Electronic Supplementary Information

for

The Influence of External Electric Fields on Charge Reorganization Energy in Organic Semiconductors

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Computational details

We calculated the internal charge reorganization energy (λ) for the self-exchange hole-transfer process via the normal mode (NM) analysis. In the NM method, the molecule is forced to vibrate around its equilibrium position in the form of translation and rotational oscillations. The NM method calculates the λ based on the structural displacement corresponding to each vibration mode when the molecule goes from a neutral state to a positively charged (for hole transport) state

$$\lambda = \sum_i \lambda_i = \sum S_i \omega_i = \sum_i \frac{1}{2} \Delta Q_i^2 \omega_i^2$$

λ_i is the reorganization energy obtained in mode i of the frequency ω_i. S_i represents the Huang-Rhys factor measuring the charge-phonon coupling strength. ΔQ_i is the displacement along the normal mode coordinate between the equilibrium positions of charged and neutral states.

For comparison, we also calculated the λ for **$OT_{0\text{-}3}$** via the Nelsen's four-point method. It is described as the vertical ionization of a neutral molecule followed by geometric relaxation, and then vertical neutralization of a charged molecule followed by geometric relaxation

$$\lambda = \lambda_1 + \lambda_2 = E_+(Q_0) - E_+(Q_+) + E_0(Q_+) - E_0(Q_0)$$

where E is energy, Q is geometry, and the subscripts 0 and + denote neutral and cationic states, respectively.

All the quantum mechanical calculations were performed with Gaussian 09 package.[1] The equilibrium structures of the neutral and cationic species for molecules studied if not specified were optimized by DFT at the M06-2X/6-31+g(d) level.[2] To mimic external electric conditions, a built-in electric dipole field was applied to the molecule along each axial direction by invoking the 'field' keyword in the same package. Field strengths were referenced by molecular systems reported elsewhere.[3] NM analysis was made by DUSHIN program.[4] Mayer bond order analysis was performed using Multiwfn software.[5]

The ab initio molecular dynamics (AIMD) simulations were carried out using Vienna ab initio simulation package.[6] The spin polarized generalized gradient approximation method of Perdew,

Burke, and Ernzerhof (PBE)[7] was used to deal with the exchange-correlation functional with the projector-augmented wave method.[8] The vdW correction was employed for enhancing accuracy. The distance between the molecule and box edge was set more than 1 nm to remove the imaginary interactions. The k-point of 1×1×1 was used. In the AIMD simulations, the Nose-Hoover thermostat[9] was applied with a target temperature of 300 K and the cutoff energy was set to 400 eV. Trajectories ran with a time step of 0.5 fs. Total 2 ps trajectory for each system was collected for further analysis. The RMSD of mutual atomic coordinates was computed using Gromacs 5.1.[10] All of initial structures were derived at the M06-2X/6-31+g(d) level from the Gaussian 09 package.

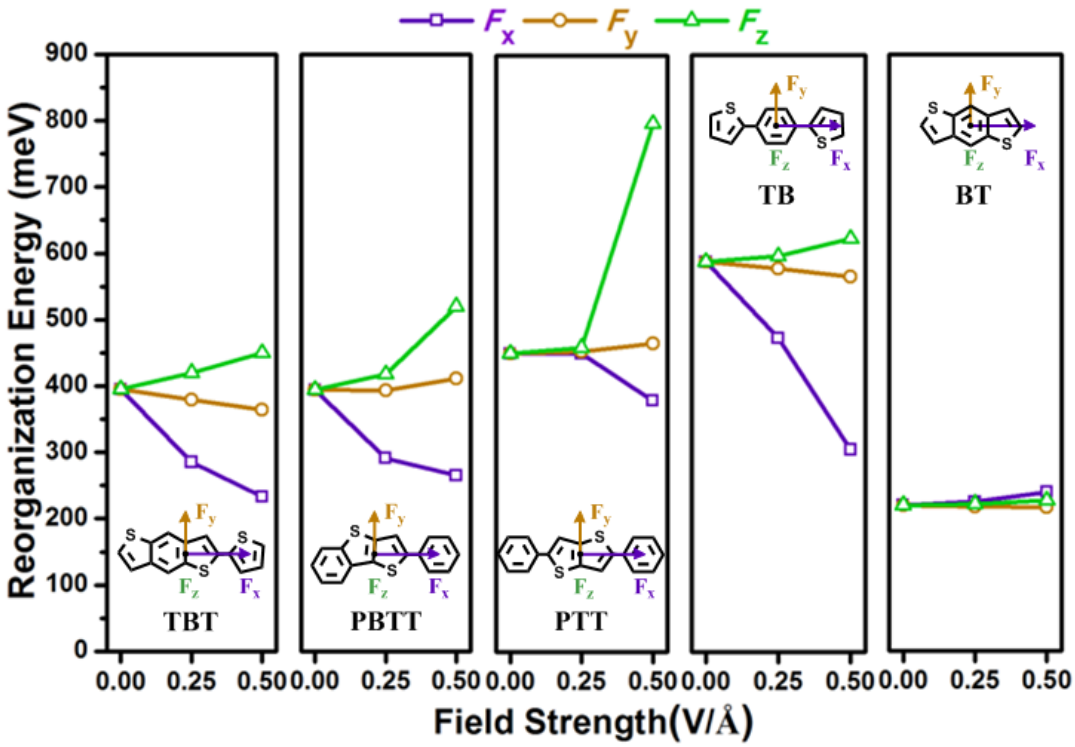

Fig.S1 λ change as a function of axial EEF for other tested linear compounds, computed via normal mode analyses at the M06-2X/6-31+g(d) level.

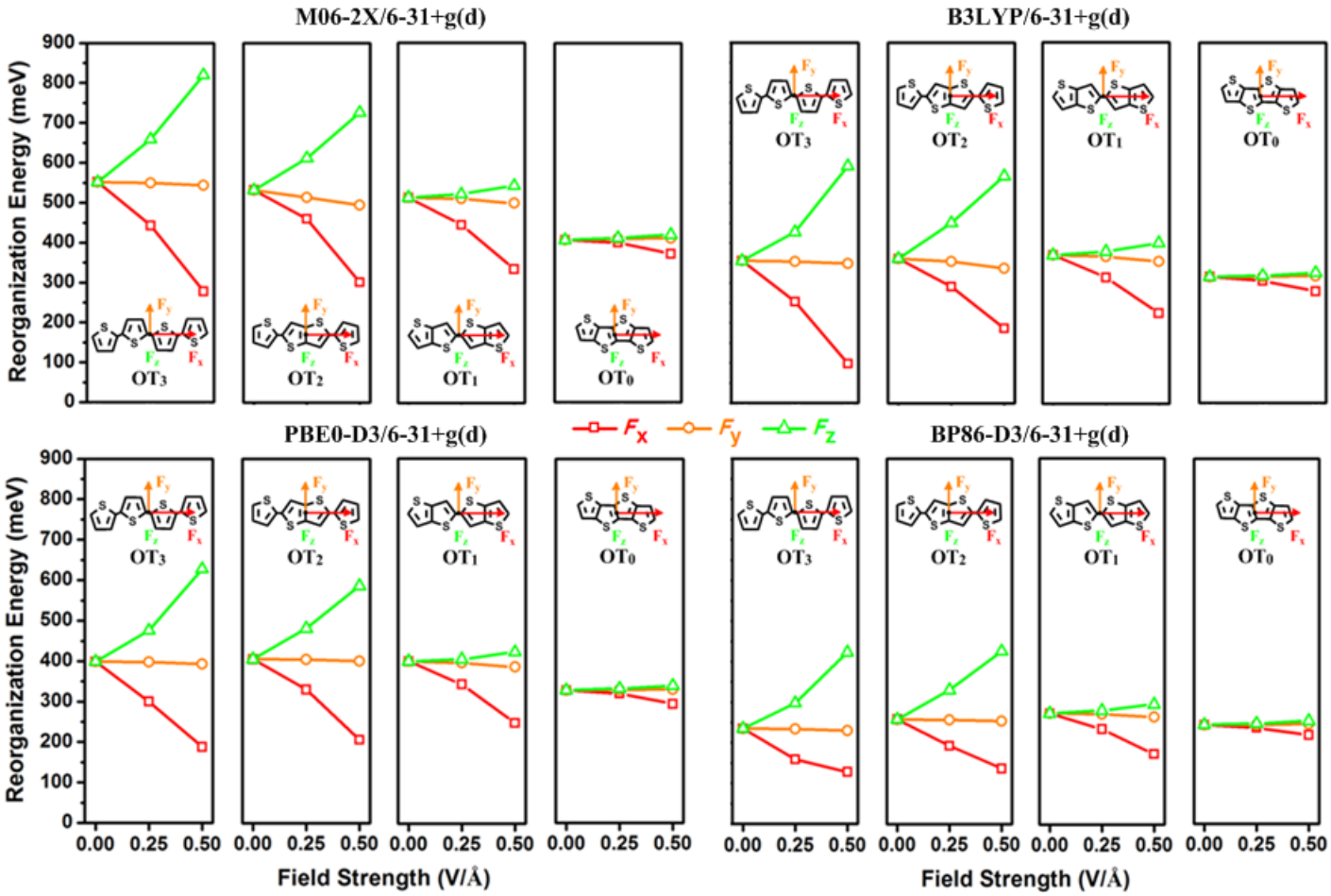

Fig.S2 λ change as a function of axial EEF for **$OT_{0\text{-}3}$** computed via Nelsen's four-point method using different DFT functionals.

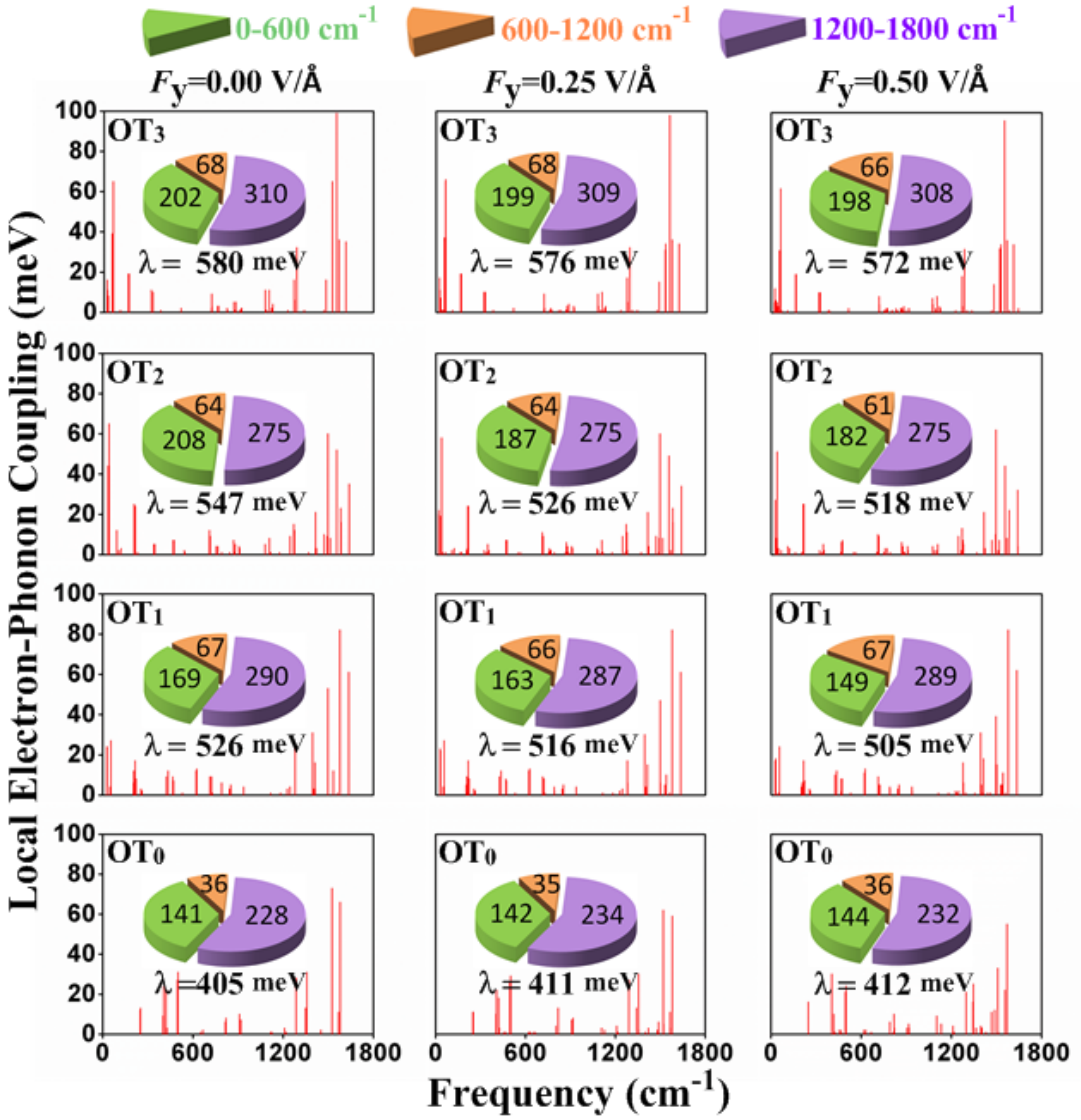

Fig.S3 Each vibrational mode contribution to λ for **OT$_{0\text{-}3}$** under F_y. Insets display the sorted contributions to λ in terms of low (0-600 cm^{-1}), medium (600-1200 cm^{-1}), high (1200-1800 cm^{-1}) frequency regions.

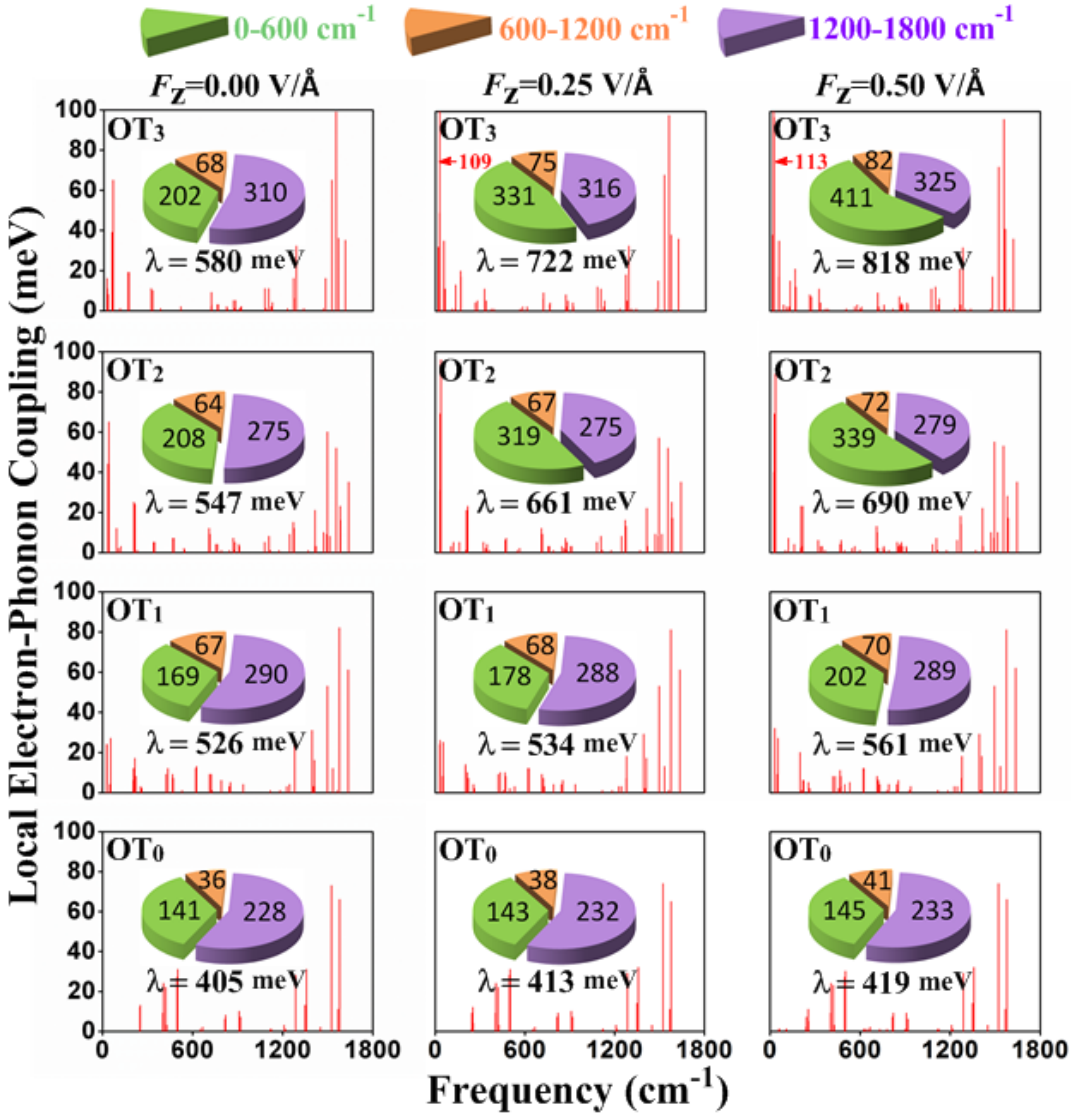

Fig.S4 Each vibrational mode contribution to λ for **$OT_{0\text{-}3}$** under F_z. Insets display the sorted contributions to λ in terms of low (0-600 cm^{-1}), medium (600-1200 cm^{-1}), high (1200-1800 cm^{-1}) frequency regions.

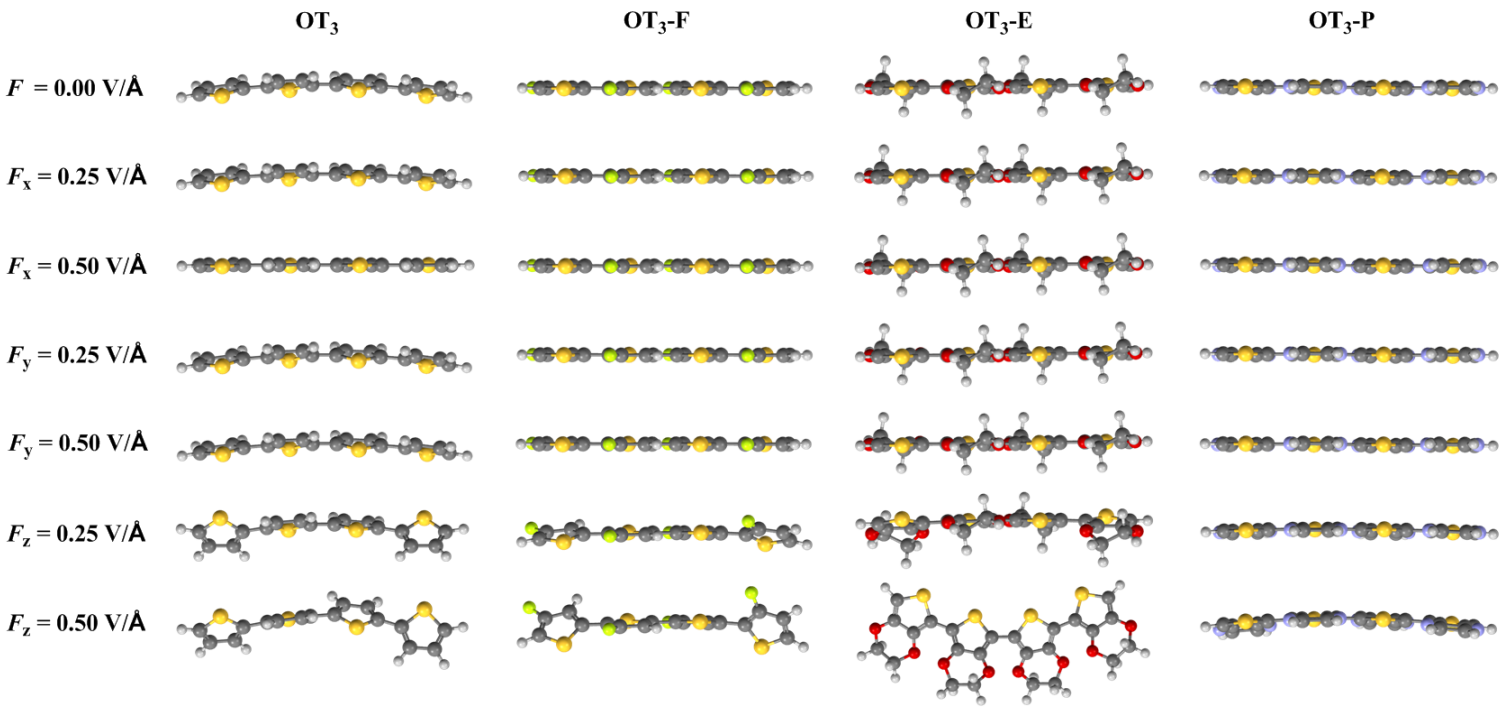

Fig.S5 Optimized neutral structures of **OT_3**, **OT_3-F**, **OT_3-E** and **OT_3-P** under axial EEF.

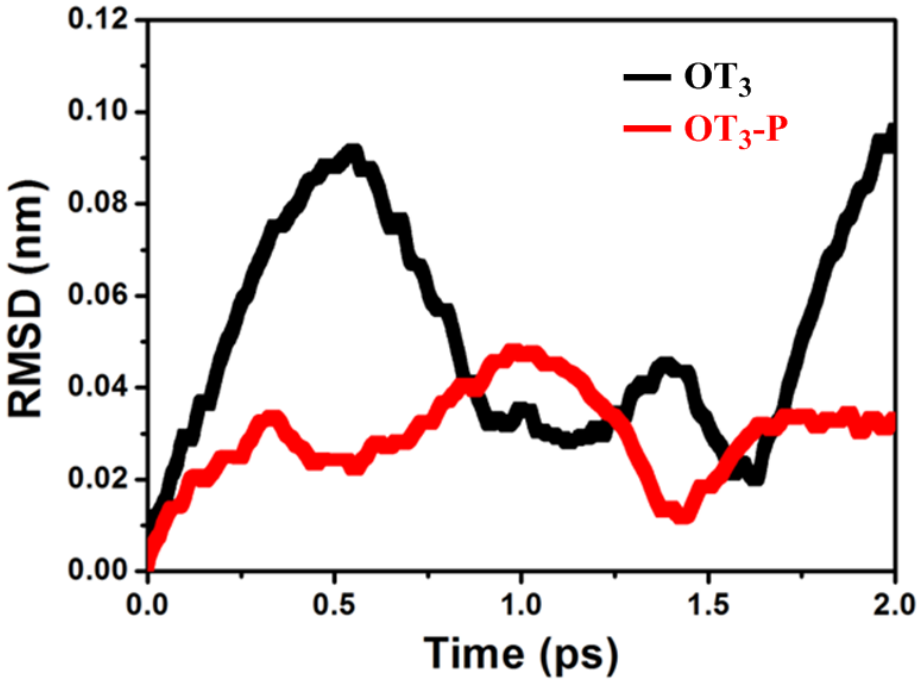

Fig.S6 RMSD of the mutual atomic coordinates for **OT_3** and **OT_3-P** during 2 ps *ab initio* molecular dynamics simulations at room temperature. (RMSD measures the similarity of the structure of a given snapshot with the reference of the M06-2X/6-31+g(d) optimised structure.)

Optimized molecular coordinates at M06-2X/6-31+g(d)

(1) OT_3 (F = 0.00 V/Å)

Neutral			
elements	x	y	z
C	-4.59718400	0.09712200	0.01264100
C	-5.18732600	1.32235100	0.20368200
C	-6.59956400	1.29511300	0.01407800
C	-7.05944200	0.05216500	-0.31514600
S	-5.78083300	-1.09757900	-0.41650200
H	-4.62971400	2.20646000	0.49374800
H	-7.24283200	2.15968400	0.12702200
H	-8.07822300	-0.25459700	-0.50872600
C	-3.19235500	-0.26042000	0.12703400
C	-2.63743300	-1.48820700	0.39124200
S	-1.95837400	0.94283500	-0.08534900
C	-1.21831800	-1.45862500	0.44895800
H	-3.23240600	-2.37728700	0.57053100
C	-0.69567600	-0.20766000	0.22901700
H	-0.60335500	-2.32236200	0.67799900
C	0.69567600	0.20765900	0.22901700
C	1.21831800	1.45862500	0.44895800
S	1.95837400	-0.94283500	-0.08535000
C	2.63743300	1.48820700	0.39124100
H	0.60335500	2.32236200	0.67799800
C	3.19235500	0.26042000	0.12703400
H	3.23240500	2.37728700	0.57053000
C	4.59718400	-0.09712200	0.01264100
C	5.18732600	-1.32235100	0.20368300
S	5.78083300	1.09757900	-0.41650100
C	6.59956400	-1.29511300	0.01407800
H	4.62971400	-2.20646000	0.49374800
C	7.05944200	-0.05216500	-0.31514600
H	7.24283200	-2.15968400	0.12702200
H	8.07822300	0.25459700	-0.50872600

Cationic			
elements	x	y	z
C	-4.56126800	0.09561100	0.13128600
C	-5.14346900	1.35792100	0.13146200
C	-6.55089600	1.31171000	0.13131300
C	-7.02874700	0.02048600	0.13111700
S	-5.78144700	-1.14680900	0.13102500
H	-4.56911800	2.27862700	0.13167900
H	-7.19207000	2.18416500	0.13138600
H	-8.06247900	-0.30061200	0.13097600
C	-3.17432300	-0.23298600	0.13133000
C	-2.59689200	-1.51472900	0.13145300
S	-1.95614100	1.00061000	0.13126200
C	-1.21276300	-1.49017600	0.13144900
H	-3.18848800	-2.42341700	0.13154600
C	-0.67767300	-0.18775600	0.13139600
H	-0.59173700	-2.37971100	0.13154800
C	0.67767300	0.18775600	0.13139600
C	1.21276300	1.49017600	0.13144900
S	1.95614100	-1.00061000	0.13126200
C	2.59689200	1.51472900	0.13145300
H	0.59173700	2.37971100	0.13154800
C	3.17432300	0.23298600	0.13133000
H	3.18848800	2.42341700	0.13154500
C	4.56126800	-0.09561100	0.13128600
C	5.14346900	-1.35792100	0.13146200
S	5.78144700	1.14680900	0.13102500
C	6.55089600	-1.31171000	0.13131300
H	4.56911800	-2.27862700	0.13167900
C	7.02874700	-0.02048600	0.13111700
H	7.19207000	-2.18416500	0.13138600
H	8.06247900	0.30061200	0.13097600

(2) OT_3 (F_x = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.60003800	0.09722700	0.02555300	C	-4.56504500	0.08504500	0.11792800
C	-5.18997500	1.32276700	0.22826700	C	-5.16045900	1.36233600	0.17167700
C	-6.60390600	1.28893300	0.07388800	C	-6.54991800	1.31207500	0.17113800
C	-7.06368100	0.04094800	-0.24125400	C	-7.02643900	0.00255700	0.11723200
S	-5.78813400	-1.10483200	-0.36615000	S	-5.79219700	-1.16351400	0.06764200
H	-4.63260900	2.21191800	0.50458500	H	-4.58567000	2.28208000	0.20926600
H	-7.25234700	2.14725900	0.20006400	H	-7.20395300	2.17468600	0.20751100
H	-8.08571500	-0.27094000	-0.41100300	H	-8.06431200	-0.31254300	0.10525600
C	-3.19473800	-0.25418900	0.11632200	C	-3.19477500	-0.22894200	0.10307300
C	-2.62984200	-1.48981700	0.33708000	C	-2.60282200	-1.51205600	0.04734000
S	-1.96761700	0.95964300	-0.07508100	S	-1.96703300	1.01038400	0.15444700
C	-1.21362800	-1.45580200	0.37531500	C	-1.22105600	-1.47699500	0.04802100
H	-3.22145700	-2.38419900	0.49704400	H	-3.18802000	-2.42457000	0.00895000
C	-0.69540800	-0.19625500	0.18472800	C	-0.69728700	-0.17240500	0.10423100
H	-0.59628700	-2.32667400	0.57175100	H	-0.59332300	-2.36066800	0.01135300
C	0.69225700	0.21740400	0.18759000	C	0.67472600	0.21062500	0.11955400
C	1.21829400	1.47833800	0.35644200	C	1.20728700	1.49233300	0.19828700
S	1.95971300	-0.94740100	-0.06005100	S	1.94779200	-0.97779900	0.02893100
C	2.63595100	1.50241700	0.31316900	C	2.61059700	1.50872400	0.19779600
H	0.60081100	2.35147200	0.53534500	H	0.59510000	2.38553100	0.26476400
C	3.19544200	0.26421400	0.11035100	C	3.16906400	0.24339900	0.11725800
H	3.22640000	2.40161300	0.45814400	H	3.20445800	2.41293900	0.27187800
C	4.59876400	-0.09761700	0.03591300	C	4.57455400	-0.10849300	0.09893400
C	5.18013700	-1.33182700	0.20445700	C	5.15376200	-1.33986700	0.30594600
S	5.80765900	1.10220800	-0.31810500	S	5.78400100	1.09990400	-0.20838800
C	6.59814100	-1.30781500	0.06094000	C	6.57250600	-1.30545400	0.22174500
H	4.60652200	-2.22071200	0.44296800	H	4.58269200	-2.23479700	0.52876200
C	7.08017400	-0.05953700	-0.21191100	C	7.04925800	-0.05193900	-0.04632900
H	7.22817100	-2.18411100	0.16545200	H	7.20799500	-2.17200100	0.35953500
H	8.10694300	0.24536400	-0.36135700	H	8.07851500	0.25942300	-0.16328400

(3) OT_3 (F_x = 0.5 V/Å)

Neutral			
elements	x	y	z
C	-4.60193300	0.09802900	0.12035400
C	-5.18768100	1.35092700	0.15779800
C	-6.60100200	1.30189600	0.14277200
C	-7.07533900	0.01461900	0.09467900
S	-5.81658900	-1.14524600	0.06620200
H	-4.62015000	2.27555000	0.19962600
H	-7.24897400	2.16935100	0.16767800
H	-8.10802600	-0.31258300	0.07351200
C	-3.20344200	-0.23802900	0.12743400
C	-2.62302400	-1.50125000	0.14937400
S	-1.97715100	0.99381700	0.10470900
C	-1.22050500	-1.46839600	0.15073800
H	-3.21121600	-2.41155800	0.16843800
C	-0.69187800	-0.18775800	0.13067400
H	-0.60429800	-2.36256100	0.17044000
C	0.68236900	0.20927200	0.13020900
C	1.21811700	1.49208400	0.13198600
S	1.96579900	-0.97585100	0.12498000
C	2.62474900	1.51128500	0.13078600
H	0.59718000	2.38055700	0.13582700
C	3.20445700	0.25727500	0.12796300
H	3.20562800	2.42955500	0.13312100
C	4.59807000	-0.09567600	0.12697400
C	5.17971700	-1.35017800	0.12499800
S	5.84278100	1.13491000	0.12768600
C	6.60167200	-1.31602700	0.12418800
H	4.59219200	-2.26134400	0.12416700
C	7.11192100	-0.04736200	0.12546000
H	7.21855200	-2.20964300	0.12261800
H	8.14800200	0.26433200	0.12506700

Cationic			
elements	x	y	z
C	-4.58538700	0.08554700	0.10296800
C	-5.18433800	1.37215400	0.14113700
C	-6.56429500	1.32280600	0.13729700
C	-7.04609000	-0.00302900	0.09626600
S	-5.81713700	-1.17002000	0.06273100
H	-4.60904800	2.29186100	0.17049600
H	-7.22700200	2.18081000	0.16232700
H	-8.08866300	-0.31249200	0.08540600
C	-3.21189900	-0.22977300	0.09632700
C	-2.62194100	-1.50728700	0.05996400
S	-1.97665200	1.00857300	0.13419600
C	-1.23013400	-1.47049000	0.06704100
H	-3.20301700	-2.42308400	0.03305600
C	-0.71296800	-0.17503500	0.10879700
H	-0.60617000	-2.35760300	0.04984500
C	0.67879600	0.21400300	0.13191200
C	1.21333400	1.47999500	0.26792600
S	1.94547600	-0.97242600	-0.02305800
C	2.62694200	1.49107100	0.26177800
H	0.60627400	2.37113100	0.38417000
C	3.17963200	0.23761900	0.11920200
H	3.22098700	2.39104600	0.38228600
C	4.58990200	-0.11783000	0.08382200
C	5.18613900	-1.33199200	0.33066700
S	5.78779100	1.08052100	-0.31238500
C	6.60587900	-1.29294100	0.21198900
H	4.62488900	-2.21710300	0.60870600
C	7.07331900	-0.05260200	-0.12040000
H	7.24668100	-2.15248400	0.37592000
H	8.09869700	0.25905100	-0.26993300

(4) OT_3 (F_y = 0.25 V/Å)

Neutral			
elements	x	y	z
C	-4.59735500	0.09824300	0.01223800
C	-5.20089100	1.32023500	0.19136300
C	-6.61243500	1.27309500	0.00408800
C	-7.05643900	0.01944000	-0.31170100
S	-5.76580400	-1.11348300	-0.40195500
H	-4.65071700	2.21136100	0.47490100
H	-7.26938800	2.12840400	0.11246000
H	-8.07110300	-0.30638700	-0.49607200
C	-3.18971100	-0.24618300	0.13219000
C	-2.62759900	-1.46961100	0.39642700
S	-1.96074100	0.96620300	-0.07817900
C	-1.20842200	-1.43274300	0.45421500
H	-3.21391600	-2.36513600	0.57230400
C	-0.69105000	-0.18059600	0.23448800
H	-0.59269700	-2.29685200	0.67987400
C	0.70012400	0.23537800	0.22976800
C	1.22778500	1.48475700	0.45321700
S	1.95637900	-0.91760800	-0.09066300
C	2.64704900	1.50767600	0.39533000
H	0.61361300	2.34755100	0.68882600
C	3.19544500	0.27654800	0.12715900
H	3.24974300	2.39065100	0.58035100
C	4.59713600	-0.09387300	0.01614700
C	5.16986000	-1.32922100	0.18550100
S	5.80199800	1.09375600	-0.38385600
C	6.58385800	-1.32013800	0.00207900
H	4.60146700	-2.21395200	0.45192500
C	7.06456700	-0.07978100	-0.30037600
H	7.21030900	-2.19896400	0.09685100
H	8.08893600	0.21123100	-0.48844400

Cationic			
elements	x	y	z
C	-4.56333100	0.09559000	0.13147000
C	-5.13864900	1.36182200	0.13110300
C	-6.54533400	1.32075300	0.13115500
C	-7.02794100	0.02948600	0.13132800
S	-5.78743500	-1.14048900	0.13205300
H	-4.55734000	2.27824900	0.13084600
H	-7.18496700	2.19445800	0.13092900
H	-8.06231200	-0.28995900	0.13133900
C	-3.17707800	-0.23865900	0.13150300
C	-2.60154300	-1.51983700	0.13219100
S	-1.95555000	0.99485600	0.13075100
C	-1.21645800	-1.49765400	0.13218500
H	-3.19144800	-2.42999300	0.13278400
C	-0.67813200	-0.19717300	0.13130000
H	-0.60016500	-2.39078800	0.13275800
C	0.67720000	0.17875900	0.13097200
C	1.20872700	1.48330000	0.13032300
S	1.95707800	-1.00602200	0.13142300
C	2.59226400	1.51053000	0.13024500
H	0.58313800	2.36959900	0.12998800
C	3.17180200	0.22835800	0.13092400
H	3.18508300	2.41834800	0.12981900
C	4.55947000	-0.09512400	0.13118100
C	5.14795100	-1.35380600	0.13185700
S	5.77622800	1.15363500	0.13023800
C	6.55646900	-1.30298900	0.13197300
H	4.58046000	-2.27893500	0.13239500
C	7.02998500	-0.01203100	0.13141200
H	7.19868400	-2.17490500	0.13258600
H	8.06314600	0.31062200	0.13142400

(5) OT_3 (F_y = 0.50 V/Å)

Neutral			
elements	x	y	z
C	-4.59812000	0.09758000	0.01641900
C	-5.21102900	1.32052300	0.16614200
C	-6.62280200	1.25483800	-0.01222600
C	-7.05546800	-0.01275300	-0.29191300
S	-5.75666800	-1.13414200	-0.35812100
H	-4.66510100	2.22227900	0.42505200
H	-7.29013700	2.10490000	0.07920800
H	-8.06704800	-0.35746900	-0.45903000
C	-3.18785000	-0.23469600	0.13919400
C	-2.61758600	-1.45498300	0.39621800
S	-1.96441200	0.98891700	-0.06278400
C	-1.19809500	-1.41047600	0.45302800
H	-3.19414500	-2.35876000	0.56379600
C	-0.68665800	-0.15562100	0.24012100
H	-0.58122900	-2.27633400	0.66996100
C	0.70396200	0.26221700	0.23173400
C	1.23602700	1.51009000	0.46005700
S	1.95470400	-0.89257400	-0.09527400
C	2.65580400	1.52715500	0.40231700
H	0.62256200	2.37177800	0.70351900
C	3.19839900	0.29322000	0.12900900
H	3.26533900	2.40449700	0.59448000
C	4.59685900	-0.08979100	0.02074700
C	5.15183700	-1.33568700	0.16186000
S	5.82353600	1.09223000	-0.34112600
C	6.56782800	-1.34400600	-0.01307700
H	4.57253700	-2.22195000	0.39927400
C	7.06963300	-0.10535600	-0.28037000
H	7.17749900	-2.23676800	0.06047200
H	8.09982100	0.17114100	-0.45823000

Cationic			
elements	x	y	z
C	-4.56562300	0.09518000	0.13184000
C	-5.13348500	1.36565500	0.13038100
C	-6.53974600	1.33042600	0.13056900
C	-7.02764400	0.03932700	0.13212700
S	-5.79439600	-1.13433300	0.13332500
H	-4.54496200	2.27785100	0.12921100
H	-7.17736500	2.20606800	0.12957600
H	-8.06279700	-0.27814100	0.13256000
C	-3.18002800	-0.24525200	0.13206500
C	-2.60638800	-1.52598500	0.13328800
S	-1.95518600	0.98853200	0.13057200
C	-1.22006900	-1.50607400	0.13313600
H	-3.19451000	-2.43795700	0.13429900
C	-0.67862100	-0.20732200	0.13172300
H	-0.60845600	-2.40303000	0.13401900
C	0.67666600	0.16961600	0.13114800
C	1.20427700	1.47656000	0.12980300
S	1.95837900	-1.01148700	0.13200000
C	2.58746600	1.50684900	0.12961300
H	0.57392900	2.35972800	0.12907400
C	3.16937800	0.22426000	0.13075700
H	3.18122000	2.41426700	0.12872700
C	4.55789100	-0.09421700	0.13091500
C	5.15252600	-1.34940600	0.13235800
S	5.77158700	1.16109600	0.12915400
C	6.56243700	-1.29420300	0.13197400
H	4.59190500	-2.27918900	0.13364600
C	7.03172300	-0.00353100	0.13023700
H	7.20555000	-2.16601900	0.13285900
H	8.06434100	0.32072700	0.12950400

(6) OT_3 (F_z = 0.25 V/Å)

Neutral			
elements	x	y	z
C	-4.58332700	0.12395600	0.15092600
C	-5.09363100	1.10596000	-0.66049800
C	-6.51902100	1.13823300	-0.66736600
C	-7.06858300	0.18261000	0.13756300
S	-5.86077500	-0.76238400	0.92590400
H	-4.46927700	1.75348400	-1.26675100
H	-7.10499500	1.82463500	-1.26681700
H	-8.11629000	-0.03286600	0.29700400
C	-3.19066500	-0.23296300	0.37387100
C	-2.65526800	-1.46627000	0.65184100
S	-1.94487300	0.96984800	0.25238600
C	-1.23905600	-1.44572400	0.76679500
H	-3.25866700	-2.36419200	0.72948400
C	-0.69919000	-0.19764800	0.57344200
H	-0.63554900	-2.32359600	0.97228100
C	0.69920000	0.19763100	0.57348900
C	1.23905800	1.44570600	0.76687100
S	1.94490500	-0.96989200	0.25262200
C	2.65527100	1.46625800	0.65193300
H	0.63554200	2.32358200	0.97231000
C	3.19067400	0.23295900	0.37393800
H	3.25866100	2.36418900	0.72954300
C	4.58333100	-0.12393400	0.15092200
C	5.09361600	-1.10594300	-0.66050900
S	5.86080300	0.76250800	0.92574400
C	6.51900500	-1.13822100	-0.66740900
H	4.46924500	-1.75349400	-1.26671600
C	7.06859000	-0.18261400	0.13752400
H	7.10496400	-1.82465200	-1.26684200
H	8.11630200	0.03283400	0.29697100

Cationic			
elements	x	y	z
C	-4.56054000	0.09059800	0.16230200
C	-5.14220200	1.35228000	0.10981900
C	-6.54779800	1.30481900	0.04104300
C	-7.02508100	0.01319900	0.04061600
S	-5.77920700	-1.15284500	0.12140400
H	-4.56770200	2.27287100	0.10048300
H	-7.18724500	2.17596400	-0.02616700
H	-8.05652600	-0.30903900	-0.02393100
C	-3.17418900	-0.23686300	0.20371200
C	-2.59479300	-1.51768700	0.19368100
S	-1.95760200	0.99805800	0.24687200
C	-1.21077700	-1.49146400	0.21632200
H	-3.18422500	-2.42666100	0.14782900
C	-0.67742000	-0.18873000	0.24522800
H	-0.58866400	-2.37990200	0.19107200
C	0.67742000	0.18873000	0.24522700
C	1.21077700	1.49146300	0.21632100
S	1.95760200	-0.99805900	0.24686700
C	2.59479300	1.51768700	0.19367900
H	0.58866400	2.37990100	0.19107400
C	3.17418900	0.23686300	0.20370600
H	3.18422500	2.42666100	0.14782800
C	4.56054000	-0.09059800	0.16229400
C	5.14220200	-1.35228000	0.10981200
S	5.77920700	1.15284600	0.12140500
C	6.54779800	-1.30481900	0.04103000
H	4.56770300	-2.27287100	0.10047600
C	7.02508000	-0.01319800	0.04059500
H	7.18724500	-2.17596400	-0.02618600
H	8.05652500	0.30904000	-0.02395900

(7) OT_3 (F_z = 0.50 V/Å)

Neutral			
elements	x	y	z
C	-4.55108800	0.13849200	0.14378900
C	-4.98307600	0.96724800	-0.85954200
C	-6.40467000	1.01451800	-0.97210100
C	-7.02972700	0.22501700	-0.05206300
S	-5.89869300	-0.58398100	0.97230300
H	-4.30618500	1.48081900	-1.53409200
H	-6.93060300	1.58213200	-1.73060700
H	-8.09044900	0.04521600	0.05855200
C	-3.18206200	-0.20811700	0.49828000
C	-2.67921200	-1.42604900	0.88570200
S	-1.91587500	0.96995700	0.36216100
C	-1.26922600	-1.41277200	1.06872300
H	-3.29788400	-2.31301100	0.96867900
C	-0.70372400	-0.18551400	0.82148200
H	-0.68335500	-2.28534200	1.33884000
C	0.70373400	0.18550600	0.82151200
C	1.26922800	1.41276400	1.06876700
S	1.91590700	-0.96999100	0.36231600
C	2.67921500	1.42604800	0.88575100
H	0.68335000	2.28533900	1.33885200
C	3.18207000	0.20812100	0.49832100
H	3.29787800	2.31301900	0.96870200
C	4.55109000	-0.13846700	0.14378500
C	4.98306100	-0.96721400	-0.85956000
S	5.89870900	0.58409800	0.97219800
C	6.40465600	-1.01451400	-0.97211800
H	4.30616000	-1.48079300	-1.53409200
C	7.02973200	-0.22505800	-0.05205700
H	6.93057700	-1.58216000	-1.73060900
H	8.09046000	-0.04531000	0.05858200

Cationic			
elements	x	y	z
C	-4.55622900	0.08145700	0.19156200
C	-5.13329700	1.34217500	0.07934500
C	-6.53058200	1.29255600	-0.08395400
C	-7.00708500	0.00005100	-0.09703000
S	-5.76976100	-1.16367900	0.08404600
H	-4.55732400	2.26196700	0.07417300
H	-7.16189900	2.16049100	-0.22760900
H	-8.02943100	-0.32435700	-0.24508000
C	-3.17325100	-0.24397400	0.29466700
C	-2.58972400	-1.52311500	0.28297600
S	-1.96074100	0.99291200	0.39356300
C	-1.20648400	-1.49377000	0.34045800
H	-3.17390900	-2.43166800	0.18717400
C	-0.67703200	-0.19066500	0.40039100
H	-0.58113100	-2.37923200	0.29554900
C	0.67703200	0.19066500	0.40039000
C	1.20648400	1.49377000	0.34045600
S	1.96074100	-0.99291200	0.39356400
C	2.58972400	1.52311500	0.28297400
H	0.58113100	2.37923200	0.29554700
C	3.17325100	0.24397400	0.29466600
H	3.17390900	2.43166800	0.18717000
C	4.55622900	-0.08145700	0.19156100
C	5.13329600	-1.34217500	0.07934200
S	5.76976100	1.16367900	0.08404100
C	6.53058200	-1.29255600	-0.08395400
H	4.55732400	-2.26196700	0.07416900
C	7.00708500	-0.00005100	-0.09702500
H	7.16189900	-2.16049200	-0.22760800
H	8.02943200	0.32435700	-0.24507100

(8) OT_2 (F = 0.00 V/Å)

Neutral			
elements	x	y	z
C	2.29467600	-0.09391100	-0.03175200
C	1.49706600	0.99793100	-0.26275100
C	0.11868500	0.66566600	-0.15276000
C	-0.11865800	-0.66559700	0.15291700
C	-2.29467100	0.09395600	0.03169700
C	-1.49705500	-0.99785900	0.26281400
H	1.88659700	1.97547600	-0.52301800
H	-1.88657900	-1.97541400	0.52306300
S	-1.36788500	1.53467000	-0.33599400
S	1.36786300	-1.53462000	0.33601400
C	3.74742200	-0.16413200	-0.05990200
C	4.54516100	-1.25074600	-0.32152100
S	4.70851200	1.24380200	0.26563100
C	5.93606200	-0.94362300	-0.27194400
H	4.14641400	-2.22955100	-0.56556900
C	6.17214700	0.36844700	0.02413700
H	7.12455800	0.87185300	0.11914000
H	6.72281900	-1.66508500	-0.45771200
C	-3.74741300	0.16414900	0.05971000
C	-4.54520800	1.25108700	0.31983000
S	-4.70847100	-1.24418800	-0.26420000
C	-5.93609800	0.94388600	0.27050900
H	-4.14651700	2.23020600	0.56271600
C	-6.17214400	-0.36852700	-0.02407500
H	-6.72288100	1.66559200	0.45524100
H	-7.12453800	-0.87207200	-0.11853500

Cationic			
elements	x	y	z
C	2.28184900	-0.11709100	-0.06494700
C	1.47095400	1.03121900	-0.00248800
C	0.12691900	0.69964500	0.02140600
C	-0.12693000	-0.69953600	-0.02189600
C	-2.28185900	0.11719900	0.06445900
C	-1.47096400	-1.03111100	0.00199900
H	1.87160800	2.03822700	0.02206100
H	-1.87161800	-2.03811800	-0.02255100
S	-1.34931300	1.60379800	0.09190000
S	1.34930200	-1.60368900	-0.09238900
C	3.70073300	-0.15951900	-0.10500100
C	4.52040600	-1.28539900	-0.17275700
S	4.65674500	1.29776200	-0.07231600
C	5.88800100	-0.96477100	-0.19723300
H	4.13676100	-2.30000700	-0.20361900
C	6.10443400	0.39659700	-0.14808500
H	7.05635800	0.91237800	-0.15312700
H	6.68760500	-1.69290800	-0.24880800
C	-3.70074300	0.15962700	0.10451300
C	-4.52041700	1.28550600	0.17227800
S	-4.65675500	-1.29765500	0.07182000
C	-5.88801100	0.96487700	0.19675400
H	-4.13677200	2.30011400	0.20314800
C	-6.10444400	-0.39649100	0.14759600
H	-6.68761500	1.69301400	0.24833500
H	-7.05636800	-0.91227200	0.15263400

(9) OT_2 (F_x = 0.25 V/Å)

Neutral			
elements	x	y	z
C	2.29545500	-0.09344100	-0.02224700
C	1.49516300	1.00599600	-0.21497600
C	0.11818100	0.67493700	-0.12039800
C	-0.12100900	-0.66746100	0.13979300
C	-2.29655100	0.09423800	0.04370600
C	-1.49691500	-1.00600000	0.23987300
H	1.88222800	1.99406500	-0.43958700
H	-1.88836500	-1.99089000	0.46536200
S	-1.36999900	1.54750100	-0.27679700
S	1.36444000	-1.54566900	0.29050300
C	3.74530600	-0.16388300	-0.06250000
C	4.54545900	-1.25647300	-0.29841400
S	4.71332800	1.25314900	0.21626400
C	5.93678100	-0.94781900	-0.26833600
H	4.14271900	-2.24075500	-0.51060500
C	6.17902500	0.37212000	-0.01345600
H	7.13217500	0.87866400	0.05349400
H	6.71946100	-1.67799600	-0.44189200
C	-3.74705800	0.16190300	0.06411000
C	-4.54598100	1.25511300	0.30201800
S	-4.70571400	-1.25389000	-0.23038000
C	-5.93456500	0.94700900	0.25526200
H	-4.15274100	2.24133900	0.52609500
C	-6.16664500	-0.37199500	-0.01586700
H	-6.72521700	1.66841300	0.42131000
H	-7.11909700	-0.87678000	-0.10864800

Cationic			
elements	x	y	z
C	2.27195300	-0.11538900	-0.04573600
C	1.47243800	1.02122300	-0.00424300
C	0.11405300	0.68824300	0.02681000
C	-0.13471400	-0.70620100	0.00860800
C	-2.29649400	0.10994800	0.07516600
C	-1.47778700	-1.04173400	0.03582300
H	1.86793000	2.03043300	-0.00441900
H	-1.87623300	-2.05027800	0.02782800
S	-1.35252300	1.59687800	0.07680500
S	1.35019400	-1.60395000	-0.04162100
C	3.71237400	-0.16468000	-0.09049200
C	4.52328900	-1.27465500	-0.21965500
S	4.66387400	1.28604700	0.01571800
C	5.90351900	-0.95119900	-0.23373300
H	4.13984100	-2.28563000	-0.30808500
C	6.12407500	0.39578500	-0.11566600
H	7.07266100	0.91553400	-0.09731100
H	6.69692000	-1.68240700	-0.32943100
C	-3.70151400	0.15134900	0.10904900
C	-4.52859800	1.29378500	0.14745500
S	-4.66960800	-1.30834500	0.10657600
C	-5.88294200	0.98128200	0.17312300
H	-4.13963600	2.30694600	0.15551900
C	-6.10306800	-0.39553400	0.15448400
H	-6.68781100	1.70558500	0.20371800
H	-7.06232900	-0.90164200	0.16740000

(10) OT_2 (F_x = 0.50 V/Å)

Neutral			
elements	x	y	z
C	2.29923500	-0.09555800	-0.02977100
C	1.48940500	1.02186400	-0.08837500
C	0.11982400	0.69153000	-0.03470200
C	-0.12733900	-0.67820200	0.06442000
C	-2.30263200	0.09654400	0.06059300
C	-1.49500200	-1.02484100	0.12321200
H	1.87381400	2.03273900	-0.18269200
H	-1.88815700	-2.02990700	0.21708300
S	-1.37020600	1.57911800	-0.07684300
S	1.35671500	-1.57397100	0.09962900
C	3.73858400	-0.16216100	-0.07879500
C	4.55010700	-1.26868400	-0.23710100
S	4.71600600	1.27648700	0.07897200
C	5.93822900	-0.95552100	-0.24084900
H	4.14916200	-2.26802800	-0.36373000
C	6.18807500	0.38051800	-0.08950200
H	7.14153800	0.89144200	-0.07209100
H	6.71823700	-1.70085800	-0.36461400
C	-3.74348200	0.15744400	0.08517900
C	-4.54956000	1.27016600	0.22438800
S	-4.70463400	-1.28286900	-0.06256800
C	-5.93186800	0.95882100	0.21380200
H	-4.16464400	2.27831900	0.34315600
C	-6.16015500	-0.38439500	0.06821400
H	-6.72744400	1.68731600	0.31180600
H	-7.11394200	-0.89591900	0.02486400

Cationic			
elements	x	y	z
C	2.27351900	-0.12066500	-0.00799600
C	1.47835100	1.00538900	-0.05160700
C	0.10639100	0.67141000	0.00755400
C	-0.13500400	-0.71121800	0.09206900
C	-2.30521600	0.09391300	0.09212600
C	-1.48798000	-1.05071500	0.14115200
H	1.86880100	2.01251900	-0.14540600
H	-1.88091000	-2.05941200	0.20708100
S	-1.35872300	1.57749600	-0.01569500
S	1.35425700	-1.60526600	0.11660000
C	3.72602200	-0.17521600	-0.05530000
C	4.53390600	-1.23955300	-0.38463700
S	4.68120700	1.22377000	0.33272100
C	5.92075300	-0.92192800	-0.33340400
H	4.14370400	-2.20873500	-0.67518400
C	6.14878500	0.37584300	0.03241200
H	7.09841800	0.88201000	0.14538500
H	6.70996100	-1.62773400	-0.56787000
C	-3.71448900	0.14212800	0.11858100
C	-4.53899300	1.29663400	0.06649200
S	-4.69420300	-1.31374400	0.22735000
C	-5.88700200	0.99863100	0.11343000
H	-4.14339900	2.30488300	-0.00360700
C	-6.11809000	-0.38935600	0.20242700
H	-6.69427500	1.72254500	0.08635800
H	-7.08592300	-0.88223400	0.25265000

(11) OT_2 (F_y = 0.25 V/Å)

Neutral			
elements	x	y	z
C	-2.29616800	0.09912100	-0.06425400
C	-1.49356200	-1.01136800	-0.07320500
C	-0.11507600	-0.65884600	-0.05830100
C	0.12161700	0.70704000	-0.04582500
C	2.29500200	-0.06698700	-0.08296300
C	1.49984500	1.05300000	-0.06396200
H	-1.87697100	-2.02478600	-0.11314400
H	1.89368600	2.06283500	-0.08369300
S	1.36720900	-1.54913500	-0.06849400
S	-1.37060700	1.59147000	-0.02922100
C	-3.74958700	0.15239700	-0.07944900
C	-4.56505800	1.15827900	-0.54026600
S	-4.68600500	-1.17650400	0.52224600
C	-5.95002700	0.84698900	-0.41828300
H	-4.18034700	2.07200300	-0.98100900
C	-6.16238100	-0.38644800	0.13089700
H	-7.10438000	-0.88187500	0.32322500
H	-6.75151600	1.50129900	-0.74083500
C	3.74784900	-0.13518100	-0.10596300
C	4.54608200	-1.16054400	-0.54692200
S	4.71147300	1.18216300	0.49190300
C	5.93804800	-0.88221900	-0.41324800
H	4.15128200	-2.07952900	-0.96685800
C	6.17696000	0.34944900	0.12290500
H	6.72141100	-1.57146100	-0.70498400
H	7.13142000	0.81037500	0.33722200

Cationic			
elements	x	y	z
C	-2.28693500	0.09378500	-0.16340400
C	-1.46265700	-1.04479300	-0.16224800
C	-0.12045500	-0.70018000	-0.16258700
C	0.12107400	0.70191600	-0.16400100
C	2.28062100	-0.10442700	-0.16351900
C	1.46190900	1.04216700	-0.16455000
H	-1.85046200	-2.05759000	-0.16112900
H	1.85764000	2.05120300	-0.16567900
S	1.36147000	-1.59528700	-0.16175200
S	-1.36650300	1.59316800	-0.16492000
C	-3.70594400	0.12710600	-0.16334700
C	-4.53309500	1.25141700	-0.16388600
S	-4.65204000	-1.33569800	-0.16257200
C	-5.89701700	0.92234600	-0.16347600
H	-4.15311000	2.26794000	-0.16443000
C	-6.10327000	-0.44400600	-0.16267000
H	-7.05117400	-0.96775800	-0.16222400
H	-6.70423400	1.64389800	-0.16367700
C	3.70108400	-0.13319400	-0.16367100
C	4.53489900	-1.24899600	-0.16411100
S	4.64068300	1.33714300	-0.16332100
C	5.90135000	-0.91357700	-0.16426000
H	4.16667300	-2.26997700	-0.16446100
C	6.10268500	0.44847800	-0.16399500
H	6.70745000	-1.63662900	-0.16461700
H	7.04955800	0.97308100	-0.16397400

(12) OT_2 (F_y = 0.50 V/Å)

Neutral			
elements	x	y	z
C	-2.29798700	0.10913100	-0.06884100
C	-1.49055600	-0.99597000	-0.09291200
C	-0.11216100	-0.63966000	-0.07825100
C	0.12418900	0.72598700	-0.05290500
C	2.29473400	-0.05484100	-0.10109500
C	1.50207500	1.06925900	-0.07086600
H	-1.86727400	-2.01203200	-0.14139400
H	1.89983000	2.07807500	-0.07771200
S	1.36554300	-1.53290400	-0.09928900
S	-1.37314900	1.60750500	-0.02227300
C	-3.75136100	0.15499700	-0.07878500
C	-4.57542900	1.17971500	-0.48350600
S	-4.67535200	-1.21562400	0.43900700
C	-5.95703500	0.84701900	-0.38504000
H	-4.19658500	2.11899500	-0.87407100
C	-6.15662200	-0.42005300	0.09047400
H	-7.09183000	-0.94165400	0.24422900
H	-6.76679600	1.50607700	-0.67727300
C	3.74718600	-0.12792700	-0.12446600
C	4.54046500	-1.18467000	-0.49093400
S	4.72125100	1.22512600	0.38007900
C	5.93523300	-0.90815900	-0.37432900
H	4.14484300	-2.13295900	-0.83973800
C	6.18378100	0.35509400	0.07351100
H	6.71090000	-1.62701000	-0.61019300
H	7.14230800	0.81802000	0.26409100

Cationic			
elements	x	y	z
C	-2.29038100	0.08897000	-0.16330400
C	-1.46340300	-1.04596400	-0.16242300
C	-0.12032400	-0.69951800	-0.16271200
C	0.12153600	0.70260800	-0.16385900
C	2.27770800	-0.11057500	-0.16354800
C	1.46186900	1.04036700	-0.16438000
H	-1.84748600	-2.06088000	-0.16153500
H	1.86174500	2.04777400	-0.16519600
S	1.35858800	-1.59762400	-0.16225600
S	-1.36860600	1.59306400	-0.16458300
C	-3.70877700	0.12458800	-0.16327800
C	-4.53278900	1.25303900	-0.16392300
S	-4.65812900	-1.33552000	-0.16240300
C	-5.89580400	0.92665400	-0.16379400
H	-4.14749300	2.26790900	-0.16453600
C	-6.10427100	-0.44193300	-0.16298800
H	-7.05255500	-0.96578100	-0.16274000
H	-6.70358000	1.64788400	-0.16428200
C	3.69901000	-0.13695900	-0.16375800
C	4.53650200	-1.24829400	-0.16287400
S	4.63522700	1.33834000	-0.16541700
C	5.90451400	-0.90905000	-0.16350000
H	4.17481600	-2.27209800	-0.16185400
C	6.10298800	0.45100800	-0.16480200
H	6.71016100	-1.63315800	-0.16300100
H	7.04913700	0.97668700	-0.16553600

(13) OT_2 (F_z = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-2.29394800	0.09353400	0.04908900	C	-2.28383400	0.09896800	-0.08928400
C	-1.50169800	-1.02572300	0.07187400	C	-1.46228500	-1.04346700	-0.07939900
C	-0.12154100	-0.68256300	0.10847600	C	-0.12077700	-0.70095000	-0.06704000
C	0.12157200	0.68263900	0.10857000	C	0.12079900	0.70105200	-0.06695300
C	2.29397500	-0.09345000	0.04893900	C	2.28385500	-0.09886300	-0.08941800
C	1.50172600	1.02580400	0.07193600	C	1.46230600	1.04357100	-0.07933600
H	-1.89588500	-2.03358500	0.01012500	H	-1.85377600	-2.05416300	-0.10128100
H	1.89591100	2.03367500	0.01031300	H	1.85379600	2.05426900	-0.10110800
S	1.36194600	-1.57625100	0.08623600	S	1.36401200	-1.59383700	-0.08125700
S	-1.36191600	1.57633100	0.08655300	S	-1.36399200	1.59394100	-0.08097700
C	-3.74515200	0.16099600	-0.03522200	C	-3.70296400	0.13016300	-0.12634800
C	-4.51875800	1.10709900	-0.65962900	C	-4.53218000	1.25048700	-0.17030500
S	-4.73468000	-1.07871100	0.67172300	S	-4.64531300	-1.33591500	-0.16947400
C	-5.91411400	0.82509600	-0.58040100	C	-5.89579600	0.91879500	-0.23363300
H	-4.09841600	1.94958300	-1.19811100	H	-4.15718100	2.26881400	-0.17391600
C	-6.17815800	-0.32690100	0.10285500	C	-6.09996900	-0.44547900	-0.23908400
H	-7.13868300	-0.78890400	0.28592000	H	-7.04556800	-0.96926400	-0.30127200
H	-6.68137700	1.43818500	-1.03795000	H	-6.70036400	1.64091300	-0.29269500
C	3.74517400	-0.16089800	-0.03546500	C	3.70298100	-0.13005200	-0.12656800
C	4.51874600	-1.10690500	-0.66005800	C	4.53219600	-1.25036800	-0.17075700
S	4.73474000	1.07870600	0.67160900	S	4.64532600	1.33603500	-0.16951700
C	5.91410600	-0.82491300	-0.58086400	C	5.89580700	-0.91866400	-0.23411800
H	4.09837600	-1.94930900	-1.19864300	H	4.15719800	-2.26869500	-0.17451200
C	6.17818800	0.32698000	0.10255300	C	6.09997800	0.44561100	-0.23936100
H	6.68134400	-1.43793400	-1.03854600	H	6.70037200	-1.64077200	-0.29334800
H	7.13872300	0.78895500	0.28563600	H	7.04557400	0.96940700	-0.30152100

(14) OT_2 (F_z = 0.50 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-2.29248900	0.10629700	0.17246800	C	-2.28428800	0.09894900	0.00945400
C	-1.50784000	-1.01744500	0.21462500	C	-1.46268700	-1.04325200	0.03452900
C	-0.12566600	-0.68199200	0.27313800	C	-0.12103400	-0.70075900	0.06225300
C	0.12571100	0.68205800	0.27323600	C	0.12106400	0.70084300	0.06234500
C	2.29252600	-0.10621800	0.17234400	C	2.28431400	-0.09886000	0.00931600
C	1.50788300	1.01752000	0.21473200	C	1.46271400	1.04334000	0.03459700
H	-1.90722300	-2.02088000	0.12219100	H	-1.85291900	-2.05363300	-0.01237600
H	1.90726300	2.02096600	0.12242100	H	1.85294400	2.05372600	-0.01218900
S	1.35286900	-1.58376400	0.22300400	S	1.36359400	-1.59398200	0.03112300
S	-1.35282700	1.58383600	0.22325600	S	-1.36356800	1.59406900	0.03141800
C	-3.73851900	0.18059200	0.01690600	C	-3.70082200	0.13052800	-0.07860100
C	-4.46367800	1.05317000	-0.75361600	C	-4.52406600	1.25038700	-0.19844400
S	-4.78029800	-0.97939600	0.78552900	S	-4.64201500	-1.33577900	-0.15087000
C	-5.86376500	0.77950300	-0.73782700	C	-5.88167900	0.91858700	-0.33855600
H	-4.00307600	1.82298500	-1.36341700	H	-4.14591200	2.26740300	-0.22036200
C	-6.18049500	-0.29086300	0.04693800	C	-6.08796100	-0.44580400	-0.32775400
H	-7.15239900	-0.74089000	0.19729000	H	-7.02703700	-0.97015100	-0.45430200
H	-6.59171000	1.32959800	-1.32229000	H	-6.67768500	1.63868600	-0.48112100
C	3.73854500	-0.18049400	0.01667100	C	3.70084200	-0.13042400	-0.07882500
C	4.46365000	-1.05296300	-0.75402700	C	4.52408100	-1.25026400	-0.19888600
S	4.78037900	0.97937600	0.78539800	S	4.64202800	1.33589700	-0.15092500
C	5.86374000	-0.77931000	-0.73828200	C	5.88168400	-0.91844100	-0.33902900
H	4.00300600	-1.82268800	-1.36390800	H	4.14592900	-2.26727700	-0.22093600
C	6.18052600	0.29093900	0.04662100	C	6.08796400	0.44595000	-0.32803300
H	6.59164500	-1.32932900	-1.32286500	H	6.67768300	-1.63851600	-0.48175100
H	7.15244400	0.74093200	0.19698300	H	7.02703300	0.97031700	-0.45455700

(15) OT_1 (F = 0.00 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-0.72612900	-0.03644400	0.01138900	C	-0.70123900	-0.05329900	-0.00785500
C	-1.62019400	0.97487900	-0.22915300	C	-1.62705000	1.01103600	-0.00787500
C	-2.96357300	0.51078300	-0.14499100	C	-2.93432200	0.54803600	-0.00781900
C	-3.07674800	-0.83882400	0.15050700	C	-3.04196400	-0.86387800	-0.00779500
C	-5.29941200	-0.28788300	-0.02626000	C	-5.24500700	-0.26458600	-0.00759900
C	-4.42338800	-1.30429400	0.21992300	C	-4.36962800	-1.32851700	-0.00766600
H	-1.32270200	1.98724400	-0.47788200	H	-1.33123600	2.05467100	-0.00788600
H	-6.37968100	-0.34285500	-0.03905300	H	-6.32671100	-0.32731700	-0.00751500
H	-4.72410600	-2.32140400	0.43829200	H	-4.68122800	-2.36500800	-0.00762400
S	-4.52387000	1.23363000	-0.34440400	S	-4.50257100	1.29289400	-0.00778000
S	-1.51661700	-1.56239000	0.35628000	S	-1.49440000	-1.62572100	-0.00793200
C	0.72615400	0.03654200	0.01132500	C	0.70123400	0.05330100	-0.00786700
C	1.62017900	-0.97483500	-0.22921600	C	1.62704500	-1.01103400	-0.00794000
S	1.51664600	1.56234900	0.35631000	S	1.49439500	1.62572200	-0.00790400
C	2.96355900	-0.51079900	-0.14487700	C	2.93431700	-0.54803400	-0.00789300
H	1.32264700	-1.98713100	-0.47816800	H	1.33123100	-2.05467000	-0.00798100
C	3.07674300	0.83880100	0.15065000	C	3.04195800	0.86388000	-0.00782300
C	4.42339800	1.30426900	0.21991900	C	4.36962200	1.32851900	-0.00770400
S	4.52385900	-1.23359400	-0.34436300	S	4.50256600	-1.29289200	-0.00791000
C	5.29936900	0.28781800	-0.02642300	C	5.24500200	0.26458800	-0.00769300
H	4.72416400	2.32138200	0.43818700	H	4.68122300	2.36501000	-0.00763400
H	6.37964500	0.34277600	-0.03931600	H	6.32670600	0.32731900	-0.00762900

(16) OT_1 (F_x = 0.25 V/Å)

Neutral			
elements	x	y	z
C	-0.72594700	-0.04856700	0.01149600
C	-1.61828400	0.97038200	-0.21056900
C	-2.96197200	0.51349000	-0.13574800
C	-3.07926900	-0.84316200	0.13588700
C	-5.29491100	-0.27671300	-0.02423000
C	-4.42589000	-1.30484200	0.20236100
H	-1.32088200	1.98811500	-0.43915700
H	-6.37609400	-0.32550200	-0.03486700
H	-4.73637100	-2.32219000	0.40343800
S	-4.51852800	1.24562800	-0.31782700
S	-1.52214800	-1.57855200	0.32417400
C	0.72401000	0.02509600	0.00889800
C	1.62463900	-0.98762500	-0.21124200
S	1.51085500	1.55956200	0.33228400
C	2.96501100	-0.51478700	-0.13068600
H	1.32859500	-2.00397900	-0.44297700
C	3.07489700	0.83989600	0.14058700
C	4.41990100	1.31024400	0.20006500
S	4.53102700	-1.23512200	-0.31658000
C	5.30513900	0.29646600	-0.02633900
H	4.71113000	2.33456400	0.39949300
H	6.38503300	0.35761700	-0.03978500

Cationic			
elements	x	y	z
C	-0.70817700	-0.07182900	-0.00786100
C	-1.63129700	1.00154900	-0.00805600
C	-2.93537700	0.54800200	-0.00780100
C	-3.05225200	-0.87262400	-0.00744300
C	-5.24552300	-0.24452500	-0.00745700
C	-4.36811400	-1.32701800	-0.00715900
H	-1.32851700	2.04324400	-0.00825300
H	-6.32900000	-0.30719900	-0.00740000
H	-4.69585700	-2.35899300	-0.00688700
S	-4.50466800	1.30333600	-0.00772600
S	-1.49817800	-1.63909600	-0.00754600
C	0.70297100	0.03392500	-0.00791600
C	1.62477800	-1.01786900	-0.00732200
S	1.49156500	1.60819000	-0.00858400
C	2.94103400	-0.54366400	-0.00760700
H	1.33732600	-2.06364300	-0.00676900
C	3.04066700	0.85618400	-0.00828500
C	4.37766200	1.33123900	-0.00854500
S	4.51077000	-1.28079400	-0.00730000
C	5.25708700	0.28242800	-0.00814900
H	4.67529500	2.37195500	-0.00902700
H	6.33774600	0.34722400	-0.00823000

(17) OT_1 (F_x = 0.50 V/Å)

Neutral			
elements	x	y	z
C	-0.72345000	-0.05917700	0.01126200
C	-1.62082100	0.97517700	-0.14231700
C	-2.96084900	0.52342900	-0.09474400
C	-3.08185200	-0.85275600	0.09166600
C	-5.29060000	-0.26453600	-0.02276100
C	-4.42611100	-1.31288100	0.13480300
H	-1.32595000	2.00757000	-0.30130800
H	-6.37330400	-0.30879900	-0.03170200
H	-4.74654900	-2.33756000	0.27186700
S	-4.51628700	1.26964100	-0.22326000
S	-1.52659300	-1.60564600	0.22271300
C	0.71844600	0.01670000	0.00741600
C	1.63046700	-1.00698800	-0.14370400
S	1.50600300	1.57248200	0.23763900
C	2.96513700	-0.52459300	-0.08589100
H	1.33704100	-2.03660200	-0.30891000
C	3.07484700	0.84651100	0.10045900
C	4.41633600	1.32081000	0.13115900
S	4.53856400	-1.25016200	-0.22139300
C	5.31323000	0.30107900	-0.02739100
H	4.69899300	2.35895800	0.26489900
H	6.39324600	0.36736200	-0.04182700

Cationic			
elements	x	y	z
C	-0.71976900	-0.08416400	-0.00762400
C	-1.63572800	0.99166000	-0.00730300
C	-2.94338300	0.54335000	-0.00704200
C	-3.06597900	-0.87860800	-0.00718400
C	-5.25867000	-0.22661000	-0.00657600
C	-4.37357400	-1.32710400	-0.00690200
H	-1.33051700	2.03271400	-0.00725000
H	-6.34449100	-0.29140500	-0.00634300
H	-4.71545600	-2.35551200	-0.00696300
S	-4.51739800	1.30903300	-0.00651800
S	-1.50296400	-1.64445100	-0.00770000
C	0.71062500	0.01813700	-0.00793100
C	1.62734200	-1.02262000	-0.00819000
S	1.49220200	1.59281700	-0.00803400
C	2.95289200	-0.53862600	-0.00847100
H	1.34673800	-2.06989000	-0.00818900
C	3.04865700	0.85192400	-0.00842000
C	4.39037000	1.33363500	-0.00872400
S	4.52581200	-1.27089400	-0.00892200
C	5.27727900	0.29550700	-0.00901400
H	4.67822600	2.37766600	-0.00873400
H	6.35773200	0.36346000	-0.00929000

(18) OT_1 (F_y = 0.25 V/Å)

Neutral			
elements	x	y	z
C	-0.72907500	-0.02684800	0.01447900
C	-1.62515800	0.98664100	-0.21903100
C	-2.96633100	0.51925900	-0.13528600
C	-3.07335700	-0.83270100	0.15161000
C	-5.30099000	-0.30100800	-0.02594800
C	-4.41766000	-1.30975800	0.21480400
H	-1.32770500	1.99945100	-0.46620300
H	-6.38041400	-0.36743700	-0.04686400
H	-4.70981400	-2.33206400	0.42065000
S	-4.53416100	1.23192400	-0.33368100
S	-1.51396300	-1.55346800	0.35135900
C	0.72310500	0.04635100	0.00714000
C	1.61569200	-0.96598300	-0.22590900
S	1.51946900	1.57657700	0.34007300
C	2.96127700	-0.50439900	-0.14536200
H	1.31902700	-1.98176100	-0.46231300
C	3.08048700	0.84684600	0.14017000
C	4.42942200	1.30172000	0.21056900
S	4.51398900	-1.24085800	-0.33350200
C	5.29819100	0.27389900	-0.02569300
H	4.73873100	2.31678100	0.42759200
H	6.37918200	0.31685500	-0.02997700

Cationic			
elements	x	y	z
C	-0.70369400	-0.05448400	-0.00784900
C	-1.62734300	1.01390200	-0.00849900
C	-2.93361800	0.55305500	-0.00832000
C	-3.04097600	-0.86038400	-0.00758500
C	-5.24658400	-0.26964200	-0.00800500
C	-4.36901700	-1.32875300	-0.00733400
H	-1.32749700	2.05619600	-0.00902400
H	-6.32810200	-0.33573100	-0.00804800
H	-4.67781800	-2.36655600	-0.00678600
S	-4.50508700	1.29416500	-0.00881000
S	-1.49741400	-1.62414900	-0.00721800
C	0.69880200	0.05221900	-0.00779400
C	1.62688900	-1.00806500	-0.00734400
S	1.49166500	1.62798800	-0.00845600
C	2.93523200	-0.54277000	-0.00739600
H	1.33525700	-2.05330000	-0.00695100
C	3.04327000	0.86771900	-0.00793500
C	4.37079300	1.32853600	-0.00790400
S	4.50011700	-1.29200100	-0.00688900
C	5.24385200	0.25953700	-0.00747100
H	4.68543700	2.36398200	-0.00828300
H	6.32578000	0.31855700	-0.00742100

(19) OT_1 (F_y = 0.50 V/Å)

Neutral			
elements	x	y	z
C	-0.73186300	-0.01878100	0.01474000
C	-1.63009200	1.00025500	-0.19607300
C	-2.96926600	0.52905000	-0.11767300
C	-3.07058400	-0.82894900	0.14173100
C	-5.30314000	-0.31234000	-0.02375900
C	-4.41272400	-1.31747600	0.19477700
H	-1.33312700	2.01750700	-0.42638300
H	-6.38173300	-0.38867200	-0.05044700
H	-4.69680400	-2.34730100	0.37508200
S	-4.54454200	1.23605500	-0.30017000
S	-1.51193100	-1.55086700	0.32261000
C	0.72006700	0.05487700	0.00152000
C	1.61235000	-0.96090700	-0.20848300
S	1.52176800	1.59478500	0.30170000
C	2.95991300	-0.50029200	-0.13594000
H	1.31780600	-1.98348900	-0.41886400
C	3.08436100	0.85635000	0.12068800
C	4.43530300	1.30232400	0.18712300
S	4.50539300	-1.25256000	-0.29970800
C	5.29731500	0.26005300	-0.02266400
H	4.75263500	2.31887600	0.38772400
H	6.37883700	0.29152300	-0.01885500

Cationic			
elements	x	y	z
C	-0.70616500	-0.05592800	-0.00775600
C	-1.62771100	1.01655100	-0.00902600
C	-2.93308400	0.55777000	-0.00882000
C	-3.04035700	-0.85728100	-0.00741300
C	-5.24860700	-0.27457700	-0.00855400
C	-4.36903200	-1.32918300	-0.00715900
H	-1.32396700	2.05775900	-0.01006600
H	-6.32998600	-0.34355500	-0.00878600
H	-4.67538200	-2.36853500	-0.00614800
S	-4.50755300	1.29588600	-0.00999000
S	-1.50076800	-1.62339300	-0.00642400
C	0.69639700	0.05108000	-0.00761200
C	1.62694300	-1.00510000	-0.00673800
S	1.48918200	1.63083900	-0.00876400
C	2.93640700	-0.53731200	-0.00691700
H	1.33968200	-2.05220200	-0.00603500
C	3.04487600	0.87186500	-0.00794700
C	4.37247400	1.32887400	-0.00801300
S	4.49785300	-1.29142200	-0.00616900
C	5.24312900	0.25462800	-0.00715800
H	4.69029900	2.36357500	-0.00874500
H	6.32530900	0.30968400	-0.00708000

(20) OT_1 (F_z = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-0.72632900	-0.03190500	0.11467300	C	-0.70131100	-0.05288600	0.09259900
C	-1.61221200	0.97617900	-0.16438600	C	-1.62616500	1.01124900	0.04592600
C	-2.95833500	0.51402000	-0.11153600	C	-2.93326100	0.54848000	0.01528800
C	-3.08181200	-0.83180100	0.19741600	C	-3.04204100	-0.86322400	0.03907400
C	-5.29310000	-0.29225200	-0.10872600	C	-5.24143300	-0.26441200	-0.08985000
C	-4.42819000	-1.30252400	0.19778000	C	-4.36819000	-1.32805600	-0.01847600
H	-1.30587900	1.97774500	-0.44420900	H	-1.32925000	2.05404300	0.01158400
H	-6.36855400	-0.35763600	-0.20582800	H	-6.32059700	-0.32784100	-0.16411300
H	-4.73533700	-2.32334600	0.38821900	H	-4.67951800	-2.36458300	-0.03060100
S	-4.50709400	1.22642700	-0.40830600	S	-4.49858600	1.29260400	-0.08956800
S	-1.52808100	-1.55287300	0.45941900	S	-1.49526400	-1.62496700	0.10280400
C	0.72633000	0.03188700	0.11467700	C	0.70130800	0.05288400	0.09258700
C	1.61221500	-0.97618500	-0.16442000	C	1.62616100	-1.01124900	0.04585800
S	1.52808200	1.55282100	0.45957000	S	1.49526100	1.62496500	0.10283100
C	2.95833800	-0.51402800	-0.11153600	C	2.93325700	-0.54847800	0.01521000
H	1.30588500	-1.97774000	-0.44428400	H	1.32924600	-2.05404200	0.01148500
C	3.08181100	0.83178100	0.19747000	C	3.04203700	0.86322400	0.03904300
C	4.42818300	1.30252000	0.19780100	C	4.36818500	1.32805800	-0.01851700
S	4.50710400	-1.22644300	-0.40824400	S	4.49857900	-1.29259900	-0.08970400
C	5.29307900	0.29230400	-0.10893200	C	5.24142700	0.26441700	-0.08994600
H	4.73532300	2.32334300	0.38824600	H	4.67951200	2.36458600	-0.03061200
H	6.36851700	0.35772600	-0.20618900	H	6.32058900	0.32784800	-0.16422700

(21) OT_1 (F_z = 0.50 V/Å)

Neutral			
elements	x	y	z
C	-0.72678900	-0.02578200	0.22879500
C	-1.60086400	0.97454600	-0.10735500
C	-2.94979100	0.51563000	-0.08717700
C	-3.08764200	-0.82131500	0.25395600
C	-5.27742900	-0.29862800	-0.20036100
C	-4.43027500	-1.29752500	0.18619300
H	-1.28125700	1.95901500	-0.43009100
H	-6.34080000	-0.37670700	-0.38438900
H	-4.74351400	-2.31907500	0.36271500
S	-4.47886700	1.21215700	-0.49864400
S	-1.54372300	-1.53606000	0.59102800
C	0.72678800	0.02578000	0.22878000
C	1.60085600	-0.97454000	-0.10741500
S	1.54373000	1.53604700	0.59103600
C	2.94978400	-0.51562500	-0.08725400
H	1.28124100	-1.95899900	-0.43017400
C	3.08764300	0.82131000	0.25391800
C	4.43027500	1.29751900	0.18615000
S	4.47885000	-1.21214100	-0.49877000
C	5.27741900	0.29863300	-0.20045800
H	4.74352000	2.31906300	0.36269800
H	6.34078700	0.37671600	-0.38450400

Cationic			
elements	x	y	z
C	-0.70154300	-0.05178500	0.19526900
C	-1.62354400	1.01173000	0.10268700
C	-2.93002600	0.54958200	0.03942600
C	-3.04185400	-0.86157900	0.08526400
C	-5.23005400	-0.26410900	-0.17410500
C	-4.36321400	-1.32706400	-0.03208900
H	-1.32325000	2.05206800	0.03574300
H	-6.30153000	-0.32962400	-0.32325200
H	-4.67365300	-2.36368100	-0.05813500
S	-4.48602500	1.29155500	-0.16999200
S	-1.49778600	-1.62291900	0.21385000
C	0.70154200	0.05178100	0.19525700
C	1.62354100	-1.01173100	0.10262400
S	1.49778500	1.62291500	0.21386900
C	2.93002100	-0.54958200	0.03935100
H	1.32324500	-2.05206600	0.03565500
C	3.04185100	0.86157800	0.08523000
C	4.36320800	1.32706700	-0.03213400
S	4.48601600	-1.29154900	-0.17012000
C	5.23004600	0.26411400	-0.17420000
H	4.67364800	2.36368300	-0.05815500
H	6.30151800	0.32963300	-0.32336600

(22) OT_0 (F = 0.00 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	4.18940900	-0.12413900	0.00013200	C	4.13751700	-0.10585500	0.00001200
C	3.46694700	-1.28132600	0.00000700	C	3.41588300	-1.28584300	0.00003700
C	2.06713600	-1.00854100	0.00004000	C	2.04174300	-1.01695800	0.00005300
C	1.76741300	0.34554700	0.00001200	C	1.74028100	0.36971900	0.00004100
S	3.20263700	1.30557400	-0.00013000	S	3.18539900	1.32907900	0.00002700
H	5.26617100	-0.02191900	0.00022000	H	5.21742900	-0.01516100	-0.00000500
H	3.91065500	-2.26925000	0.00001400	H	3.87157600	-2.26794400	0.00004000
C	0.36435700	0.58987700	0.00002400	C	0.37540900	0.61121100	0.00004400
S	0.63882400	-2.01330400	0.00004300	S	0.62240900	-2.03734600	0.00008000
C	-0.36405200	-0.58969400	0.00003800	C	-0.37524300	-0.61116500	0.00006100
C	-1.76723000	-0.34581400	0.00001700	C	-1.74012700	-0.36970300	0.00006600
S	-0.63923600	2.01335500	0.00003800	S	-0.62226200	2.03737800	0.00005000
C	-2.06687200	1.00857500	0.00000800	C	-2.04157500	1.01697100	0.00005400
S	-3.20269300	-1.30574200	-0.00016000	S	-3.18524200	-1.32904900	0.00008500
C	-3.46668300	1.28138300	-0.00001000	C	-3.41572300	1.28587400	0.00004900
C	-4.18931400	0.12442500	0.00019200	C	-4.13735800	0.10590100	0.00005300
H	-3.90999800	2.26948800	-0.00003300	H	-3.87139000	2.26798700	0.00004000
H	-5.26601300	0.02178200	0.00038600	H	-5.21726700	0.01518000	0.00005100

(23) OT_0 (F_x = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	4.19445200	-0.12652800	0.00009300	C	4.14358500	-0.11026700	0.00003300
C	3.46609200	-1.28086700	0.00005900	C	3.42409700	-1.28184300	0.00003700
C	2.06676700	-1.00871800	0.00002400	C	2.03932900	-1.01256800	0.00004100
C	1.76648800	0.34599700	0.00000100	C	1.74108500	0.36541100	0.00003100
S	3.20518600	1.30497600	-0.00002500	S	3.18377000	1.32473700	0.00000500
H	5.27140200	-0.02675700	0.00014200	H	5.22253600	-0.01751900	0.00003400
H	3.90370400	-2.27208000	0.00008500	H	3.87403800	-2.26652100	0.00004600
C	0.36528700	0.59655800	-0.00001900	C	0.36903400	0.61166500	0.00003700
S	0.63687200	-2.00923000	-0.00001400	S	0.62540300	-2.03431100	0.00005900
C	-0.36396100	-0.58341500	-0.00000400	C	-0.37979000	-0.60952300	0.00005200
C	-1.76780600	-0.34646600	0.00001500	C	-1.74258900	-0.37164300	0.00005900
S	-0.64119300	2.01747300	-0.00005600	S	-0.61963000	2.03860700	0.00003000
C	-2.06823500	1.00829500	0.00001400	C	-2.04644800	1.02178100	0.00004800
S	-3.20143900	-1.30705400	0.00000300	S	-3.19202600	-1.33217000	0.00007600
C	-3.46739500	1.28199900	0.00006500	C	-3.41025900	1.29084700	0.00005400
C	-4.18567000	0.12204800	0.00014500	C	-4.13745800	0.09990600	0.00007100
H	-3.91636900	2.26719600	0.00008700	H	-3.87394700	2.26979800	0.00004700
H	-5.26272400	0.01685100	0.00022200	H	-5.21927200	0.01389100	0.00007800

(24) OT_0 (F_x = 0.50 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	4.20068300	-0.12847800	0.00038600	C	4.15430200	-0.11410900	0.00019500
C	3.46452500	-1.28025800	0.00006700	C	3.43351900	-1.27901700	0.00000300
C	2.06713500	-1.00937900	-0.00006900	C	2.04050400	-1.00925800	-0.00004800
C	1.76464700	0.34756000	-0.00012800	C	1.74453300	0.36055600	-0.00006100
S	3.20838700	1.30490500	-0.00023700	S	3.18604400	1.32064700	-0.00022600
H	5.27842200	-0.03228900	0.00069700	H	5.23304400	-0.02024300	0.00036500
H	3.89670300	-2.27469300	0.00015100	H	3.87812900	-2.26647300	0.00006100
C	0.36732300	0.60400600	-0.00018300	C	0.36309400	0.61162300	-0.00002400
S	0.63468000	-2.00572500	-0.00023000	S	0.62800900	-2.03001000	-0.00006500
C	-0.36512700	-0.57793900	-0.00015200	C	-0.38179100	-0.60566800	-0.00000500
C	-1.76766200	-0.34853200	-0.00016900	C	-1.74759800	-0.37045900	0.00003900
S	-0.64380200	2.02213600	-0.00033400	S	-0.61799200	2.03840600	-0.00004800
C	-2.07017900	1.00860800	-0.00016700	C	-2.05201400	1.02526700	0.00003500
S	-3.20131000	-1.30900700	-0.00041900	S	-3.20179100	-1.33437600	0.00007700
C	-3.46719800	1.28263600	0.00002000	C	-3.40835500	1.29571300	0.00009000
C	-4.18267600	0.11927200	0.00050000	C	-4.14316800	0.09316500	0.00014800
H	-3.92238600	2.26492300	0.00015700	H	-3.87945900	2.27211900	0.00010400
H	-5.26070600	0.01253000	0.00095000	H	-5.22755100	0.01239400	0.00019900

(25) OT_0 (F_y = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	4.19292500	-0.13361500	0.00004600	C	4.13959800	-0.11225100	0.00002700
C	3.46283400	-1.28359600	0.00006800	C	3.41376400	-1.28722500	0.00004400
C	2.06333200	-1.00174500	0.00004200	C	2.03901300	-1.01347900	0.00004500
C	1.76916000	0.35399600	0.00002300	C	1.74053300	0.37570000	0.00003300
S	3.21269900	1.30628100	0.00002500	S	3.18998800	1.33053000	0.00001600
H	5.27041800	-0.04024800	0.00004700	H	5.21987800	-0.02640200	0.00002100
H	3.89855600	-2.27520900	0.00008500	H	3.86590900	-2.27150500	0.00005200
C	0.36782100	0.59948000	-0.00000100	C	0.37833300	0.61684800	0.00003400
S	0.63704000	-2.00303600	0.00001300	S	0.62138000	-2.03163600	0.00005800
C	-0.36048900	-0.57997300	0.00001200	C	-0.37235400	-0.60569800	0.00005000
C	-1.76584500	-0.33735900	0.00003600	C	-1.73997700	-0.36376200	0.00005800
S	-0.64095900	2.02382300	-0.00002600	S	-0.62331400	2.04363400	0.00002600
C	-2.07105300	1.01507000	0.00003400	C	-2.04443200	1.02057200	0.00004800
S	-3.19303100	-1.30554200	0.00005300	S	-3.18077000	-1.32799000	0.00007500
C	-3.47141300	1.27945400	0.00007300	C	-3.41812000	1.28468300	0.00005600
C	-4.18627500	0.11527700	0.00009800	C	-4.13552900	0.09960400	0.00006900
H	-3.92212800	2.26437300	0.00008200	H	-3.87739500	2.26490500	0.00005100
H	-5.26213200	0.00284600	0.00012900	H	-5.21504500	0.00375100	0.00007500

(26) OT_0 (F_y = 0.50 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	4.19639000	-0.14291100	0.00012100	C	4.14199100	-0.11849900	0.00003400
C	3.45885200	-1.28596000	0.00008600	C	3.41190900	-1.28885200	0.00004400
C	2.05960600	-0.99528600	0.00002100	C	2.03627700	-1.01019200	0.00004500
C	1.77084500	0.36231900	-0.00000500	C	1.74103700	0.38170300	0.00003300
S	3.22252300	1.30717300	-0.00000500	S	3.19523000	1.33215300	0.00001900
H	5.27457200	-0.05855100	0.00017900	H	5.22271100	-0.03811100	0.00003100
H	3.88719900	-2.28127800	0.00011700	H	3.86125800	-2.27531200	0.00005100
C	0.37147300	0.60927900	-0.00004900	C	0.38120200	0.62287100	0.00003300
S	0.63513700	-1.99346900	-0.00006100	S	0.62044500	-2.02639100	0.00005500
C	-0.35706000	-0.57046900	-0.00003700	C	-0.36926700	-0.60046200	0.00004800
C	-1.76440600	-0.32916900	-0.00002900	C	-1.73985700	-0.35772800	0.00004900
S	-0.64309500	2.03494900	-0.00011000	S	-0.62452800	2.05049600	0.00002100
C	-2.07518200	1.02183000	-0.00002400	C	-2.04736900	1.02445900	0.00003800
S	-3.18347600	-1.30577500	-0.00010000	S	-3.17675600	-1.32715100	0.00004200
C	-3.47612000	1.27765400	0.00005200	C	-3.42094100	1.28374500	0.00004600
C	-4.18321500	0.10623800	0.00021600	C	-4.13400400	0.09307300	0.00008900
H	-3.93444600	2.25958200	0.00009500	H	-3.88467800	2.26199700	0.00004500
H	-5.25814100	-0.01587800	0.00037000	H	-5.21320200	-0.00752200	0.00011400

(27) OT_0 (F_z = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	4.18761300	-0.12408500	-0.04291400	C	4.13662700	-0.10534000	-0.03064600
C	3.46554200	-1.28124700	-0.02089100	C	3.41536200	-1.28589600	-0.00818100
C	2.06697700	-1.00841600	0.04237100	C	2.04165400	-1.01710200	0.03017000
C	1.76757900	0.34553900	0.06277900	C	1.74036500	0.36960400	0.04073400
S	3.20170300	1.30592800	0.00546600	S	3.18518300	1.32895500	-0.00721800
H	5.26184100	-0.02092300	-0.11586500	H	5.21562000	-0.01561300	-0.07856200
H	3.90719800	-2.26874200	-0.07248100	H	3.87143100	-2.26740700	-0.03825500
C	0.36433400	0.58962700	0.08614000	C	0.37526000	0.61134000	0.05490900
S	0.63864400	-2.01314400	0.05573600	S	0.62240000	-2.03732700	0.03738800
C	-0.36417100	-0.58959800	0.08615400	C	-0.37509700	-0.61130800	0.05492400
C	-1.76741600	-0.34550800	0.06280100	C	-1.74020300	-0.36957200	0.04075800
S	-0.63847700	2.01317600	0.05570400	S	-0.62223800	2.03735800	0.03735700
C	-2.06681500	1.00844700	0.04237100	C	-2.04149100	1.01713200	0.03017200
S	-3.20154200	-1.30589600	0.00551500	S	-3.18502100	-1.32892400	-0.00716200
C	-3.46538000	1.28127800	-0.02088300	C	-3.41520000	1.28592700	-0.00817000
C	-4.18745200	0.12411400	-0.04287200	C	-4.13646500	0.10537000	-0.03060700
H	-3.90703700	2.26877100	-0.07248500	H	-3.87126900	2.26743700	-0.03825800
H	-5.26168200	0.02095400	-0.11580700	H	-5.21545900	0.01564300	-0.07851100

(28) OT_0 (F_z = 0.50 V/Å)

Neutral			
elements	x	y	z
C	4.18104900	-0.12302700	-0.08924700
C	3.46060100	-1.28067100	-0.04273500
C	2.06624800	-1.00861400	0.08706200
C	1.76771200	0.34520000	0.12840600
S	3.19761300	1.30642700	0.00916600
H	5.24756000	-0.01882400	-0.23738500
H	3.89740900	-2.26625400	-0.14687200
C	0.36475900	0.58943400	0.17650400
S	0.63744700	-2.01308000	0.11544800
C	-0.36459500	-0.58940200	0.17651900
C	-1.76754900	-0.34516800	0.12842700
S	-0.63728100	2.01311300	0.11541800
C	-2.06608500	1.00864500	0.08706200
S	-3.19745200	-1.30639500	0.00921400
C	-3.46043900	1.28070100	-0.04273000
C	-4.18088900	0.12305700	-0.08920900
H	-3.89724800	2.26628200	-0.14688000
H	-5.24740200	0.01885300	-0.23733100

Cationic			
elements	x	y	z
C	4.13357300	-0.10484100	-0.06480000
C	3.41348000	-1.28581100	-0.01764400
C	2.04166700	-1.01720800	0.06287400
C	1.74049000	0.36960800	0.08479900
S	3.18267600	1.32924400	-0.01523800
H	5.20920100	-0.01502800	-0.16402300
H	3.86777400	-2.26676000	-0.07938800
C	0.37542500	0.61118500	0.11460700
S	0.62208800	-2.03734400	0.07915900
C	-0.37526200	-0.61115300	0.11462100
C	-1.74032700	-0.36957600	0.08482200
S	-0.62192600	2.03737600	0.07912700
C	-2.04150400	1.01724000	0.06287400
S	-3.18251400	-1.32921400	-0.01518400
C	-3.41331800	1.28584200	-0.01763600
C	-4.13341200	0.10487100	-0.06476400
H	-3.86761200	2.26679000	-0.07939400
H	-5.20904000	0.01505700	-0.16397600

(29) OP (F = 0.00 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	3.57368300	0.00000700	0.00000700	C	3.57035200	-0.00000500	-0.00000200
C	2.85281000	-1.13276200	-0.39849000	C	2.83590200	-1.19547000	-0.20796200
C	1.46229800	-1.13279000	-0.39839500	C	1.46226800	-1.19773900	-0.20457200
C	0.74125700	0.00007100	0.00008900	C	0.72108800	-0.00000300	-0.00000300
C	1.46235600	1.13288200	0.39856100	C	1.46227000	1.19773200	0.20456600
C	2.85287100	1.13279100	0.39856900	C	2.83590300	1.19546100	0.20795700
C	5.05731600	-0.00000600	-0.00002400	C	5.03052300	-0.00000600	-0.00000200
C	5.77361500	-1.12967900	0.41648400	C	5.74976100	-1.15453700	0.37133400
C	7.16626000	-1.13059600	0.41613400	C	7.13684900	-1.14940400	0.38004900
C	7.86816500	-0.00005300	-0.00007300	C	7.83442800	-0.00000800	-0.00000100
C	7.16628200	1.13051100	-0.41626200	C	7.13685200	1.14938800	-0.38005100
C	5.77363700	1.12964200	-0.41656500	C	5.74976300	1.15452300	-0.37133700
H	3.38847100	-2.01253700	-0.74520100	H	3.36527500	-2.11797300	-0.42028200
H	0.92687400	-2.01256000	-0.74553400	H	0.94338100	-2.12563900	-0.41677900
H	0.92699200	2.01266000	0.74577400	H	0.94338400	2.12563300	0.41677400
H	3.38859400	2.01252700	0.74527900	H	3.36527700	2.11796300	0.42027800
H	5.23300000	-2.00493000	0.76703300	H	5.21982700	-2.04471200	0.69541100
H	7.70405300	-2.01304500	0.75030000	H	7.67822800	-2.03806200	0.68732500
H	8.95400000	-0.00007000	-0.00009200	H	8.91985300	-0.00000900	-0.00000100
H	7.70409200	2.01294000	-0.75045100	H	7.67823200	2.03804500	-0.68732700
H	5.23304200	2.00490700	-0.76710600	H	5.21983100	2.04470000	-0.69541500
C	-5.05731600	0.00000400	-0.00002600	C	-5.03052400	-0.00000300	-0.00000500
C	-5.77359000	-1.12967500	-0.41656000	C	-5.74976200	-1.15453300	-0.37134000
C	-7.16623600	-1.13060100	-0.41625900	C	-7.13685000	-1.14940000	-0.38005500
C	-7.86816500	-0.00006400	-0.00007500	C	-7.83442800	-0.00000300	-0.00000600
C	-7.16630700	1.13050700	0.41613600	C	-7.13685100	1.14939300	0.38004400
C	-5.77366100	1.12964600	0.41648900	C	-5.74976300	1.15452700	0.37133000
C	-3.57368300	0.00003600	0.00001700	C	-3.57035200	-0.00000200	-0.00000400
C	-2.85284500	-1.13274100	0.39855200	C	-2.83590300	-1.19546800	0.20795500
C	-1.46233200	-1.13280500	0.39854100	C	-1.46226900	-1.19773800	0.20456500
C	-0.74125700	0.00003200	0.00009700	C	-0.72108800	-0.00000300	-0.00000300
C	-1.46232200	1.13286800	-0.39841500	C	-1.46226900	1.19773300	-0.20457200
C	-2.85283600	1.13281200	-0.39850700	C	-2.83590200	1.19546300	-0.20796300
H	-5.23295800	-2.00492200	-0.76708900	H	-5.21982800	-2.04470900	-0.69541800
H	-7.70401000	-2.01305400	-0.75044300	H	-7.67822900	-2.03805700	-0.68733100
H	-8.95400000	-0.00009100	-0.00009300	H	-8.91985300	-0.00000400	-0.00000600
H	-7.70413600	2.01293100	0.75030700	H	-7.67823100	2.03805000	0.68732000
H	-5.23308400	2.00491400	0.76705100	H	-5.21983000	2.04470300	0.69540900
H	-3.38855000	-2.01250000	0.74523300	H	-3.36527700	-2.11797100	0.42027600
H	-0.92694900	-2.01258800	0.74571300	H	-0.94338300	-2.12563900	0.41677300
H	-0.92691800	2.01263200	-0.74559600	H	-0.94338300	2.12563300	-0.41678000

H	-3.38851500	2.01256400	-0.74524600	H	-3.36527600	2.11796600	-0.42028500

(30) OP (F_x = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	3.57414000	-0.00000900	-0.00000100	C	3.56255300	-0.00000500	-0.00000200
C	2.85301600	-1.13880500	-0.38123400	C	2.84230600	-1.13052900	-0.41281500
C	1.46288500	-1.13710900	-0.38466600	C	1.45467000	-1.13509300	-0.40655500
C	0.73750100	-0.00001500	-0.00000300	C	0.73134500	-0.00000400	-0.00000300
C	1.46287900	1.13708200	0.38465600	C	1.45467100	1.13508400	0.40655000
C	2.85301100	1.13878400	0.38122600	C	2.84230700	1.13051900	0.41281000
C	5.05643200	-0.00000600	-0.00000100	C	5.04583400	-0.00000600	-0.00000200
C	5.77789400	-1.13127900	0.40835200	C	5.76172800	-1.14231000	0.38352700
C	7.17052700	-1.13325100	0.40616200	C	7.15419000	-1.14211500	0.38459400
C	7.87489900	0.00000400	0.00000000	C	7.85550000	-0.00000700	-0.00000100
C	7.17052000	1.13325400	-0.40616100	C	7.15419200	1.14210100	-0.38459600
C	5.77788700	1.13127300	-0.40835200	C	5.76172900	1.14229700	-0.38353000
H	3.38582600	-2.02508300	-0.71733100	H	3.37639600	-2.00501000	-0.77329500
H	0.92647500	-2.01947100	-0.72219500	H	0.92803600	-2.01394900	-0.76600500
H	0.92646600	2.01944400	0.72217900	H	0.92803800	2.01394100	0.76599900
H	3.38581600	2.02506600	0.71732100	H	3.37639700	2.00500000	0.77329100
H	5.23636000	-2.00802100	0.75291200	H	5.22315100	-2.02808600	0.70885300
H	7.70568900	-2.02072800	0.73369700	H	7.69089200	-2.03411400	0.69450900
H	8.96180200	0.00000800	0.00000100	H	8.94187600	-0.00000800	-0.00000100
H	7.70567600	2.02073500	-0.73369400	H	7.69089500	2.03410000	-0.69451100
H	5.23634700	2.00801100	-0.75291100	H	5.22315400	2.02807400	-0.70885700
C	-5.05998300	-0.00000500	-0.00000400	C	-5.02741200	-0.00000300	-0.00000500
C	-5.77365300	-1.13334400	-0.41078700	C	-5.76448300	-1.21245800	-0.19059300
C	-7.16609900	-1.13292400	-0.41236800	C	-7.13918900	-1.20824200	-0.20035700
C	-7.86659700	0.00001000	-0.00000300	C	-7.83927000	-0.00000300	-0.00000500
C	-7.16608700	1.13293800	0.41236000	C	-7.13918900	1.20823700	0.20034600
C	-5.77364100	1.13334300	0.41077700	C	-5.76448300	1.21245200	0.19058400
C	-3.57749400	-0.00001000	-0.00000700	C	-3.58743600	-0.00000300	-0.00000400
C	-2.85374000	-1.13615000	0.38894000	C	-2.84314600	-1.19704900	0.21549300
C	-1.46371600	-1.13808400	0.38535000	C	-1.46764900	-1.19210800	0.22055700
C	-0.74333200	-0.00001500	-0.00000700	C	-0.73800600	-0.00000400	-0.00000300
C	-1.46371200	1.13805800	-0.38535900	C	-1.46764900	1.19210100	-0.22056400
C	-2.85373600	1.13612800	-0.38894900	C	-2.84314500	1.19704300	-0.21550100
H	-5.23537200	-2.01144100	-0.75860300	H	-5.23961600	-2.14242900	-0.37602000
H	-7.70661500	-2.01433100	-0.74319700	H	-7.69004200	-2.12756400	-0.36760200
H	-8.95193200	0.00001600	-0.00000300	H	-8.92523000	-0.00000300	-0.00000600
H	-7.70659300	2.01435000	0.74318800	H	-7.69004300	2.12755900	0.36759100
H	-5.23535000	2.01143500	0.75858900	H	-5.23961700	2.14242400	0.37601100
H	-3.39086800	-2.01717900	0.72867700	H	-3.36022300	-2.12402000	0.43456500

H	-0.93133800	-2.02319000	0.72493900	H	-0.93690700	-2.11276800	0.43976500
H	-0.93133000	2.02316400	-0.72494200	H	-0.93690600	2.11276100	-0.43977200
H	-3.39086200	2.01716100	-0.72868100	H	-3.36022100	2.12401400	-0.43457400

(31) OP (F_x = 0.50 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	3.58136800	0.00000100	-0.00000400	C	3.57365400	-0.00000600	-0.00000200
C	2.85385300	-1.15667500	-0.32142700	C	2.85179800	-1.11481000	-0.44672600
C	1.46582900	-1.15433500	-0.32859500	C	1.46058100	-1.11537800	-0.44666300
C	0.72999700	0.00001200	-0.00000600	C	0.73570800	-0.00000700	-0.00000300
C	1.46583800	1.15435300	0.32858900	C	1.46058000	1.11536400	0.44665700
C	2.85386100	1.15668200	0.32142200	C	2.85179700	1.11479700	0.44672100
C	5.05793400	-0.00000600	-0.00000100	C	5.05914600	-0.00000600	-0.00000200
C	5.78925000	-1.14139200	0.37535900	C	5.78289300	-1.15364500	0.33903300
C	7.18140500	-1.14391900	0.37089200	C	7.17612500	-1.15529600	0.33711300
C	7.89084600	-0.00002500	-0.00000100	C	7.88136000	-0.00000400	0.00000000
C	7.18142000	1.14387800	-0.37089500	C	7.17612400	1.15528700	-0.33711500
C	5.78926500	1.14136900	-0.37536300	C	5.78289200	1.15363400	-0.33903500
H	3.38041300	-2.06107900	-0.61886700	H	3.38230500	-1.98106700	-0.83416300
H	0.93259500	-2.05129800	-0.62877300	H	0.92993600	-1.98102400	-0.83236100
H	0.93261100	2.05131700	0.62877200	H	0.92993400	1.98101000	0.83235300
H	3.38042800	2.06108100	0.61886800	H	3.38230300	1.98105400	0.83415700
H	5.25007800	-2.02750600	0.69785800	H	5.24415300	-2.05111600	0.62968700
H	7.71334200	-2.04367600	0.67306700	H	7.71032500	-2.06184500	0.61090800
H	8.97938200	-0.00003200	0.00000000	H	8.96940900	-0.00000300	0.00000000
H	7.71336900	2.04362800	-0.67307000	H	7.71032300	2.06183700	-0.61090800
H	5.25010500	2.02748900	-0.69786400	H	5.24415100	2.05110500	-0.62969000
C	-5.06539600	-0.00000100	-0.00000400	C	-5.04887700	-0.00000400	-0.00000400
C	-5.77982400	-1.14495100	-0.38368700	C	-5.78405500	-1.21820500	-0.19647000
C	-7.17140900	-1.14295800	-0.38805600	C	-7.15388800	-1.21858000	-0.20613100
C	-7.87143500	-0.00002100	-0.00000700	C	-7.86237600	0.00000200	-0.00000500
C	-7.17142600	1.14292500	0.38804500	C	-7.15388300	1.21858100	0.20612100
C	-5.77984100	1.14493900	0.38368000	C	-5.78405000	1.21820000	0.19646000
C	-3.58809200	0.00000700	0.00000000	C	-3.59235400	-0.00000600	-0.00000500
C	-2.85683400	-1.15188900	0.34138600	C	-2.85737500	-1.17135000	0.30314600
C	-1.46911900	-1.15493500	0.33394400	C	-1.47189800	-1.16509300	0.31096600
C	-0.74325200	0.00001300	-0.00000300	C	-0.74969400	-0.00000700	-0.00000400
C	-1.46912500	1.15495700	-0.33395300	C	-1.47189700	1.16507900	-0.31097400
C	-2.85683900	1.15190400	-0.34139300	C	-2.85737400	1.17133800	-0.30315500
H	-5.24609100	-2.03214500	-0.71542000	H	-5.25101500	-2.14335500	-0.38517100
H	-7.71482300	-2.02887700	-0.70061800	H	-7.71093400	-2.13424300	-0.37762100
H	-8.95687300	-0.00002900	-0.00000700	H	-8.94976600	0.00000500	-0.00000500
H	-7.71485400	2.02883600	0.70060900	H	-7.71092500	2.13424700	0.37761100

H	-5.24612200	2.03213900	0.71541900	H	-5.25100500	2.14334800	0.38516000
H	-3.39256100	-2.04480600	0.64913500	H	-3.37539200	-2.08171300	0.58477400
H	-0.94334700	-2.05595300	0.64147700	H	-0.94167800	-2.06966100	0.59430900
H	-0.94335800	2.05597500	-0.64149400	H	-0.94167600	2.06964700	-0.59431500
H	-3.39257200	2.04481600	-0.64914900	H	-3.37539100	2.08170200	-0.58478100

(32) OP (F_y = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	3.57393800	0.01062800	-0.00275700	C	3.57048300	-0.00653700	0.00557100
C	2.84975100	-1.11945100	-0.40332800	C	2.84033600	-1.20335800	-0.20471600
C	1.45934900	-1.11575000	-0.40301100	C	1.46563200	-1.20954800	-0.20254900
C	0.74127100	0.01848200	-0.00282900	C	0.72111500	-0.01430000	0.00176000
C	1.46536500	1.14931800	0.39590300	C	1.45880800	1.18527900	0.21134200
C	2.85614000	1.14526400	0.39627300	C	2.83152500	1.18663500	0.21707700
C	5.05758600	0.00248600	0.00278900	C	5.03075200	0.00208500	0.00577300
C	5.76497800	-1.13559500	0.41203000	C	5.75750700	-1.15039300	0.36774100
C	7.15749600	-1.14853200	0.41102500	C	7.14542000	-1.13850600	0.37212900
C	7.86854900	-0.02095900	0.00229400	C	7.83489200	0.01668900	-0.00226800
C	7.17582600	1.11840200	-0.40558300	C	7.12916300	1.16548400	-0.37215000
C	5.78300700	1.12934300	-0.40577500	C	5.74275000	1.16354900	-0.35967300
H	3.38053600	-2.00309500	-0.74668400	H	3.37025600	-2.12583300	-0.41567700
H	0.92384800	-1.99661800	-0.74628000	H	0.95121700	-2.14022400	-0.41365700
H	0.93020500	2.02763200	0.74870900	H	0.93525500	2.10964800	0.42850700
H	3.39621600	2.02049400	0.74914700	H	3.35973200	2.10853200	0.43578000
H	5.21973000	-2.01170900	0.75206800	H	5.23551500	-2.04799700	0.68345100
H	7.68660700	-2.04035200	0.73254200	H	7.69126200	-2.02863900	0.66638200
H	8.95428300	-0.03484300	-0.00409100	H	8.92029900	0.01929800	-0.01030200
H	7.72219000	1.99614300	-0.74051900	H	7.66588700	2.05719300	-0.68029700
H	5.24755800	2.00859500	-0.75582600	H	5.20554800	2.05082100	-0.68091500
C	-5.05758700	0.00248900	-0.00279700	C	-5.03075200	0.00208800	-0.00578000
C	-5.76497800	-1.13559100	-0.41204000	C	-5.75750700	-1.15038900	-0.36774900
C	-7.15749700	-1.14852700	-0.41103700	C	-7.14542100	-1.13850200	-0.37213700
C	-7.86854900	-0.02095400	-0.00230500	C	-7.83489200	0.01669400	0.00226100
C	-7.17582500	1.11840600	0.40557400	C	-7.12916200	1.16548800	0.37214500
C	-5.78300700	1.12934600	0.40576800	C	-5.74274900	1.16355200	0.35966800
C	-3.57393800	0.01063000	0.00275100	C	-3.57048300	-0.00653400	-0.00557700
C	-2.84975300	-1.11944900	0.40332200	C	-2.84033700	-1.20335600	0.20470900
C	-1.45935000	-1.11575000	0.40300800	C	-1.46563300	-1.20954700	0.20254200
C	-0.74127100	0.01848100	0.00282900	C	-0.72111500	-0.01430000	-0.00176600
C	-1.46536400	1.14931900	-0.39590300	C	-1.45880700	1.18528000	-0.21134700
C	-2.85613800	1.14526600	-0.39627600	C	-2.83152400	1.18663700	-0.21708200
H	-5.21973100	-2.01170600	-0.75207900	H	-5.23551600	-2.04799300	-0.68346000
H	-7.68660800	-2.04034600	-0.73255600	H	-7.69126300	-2.02863400	-0.66639100

H	-8.95428300	-0.03483800	0.00407900	H	-8.92029900	0.01930300	0.01029500
H	-7.72218900	1.99614700	0.74051100	H	-7.66588600	2.05719700	0.68029300
H	-5.24755700	2.00859600	0.75582100	H	-5.20554700	2.05082300	0.68091100
H	-3.38053800	-2.00309400	0.74667700	H	-3.37025700	-2.12583100	0.41566800
H	-0.92385200	-1.99662000	0.74627800	H	-0.95121800	-2.14022300	0.41364900
H	-0.93020100	2.02763200	-0.74870600	H	-0.93525400	2.10964900	-0.42851100
H	-3.39621400	2.02049700	-0.74915000	H	-3.35973100	2.10853500	-0.43578400

(33) OP (F_y = 0.50 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	3.57475200	0.02121000	-0.00621800	C	3.57081800	-0.01377800	0.01066900
C	2.84670700	-1.10550200	-0.41036000	C	2.84519800	-1.21156000	-0.20615600
C	1.45626000	-1.09804100	-0.40906600	C	1.46926000	-1.22250800	-0.20406600
C	0.74131500	0.03735600	-0.00589500	C	0.72113700	-0.03042000	0.00351700
C	1.46877800	1.16584300	0.39390800	C	1.45479000	1.17078500	0.22154400
C	2.85993600	1.15740200	0.39480700	C	2.82672700	1.17606300	0.23032700
C	5.05854100	0.00456800	0.00488100	C	5.03140100	0.00413600	0.01078700
C	5.75700600	-1.14646500	0.39396400	C	5.76657100	-1.14970300	0.35059300
C	7.14947500	-1.17151700	0.39226900	C	7.15546000	-1.13037000	0.35047100
C	7.86984400	-0.04215700	0.00486400	C	7.83618900	0.03528900	-0.00447500
C	7.18647800	1.11070600	-0.38121900	C	7.12164600	1.18708300	-0.35097700
C	5.79343600	1.13325400	-0.38217900	C	5.73575600	1.17686300	-0.33568800
H	3.37184200	-1.99287100	-0.75232600	H	3.37553200	-2.13338400	-0.41960400
H	0.92057000	-1.97985100	-0.74929800	H	0.95944800	-2.15567100	-0.41675800
H	0.93407700	2.04245900	0.75379800	H	0.92595200	2.09074800	0.44674100
H	3.40407600	2.02753800	0.75599500	H	3.35290500	2.09698100	0.45947900
H	5.20760000	-2.02719200	0.71430100	H	5.25363600	-2.05845400	0.64860700
H	7.66963700	-2.07615300	0.69128900	H	7.70613300	-2.02486600	0.62195700
H	8.95529300	-0.06953000	-0.00711600	H	8.92155200	0.04160500	-0.01971000
H	7.74145900	1.98806200	-0.70599500	H	7.65308700	2.08621200	-0.64913900
H	5.26377300	2.02076200	-0.72223800	H	5.19137900	2.06482900	-0.64441200
C	-5.05854100	0.00457100	-0.00488800	C	-5.03140100	0.00413900	-0.01079300
C	-5.75700700	-1.14646100	-0.39397400	C	-5.76657100	-1.14969900	-0.35060300
C	-7.14947600	-1.17151200	-0.39227800	C	-7.15546100	-1.13036400	-0.35048000
C	-7.86984400	-0.04215200	-0.00487000	C	-7.83618900	0.03529400	0.00446900
C	-7.18647700	1.11070900	0.38121600	C	-7.12164500	1.18708600	0.35097400
C	-5.79343500	1.13325600	0.38217600	C	-5.73575500	1.17686600	0.33568500
C	-3.57475200	0.02121200	0.00621200	C	-3.57081800	-0.01377600	-0.01067500
C	-2.84670800	-1.10550100	0.41035000	C	-2.84519900	-1.21155900	0.20614600
C	-1.45626000	-1.09804100	0.40905600	C	-1.46926100	-1.22250800	0.20405700
C	-0.74131500	0.03735600	0.00588900	C	-0.72113700	-0.03042000	-0.00352300
C	-1.46877800	1.16584500	-0.39391200	C	-1.45478900	1.17078700	-0.22154800
C	-2.85993500	1.15740400	-0.39481000	C	-2.82672600	1.17606500	-0.23033100

H	-5.20760200	-2.02718800	-0.71431200	H	-5.25363700	-2.05844900	-0.64861900
H	-7.66963900	-2.07614700	-0.69130000	H	-7.70613500	-2.02486000	-0.62196800
H	-8.95529300	-0.06952400	0.00711000	H	-8.92155200	0.04161000	0.01970400
H	-7.74145700	1.98806500	0.70599400	H	-7.65308600	2.08621500	0.64913800
H	-5.26377100	2.02076400	0.72223600	H	-5.19137800	2.06483000	0.64441100
H	-3.37184300	-1.99287100	0.75231500	H	-3.37553300	-2.13338300	0.41959200
H	-0.92057100	-1.97985300	0.74928700	H	-0.95944900	-2.15567100	0.41674700
H	-0.93407600	2.04246100	-0.75379900	H	-0.92595100	2.09075000	-0.44674200
H	-3.40407500	2.02754100	-0.75599600	H	-3.35290300	2.09698400	-0.45948000

(34) OP (F_z = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	3.57329400	-0.00589600	0.07707000	C	3.57039400	0.00305100	0.02353800
C	2.84373000	-1.13966400	-0.30270800	C	2.83761800	-1.19338200	-0.18463300
C	1.45341400	-1.13890000	-0.27360200	C	1.46373500	-1.19679700	-0.18373900
C	0.74130200	-0.00451800	0.13692800	C	0.72113000	0.00025200	0.02062000
C	1.47131300	1.12740700	0.52149900	C	1.46106700	1.19943700	0.22143400
C	2.86160800	1.12681100	0.49178200	C	2.83455800	1.19857800	0.22611200
C	5.05562000	0.00135800	0.01511700	C	5.03053600	0.00529800	0.01963000
C	5.79577400	-1.12380800	0.40070500	C	5.75254700	-1.14787600	0.38985200
C	7.18585600	-1.12595800	0.31467900	C	7.13936500	-1.14672900	0.37538200
C	7.86094500	-0.00094600	-0.15737900	C	7.83387000	-0.00294200	-0.02781200
C	7.13513400	1.12579400	-0.54186400	C	7.13354900	1.14583200	-0.40391200
C	5.74507800	1.12645000	-0.45578500	C	5.74646900	1.15539000	-0.37131700
H	3.37026700	-2.01394400	-0.67589000	H	3.36779100	-2.11283300	-0.40813100
H	0.91150300	-2.01264700	-0.62540600	H	0.94687800	-2.12285900	-0.40861400
H	0.94242400	2.01379500	0.86248400	H	0.94056900	2.12987000	0.41797300
H	3.40599600	2.01271500	0.80881000	H	3.36372600	2.12474100	0.42279700
H	5.27512900	-2.00131500	0.77584100	H	5.22395300	-2.03814800	0.71640700
H	7.74253300	-2.01184100	0.60695100	H	7.68354400	-2.03937800	0.66618300
H	8.94325700	-0.00843300	-0.24408100	H	8.91871200	-0.01121100	-0.06267400
H	7.64992900	1.99672300	-0.93636200	H	7.67150300	2.02507700	-0.74241800
H	5.18413000	1.99167400	-0.79882700	H	5.21430500	2.03998500	-0.70671700
C	-5.05562000	-0.00136700	0.01511400	C	-5.03053700	-0.00530700	0.01962700
C	-5.74507400	-1.12646100	-0.45578700	C	-5.74646800	-1.15539900	-0.37131800
C	-7.13513000	-1.12580900	-0.54186700	C	-7.13354900	-1.14584100	-0.40391500
C	-7.86094500	0.00093000	-0.15738400	C	-7.83387000	0.00293300	-0.02781600
C	-7.18585900	1.12594400	0.31467400	C	-7.13936500	1.14672100	0.37537600
C	-5.79577800	1.12379800	0.40070100	C	-5.75254700	1.14786800	0.38984700
C	-3.57329400	0.00589100	0.07706900	C	-3.57039400	-0.00306000	0.02353600
C	-2.86160700	-1.12681500	0.49178100	C	-2.83455900	-1.19858700	0.22611200
C	-1.47131200	-1.12741000	0.52149900	C	-1.46106700	-1.19944500	0.22143400
C	-0.74130200	0.00451700	0.13692900	C	-0.72113000	-0.00026000	0.02062000

C	-1.45341500	1.13889700	-0.27360400	C	-1.46373500	1.19678900	-0.18374100
C	-2.84373200	1.13965900	-0.30271100	C	-2.83761800	1.19337300	-0.18463600
H	-5.18412400	-1.99168400	-0.79882600	H	-5.21430400	-2.03999500	-0.70671700
H	-7.64992300	-1.99674000	-0.93636400	H	-7.67150200	-2.02508700	-0.74241900
H	-8.94325700	0.00841400	-0.24408700	H	-8.91871200	0.01120200	-0.06268000
H	-7.74253900	2.01182600	0.60694500	H	-7.68354500	2.03937100	0.66617600
H	-5.27513500	2.00130700	0.77583700	H	-5.22395300	2.03814000	0.71640100
H	-3.40599500	-2.01272000	0.80880900	H	-3.36372600	-2.12474900	0.42279700
H	-0.94242200	-2.01379700	0.86248300	H	-0.94057000	-2.12987800	0.41797500
H	-0.91150600	2.01264400	-0.62541000	H	-0.94687800	2.12285000	-0.40861700
H	-3.37026900	2.01393800	-0.67589600	H	-3.36779100	2.11282400	-0.40813600

(35) OP (F_z = 0.50 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	3.57137500	-0.01282700	0.17027400	C	3.57081600	0.00669100	0.05467100
C	2.83121200	-1.14891200	-0.18173000	C	2.83962000	-1.19261300	-0.14178600
C	1.44193400	-1.14705000	-0.11453600	C	1.46539800	-1.19707700	-0.14112800
C	0.74143100	-0.01008400	0.30973700	C	0.72131000	0.00050400	0.05704900
C	1.48290800	1.12091900	0.67533500	C	1.46069000	1.20227100	0.24591200
C	2.87214000	1.12005000	0.60544100	C	2.83417600	1.20347400	0.24619700
C	5.04835400	0.00304300	0.02852800	C	5.03074200	0.01160100	0.03890300
C	5.81827600	-1.10839000	0.39491000	C	5.75779400	-1.13257700	0.42695300
C	7.19816000	-1.11258100	0.20380400	C	7.14375700	-1.13599200	0.38051300
C	7.83168900	-0.00391600	-0.35700500	C	7.83149100	-0.00728200	-0.07536400
C	7.07586300	1.10971100	-0.72190100	C	7.12590600	1.13288500	-0.46711100
C	5.69632900	1.11346100	-0.52864700	C	5.73956300	1.14867700	-0.40014800
H	3.34545500	-2.01818200	-0.58267100	H	3.37081900	-2.11036500	-0.37055200
H	0.89108900	-2.01498600	-0.46665200	H	0.95090700	-2.12303500	-0.37163200
H	0.96256900	2.01455100	1.01161500	H	0.93966600	2.13629000	0.42278500
H	3.42643500	2.01270800	0.88538900	H	3.36411400	2.13433100	0.41818100
H	5.32606100	-1.98051600	0.81916400	H	5.23195500	-2.01568700	0.77763000
H	7.77666800	-1.99459800	0.46453200	H	7.69249500	-2.02634800	0.67054500
H	8.90096300	-0.02082900	-0.54452500	H	8.91408200	-0.02564900	-0.15227100
H	7.55407300	1.95930300	-1.19973900	H	7.65690400	1.99403800	-0.85891900
H	5.10723000	1.95991000	-0.87136200	H	5.20160900	2.02000300	-0.76046800
C	-5.04835400	-0.00305100	0.02852500	C	-5.03074200	-0.01161000	0.03890000
C	-5.69632900	-1.11347100	-0.52864800	C	-5.73956200	-1.14868700	-0.40014800
C	-7.07586300	-1.10972000	-0.72190300	C	-7.12590600	-1.13289500	-0.46711300
C	-7.83168900	0.00390800	-0.35700900	C	-7.83149100	0.00727300	-0.07536900
C	-7.19815900	1.11257400	0.20379800	C	-7.14375700	1.13598400	0.38050600
C	-5.81827500	1.10838300	0.39490300	C	-5.75779400	1.13256900	0.42694800
C	-3.57137500	0.01281800	0.17027200	C	-3.57081600	-0.00670000	0.05466900
C	-2.87214100	-1.12005900	0.60544200	C	-2.83417600	-1.20348200	0.24619700

C	-1.48290900	-1.12092800	0.67533700	C	-1.46069000	-1.20228000	0.24591300
C	-0.74143100	0.01007400	0.30973600	C	-0.72131000	-0.00051200	0.05704900
C	-1.44193400	1.14704000	-0.11453900	C	-1.46539700	1.19706800	-0.14113100
C	-2.83121200	1.14890200	-0.18173400	C	-2.83962000	1.19260400	-0.14179000
H	-5.10723100	-1.95992100	-0.87136200	H	-5.20160900	-2.02001400	-0.76046600
H	-7.55407400	-1.95931300	-1.19973900	H	-7.65690400	-1.99404900	-0.85891900
H	-8.90096200	0.02082200	-0.54453000	H	-8.91408200	0.02564000	-0.15227600
H	-7.77666700	1.99459200	0.46452300	H	-7.69249600	2.02634100	0.67053700
H	-5.32606000	1.98050900	0.81915600	H	-5.23195500	2.01568000	0.77762200
H	-3.42643600	-2.01271600	0.88539200	H	-3.36411400	-2.13433900	0.41818300
H	-0.96257000	-2.01456000	1.01161900	H	-0.93966700	-2.13629800	0.42278900
H	-0.89108800	2.01497400	-0.46665700	H	-0.95090600	2.12302500	-0.37163600
H	-3.34545300	2.01817100	-0.58267700	H	-3.37081900	2.11035600	-0.37055800

(36) OA (F = 0.00 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.87824900	0.71756400	-0.00003500	C	-4.87705900	0.70744200	0.00000000
C	-3.70573400	1.40877400	-0.00003500	C	-3.69073000	1.40873700	0.00000100
C	-2.44256900	0.72251200	-0.00001000	C	-2.45212000	0.71871000	0.00000000
C	-2.44256400	-0.72252300	-0.00000200	C	-2.45212200	-0.71871300	-0.00000200
C	-3.70569100	-1.40883600	-0.00001000	C	-3.69073900	-1.40873500	-0.00000300
C	-4.87825100	-0.71768100	-0.00002000	C	-4.87706300	-0.70743400	-0.00000100
H	-1.23334700	2.49251400	-0.00002900	H	-1.22774600	2.49492800	0.00000200
H	-5.82549100	1.24836100	-0.00003900	H	-5.82195800	1.24084600	0.00000100
H	-3.70133800	2.49600900	-0.00003700	H	-3.69114000	2.49501700	0.00000200
C	-1.23396400	1.40403600	-0.00001800	C	-1.22530400	1.40703200	0.00000100
C	-1.23389700	-1.40391000	0.00000100	C	-1.22531500	-1.40704100	-0.00000200
H	-3.70126500	-2.49606800	0.00001200	H	-3.69115000	-2.49501400	-0.00000400
H	-5.82548000	-1.24848800	-0.00001200	H	-5.82196500	-1.24083100	-0.00000200
C	0.00034600	-0.72135500	0.00001600	C	0.00000000	-0.72289400	-0.00000200
C	0.00009200	0.72175000	0.00001600	C	0.00000600	0.72287600	-0.00000100
H	-1.23335600	-2.49239700	-0.00000900	H	-1.22775400	-2.49493700	-0.00000400
C	1.23387900	1.40389700	0.00012600	C	1.22530700	1.40702900	-0.00000400
C	2.44276900	0.72230700	0.00008200	C	2.45213000	0.71869700	-0.00000300
C	2.44272200	-0.72236000	0.00007000	C	2.45212900	-0.71872100	-0.00000400
C	1.23361500	-1.40399000	0.00008800	C	1.22530100	-1.40704600	-0.00000600
H	3.70135800	2.49586300	-0.00001800	H	3.69115900	2.49499900	0.00000100
H	1.23371700	2.49238900	0.00014100	H	1.22776700	2.49492500	-0.00000200
C	3.70548400	1.40863800	-0.00006600	C	3.69073400	1.40871900	0.00000100
C	3.70548200	-1.40868200	-0.00006600	C	3.69072600	-1.40874700	-0.00000200
H	1.23337500	-2.49243400	0.00007200	H	1.22775800	-2.49494200	-0.00000600
C	4.87826600	-0.71747800	-0.00006300	C	4.87706600	-0.70744600	-0.00000300
C	4.87825100	0.71737700	-0.00006300	C	4.87707100	0.70741600	-0.00000100
H	3.70127700	-2.49591500	-0.00005900	H	3.69115400	-2.49502600	-0.00000400
H	5.82533500	-1.24858900	-0.00005500	H	5.82195700	-1.24086500	-0.00000400
H	5.82529200	1.24852400	-0.00003200	H	5.82196500	1.24082900	-0.00000200

(37) OA (F_x = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.87701400	0.71766100	0.00000100	C	-4.88115100	0.70543600	0.00000000
C	-3.70578500	1.41051500	-0.00000200	C	-3.68895900	1.40978800	0.00000100
C	-2.44388000	0.72310400	-0.00000600	C	-2.45075600	0.72128300	0.00000000
C	-2.44385400	-0.72307200	-0.00000400	C	-2.45075900	-0.72128600	-0.00000200
C	-3.70573900	-1.41052800	0.00000500	C	-3.68896600	-1.40978600	-0.00000300
C	-4.87699400	-0.71772400	0.00000500	C	-4.88115400	-0.70542900	-0.00000200
H	-1.23557600	2.49307100	-0.00001400	H	-1.23198800	2.49558900	0.00000100
H	-5.82479900	1.24634300	0.00000000	H	-5.82599400	1.23934100	0.00000100
H	-3.70323500	2.49736000	-0.00000300	H	-3.69377400	2.49612600	0.00000200
C	-1.23479900	1.40477400	-0.00000400	C	-1.22986300	1.40769600	0.00000000
C	-1.23475000	-1.40468200	-0.00000600	C	-1.22987000	-1.40770400	-0.00000300
H	-3.70314900	-2.49737400	0.00000800	H	-3.69378400	-2.49612300	-0.00000400
H	-5.82476000	-1.24643500	0.00000600	H	-5.82600000	-1.23932900	-0.00000200
C	-0.00120800	-0.72195500	-0.00000600	C	0.00769500	-0.72232300	-0.00000200
C	-0.00129400	0.72211200	-0.00000500	C	0.00769900	0.72230900	-0.00000100
H	-1.23549200	-2.49297800	-0.00001400	H	-1.23199800	-2.49559700	-0.00000400
C	1.23327300	1.40359200	-0.00002000	C	1.22428300	1.40638100	0.00000000
C	2.44288500	0.72232600	-0.00000500	C	2.45304900	0.71695200	-0.00000100
C	2.44288700	-0.72237500	-0.00000900	C	2.45304600	-0.71697500	-0.00000300
C	1.23322100	-1.40359000	-0.00002100	C	1.22427700	-1.40639800	-0.00000300
H	3.70041500	2.49463900	0.00002800	H	3.69307100	2.49362000	0.00000000
H	1.23189200	2.49221600	0.00000500	H	1.22619400	2.49423000	0.00000100
C	3.70666000	1.40699500	0.00003800	C	3.69608200	1.40718900	-0.00000200
C	3.70663100	-1.40706700	0.00002200	C	3.69607600	-1.40721700	-0.00000400
H	1.23181000	-2.49219500	-0.00000400	H	1.22618400	-2.49424800	-0.00000400
C	4.88198600	-0.71762500	-0.00000300	C	4.87855300	-0.70958600	-0.00000400
C	4.88199300	0.71752100	0.00000600	C	4.87855600	0.70955400	-0.00000200
H	3.70034300	-2.49471400	0.00000600	H	3.69306200	-2.49364700	-0.00000500
H	5.82919300	-1.25081400	-0.00003500	H	5.82362500	-1.24371200	-0.00000400
H	5.82920400	1.25070900	-0.00002200	H	5.82363100	1.24367500	-0.00000200

(38) OA (F_x = 0.50 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.87725500	0.71776300	-0.00000400	C	-4.89033800	0.70398300	0.00000000
C	-3.70597300	1.41266400	-0.00000100	C	-3.69135300	1.41007500	0.00000000
C	-2.44629000	0.72450600	0.00000100	C	-2.44792100	0.72385100	-0.00000100
C	-2.44628500	-0.72450100	0.00000000	C	-2.44792400	-0.72385400	-0.00000200
C	-3.70596900	-1.41266800	-0.00000300	C	-3.69135900	-1.41007300	-0.00000300
C	-4.87725400	-0.71777500	-0.00000500	C	-4.89034100	-0.70397600	-0.00000200
H	-1.23826400	2.49379600	0.00000300	H	-1.23701600	2.49668400	0.00000100
H	-5.82702100	1.24311100	-0.00000500	H	-5.83529100	1.23952800	0.00000100
H	-3.70652500	2.49910000	0.00000000	H	-3.70076600	2.49662500	0.00000200
C	-1.23502700	1.40563900	0.00000300	C	-1.23560300	1.40882500	0.00000000
C	-1.23502500	-1.40562300	0.00000000	C	-1.23560900	-1.40883300	-0.00000300
H	-3.70650900	-2.49910400	-0.00000500	H	-3.70077600	-2.49662300	-0.00000400
H	-5.82701800	-1.24312500	-0.00000600	H	-5.83529600	-1.23951700	-0.00000200
C	-0.00206200	-0.72387400	0.00000400	C	0.01260200	-0.72132000	-0.00000200
C	-0.00206900	0.72389700	0.00000500	C	0.01260500	0.72130700	-0.00000100
H	-1.23823900	-2.49378000	-0.00000200	H	-1.23702600	-2.49669200	-0.00000400
C	1.23333500	1.40377800	0.00000800	C	1.22664600	1.40542000	0.00000000
C	2.44462400	0.72345800	-0.00000100	C	2.45469700	0.71650100	-0.00000200
C	2.44462900	-0.72348700	-0.00000200	C	2.45469400	-0.71652400	-0.00000300
C	1.23332100	-1.40377900	0.00000500	C	1.22664000	-1.40543800	-0.00000300
H	3.69984800	2.49307600	-0.00000500	H	3.69847700	2.49222600	0.00000000
H	1.22985500	2.49272200	0.00000600	H	1.22744400	2.49324600	0.00000100
C	3.70832600	1.40468500	-0.00001100	C	3.70348600	1.40544900	-0.00000100
C	3.70831300	-1.40472500	-0.00001500	C	3.70348000	-1.40547600	-0.00000400
H	1.22981100	-2.49272200	0.00000100	H	1.22743400	-2.49326400	-0.00000500
C	4.88796000	-0.71782400	-0.00000700	C	4.88481100	-0.71139200	-0.00000400
C	4.88796200	0.71777200	-0.00000500	C	4.88481400	0.71136000	-0.00000200
H	3.69982300	-2.49311500	-0.00001100	H	3.69846700	-2.49225400	-0.00000500
H	5.83451800	-1.25543300	-0.00000300	H	5.83019000	-1.24736500	-0.00000400
H	5.83452400	1.25537700	0.00000100	H	5.83019500	1.24732800	-0.00000200

(39) OA (F_y = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.87945600	0.71029400	-0.00000200	C	-4.87711600	0.70527700	0.00000000
C	-3.70959600	1.40723100	0.00000000	C	-3.69224900	1.40832400	0.00000000
C	-2.44359000	0.72667400	0.00000100	C	-2.45214000	0.72094300	-0.00000100
C	-2.44201300	-0.71817100	-0.00000200	C	-2.45236300	-0.71660200	-0.00000200
C	-3.70181100	-1.41045300	-0.00000500	C	-3.68933900	-1.40939100	-0.00000300
C	-4.87742700	-0.72459800	-0.00000300	C	-4.87740300	-0.70953100	-0.00000200
H	-1.23707500	2.49927200	0.00000200	H	-1.22856900	2.49703400	0.00000100
H	-5.82966800	1.23689200	-0.00000100	H	-5.82343700	1.23661700	0.00000100
H	-3.70906500	2.49526700	0.00000100	H	-3.69283400	2.49502500	0.00000200
C	-1.23545100	1.41003400	0.00000100	C	-1.22592900	1.40879500	0.00000000
C	-1.23234600	-1.39813100	-0.00000200	C	-1.22471500	-1.40556300	-0.00000300
H	-3.69360400	-2.49719100	-0.00000600	H	-3.68972400	-2.49558900	-0.00000400
H	-5.82174100	-1.25964500	-0.00000400	H	-5.82087700	-1.24522200	-0.00000200
C	0.00004400	-0.71300000	0.00000000	C	0.00000100	-0.71963700	-0.00000300
C	0.00004000	0.73031600	0.00000100	C	0.00000400	0.72627800	-0.00000100
H	-1.23015900	-2.48612500	-0.00000400	H	-1.22698500	-2.49343800	-0.00000400
C	1.23539200	1.41001700	0.00000600	C	1.22593600	1.40879000	-0.00000100
C	2.44364900	0.72662000	0.00000200	C	2.45214800	0.72093200	-0.00000200
C	2.44207200	-0.71814400	-0.00000100	C	2.45236500	-0.71661100	-0.00000300
C	1.23227100	-1.39813000	0.00000400	C	1.22471100	-1.40556800	-0.00000400
H	3.70908600	2.49522000	-0.00000400	H	3.69285000	2.49500900	0.00000000
H	1.23712000	2.49925500	0.00000500	H	1.22858600	2.49703000	0.00000100
C	3.70955800	1.40718500	-0.00001000	C	3.69225700	1.40830800	-0.00000100
C	3.70176200	-1.41044000	-0.00001400	C	3.68933600	-1.40940600	-0.00000400
H	1.23018000	-2.48612300	0.00000000	H	1.22698200	-2.49344300	-0.00000500
C	4.87744300	-0.72457000	-0.00000700	C	4.87740500	-0.70954900	-0.00000300
C	4.87947900	0.71023000	-0.00000600	C	4.87712400	0.70525500	-0.00000200
H	3.69361000	-2.49717700	-0.00000800	H	3.68971900	-2.49560400	-0.00000500
H	5.82171100	-1.25969800	0.00000000	H	5.82087500	-1.24524900	-0.00000400
H	5.82965100	1.23690100	0.00000100	H	5.82344500	1.23659600	-0.00000100

(40) OA (F_y = 0.50 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.88107900	0.70272000	-0.00000100	C	-4.87758300	0.70304500	0.00000000
C	-3.71379200	1.40584800	0.00000000	C	-3.69391700	1.40814900	0.00000100
C	-2.44488300	0.73111700	0.00000100	C	-2.45242700	0.72330700	-0.00000100
C	-2.44168500	-0.71397500	-0.00000200	C	-2.45285500	-0.71460600	-0.00000200
C	-3.69807400	-1.41234400	-0.00000500	C	-3.68806600	-1.41029900	-0.00000300
C	-4.87695600	-0.73153400	-0.00000400	C	-4.87814200	-0.71157300	-0.00000200
H	-1.24067600	2.50684800	0.00000200	H	-1.22944300	2.49975900	0.00000100
H	-5.83431200	1.22525500	-0.00000100	H	-5.82533200	1.23252500	0.00000100
H	-3.71738000	2.49507800	0.00000200	H	-3.69480600	2.49562300	0.00000200
C	-1.23708500	1.41645000	0.00000200	C	-1.22659000	1.41084200	0.00000000
C	-1.23082600	-1.39247700	-0.00000300	C	-1.22415300	-1.40436300	-0.00000300
H	-3.68617300	-2.49895200	-0.00000700	H	-3.68854900	-2.49674800	-0.00000400
H	-5.81832300	-1.27110900	-0.00000400	H	-5.82018800	-1.24978100	-0.00000200
C	0.00004200	-0.70446200	0.00000100	C	0.00000100	-0.71652200	-0.00000300
C	0.00004100	0.73931800	0.00000200	C	0.00000400	0.72982400	-0.00000100
H	-1.22677200	-2.48035600	-0.00000400	H	-1.22626500	-2.49252900	-0.00000500
C	1.23702700	1.41643500	0.00000400	C	1.22659800	1.41083700	0.00000000
C	2.44494400	0.73106800	0.00000100	C	2.45243500	0.72329600	-0.00000100
C	2.44174000	-0.71394500	-0.00000200	C	2.45285700	-0.71461600	-0.00000300
C	1.23075000	-1.39247400	0.00000300	C	1.22415000	-1.40436900	-0.00000400
H	3.71740600	2.49503300	-0.00000400	H	3.69482300	2.49560700	0.00000100
H	1.24072100	2.50683300	0.00000500	H	1.22946000	2.49975400	0.00000100
C	3.71375800	1.40580500	-0.00000800	C	3.69392400	1.40813300	-0.00000100
C	3.69802200	-1.41233000	-0.00001300	C	3.68806200	-1.41031400	-0.00000400
H	1.22679200	-2.48035300	-0.00000100	H	1.22626200	-2.49253500	-0.00000500
C	4.87696900	-0.73150600	-0.00000600	C	4.87814400	-0.71159200	-0.00000300
C	4.88110500	0.70265900	-0.00000600	C	4.87759100	0.70302300	-0.00000200
H	3.68617500	-2.49893700	-0.00000600	H	3.68854400	-2.49676200	-0.00000500
H	5.81828800	-1.27116500	0.00000000	H	5.82018500	-1.24980700	-0.00000400
H	5.83429900	1.22526300	0.00000100	H	5.82534000	1.23250300	-0.00000100

(41) OA (F_z = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.87682900	0.71757300	-0.04508400	C	-4.87640100	0.70746200	-0.03201800
C	-3.70492800	1.40882100	-0.00263000	C	-3.69041400	1.40878800	-0.00034100
C	-2.44264700	0.72239900	0.04010800	C	-2.45213300	0.71874900	0.02974300
C	-2.44264900	-0.72240100	0.04010900	C	-2.45213600	-0.71875200	0.02974300
C	-3.70493200	-1.40881900	-0.00262800	C	-3.69042000	-1.40878600	-0.00034100
C	-4.87683100	-0.71756800	-0.04508300	C	-4.87640400	-0.70745400	-0.03201800
H	-1.23342400	2.49227600	0.03932000	H	-1.22765900	2.49487300	0.02575600
H	-5.82249300	1.24820300	-0.10119500	H	-5.82046600	1.24082600	-0.07296700
H	-3.69989900	2.49584500	-0.02332500	H	-3.69052900	2.49498400	-0.01535400
C	-1.23389100	1.40396900	0.05805500	C	-1.22532700	1.40705000	0.03999900
C	-1.23389600	-1.40397300	0.05805600	C	-1.22533300	-1.40705700	0.03999900
H	-3.69990700	-2.49584300	-0.02332100	H	-3.69053900	-2.49498200	-0.01535300
H	-5.82249700	-1.24819500	-0.10119200	H	-5.82047200	-1.24081500	-0.07296700
C	0.00002600	-0.72160400	0.06948100	C	0.00000100	-0.72290900	0.05035500
C	0.00002600	0.72159800	0.06948100	C	0.00000400	0.72289600	0.05035500
H	-1.23342900	-2.49228000	0.03932300	H	-1.22766900	-2.49488100	0.02575700
C	1.23386000	1.40395700	0.05805400	C	1.22533500	1.40704500	0.03999800
C	2.44268400	0.72236200	0.04010500	C	2.45214100	0.71873800	0.02974100
C	2.44268400	-0.72238900	0.04010400	C	2.45213800	-0.71876100	0.02974100
C	1.23385100	-1.40397400	0.05805400	C	1.22533000	-1.40706200	0.03999800
H	3.69991600	2.49581100	-0.02332400	H	3.69054500	2.49496900	-0.01535700
H	1.23345900	2.49226300	0.03932000	H	1.22767400	2.49486900	0.02575500
C	3.70490800	1.40878700	-0.00263000	C	3.69042200	1.40877300	-0.00034400
C	3.70490300	-1.40881700	-0.00263100	C	3.69041700	-1.40880000	-0.00034400
H	1.23343800	-2.49228000	0.03931900	H	1.22766400	-2.49488600	0.02575600
C	4.87684200	-0.71756000	-0.04508900	C	4.87640500	-0.70747300	-0.03202200
C	4.87684400	0.71752600	-0.04508800	C	4.87640800	0.70744100	-0.03202200
H	3.69990800	-2.49584000	-0.02332600	H	3.69053400	-2.49499600	-0.01535600
H	5.82248100	-1.24823400	-0.10119800	H	5.82047000	-1.24084000	-0.07297200
H	5.82248500	1.24819700	-0.10119700	H	5.82047500	1.24080400	-0.07297200

(42) OA (F_z = 0.50 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.87210700	0.71765100	-0.09421600	C	-4.87412200	0.70752900	-0.06769800
C	-3.70263100	1.40903700	-0.00614300	C	-3.68932400	1.40894700	-0.00145200
C	-2.44259300	0.72248600	0.08202100	C	-2.45213700	0.71887400	0.06118600
C	-2.44259500	-0.72248900	0.08202400	C	-2.45214000	-0.71887700	0.06118800
C	-3.70263800	-1.40903500	-0.00613500	C	-3.68932900	-1.40894500	-0.00144800
C	-4.87211000	-0.71764300	-0.09421100	C	-4.87412500	-0.70752200	-0.06769600
H	-1.23289300	2.49191100	0.08200700	H	-1.22736600	2.49470300	0.05484000
H	-5.81282900	1.24785900	-0.20788100	H	-5.81553700	1.24074400	-0.15135600
H	-3.69576300	2.49551000	-0.04729900	H	-3.68849700	2.49489700	-0.03131200
C	-1.23397200	1.40402000	0.11977300	C	-1.22539900	1.40709700	0.08336100
C	-1.23397900	-1.40402900	0.11977900	C	-1.22540400	-1.40710400	0.08336500
H	-3.69577500	-2.49550800	-0.04728500	H	-3.68850700	-2.49489500	-0.03130500
H	-5.81283500	-1.24784700	-0.20787300	H	-5.81554200	-1.24073400	-0.15135200
C	0.00002000	-0.72166800	0.14342500	C	0.00000100	-0.72296400	0.10483400
C	0.00002500	0.72165400	0.14342300	C	0.00000400	0.72295200	0.10483200
H	-1.23290200	-2.49192000	0.08202100	H	-1.22737600	-2.49471000	0.05484800
C	1.23394800	1.40401100	0.11977300	C	1.22540800	1.40709200	0.08335900
C	2.44262600	0.72245500	0.08201700	C	2.45214500	0.71886400	0.06118300
C	2.44262500	-0.72248000	0.08201700	C	2.45214200	-0.71888600	0.06118500
C	1.23394200	-1.40402800	0.11977400	C	1.22540200	-1.40711000	0.08336300
H	3.69577900	2.49548000	-0.04729700	H	3.68851200	2.49488200	-0.03131700
H	1.23292600	2.49190100	0.08200600	H	1.22738200	2.49469800	0.05483900
C	3.70261600	1.40900700	-0.00614200	C	3.68933200	1.40893100	-0.00145700
C	3.70261200	-1.40903500	-0.00614100	C	3.68932700	-1.40895900	-0.00145200
H	1.23290800	-2.49191900	0.08200900	H	1.22737200	-2.49471600	0.05484600
C	4.87211800	-0.71763900	-0.09422000	C	4.87412700	-0.70754100	-0.06770200
C	4.87212000	0.71760800	-0.09422000	C	4.87413000	0.70750800	-0.06770400
H	3.69577400	-2.49550800	-0.04729600	H	3.68850200	-2.49491000	-0.03130900
H	5.81282100	-1.24788200	-0.20788200	H	5.81554000	-1.24075900	-0.15135900
H	5.81282500	1.24784800	-0.20788200	H	5.81554600	1.24072200	-0.15136300

(43) PT (F = 0.00 V/Å)

Neutral			
elements	x	y	z
C	-3.19028100	-0.32517000	0.16809500
C	-2.60896500	-1.53916200	0.43523400
S	-1.97748700	0.90225700	-0.02782400
C	-1.19049600	-1.48200900	0.50365400
H	-3.18553400	-2.43928600	0.61762300
C	-0.69209300	-0.22103600	0.28547900
H	-0.55925000	-2.33271500	0.73764400
C	0.69209300	0.22103700	0.28547800
C	1.19049600	1.48201100	0.50364800
S	1.97748700	-0.90225600	-0.02782600
C	2.60896500	1.53916300	0.43522800
H	0.55925100	2.33271800	0.73763700
C	3.19028100	0.32517000	0.16809500
H	3.18553400	2.43928800	0.61761500
C	-4.62005100	-0.01199500	0.03841400
C	-5.12596000	1.24848000	0.38500300
C	-5.51025700	-0.98683900	-0.43507700
C	-6.48496100	1.52475000	0.26514000
H	-4.45308800	2.01028500	0.77030900
C	-6.86991000	-0.71227700	-0.54311100
H	-5.12682100	-1.95655600	-0.73933900
C	-7.36343600	0.54513400	-0.19536600
H	-6.85923800	2.50598900	0.54134400
H	-7.54433500	-1.47878900	-0.91320800
H	-8.42369900	0.76046400	-0.28571000
C	4.62005100	0.01199400	0.03841600
C	5.12595800	-1.24848100	0.38500600
C	5.51025800	0.98683800	-0.43507400
C	6.48496000	-1.52475200	0.26514500
H	4.45308600	-2.01028500	0.77031200
C	6.86991100	0.71227500	-0.54310600
H	5.12682300	1.95655500	-0.73933800
C	7.36343600	-0.54513600	-0.19536000
H	6.85923600	-2.50599000	0.54135000
H	7.54433700	1.47878700	-0.91320200
H	8.42369900	-0.76046700	-0.28570300

Cationic			
elements	x	y	z
C	-3.16921800	-0.30655000	0.09321500
C	-2.56077600	-1.57316600	0.10959100
S	-1.98044500	0.95039500	0.07426900
C	-1.17706100	-1.51942300	0.11780100
H	-3.12672600	-2.49557300	0.14532000
C	-0.67267900	-0.20379500	0.10377000
H	-0.53575500	-2.39404700	0.14663900
C	0.67267900	0.20379500	0.10377000
C	1.17706100	1.51942300	0.11779900
S	1.98044500	-0.95039600	0.07427200
C	2.56077600	1.57316600	0.10958900
H	0.53575500	2.39404700	0.14663500
C	3.16921800	0.30654900	0.09321600
H	3.12672600	2.49557300	0.14531700
C	-4.58745200	-0.00835000	0.08809400
C	-5.06247800	1.27879600	0.40747900
C	-5.51475000	-1.01598100	-0.24475000
C	-6.42272000	1.54740600	0.39765200
H	-4.36623500	2.06513800	0.68748300
C	-6.87417400	-0.74006500	-0.25583000
H	-5.16949000	-2.00724200	-0.51963500
C	-7.33178900	0.53948500	0.06620600
H	-6.77861700	2.53971200	0.65367100
H	-7.57976500	-1.52019200	-0.52137200
H	-8.39610600	0.75182000	0.05869200
C	4.58745200	0.00835000	0.08809600
C	5.06247800	-1.27879600	0.40748500
C	5.51475000	1.01598000	-0.24474900
C	6.42272000	-1.54740600	0.39765800
H	4.36623400	-2.06513700	0.68748900
C	6.87417400	0.74006400	-0.25582800
H	5.16949100	2.00724000	-0.51963600
C	7.33178900	-0.53948600	0.06621100
H	6.77861700	-2.53971100	0.65368000
H	7.57976500	1.52019100	-0.52137100
H	8.39610600	-0.75182000	0.05869800

(44) PT (F_x = 0.25 V/Å)

Neutral			
elements	x	y	z
C	-3.19469900	-0.32807000	0.15430400
C	-2.60675200	-1.54595900	0.40146600
S	-1.98750700	0.90180700	-0.05197300
C	-1.18987400	-1.48767400	0.44394500
H	-3.18252600	-2.44543200	0.58647600
C	-0.69478500	-0.22325500	0.22740600
H	-0.55725000	-2.34253700	0.66161400
C	0.68578700	0.21872400	0.22044500
C	1.18267600	1.49435200	0.36070900
S	1.98046600	-0.91867500	-0.00139900
C	2.59939700	1.55042700	0.30489700
H	0.54564000	2.35595300	0.52713200
C	3.19127600	0.32407100	0.12542200
H	3.16500800	2.46710700	0.43477700
C	-4.62563400	-0.01207600	0.04909600
C	-5.12372200	1.24146000	0.42953700
C	-5.51867900	-0.98145900	-0.42943400
C	-6.48484600	1.51688000	0.33793400
H	-4.44720100	1.99563700	0.82438500
C	-6.87979300	-0.70589300	-0.51204700
H	-5.14082900	-1.94597600	-0.75680000
C	-7.36735600	0.54391200	-0.12970400
H	-6.86013000	2.48868200	0.64283700
H	-7.56164800	-1.46381800	-0.88449700
H	-8.42926400	0.75764600	-0.19615700
C	4.62074800	0.01404100	0.04245300
C	5.11967800	-1.25507300	0.37700700
C	5.53590500	0.99372000	-0.37860600
C	6.48128800	-1.53220400	0.29800700
H	4.43331600	-2.02601500	0.71689300
C	6.89768300	0.71889300	-0.44365500
H	5.16674400	1.97042400	-0.67735000
C	7.38067900	-0.54673000	-0.10771300
H	6.83928200	-2.52340500	0.56263700
H	7.58326700	1.49444300	-0.77525900
H	8.44365800	-0.76393500	-0.16816000

Cationic			
elements	x	y	z
C	-3.19066800	-0.29439000	0.03465400
C	-2.56452000	-1.55516100	-0.12446700
S	-1.98797500	0.95751900	0.19962700
C	-1.18554800	-1.49365300	-0.10957700
H	-3.11945100	-2.47699500	-0.24322000
C	-0.68960600	-0.18584100	0.06094800
H	-0.53925000	-2.35826900	-0.21514200
C	0.67075900	0.22291100	0.12074300
C	1.17335200	1.50828900	0.30597200
S	1.97357100	-0.92285900	-0.04941200
C	2.57529300	1.55455800	0.31549200
H	0.53893300	2.37774700	0.44272900
C	3.16508200	0.31278900	0.14109100
H	3.14719200	2.46043200	0.47840000
C	-4.58767800	-0.00892100	0.06636200
C	-5.06287400	1.31893000	0.24861400
C	-5.53564000	-1.05981000	-0.08489200
C	-6.41580300	1.58030800	0.27860100
H	-4.35969300	2.13915100	0.36754300
C	-6.88870200	-0.78972600	-0.05410000
H	-5.20272600	-2.08179800	-0.22680600
C	-7.33528400	0.52781000	0.12755500
H	-6.77364000	2.59449100	0.41868500
H	-7.60737000	-1.59372600	-0.17008200
H	-8.40048200	0.73654100	0.15179400
C	4.59895800	0.00429500	0.10556000
C	5.08547500	-1.25100000	0.49945900
C	5.51121400	0.98025400	-0.32510600
C	6.44977800	-1.52130400	0.46666800
H	4.39640400	-2.01222400	0.85544900
C	6.87462200	0.70780800	-0.35166000
H	5.14703400	1.94548300	-0.66390500
C	7.34880300	-0.54311900	0.04356900
H	6.80999200	-2.49641000	0.77967800
H	7.56688900	1.47154500	-0.69311300
H	8.41356100	-0.75566400	0.01891600

(45) PT (F_x = 0.50 V/Å)

Neutral			
elements	x	y	z
C	-3.20335800	-0.32740900	0.11676800
C	-2.60339900	-1.56671100	0.26991200
S	-1.99936300	0.91058800	-0.04895400
C	-1.19686800	-1.51228800	0.26902200
H	-3.17656500	-2.47418100	0.41660700
C	-0.69494200	-0.23212500	0.11396400
H	-0.56445500	-2.38499000	0.40442700
C	0.67397000	0.19789600	0.08943200
C	1.17303500	1.49225400	0.05381100
S	1.98767200	-0.94762700	0.09408000
C	2.57946500	1.54917900	0.03877700
H	0.52796600	2.36346900	0.05406100
C	3.19777400	0.31388900	0.06222200
H	3.12471400	2.48754000	0.03454400
C	-4.63004500	-0.00983700	0.07950100
C	-5.10459400	1.25993500	0.44626100
C	-5.55074600	-0.99356100	-0.31971600
C	-6.46663400	1.53611800	0.41946500
H	-4.40919000	2.02492800	0.78481400
C	-6.91213300	-0.71380600	-0.34267400
H	-5.19896700	-1.97121900	-0.63646000
C	-7.37441200	0.55046200	0.02735600
H	-6.82771900	2.51562400	0.71554700
H	-7.61720700	-1.47720700	-0.65515200
H	-8.43825200	0.76549400	0.01123900
C	4.61906200	0.01889800	0.06425400
C	5.11393000	-1.27810200	0.32002900
C	5.57453300	1.02704500	-0.19533800
C	6.47788600	-1.54723100	0.32118300
H	4.41352800	-2.08204200	0.52885200
C	6.93638000	0.75568300	-0.18316500
H	5.23379400	2.03264600	-0.42146800
C	7.40834700	-0.53542600	0.07411100
H	6.81396700	-2.56188300	0.52281000
H	7.63748800	1.56257400	-0.38952600
H	8.47534200	-0.74858500	0.07602800

Cationic			
elements	x	y	z
C	-3.21032900	-0.29031300	0.03739200
C	-2.58501700	-1.54605400	-0.10890000
S	-1.99689500	0.96247600	0.19084800
C	-1.19631900	-1.48189300	-0.09319200
H	-3.13594200	-2.47157200	-0.21964100
C	-0.70724000	-0.18269500	0.06379600
H	-0.55350500	-2.35024600	-0.18974900
C	0.67490200	0.23205000	0.12235100
C	1.18055400	1.50457500	0.30473600
S	1.97017500	-0.91926500	-0.04984900
C	2.59362600	1.54551200	0.30882200
H	0.55220600	2.37785500	0.44245100
C	3.17853000	0.31104900	0.13223400
H	3.16327100	2.45394300	0.47062900
C	-4.60494600	-0.00664000	0.06650000
C	-5.08770700	1.33099900	0.23510100
C	-5.55887500	-1.06939400	-0.07324800
C	-6.43459000	1.58833900	0.26333200
H	-4.38394000	2.15204900	0.34358100
C	-6.90639800	-0.80669400	-0.04480400
H	-5.22089200	-2.09105700	-0.20367600
C	-7.35909300	0.52206800	0.12383400
H	-6.80298900	2.60065300	0.39197700
H	-7.62856200	-1.60983400	-0.15059500
H	-8.42612300	0.72852000	0.14687400
C	4.61489200	0.00151100	0.09656300
C	5.10941300	-1.25799100	0.47106000
C	5.53708000	0.98047400	-0.31152200
C	6.47544300	-1.52652800	0.44351000
H	4.41944600	-2.02832800	0.80427500
C	6.90251300	0.71354100	-0.32702200
H	5.17422600	1.94990700	-0.63941900
C	7.38100800	-0.54210900	0.04927200
H	6.83053500	-2.50969400	0.73988400
H	7.59383400	1.48796000	-0.65019600
H	8.44770900	-0.75318300	0.02941700

(46) PT (F_y = 0.25 V/Å)

Neutral			
elements	x	y	z
C	-3.18811500	-0.30913100	0.16560100
C	-2.59967500	-1.52040100	0.42467000
S	-1.98009600	0.92912700	-0.01698000
C	-1.18144800	-1.45622000	0.49537500
H	-3.16683900	-2.42843300	0.59610200
C	-0.68829000	-0.19245100	0.28793500
H	-0.54963100	-2.30897300	0.72013500
C	0.69574400	0.25028500	0.28909800
C	1.19958000	1.50651500	0.52813600
S	1.97453700	-0.87170700	-0.04435800
C	2.61849000	1.55707900	0.46137900
H	0.56932000	2.35289500	0.78079500
C	3.19275200	0.34295400	0.17433200
H	3.20342700	2.44810400	0.66305000
C	-4.61958600	-0.00753600	0.03256100
C	-5.13550500	1.25537400	0.35523900
C	-5.50418400	-0.99944900	-0.41658300
C	-6.49785000	1.51652400	0.23670200
H	-4.46656000	2.02865300	0.72517900
C	-6.86677800	-0.74014900	-0.52221800
H	-5.11746000	-1.97409600	-0.69875400
C	-7.37025400	0.51975100	-0.19795900
H	-6.88097700	2.49885200	0.49961100
H	-7.53512800	-1.52332900	-0.86650300
H	-8.43428700	0.71918100	-0.28170900
C	4.62039100	0.01848100	0.04329700
C	5.11180200	-1.25160800	0.37553900
C	5.52071200	0.98764300	-0.42236800
C	6.46678200	-1.54407600	0.24847200
H	4.43240400	-2.01238000	0.75080800
C	6.87661400	0.69673200	-0.53784300
H	5.14534000	1.96310600	-0.72026600
C	7.35551300	-0.57047700	-0.20496100
H	6.82791900	-2.53431100	0.50780700
H	7.56014600	1.45569600	-0.90836000
H	8.41118800	-0.80223100	-0.30633700

Cationic			
elements	x	y	z
C	-3.17206300	-0.32723500	0.09352000
C	-2.57268700	-1.59707400	0.11537800
S	-1.97205700	0.92216500	0.07259400
C	-1.18734600	-1.55393700	0.12433400
H	-3.14203300	-2.51770900	0.15156200
C	-0.67223600	-0.24291600	0.10686600
H	-0.55567700	-2.43582100	0.15576300
C	0.67307500	0.16529700	0.10858000
C	1.16616500	1.48564700	0.12772200
S	1.98930800	-0.97718900	0.07585400
C	2.54837500	1.55061600	0.12177700
H	0.51519000	2.35288300	0.15972400
C	3.16686200	0.28769100	0.10056400
H	3.10912800	2.47583500	0.16225500
C	-4.58690200	-0.01113000	0.08394000
C	-5.04280200	1.29206900	0.36583100
C	-5.52993700	-1.01463500	-0.21340300
C	-6.39863400	1.57916600	0.35290900
H	-4.33326700	2.07562900	0.61984600
C	-6.88653900	-0.72019400	-0.22657800
H	-5.20305000	-2.02062700	-0.45404100
C	-7.32417900	0.57435000	0.05705600
H	-6.73991400	2.58352000	0.58260000
H	-7.60302400	-1.50048300	-0.45989900
H	-8.38603200	0.79909700	0.05077000
C	4.58846200	0.00711500	0.09312000
C	5.08079900	-1.27741800	0.39578600
C	5.50260600	1.03114800	-0.22874400
C	6.44492800	-1.52924800	0.38018200
H	4.39709100	-2.07870700	0.66378900
C	6.86447200	0.77267700	-0.24516500
H	5.14255000	2.02005700	-0.49441800
C	7.33967800	-0.50574200	0.05990600
H	6.81304300	-2.52129100	0.61869200
H	7.56059500	1.56324100	-0.50620600
H	8.40605100	-0.70685500	0.04415800

(47) PT (F_y = 0.50 V/Å)

Neutral			
elements	x	y	z
C	-3.18650400	-0.29595500	0.16669500
C	-2.58950700	-1.50285900	0.42257300
S	-1.98389100	0.95355600	-0.00869500
C	-1.17128200	-1.43028400	0.49406800
H	-3.14556500	-2.41899500	0.58755700
C	-0.68450600	-0.16415200	0.29197900
H	-0.53822900	-2.28381800	0.71334400
C	0.69893800	0.28082200	0.29327000
C	1.20816300	1.53099900	0.55803200
S	1.97131800	-0.83793600	-0.06590800
C	2.62774400	1.57543300	0.49253000
H	0.57920700	2.37132900	0.83496300
C	3.19536100	0.36293100	0.18004700
H	3.22019200	2.45635500	0.71849400
C	-4.61960400	-0.00611600	0.02887500
C	-5.14159400	1.26705600	0.29895900
C	-5.50230800	-1.02152400	-0.37065900
C	-6.50657600	1.51487200	0.17749700
H	-4.47394300	2.05839600	0.63278000
C	-6.86712100	-0.77548500	-0.47760600
H	-5.11618900	-2.00762200	-0.60972500
C	-7.37631700	0.49492100	-0.20623100
H	-6.89503400	2.50565900	0.40291100
H	-7.53175300	-1.57953700	-0.77762300
H	-8.44314400	0.68068700	-0.28782800
C	4.62049000	0.02639400	0.04590400
C	5.09254000	-1.26159600	0.33594500
C	5.53591100	0.99755500	-0.38524600
C	6.44300400	-1.57118300	0.19989100
H	4.40353200	-2.02763300	0.68177300
C	6.88765600	0.68939500	-0.50904700
H	5.17349100	1.98691800	-0.65489600
C	7.34673300	-0.59599300	-0.21956100
H	6.78710100	-2.57644800	0.42135500
H	7.58417700	1.44788400	-0.85788800
H	8.39750700	-0.84403200	-0.33190700

Cationic			
elements	x	y	z
C	-3.17577500	-0.35246800	0.08947400
C	-2.58479800	-1.62576900	0.09678300
S	-1.96307700	0.88938300	0.08773100
C	-1.19765500	-1.59381100	0.10526500
H	-3.15541800	-2.54664400	0.11302900
C	-0.67161000	-0.28734600	0.10570700
H	-0.57636800	-2.48408300	0.12188200
C	0.67348700	0.12279900	0.11677400
C	1.15364700	1.44762300	0.16644600
S	1.99965200	-1.00566900	0.06050900
C	2.53448000	1.52555800	0.16498800
H	0.49244400	2.30627400	0.21804500
C	3.16461400	0.26801500	0.11467500
H	3.08785700	2.45406200	0.22787700
C	-4.58671300	-0.01644200	0.07878900
C	-5.01690000	1.31533700	0.25028600
C	-5.55316100	-1.02457700	-0.10611800
C	-6.36717800	1.62482300	0.23669100
H	-4.28951100	2.10757500	0.41111900
C	-6.90605300	-0.70796800	-0.11819700
H	-5.25320300	-2.05666700	-0.25145700
C	-7.31621200	0.61415700	0.05292400
H	-6.68686000	2.65323500	0.37821300
H	-7.63847300	-1.49543900	-0.26038300
H	-8.37464100	0.85509800	0.04727000
C	4.58995900	0.00634300	0.09873200
C	5.10002700	-1.28362600	0.34346700
C	5.49093600	1.05682600	-0.17479700
C	6.46827400	-1.51705800	0.31783100
H	4.42954000	-2.10850800	0.57062800
C	6.85548600	0.81772500	-0.19984800
H	5.11676600	2.05168000	-0.39764300
C	7.34859900	-0.46778700	0.04667900
H	6.84855100	-2.51519100	0.50770400
H	7.54206200	1.62810300	-0.42553800
H	8.41722400	-0.65556700	0.02108300

(48) PT (F_z = 0.25 V/Å)

Neutral			
elements	x	y	z
C	-3.18991700	-0.34570700	0.07649300
C	-2.60048900	-1.53930400	-0.25492700
S	-1.98452600	0.87577400	0.34726900
C	-1.18087800	-1.47439000	-0.30117500
H	-3.16927000	-2.43901400	-0.46226100
C	-0.69083100	-0.22706400	-0.00395600
H	-0.54347100	-2.30537600	-0.58379800
C	0.69083700	0.22715200	-0.00389300
C	1.18090500	1.47448500	-0.30104800
S	1.98449900	-0.87565900	0.34753600
C	2.60051500	1.53937900	-0.25477300
H	0.54351700	2.30547400	-0.58370700
C	3.18992000	0.34575600	0.07659700
H	3.16931400	2.43907500	-0.46211600
C	-4.62404200	-0.03815800	0.17504800
C	-5.10493800	0.93448700	1.06237000
C	-5.54106400	-0.71559300	-0.64175200
C	-6.46570300	1.22043200	1.13142700
H	-4.40698900	1.46595600	1.70486900
C	-6.90190800	-0.43628400	-0.56315700
H	-5.17878000	-1.43820100	-1.36700400
C	-7.37035100	0.53440200	0.32221400
H	-6.81955000	1.98641200	1.81582100
H	-7.59448000	-0.95892300	-1.21577800
H	-8.43022500	0.76583100	0.36620700
C	4.62403900	0.03815800	0.17509100
C	5.10493800	-0.93447700	1.06242200
C	5.54105200	0.71553700	-0.64176700
C	6.46569500	-1.22046800	1.13143100
H	4.40699600	-1.46590100	1.70496600
C	6.90188900	0.43618300	-0.56322000
H	5.17876400	1.43813700	-1.36702500
C	7.37033400	-0.53449400	0.32216000
H	6.81954400	-1.98644100	1.81583200
H	7.59445200	0.95877800	-1.21588600
H	8.43020100	-0.76596000	0.36611500

Cationic			
elements	x	y	z
C	-3.16900000	-0.30554700	0.07210000
C	-2.56149700	-1.57187500	0.02770400
S	-1.98013600	0.95126000	0.07422600
C	-1.17768600	-1.51886300	0.01954600
H	-3.12801900	-2.49462100	0.01965100
C	-0.67277300	-0.20356900	0.04762200
H	-0.53679500	-2.39371600	-0.01227900
C	0.67277300	0.20356800	0.04762400
C	1.17768600	1.51886300	0.01955900
S	1.98013600	-0.95126100	0.07422200
C	2.56149700	1.57187500	0.02771800
H	0.53679500	2.39371600	-0.01226100
C	3.16900000	0.30554600	0.07210500
H	3.12801900	2.49462100	0.01967200
C	-4.58715100	-0.00746000	0.10974600
C	-5.05389300	1.26444500	0.49553500
C	-5.52157300	-0.99607400	-0.25785000
C	-6.41310600	1.53715500	0.51388000
H	-4.35022700	2.03830000	0.79164600
C	-6.88043500	-0.71554200	-0.24127100
H	-5.18296900	-1.97010200	-0.59541100
C	-7.32962600	0.54909600	0.14428800
H	-6.76202900	2.52208000	0.80603000
H	-7.59050200	-1.47548100	-0.54978200
H	-8.39236700	0.76940600	0.14288400
C	4.58715100	0.00745900	0.10975000
C	5.05389200	-1.26444800	0.49553100
C	5.52157300	0.99607600	-0.25783900
C	6.41310600	-1.53715800	0.51387400
H	4.35022700	-2.03830500	0.79163600
C	6.88043500	0.71554300	-0.24126100
H	5.18296900	1.97010600	-0.59539400
C	7.32962600	-0.54909600	0.14429000
H	6.76202900	-2.52208500	0.80601800
H	7.59050200	1.47548500	-0.54976800
H	8.39236700	-0.76940700	0.14288400

(49) PT (F_z = 0.50 V/Å)

Neutral			
elements	x	y	z
C	-3.19014700	-0.35560700	0.12414500
C	-2.59952400	-1.51606000	-0.30582100
S	-1.98569000	0.83900400	0.50311100
C	-1.17865700	-1.44887400	-0.33852500
H	-3.16827800	-2.38717800	-0.61243200
C	-0.69045900	-0.23141300	0.06359300
H	-0.54043500	-2.24445800	-0.70773900
C	0.69046300	0.23145500	0.06362200
C	1.17867200	1.44893100	-0.33843700
S	1.98567900	-0.83896500	0.50317600
C	2.59953800	1.51610600	-0.30571900
H	0.54045900	2.24452800	-0.70764000
C	3.19015000	0.35562900	0.12419900
H	3.16830100	2.38722700	-0.61230500
C	-4.62581700	-0.04819300	0.21180100
C	-5.13576100	0.79522100	1.20841300
C	-5.51014500	-0.58368000	-0.73604000
C	-6.49514900	1.09428200	1.25529800
H	-4.45769800	1.22179100	1.94457600
C	-6.86980200	-0.29099300	-0.68181100
H	-5.12169500	-1.19428000	-1.54577000
C	-7.36774700	0.55062600	0.31299500
H	-6.87227300	1.76835300	2.02058200
H	-7.53379700	-0.69270700	-1.44080200
H	-8.42404300	0.80141000	0.33246100
C	4.62581600	0.04819000	0.21182800
C	5.13575900	-0.79525300	1.20841700
C	5.51014100	0.58368300	-0.73601200
C	6.49514200	-1.09433700	1.25527700
H	4.45769800	-1.22182800	1.94457800
C	6.86979300	0.29097300	-0.68180700
H	5.12169000	1.19430600	-1.54572500
C	7.36773700	-0.55067500	0.31297500
H	6.87226500	-1.76843100	2.02054200
H	7.53378500	0.69269100	-1.44079900
H	8.42402900	-0.80147900	0.33242100

Cationic			
elements	x	y	z
C	-3.16721100	-0.30063500	0.02968200
C	-2.56610400	-1.56392500	-0.09725300
S	-1.97686700	0.95323600	0.06203600
C	-1.18184900	-1.51405500	-0.12471400
H	-3.13788800	-2.48185000	-0.15708800
C	-0.67326800	-0.20239400	-0.03954700
H	-0.54434100	-2.38559200	-0.23120700
C	0.67326900	0.20239500	-0.03953900
C	1.18184900	1.51405900	-0.12466000
S	1.97686800	-0.95323700	0.06200800
C	2.56610300	1.56392900	-0.09719300
H	0.54434000	2.38560000	-0.23112500
C	3.16721100	0.30063500	0.02970000
H	3.13788700	2.48185600	-0.15699600
C	-4.58401500	-0.00411800	0.12901000
C	-5.03545700	1.21767300	0.66491700
C	-5.52892000	-0.93966300	-0.33563100
C	-6.39274800	1.49296300	0.73425100
H	-4.31989100	1.95108000	1.02839900
C	-6.88627700	-0.65433500	-0.27019000
H	-5.20051000	-1.86388700	-0.80007600
C	-7.32110600	0.55980000	0.26427700
H	-6.73080800	2.44486300	1.13117500
H	-7.60406900	-1.36338100	-0.66881800
H	-8.38153300	0.79005000	0.28892600
C	4.58401500	0.00411600	0.12902200
C	5.03545700	-1.21769300	0.66488700
C	5.52892000	0.93967800	-0.33558400
C	6.39274800	-1.49298400	0.73421500
H	4.31989100	-1.95111400	1.02834100
C	6.88627700	0.65434900	-0.27014900
H	5.20051000	1.86391800	-0.79999900
C	7.32110700	-0.55980300	0.26427600
H	6.73080800	-2.44489800	1.13110600
H	7.60407000	1.36341000	-0.66875100
H	8.38153400	-0.79005400	0.28892000

(50) TA (F = 0.00 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	2.15480700	0.83521200	-0.00012400	C	2.14690200	0.82050700	-0.00011300
C	1.75104200	-0.51980800	0.00017200	C	1.74975000	-0.53750100	-0.00009600
C	2.72559700	-1.52879100	0.00013400	C	2.72527700	-1.54671000	-0.00006800
C	4.06636700	-1.17795200	-0.00020900	C	4.06781200	-1.18377100	-0.00007200
C	4.45474400	0.17216000	-0.00046600	C	4.43858600	0.16359200	-0.00009900
C	3.50641300	1.18630600	-0.00038800	C	3.47866100	1.18792700	-0.00011800
H	2.42515800	-2.57295300	0.00039200	H	2.43340200	-2.59285600	-0.00004200
H	4.82540900	-1.95381600	-0.00023600	H	4.83337200	-1.95170500	-0.00004900
H	5.50965000	0.42809500	-0.00066500	H	5.49057700	0.42980100	-0.00010200
H	3.80801000	2.22943300	-0.00050000	H	3.78220100	2.22978600	-0.00013300
C	-2.15478300	-0.83526600	-0.00007700	C	-2.14693400	-0.82054200	-0.00012600
C	-1.75120000	0.51981000	0.00020400	C	-1.74978100	0.53746800	-0.00010000
C	-2.72568800	1.52875500	0.00014400	C	-2.72530600	1.54667900	-0.00007000
C	-4.06648200	1.17786700	-0.00022600	C	-4.06784400	1.18374400	-0.00008000
C	-4.45474700	-0.17222100	-0.00046300	C	-4.43861900	-0.16361800	-0.00011400
C	-3.50635700	-1.18636800	-0.00040100	C	-3.47869500	-1.18795600	-0.00013600
C	0.31644900	-0.60769300	0.00062600	C	0.32623700	-0.63553600	-0.00007600
C	-0.31643300	0.60792900	0.00063600	C	-0.32626900	0.63550600	-0.00007300
H	-2.42531400	2.57292700	0.00040600	H	-2.43342800	2.59282400	-0.00003700
H	-4.82553400	1.95372100	-0.00026500	H	-4.83340000	1.95168200	-0.00005600
H	-5.50962700	-0.42825200	-0.00070500	H	-5.49060800	-0.42983000	-0.00012300
H	-3.80797600	-2.22949200	-0.00055600	H	-3.78224100	-2.22981300	-0.00015800
S	0.79573000	1.94928400	0.00014700	S	0.76382000	1.93959000	-0.00010800
S	-0.79561500	-1.94924000	0.00015000	S	-0.76385100	-1.93962000	-0.00012200

(51) TA (F_x = 0.25 V/Å)

Neutral			
elements	x	y	z
C	2.15446600	0.83655600	-0.00008200
C	1.74953300	-0.52053100	-0.00000100
C	2.72665400	-1.52735000	-0.00001700
C	4.06849500	-1.17683600	-0.00013000
C	4.45774900	0.17293400	-0.00021400
C	3.50621900	1.18568700	-0.00018500
H	2.42482200	-2.57112200	0.00005500
H	4.82613200	-1.95527100	-0.00014600
H	5.51328400	0.43035100	-0.00029100
H	3.80428900	2.23030700	-0.00022300
C	-2.15567800	-0.83430300	-0.00009800
C	-1.75234400	0.51993200	-0.00001000
C	-2.72546600	1.53084000	-0.00002300
C	-4.06532200	1.17932100	-0.00014000
C	-4.45301300	-0.17147400	-0.00023000
C	-3.50686700	-1.18718600	-0.00020500
C	0.31677300	-0.61272100	0.00011900
C	-0.31699100	0.60343700	0.00012000
H	-2.42695300	2.57556300	0.00006000
H	-4.82644100	1.95250800	-0.00015200
H	-5.50788900	-0.42593700	-0.00030700
H	-3.81224600	-2.22886200	-0.00024600
S	0.79602300	1.94617000	0.00004500
S	-0.79561000	-1.95236500	0.00003200

Cationic			
elements	x	y	z
C	2.14404700	0.81899700	-0.00009500
C	1.75156100	-0.53900100	-0.00009500
C	2.72775500	-1.54535000	-0.00008800
C	4.06847500	-1.18136000	-0.00008400
C	4.43957400	0.16809100	-0.00008600
C	3.48150800	1.18516500	-0.00009100
H	2.43715300	-2.59174300	-0.00008500
H	4.83382600	-1.95009400	-0.00007900
H	5.49189500	0.43461600	-0.00008400
H	3.77940900	2.22872000	-0.00009200
C	-2.14805600	-0.82562100	-0.00010700
C	-1.74562900	0.53352400	-0.00010000
C	-2.72459000	1.54660100	-0.00009200
C	-4.06946800	1.18730200	-0.00009300
C	-4.44076100	-0.15806800	-0.00010200
C	-3.47630500	-1.19111300	-0.00010800
C	0.32152200	-0.63993500	-0.00009400
C	-0.33045700	0.62889800	-0.00009300
H	-2.43115600	2.59249900	-0.00008300
H	-4.83452600	1.95572400	-0.00008700
H	-5.49285200	-0.42517900	-0.00010400
H	-3.78720300	-2.23108000	-0.00011500
S	0.76804200	1.94009000	-0.00009800
S	-0.76414600	-1.94203600	-0.00011200

(52) TA (F_x = 0.50 V/Å)

Neutral			
elements	x	y	z
C	2.15471200	0.83816000	-0.00008600
C	1.74723400	-0.52207600	0.00000200
C	2.72870900	-1.52639400	-0.00001400
C	4.07167100	-1.17600600	-0.00013000
C	4.46245000	0.17386500	-0.00021600
C	3.50639000	1.18509200	-0.00018800
H	2.42602500	-2.56998100	0.00005900
H	4.82825400	-1.95722500	-0.00014900
H	5.51913900	0.43313200	-0.00029600
H	3.80105000	2.23135200	-0.00022800
C	-2.15723100	-0.83398100	-0.00010000
C	-1.75298400	0.52062800	-0.00001000
C	-2.72612300	1.53333500	-0.00002000
C	-4.06514600	1.18138300	-0.00014100
C	-4.45261800	-0.17061400	-0.00023300
C	-3.50788600	-1.18809400	-0.00020700
C	0.31810500	-0.61836800	0.00013200
C	-0.31877000	0.59948500	0.00013000
H	-2.42965300	2.57869700	0.00006700
H	-4.82863100	1.95209400	-0.00015200
H	-5.50799500	-0.42381400	-0.00031300
H	-3.81757600	-2.22833000	-0.00025100
S	0.79620100	1.94315600	0.00004100
S	-0.79570700	-1.95585000	0.00003300

Cationic			
elements	x	y	z
C	2.14287700	0.82010300	-0.00008800
C	1.75203700	-0.53864300	-0.00008500
C	2.73157100	-1.54234400	-0.00008800
C	4.07167300	-1.17942000	-0.00009700
C	4.44469700	0.17169300	-0.00010100
C	3.48672800	1.18303200	-0.00009600
H	2.44193500	-2.58900800	-0.00008500
H	4.83605600	-1.95031700	-0.00009900
H	5.49799000	0.43887300	-0.00010500
H	3.78067400	2.22807300	-0.00009500
C	-2.14668300	-0.83294700	-0.00009700
C	-1.74049600	0.52676600	-0.00008300
C	-2.72778000	1.54446800	-0.00008700
C	-4.07501200	1.19194000	-0.00010400
C	-4.44807200	-0.15171500	-0.00011700
C	-3.47573700	-1.19347700	-0.00011500
C	0.31750700	-0.64194400	-0.00007700
C	-0.33218700	0.62061300	-0.00007400
H	-2.43266600	2.59020000	-0.00008100
H	-4.83849500	1.96257500	-0.00010900
H	-5.50039700	-0.42207400	-0.00012900
H	-3.79525900	-2.23149300	-0.00012000
S	0.77690300	1.94135200	-0.00007100
S	-0.76824500	-1.94666100	-0.00006900

(53) TA (F_y = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	2.15986500	0.84017200	-0.00008200	C	2.14717700	0.82024000	-0.00009400
C	1.75102300	-0.51229100	-0.00000500	C	1.74953700	-0.53722000	-0.00009300
C	2.71978600	-1.52635200	-0.00002100	C	2.72548600	-1.54602700	-0.00008900
C	4.06252100	-1.18229000	-0.00013000	C	4.06895900	-1.18248500	-0.00008800
C	4.45631100	0.16559600	-0.00021200	C	4.43901900	0.16431600	-0.00009000
C	3.51234000	1.18497700	-0.00018200	C	3.47862100	1.18782900	-0.00009200
H	2.41612100	-2.56931600	0.00005000	H	2.43671900	-2.59304600	-0.00008600
H	4.81623800	-1.96281600	-0.00014400	H	4.83336700	-1.95155300	-0.00008400
H	5.51317200	0.41419900	-0.00028700	H	5.49136800	0.42940400	-0.00008900
H	3.81876900	2.22719700	-0.00021900	H	3.78027300	2.23039500	-0.00009200
C	-2.14979200	-0.83033500	-0.00009900	C	-2.14696000	-0.82092600	-0.00010700
C	-1.75151200	0.52762000	-0.00000900	C	-1.75028500	0.53777500	-0.00009600
C	-2.73158200	1.53169900	-0.00002100	C	-2.72520000	1.54756400	-0.00008800
C	-4.07060100	1.17358600	-0.00013800	C	-4.06707200	1.18510100	-0.00009400
C	-4.45321100	-0.17874200	-0.00022700	C	-4.43857000	-0.16287100	-0.00010600
C	-3.50043700	-1.18799300	-0.00020500	C	-3.47905700	-1.18833500	-0.00011200
C	0.31447100	-0.59849100	0.00011200	C	0.32359600	-0.63779900	-0.00009000
C	-0.31837100	0.61725000	0.00011700	C	-0.32892900	0.63322400	-0.00008800
H	-2.43471400	2.57746400	0.00006100	H	-2.43032500	2.59315500	-0.00007700
H	-4.83529700	1.94476200	-0.00015000	H	-4.83370800	1.95226000	-0.00008700
H	-5.50617900	-0.44195300	-0.00030200	H	-5.49023300	-0.43024900	-0.00011000
H	-3.79723700	-2.23229300	-0.00024500	H	-3.78458800	-2.22976900	-0.00012000
S	0.79969900	1.95843100	0.00004400	S	0.76397400	1.93918900	-0.00009000
S	-0.79176300	-1.94043600	0.00002500	S	-0.76354900	-1.94052700	-0.00010600

(54) TA (F_y = 0.50 V/Å)

Neutral			
elements	x	y	z
C	2.16507400	0.84519900	-0.00008500
C	1.75099600	-0.50486400	-0.00000400
C	2.71410300	-1.52415600	-0.00001900
C	4.05895200	-1.18679200	-0.00013000
C	4.45812400	0.15899000	-0.00021400
C	3.51849400	1.18377200	-0.00018300
H	2.40731000	-2.56627600	0.00005500
H	4.80730800	-1.97226300	-0.00014500
H	5.51686300	0.40048500	-0.00029100
H	3.82985900	2.22539800	-0.00022500
C	-2.14492300	-0.82549700	-0.00010200
C	-1.75195200	0.53555000	-0.00000600
C	-2.73762200	1.53489400	-0.00001400
C	-4.07506500	1.16938600	-0.00013700
C	-4.45190300	-0.18521900	-0.00023000
C	-3.49465600	-1.18977900	-0.00020900
C	0.31264400	-0.58930400	0.00011900
C	-0.32042200	0.62679400	0.00013100
H	-2.44443300	2.58264300	0.00007400
H	-4.84536200	1.93617600	-0.00014700
H	-5.50286200	-0.45591300	-0.00030800
H	-3.78678200	-2.23554000	-0.00025100
S	0.80357500	1.96810400	0.00003700
S	-0.78769800	-1.93214000	0.00001500

Cationic			
elements	x	y	z
C	2.14769600	0.82004500	-0.00009400
C	1.74959900	-0.53702700	-0.00009400
C	2.72587900	-1.54558600	-0.00009000
C	4.07048700	-1.18124700	-0.00008800
C	4.43979300	0.16512200	-0.00009000
C	3.47885100	1.18804100	-0.00009200
H	2.44035100	-2.59379800	-0.00008700
H	4.83375000	-1.95172200	-0.00008500
H	5.49253000	0.42914800	-0.00008800
H	3.77864400	2.23162700	-0.00009100
C	-2.14732800	-0.82149000	-0.00010800
C	-1.75108000	0.53802600	-0.00009700
C	-2.72511100	1.54861600	-0.00008600
C	-4.06664200	1.18656600	-0.00009200
C	-4.43891300	-0.16199600	-0.00010500
C	-3.47978400	-1.18898000	-0.00011300
C	0.32100700	-0.64014900	-0.00009100
C	-0.33159500	0.63080800	-0.00008700
H	-2.42727700	2.59396000	-0.00007400
H	-4.83423800	1.95335400	-0.00008300
H	-5.49029500	-0.43054300	-0.00010900
H	-3.78748100	-2.23024600	-0.00012300
S	0.76392300	1.93919500	-0.00009000
S	-0.76314300	-1.94207900	-0.00011100

(55) TA (F_z = 0.25 V/Å)

Neutral			
elements	x	y	z
C	2.15468200	0.83529400	0.04957600
C	1.75119400	-0.51980400	0.06027700
C	2.72486300	-1.52882900	0.01996900
C	4.06480500	-1.17782900	-0.02973500
C	4.45297200	0.17229600	-0.03964600
C	3.50537800	1.18654400	-0.00001100
H	2.42393200	-2.57276200	0.00522400
H	4.82236400	-1.95325200	-0.08434700
H	5.50608400	0.42812100	-0.10184800
H	3.80604400	2.22948100	-0.03122500
C	-2.15471600	-0.83532300	0.04956500
C	-1.75122300	0.51977400	0.06027100
C	-2.72489400	1.52880000	0.01996400
C	-4.06483400	1.17780100	-0.02974500
C	-4.45300400	-0.17232500	-0.03966100
C	-3.50541100	-1.18657300	-0.00002700
C	0.31647300	-0.60779500	0.08461400
C	-0.31650500	0.60775900	0.08461400
H	-2.42396200	2.57273200	0.00522300
H	-4.82239300	1.95322400	-0.08435600
H	-5.50611600	-0.42814800	-0.10186700
H	-3.80607800	-2.22951000	-0.03124500
S	0.79554000	1.94927100	0.06607700
S	-0.79557500	-1.94930100	0.06606800

Cationic			
elements	x	y	z
C	2.14700300	0.82042400	0.01318000
C	1.74963200	-0.53734600	0.01939700
C	2.72514800	-1.54648100	0.01399900
C	4.06776600	-1.18372100	0.00307300
C	4.43871700	0.16365100	-0.00581400
C	3.47868900	1.18791000	-0.00073500
H	2.43339500	-2.59268800	0.00537900
H	4.83278200	-1.95198400	-0.01568800
H	5.49038500	0.43001400	-0.03102600
H	3.78194600	2.22965500	-0.02274200
C	-2.14703400	-0.82045400	0.01317000
C	-1.74966400	0.53731600	0.01939300
C	-2.72518000	1.54645200	0.01399500
C	-4.06779800	1.18369200	0.00306300
C	-4.43874800	-0.16368000	-0.00582900
C	-3.47872000	-1.18794000	-0.00075000
C	0.32599800	-0.63558000	0.01738900
C	-0.32603000	0.63555100	0.01739000
H	-2.43342700	2.59265900	0.00537800
H	-4.83281400	1.95195500	-0.01569900
H	-5.49041700	-0.43004400	-0.03104600
H	-3.78197700	-2.22968500	-0.02276200
S	0.76378200	1.93971400	0.00251000
S	-0.76381400	-1.93974300	0.00250200

(56) TA (F_z = 0.50 V/Å)

Neutral			
elements	x	y	z
C	2.15434700	0.83555200	0.10115600
C	1.75116700	-0.51953800	0.12422000
C	2.72243500	-1.52866800	0.04212700
C	4.05950800	-1.17758600	-0.06134700
C	4.44727500	0.17267700	-0.08332900
C	3.50213500	1.18706500	-0.00194300
H	2.41973100	-2.57189900	0.01413100
H	4.81195600	-1.95209800	-0.17156900
H	5.49446800	0.42848000	-0.21093300
H	3.79985600	2.22943600	-0.06568100
C	-2.15437900	-0.83558100	0.10114800
C	-1.75119900	0.51950900	0.12421500
C	-2.72246800	1.52863900	0.04212000
C	-4.05953900	1.17755700	-0.06135800
C	-4.44730600	-0.17270700	-0.08334300
C	-3.50216600	-1.18709500	-0.00195600
C	0.31680300	-0.60768800	0.17517400
C	-0.31683500	0.60765700	0.17517400
H	-2.41976400	2.57187000	0.01412700
H	-4.81198800	1.95206800	-0.17158100
H	-5.49449900	-0.42850900	-0.21095100
H	-3.79988600	-2.22946600	-0.06569600
S	0.79486400	1.94952100	0.13691300
S	-0.79489700	-1.94955000	0.13691100

Cationic			
elements	x	y	z
C	2.14709900	0.82061400	0.02694000
C	1.74973800	-0.53723500	0.03989800
C	2.72533700	-1.54648000	0.02874900
C	4.06793700	-1.18381000	0.00591200
C	4.43878100	0.16368000	-0.01254100
C	3.47869200	1.18806700	-0.00194900
H	2.43341500	-2.59260300	0.01192700
H	4.83238800	-1.95203100	-0.03196400
H	5.48963900	0.42976900	-0.06383400
H	3.78147800	2.22930900	-0.04650200
C	-2.14713100	-0.82064300	0.02693300
C	-1.74977000	0.53720600	0.03989300
C	-2.72536900	1.54645000	0.02874200
C	-4.06796900	1.18378100	0.00590100
C	-4.43881300	-0.16371000	-0.01255500
C	-3.47872400	-1.18809700	-0.00196100
C	0.32605200	-0.63563300	0.03624000
C	-0.32608400	0.63560300	0.03623900
H	-2.43344600	2.59257300	0.01192300
H	-4.83241900	1.95200200	-0.03197700
H	-5.48967100	-0.42979800	-0.06385200
H	-3.78151000	-2.22933800	-0.04651600
S	0.76362900	1.93976800	0.00604400
S	-0.76366100	-1.93979800	0.00603900

(57) OT_3-F (F = 0.00 V/Å)

Neutral			
elements	x	y	z
C	-4.97557500	-0.41668900	-0.00695700
C	-5.67014000	0.76376300	-0.01789100
C	-7.08323700	0.64689900	-0.02009800
C	-7.45612900	-0.66483300	-0.01051500
S	-6.10561200	-1.73558700	0.00105200
H	-7.75785700	1.49319000	-0.02829900
H	-8.45849400	-1.07003300	-0.00953100
C	-3.54273800	-0.62686500	-0.00212400
C	-2.87735800	-1.82827600	0.00897000
S	-2.43331900	0.71569800	-0.01067000
C	-1.47867000	-1.63966400	0.01044500
H	-3.34881100	-2.80385100	0.01584500
C	-1.05178600	-0.33815500	0.00086700
C	0.30014500	0.17482100	-0.00045400
C	0.69167900	1.49175400	-0.01032900
S	1.67386200	-0.89670900	0.01111600
C	2.09860100	1.60802700	-0.00845600
H	0.02151600	2.34325400	-0.01859300
C	2.79559500	0.42981300	0.00251800
C	4.22879400	0.21832300	0.00702000
C	4.89092800	-0.98538100	0.01884100
S	5.34489100	1.55381800	-0.00297500
C	6.29604600	-0.79963100	0.01952700
H	4.41562500	-1.95932000	0.02672200
C	6.70517000	0.49706900	0.00867500
H	7.71721600	0.87434300	0.00702800
F	-5.05184800	1.95355300	-0.02601700
F	-0.62266200	-2.67128400	0.02054700
F	2.71207900	2.80023900	-0.01699700
F	7.14110200	-1.84058800	0.03013900

Cationic			
elements	x	y	z
C	-4.93416100	-0.42349600	-0.00694300
C	-5.63139300	0.77374400	-0.01801400
C	-7.03278900	0.65924400	-0.02014300
C	-7.39884900	-0.66211400	-0.01049000
S	-6.06838600	-1.74331000	0.00118100
H	-7.71385200	1.50012100	-0.02828200
H	-8.40455000	-1.06223600	-0.00955300
C	-3.52194100	-0.61091800	-0.00227600
C	-2.84777300	-1.83608900	0.00952000
S	-2.42552000	0.74080600	-0.01121900
C	-1.47752300	-1.65199700	0.01095800
H	-3.32748600	-2.80743200	0.01668900
C	-1.03850000	-0.31791200	0.00070000
C	0.28372200	0.15323700	-0.00041300
C	0.68937100	1.50083000	-0.01071000
S	1.66006000	-0.93047400	0.01140500
C	2.06165600	1.61280900	-0.00880300
H	0.01549400	2.34973300	-0.01901600
C	2.77503000	0.39789400	0.00271300
C	4.17962300	0.21585800	0.00698800
C	4.85839800	-1.00138300	0.01823500
S	5.29478100	1.56419900	-0.00200500
C	6.24313500	-0.80845900	0.01917700
H	4.38947800	-1.97893300	0.02537100
C	6.63479900	0.51314200	0.00906400
H	7.64897100	0.89048000	0.00784400
F	-4.99607200	1.94245900	-0.02591800
F	-0.60573100	-2.65046200	0.02129700
F	2.70191200	2.77323100	-0.01697200
F	7.10711000	-1.81487200	0.02901900

(58) OT_3-F (F_x = 0.25 V/Å)

Neutral			
elements	x	y	z
C	-4.97819200	-0.42462500	-0.00690000
C	-5.66231200	0.76546200	-0.01823400
C	-7.07324400	0.66375300	-0.02041000
C	-7.45440200	-0.64727800	-0.01034900
S	-6.11974200	-1.73389700	0.00143700
H	-7.74591400	1.51158100	-0.02877200
H	-8.46150600	-1.04299800	-0.00914200
C	-3.54983700	-0.63471800	-0.00206100
C	-2.88057700	-1.83925500	0.00930500
S	-2.44288800	0.71130300	-0.01081100
C	-1.48681600	-1.64654800	0.01064600
H	-3.35518800	-2.81293100	0.01638400
C	-1.05839300	-0.34296600	0.00083100
C	0.29010500	0.16298400	-0.00052500
C	0.68816700	1.48209600	-0.01033500
S	1.66373300	-0.91453000	0.01085800
C	2.09225100	1.59127800	-0.00840600
H	0.01726000	2.33258300	-0.01842900
C	2.79100500	0.41261000	0.00249400
C	4.22132000	0.21067100	0.00701000
C	4.90101800	-0.98591700	0.01828400
S	5.32756600	1.56010400	-0.00229500
C	6.30300300	-0.78180300	0.01921400
H	4.43243400	-1.96276600	0.02561700
C	6.70384500	0.51653900	0.00914400
H	7.71231000	0.90210600	0.00794800
F	-5.02130500	1.94219700	-0.02663000
F	-0.61997100	-2.67158600	0.02086300
F	2.71691700	2.78040900	-0.01677000
F	7.16836600	-1.81615800	0.02944000

Cationic			
elements	x	y	z
C	-4.93740200	-0.43798800	-0.00674700
C	-5.64088500	0.78400800	-0.01890000
C	-7.02708400	0.67828700	-0.02116500
C	-7.39677800	-0.65508800	-0.01060600
S	-6.08755900	-1.75380100	0.00188000
H	-7.71475800	1.51489000	-0.02982500
H	-8.40978700	-1.04333400	-0.00957700
C	-3.54602500	-0.61529400	-0.00199800
C	-2.85694700	-1.84825900	0.01028400
S	-2.43556000	0.74089800	-0.01124900
C	-1.49572100	-1.65980700	0.01163600
H	-3.33537400	-2.82088000	0.01774800
C	-1.05960600	-0.31870600	0.00099800
C	0.27340900	0.15511500	-0.00012900
C	0.68005000	1.48925500	-0.00997300
S	1.65108800	-0.92666300	0.01119400
C	2.06737300	1.59598500	-0.00809500
H	0.01340400	2.34416700	-0.01794400
C	2.76408600	0.39568700	0.00281300
C	4.19290800	0.20471600	0.00699700
C	4.87355500	-0.99495500	0.01728900
S	5.29156300	1.55734800	-0.00134000
C	6.27068200	-0.78864300	0.01831700
H	4.41286100	-1.97604500	0.02385200
C	6.65751900	0.51922300	0.00918200
H	7.66518400	0.90900200	0.00820100
F	-4.98221900	1.93021000	-0.02714900
F	-0.61217900	-2.65055500	0.02221000
F	2.70396500	2.76712500	-0.01612100
F	7.13924900	-1.80819600	0.02762300

(59) OT_3-F (F_x = 0.50 V/Å)

Neutral			
elements	x	y	z
C	-4.97874400	-0.42887600	-0.00737100
C	-5.66177000	0.77241200	-0.01884700
C	-7.06595000	0.68053700	-0.02087100
C	-7.45099900	-0.63469000	-0.01058800
S	-6.13138800	-1.73278300	0.00134500
H	-7.74232600	1.52603600	-0.02921100
H	-8.46324900	-1.02214000	-0.00925000
C	-3.56180400	-0.63072400	-0.00280300
C	-2.88554900	-1.84580600	0.00863100
S	-2.45134700	0.71556300	-0.01170100
C	-1.50398400	-1.65466600	0.00991600
H	-3.36726900	-2.81584400	0.01573200
C	-1.06229100	-0.34422800	0.00008800
C	0.27646000	0.14200900	-0.00074800
C	0.68880300	1.46965300	-0.00998500
S	1.65546100	-0.94195700	0.01032500
C	2.08237900	1.56986100	-0.00786500
H	0.01788100	2.31987500	-0.01764000
C	2.79191700	0.38822100	0.00259600
C	4.21188200	0.20166600	0.00740500
C	4.91869800	-0.98859900	0.01831200
S	5.31127100	1.56917100	-0.00056900
C	6.31369000	-0.76135800	0.01977600
H	4.46084500	-1.97012800	0.02494300
C	6.70764500	0.54005100	0.01056500
H	7.71269400	0.93469500	0.01015500
F	-5.00052100	1.93465700	-0.02730800
F	-0.62804400	-2.67254800	0.02012800
F	2.72061600	2.75474800	-0.01555400
F	7.20400200	-1.78710800	0.02979900

Cationic			
elements	x	y	z
C	-4.96035600	-0.44697900	-0.00726400
C	-5.66419300	0.79496800	-0.01932200
C	-7.03981300	0.70093100	-0.02140300
C	-7.41930800	-0.64366200	-0.01078100
S	-6.12185100	-1.75798600	0.00137600
H	-7.73246900	1.53566600	-0.02983000
H	-8.44000300	-1.02072300	-0.00967600
C	-3.56914400	-0.62454200	-0.00268700
C	-2.87831300	-1.85408400	0.00933900
S	-2.44830900	0.73035400	-0.01174700
C	-1.51032000	-1.66134900	0.01066400
H	-3.35338300	-2.82887700	0.01670800
C	-1.08077100	-0.32980600	0.00031300
C	0.27384300	0.14990200	-0.00060300
C	0.68305400	1.47132600	-0.01001300
S	1.64373800	-0.93862300	0.01086600
C	2.08241400	1.57031300	-0.00777900
H	0.02260400	2.33078200	-0.01795200
C	2.77226300	0.37931100	0.00297900
C	4.20877600	0.19102100	0.00765500
C	4.90987900	-0.99465700	0.01759800
S	5.29192500	1.55982100	0.00078000
C	6.30730800	-0.76511700	0.01917000
H	4.46157400	-1.98100300	0.02345800
C	6.68281000	0.54184500	0.01084200
H	7.68498700	0.94486000	0.01040100
F	-4.98242200	1.92306400	-0.02741000
F	-0.62432500	-2.65640800	0.02108000
F	2.72100500	2.74660800	-0.01557800
F	7.19780800	-1.77925700	0.02822200

(60) OT_3-F (F_y = 0.25 V/Å)

Neutral			
elements	x	y	z
C	-4.97599100	-0.41303200	-0.00707000
C	-5.68454200	0.75942400	-0.01699000
C	-7.09466900	0.62532100	-0.01972100
C	-7.45044100	-0.69297200	-0.01155300
S	-6.08950200	-1.74444500	-0.00087500
H	-7.78186200	1.46143200	-0.02739900
H	-8.44664600	-1.11356600	-0.01140400
C	-3.54140400	-0.61422200	-0.00207500
C	-2.87106900	-1.81165400	0.00892600
S	-2.43732700	0.73588800	-0.01074600
C	-1.47238800	-1.61718500	0.01055400
H	-3.33525700	-2.79105900	0.01564200
C	-1.05110600	-0.31360400	0.00110900
C	0.30140400	0.19567800	-0.00011800
C	0.69867300	1.51234000	-0.01019100
S	1.66962000	-0.88011700	0.01158500
C	2.10535900	1.62134000	-0.00839400
H	0.02905600	2.36405000	-0.01875100
C	2.79763400	0.44056400	0.00269200
C	4.22916400	0.21513200	0.00706800
C	4.88059700	-0.99283500	0.01979200
S	5.35939400	1.54221600	-0.00448700
C	6.28935300	-0.82166800	0.01980100
H	4.39956900	-1.96435100	0.02862700
C	6.71072900	0.47105600	0.00756200
H	7.72808800	0.83317400	0.00495500
F	-5.08121800	1.96393200	-0.02373200
F	-0.61198600	-2.63761800	0.02075000
F	2.72332900	2.81876500	-0.01721800
F	7.12245400	-1.86428600	0.03106600

Cationic			
elements	x	y	z
C	-4.93499200	-0.42039300	-0.00704200
C	-5.63623100	0.77589600	-0.01736100
C	-7.03427400	0.65668200	-0.02008000
C	-7.39566200	-0.66905000	-0.01168200
S	-6.06548100	-1.74331000	-0.00062300
H	-7.72002800	1.49347400	-0.02784900
H	-8.39972200	-1.07409400	-0.01160100
C	-3.52368300	-0.60894000	-0.00204200
C	-2.84896600	-1.83345100	0.00969800
S	-2.42609400	0.74638800	-0.01069300
C	-1.47849000	-1.64918300	0.01134800
H	-3.32589100	-2.80684500	0.01663600
C	-1.03936600	-0.31277000	0.00122200
C	0.28313800	0.15381200	0.00008100
C	0.69019100	1.50193400	-0.01034400
S	1.65860000	-0.92914700	0.01168700
C	2.06191900	1.61167400	-0.00865000
H	0.01518900	2.34956000	-0.01870600
C	2.77380100	0.39747000	0.00282700
C	4.18009100	0.21164800	0.00694600
C	4.85871200	-1.00304900	0.01900200
S	5.29564600	1.56096700	-0.00359900
C	6.24712900	-0.81138500	0.01928300
H	4.39296500	-1.98264900	0.02710000
C	6.63831800	0.50839200	0.00779300
H	7.65332500	0.88238600	0.00564600
F	-5.00530300	1.95338000	-0.02403900
F	-0.60485000	-2.63836700	0.02169700
F	2.70050800	2.78027900	-0.01700700
F	7.10851600	-1.81361300	0.02975700

(61) OT_3-F (F_y = 0.50 V/Å)

Neutral			
elements	x	y	z
C	-4.97630100	-0.41019100	-0.00631500
C	-5.69872300	0.75429800	-0.01355300
C	-7.10590800	0.60316400	-0.01573200
C	-7.44454300	-0.72152500	-0.00994400
S	-6.07359300	-1.75422300	-0.00214300
H	-7.80539200	1.42933600	-0.02147300
H	-8.43441000	-1.15751200	-0.01009400
C	-3.54001200	-0.60252200	-0.00260000
C	-2.86418300	-1.79576600	0.00538500
S	-2.44158400	0.75600800	-0.00878400
C	-1.46536000	-1.59462800	0.00642200
H	-3.32036000	-2.77959700	0.01019900
C	-1.04998000	-0.28865400	-0.00061900
C	0.30268700	0.21804200	-0.00194900
C	0.70540200	1.53470800	-0.01174400
S	1.66588300	-0.86171100	0.00905800
C	2.11219100	1.63692500	-0.00958200
H	0.03640300	2.38698200	-0.02043300
C	2.80011600	0.45375900	0.00146600
C	4.22967200	0.21307600	0.00646100
C	4.86888400	-0.99984600	0.02787200
S	5.37579000	1.53045400	-0.01771500
C	6.28154800	-0.84511500	0.02436100
H	4.38126700	-1.96863600	0.04528000
C	6.71675500	0.44293300	0.00123400
H	7.73961000	0.78874700	-0.00607300
F	-5.11087800	1.97385200	-0.01830300
F	-0.60062300	-2.60426400	0.01380600
F	2.73381300	2.84047000	-0.01807000
F	7.10084100	-1.89086500	0.04298600

Cationic			
elements	x	y	z
C	-4.93584900	-0.41848300	-0.00640000
C	-5.63909200	0.77797800	-0.01650300
C	-7.03422500	0.65650500	-0.01960200
C	-7.39316400	-0.67310800	-0.01172300
S	-6.06483500	-1.74311800	-0.00092100
H	-7.72320500	1.49063000	-0.02735100
H	-8.39634700	-1.08136100	-0.01212800
C	-3.52537800	-0.60966400	-0.00119000
C	-2.85042600	-1.83372100	0.01084200
S	-2.42642700	0.74932700	-0.01026500
C	-1.47912300	-1.64898300	0.01240400
H	-3.32457700	-2.80942600	0.01800000
C	-1.04013900	-0.31041400	0.00184500
C	0.28268900	0.15326500	0.00033600
C	0.68951400	1.50209400	-0.01067500
S	1.65786200	-0.92818500	0.01179900
C	2.06123000	1.61070500	-0.00944000
H	0.01251200	2.34793700	-0.01923500
C	2.77245000	0.39783300	0.00227500
C	4.18071100	0.20881900	0.00611300
C	4.85896900	-1.00357500	0.01985000
S	5.29675300	1.55951300	-0.00804300
C	6.25134300	-0.81308300	0.01919000
H	4.39622000	-1.98533800	0.03001000
C	6.64219700	0.50498900	0.00519800
H	7.65819800	0.87541800	0.00171900
F	-5.01111500	1.96391000	-0.02261000
F	-0.60423400	-2.62972100	0.02300200
F	2.69673400	2.78852000	-0.01843300
F	7.10976900	-1.81156200	0.03134000

(62) OT_3-F (F_z = 0.25 V/Å)

Neutral			
elements	x	y	z
C	-4.97380000	-0.41187100	-0.01930300
C	-5.68908200	0.71941200	0.27083800
C	-7.09087400	0.62426400	0.08311900
C	-7.43220900	-0.61950300	-0.36295000
S	-6.06530800	-1.64747600	-0.56320500
H	-7.77973200	1.44132900	0.25431200
H	-8.41722900	-0.98586400	-0.61736000
C	-3.54198000	-0.62634500	0.05008200
C	-2.87760100	-1.82794700	0.04833100
S	-2.43357000	0.71529800	0.07170200
C	-1.47831800	-1.63920100	0.06184300
H	-3.35131000	-2.80218300	0.02648400
C	-1.05130400	-0.33763300	0.07020400
C	0.30095300	0.17539600	0.05152100
C	0.69096000	1.49026400	-0.03083400
S	1.67566200	-0.89415500	0.08706700
C	2.09786700	1.60759900	-0.05287000
H	0.01959800	2.33825400	-0.09805500
C	2.79560200	0.43145300	0.00749800
C	4.22921200	0.21934300	-0.01306400
C	4.89990300	-0.94992400	0.25376900
S	5.32838900	1.49352900	-0.45199100
C	6.29902000	-0.78574300	0.09948800
H	4.43241900	-1.88639000	0.53472700
C	6.69485200	0.46092500	-0.27287900
H	7.69863100	0.81079000	-0.46505000
F	-5.10126200	1.84435100	0.70953100
F	-0.62197400	-2.67072600	0.07349000
F	2.70921800	2.79811300	-0.12840300
F	7.15227900	-1.79766500	0.32136400

Cationic			
elements	x	y	z
C	-4.93325600	-0.42426700	-0.00435300
C	-5.63387900	0.76839800	0.07529300
C	-7.03116300	0.65886100	-0.03306900
C	-7.39024600	-0.65391500	-0.20334000
S	-6.05822700	-1.73240300	-0.23049800
H	-7.71368400	1.49818100	-0.00686800
H	-8.39006700	-1.04599500	-0.33892300
C	-3.52186200	-0.61248500	0.04825200
C	-2.84767100	-1.83770200	0.05315400
S	-2.42605400	0.73916000	0.08258800
C	-1.47756200	-1.65315900	0.08496600
H	-3.32717600	-2.80873500	0.02482700
C	-1.03888100	-0.31931000	0.09715500
C	0.28349600	0.15210300	0.08384900
C	0.68796400	1.49957900	0.04810300
S	1.65983800	-0.93138200	0.06927500
C	2.06003600	1.61154600	0.01120800
H	0.01329200	2.34770900	0.03246600
C	2.77377300	0.39713000	0.02095800
C	4.17823300	0.21595400	-0.01059600
C	4.86099300	-0.99453200	0.09877700
S	5.28542200	1.55232900	-0.23008000
C	6.24308300	-0.80425900	0.01181000
H	4.39549600	-1.96492100	0.22921000
C	6.62839200	0.50705100	-0.17026300
H	7.63861000	0.87747600	-0.28640200
F	-5.00492200	1.92859000	0.25003500
F	-0.60592600	-2.65186400	0.10664600
F	2.69963400	2.77176400	-0.01972500
F	7.11132600	-1.80321000	0.10495100

(63) OT_3-F (F_z = 0.50 V/Å)

Neutral			
elements	x	y	z
C	-4.97272400	-0.37655300	-0.05389800
C	-5.77976000	0.44265800	0.68785100
C	-7.13865700	0.48164700	0.28862300
C	-7.34656600	-0.33510200	-0.78839400
S	-5.91150400	-1.11857700	-1.30963400
H	-7.89363900	1.09579400	0.76248900
H	-8.26881200	-0.49570500	-1.33082100
C	-3.53949500	-0.61027400	0.06181500
C	-2.88163200	-1.81250500	0.03945900
S	-2.42807700	0.72516500	0.10361900
C	-1.47945200	-1.62914600	0.07322800
H	-3.36534800	-2.77989000	-0.02239300
C	-1.04807600	-0.32922300	0.10259800
C	0.30818800	0.17840000	0.05796800
C	0.69799900	1.48341400	-0.12287200
S	1.68151700	-0.88753200	0.14573100
C	2.10603700	1.59981900	-0.16779600
H	0.02600900	2.32188100	-0.26499500
C	2.80070600	0.42899300	-0.03174200
C	4.23657300	0.20427500	-0.07065100
C	4.95216600	-0.72162800	0.65045100
S	5.25362800	1.07914600	-1.16789600
C	6.32514000	-0.68510900	0.30381400
H	4.52605400	-1.39808200	1.38182900
C	6.65460000	0.22743700	-0.65066100
H	7.62422400	0.41948800	-1.08797100
F	-5.32605200	1.15156100	1.74428800
F	-0.62605200	-2.66348100	0.08043400
F	2.71093300	2.78426000	-0.32010700
F	7.22108300	-1.49343100	0.90504000

Cationic			
elements	x	y	z
C	-4.92982300	-0.42432300	-0.00420600
C	-5.64209700	0.75181800	0.16772200
C	-7.02512600	0.66080600	-0.05985900
C	-7.36085200	-0.62020900	-0.42253700
S	-6.02448500	-1.68966800	-0.48240400
H	-7.71217000	1.49459700	0.00171500
H	-8.34097800	-0.98459300	-0.70376100
C	-3.52184700	-0.61680900	0.10655600
C	-2.84686200	-1.84132500	0.10976200
S	-2.42802100	0.73447400	0.19044400
C	-1.47770000	-1.65631100	0.18058100
H	-3.32463600	-2.81141300	0.04312200
C	-1.03975900	-0.32290800	0.21579200
C	0.28263700	0.14964200	0.18785000
C	0.68467100	1.49637100	0.11735400
S	1.65943100	-0.93334000	0.14850500
C	2.05510700	1.60856500	0.03361700
H	0.00850000	2.34315700	0.09168400
C	2.77008900	0.39501700	0.04524500
C	4.17288500	0.21371100	-0.03084200
C	4.86803900	-0.97594700	0.18411600
S	5.25559000	1.51034800	-0.48351400
C	6.24082900	-0.79760000	-0.00328400
H	4.41526000	-1.92365400	0.45253700
C	6.60585400	0.48045900	-0.37459400
H	7.60217700	0.82908300	-0.61546000
F	-5.03517400	1.88046100	0.53855800
F	-0.60615400	-2.65530500	0.21900700
F	2.69267600	2.76814400	-0.03105100
F	7.12095300	-1.77554700	0.17675200

(64) OT_3-E (F = 0.00 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.74125000	-0.10817600	-0.16976400	C	-4.69471300	-0.11872100	-0.17075700
C	-5.40640800	1.09290400	-0.15447500	C	-5.36530200	1.09948500	-0.17581400
C	-6.82921700	0.96320900	-0.18217000	C	-6.77882700	0.96725400	-0.20499800
C	-7.23658200	-0.33519600	-0.22267300	C	-7.17447400	-0.34179500	-0.23195100
S	-5.89258700	-1.41908100	-0.22353700	S	-5.84914300	-1.43545000	-0.21799900
H	-8.25166100	-0.70389600	-0.24968700	H	-8.19209000	-0.70781100	-0.25287800
C	-3.31251300	-0.32019600	-0.15773100	C	-3.28987100	-0.30784200	-0.15132900
C	-2.65421700	-1.52442800	-0.17388600	C	-2.62140800	-1.53653700	-0.15973800
S	-2.16290600	0.99453000	-0.13892700	S	-2.15327700	1.01952900	-0.13291500
C	-1.23955600	-1.40082600	-0.16787300	C	-1.23448300	-1.41549100	-0.14798400
C	-0.80037300	-0.09956100	-0.15119400	C	-0.78363500	-0.08274300	-0.13884800
C	0.56681100	0.36011700	-0.13118100	C	0.54953100	0.34225200	-0.11940700
C	1.00608500	1.66135400	-0.11510400	C	1.00008300	1.67489000	-0.09427500
S	1.92881800	-0.73438400	-0.10559500	S	1.91896200	-0.76010600	-0.10049300
C	2.42049100	1.78470800	-0.08548700	C	2.38684800	1.79601700	-0.07139500
C	3.07837000	0.58019300	-0.07457300	C	3.05529500	0.56727400	-0.06901200
C	4.50699700	0.36782000	-0.05683500	C	4.46025600	0.37835300	-0.05947900
C	5.17147200	-0.83368200	-0.04589900	C	5.13109900	-0.83969700	-0.06879800
S	5.65947600	1.67882100	-0.06251700	S	5.61517900	1.69553800	-0.06011800
C	6.59456400	-0.70433700	-0.03839900	C	6.54488400	-0.70719000	-0.06420900
C	7.00294500	0.59435500	-0.04821300	C	6.94073300	0.60207900	-0.06173500
H	8.01842200	0.96294200	-0.04558700	H	7.95847500	0.96826600	-0.05410600
C	-6.98695600	3.23016400	0.23798200	C	-6.94608700	3.21951500	0.24665700
C	-5.64918100	3.36992100	-0.46851400	C	-5.61273700	3.38769100	-0.45995800
H	-6.83325200	3.19441100	1.32491100	H	-6.79774200	3.15575300	1.33207700
H	-7.64801000	4.06296700	-0.00918800	H	-7.61163200	4.05264500	0.01800400
H	-5.79602100	3.36101500	-1.55664300	H	-5.75476600	3.42350500	-1.54583900
H	-5.14376700	4.29160900	-0.17462200	H	-5.09578900	4.28680300	-0.12381400
O	-7.65663000	2.04857900	-0.18815900	O	-7.60689300	2.04075700	-0.21116600
O	-4.78022000	2.30334400	-0.09977200	O	-4.73766700	2.28982500	-0.14987700
C	-2.40976300	-3.78942700	-0.56928700	C	-2.38820100	-3.79022600	-0.58318900
C	-1.08748100	-3.68219000	0.17157200	C	-1.07140800	-3.70028800	0.16940300
H	-2.23850400	-3.73903300	-1.65256800	H	-2.21865900	-3.72387000	-1.66435800
H	-2.92398900	-4.71990200	-0.32225900	H	-2.90941300	-4.71838300	-0.34781400
H	-1.26257900	-3.68703400	1.25547200	H	-1.24259600	-3.73916500	1.25092400
H	-0.42056000	-4.50386400	-0.09550600	H	-0.39186700	-4.49929200	-0.12735700
O	-3.28394700	-2.73432700	-0.17913000	O	-3.26058300	-2.72773100	-0.18430400
O	-0.41027600	-2.48346000	-0.19305700	O	-0.39890500	-2.46996200	-0.14264900
C	0.84562400	3.93610800	0.26153900	C	0.82887100	3.95332600	0.26130700
C	2.18493600	4.05663800	-0.44598700	C	2.16275200	4.05726500	-0.45873400
H	0.99516200	3.92075400	1.34915500	H	0.97487500	3.97170400	1.34706000

H	0.18502700	4.76276400	-0.00587700	H	0.15616600	4.75788100	-0.03601700
H	2.03907000	4.02611800	-1.53371800	H	2.01826200	4.01124200	-1.54459200
H	2.69312200	4.98230900	-0.17005400	H	2.67814300	4.98076800	-0.19402000
O	0.17752900	2.74451400	-0.14123300	O	0.16429500	2.72920200	-0.08955900
O	3.05000000	2.99435700	-0.05486700	O	3.02606600	2.98737500	-0.05981500
C	5.42111200	-3.10510300	-0.39253800	C	5.38539300	-3.12330100	-0.38271600
C	6.74202300	-2.97817300	0.34725200	C	6.70250200	-2.96614400	0.35613800
H	5.59324200	-3.07755000	-1.47664400	H	5.55177900	-3.14247600	-1.46556300
H	4.90886300	-4.03141600	-0.12634900	H	4.86119200	-4.02739400	-0.07211700
H	6.56290900	-2.96075800	1.43074500	H	6.52988100	-2.91899000	1.43881800
H	7.40855100	-3.80703300	0.10154500	H	7.37319900	-3.79574300	0.12972000
O	4.54401800	-2.04453300	-0.02575200	O	4.50330600	-2.03021700	-0.07558900
O	7.42174000	-1.78990600	-0.04296600	O	7.37311400	-1.78057500	-0.06864900

(65) OT_3-E (F_x = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.73601300	-0.10757800	-0.16504400	C	-4.69485500	-0.11990800	-0.18486100
C	-5.40786600	1.09293500	-0.16640500	C	-5.38199600	1.11230500	-0.19106600
C	-6.82858600	0.95174500	-0.19712600	C	-6.78442100	0.97234300	-0.22204000
C	-7.22232300	-0.35235200	-0.22479300	C	-7.16871400	-0.34938400	-0.25091000
S	-5.87850300	-1.42820400	-0.21052000	S	-5.84946100	-1.44712700	-0.23663800
H	-8.23592000	-0.72782900	-0.24845200	H	-8.18856400	-0.71600200	-0.27188100
C	-3.30901100	-0.30852400	-0.14979100	C	-3.30737600	-0.29477400	-0.16721000
C	-2.64503800	-1.51352900	-0.15104900	C	-2.62708100	-1.53168500	-0.18309800
S	-2.16695000	1.00967000	-0.14561000	S	-2.15721800	1.03078000	-0.14612200
C	-1.23480000	-1.38677800	-0.14779700	C	-1.24202300	-1.40809800	-0.16825800
C	-0.79647800	-0.08173300	-0.14803400	C	-0.79827300	-0.07963100	-0.14995800
C	0.56774100	0.37172500	-0.13311500	C	0.54977700	0.35053700	-0.12278100
C	1.01732500	1.67305300	-0.13180700	C	0.99828000	1.66796500	-0.09350500
S	1.92448500	-0.72865200	-0.09721700	S	1.91550900	-0.75156800	-0.10132300
C	2.42926100	1.79022800	-0.10255900	C	2.40211000	1.78507600	-0.06588500
C	3.08618500	0.58246600	-0.07768300	C	3.05568000	0.56789000	-0.06467300
C	4.50998200	0.36482100	-0.05995900	C	4.48044700	0.36473400	-0.05252300
C	5.17595900	-0.83766800	-0.03504000	C	5.14912300	-0.83920600	-0.05480700
S	5.67216600	1.67028600	-0.07899900	S	5.62941300	1.68045900	-0.04726200
C	6.59793400	-0.71521000	-0.03116900	C	6.56975900	-0.70548900	-0.04575800
C	7.01852400	0.58004900	-0.05507800	C	6.97106400	0.59706700	-0.04357700
H	8.03561000	0.94330000	-0.06038400	H	7.98599500	0.96768900	-0.03576200
C	-7.01321700	3.20872800	0.23142600	C	-6.97751000	3.21288000	0.24884100
C	-5.67726200	3.37481900	-0.47214300	C	-5.64474900	3.40441000	-0.45343300
H	-6.86564200	3.16003300	1.31848100	H	-6.83770400	3.14007000	1.33415100
H	-7.68430900	4.03517400	-0.00722800	H	-7.65383200	4.03750800	0.02304700
H	-5.82275900	3.38531000	-1.55933300	H	-5.77948600	3.46414700	-1.53785800

H	-5.17751700	4.29254500	-0.15796700	H	-5.12572300	4.29093300	-0.09029600
O	-7.66217200	2.02461700	-0.21528800	O	-7.61961900	2.02647400	-0.22213500
O	-4.78987500	2.30333900	-0.13091100	O	-4.75814600	2.29115600	-0.17770000
C	-2.40583100	-3.76894100	-0.56245000	C	-2.39767200	-3.80060000	-0.55123300
C	-1.08102500	-3.67675500	0.17629500	C	-1.08531700	-3.68030300	0.20472900
H	-2.24066700	-3.69592000	-1.64580600	H	-2.22509600	-3.78400800	-1.63310600
H	-2.91749400	-4.70512000	-0.33294200	H	-2.93201300	-4.70973500	-0.27555400
H	-1.25408200	-3.70593100	1.25948600	H	-1.26354300	-3.67195900	1.28611900
H	-0.41140000	-4.48931500	-0.11188700	H	-0.41120200	-4.49736800	-0.05305700
O	-3.27188200	-2.72457100	-0.14196000	O	-3.26613300	-2.71014800	-0.21159200
O	-0.40124000	-2.46475100	-0.15742100	O	-0.40497300	-2.47012700	-0.16032800
C	0.85715500	3.93729400	0.26320800	C	0.83769200	3.95052600	0.25924400
C	2.19572000	4.07204600	-0.44402700	C	2.17502000	4.05072400	-0.45312900
H	1.00709300	3.89644900	1.35066600	H	0.97901400	3.96757000	1.34608800
H	0.19940300	4.77250600	0.01654600	H	0.16972000	4.75897300	-0.03870700
H	2.04512400	4.06747200	-1.53106400	H	2.03425700	4.00156300	-1.53971700
H	2.70840200	4.98904900	-0.14717400	H	2.68707200	4.97689200	-0.18958800
O	0.19284500	2.76012800	-0.17085400	O	0.17300300	2.73264500	-0.09986500
O	3.06601700	2.99638800	-0.08641800	O	3.03857600	2.98518000	-0.04452200
C	5.40329600	-3.10326200	-0.39014200	C	5.40339800	-3.10960900	-0.41036000
C	6.73007400	-2.99829500	0.34420600	C	6.72198800	-2.98031400	0.33250300
H	5.57072600	-3.05672800	-1.47548000	H	5.57510300	-3.08356700	-1.49400400
H	4.88932300	-4.03346500	-0.14003700	H	4.88926500	-4.03372900	-0.14255000
H	6.55144000	-2.99567700	1.42811500	H	6.54303200	-2.96538700	1.41559900
H	7.38873900	-3.83048100	0.08455400	H	7.39011200	-3.80705900	0.08424100
O	4.54320900	-2.04970200	0.00703600	O	4.52549900	-2.04537100	-0.04819300
O	7.42309600	-1.81015200	-0.02767800	O	7.40176500	-1.78728200	-0.05356100

(66) OT_3-E (F_x = 0.50 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.72509300	-0.10306200	-0.08679900	C	-4.71565200	-0.10428800	-0.09609200
C	-5.41642300	1.09921000	-0.10869800	C	-5.41635000	1.12390000	-0.09623700
C	-6.82946500	0.93948500	-0.14591100	C	-6.80877400	0.96669400	-0.12345400
C	-7.20310100	-0.37570500	-0.15925000	C	-7.18353100	-0.37695400	-0.15724700
S	-5.85934400	-1.44020700	-0.12418800	S	-5.86057400	-1.45871400	-0.14303300
H	-8.21556900	-0.75976200	-0.18171700	H	-8.20541100	-0.74652300	-0.17681800
C	-3.31093200	-0.28435800	-0.06909300	C	-3.32520100	-0.27816600	-0.08687800
C	-2.63692400	-1.49999500	-0.06185500	C	-2.64747400	-1.51239300	-0.10673900
S	-2.16856300	1.03451300	-0.07368300	S	-2.16616400	1.04351900	-0.07123700
C	-1.24151900	-1.37711100	-0.06319200	C	-1.25116700	-1.38829900	-0.09671200
C	-0.78736200	-0.06238900	-0.07386000	C	-0.81189500	-0.07098800	-0.07941200
C	0.56403600	0.36692700	-0.06254400	C	0.55676600	0.35760200	-0.05409900
C	1.03420600	1.67650200	-0.06123800	C	1.01411500	1.66166200	-0.02663800

S	1.92443200	-0.74023300	-0.03376100	S	1.91104500	-0.75488600	-0.03791700
C	2.43229100	1.78672900	-0.03556300	C	2.42588900	1.76853500	-0.00007100
C	3.10289400	0.57222300	-0.01336400	C	3.07278600	0.55239500	0.00059600
C	4.51161800	0.36035300	-0.01170900	C	4.50118000	0.34540200	0.00961700
C	5.19647600	-0.84325900	0.00048100	C	5.18516000	-0.84893200	0.00702200
S	5.68535500	1.66903300	-0.03288500	S	5.64529900	1.66839700	0.01714100
C	6.61098000	-0.71827300	-0.01186200	C	6.60538000	-0.70479500	0.01341400
C	7.04448700	0.57673300	-0.02996100	C	7.00519400	0.59764700	0.01717600
H	8.06223000	0.93767300	-0.05536800	H	8.01765000	0.97498300	0.02030400
C	-7.05910500	3.18566000	0.28404500	C	-7.05302200	3.21587800	0.28915400
C	-5.72310200	3.38309800	-0.41134600	C	-5.72164600	3.39826200	-0.42032400
H	-6.92399200	3.13115300	1.37196000	H	-6.92292800	3.20171500	1.37698800
H	-7.74533400	3.99893600	0.04459900	H	-7.75405900	4.00434800	0.01452600
H	-5.86146400	3.41130300	-1.49778400	H	-5.85405300	3.40745200	-1.50646700
H	-5.23185500	4.29653500	-0.07417000	H	-5.22299600	4.30989500	-0.09383500
O	-7.67701200	1.99086100	-0.17851700	O	-7.66471800	1.98193100	-0.11222800
O	-4.81345100	2.30774600	-0.09575400	O	-4.80877500	2.31275100	-0.09536700
C	-2.41928100	-3.74759900	-0.49089700	C	-2.41853900	-3.78924900	-0.45655200
C	-1.09125400	-3.67270400	0.24553100	C	-1.10325100	-3.66248700	0.29131900
H	-2.26015800	-3.65886000	-1.57402400	H	-2.25367000	-3.78754100	-1.53969300
H	-2.93570000	-4.68369000	-0.27274200	H	-2.95714100	-4.69134400	-0.16617000
H	-1.26168500	-3.72211500	1.32765700	H	-1.27630500	-3.64081200	1.37341600
H	-0.42137700	-4.47813900	-0.06174200	H	-0.43365900	-4.48552300	0.03974200
O	-3.27152900	-2.70435700	-0.04882800	O	-3.27922800	-2.69043400	-0.12600000
O	-0.40680700	-2.45033100	-0.06033300	O	-0.41876700	-2.45911600	-0.09300900
C	0.86703200	3.92766600	0.36545500	C	0.87102000	3.93180900	0.37599400
C	2.20215100	4.07615800	-0.34812100	C	2.20689100	4.05208400	-0.33609800
H	1.02413700	3.86297000	1.45119900	H	1.01773800	3.90279200	1.46282700
H	0.20900100	4.76909900	0.14155100	H	0.21183400	4.76094000	0.11718300
H	2.04132700	4.09503700	-1.43322600	H	2.06062300	4.04415200	-1.42283300
H	2.71973500	4.98553300	-0.03506200	H	2.72753000	4.96402200	-0.03989300
O	0.20590900	2.76253200	-0.09180700	O	0.20049300	2.74236200	-0.03842400
O	3.07727300	2.98966500	-0.02550100	O	3.07072700	2.96588600	0.02555600
C	5.40640900	-3.09274600	-0.41058300	C	5.44972900	-3.10345300	-0.39224200
C	6.74916200	-3.01771900	0.30199300	C	6.77446600	-2.99294000	0.34515200
H	5.55595400	-3.00009400	-1.49708400	H	5.61747400	-3.03427100	-1.47610500
H	4.90062800	-4.03598900	-0.19186600	H	4.94924300	-4.04509200	-0.16014700
H	6.58451700	-3.05708600	1.38792400	H	6.59827000	-3.01484600	1.42893200
H	7.40132200	-3.84320800	0.00053100	H	7.44538500	-3.80968800	0.06702000
O	4.56398400	-2.06289300	0.05160500	O	4.57367100	-2.06902400	0.02277100
O	7.44301500	-1.81870100	-0.03233300	O	7.45084800	-1.78569600	-0.00266700

(67) OT_3-E (F_y = 0.25 V/Å)

Neutral			
elements	x	y	z
C	-4.73084900	-0.10389100	-0.17567100
C	-5.41442700	1.08723800	-0.15546100
C	-6.83274300	0.93533900	-0.18511300
C	-7.22125200	-0.36869900	-0.23072100
S	-5.86228700	-1.42951400	-0.23451400
H	-8.22924800	-0.75659300	-0.26094500
C	-3.30024400	-0.30237700	-0.16085400
C	-2.63786400	-1.50465000	-0.17653200
S	-2.15750400	1.02002300	-0.14455600
C	-1.22158200	-1.37447000	-0.16967500
C	-0.78987200	-0.07035500	-0.15631900
C	0.57687600	0.39037800	-0.13360900
C	1.02335800	1.68921200	-0.12057300
S	1.93455500	-0.70759000	-0.10593900
C	2.43686200	1.80653300	-0.08921400
C	3.09106500	0.60006100	-0.07676800
C	4.51734000	0.37265500	-0.05394900
C	5.16269700	-0.83919600	-0.04467900
S	5.69065600	1.66815300	-0.05522500
C	6.59048400	-0.73301200	-0.03243300
C	7.01819800	0.55951600	-0.03910600
H	8.04046600	0.90844900	-0.03113400
C	-7.02812700	3.19342700	0.24697400
C	-5.69148700	3.35726800	-0.46034900
H	-6.86710700	3.15013200	1.33366600
H	-7.69980300	4.02273700	0.01095300
H	-5.84454000	3.34417500	-1.54884200
H	-5.20497500	4.29182300	-0.16999300
O	-7.68095600	2.01371200	-0.19018000
O	-4.80559100	2.31429800	-0.08982800
C	-2.38248600	-3.77498000	-0.56525800
C	-1.06175200	-3.66033600	0.17349000
H	-2.21878100	-3.73450000	-1.64896900
H	-2.89733900	-4.70081300	-0.30658300
H	-1.22855200	-3.66919600	1.25746300
H	-0.38851300	-4.47323800	-0.10047900
O	-3.26012000	-2.70966400	-0.18472200
O	-0.39131900	-2.44725100	-0.18682600
C	0.86982000	3.96035700	0.25378400
C	2.21199900	4.07524300	-0.45318200
H	1.02497900	3.93968700	1.34185200

Cationic			
elements	x	y	z
C	-4.69104900	-0.11439600	-0.17562000
C	-5.36743400	1.09950900	-0.17604100
C	-6.77684600	0.95924900	-0.20615200
C	-7.16728900	-0.35260200	-0.23667400
S	-5.83774400	-1.43514600	-0.22489100
H	-8.18193000	-0.72737700	-0.25979600
C	-3.28419300	-0.30237000	-0.15478300
C	-2.61773000	-1.53041700	-0.16175400
S	-2.14991800	1.02918900	-0.13799600
C	-1.22726100	-1.40791700	-0.14792500
C	-0.77910700	-0.07361400	-0.14220300
C	0.55379400	0.35231500	-0.12116000
C	1.00670900	1.68394000	-0.09768200
S	1.92261600	-0.74928600	-0.10055400
C	2.39074500	1.80409400	-0.07156100
C	3.06129400	0.57484300	-0.06834100
C	4.46413400	0.38338600	-0.05581700
C	5.12882200	-0.83953700	-0.07015700
S	5.62762400	1.69618700	-0.05138300
C	6.54742700	-0.71563400	-0.06217900
C	6.94885500	0.59055300	-0.05428900
H	7.96945600	0.94799600	-0.04219600
C	-6.95945400	3.20676600	0.24947700
C	-5.62635700	3.38160900	-0.45961200
H	-6.80341000	3.14106400	1.33457400
H	-7.62794700	4.04053600	0.02717200
H	-5.77616200	3.40981400	-1.54579500
H	-5.11952900	4.29115100	-0.13243700
O	-7.61529300	2.03330800	-0.21111100
O	-4.74457800	2.30173100	-0.14115000
C	-2.38102200	-3.78991700	-0.57812500
C	-1.06460600	-3.69812700	0.17181500
H	-2.21915700	-3.73174600	-1.66011600
H	-2.90511200	-4.71322800	-0.33251500
H	-1.22663200	-3.74019500	1.25370300
H	-0.38150100	-4.49028400	-0.13272100
O	-3.25362800	-2.71545400	-0.18650200
O	-0.39459700	-2.45484800	-0.13454900
C	0.83444300	3.95750800	0.26038700
C	2.16986600	4.06221100	-0.45989200
H	0.98722700	3.97000500	1.34634700

H	0.21563400	4.79606900	-0.00705200	H	0.16508600	4.76935600	-0.02832700
H	2.06079800	4.03809400	-1.54127700	H	2.01959900	4.01252200	-1.54575600
H	2.71927500	5.00553000	-0.18515800	H	2.68216000	4.99019800	-0.20076600
O	0.19655400	2.78286400	-0.15611400	O	0.16869600	2.74627100	-0.10014700
O	3.07292100	3.02165400	-0.05394100	O	3.03238000	3.00225400	-0.05654300
C	5.37826400	-3.11968800	-0.39251100	C	5.37165800	-3.13076500	-0.38466200
C	6.69867300	-3.01453900	0.34779900	C	6.68836300	-2.98038600	0.35277500
H	5.54563000	-3.10139600	-1.47641100	H	5.53077300	-3.15859800	-1.46743100
H	4.84625100	-4.03156900	-0.11929400	H	4.83625200	-4.02401500	-0.06457800
H	6.52547400	-3.00135000	1.43127000	H	6.52295600	-2.93565600	1.43587800
H	7.35514000	-3.84780200	0.09421100	H	7.35636700	-3.80967200	0.12005500
O	4.51850700	-2.03299500	-0.03342600	O	4.49680000	-2.01811100	-0.08776600
O	7.39581600	-1.82590900	-0.03390000	O	7.36435400	-1.78921300	-0.06835000

(68) OT_3-E (F_y = 0.50 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.72097900	-0.10045500	-0.18003200	C	-4.68796000	-0.11074100	-0.17967900
C	-5.42142800	1.08168000	-0.15771800	C	-5.36905400	1.09975200	-0.17568800
C	-6.83571000	0.90927200	-0.18723000	C	-6.77521300	0.95266300	-0.20670700
C	-7.20679700	-0.39991900	-0.23379200	C	-7.16153600	-0.36150700	-0.24048100
S	-5.83437100	-1.43966300	-0.23925400	S	-5.82836600	-1.43468900	-0.23091200
H	-8.20777200	-0.80620300	-0.26528200	H	-8.17333900	-0.74461800	-0.26570100
C	-3.28893500	-0.28728200	-0.16300000	C	-3.27916200	-0.29947600	-0.15762000
C	-2.62237900	-1.48781900	-0.17797500	C	-2.61500200	-1.52692100	-0.16379400
S	-2.15284800	1.04325000	-0.15019600	S	-2.14683100	1.03682400	-0.14239300
C	-1.20372700	-1.35085700	-0.17016600	C	-1.21998500	-1.40285900	-0.14825900
C	-0.77959600	-0.04348100	-0.16060800	C	-0.77450600	-0.06650900	-0.14558300
C	0.58585800	0.42046600	-0.13487200	C	0.55762900	0.36222100	-0.12297200
C	1.03898700	1.71730900	-0.12364600	C	1.01225000	1.69335100	-0.10149100
S	1.94030300	-0.68053300	-0.10672700	S	1.92678900	-0.73798800	-0.10011600
C	2.45237500	1.82935500	-0.09143000	C	2.39436300	1.81346400	-0.07210400
C	3.10360900	0.62111700	-0.07886600	C	3.06756600	0.58411100	-0.06755300
C	4.52715300	0.37788700	-0.05127300	C	4.46825100	0.38926000	-0.05204600
C	5.15366400	-0.84434900	-0.04540000	C	5.12696200	-0.83895600	-0.07074200
S	5.72111100	1.65829000	-0.04703300	S	5.64059100	1.69783500	-0.04416700
C	6.58630900	-0.76088400	-0.02866200	C	6.55100400	-0.72350900	-0.05997700
C	7.03271300	0.52550600	-0.03116500	C	6.95783300	0.57968400	-0.04780700
H	8.06121000	0.85534700	-0.01756500	H	7.98103900	0.92900200	-0.03180900
C	-7.06575500	3.16028100	0.25021600	C	-6.97143000	3.19651800	0.25254100
C	-5.73062600	3.34492000	-0.45856700	C	-5.63784700	3.37738500	-0.45765100
H	-6.89757600	3.11302600	1.33683000	H	-6.80913400	3.12912000	1.33758200
H	-7.74727700	3.98623700	0.02253500	H	-7.64205600	4.03184700	0.03559600
H	-5.88974900	3.32578100	-1.54747400	H	-5.79393800	3.39944600	-1.54435400

H	-5.26216800	4.29241100	-0.17327800	H	-5.14057800	4.29666400	-0.13763000
O	-7.70297700	1.98164100	-0.19417100	O	-7.62261300	2.02854300	-0.21143600
O	-4.82935200	2.32494900	-0.08462100	O	-4.75076600	2.31372700	-0.13149000
C	-2.35618400	-3.76479500	-0.55919800	C	-2.37495900	-3.79342100	-0.57432900
C	-1.03617900	-3.64280000	0.17595400	C	-1.05788100	-3.70057900	0.17117800
H	-2.20170200	-3.73540100	-1.64359100	H	-2.22269400	-3.74360200	-1.65742300
H	-2.87160500	-4.68601300	-0.28734100	H	-2.90179300	-4.71218200	-0.31766800
H	-1.19295300	-3.65671200	1.26029400	H	-1.20861100	-3.74754700	1.25372600
H	-0.35681100	-4.44678700	-0.10680700	H	-0.37118900	-4.48522800	-0.14373900
O	-3.23666800	-2.68830700	-0.18823700	O	-3.24703100	-2.70632900	-0.18859400
O	-0.37312100	-2.41425300	-0.17943200	O	-0.39103000	-2.44264300	-0.12810700
C	0.89142400	3.98575200	0.25014500	C	0.83760300	3.96350100	0.25766600
C	2.23707800	4.09668200	-0.45475700	C	2.17539200	4.06974900	-0.46116000
H	1.05073300	3.95905900	1.33896200	H	0.99524600	3.97109800	1.34417700
H	0.24352400	4.83080900	-0.00442900	H	0.17128300	4.78223300	-0.02418100
H	2.08183900	4.05562100	-1.54360400	H	2.02095400	4.01758200	-1.54740800
H	2.74284400	5.03176700	-0.19180500	H	2.68379000	5.00281100	-0.20600100
O	0.21427700	2.82188500	-0.16855200	O	0.17215400	2.76379600	-0.11244300
O	3.09377800	3.05083400	-0.04892400	O	3.03713600	3.01941500	-0.05322600
C	5.33659000	-3.13473800	-0.39481200	C	5.35897300	-3.13952400	-0.38386700
C	6.65675700	-3.05043000	0.34475500	C	6.67604500	-2.99488800	0.35043800
H	5.49756100	-3.12641300	-1.47874400	H	5.50886700	-3.17735800	-1.46681100
H	4.78561200	-4.03195900	-0.11305900	H	4.81258600	-4.02137100	-0.05213900
H	6.49099500	-3.04236100	1.42848100	H	6.51956700	-2.95267600	1.43424300
H	7.30366300	-3.88762800	0.08199300	H	7.34155200	-3.82392400	0.11049100
O	4.49440200	-2.02151200	-0.04393600	O	4.49173900	-2.00602800	-0.09805100
O	7.36984600	-1.86052800	-0.02875900	O	7.35631000	-1.79747800	-0.06815600

(69) OT_3-E (F_z = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.74480200	-0.08460000	0.12411300	C	-4.69639500	-0.12166600	-0.03480900
C	-5.39309900	1.09446800	-0.14921700	C	-5.36517000	1.09543000	-0.10954900
C	-6.81745200	0.97439800	-0.18221400	C	-6.77731200	0.96302600	-0.17487900
C	-7.24199000	-0.29397000	0.07449700	C	-7.17340700	-0.34670200	-0.15738800
S	-5.91196600	-1.36162400	0.34786800	S	-5.85004900	-1.43905900	-0.06343800
H	-8.25886200	-0.65874500	0.06710000	H	-8.18917200	-0.71410000	-0.21492400
C	-3.31865300	-0.30766000	0.19709200	C	-3.29204900	-0.31066600	0.00453100
C	-2.66664600	-1.51532200	0.20712200	C	-2.62285800	-1.53851400	-0.00999000
S	-2.16424200	1.00014900	0.24146000	S	-2.15634900	1.01752700	0.03548300
C	-1.25168600	-1.39919300	0.24917200	C	-1.23590200	-1.41723100	0.00399000
C	-0.80630000	-0.09973100	0.27589600	C	-0.78554900	-0.08394000	0.02903400
C	0.56298900	0.35421800	0.29615300	C	0.54734500	0.34160100	0.04893000
C	1.00902200	1.65371600	0.30325400	C	0.99807800	1.67478800	0.05773200

S	1.92120200	-0.74551700	0.27464300	S	1.91785200	-0.76007100	0.06963500
C	2.42457600	1.76984700	0.29644300	C	2.38525900	1.79576000	0.07919600
C	3.07659600	0.56225900	0.28027000	C	3.05366200	0.56796700	0.08865900
C	4.50394100	0.33948300	0.23606500	C	4.45913400	0.37874200	0.07956300
C	5.15781900	-0.83558600	-0.04114800	C	5.12912800	-0.83676800	-0.00114700
S	5.66646800	1.61195200	0.50591800	S	5.61314400	1.69569900	0.10234000
C	6.58263400	-0.71623400	-0.04018000	C	6.54276200	-0.70406300	-0.03036600
C	7.00200200	0.54752500	0.24597600	C	6.93862700	0.60464200	0.02033400
H	8.01896500	0.91146200	0.26715900	H	7.95541700	0.97259000	-0.00653500
C	-6.95363900	3.27542200	-0.49021200	C	-6.95329200	3.25834100	0.04676400
C	-5.58842600	3.15832600	-1.14492900	C	-5.59586600	3.33415700	-0.62883700
H	-6.83713000	3.62909200	0.54368200	H	-6.83728200	3.34175800	1.13565800
H	-7.59365900	3.96622900	-1.04219600	H	-7.60876700	4.05222900	-0.31329600
H	-5.68440600	2.77512500	-2.16836100	H	-5.69415100	3.22319700	-1.71401300
H	-5.07880000	4.12281900	-1.16297400	H	-5.08972700	4.27140900	-0.39748200
O	-7.63228200	2.02277400	-0.48637200	O	-7.60764600	2.02960800	-0.26321000
O	-4.76049600	2.27861500	-0.38409100	O	-4.74027500	2.28786000	-0.13428400
C	-2.42123500	-3.73360700	-0.34624100	C	-2.38777200	-3.75257300	-0.57611300
C	-1.10567900	-3.71433700	0.41337800	C	-1.06377900	-3.72645000	0.16846800
H	-2.24907600	-3.55672500	-1.41528100	H	-2.23545400	-3.58579900	-1.64843900
H	-2.93634500	-4.68625300	-0.21239700	H	-2.90260300	-4.70089700	-0.42173600
H	-1.29611600	-3.85697100	1.48604000	H	-1.22681900	-3.87409200	1.24233200
H	-0.43274200	-4.49489100	0.05339100	H	-0.38180200	-4.48713100	-0.21210500
O	-3.29169100	-2.72781800	0.16836200	O	-3.25502400	-2.73324500	-0.06336600
O	-0.42176100	-2.48019600	0.21896400	O	-0.39729600	-2.46751400	-0.01846900
C	0.85932100	3.96539900	0.50556000	C	0.82197500	3.98131400	0.25489500
C	2.19211700	3.99772000	-0.22293000	C	2.16355500	4.01840400	-0.45698300
H	1.02505600	4.08844700	1.58477700	H	0.95922800	4.11247700	1.33450500
H	0.19504200	4.75284600	0.14445000	H	0.14923800	4.74793800	-0.13021100
H	2.04464500	3.83999400	-1.29864400	H	2.03712700	3.86783800	-1.53508100
H	2.70391000	4.94768100	-0.06023100	H	2.67414400	4.96432900	-0.27599000
O	0.17999600	2.73560900	0.27290900	O	0.16029000	2.72570100	0.03276900
O	3.05053700	2.98265300	0.29359100	O	3.01823800	2.99153700	0.06133500
C	5.37432000	-2.88355500	-1.06485900	C	5.37157100	-3.06543300	-0.55668800
C	6.72438500	-3.01237800	-0.38160300	C	6.71264500	-3.00359600	0.15207800
H	5.49349200	-2.48409700	-2.07961400	H	5.49548500	-2.93374300	-1.63694000
H	4.86464100	-3.84712900	-1.10984100	H	4.86009000	-4.00673400	-0.35549800
H	6.58447100	-3.38238300	0.64360400	H	6.57093100	-3.10785500	1.23612200
H	7.37630800	-3.69482000	-0.93004800	H	7.37620000	-3.79092700	-0.20758800
O	4.53015900	-2.01537900	-0.30873300	O	4.50492300	-2.02845600	-0.06224500
O	7.40353900	-1.76045200	-0.34241800	O	7.37468800	-1.76958800	-0.11858000

(70) OT_3-E (F_z = 0.50 V/Å)

Neutral			
elements	x	y	z
C	-4.65946400	0.11616700	1.62330400
C	-5.74772700	0.57205200	0.92761600
C	-6.96271600	0.56665900	1.69620000
C	-6.77901000	0.12804300	2.97296100
S	-5.12600800	-0.31865600	3.24996800
H	-7.52864300	0.03801900	3.74546700
C	-3.31646500	-0.04351700	1.10585400
C	-2.98013900	-0.53680000	-0.12797300
S	-1.89187300	0.49653800	1.96009100
C	-1.56922200	-0.49878800	-0.39022700
C	-0.84130600	0.02647500	0.64566800
C	0.59129500	0.23205100	0.66131500
C	1.34113600	0.76083800	-0.35694300
S	1.61373100	-0.24210200	1.99630900
C	2.74608200	0.79805100	-0.06470100
C	3.05611200	0.30105600	1.17460700
C	4.38779700	0.13942600	1.71981500
C	5.49014200	-0.31573400	1.04621700
S	4.82039800	0.56910500	3.35717300
C	6.68851400	-0.31382600	1.84016400
C	6.47851100	0.12141300	3.11408000
H	7.21162800	0.20771800	3.90270400
C	-8.02560400	1.64113600	-0.08253500
C	-6.98748500	0.97794200	-0.96754700
H	-7.74341800	2.68366300	0.10823400
H	-9.01294600	1.60777100	-0.54459300
H	-7.24861800	-0.06984400	-1.16057300
H	-6.89172400	1.50872100	-1.91536400
O	-8.15199900	0.95696500	1.17493500
O	-5.70499400	1.03527200	-0.33975000
C	-3.31689100	-1.09541900	-2.34193700
C	-1.94087800	-1.73043800	-2.33014500
H	-3.27209900	-0.07334200	-2.73546200
H	-4.01283400	-1.68664200	-2.93731300
H	-1.99521600	-2.74804900	-1.92476800
H	-1.51479900	-1.76018100	-3.33345800
O	-3.85550600	-1.05932700	-1.00986700
O	-1.03004100	-0.96088300	-1.53370100
C	1.75309600	1.99974900	-2.28371500
C	3.12915000	1.36479800	-2.26918500
H	1.79881200	3.01570100	-1.87304000

Cationic			
elements	x	y	z
C	-4.48124400	-0.00620600	1.53380800
C	-5.72428700	0.40640100	1.09461000
C	-6.73133200	0.32926500	2.11678800
C	-6.24407000	-0.13007000	3.30377500
S	-4.55708800	-0.48984100	3.21420600
H	-6.80301800	-0.28758300	4.21500200
C	-3.24902400	-0.04017200	0.80248800
C	-3.05156600	-0.28806700	-0.54665500
S	-1.73671200	0.28019400	1.62281900
C	-1.68622300	-0.22897800	-0.93185900
C	-0.81786400	0.08340400	0.13884800
C	0.57947300	0.18229600	0.15456500
C	1.47077300	0.50037700	-0.89492200
S	1.46586300	-0.02105600	1.65736500
C	2.82787400	0.55864600	-0.47895300
C	2.99522900	0.30452800	0.87214500
C	4.21301300	0.26611800	1.62893200
C	5.46092400	-0.15509600	1.21489500
S	4.25976200	0.75461500	3.30861500
C	6.44913000	-0.08081000	2.25553500
C	5.94261000	0.38501800	3.43183900
H	6.48492500	0.54186000	4.35315400
C	-8.17449200	1.48693800	0.71108800
C	-7.37723700	0.91097600	-0.44167100
H	-7.84626900	2.51003000	0.93006300
H	-9.24078600	1.48372800	0.48482700
H	-7.69049600	-0.11508400	-0.66320200
H	-7.47867300	1.52577600	-1.33569400
O	-8.01594600	0.68618500	1.89480300
O	-5.97597000	0.90513100	-0.11907700
C	-3.61554900	-0.47287000	-2.77813200
C	-2.27221600	-1.13251700	-3.00492300
H	-3.57806100	0.59741900	-3.00813800
H	-4.38605300	-0.95135900	-3.38176100
H	-2.31249200	-2.20281600	-2.78179200
H	-1.91472400	-0.97889500	-4.02258400
O	-4.01828600	-0.63622700	-1.40335000
O	-1.26513100	-0.54429200	-2.14055600
C	2.10266000	1.41154600	-2.95119000
C	3.44067100	0.75122000	-2.69674700
H	2.13787300	2.48113400	-2.72378800

H	1.34831000	2.03377600	-3.29567900	H	1.76773600	1.26123000	-3.97700000
H	3.09250300	0.34424300	-2.66746100	H	3.40816200	-0.31840000	-2.93071000
H	3.83743600	1.95822600	-2.84757300	H	4.22410000	1.23143700	-3.28210100
O	0.82613700	1.22673400	-1.51008500	O	1.07685500	0.82055700	-2.11136400
O	3.63999400	1.32342000	-0.92625300	O	3.81321300	0.91075400	-1.31315600
C	6.76846100	-0.71948100	-0.82337100	C	7.13894700	-0.67041900	-0.28926900
C	7.78664400	-1.38633200	0.08194900	C	7.91216000	-1.24868100	0.87878600
H	7.03554300	0.32828300	-1.00848400	H	7.46087300	0.35417400	-0.50548900
H	6.69188900	-1.24798800	-1.77421600	H	7.25522600	-1.28633700	-1.18075300
H	7.49819100	-2.42856700	0.26490600	H	7.57474000	-2.26991900	1.09252900
H	8.78350000	-1.35436900	-0.35936600	H	8.98248400	-1.25109900	0.67220900
O	5.47331200	-0.77614300	-0.22297000	O	5.73252700	-0.65916600	0.00684300
O	7.88827400	-0.70452900	1.34289600	O	7.73597700	-0.44594500	2.05847400

(71) OT_3-P (F = 0.00 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.61836200	0.13010800	0.39929500	C	-4.57788300	0.12454400	0.39878300
C	-5.19675800	1.40309900	0.38141200	C	-5.16443900	1.41246100	0.38111400
C	-6.63382400	1.37581500	0.39276400	C	-6.58687000	1.37831900	0.39188600
C	-7.12995300	0.08802100	0.41906600	C	-7.07684100	0.07261600	0.41750700
S	-5.87120100	-1.06252100	0.42952000	S	-5.83787000	-1.08074700	0.42818200
H	-8.16690000	-0.21749700	0.43225100	H	-8.11739000	-0.22642700	0.43003800
C	-3.21915700	-0.19783300	0.39466900	C	-3.20455900	-0.17741300	0.39419000
C	-2.65272800	-1.47569100	0.41260400	C	-2.62699000	-1.48427500	0.41283600
S	-1.97125500	1.00103900	0.36486400	S	-1.96231000	1.03637800	0.36422400
C	-1.22330100	-1.45788500	0.40201400	C	-1.21907500	-1.46837100	0.40260400
C	-0.68874100	-0.16426100	0.37592000	C	-0.67075700	-0.14790800	0.37566800
C	0.69751500	0.19968100	0.35971800	C	0.67953400	0.18331900	0.36018700
C	1.23209600	1.49328100	0.33368000	C	1.22785200	1.50378200	0.33325200
S	1.98003800	-0.96564600	0.37057200	S	1.97108700	-1.00096600	0.37163800
C	2.66151100	1.51109000	0.32311100	C	2.63576700	1.51968700	0.32302200
C	3.22795000	0.23326200	0.34100500	C	3.21333600	0.21282500	0.34167000
C	4.62715700	-0.09468500	0.33639500	C	4.58666100	-0.08913200	0.33708300
C	5.20554300	-1.36767300	0.35438000	C	5.17321800	-1.37704800	0.35475600
S	5.88000400	1.09794200	0.30621700	S	5.84664700	1.11616100	0.30769400
C	6.64260700	-1.34040000	0.34308500	C	6.59564900	-1.34290400	0.34398200
C	7.13875200	-0.05261500	0.31672100	C	7.08561900	-0.03720200	0.31835600
H	8.17569400	0.25291300	0.30348800	H	8.12616700	0.26184200	0.30582300
N	-4.50028800	2.57519000	0.35559900	N	-4.47162000	2.57700000	0.35633400
C	-5.23269100	3.65373100	0.34228300	C	-5.21419200	3.65655800	0.34330300
C	-6.67562500	3.62716100	0.35368500	C	-6.65192100	3.62262800	0.35420000
N	-7.37475000	2.52935100	0.37816200	N	-7.34012500	2.51252000	0.37799800
H	-4.71760400	4.61165900	0.32148300	H	-4.70252100	4.61545000	0.32322600
H	-7.22034600	4.56906800	0.34121800	H	-7.20590100	4.55768600	0.34218300
N	-0.49427600	-2.60661300	0.41667500	N	-0.49013900	-2.60083300	0.41733000
C	-1.19063200	-3.71156400	0.44076600	C	-1.18839800	-3.71672300	0.44182100
C	-2.62789000	-3.72982600	0.45144300	C	-2.61370900	-3.73281500	0.45219700
N	-3.35308500	-2.64367700	0.43788700	N	-3.33315400	-2.63123200	0.43798100
H	-0.64256200	-4.65086800	0.45316500	H	-0.63577700	-4.65205600	0.45441800
H	-3.15111300	-4.68318800	0.47184500	H	-3.14620100	-4.67951300	0.47272100
N	3.36187000	2.67911600	0.29799400	N	3.34193100	2.66664400	0.29787400
C	2.63665700	3.76522000	0.28459400	C	2.62248700	3.76822600	0.28365500
C	1.19936200	3.74695000	0.29527200	C	1.19717500	3.75213300	0.29403000
N	0.50302200	2.64201200	0.31921000	N	0.49891600	2.63624500	0.31852300
H	3.15983300	4.71861500	0.26437600	H	3.15497800	4.71492400	0.26313000
H	0.65131500	4.68626900	0.28302100	H	0.64455400	4.68746700	0.28142900
N	7.38354100	-2.49394000	0.35778100	N	7.34890500	-2.47710500	0.35786900

C	6.68441400	-3.59174700	0.38232100	C	6.66070200	-3.58721400	0.38166800
C	5.24147300	-3.61830700	0.39367300	C	5.22297400	-3.62114500	0.39256500
N	4.50907400	-2.53977100	0.38024800	N	4.48040000	-2.54158800	0.37953600
H	7.22912500	-4.53366000	0.39486000	H	7.21468300	-4.52227100	0.39368400
H	4.72639200	-4.57623800	0.41450100	H	4.71130300	-4.58003800	0.41264300

(72) OT_3-P (F_x = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.61343800	0.13279400	0.39923300	C	-4.57421600	0.12844800	0.39851600
C	-5.18916300	1.41271500	0.38196300	C	-5.16439900	1.42888100	0.38075600
C	-6.61872600	1.38496300	0.39252100	C	-6.57833500	1.39109400	0.39105500
C	-7.11522700	0.08850300	0.41758400	C	-7.06694100	0.07127100	0.41629700
S	-5.87272000	-1.06204300	0.42791200	S	-5.84630300	-1.08432700	0.42723800
H	-8.15594000	-0.21018400	0.42973700	H	-8.11283500	-0.22017100	0.42808500
C	-3.22315200	-0.18550600	0.39469900	C	-3.21674900	-0.16582000	0.39431000
C	-2.65069400	-1.47775900	0.41258400	C	-2.63324400	-1.48707700	0.41333500
S	-1.98002200	1.01091200	0.36520900	S	-1.97006200	1.04883700	0.36461000
C	-1.22761100	-1.46151300	0.40215300	C	-1.22933300	-1.47247300	0.40347300
C	-0.68854400	-0.16534200	0.37621900	C	-0.67675000	-0.14790400	0.37646500
C	0.68698200	0.18306300	0.36023500	C	0.67061700	0.17362600	0.36115400
C	1.23446100	1.48759800	0.33341300	C	1.22690500	1.49578800	0.33393300
S	1.96761700	-0.98516600	0.37156000	S	1.96271900	-1.01390200	0.37250800
C	2.66276300	1.50061400	0.32295300	C	2.63879500	1.50581500	0.32360300
C	3.22906400	0.22297500	0.34143100	C	3.21031900	0.20297100	0.34225900
C	4.61961100	-0.09649800	0.33689700	C	4.59143900	-0.09785000	0.33733800
C	5.21791600	-1.36939700	0.35496700	C	5.19073900	-1.37647600	0.35472800
S	5.86921200	1.10597500	0.30636200	S	5.84020000	1.11442900	0.30742700
C	6.66086900	-1.32995500	0.34350700	C	6.62179400	-1.33200500	0.34327300
C	7.14884000	-0.04402500	0.31712400	C	7.10312400	-0.03212800	0.31749100
H	8.18201500	0.27202600	0.30342800	H	8.13848300	0.27948100	0.30414100
N	-4.49367200	2.58342900	0.35739800	N	-4.47608100	2.58815300	0.35662600
C	-5.23663100	3.65926800	0.34444600	C	-5.23089600	3.66799900	0.34355700
C	-6.67749400	3.63112200	0.35512700	C	-6.66365500	3.62962600	0.35401700
N	-7.36697500	2.52550900	0.37869500	N	-7.34121400	2.50789800	0.37757600
H	-4.72554100	4.61919200	0.32450100	H	-4.72225400	4.62814300	0.32380500
H	-7.22928200	4.56784700	0.34311100	H	-7.22871600	4.55748500	0.34216300
N	-0.50424700	-2.61279300	0.41668900	N	-0.50483500	-2.60459800	0.41838200
C	-1.21292100	-3.71489900	0.44038500	C	-1.21100500	-3.72090200	0.44264300
C	-2.64458500	-3.72966200	0.45087700	C	-2.63083800	-3.73437600	0.45260400
N	-3.35718900	-2.63070600	0.43736300	N	-3.34268900	-2.62241100	0.43812400
H	-0.66903500	-4.65679300	0.45255500	H	-0.66005400	-4.65704100	0.45528400
H	-3.17852000	-4.67604800	0.47088200	H	-3.17244200	-4.67543300	0.47285700
N	3.35902800	2.67223600	0.29713700	N	3.34392100	2.65589900	0.29821000

C	2.62390000	3.75711300	0.28297300	C	2.62005300	3.75714800	0.28382200
C	1.19438200	3.74095700	0.29350500	C	1.19875400	3.74537800	0.29425400
N	0.50659000	2.62442300	0.31839300	N	0.50215000	2.62528100	0.31918300
H	3.14621000	4.71170100	0.26199400	H	3.15327800	4.70377100	0.26298700
H	0.63863400	4.67483100	0.28062100	H	0.64390000	4.67899900	0.28151200
N	7.40214800	-2.48909000	0.35840400	N	7.37580700	-2.47309200	0.35706000
C	6.69889700	-3.58726600	0.38284400	C	6.68553200	-3.58169700	0.38090700
C	5.26127500	-3.62303100	0.39424500	C	5.24894900	-3.62457200	0.39239400
N	4.53173700	-2.53862400	0.38074400	N	4.50709900	-2.54606300	0.37976300
H	7.24627900	-4.52923600	0.39529200	H	7.24127600	-4.51686000	0.39260200
H	4.74480000	-4.57974500	0.41494100	H	4.73989300	-4.58476200	0.41248300

(73) OT_3-P (F_x = 0.50 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.59182200	0.15368700	0.39804700	C	-4.57617900	0.14185600	0.39810900
C	-5.18882400	1.45047300	0.38152300	C	-5.18318700	1.45401100	0.38033800
C	-6.60467600	1.40509200	0.39192300	C	-6.58989600	1.40280500	0.39091600
C	-7.08981500	0.08442700	0.41584000	C	-7.07254100	0.06646500	0.41626300
S	-5.86588100	-1.06224400	0.42563900	S	-5.86478700	-1.08959300	0.42721100
H	-8.13643200	-0.20912800	0.42720200	H	-8.12407800	-0.22104100	0.42797300
C	-3.23248100	-0.14402600	0.39370300	C	-3.23798700	-0.14456000	0.39400700
C	-2.65740300	-1.47275000	0.41238600	C	-2.64617100	-1.47939300	0.41336200
S	-1.97117100	1.05132600	0.36444900	S	-1.97146500	1.07885500	0.36390900
C	-1.24869900	-1.47619800	0.40299200	C	-1.24743900	-1.46977100	0.40380100
C	-0.67272100	-0.16511500	0.37649100	C	-0.67933500	-0.13467300	0.37636400
C	0.67510900	0.13390300	0.36152300	C	0.66125800	0.16069900	0.36166600
C	1.24352700	1.46484200	0.33324200	C	1.23607500	1.48479100	0.33406600
S	1.97178800	-1.05498300	0.37357400	S	1.96053500	-1.04717900	0.37364800
C	2.66579800	1.47623400	0.32270100	C	2.64732600	1.48545700	0.32400200
C	3.24851100	0.18406500	0.34193800	C	3.21786600	0.17016300	0.34311200
C	4.61417500	-0.09650000	0.33718600	C	4.59121500	-0.11265300	0.33796200
C	5.25376100	-1.38074300	0.35545700	C	5.21755200	-1.39104900	0.35498100
S	5.86180300	1.13845500	0.30651000	S	5.83371900	1.12185900	0.30790300
C	6.70815600	-1.31071900	0.34409400	C	6.65533400	-1.32536100	0.34343500
C	7.17360700	-0.02171300	0.31829600	C	7.11945200	-0.02159000	0.31823200
H	8.20210200	0.31210600	0.30343500	H	8.15098500	0.30261200	0.30448000
N	-4.51143900	2.61786700	0.35847000	N	-4.50832200	2.61103800	0.35651700
C	-5.27990900	3.68944800	0.34655600	C	-5.28197100	3.68873300	0.34371400
C	-6.71174700	3.64222100	0.35712200	C	-6.70862000	3.63631400	0.35443500
N	-7.37739600	2.51387400	0.37974000	N	-7.36902100	2.49748600	0.37816000
H	-4.78096300	4.65487500	0.32766600	H	-4.78226500	4.65310300	0.32404600
H	-7.28714300	4.56402700	0.34627800	H	-7.29170400	4.55327400	0.34301600
N	-0.54707700	-2.62454100	0.41793100	N	-0.52741000	-2.59721100	0.41885100

C	-1.27749400	-3.72799500	0.44133800	C	-1.23810800	-3.71790100	0.44312700
C	-2.69252300	-3.72174100	0.45071500	C	-2.65115000	-3.72699800	0.45277100
N	-3.38224000	-2.59413100	0.43642400	N	-3.35751700	-2.60499600	0.43801000
H	-0.74213800	-4.67368500	0.45372000	H	-0.68765900	-4.65382500	0.45581700
H	-3.25431200	-4.65090500	0.47019600	H	-3.20225200	-4.66252500	0.47288500
N	3.35280400	2.63885700	0.29642300	N	3.35787700	2.62477300	0.29861100
C	2.60635400	3.73562200	0.28136200	C	2.63851300	3.73812000	0.28354600
C	1.20023500	3.71868000	0.29182500	C	1.22745900	3.73636000	0.29360600
N	0.51671000	2.57887500	0.31802300	N	0.52265600	2.61343800	0.31898900
H	3.13380000	4.68727400	0.25959900	H	3.18159900	4.67905300	0.26244700
H	0.62872500	4.64185500	0.27855100	H	0.67336200	4.67021500	0.28047600
N	7.45595400	-2.47062000	0.35893200	N	7.41828100	-2.46184000	0.35685700
C	6.74716700	-3.58031500	0.38288500	C	6.73034200	-3.58057300	0.38014700
C	5.33228300	-3.63862300	0.39391300	C	5.30647200	-3.64160600	0.39152200
N	4.59150600	-2.53615900	0.38022300	N	4.55379900	-2.55900000	0.37929600
H	7.30789800	-4.51754700	0.39491600	H	7.29766400	-4.51027700	0.39127700
H	4.81443500	-4.59322000	0.41385400	H	4.80162600	-4.60337800	0.41094800

(74) OT_3-P (F_y = 0.25 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.60928200	0.13034700	0.39949200	C	-4.57323400	0.12583600	0.39862700
C	-5.20503300	1.39768200	0.38287700	C	-5.16816200	1.40927600	0.38129800
C	-6.64536400	1.34827100	0.39267300	C	-6.59382400	1.36164600	0.39002000
C	-7.12086500	0.05241100	0.41642900	C	-7.07117700	0.05025000	0.41361100
S	-5.84503900	-1.07761700	0.42638200	S	-5.82142900	-1.08816300	0.42481600
H	-8.15154100	-0.27391900	0.42764700	H	-8.10766100	-0.26297200	0.42401100
C	-3.20743700	-0.18404200	0.39547500	C	-3.19588700	-0.17112600	0.39532300
C	-2.63383300	-1.45820000	0.41257400	C	-2.61515900	-1.47403800	0.41392500
S	-1.96567900	1.02299800	0.36678500	S	-1.95813300	1.04782500	0.36650900
C	-1.20826700	-1.43377000	0.40245800	C	-1.20902400	-1.45425300	0.40466700
C	-0.67877000	-0.13818300	0.37735400	C	-0.66431000	-0.13299900	0.37833100
C	0.70722300	0.22702000	0.36101800	C	0.68652100	0.20012100	0.36280800
C	1.24593300	1.51909300	0.33388100	C	1.23507400	1.51987300	0.33523000
S	1.98614300	-0.94249900	0.37222200	S	1.97492500	-0.98700200	0.37392200
C	2.68040200	1.53093300	0.32289300	C	2.64786100	1.53286900	0.32403400
C	3.24012700	0.24913200	0.34175500	C	3.22093600	0.22240300	0.34281500
C	4.63592600	-0.09347500	0.33683700	C	4.59108900	-0.08695600	0.33707500
C	5.19599200	-1.37304300	0.35591200	C	5.16708800	-1.38030700	0.35506500
S	5.90692100	1.08304500	0.30360900	S	5.86292300	1.10859800	0.30448500
C	6.63050900	-1.36867400	0.34341900	C	6.58814400	-1.36068000	0.34224900
C	7.14744600	-0.08966900	0.31501000	C	7.09071600	-0.06134500	0.31464100
H	8.19041800	0.19465700	0.30010000	H	8.13532500	0.22340100	0.29997600
N	-4.52913700	2.57902900	0.35944900	N	-4.48842500	2.58114900	0.35851100

C	-5.27764500	3.64824800	0.34638600	C	-5.24134100	3.65388500	0.34499900
C	-6.71542800	3.60018000	0.35616800	C	-6.67406400	3.60665900	0.35380100
N	-7.40011700	2.49188500	0.37882200	N	-7.35396500	2.49028000	0.37601800
H	-4.77420600	4.61340300	0.32715100	H	-4.73641600	4.61711400	0.32620900
H	-7.27602400	4.53408500	0.34408400	H	-7.23869600	4.53612800	0.34154400
N	-0.47140000	-2.57889200	0.41621300	N	-0.47505800	-2.58395400	0.41940300
C	-1.16139100	-3.68707800	0.43862700	C	-1.16931200	-3.70237000	0.44262000
C	-2.60308600	-3.71212100	0.44886200	C	-2.59926900	-3.72275600	0.45203900
N	-3.33158000	-2.62896300	0.43649800	N	-3.32031000	-2.62276400	0.43810900
H	-0.61128300	-4.62459700	0.44998500	H	-0.61566900	-4.63688200	0.45497000
H	-3.12013200	-4.66829000	0.46782900	H	-3.12785100	-4.67156200	0.47152200
N	3.38234700	2.69638000	0.29634600	N	3.35302900	2.67864800	0.29795600
C	2.66035000	3.78600200	0.28154700	C	2.63398900	3.78234400	0.28337200
C	1.22713100	3.77387000	0.29255500	C	1.21397600	3.76950700	0.29463600
N	0.52492000	2.67144400	0.31827900	N	0.51169600	2.65487000	0.32044500
H	3.18948500	4.73728500	0.25971900	H	3.17095300	4.72708900	0.26173900
H	0.68072600	4.71533400	0.27901600	H	0.66078100	4.70516400	0.28168800
N	7.35656800	-2.53244100	0.35869100	N	7.33274400	-2.50099900	0.35596800
C	6.64284700	-3.61967900	0.38451700	C	6.63539000	-3.60492100	0.38124600
C	5.19487200	-3.62375000	0.39716300	C	5.19320300	-3.62419800	0.39424800
N	4.47926400	-2.53486400	0.38366700	N	4.46131600	-2.53628500	0.38178600
H	7.17133500	-4.57004600	0.39727100	H	7.17929000	-4.54560400	0.39296000
H	4.66755900	-4.57443300	0.41916500	H	4.67331000	-4.57830900	0.41558500

(75) OT_3-P (F_y = 0.50 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.59964600	0.12937700	0.39935100	C	-4.56874200	0.12679400	0.39832300
C	-5.21159000	1.39203000	0.38329500	C	-5.17213400	1.40620900	0.38117900
C	-6.65591300	1.32134400	0.39108900	C	-6.60156100	1.34503500	0.38774500
C	-7.11113000	0.01827900	0.41269800	C	-7.06609000	0.02840100	0.40940100
S	-5.81937500	-1.09320600	0.42303500	S	-5.80598500	-1.09628700	0.42131500
H	-8.13537300	-0.32833700	0.42184400	H	-8.09831600	-0.29916500	0.41770400
C	-3.19590900	-0.17252700	0.39657900	C	-3.18801800	-0.16555200	0.39652000
C	-2.61480400	-1.44324000	0.41358700	C	-2.60340800	-1.46455100	0.41532800
S	-1.96056800	1.04359700	0.36882900	S	-1.95464500	1.05977000	0.36879900
C	-1.19193600	-1.41153600	0.40430000	C	-1.19877000	-1.44044600	0.40712500
C	-0.66854500	-0.11346400	0.37976400	C	-0.65743500	-0.11815600	0.38122300
C	0.71656500	0.25557300	0.36346700	C	0.69332600	0.21782300	0.36566000
C	1.25833300	1.54652600	0.33551900	C	1.24241600	1.53688800	0.33739300
S	1.99274000	-0.91834400	0.37503000	S	1.97962700	-0.97298700	0.37648900
C	2.69900200	1.55320500	0.32399300	C	2.66043100	1.54736000	0.32523500
C	3.25257100	0.26706000	0.34335800	C	3.22968700	0.23320600	0.34417700
C	4.64393300	-0.09130800	0.33756100	C	4.59586100	-0.08447500	0.33727100

C	5.18468600	-1.37839600	0.35694900	C	5.16096300	-1.38402600	0.35537800
S	5.93407900	1.06836600	0.30117300	S	5.88085800	1.10111800	0.30144900
C	6.61730400	-1.39763400	0.34237800	C	6.58118300	-1.37938600	0.34035900
C	7.15507100	-0.12800800	0.31201900	C	7.09656600	-0.08699900	0.31083800
H	8.20374000	0.13491400	0.29474700	H	8.14511600	0.18324300	0.29387400
N	-4.55614700	2.58151200	0.36200300	N	-4.50614300	2.58537700	0.36039200
C	-5.31987700	3.64255100	0.34863400	C	-5.26927700	3.65168200	0.34634400
C	-6.75259900	3.57411800	0.35637000	C	-6.69754100	3.59118900	0.35295300
N	-7.42330300	2.45573200	0.37730700	N	-7.36861200	2.46824400	0.37352800
H	-4.82745000	4.61495400	0.33071100	H	-4.77149600	4.61997300	0.32882900
H	-7.32841100	4.50074500	0.34411100	H	-7.27243600	4.51578300	0.34034500
N	-0.44742000	-2.55284700	0.41787800	N	-0.45964000	-2.56744500	0.42208100
C	-1.13062800	-3.66504700	0.43896000	C	-1.14927800	-3.68885500	0.44415600
C	-2.57700500	-3.69749800	0.44838100	C	-2.58475200	-3.71399800	0.45253500
N	-3.30899400	-2.61680000	0.43649200	N	-3.30724100	-2.61533200	0.43867500
H	-0.57801000	-4.60103500	0.44993400	H	-0.59475600	-4.62320700	0.45648000
H	-3.08773300	-4.65708700	0.46629300	H	-3.10863900	-4.66592300	0.47113700
N	3.40139600	2.71633700	0.29627200	N	3.36430700	2.69236900	0.29824200
C	2.68253100	3.80995700	0.28043500	C	2.64585500	3.79839300	0.28329900
C	1.25286900	3.80317600	0.29188600	C	1.23011500	3.78838800	0.29544000
N	0.54541900	2.70259800	0.31914200	N	0.52441600	2.67475000	0.32254400
H	3.21727900	4.75996900	0.25712100	H	3.18641900	4.74231700	0.26050200
H	0.70770000	4.74723100	0.27724800	H	0.67664200	4.72521000	0.28208100
N	7.32753200	-2.57167700	0.35723700	N	7.31678900	-2.52600100	0.35362300
C	6.59921100	-3.64846700	0.38416500	C	6.61059600	-3.62403800	0.38019400
C	5.14645700	-3.62913400	0.39895400	C	5.16358300	-3.62813200	0.39545100
N	4.44815900	-2.52891700	0.38642800	N	4.44272700	-2.53109600	0.38387900
H	7.11128500	-4.60762200	0.39634000	H	7.14389400	-4.57108600	0.39139500
H	4.60640600	-4.57253800	0.42194700	H	4.63544000	-4.57789700	0.41792200

(76) OT_3-P (F_z = 0.25 V/Å)

Neutral			
elements	x	y	z
C	-4.61802300	0.13060800	0.45578200
C	-5.19593500	1.40328700	0.41497000
C	-6.63233600	1.37531500	0.37240500
C	-7.12882600	0.08737300	0.38333900
S	-5.87043300	-1.06283700	0.43029100
H	-8.16422700	-0.21875300	0.32715300
C	-3.21886100	-0.19704900	0.48221500
C	-2.65203800	-1.47482600	0.48066000
S	-1.97084800	1.00241800	0.47648400
C	-1.22249400	-1.45664200	0.48504800
C	-0.68798100	-0.16273000	0.48877300

Cationic			
elements	x	y	z
C	-4.57608600	0.12391600	0.40884000
C	-5.16230200	1.41198200	0.39543800
C	-6.58266800	1.37774400	0.31041900
C	-7.07024700	0.07196300	0.25414800
S	-5.83180700	-1.08098000	0.30185000
H	-8.10709600	-0.22676200	0.16260700
C	-3.20305400	-0.17794900	0.46022800
C	-2.62547900	-1.48437100	0.47573700
S	-1.96154900	1.03669100	0.47822300
C	-1.21675100	-1.46737800	0.50569700
C	-0.67009500	-0.14651000	0.50764400

C	0.69824800	0.20180300	0.47226900	C	0.68071500	0.18638600	0.49205800
C	1.23222500	1.49459800	0.41610600	C	1.22700900	1.50630500	0.43707600
S	1.98117900	-0.96346700	0.48128200	S	1.97187600	-0.99753100	0.48433500
C	2.66138600	1.51232100	0.39013900	C	2.63498500	1.52186900	0.38606600
C	3.22862300	0.23520200	0.42744600	C	3.21266900	0.21543400	0.40676200
C	4.62738600	-0.09325700	0.39218600	C	4.58475000	-0.08823300	0.34553800
C	5.20512300	-1.36674500	0.38719700	C	5.17115600	-1.37620500	0.36873000
S	5.87877400	1.09839700	0.30792500	S	5.83831000	1.11196200	0.17703000
C	6.64080400	-1.34026200	0.32351000	C	6.59002200	-1.34510900	0.26134800
C	7.13674000	-0.05260900	0.28289800	C	7.07610900	-0.04196300	0.15148600
H	8.17109200	0.25154900	0.20181900	H	8.11136100	0.25332000	0.03403400
N	-4.49910500	2.57553800	0.39862200	N	-4.47156100	2.57662600	0.44867800
C	-5.23000700	3.65222600	0.31811100	C	-5.21264100	3.65636100	0.39358500
C	-6.67257300	3.62495900	0.27667200	C	-6.64755900	3.62238000	0.30972700
N	-7.37247300	2.52805000	0.31497100	N	-7.33512400	2.51177000	0.27976300
H	-4.71412700	4.60928500	0.28253300	H	-4.70115100	4.61526000	0.41670000
H	-7.21606600	4.56537900	0.21137600	H	-7.20096900	4.55701200	0.27032900
N	-0.49328000	-2.60540500	0.47050200	N	-0.48770500	-2.59966700	0.51748600
C	-1.18932000	-3.71006800	0.42954300	C	-1.18501700	-3.71620200	0.47813900
C	-2.62673600	-3.72872300	0.42516600	C	-2.60951900	-3.73337900	0.44745200
N	-3.35214300	-2.64325200	0.46179400	N	-3.33021500	-2.63214700	0.45658700
H	-0.64102400	-4.64876400	0.39683000	H	-0.63103600	-4.65074000	0.46929600
H	-3.14974400	-4.68176300	0.38944400	H	-3.14153300	-4.67998700	0.41484500
N	3.36100100	2.67908400	0.32072700	N	3.33927300	2.66798200	0.31758400
C	2.63504500	3.76291000	0.25725500	C	2.61843500	3.76855800	0.28136200
C	1.19768800	3.74475200	0.28332700	C	1.19437600	3.75283600	0.33320900
N	0.50248000	2.64244200	0.37259600	N	0.49787800	2.63851600	0.42073900
H	3.15727100	4.71397700	0.18110900	H	3.14976500	4.71334100	0.20892300
H	0.64888900	4.68198200	0.22629900	H	0.64024200	4.68674300	0.30041800
N	7.38058700	-2.49418000	0.29557900	N	7.34243900	-2.47940800	0.25980300
C	6.68081200	-3.59184000	0.30523000	C	6.65595500	-3.58831400	0.33956500
C	5.23915200	-3.61765700	0.36797600	C	5.22266400	-3.61920100	0.44585100
N	4.50879400	-2.53885200	0.42135500	N	4.48187300	-2.53814000	0.47352200
H	7.22391500	-4.53388600	0.26483000	H	7.20931000	-4.52369600	0.32532200
H	4.72329200	-4.57540000	0.37306900	H	4.71189900	-4.57660100	0.51063300

(77) OT_3-P (F_z = 0.50 V/Å)

Neutral				Cationic			
elements	x	y	z	elements	x	y	z
C	-4.61490000	0.13287400	0.53152900	C	-4.56558000	0.12113100	0.41175600
C	-5.18448300	1.40040400	0.37686000	C	-5.15262800	1.40935000	0.38824600
C	-6.61602000	1.37049300	0.25828700	C	-6.55592000	1.37784800	0.15398700
C	-7.11882000	0.08666300	0.32920400	C	-7.02911800	0.07458900	-0.00990200
S	-5.86864700	-1.06013900	0.50571600	S	-5.79730100	-1.07820100	0.11644100

H	-8.14775300	-0.22266900	0.20670600	H	-8.04534500	-0.21863900	-0.24411200
C	-3.21836600	-0.19503200	0.62690000	C	-3.19946700	-0.18018100	0.55641700
C	-2.65109600	-1.47247300	0.65188700	C	-2.61934700	-1.48538800	0.58247300
S	-1.96994200	1.00447300	0.63832100	S	-1.96182700	1.03624700	0.64762700
C	-1.22154600	-1.45382200	0.69316200	C	-1.21293600	-1.46649700	0.67621800
C	-0.68690100	-0.16013600	0.70246500	C	-0.66874100	-0.14516300	0.71122400
C	0.69977700	0.20486900	0.68623900	C	0.68188400	0.19049300	0.69553000
C	1.23335700	1.49741500	0.62615500	C	1.22486700	1.50991100	0.60715500
S	1.98249100	-0.96131600	0.64185900	S	1.97450000	-0.99252500	0.65353200
C	2.66176700	1.51488100	0.56299800	C	2.62933400	1.52563400	0.49202900
C	3.22958500	0.23727200	0.57180100	C	3.20989300	0.22014600	0.50195800
C	4.62484600	-0.09271000	0.46619200	C	4.57371100	-0.08538700	0.34788000
C	5.19376800	-1.36469500	0.34941700	C	5.16168600	-1.37360800	0.36085200
S	5.87599900	1.09969200	0.37562200	S	5.79996800	1.10375500	-0.00650300
C	6.62319300	-1.33755400	0.20645300	C	6.56137100	-1.34924800	0.10567800
C	7.12469400	-0.05111800	0.22104000	C	7.03061500	-0.05169300	-0.11040300
H	8.15102000	0.25489100	0.07113400	H	8.04322200	0.23403800	-0.36868400
N	-4.48138100	2.56759100	0.30315900	N	-4.47586100	2.57204300	0.55204300
C	-5.19965900	3.63063600	0.07049500	C	-5.20906500	3.65298700	0.43459100
C	-6.63917100	3.60154500	-0.04589800	C	-6.62691600	3.62160300	0.20158500
N	-7.34672900	2.51506500	0.06853800	N	-7.30569300	2.51099100	0.08438100
H	-4.67658600	4.57845100	-0.03573200	H	-4.70395200	4.61125000	0.52661000
H	-7.17200700	4.53086800	-0.23575000	H	-7.17529800	4.55646900	0.11974500
N	-0.49213000	-2.60311800	0.69040800	N	-0.48278200	-2.59846900	0.69916200
C	-1.18606100	-3.70656500	0.60296800	C	-1.17389100	-3.71415100	0.58716200
C	-2.62309600	-3.72561300	0.56201200	C	-2.59558500	-3.73311800	0.49131600
N	-3.34976100	-2.64134900	0.60918500	N	-3.31943700	-2.63398500	0.50885000
H	-0.63632800	-4.64405400	0.55924500	H	-0.61691000	-4.64682700	0.56873500
H	-3.14439500	-4.67736400	0.48724600	H	-3.12240900	-4.67876500	0.39917100
N	3.35934100	2.68148300	0.47129700	N	3.32794200	2.67079700	0.36905700
C	2.63183900	3.76373500	0.39911100	C	2.60366200	3.76887700	0.32473300
C	1.19528900	3.74590000	0.46200500	C	1.18324400	3.75313600	0.44188500
N	0.50316300	2.64608800	0.59624700	N	0.49437800	2.64194600	0.60201300
H	3.15148300	4.71248900	0.28570400	H	3.12865300	4.71084500	0.19325400
H	0.64472400	4.68154600	0.39575000	H	0.62576900	4.68473300	0.39984600
N	7.35276500	-2.48733500	0.04806200	N	7.31152200	-2.48319200	0.06530800
C	6.64555900	-3.57836300	-0.01387600	C	6.63611400	-3.58975000	0.23160400
C	5.20850200	-3.60478000	0.12672500	C	5.22216300	-3.61407600	0.48565800
N	4.49182700	-2.53467000	0.33083500	N	4.48897100	-2.53027800	0.57513400
H	7.17723300	-4.51341000	-0.17721000	H	7.18482300	-4.52628600	0.17495100
H	4.68546100	-4.55655000	0.06434200	H	4.71961700	-4.56890300	0.61862000

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