0.47805000
N	1.29563900	1.16472900	0.44155000
N	-0.93769100	1.43766100	0.47841300
N	-1.29552800	-1.16447500	0.44235200
C	0.11399800	0.79232700	1.23842700
H	0.17343100	1.18422000	2.25078800
C	-0.11340600	-0.79198600	1.23861800
H	-0.17235600	-1.18382800	2.25102400
N	1.24086200	-0.20269900	-1.57128000
N	-1.24185000	0.20258600	-1.57051600
N	-2.43269000	0.40853600	-2.37141100
O	-2.71728600	1.56792800	-2.58261400
O	-2.97451900	-0.60378500	-2.76008900

N	2.43204300	-0.40891800	-2.37197500
O	2.71658900	-1.56834300	-2.58283400
O	2.97386000	0.60331300	-2.76084100
N	1.27534700	-2.80143400	0.94639800
O	1.74154500	-3.53318000	0.10430200
O	1.11122800	-2.99255200	2.13286600
N	-2.54273600	-1.02621700	0.91744800
O	-3.48880900	-1.18087200	0.12819000
N	-1.27418900	2.80205900	0.94640800
O	-1.74068300	3.53369200	0.10434500
O	-1.10919900	2.99367100	2.13269500
N	2.54311600	1.02629100	0.91608500
O	3.48886000	1.18097300	0.12659700
O	-2.69027200	-0.78977300	2.12740300
Na	-5.18282400	-0.99525600	1.83439800
O	2.69107100	0.78995900	2.12612300
Na	5.18137000	0.99393000	1.83532600

CL-20-A_K

E = -2390.93941604

C	0.12460400	0.11277700	-1.52369500
C	-1.40312600	0.43492400	-1.22696000
H	0.41224100	0.28285800	-2.55806400
H	-1.93872500	0.80081400	-2.10074800
C	0.06891500	-1.66474100	0.17639300
H	0.34900500	-2.70581900	0.31590400
C	-1.47393200	-1.38788600	0.42322200
H	-2.04272900	-2.28983600	0.63635700
N	-1.38569600	1.48707200	-0.18221700
N	-1.39729200	-0.50791200	1.60097900
N	0.78174400	-0.81280900	1.16099700
N	0.78332000	1.09602100	-0.61534000
C	-0.14071200	0.23370500	1.58922100
H	0.11424500	0.60976200	2.57523900
C	-0.11853900	1.41713900	0.51283100
H	0.13412800	2.37028500	0.96751200
N	-2.02698400	-0.76263300	-0.75149300
N	0.39802300	-1.25160500	-1.16778700
N	1.36114500	-1.99352600	-1.92025800
O	1.76195100	-3.01866600	-1.40059000
O	1.64214100	-1.54055300	-3.01388800
N	-3.33867200	-1.11441700	-1.21173800
O	-3.80216600	-0.38995900	-2.07194000
O	-3.81317800	-2.11953000	-0.72493000
N	-1.75990600	2.82744200	-0.63645300
O	-2.51545300	2.86336500	-1.58424400
O	-1.31991500	3.74763900	0.02332400
N	2.11774100	1.11778900	-0.44907800
O	2.82293800	0.59186200	-1.32295700
N	1.47989400	-1.50447900	2.22352400
O	1.80882600	-2.65045100	1.98454700
O	1.73955400	-0.83322000	3.20505500
N	-2.55393800	0.14509700	2.06804100
O	-2.35173200	1.14802700	2.73738500
O	-3.61356200	-0.38159400	1.78181900
O	2.56623800	1.69193300	0.55566600
K	5.26356800	1.16333300	-0.09107800

CL-20-B'$_K$

E = -2390.94422029

C	-1.34166700	1.01286800	-1.23023200
C	0.20095000	1.34434000	-1.01676600
H	-1.82794500	1.69351500	-1.92524100
H	0.54686600	2.19003200	-1.60667800
C	-1.50937900	0.27436600	1.10657500
H	-2.12373200	0.42005600	1.99318400
C	0.02003400	0.63171700	1.34507100
H	0.22616900	1.01201900	2.34291400
N	0.82967100	0.08426400	-1.46091500
N	0.63555800	-0.69653700	1.13483200
N	-1.52326800	-1.15965200	0.72778900
N	-1.27288500	-0.35494900	-1.78514200
C	-0.20657800	-1.51119600	0.23716500
H	-0.00828100	-2.57328800	0.34850600
C	-0.08252200	-1.04172500	-1.31054600
H	0.18936300	-1.87768800	-1.94926400
N	0.45804700	1.59905600	0.37428800
N	-1.99677000	1.10867900	0.04724300
N	-3.32282300	1.66682800	0.13218400
O	-3.89859800	1.47931400	1.18501500
O	-3.68419000	2.30142900	-0.83597500
N	1.20751300	2.74823200	0.77637000
O	1.55401300	3.49077500	-0.12199000
O	1.39419200	2.86311600	1.97180100
N	2.17103400	-0.05844200	-1.59713100
O	2.86432600	0.94592300	-1.39693900
N	-2.44908100	-1.11401100	-1.94701500
O	-3.47958000	-0.47398400	-2.03796000
N	-2.05921000	-2.07351100	1.74508800
O	-2.87345000	-1.58797400	2.50008700

O	-1.67088400	-3.22086900	1.67181900
N	1.97864000	-0.87863000	1.22546100
O	2.43147100	-1.94941700	0.80185500
O	2.65042100	0.03660800	1.71136800
O	-2.28321400	-2.32237000	-2.01236600
O	2.60086700	-1.17901200	-1.88486300
K	4.89866100	-0.75234000	-0.10616800

CL-20-C'$_K$

E = -2390.94396357

C	-0.36604500	-1.37512800	0.02891500
C	1.20798200	-1.38427900	-0.14746800
H	-0.80692600	-2.36750800	0.01367000
H	1.62332400	-2.38813100	-0.21474300
C	-0.46470400	0.78882700	-1.19372500
H	-0.99250800	1.28178900	-2.00579800
C	1.10295800	0.72047900	-1.41765700
H	1.41362100	1.12223100	-2.37945400
N	1.73277600	-0.71346900	1.06295500
N	1.55323900	1.57062700	-0.30578000
N	-0.66039100	1.53775700	0.06217900
N	-0.49741700	-0.73877900	1.34972400
C	0.60065300	1.49510800	0.79957600
H	0.69526200	2.34370900	1.47046100
C	0.68104000	0.11921500	1.60944700
H	0.82291500	0.28767000	2.67309200
N	1.52865800	-0.65565300	-1.33875600
N	-0.95316600	-0.58017000	-1.05115900
N	-2.26090700	-0.85795200	-1.40783600
O	-2.94408000	0.06708900	-1.84856800
N	2.55509600	-1.14411000	-2.21734800
O	3.01741900	-2.23013100	-1.92629600
O	2.80192400	-0.44095700	-3.17467700
N	2.38158900	-1.60091300	2.03463400
O	2.86511100	-2.61281100	1.57181300
O	2.41370900	-1.19131700	3.17561300
N	-1.72661200	-0.36213000	1.84094600
O	-2.71423000	-0.89971100	1.31275200
N	-1.25945000	2.85937600	-0.07977100
O	-1.99558600	2.99677200	-1.03888500
O	-1.02091000	3.64431100	0.81228100
N	2.92728300	1.66213700	-0.00697000
O	3.19060500	2.02170100	1.12976000
O	3.68594700	1.40623400	-0.92490000
O	-1.74234900	0.43353200	2.75915500
O	-2.64949000	-2.01709900	-1.26682700
K	-5.04402300	-0.98542200	-0.09901300

TNCB

E = -860.04824522

C	-0.32137500	1.19957400	0.00337900
C	-1.05670000	-0.00002100	-0.01237100
C	-0.32131500	-1.19959500	0.00338600
C	1.06824400	-1.21191100	0.02416100
C	1.74370400	0.00003400	0.04917200
C	1.06818800	1.21194900	0.02420200
H	1.60902100	-2.14957500	0.01311400
H	1.60891700	2.14963800	0.01318000
O	3.77648200	1.09300800	0.09783600
O	3.77652900	-1.09285300	0.09779900
O	-0.43304100	-3.39520200	-0.67728500
O	-1.97000500	-2.67134600	0.69998600
O	-0.43292800	3.39535600	-0.67681200
O	-1.97053200	2.67102600	0.69948200
N	-0.97616400	2.52854900	0.00200200
N	-0.97600700	-2.52861400	0.00202400
N	3.21868800	0.00006600	0.08407300
Cl	-2.77294500	-0.00001000	-0.18368300

TNCB-A$_{Li}$

E = -867.39817478

C	-0.45393900	-1.20771500	-0.00208200
C	0.92793100	-1.22386100	-0.02308900
C	1.60660000	0.00000400	-0.04684500
C	0.92795000	1.22387500	-0.02312200
C	-0.45393000	1.20772900	-0.00214400
C	-1.19189500	0.00001400	0.01940900
H	1.45480700	2.17006300	-0.00454400
O	-2.12158800	2.66729300	-0.67205400
O	-0.53020200	3.41554800	0.63622700
O	3.66195800	1.07892300	-0.07909800
O	-2.12171100	-2.66715600	-0.67202000
O	-0.53012300	-3.41578500	0.63576300
N	-1.10803800	-2.54600000	-0.00545400
N	3.02942400	-0.00000900	-0.06921500
N	-1.10799900	2.54594600	-0.00536700
O	3.66198100	-1.07893200	-0.07779500
Li	5.38914100	0.00012400	-0.09270000
H	1.45475400	-2.17007100	-0.00466400
Cl	-2.88879500	0.00003900	0.18509500

TNCB-B_{Li}

E = -867.39703677

C	0.13857700	1.32917000	0.01095800
C	-0.94317400	0.43261200	-0.00891800
C	-0.61250700	-0.95527000	-0.00232800
C	0.72091100	-1.39834600	0.02222800
C	1.73098800	-0.46086500	0.02839700
C	1.46193400	0.90457900	0.00619800
H	0.96071000	-2.45362200	0.03538000
H	2.27111400	1.62659300	-0.01711900
O	3.99950500	-0.05755900	0.04668300
O	3.31291900	-2.13878700	0.06620400
O	-1.23117900	-3.18756700	-0.12428200
O	0.65237700	3.43947200	-0.73182000
O	-0.88577000	3.23904000	0.81955800
N	-0.06454600	2.80375100	0.02858900
N	-1.60101500	-1.99491700	-0.01364600
N	3.13955800	-0.92654700	0.04888100
O	-2.81761200	-1.75445300	0.09510100
Li	-3.17105100	-3.76630900	-0.02054200
Cl	-2.54464300	1.03044100	-0.12436200

TNCB-A_{Na}

E = -1022.17710682

C	0.80552000	-1.20538300	0.00113100
C	-0.57841000	-1.22002600	0.01624200
C	-1.25570800	0.00079100	0.03685600
C	-0.57736800	1.22105800	0.01616100
C	0.80653600	1.20518700	0.00110700
C	1.54423000	-0.00042600	-0.01608000
H	-1.10365100	2.16710500	-0.00388300
O	2.46904700	2.66857800	0.67734600
O	0.88476800	3.41220500	-0.64073600
O	-3.30268700	1.08575400	0.05906600
O	2.46718400	-2.67013600	0.67671600
O	0.88149800	-3.41267100	-0.64021500
N	1.45671300	-2.54355900	0.00565600
N	-2.69263400	0.00142900	0.05294900
N	1.45884500	2.54276700	0.00571100
O	-3.30357000	-1.08252100	0.05881600
Na	-5.43310200	-0.00053400	0.05964600
H	-1.10545400	-2.16565000	-0.00365300
Cl	3.24553100	-0.00099500	-0.17407200

TNCB-B_{Na}

E = -1022.17617174

C	-1.29977300	-0.95514200	0.01188000
C	0.10490800	-0.98651300	-0.00817300
C	0.76427600	0.27216700	0.00137700
C	0.05582500	1.47961500	0.02179300
C	-1.32443800	1.43810000	0.03664200
C	-2.01932100	0.23433900	0.01702500
H	0.57089200	2.43137800	0.03115800
H	-3.10343300	0.22090100	0.00036000
O	-3.29719700	2.62971900	0.06444100
O	-1.41013600	3.74246100	0.08285800
O	2.70069200	1.49666600	-0.33347500
O	-3.08788800	-2.19870400	-0.71681900
O	-1.76078000	-3.08568700	0.78668100
N	-2.11217900	-2.20118900	0.02180500
N	2.20768700	0.40151400	-0.00232600
N	-2.07723700	2.71464200	0.06370700
O	2.92924200	-0.54566600	0.33788500
Na	4.93526300	0.72406700	-0.00413100
Cl	0.93155500	-2.48397100	-0.16613000

TNCB-A_{K}

E = -1459.80322575

C	1.17346000	-1.20348900	0.00202600
C	-0.21201000	-1.21796700	0.01583400
C	-0.88911600	-0.00009000	0.03564600
C	-0.21210100	1.21788400	0.01571000
C	1.17335400	1.20353100	0.00193700
C	1.91155100	0.00001600	-0.01370800
H	-0.74026200	2.16260200	-0.00381300
O	2.83213600	2.67102000	0.67994300
O	1.25174400	3.40956400	-0.64429800
O	-2.93336600	1.08574800	0.05483300
O	2.83239200	-2.67095900	0.67979600
O	1.25179500	-3.40945700	-0.64426900
N	1.82387500	-2.54061100	0.00582800
N	-2.33640200	-0.00020600	0.04994000
N	1.82370700	2.54069500	0.00584000
O	-2.93316600	-1.08624500	0.05479800
K	-5.53977400	0.00012600	0.03622000
H	-0.74010500	-2.16273300	-0.00356500
Cl	3.61616000	0.00011200	-0.17077400

TNCB-B_{K}

E = -1459.80262270

C	-1.70202300	-0.88580900	0.01016000
C	-0.30203000	-1.00487000	-0.00987000
C	0.43531900	0.20440300	0.00278800
C	-0.18924300	1.45308600	0.02226500
C	-1.57137000	1.50227800	0.04055300
C	-2.34342400	0.34771400	0.02083900
H	0.38920400	2.36765400	0.02738100
H	-3.42582800	0.40454700	0.00698300
O	-3.46122200	2.82254400	0.07440700
O	-1.50535300	3.80753200	0.08753500
O	2.45083200	1.25020800	-0.43874400
O	-3.57469100	-2.00740700	-0.70729200
O	-2.28626200	-2.99221900	0.76749300
N	-2.59039000	-2.07725900	0.01731100
N	1.89423900	0.23471800	0.00459800
N	-2.23789300	2.82445500	0.07003200
O	2.52762700	-0.71887000	0.46494300
K	5.10285600	0.35190200	-0.00378900
Cl	0.43822600	-2.54863900	-0.18312400

TNT

E = -885.04550439

C	0.51514400	-1.18434800	-0.02815900
C	1.28239200	-0.00065300	-0.06354600
C	0.51629900	1.18392700	-0.02813600
C	-0.87359500	1.20932700	0.00903600
C	-1.55213500	0.00078900	0.03686100
C	-0.87485900	-1.20840400	0.00915000
H	-1.41001700	2.14904300	0.01367000
H	-1.41203600	-2.14766700	0.01359800
C	2.78405000	-0.00129400	-0.21071900
H	3.26426700	-0.00054100	0.77269800
H	3.12350200	-0.89159500	-0.73890700
H	3.12416500	0.88833300	-0.73969800
O	-3.58658000	-1.09041300	0.11222700
O	-3.58540500	1.09432100	0.11143300
O	0.56124900	3.43354500	-0.56098400
O	2.24188400	2.61892300	0.56789800
O	0.55699800	-3.43378900	-0.56152200
O	2.23859400	-2.62204900	0.56807800
N	1.16244500	-2.51635400	-0.01451900
N	1.16536400	2.51498100	-0.01444200
N	-3.02603700	0.00166500	0.09105600

TNT-A_{Li}

E = -892.39906489

C	0.65012100	-1.19213100	-0.03127400
C	-0.73207300	-1.22139700	0.00546400
C	-1.41275700	-0.00036500	0.03218300
C	-0.73261300	1.22097600	0.00558000
C	0.64958500	1.19228600	-0.03112100
C	1.41639600	0.00027300	-0.07220300
H	-1.25605800	2.16880900	0.00201600
O	2.36946900	2.62278400	0.57468600
O	0.68189400	3.44230500	-0.55078400
O	-3.46861100	1.07773500	0.08983300
O	2.37113400	-2.62183900	0.57343800
O	0.68246200	-3.44245200	-0.54951300
N	1.29944100	-2.53116700	-0.01053000
N	-2.83468300	-0.00075900	0.07269900
N	1.29846400	2.53155100	-0.01050400
O	-3.46806600	-1.07935100	0.08939100
Li	-5.18924400	0.00172700	0.12657700
H	-1.25512300	-2.16944400	0.00193400
C	2.91082300	0.00069400	-0.21803900
H	3.25516200	0.89368600	-0.73837000
H	3.38236800	0.00053800	0.77215200
H	3.25568500	-0.89163200	-0.73907100

TNT-B_{Li}

E = -892.39605441

C	0.71802900	1.18555100	-0.01805400
C	-0.68173300	1.04993100	-0.06987000
C	-1.12574400	-0.30650300	-0.03852600
C	-0.26179400	-1.41445200	-0.00056700
C	1.09493700	-1.17892300	0.01938900
C	1.60607500	0.11418400	0.00293700
H	-0.63832800	-2.42870300	0.02302200
H	2.67682000	0.28462200	0.00515900
C	-1.59875900	2.23398700	-0.22694100
H	-2.05193600	2.50110500	0.73466600
H	-1.05558300	3.10612400	-0.58255700
H	-2.41235900	2.00776600	-0.91814800
O	3.21957400	-2.07253300	0.07201700
O	1.51377100	-3.44679200	0.08398500
O	-2.88260500	-1.82259900	-0.20435800
O	2.41182200	2.64389200	-0.58677000
O	0.80057200	3.38863800	0.69498500
N	1.35825000	2.52755800	0.02379100

N	-2.51996600	-0.63679400	-0.02062600
N	2.02487900	-2.33352100	0.06254600
O	-3.39749300	0.22404500	0.20246700
Li	-4.79731900	-1.26382100	0.05635300

TNT-A_{Na}

E = -1047.17754398

C	1.01213300	-1.18975200	-0.03129800
C	-0.37225400	-1.21784600	-0.00399800
C	-1.05199500	-0.00004200	0.01765600
C	-0.37232600	1.21781800	-0.00415800
C	1.01206400	1.18978800	-0.03130700
C	1.77922200	0.00001900	-0.06602700
H	-0.89554900	2.16532900	-0.01041200
O	2.72797800	2.62363400	0.58119800
O	1.04455300	3.44041000	-0.55053000
O	-3.10003900	1.08369500	0.05994300
O	2.72831300	-2.62361100	0.58065400
O	1.04438500	-3.44039100	-0.55033700
N	1.65894100	-2.52866700	-0.00777400
N	-2.48828400	-0.00012800	0.04843200
N	1.65884600	2.52869200	-0.00766800
O	-3.09989000	-1.08400700	0.06060700
Na	-5.22440500	0.00016200	0.08285800
H	-0.89537900	-2.16541600	-0.01004300
C	3.27655200	0.00012200	-0.20122000
H	3.62371100	0.89214800	-0.72125500
H	3.74257800	-0.00004300	0.79089900
H	3.62379500	-0.89156400	-0.72173500

TNT-B_{Na}

E = -1047.17455280

C	1.29944600	-1.02156700	0.01989300
C	-0.09850000	-1.18166900	0.07786900
C	-0.81577400	0.04645100	0.04891000
C	-0.20754000	1.30798000	0.00853100
C	1.17036200	1.36542000	-0.02313300
C	1.94334300	0.21143800	-0.01068100
H	-0.79053100	2.21918300	-0.00895800
H	3.02556700	0.26927700	-0.02240900
C	-0.74703500	-2.53196700	0.24565100
H	-1.07051600	-2.92745400	-0.72339100
H	-0.04892200	-3.24997400	0.67068700
H	-1.62819800	-2.46563100	0.88501800
O	3.05534100	2.69235300	-0.09457100
O	1.09649200	3.67076000	-0.09084400
O	-2.84817500	1.13462000	0.33220900
O	3.27358200	-2.08726600	0.56069500
O	1.82129500	-3.17368100	-0.66345600
N	2.20319500	-2.20096800	-0.02137200
N	-2.26339600	0.07455700	0.03676100
N	1.83220200	2.69018800	-0.07416100
O	-2.91234400	-0.93276000	-0.29396100
Na	-5.00425000	0.23631100	-0.05385000

TNT-A_{K}

E = -1484.80509288

C	1.38670000	-1.18807000	-0.03030100
C	0.00076500	-1.21536100	-0.00699800
C	-0.67838900	-0.00009400	0.01257000
C	0.00061200	1.21527800	-0.00717100
C	1.38655300	1.18814000	-0.03029400
C	2.15406600	0.00006000	-0.06185000
H	-0.52399200	2.16173400	-0.01382500
O	3.10059500	2.62474400	0.58376500
O	1.41882100	3.43889900	-0.55069800
O	-2.72371500	1.08531500	0.04868800
O	3.10115300	-2.62458500	0.58306000
O	1.41877800	-3.43885800	-0.55045000
N	2.03212800	-2.52645700	-0.00639100
N	-2.12465700	-0.00023600	0.03940700
N	2.03188100	2.52654600	-0.00624100
O	-2.72346100	-1.08590000	0.04967800
K	-5.30558300	0.00012100	0.05529500
H	-0.52367600	-2.16191300	-0.01342000
C	3.65318700	0.00022400	-0.19224900
H	4.00123100	0.89174000	-0.71255200
H	4.11733500	0.00006300	0.80026500
H	4.00138600	-0.89088400	-0.71308700

TNT-B_{K}

E = -1484.80225952

C	-1.68743300	-0.99550600	-0.02032700
C	-0.29346300	-1.19020800	-0.08509900
C	0.45411300	0.01573400	-0.05995900
C	-0.11921700	1.29000100	-0.01576400
C	-1.49643500	1.38479900	0.02561400
C	-2.29989200	0.25294600	0.01677600
H	0.48953200	2.18409500	-0.00485400
H	-3.37985600	0.33849100	0.03609200

C	0.32193900	-2.55646400	-0.25636600
H	0.60748200	-2.97525400	0.71436000
H	-0.38518800	-3.24786000	-0.71068700
H	1.22054600	-2.50598800	-0.87187800
O	-3.34434900	2.76302700	0.11115500
O	-1.36059700	3.68771200	0.09496100
O	2.51137000	1.03108600	-0.41363300
O	-3.69572200	-2.00867500	-0.53991200
O	-2.25185800	-3.14151700	0.64989000
N	-2.61862800	-2.15206000	0.02389600
N	1.91178400	0.00506600	-0.05585500
N	-2.12152200	2.72573300	0.08223100
O	2.52002500	-1.00197500	0.33154100
K	5.10197000	0.12159300	0.05177900

6. The Natural atomic charges of CL-20, TNCB and TNT

Table S1 The Natural atomic charges of CL-20

Serial number	The charge of Cl-20
1a	0.080
1b	0.080
2a	-0.358
2b	-0.358
3a	0.077
3b	0.077
4a	0.080
4b	0.080
5a	-0.337
5b	-0.337
6a	0.660
6b	0.664
7a	-0.379
7b	-0.354
8a	-0.372
8b	-0.357
9a	0.664
9b	0.660
10a	-0.357
10b	-0.372
11a	-0.354
11b	-0.379
12	-0.340
13	0.673
14	-0.363
15	-0.369
16	-0.340
17	0.673
18	-0.369
19	-0.363

Table S2 The Natural atomic charges of TNCB

Serial number	The charge of TNCB
1	-0.040
2	0.037
3	-0.173
4	0.062
5	-0.173
6	0.067
7	0.307
8	0.307
9	-0.367
10	-0.367
11	-0.362
12	-0.340
13	-0.362
14	-0.340
15	0.528
16	0.528
17	0.531
18	0.129

Table S3 The Natural atomic charges of TNT

Serial number	The charge of TNT
1	0.036
2	0.077
3	-0.173
4	0.059
5	-0.173
6	0.077
7	0.306
8	0.306
9	-0.702
10	0.285
11	0.262
12	0.262
13	-0.363
14	-0.363
15	-0.360
16	-0.359
17	-0.359
18	-0.360
19	0.512
20	0.512
21	0.515