Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Controlling Electronic Effects and Intermolecular Packing in Contorted Polyaromatic Hydrocarbons: Towards High Mobility Field Effect Transistors

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1.

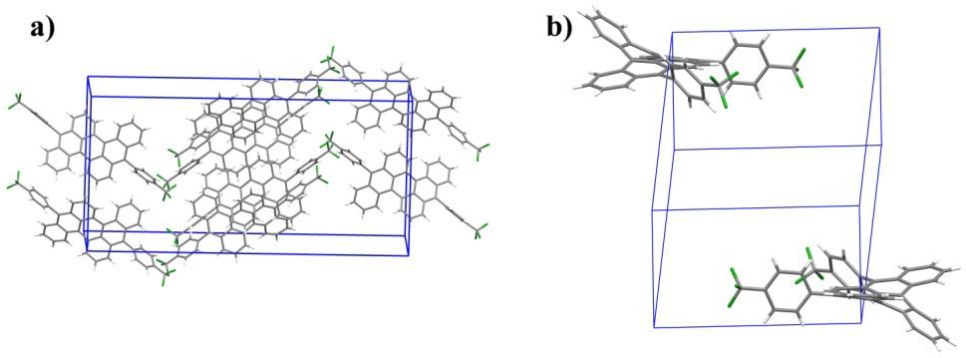


Figure S1 : Unit Cell of (a) DBP(**1**) and (b) 9,10-dioxoTBP(**3**) .

2. Molecular Dynamics simulations of 9,10-dioxoTBP derevative :

The unit cell of 9,10-dioxo TBP (**3)** contains two molecules each containing 44 atoms (88 atoms in unit cell). We have taken a 2×2×2 supercell of **3** containing 704 atoms for molecular dynamics simulation. Periodic boundary conditions were given in all three directions and the size of the simulation box was 30Å×30 Å×30Å. The system was first equilibrated for 10000 steps using conjugate gradient method and minimization was confirmed by convergence of the total potential energy of the system. Then heating up to 300K was performed, starting from 0K and temperature was allowed to increase in an extent of 1K after each 1ps of equilibration of the system with NVT ensemble. To equilibrate the system, we performed a 500ps MD simulation using NVT ensemble at 300 K. Equilibration was characterized by the approximate constancy of the RMSD value. Further, production simulation was carried out for 50ns with NVT ensemble at 300K. Constant temperature of the simulation system was maintained using Langevin dynamics with a damping coefficient of 5 ps^{-1}. With the particle-mesh Ewald method, full electrostatics was employed with a 1 Å grid width. The cut off for the van der Waals interaction was set to 12Å and switching functions were employed at 10Å. Using a group based cutoff, nonbonded interactions were updated at each time steps. We used

SHAKE algorithm to hold rigid covalent bonds involving hydrogen. Newton's equations of motion were integrated using the velocity verlet algorithm with a time step of 2 fs for all simulations, and we saved atomic coordinates by every 1 ps for the trajectory analysis.

$$U\left(b,\theta,\chi,\phi,r_{ij}\right) = \sum_{bonds} K_b(b-b_0)^2 + \sum_{angles} K_\theta(\theta-\theta_0)^2 + \sum_{dihedrals} K_\chi\left(1+cos(n\chi-\delta)\right) + \sum_{impropers} K_\phi(\phi-\phi_0)^2 + \sum_{nonbonded} \varepsilon_{ij}\left[\left(\frac{R_{ij}^{min}}{r_{ij}}\right)^2 - \left(\frac{R_{ij}^{min}}{r_{ij}}\right)^6\right] + \frac{q_i q_j}{\varepsilon_0 r_{ij}}$$

Where K_b (bond), K_θ (angle), K_χ (dihedral), and K_φ(improper) are force constants. The equilibrium values of bond (b), angle (θ), dihedral (χ), and improper (φ) are represented by the subscript 0, and n determining the periodicity of the dihedral potential in the interval [0,2π]. Lennard−Jones (LJ) 6−12 and Coulombic terms determine the nonbonded interaction; ε_0 is the effective dielectric constant, q_i is the partial atomic charge, r_{ij} is the distance between atoms i and j, R_{ij}^{min} is the distance at the LJ minimum, and ε_{ij} is the LJ well depth. The geometric mean ($\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}$) and arithmetic mean ($R_{ij}^{min} = \frac{R_i^{min} + R_j^{min}}{2}$) was used for calculating ε_{ij} *and* R_{ij}^{min} respectively. The MD simulations were carried out NAMD2 package with CHARMM general force field.

3. MD snapshot and RMSD plot of 9,10-dioxoTBP (**3**)geometries.

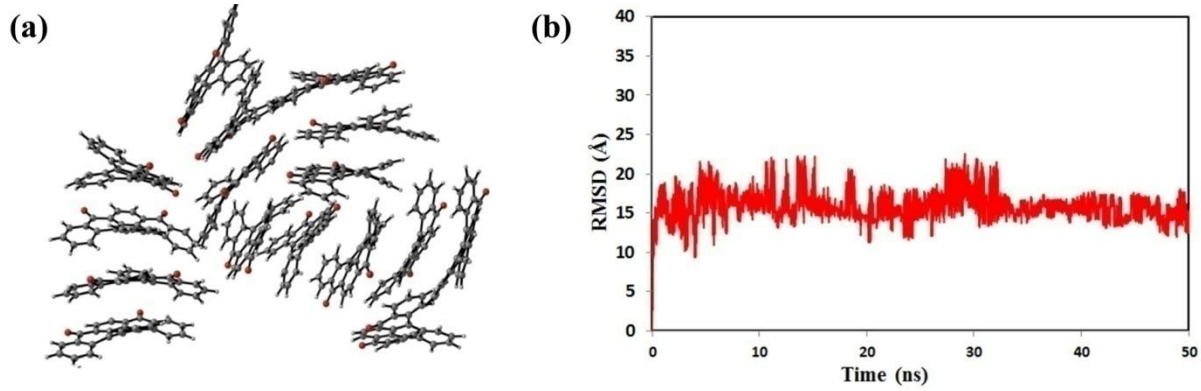
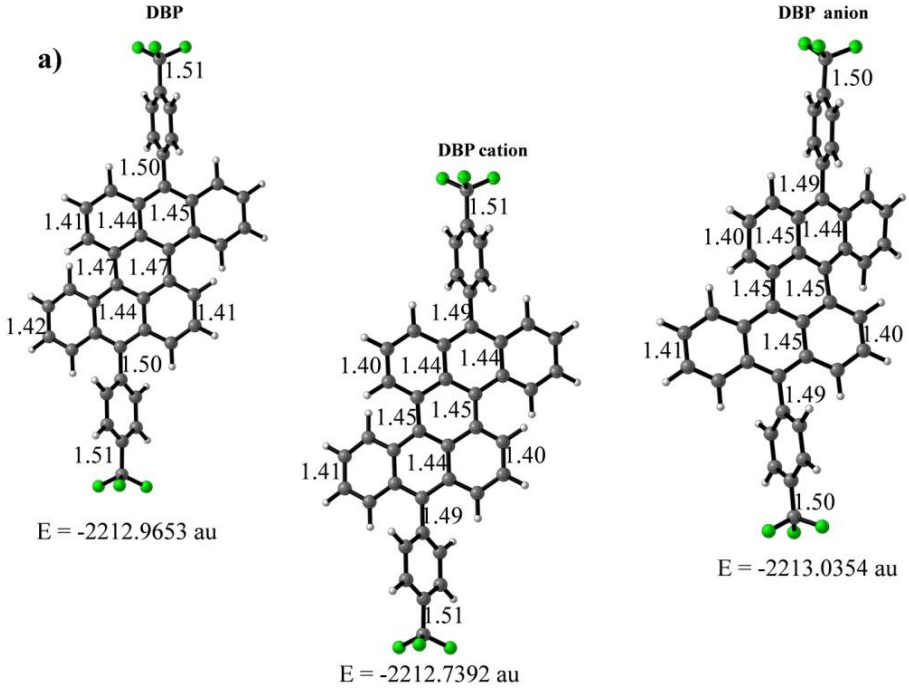


Figure S2 : (a) MD snapshot of 9,10-dioxoTBP geometries after 50 ns of production run. (b) RMSD plot of 9,10-dioxoTBP geometries.

4. Optimized Structure of DBP (**1**) and 9,10- dioxo TBP (**3**)molecule.



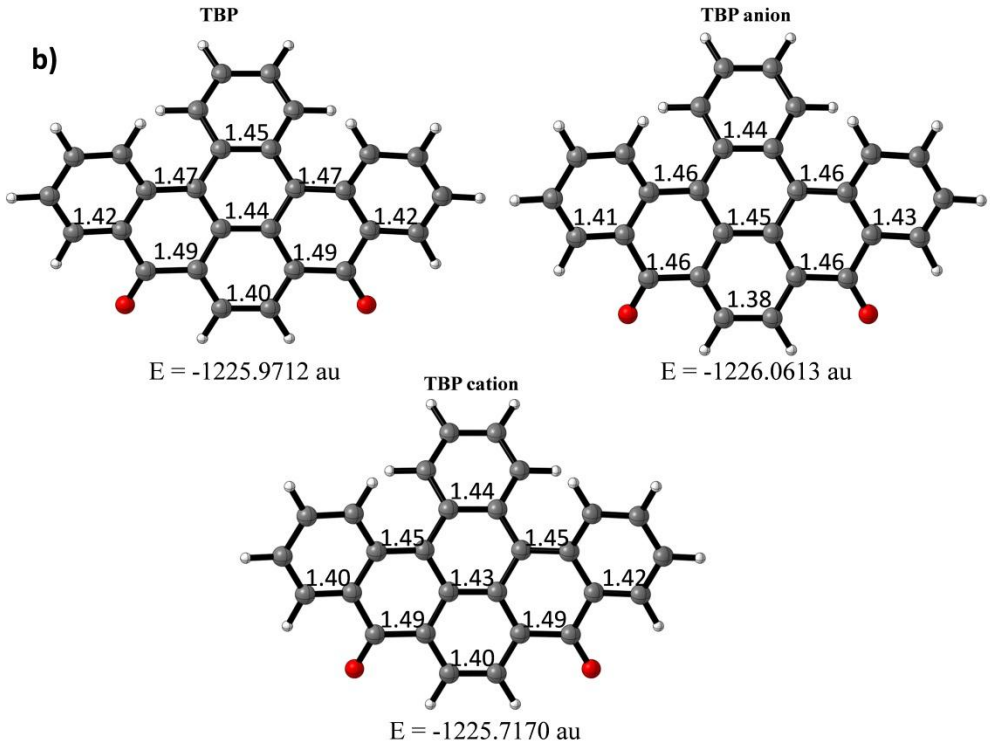


Figure S3. Ground state optimized geometries for the neutral, anionic and cationic structures of DBP (a) and TBP (b). The corresponding energies are reported in Hartree.

5. Cartesian coordinates for optimized structure and their energies in hartree and low frequencies calculated at B3LYP/6-31++G(d,p) level of theory. All calculations have been performed in gas- phase.

Dibenzoperylene molecule (DBP, **1**)

Neutral structure of **1**

Atom	X	Y	Z
F	10.17601600	-0.40307500	0.09209700
F	9.78708300	0.73818100	1.90525100
F	9.84788000	1.74563800	-0.02975900
F	-9.78689900	-0.73919000	1.90520500
F	-9.84806800	-1.74515600	-0.03055500

F	-10.17594000	0.40352200	0.09299500
C	3.76321400	-0.44033300	-0.12366900
C	3.34044300	-1.72392400	-0.54175000
C	4.28592200	-2.73536000	-0.91206200
H	5.34371500	-2.51108700	-0.83708200
C	3.88121400	-3.95679900	-1.38744000
H	4.61844600	-4.70042900	-1.67531200
C	2.49773800	-4.23092500	-1.54609400
H	2.17926900	-5.16936200	-1.99029400
C	1.55894000	-3.30175400	-1.16578900
H	0.51116400	-3.51160300	-1.33810300
C	1.92963400	-2.03510100	-0.61479400
C	0.97312700	-1.05189100	-0.21429300
C	-0.43678400	-1.34733100	0.07673400
C	-0.87175600	-2.59556100	0.50521400
H	-0.15245800	-3.38222300	0.69522400
C	-2.24199600	-2.86097200	0.72977200
H	-2.54098600	-3.84646000	1.07460500
C	-3.19201200	-1.89750700	0.49665700
H	-4.24218400	-2.12524600	0.63539900
C	-2.81079300	-0.57894800	0.09536700
C	-3.76319900	0.44036100	-0.12368800
C	-3.34044500	1.72397000	-0.54167700
C	-4.28594400	2.73549400	-0.91173700
H	-5.34373400	2.51125600	-0.83657100
C	-3.88125400	3.95694900	-1.38707100
H	-4.61848400	4.70066400	-1.67473200

C	-2.49778000	4.23101500	-1.54592100
H	-2.17934100	5.16945200	-1.99014400
C	-1.55896700	3.30180200	-1.16577300
H	-0.51120200	3.51162700	-1.33819800
C	-1.92963300	2.03513300	-0.61478100
C	-0.97313000	1.05192100	-0.21430700
C	0.43677700	1.34735400	0.07677600
C	0.87172400	2.59555200	0.50536000
H	0.15243300	3.38222200	0.69534900
C	2.24194500	2.86091000	0.73010900
H	2.54091000	3.84634200	1.07512200
C	3.19196800	1.89745800	0.49700300
H	4.24211400	2.12515200	0.63600000
C	2.81079500	0.57895000	0.09547100
C	1.40354100	0.28055000	-0.02978900
C	-1.40354200	-0.28053100	-0.02983200
C	5.22042200	-0.15623100	0.06437800
C	5.95674300	0.52192600	-0.91983800
H	5.46047200	0.84215800	-1.83103800
C	7.31491600	0.78704100	-0.74370000
H	7.87010300	1.31392300	-1.51247500
C	7.95674300	0.37836400	0.42960500
C	7.23833300	-0.29933000	1.41975000
H	7.73349600	-0.61316200	2.33245900
C	5.88121600	-0.56240100	1.23437200
H	5.32480300	-1.08521900	2.00651900
C	9.43244200	0.61890700	0.60149400

C	-5.22041700	0.15622200	0.06437200
C	-5.95700200	-0.52082700	-0.92040200
H	-5.46094700	-0.84018600	-1.83202800
C	-7.31517200	-0.78597400	-0.74426100
H	-7.87057300	-1.31202100	-1.51345200
C	-7.95670800	-0.37844600	0.42960400
C	-7.23802000	0.29812700	1.42031100
H	-7.73296500	0.61105200	2.33344800
C	-5.88090600	0.56123100	1.23493200
H	-5.32427000	1.08318600	2.00750100
C	-9.43240800	-0.61897700	0.60150700

Energy = -2212.9653 Hartree

Low Frequencies (cm^{-1}) : 11.8875 17.8361 18.8227 19.6037 29.1888 31.3634 32.8304 34.4749 49.0603 74.0653 90.1218 99.6565 103.3025 114.1553 114.5867

cation structure of **1**

Atom	X	Y	Z
F	10.14986900	-0.40617200	0.20215900
F	9.72893600	0.72725200	2.01424200
F	9.82361700	1.74478800	0.08589100
F	-9.72899900	-0.72739100	2.01413300
F	-9.82357800	-1.74492400	0.08577600
F	-10.14988300	0.40602700	0.20203500
C	3.76049900	-0.45357400	-0.11635200
C	3.34496600	-1.75073700	-0.52544700
C	4.30137000	-2.75403400	-0.86320100

H	5.35551000	-2.53138600	-0.75138200
C	3.90977300	-3.97706600	-1.36280200
H	4.65411400	-4.72114400	-1.62679900
C	2.54044600	-4.23831700	-1.57891600
H	2.23377800	-5.17282600	-2.03825800
C	1.58427000	-3.29865600	-1.23729900
H	0.54739500	-3.50066500	-1.47358000
C	1.94132400	-2.05266300	-0.65981300
C	0.96704300	-1.05667100	-0.29103900
C	-0.43108200	-1.34494900	-0.03081800
C	-0.87464000	-2.61622800	0.38066200
H	-0.15194500	-3.40095400	0.56439800
C	-2.22659200	-2.87725900	0.62291900
H	-2.52943400	-3.86123300	0.96543400
C	-3.17641700	-1.88692300	0.43565200
H	-4.22222900	-2.10359700	0.61583000
C	-2.79625300	-0.57434700	0.04888800
C	-3.76050600	0.45357300	-0.11624900
C	-3.34497100	1.75081900	-0.52508300
C	-4.30137400	2.75418400	-0.86264200
H	-5.35551500	2.53151200	-0.75087900
C	-3.90977500	3.97731600	-1.36199600
H	-4.65411500	4.72144500	-1.62585000
C	-2.54044700	4.23861100	-1.57804800
H	-2.23377700	5.17321400	-2.03719900
C	-1.58427200	3.29888200	-1.23661700
H	-0.54739600	3.50093900	-1.47285200

C	-1.94132900	2.05277200	-0.65938500
C	-0.96704900	1.05670300	-0.29081600
C	0.43107600	1.34492600	-0.03053800
C	0.87463400	2.61612100	0.38120200
H	0.15193900	3.40080700	0.56510600
C	2.22658900	2.87710600	0.62349900
H	2.52943200	3.86101100	0.96620900
C	3.17641400	1.88680900	0.43602000
H	4.22222900	2.10344800	0.61622500
C	2.79624600	0.57431000	0.04899900
C	1.39313700	0.27995800	-0.11107200
C	-1.39314400	-0.27996300	-0.11112800
C	5.21065100	-0.16518700	0.09504000
C	5.94021000	0.57557200	-0.84817100
H	5.45032900	0.93951400	-1.74636000
C	7.29594900	0.83764000	-0.64885100
H	7.85226900	1.40783000	-1.38476100
C	7.93237200	0.37072200	0.50441400
C	7.21603700	-0.36599500	1.45266100
H	7.70908300	-0.72269200	2.35051100
C	5.86389500	-0.63642900	1.24519300
H	5.31127400	-1.20742900	1.98522100
C	9.40939600	0.61535400	0.70428500
C	-5.21065700	0.16515100	0.09509200
C	-5.94020900	-0.57548700	-0.84822100
H	-5.45032200	-0.93930900	-1.74645600
C	-7.29594800	-0.83758300	-0.64894600

H	-7.85226100	-1.40767800	-1.38493500
C	-7.93238200	-0.37081800	0.50437600
C	-7.21605600	0.36577700	1.45272300
H	-7.70910900	0.72235500	2.35061700
C	-5.86391300	0.63624200	1.24530000
H	-5.31130000	1.20714800	1.98540700
C	-9.40940800	-0.61548200	0.70419200

Energy = -2212.7392 Hartree

Low Frequency (cm^{-1}): 11.6898 18.3275 19.2960 20.2189 29.4789 30.5839 32.8071 35.9316 51.4414 74.3017 91.5691 97.6837 101.8613 115.1668 115.5540

Anion structure of **1**

Atom	X	Y	Z
F	10.08009400	-0.52378100	1.06772500
F	9.62358600	1.45316500	1.85335600
F	10.03617100	1.18907300	-0.27447200
F	-9.62349200	-1.45404900	1.85285900
F	-10.03655500	-1.18800900	-0.27464100
F	-10.07987800	0.52366800	1.06905800
C	3.76564800	-0.45184400	-0.15465600
C	3.35412200	-1.74338200	-0.58299300
C	4.28893600	-2.78806100	-0.87191000
H	5.34380300	-2.61054600	-0.69466700
C	3.88954700	-4.00212400	-1.39025300
H	4.63127700	-4.76660800	-1.60937000

C	2.52361200	-4.23741100	-1.65989600
H	2.20625800	-5.16378400	-2.13114600
C	1.58700900	-3.27736600	-1.31984700
H	0.54319100	-3.46010800	-1.54366600
C	1.94728400	-2.03885500	-0.72301400
C	0.96912600	-1.05014400	-0.32599100
C	-0.42609500	-1.35564000	-0.06532500
C	-0.86913600	-2.64166900	0.30897700
H	-0.14497200	-3.42672600	0.48644900
C	-2.22633500	-2.91076000	0.49490800
H	-2.53622400	-3.91295300	0.78288100
C	-3.18586800	-1.92543200	0.30708200
H	-4.23611700	-2.17389400	0.40750200
C	-2.80845400	-0.58865900	0.00342500
C	-3.76573700	0.45182900	-0.15495600
C	-3.35410400	1.74343700	-0.58309200
C	-4.28876600	2.78832300	-0.87176100
H	-5.34364600	2.61099600	-0.69444500
C	-3.88924100	4.00243000	-1.38990300
H	-4.63089200	4.76704700	-1.60882300
C	-2.52329300	4.23760300	-1.65956300
H	-2.20583500	5.16400800	-2.13067700
C	-1.58681200	3.27740300	-1.31963100
H	-0.54295900	3.46006100	-1.54336100
C	-1.94724000	2.03884800	-0.72298200
C	-0.96913900	1.05008000	-0.32596600
C	0.42602900	1.35553900	-0.06505200

C	0.86902600	2.64150500	0.30955100
H	0.14483000	3.42653600	0.48702100
C	2.22618900	2.91055100	0.49582700
H	2.53600700	3.91267600	0.78411800
C	3.18576300	1.92527100	0.30796700
H	4.23600200	2.17366300	0.40871900
C	2.80838000	0.58858400	0.00385900
C	1.39607400	0.28959800	-0.13909200
C	-1.39612900	-0.28968700	-0.13931900
C	5.20821000	-0.16204900	0.07997100
C	6.13162900	-0.11406700	-0.98117900
H	5.77725000	-0.28457200	-1.99321200
C	7.48153600	0.15715200	-0.76113400
H	8.17173700	0.19657900	-1.59769700
C	7.94262900	0.39462300	0.53870100
C	7.04188500	0.35564800	1.61103700
H	7.39250300	0.53939700	2.62168400
C	5.69532400	0.08453700	1.37772600
H	4.99947000	0.06003100	2.21090000
C	9.40008700	0.63173100	0.79128700
C	-5.20825200	0.16205000	0.07970800
C	-6.13208000	0.11553900	-0.98116800
H	-5.77804400	0.28712700	-1.99313600
C	-7.48196400	-0.15567300	-0.76098600
H	-8.17243400	-0.19395900	-1.59738300
C	-7.94269000	-0.39463600	0.53870200
C	-7.04154800	-0.35716500	1.61077500

H	-7.39185400	-0.54205500	2.62132200
C	-5.69502200	-0.08607100	1.37733500
H	-4.99888800	-0.06274000	2.21030900
C	-9.40010800	-0.63171400	0.79144900

Energy = -2213.0354 Hartree

Low Frequency (cm^{-1}) : 11.4305 18.8765 21.4256 21.6982 30.2692 30.4837 33.4077 37.5105 48.2248 72.1502 82.4426 102.8119 108.6868 110.7855 120.2655

9,10 -dioxo tetrabenzopyrene (9,10-dioxoTBP,3)

Neutral structure of 3

Atom	X	Y	Z
C	2.89444800	-2.03918600	-0.27343400
C	1.40648700	-1.99661500	-0.25846000
C	0.70234800	-3.18090000	-0.39951500
H	1.26261900	-4.10244100	-0.51817800
C	-0.70224600	-3.18092800	-0.39938800
H	-1.26250400	-4.10250100	-0.51786700
C	-1.40642300	-1.99667400	-0.25826200
C	-2.89438300	-2.03936600	-0.27290700
C	-3.58817400	-0.79204900	0.12688100
C	-4.95549600	-0.86019000	0.43065500
H	-5.46355700	-1.80541500	0.27020700
C	-5.62199900	0.24284600	0.95241500
H	-6.67882600	0.18315700	1.19349000
C	-4.90173300	1.41677800	1.20460700
H	-5.39302300	2.26847500	1.66641100
C	-3.54937600	1.50218400	0.88301900

H	-3.01049800	2.40787800	1.13162700
C	-2.86579600	0.41790800	0.29151100
C	-1.43596700	0.47304200	-0.06263100
C	-0.72602600	1.67305200	-0.36123900
C	-1.39617700	2.87098300	-0.76772100
H	-2.47348100	2.85955900	-0.86544000
C	-0.70850600	4.00181800	-1.13240800
H	-1.25140100	4.87885000	-1.47189200
C	0.70852600	4.00186300	-1.13225200
H	1.25144200	4.87893700	-1.47159700
C	1.39618700	2.87105900	-0.76745600
H	2.47351100	2.85970000	-0.86495100
C	0.72601500	1.67307500	-0.36115300
C	1.43595600	0.47306800	-0.06258200
C	2.86577200	0.41792300	0.29162000
C	3.54927200	1.50210800	0.88337500
H	3.01034900	2.40775200	1.13208300
C	4.90160300	1.41665900	1.20507600
H	5.39284100	2.26827400	1.66708500
C	5.62190700	0.24278500	0.95272900
H	6.67870800	0.18306200	1.19391100
C	4.95548400	-0.86015700	0.43066200
H	5.46359200	-1.80532600	0.27003300
C	3.58819100	-0.79197500	0.12677400
C	-0.71879000	-0.74641400	-0.14931800
C	0.71880600	-0.74639900	-0.14935600
O	3.50671200	-3.07344500	-0.54064900

O	-3.50661600	-3.07377300	-0.53964700

Energy = -1225.9712 Hartree

Low Frequencies (cm^{-1}) : 43.1803 43.5881 84.6380 89.5439 100.6589 126.7613 130.1889 158.3597 159.5698 233.6949

Cation structures of 3

Atom	X	Y	Z
C	2.89515200	-2.03554200	-0.28427100
C	1.40275100	-2.00458900	-0.31890300
C	0.69994100	-3.19202600	-0.50433900
H	1.26119000	-4.11067800	-0.64042600
C	-0.69990300	-3.19203300	-0.50435200
H	-1.26114100	-4.11069000	-0.64044600
C	-1.40272900	-2.00460200	-0.31893400
C	-2.89513000	-2.03557000	-0.28433300
C	-3.57066400	-0.79104900	0.16687700
C	-4.92659100	-0.84396300	0.49046800
H	-5.45930900	-1.77533700	0.32991100
C	-5.56714500	0.27158800	1.03596700
H	-6.61948900	0.21983900	1.29599700
C	-4.83734000	1.43966600	1.28449500
H	-5.31569800	2.28891700	1.76172000
C	-3.49175000	1.51543500	0.93666300
H	-2.93486000	2.41087100	1.18386200
C	-2.83490100	0.41786000	0.32996300
C	-1.43549100	0.46256000	-0.06412800

C	-0.72170600	1.67218500	-0.38157100
C	-1.39582500	2.83982500	-0.81836000
H	-2.47317700	2.82608100	-0.91746900
C	-0.70101500	3.97378100	-1.21590300
H	-1.24659300	4.84212300	-1.57066300
C	0.70102100	3.97378900	-1.21587400
H	1.24660400	4.84213700	-1.57060900
C	1.39582600	2.83984000	-0.81830400
H	2.47318200	2.82610700	-0.91737000
C	0.72170200	1.67219100	-0.38154300
C	1.43548500	0.46257200	-0.06407900
C	2.83488200	0.41787700	0.33006100
C	3.49169800	1.51544700	0.93680500
H	2.93479200	2.41087500	1.18399600
C	4.83727600	1.43968300	1.28468900
H	5.31560900	2.28892900	1.76194600
C	5.56709900	0.27161500	1.03617000
H	6.61943300	0.21986900	1.29624300
C	4.92657500	-0.84393200	0.49062600
H	5.45930700	-1.77529800	0.33007300
C	3.57066100	-0.79102300	0.16698400
C	-0.71347700	-0.77148800	-0.19368200
C	0.71348500	-0.77148200	-0.19366300
O	3.51393900	-3.05663700	-0.55419600
O	-3.51389900	-3.05668300	-0.55423300

Energy = -1225.7170 Hartree

Low Frequncy (cm^{-1}) : 42.6143 44.2384 83.5530 88.9010 100.8011
123.6366 129.5080 154.6835 156.8496 228.0083

Anion structure of 3

Atom	X	Y	Z
C	2.87668300	-2.05070600	-0.25258500
C	1.41606300	-1.99269300	-0.29315100
C	0.69118200	-3.19082600	-0.44930800
H	1.25827500	-4.10984000	-0.55574100
C	-0.69115300	-3.19083100	-0.44933000
H	-1.25823700	-4.10984800	-0.55578000
C	-1.41604800	-1.99270200	-0.29319700
C	-2.87666800	-2.05072600	-0.25267800
C	-3.56205000	-0.80789700	0.15084200
C	-4.93397600	-0.87282300	0.46258700
H	-5.42916800	-1.82736500	0.31374100
C	-5.61015900	0.22698000	0.96700200
H	-6.66685300	0.16129600	1.21333900
C	-4.89675700	1.41827100	1.19791300
H	-5.39346200	2.27263000	1.65205300
C	-3.55196300	1.50806800	0.87036200
H	-3.01822500	2.42132400	1.10417900
C	-2.84666800	0.41773100	0.29306200
C	-1.43419000	0.48006400	-0.05829000
C	-0.72143400	1.70027000	-0.34930500
C	-1.38818800	2.88642100	-0.76909400

H	-2.46614200	2.87231800	-0.86734800
C	-0.70421000	4.02941600	-1.13829500
H	-1.25466700	4.90424500	-1.47521900
C	0.70422300	4.02942200	-1.13826100
H	1.25468900	4.90425600	-1.47515800
C	1.38819400	2.88643200	-0.76903000
H	2.46615300	2.87233800	-0.86723400
C	0.72143000	1.70027500	-0.34927500
C	1.43418100	0.48007300	-0.05823700
C	2.84664800	0.41774800	0.29316300
C	3.55191500	1.50809100	0.87048600
H	3.01816400	2.42134300	1.10428200
C	4.89669900	1.41830200	1.19808400
H	5.39338300	2.27266500	1.65224000
C	5.61011700	0.22701600	0.96719800
H	6.66680200	0.16133800	1.21357100
C	4.93395900	-0.87279100	0.46275700
H	5.42916200	-1.82733000	0.31392600
C	3.56204300	-0.80787400	0.15096500
C	-0.72416200	-0.74401000	-0.18808300
C	0.72416600	-0.74400600	-0.18805700
O	3.51446300	-3.10350100	-0.47655500
O	-3.51443400	-3.10352400	-0.47667300

Energy = -1226.0613 Hartree

Low Frequency (cm^{-1}) : 43.2624 46.5405 87.6697 91.1769 106.0796 128.3283 129.6204 164.7338 167.0499 235.0444

5. Complete reference of G09.

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