Electronic Supplementary Information (ESI)

Triptycene-based Quinone Molecules Showing Multi-Electron Redox Reactions for a Large Capacity and High Energy Organic Cathode Material in Li-ion Battery

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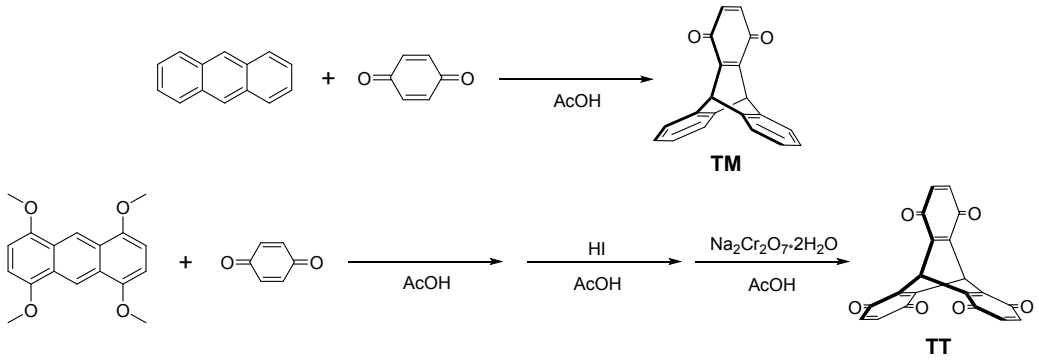
Contents

Materials preparation

All reagents and materials were obtained from commercial suppliers and used without further purification unless otherwise noted. All glassware, syringes, magnetic stirring bars, and needles were thoroughly dried in a convection oven. Reactions were monitored using thin layer chromatography (TLC) with commercial TLC plates (silica gel 60 F254, Merck Co.). 9,10-Dihydro-9,10-o-benzenoanthracene-1,4-dione (triptycene monobenzoquinone, TM) and 9,10-dihydro-9,10-o-Benzenoanthracene-1,4,5,8,13,16-hexone (triptycene tribenzoquinone, TT) were prepared according to the reported procedures.[S1] ^{1}H-NMR spectra were recorded on a Bruker Ascend 500 spectrometer. ATR/FT-IR spectra were recorded on a Bruker TENSOR II. Mass spectra were acquired through the JEOL JMS-700 instrument.



Scheme S1. Synthetic route of TM and TT.

9,10-Dihydro-9,10-o-benzenoanthracene-1,4-dione (triptycene monobenzoquinone, TM). A mixture of anthracene (10.00 g, 56.1 mmol) and *p*-benzoquinone (21.23 g, 196.4 mmol) in acetic acid (500 mL) was stirred at 120 ^{o}C for 3 h. The reaction mixture was poured into water, and then the precipitate was filtered, washed with hot water. The crude product was purified by flash chromatography on silica gel using dichloromethane as an eluent (11.17 g, 70 %). ^{1}H-NMR (500 MHz, $CDCl_3$) δ(ppm) 7.44−7.42 (m, 4H), 7.05−7.03 (m, 4H), 6.60 (s, 2H), 5.80 (s, 2H); IR (*v,* cm^{-1}) 1650 (C=O stretching); MS (EI) m/z: calcd for $C_{20}H_8O_6$ 284.08, found 284.00 $(M)^+$.

9,10-dihydro-9,10-o-Benzenoanthracene-1,4,5,8,13,16-hexone (triptycene tribenzoquinone, TT). The compound TT was prepared by the following three steps. (Step 1) A mixture of 1,4,5,8-tetramethoxyanthracene[S2] (1.26 g, 4.25 mmol) and 1,4-benzoquinone (2.28 g, 21 mmol) in acetic acid (130 mL) was refluxed for 48 h. The resulting mixture was cooled, filtrated, and washed with *N,N*-dimethylformamide (DMF) and acetone to give red powders (1.4 g). (Step 2) The resulting powders (1.4g) were then dissolved in HI (40 mL) and acetic acid (100 mL) and refluxed for 8 h. The reaction mixture was cooled, filtrated, and washed with acetone to give a grey solid (1.3 g). (Step 3) 0.87 g of the solid obtained in the step 2 was stirred with sodium dichromate dihydrate (0.75 g, 2.5 mmol) in acetic acid for 2h. The reaction mixture was poured into water and neutralized with an aqueous $NaHCO_3$ solution. The neutralized solution was then extracted with dichloromethane, and the organic layer was dried over anhydrous $MgSO_4$. After removal of the solvent, the product was purified by flash chromatography on silica gel using ethyl acetate: dichloromethane (1:30) as an eluent (0.73 g). ^{1}H-NMR (500 MHz, $CDCl_3$) δ(ppm) 6.70 (s, 6H), 6.60 (s, 2H); IR (*v,* cm^{-1}) 1650 (C=O stretching); MS (EI) m/z: calcd for $C_{20}H_8O_6$ 344.03, found 344.00 $(M)^+$.

Single crystal X-ray crystallography

Data Collection. A crystal with approximate dimensions 0.1 × 0.15 × 0.2 mm^3 was selected under oil at ambient conditions and attached to the tip of a MiTeGen MicroMount©. The crystal was mounted and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker D8 Venture diffractometer with Mo K_α (λ = 0.71073 Å) radiation and the diffractometer to crystal distance of 4.00 cm.

The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 12 frames collected at intervals of 0.5º in 6 range about ω with the exposure time of 5 seconds per frame. The reflections were successfully indexed by an automated indexing routine built in the APEXII program. The final cell constants were calculated from a set of 4244 strong reflections from the actual data collection.

The data were collected by using the full sphere data collection routine to survey the reciprocal space to the extent of a full sphere to a resolution of 0.81 Å. A total of 10224 were harvested by collecting 7 set of frames with 0.5º scans in ω and φ with an exposure time 5 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements.[S3]

Structure Solution and Refinement. The systematic absences in the diffraction data were uniquely consistent for tetragonal, space group $I4_1md$ that yielded chemically reasonable and computationally stable results of refinement.[S4-S5]

A successful solution by the direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

The final least-squares refinement of 67 parameters against 1006 data resulted in

residuals *R* (based on F^2 for $I \geq 2\sigma$) and *wR* (based on F^2 for all data) of 0.0394 and 0.0942 respectively. The final difference Fourier map was featureless.

Crystal Data for $C_{20}H_8O_6$ (*M* =344.26 g/mol): tetragonal, space group $I4_1md$ (no. 109), a = 10.8498(4) Å, c = 12.7484(5) Å, V = 1500.72(13) Å^3, Z = 4, T = 304.5 K, μ(MoKα) = 0.115 mm^{-1}, *Dcalc* = 1.524 g/cm^3, 10224 reflections measured ($4.93° \leq 2\Theta \leq 56.472°$), 1006 unique ($R_{int}$ = 0.0515, R_{sigma} = 0.0273) which were used in all calculations. The final R_1 was 0.0394 ($I > 2\sigma(I)$) and wR_2 was 0.0942 (all data). Crystallographic data for the structure has been deposited with the Cambridge Crystallographic Data Centre, CCDC No. 1574417, and can be obtained free of charge via http://www.ccdc.cam.ac.uk/structures/.

References

S1. Zhu, X. Z.; Chen, C. F. Iptycene quinones: Synthesis and structure. *J. Org. Chem.* **2005**, *70*, 917-924.

S2. Quast H.; Fuchabauer, H. –L. *Chem. Ber.* (1986) **119**, 1016-1038.

S3. Bruker-AXS. (2007-2013) APEX2 (Ver. 2013.2-0), SADABS (2012-1), and SAINT+ (Ver. 8.30C) Software Reference Manuals. Bruker-AXS, Madison, Wisconsin, USA.

S4. Sheldrick, G. M. SHELXL. *Acta. Cryst.* **2008**, *A64*, 112-122.

S5. Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H. OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Cryst.* **2009**, *42*, 339-341.

Table S1. X-ray data collection and structure refinements for TT.

Empirical formula	$C_{20}H_8O_6$	
Formula weight	344.26	
Temperature (K)	304.5	
Wavelength	λ=0.71073 (Mo K_α)	
Crystal system	Tetragonal	
Space group	$I4_1md$	
Unit cell dimensions	a/Å	10.8498(4)
	b/Å	10.8498(4)
	c/Å	12.7484(5)
	α/°	90
	β/°	90
	γ/°	90
Volume (Å^3)	1500.72(13)	
Z	4	
Density (calculated)	1.524	
Absorption coefficient	0.115	
Reflections collected	10224	
Independent reflections	1006 [R_{int}=0.0515, R_{sigma}=0.0273]	
Data / restraints / parameters	1006/1/67	
Goodness-of-fit on F^2	1.080	
Final R indices [I > 2sigma(I)]	R_1 = 0.0394, wR_2 = 0.0875	
R indices (all data)	R_1 = 0.0544, wR_2 = 0.0942	

Table S2. Electrochemical properties from the cyclic voltammetry (CV) measurement of BQ, TM, and TT in acetonitrile solution.

Compound	E_{red1}[a)]			E_{red2}[a)]		
	E_{pc} (V)	E_{pa} (V)	$E_{1/2}$ (V)	E_{pc} (V)	E_{pa} (V)	$E_{1/2}$ (V)
BQ	-0.93	-0.64	-0.79	-1.58	-1.28	-1.43
TM	-0.84	-0.61	-0.73	-1.52	-1.28	-1.40
TT	-0.69	-0.43	-0.56	-	-1.24	-
	-0.88	-0.61	-0.75	-1.72	-	-
	-1.03	-0.78	-0.90	-	-	-

a) Voltage values are presented *vs.* Ag/Ag^{+}.

Table S3. Electrochemical properties from the differential pulse voltammetry (DPV) measurement of BQ, TM, and TT in acetonitrile solution.

Compound	E_{red1}[a)] (V)	E_{red2}[a)] (V)
BQ	-0.81 (2.76)	-1.49 (2.08)
TM	-0.74 (2.83)	-1.48 (2.09)
TT	-0.58 (2.99)	-1.44 (2.13)
	-0.77 (2.80)	-1.59 (1.98)
	-0.94 (2.63)	

a) Voltage values are presented *vs.* Ag/Ag^+. Voltage values in parentheses are presented *vs.* Li/Li^+.

Table S4. Battery performance of the triptycene quinone electrodes.

Compound	Maximum specific capacity at 1 C (mAh/g)	Specific capacity after 100 cycles at 1 C (mAh/g)	Retention (%)	Specific capacity at various C-rate[a] (mAh/g)
TT	347	37	11	393 (0.1 C) 337 (0.2 C) 294 (0.5 C) 263 (1 C)
TT-CMK3-11	340	111	33	-
TT-CMK3-23	252	207	82	319 (0.1 C) 275 (0.2 C) 242 (0.5 C) 223 (1 C)
TT-CMK3-12	294	224	76	366 (0.1 C) 307 (0.2 C) 279 (0.5 C) 262 (1 C)

a) Values in the parentheses indicate the current rate.

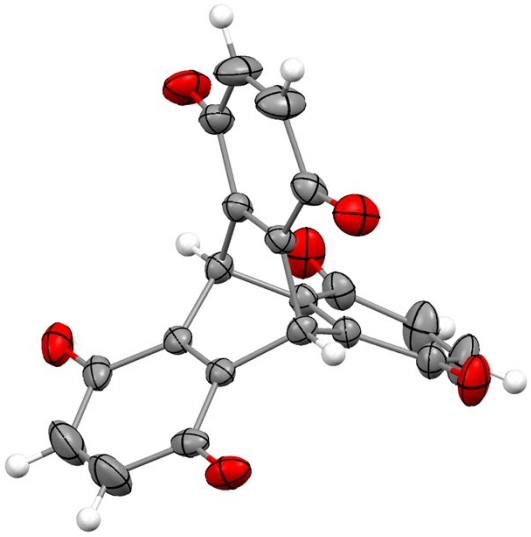


Figure S1. Single crystal structure of TT. Thermal ellipsoids are shown at 50% probability. The gray, red, and white colored atoms indicate carbon, oxygen, and hydrogen, respectively.

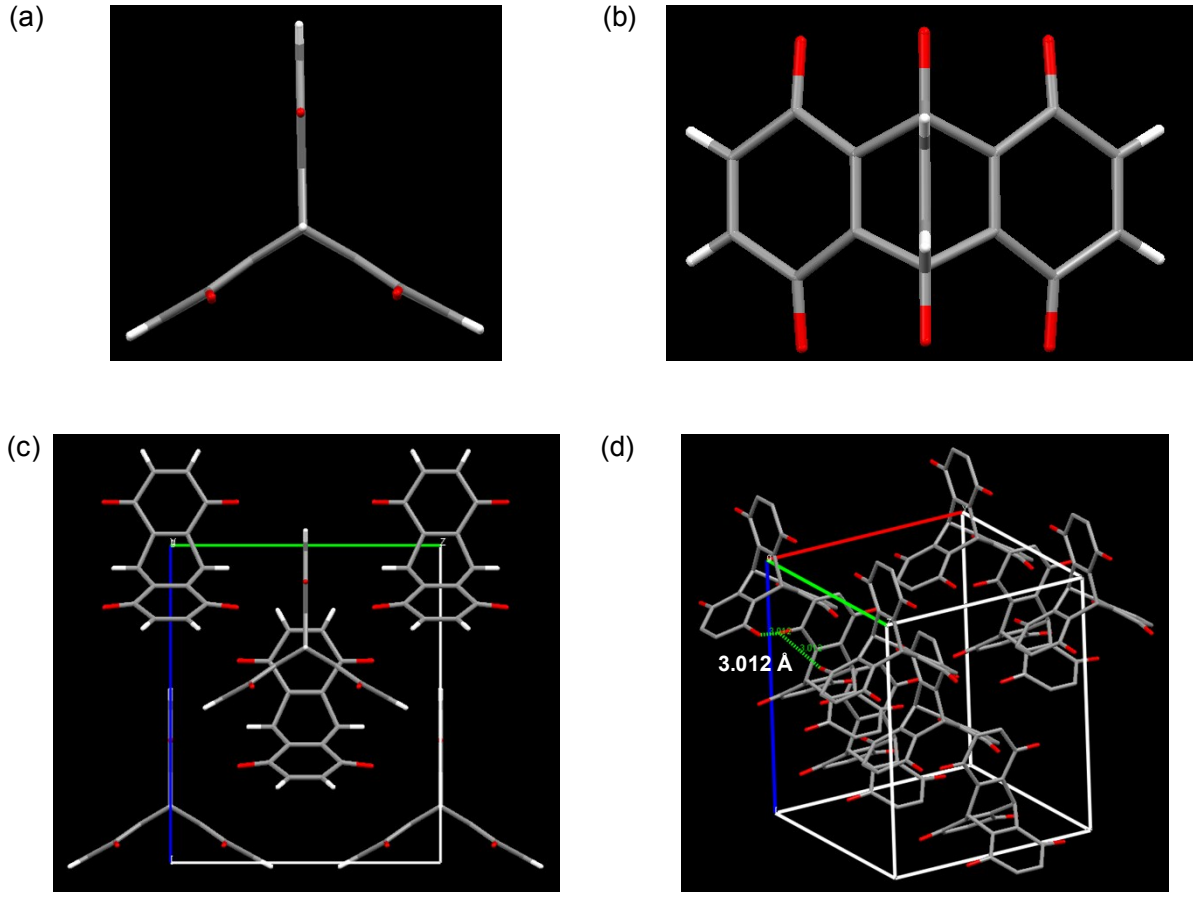


Figure S2. Single crystal structure of TT: (a) Side view and (b) top view of the molecule. Molecular packing structures of the TT single crystal: (c) along the *a* axis and (d) side view.

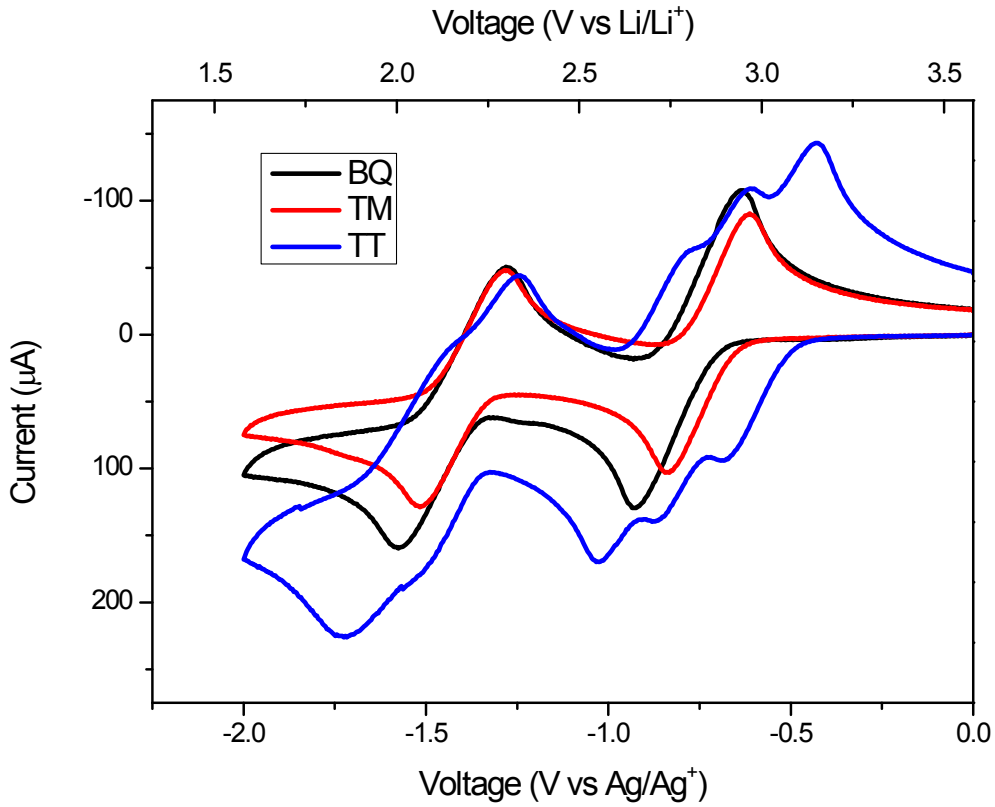


Figure S3. Cyclic voltammetry of BQ, TM, and TT with 0.1 M tetrabutylammonium hexafluorophosphate as a supporting electrolyte in acetonitrile. The potential values are linearly rescaled with respected to Li/Li^+ from the measured value *vs.* $Ag/AgNO_3$ reference electrode (Fc/Fc^+ = 0.13 V *vs.* Ag/Ag^+).

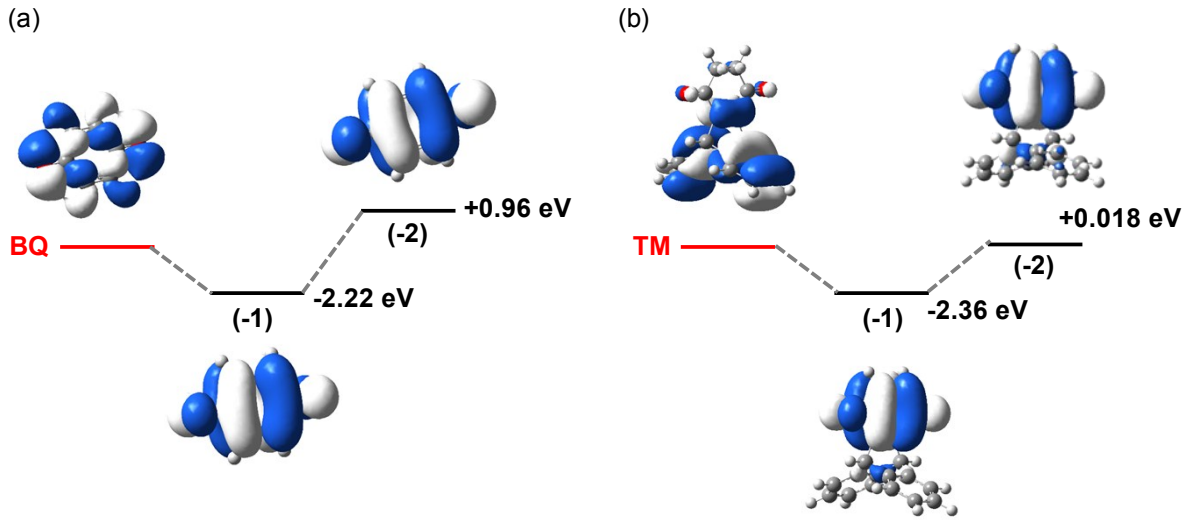


Figure S4. Relative energies and HOMO orbital diagrams of the reduced forms of (a) BQ and (b) TM.

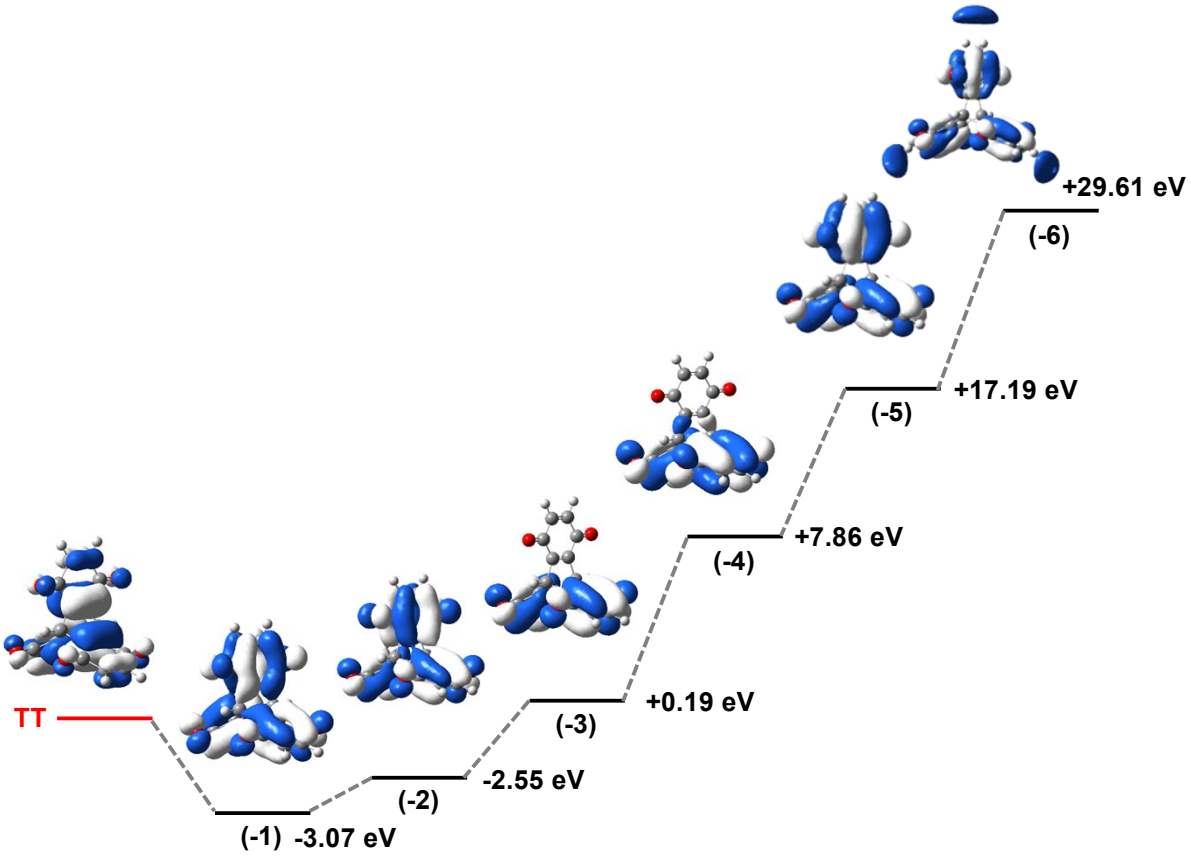


Figure S5. Relative energies and HOMO orbital diagrams of the reduced forms of TT.

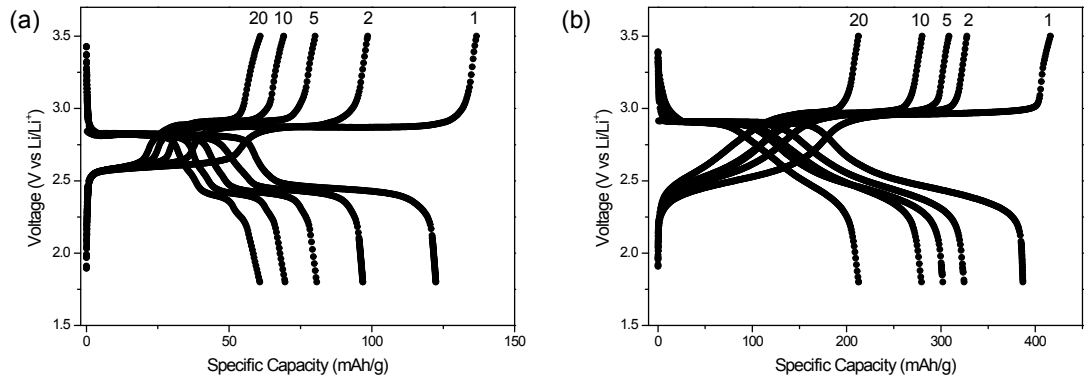


Figure S6. Representative capacity-voltage profiles of (a) TM and (b) TT electrodes at 0.1 C-rate. The numbers in the graphs indicate cycle numbers.

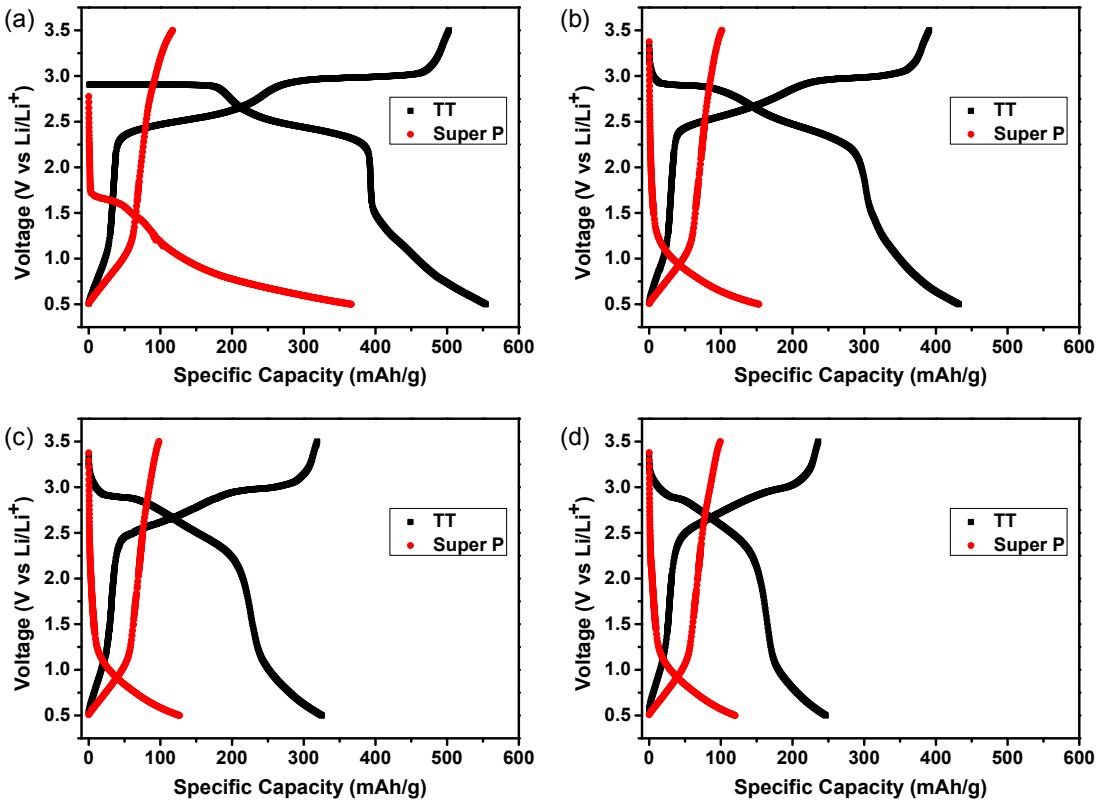


Figure S7. The Capacity-voltage profiles of TT and Super-P electrodes between 0.5–3.5 V vs Li/Li^+ at (a) 1st, (b) 2nd, (c) 5th, and (d) 10th cycle.

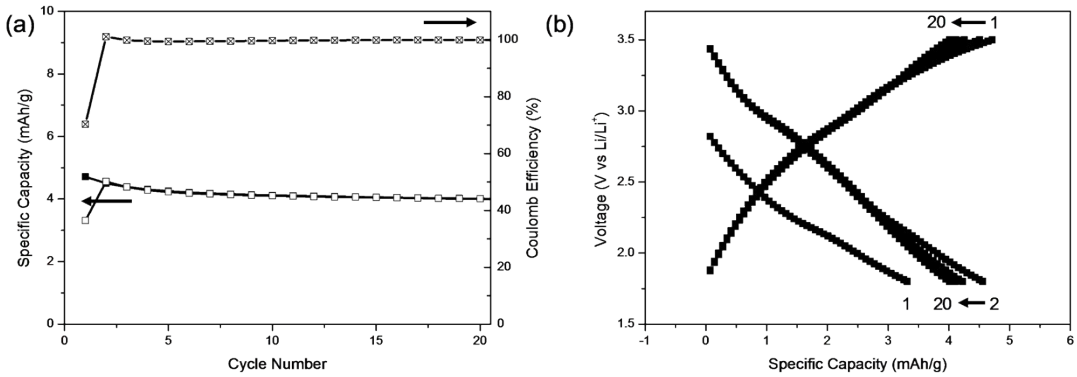


Figure S8. (a) Cycle performance and (b) representative capacity-voltage profiles of the BQ electrode at 0.1 C-rate. The numbers in the graphs indicate cycle numbers.

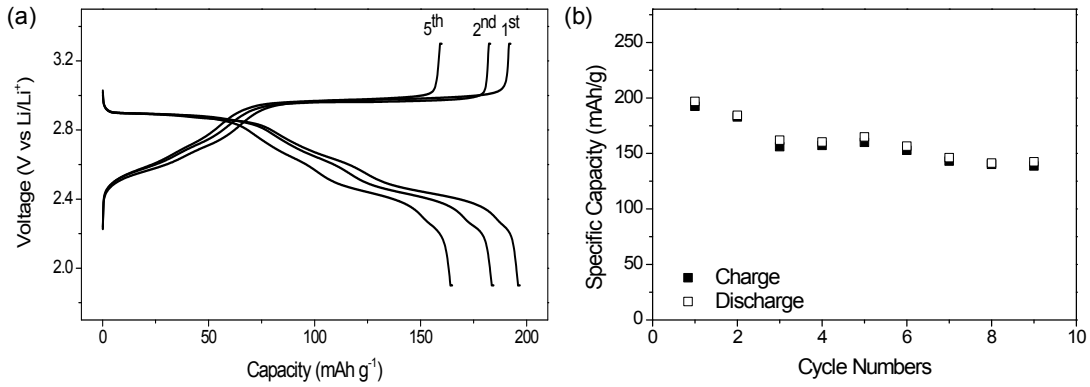


Figure S9. (a) Representative capacity-voltage profiles and (b) cycle performance of TT electrodes at 0.2 C-rate in the composite polymer electrolyte (CPE). The numbers in the graphs indicate cycle numbers.

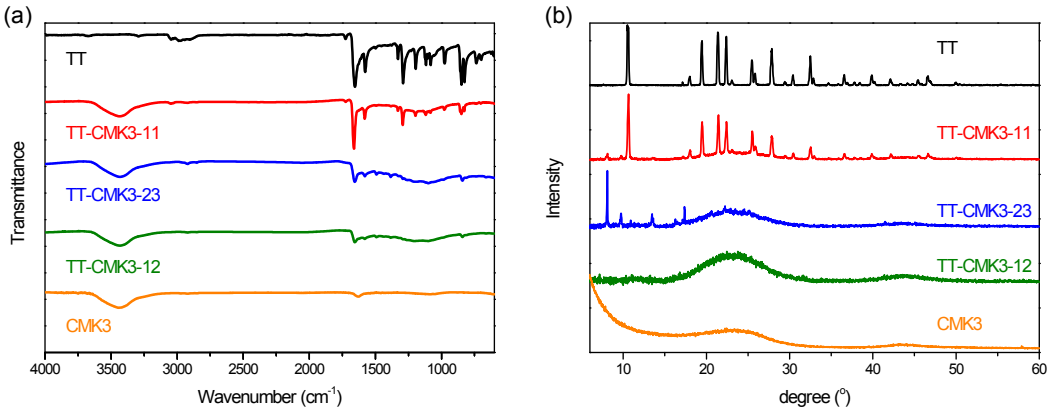


Figure S10. (a) FT-IR and (b) XRD spectra of TT, TT-CMK3 composites with different mixing ratio, and CMK3.

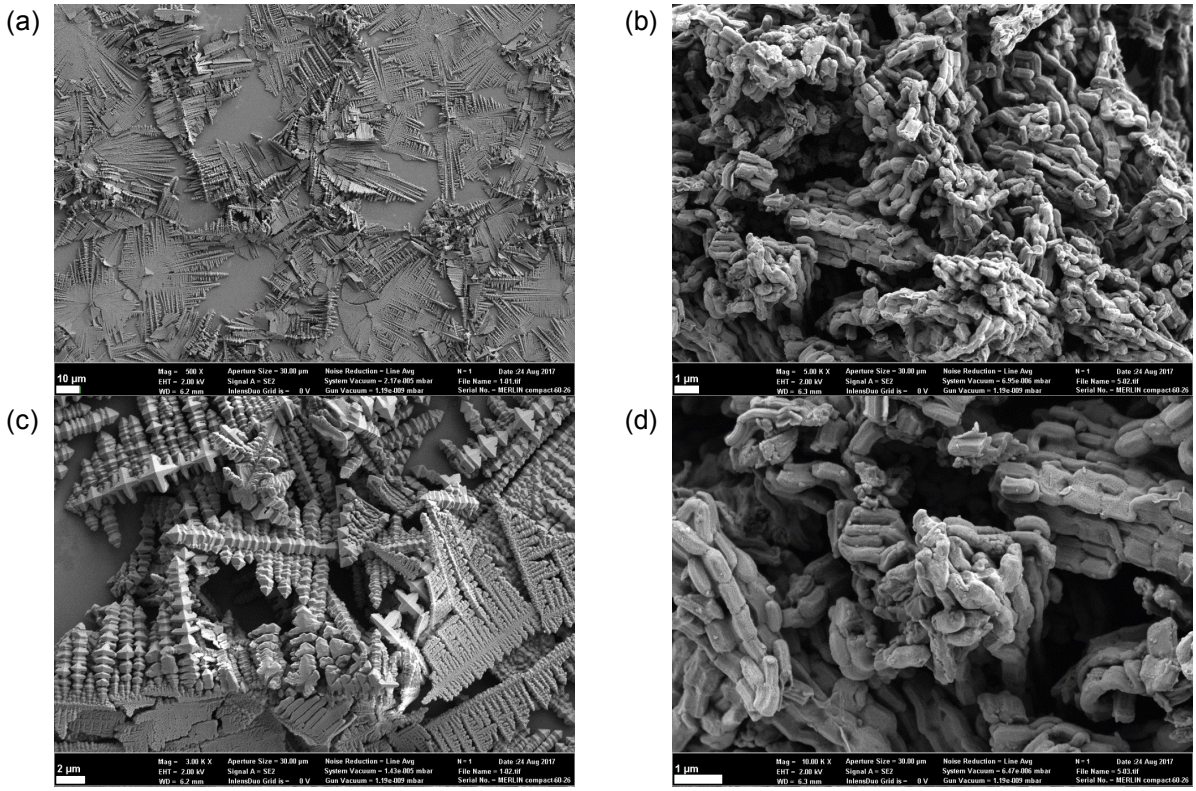


Figure S11. FE-SEM images of (a, c) TT and (b, d) CMK-3.

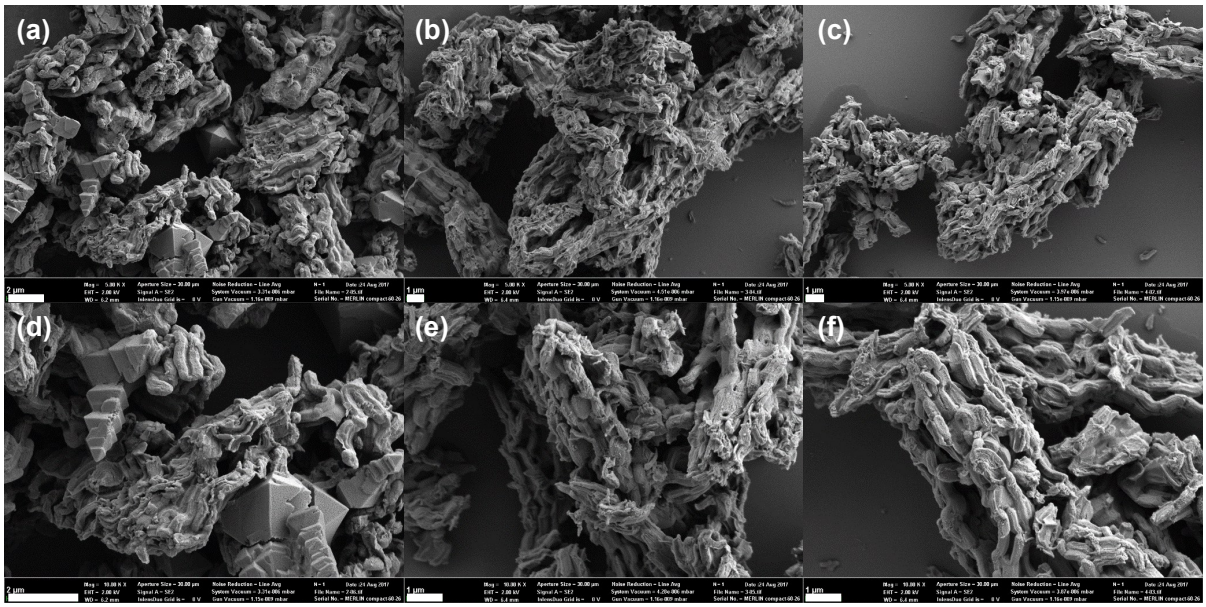


Figure S12. FE-SEM images of (a, d) TT-CMK3-11, (b, e) TT-CMK3-23, and (c,f) TT-CMK3-12 composites.

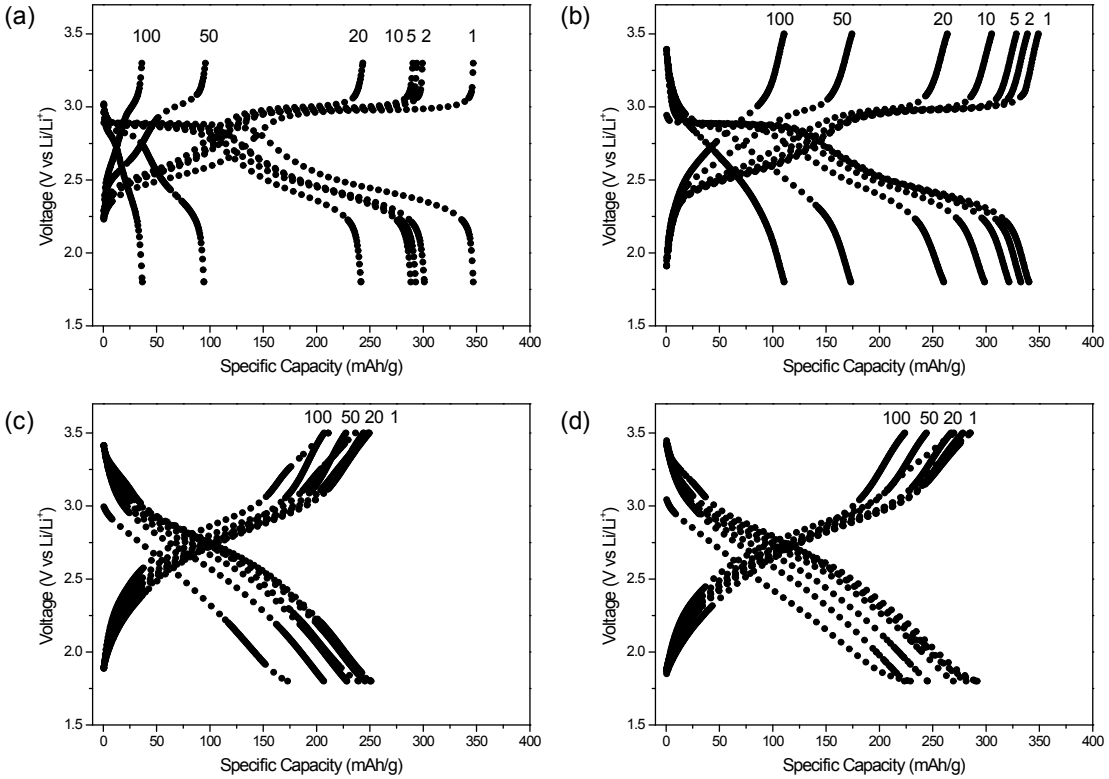


Figure S13. Representative capacity-voltage profiles of (a) TT, (b) TT-CMK3-11, (c) TT-CMK3-23, and (d) TT-CMK3-12 electrodes at 1 C-rate. The numbers in the graphs indicate cycle numbers.

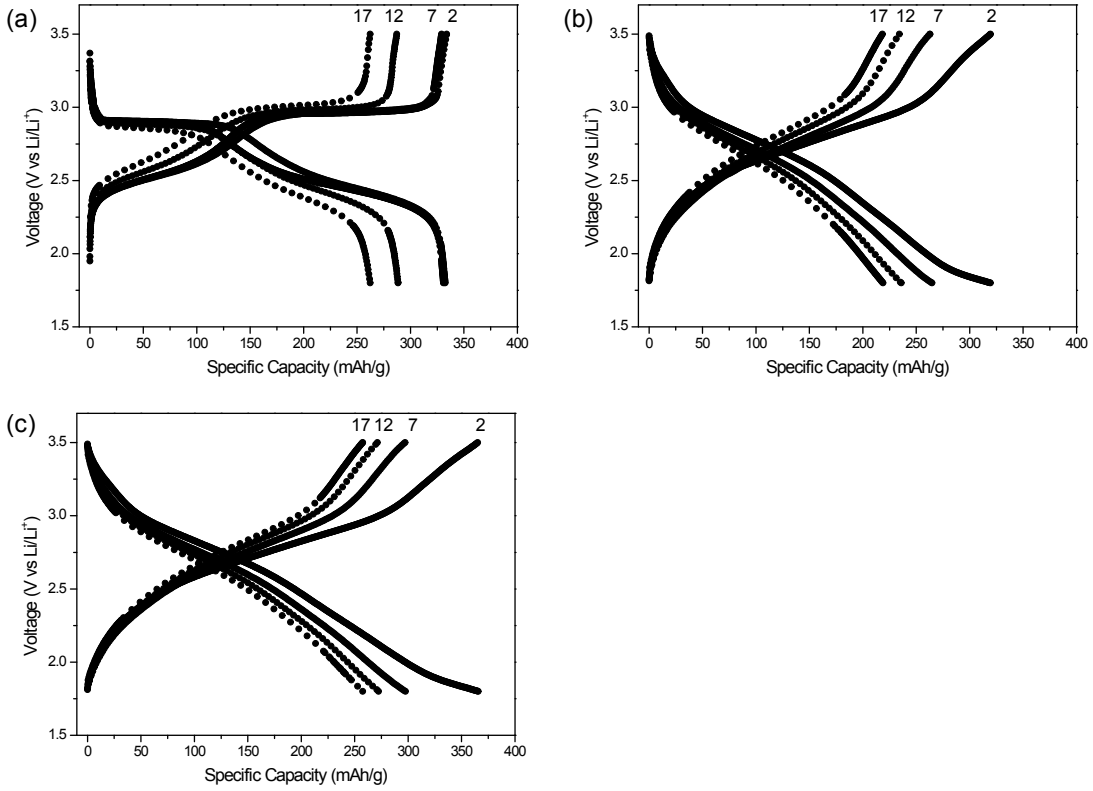


Figure S14. Representative capacity-voltage profiles of (a) TT, (b) TT-CMK3-23, and (c) TT-CMK3-12 electrodes at various C-rate. The numbers in the graphs indicate cycle numbers.

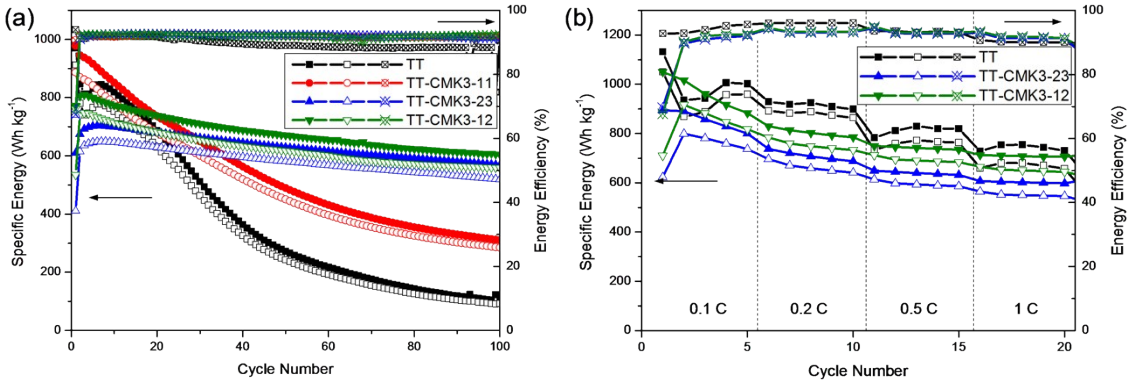


Figure S15. Specific energy with the corresponding energy efficiencies of TT (black squares), TT-CMK3-11 (red circles), TT-CMK3-23 (blue up-pointing triangles) and TT-CMK3-12 (green down-pointing triangles) composite electrodes at (a) 1 C-rate and (b) various C-rate. The symbols with an x mark in (a) and (b) indicate the energy efficiency respectively.

Optimized geometries by DFT calculation

BQ

E = −381.47650238 hartrees

Symbol	X	Y	Z
C	0.6723350	-1.2707760	0.0000700
C	-0.6723420	-1.2707780	0.0000810
C	-1.4436190	-0.0000070	0.0000270
C	-0.6723350	1.2707850	0.0000780
C	0.6723400	1.2707840	0.0000730
C	1.4436180	-0.0000020	0.0000530
H	1.2587550	-2.1851020	0.0000840
H	-1.2587570	-2.1851070	0.0001350
H	-1.2587720	2.1851000	0.0001220
H	1.2587730	2.1851030	0.0000950
O	-2.6706720	0.0000020	-0.0001690
O	2.6706750	-0.0000060	-0.0001720

BQ^-

E = −381.55622438 hartrees

Symbol	X	Y	Z
C	0.6874430	-1.2247660	0.0000070
C	-0.6874430	-1.2247660	-0.0000060
C	-1.4672830	0.0000000	-0.0000390
C	-0.6874430	1.2247660	-0.0000060
C	0.6874430	1.2247660	0.0000070
C	1.4672830	0.0000000	0.0000110
H	1.2482660	-2.1581740	0.0000190
H	-1.2482660	-2.1581740	0.0000000
H	-1.2482670	2.1581740	0.0000000
H	1.2482670	2.1581740	0.0000190
O	-2.7397670	0.0000000	0.0000210
O	2.7397670	0.0000000	-0.0000060

BQ^{2-}

E = −381.43718070 hartrees

Symbol	X	Y	Z
C	-0.0000010	0.7046460	1.1899160
C	-0.0000010	-0.7046460	1.1899160
C	-0.0000400	-1.5051820	0.0000000
C	-0.0000010	-0.7046460	-1.1899160
C	-0.0000010	0.7046460	-1.1899160
C	-0.0000330	1.5051820	0.0000000
H	0.0000240	1.2402990	2.1450400
H	0.0000250	-1.2402990	2.1450400
H	0.0000250	-1.2402990	-2.1450400
H	0.0000240	1.2402990	-2.1450400
O	0.0000320	-2.8203790	0.0000000
O	0.0000130	2.8203790	0.0000000

TM

E = −919.82976194 hartrees

Symbol	X	Y	Z
C	2.3946890	0.0004410	-1.4549280
C	1.1377330	0.0002180	-0.6762950
C	1.1377340	0.0002180	0.6762950
C	2.3946890	0.0004440	1.4549280
C	3.6634330	0.0004010	0.6721200
C	3.6634330	0.0004010	-0.6721200
C	-0.2523740	-0.0000050	-1.2989160
C	-0.2523740	-0.0000060	1.2989160
C	-1.5758550	2.2517400	-1.4078800
C	-2.1930670	3.2934210	-0.6978280
C	-2.1930670	3.2934210	0.6978290
C	-1.5758550	2.2517390	1.4078810
C	-0.9649600	1.2213710	0.7025640
C	-0.9649590	1.2213720	-0.7025630
C	-1.5751470	-2.2521640	-1.4078800
C	-2.1920240	-3.2940440	-0.6978290
C	-2.1920240	-3.2940440	0.6978280
C	-1.5751460	-2.2521650	1.4078800
C	-0.9645710	-1.2216060	0.7025630
C	-0.9645710	-1.2216060	-0.7025640
O	2.4079440	0.0002710	-2.6833430
O	2.4079440	0.0002670	2.6833430
H	4.5789960	0.0003920	1.2564980
H	4.5789950	0.0003920	-1.2564980
H	-0.2216410	0.0000020	-2.3886350
H	-0.2216410	0.0000010	2.3886350
H	-2.6709560	4.1041450	-1.2398920
H	-2.6709560	4.1041440	1.2398940
H	-2.6696580	-4.1049180	-1.2398930
H	-2.6696580	-4.1049180	1.2398920
H	-1.5740720	2.2524870	-2.4945980
H	-1.5740720	2.2524860	2.4945990
H	-1.5733750	-2.2529020	-2.4945990
H	-1.5733730	-2.2529040	2.4945980

TM^{-}

E = −919.91448765 hartrees

Symbol	X	Y	Z
C	-2.3707790	-0.0000090	-1.4782650
C	-1.1579160	-0.0000050	-0.6882330
C	-1.1579160	-0.0000050	0.6882330
C	-2.3707790	-0.0000100	1.4782650
C	-3.5918600	-0.0000100	0.6868920
C	-3.5918600	-0.0000110	-0.6868920
C	0.2472270	0.0000000	-1.2967660
C	0.2472270	0.0000010	1.2967660
C	1.5593100	-2.2582260	-1.4048720
C	2.1616010	-3.3121030	-0.6980790
C	2.1616010	-3.3121030	0.6980820
C	1.5593100	-2.2582250	1.4048740
C	0.9606480	-1.2160430	0.7048050
C	0.9606480	-1.2160440	-0.7048040
C	1.5592930	2.2582350	-1.4048730
C	2.1615760	3.3121170	-0.6980820
C	2.1615760	3.3121180	0.6980790
C	1.5592930	2.2582360	1.4048720
C	0.9606380	1.2160490	0.7048040
C	0.9606390	1.2160490	-0.7048050
O	-2.3720440	-0.0000090	-2.7487060
O	-2.3720440	-0.0000020	2.7487060
H	-4.5264280	-0.0000130	1.2447640
H	-4.5264280	-0.0000140	-1.2447640
H	0.2148180	-0.0000010	-2.3873780
H	0.2148180	0.0000010	2.3873780
H	2.6247020	-4.1320500	-1.2417240
H	2.6247020	-4.1320490	1.2417270
H	2.6246720	4.1320660	-1.2417270
H	2.6246720	4.1320670	1.2417240
H	1.5500890	-2.2603910	-2.4923390
H	1.5500890	-2.2603890	2.4923410
H	1.5500720	2.2603990	-2.4923400
H	1.5500720	2.2604010	2.4923390

TM^{2-}

E = −919.82356691 hartrees

Symbol	X	Y	Z
C	2.3188220	-0.0000430	1.5123060
C	1.1422810	-0.0000220	0.7056820
C	1.1422810	-0.0000220	-0.7056820
C	2.3188220	-0.0000450	-1.5123060
C	3.5114010	-0.0000560	-0.6990380
C	3.5114010	-0.0000560	0.6990380
C	-0.2752440	0.0000030	1.2986980
C	-0.2752440	0.0000040	-1.2986980
C	-1.5252240	-2.2928030	1.4027930
C	-2.0859440	-3.3738350	0.6993300
C	-2.0859440	-3.3738340	-0.6993330
C	-1.5252250	-2.2928020	-1.4027950
C	-0.9704390	-1.2203800	-0.7086760
C	-0.9704380	-1.2203810	0.7086750
C	-1.5251420	2.2928540	1.4027950
C	-2.0858220	3.3739060	0.6993330
C	-2.0858220	3.3739070	-0.6993300
C	-1.5251410	2.2928550	-1.4027930
C	-0.9703940	1.2204120	-0.7086750
C	-0.9703950	1.2204110	0.7086760
O	2.3265310	-0.0000400	2.8165770
O	2.3265310	-0.0000330	-2.8165770
H	4.4634380	-0.0000650	-1.2357620
H	4.4634380	-0.0000660	1.2357620
H	-0.2392030	0.0000020	2.3907960
H	-0.2392030	0.0000030	-2.3907960
H	-2.5145240	-4.2132570	1.2454170
H	-2.5145240	-4.2132560	-1.2454200
H	-2.5143710	4.2133430	1.2454200
H	-2.5143710	4.2133440	-1.2454170
H	-1.5067190	-2.2977710	2.4912650
H	-1.5067200	-2.2977690	-2.4912670
H	-1.5066360	2.2978200	2.4912670
H	-1.5066360	2.2978220	-2.4912650

TT

E = −1218.23840156 hartrees

Symbol	X	Y	Z
C	-1.7229810	2.0216740	-1.4599640
C	-0.9070840	1.0656760	-0.6744610
C	-0.9070840	1.0656860	0.6744440
C	-1.7229990	2.0216800	1.4599320
C	-2.5446790	2.9837440	0.6722040
C	-2.5446810	2.9837320	-0.6722510
C	0.0007050	0.0003890	-1.2998030
C	0.0007080	0.0004120	1.2998030
C	-0.8903910	-2.5021320	-1.4598650
C	-1.3151590	-3.6939770	-0.6721980
C	-1.3151580	-3.6939640	0.6722690
C	-0.8903840	-2.5021060	1.4599140
C	-0.4681390	-1.3183130	0.6744610
C	-0.4681410	-1.3183250	-0.6744360
C	2.6134350	0.4804750	-1.4599150
C	3.8580480	0.7081750	-0.6722470
C	3.8580500	0.7081870	0.6722230
C	2.6134470	0.4804590	1.4598980
C	1.3772510	0.2535970	0.6744450
C	1.3772480	0.2535900	-0.6744540
O	-1.7287100	2.0282300	-2.6852630
O	-1.7286630	2.0283110	2.6852310
O	-0.8935630	-2.5101760	-2.6851730
O	-0.8935620	-2.5101250	2.6852220
O	2.6217760	0.4826720	-2.6852250
O	2.6217700	0.4827920	2.6852090
H	-3.1394150	3.6804540	1.2555440
H	-3.1394230	3.6804290	-1.2556010
H	0.0008660	0.0004340	-2.3880000
H	0.0008730	0.0004750	2.3880000
H	-1.6227700	-4.5568000	-1.2555690
H	-1.6227670	-4.5567760	1.2556580
H	4.7590940	0.8730820	-1.2556340
H	4.7590970	0.8731110	1.2556040

TT^{-}

E = −1218.34863408 hartrees

Symbol	X	Y	Z
C	0.0001110	-2.5937480	-1.4684020
C	0.0000190	-1.3596520	-0.6823630
C	0.0000580	-1.3596120	0.6824480
C	0.0001200	-2.5936600	1.4685630
C	-0.0006880	-3.8438020	0.6765920
C	-0.0007440	-3.8438430	-0.6763560
C	-0.0000270	0.0503150	-1.2973060
C	0.0000590	0.0503920	1.2973040
C	2.3311040	1.2926290	-1.4636500
C	3.4431710	1.8750160	-0.6754650
C	3.4432160	1.8750590	0.6751150
C	2.3312040	1.2927160	1.4634100
C	1.2260960	0.7228710	0.6807060
C	1.2260510	0.7228290	-0.6808370
C	-2.3312260	1.2925060	-1.4634910
C	-3.4425830	1.8761490	-0.6752300
C	-3.4425380	1.8761880	0.6753490
C	-2.3312110	1.2924370	1.4635710
C	-1.2260510	0.7227990	0.6807940
C	-1.2260840	0.7227810	-0.6807530
O	-0.0006980	-2.6193350	-2.7109510
O	-0.0002530	-2.6191720	2.7111130
O	2.3537790	1.3046600	-2.7020900
O	2.3539530	1.3048370	2.7018480
O	-2.3535530	1.3053660	-2.7019270
O	-2.3532290	1.3058080	2.7020070
H	-0.0012020	-4.7659120	1.2522280
H	-0.0013200	-4.7659870	-1.2519360
H	-0.0000620	0.0490070	-2.3850540
H	0.0000960	0.0491470	2.3850510
H	4.2654230	2.2875160	-1.2542570
H	4.2655050	2.2875950	1.2538260
H	-4.2644410	2.2895080	-1.2539680
H	-4.2643480	2.2896010	1.2541180

TT^{2-}

E = −1218.32809584 hartrees

Symbol	X	Y	Z
C	-0.0000170	2.5515400	-1.4758740
C	0.0000040	1.3292120	-0.6890250
C	-0.0000130	1.3291840	0.6890820
C	-0.0000060	2.5514800	1.4759820
C	-0.0001370	3.7924280	0.6798920
C	-0.0001070	3.7924560	-0.6797340
C	0.0000270	-0.0894950	-1.2948520
C	-0.0000190	-0.0895460	1.2948490
C	-2.3531240	-1.2687270	-1.4711920
C	-3.4661820	-1.8190530	-0.6802640
C	-3.4662070	-1.8190800	0.6800630
C	-2.3531800	-1.2687800	1.4710520
C	-1.2414120	-0.7394290	0.6873310
C	-1.2413870	-0.7394040	-0.6874090
C	2.3531770	-1.2687490	-1.4711070
C	3.4663160	-1.8188620	-0.6801390
C	3.4662920	-1.8188890	0.6801890
C	2.3531750	-1.2687090	1.4711390
C	1.2414100	-0.7394070	0.6873780
C	1.2414250	-0.7393940	-0.6873620
O	0.0000320	2.5960040	-2.7311310
O	-0.0002090	2.5958930	2.7312400
O	-2.3884420	-1.2862010	-2.7252150
O	-2.3885380	-1.2863120	2.7250740
O	2.3886580	-1.2859750	-2.7251300
O	2.3884790	-1.2862620	2.7251620
H	-0.0002290	4.7194440	1.2510860
H	-0.0001640	4.7194950	-1.2508900
H	0.0000460	-0.0874020	-2.3824130
H	-0.0000370	-0.0874950	2.3824090
H	-4.3111480	-2.1985980	-1.2523720
H	-4.3111940	-2.1986470	1.2521250
H	4.3113580	-2.1982850	-1.2522150
H	4.3113090	-2.1983480	1.2522790

TT^{3-}

E = −1218.22549473 hartrees

Symbol	X	Y	Z
C	0.0137780	2.6380420	-1.4772750
C	0.0072650	1.4131740	-0.6903690
C	0.0072690	1.4131790	0.6903560
C	0.0137740	2.6380550	1.4772520
C	0.0202190	3.8590230	0.6881530
C	0.0202130	3.8590170	-0.6881860
C	-0.0000880	-0.0052450	-1.2891900
C	-0.0000780	-0.0052340	1.2891910
C	-2.3004400	-1.3069880	-1.4771590
C	-3.3643480	-1.9056370	-0.6882450
C	-3.3643430	-1.9056300	0.6882900
C	-2.3004290	-1.3069750	1.4771890
C	-1.2331900	-0.7052670	0.6902880
C	-1.2331950	-0.7052740	-0.6902710
C	2.2866430	-1.3307890	-1.4771730
C	3.3443050	-1.9404130	-0.6882720
C	3.3443100	-1.9404090	0.6882610
C	2.2866400	-1.3308020	1.4771650
C	1.2256900	-0.7180580	0.6902760
C	1.2256870	-0.7180590	-0.6902800
O	0.0140280	2.6789970	-2.7511810
O	0.0140810	2.6790200	2.7511570
O	-2.3353690	-1.3279250	-2.7511370
O	-2.3353500	-1.3278960	2.7511690
O	2.3213770	-1.3520200	-2.7511530
O	2.3214210	-1.3519600	2.7511450
H	0.0251120	4.7932330	1.2523920
H	0.0250990	4.7932230	-1.2524330
H	-0.0001080	-0.0055740	-2.3766980
H	-0.0000890	-0.0055550	2.3766980
H	-4.1794400	-2.3622410	-1.2523880
H	-4.1794310	-2.3622280	1.2524430
H	4.1546250	-2.4054280	-1.2524200
H	4.1546350	-2.4054170	1.2524060

TT^{4-}

E = −1217.94034905 hartrees

Symbol	X	Y	Z
C	-0.0275220	2.6409440	1.4891710
C	-0.0147290	1.4229560	0.6982930
C	-0.0147360	1.4229620	-0.6982800
C	-0.0275270	2.6409570	-1.4891470
C	-0.0402650	3.8542660	-0.6930050
C	-0.0402530	3.8542610	0.6930380
C	0.0000780	-0.0020280	1.2868040
C	0.0000650	-0.0020180	-1.2868040
C	2.3045000	-1.2967910	1.4891820
C	3.3634950	-1.8887690	0.6930320
C	3.3634890	-1.8887610	-0.6930860
C	2.3044870	-1.2967740	-1.4892200
C	1.2420270	-0.7011450	-0.6982910
C	1.2420330	-0.7011540	0.6982700
C	-2.2769330	-1.3444330	1.4892040
C	-3.3234170	-1.9582720	0.6930680
C	-3.3234230	-1.9582680	-0.6930470
C	-2.2769310	-1.3444530	-1.4891890
C	-1.2270790	-0.7268550	-0.6982760
C	-1.2270760	-0.7268520	0.6982840
O	-0.0281530	2.6989620	2.7764060
O	-0.0282270	2.6989850	-2.7763820
O	2.3547220	-1.3258450	2.7765050
O	2.3546980	-1.3258120	-2.7765430
O	-2.3265740	-1.3744500	2.7765270
O	-2.3266250	-1.3743910	-2.7765120
H	-0.0500990	4.7952000	-1.2528600
H	-0.0500760	4.7951900	1.2529010
H	0.0001080	-0.0023410	2.3747250
H	0.0000820	-0.0023220	-2.3747250
H	4.1850110	-2.3477710	1.2527790
H	4.1850000	-2.3477560	-1.2528460
H	-4.1352200	-2.4342300	1.2528220
H	-4.1352340	-2.4342180	-1.2527960

TT^{5-}

E = −1217.59790992 hartrees

Symbol	X	Y	Z
C	0.8094890	2.5303760	1.4750350
C	0.4404870	1.3587590	0.6922780
C	0.4392160	1.3590500	-0.6925090
C	0.8270320	2.5244440	-1.4754650
C	1.2037810	3.6887990	-0.6903070
C	1.1875650	3.6941670	0.6896740
C	-0.0001470	-0.0000270	1.2831360
C	-0.0001820	-0.0002380	-1.2831410
C	1.7868680	-1.9659740	1.4753970
C	2.6066570	-2.8745750	0.6902000
C	2.5939460	-2.8861520	-0.6897850
C	1.7730580	-1.9786540	-1.4751180
C	0.9573710	-1.0602670	-0.6923230
C	0.9564210	-1.0610250	0.6924690
C	-2.5964140	-0.5639990	1.4753120
C	-3.7933090	-0.8189210	0.6901050
C	-3.7968740	-0.8024310	-0.6898760
C	-2.6002830	-0.5463150	-1.4751610
C	-1.3970540	-0.2993420	-0.6923550
C	-1.3973110	-0.2979390	0.6924280
O	0.8107640	2.5716520	2.7588080
O	0.8498060	2.5585370	-2.7592500
O	1.8217640	-1.9876650	2.7591850
O	1.7910460	-2.0157990	-2.7588980
O	-2.6327240	-0.5830450	2.7591050
O	-2.6413140	-0.5436400	-2.7589490
H	1.4884320	4.5904340	-1.2362600
H	1.4863470	4.5913070	1.2354810
H	-0.0000260	0.0000060	2.3708990
H	-0.0000750	-0.0003660	-2.3709050
H	3.2349620	-3.5811260	1.2361470
H	3.2332470	-3.5828490	-1.2356300
H	-4.7195230	-1.0089940	1.2360060
H	-4.7200000	-1.0071460	-1.2357150

TT^{6-}

E = −1217.13918692 hartrees

Symbol	X	Y	Z
C	-1.6945190	-2.0597910	-1.4874880
C	-0.9036870	-1.1211960	-0.6975650
C	-0.8948490	-1.1282240	0.6975640
C	-1.6400100	-2.1034680	1.4874630
C	-2.3980160	-3.0490460	0.6974290
C	-2.4565000	-3.0020200	-0.6973830
C	-0.0000600	0.0002670	-1.2805180
C	0.0019440	-0.0012580	1.2805490
C	2.6319820	-0.4332000	-1.4896530
C	3.8300810	-0.6191940	-0.7005860
C	3.8420430	-0.5482380	0.6943580
C	2.6439840	-0.3707480	1.4854020
C	1.4262090	-0.2129340	0.6964270
C	1.4236630	-0.2217290	-0.6987310
C	-0.9414700	2.4961520	-1.4854260
C	-1.3800400	3.6252210	-0.6944560
C	-1.4458370	3.5982360	0.7005760
C	-0.9995280	2.4709230	1.4896960
C	-0.5270820	1.3388580	0.6987750
C	-0.5193810	1.3430840	-0.6964040
O	-1.7507580	-2.0733630	-2.7855960
O	-1.6397140	-2.1624760	2.7855100
O	2.6711090	-0.4733280	-2.7878350
O	2.6951210	-0.3457110	2.7835410
O	-0.9269430	2.5520710	-2.7835410
O	-1.0464170	2.5006590	2.7879170
H	-3.0230600	-3.7635630	1.2416010
H	-3.0206840	-3.7655380	-1.2415010
H	-0.0006110	0.0007700	-2.3686380
H	0.0029440	-0.0021770	2.3686750
H	4.7734290	-0.7216390	-1.2454420
H	4.7742570	-0.7302460	1.2376230
H	-1.7643970	4.4937930	-1.2377520
H	-1.7546190	4.4956090	1.2452760