

Two-electron mediation enables fast alkali peroxide cycling and suppresses side reactions in metal-O₂ cells

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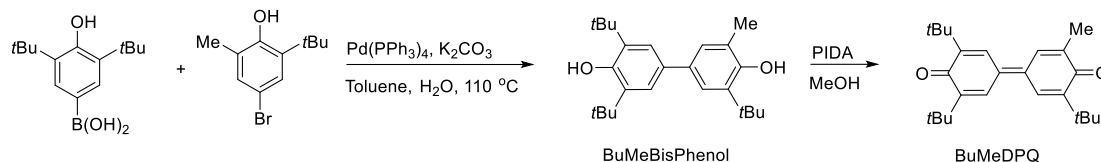
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SUPPLEMENTARY METHODS

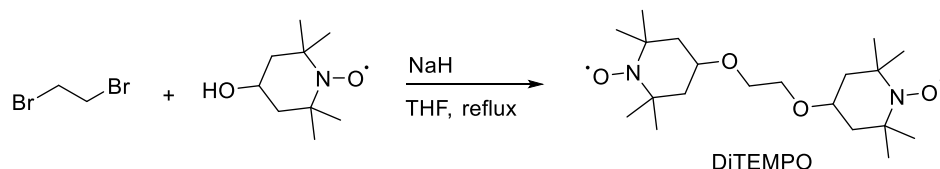
Syntheses

BuMeDPQ



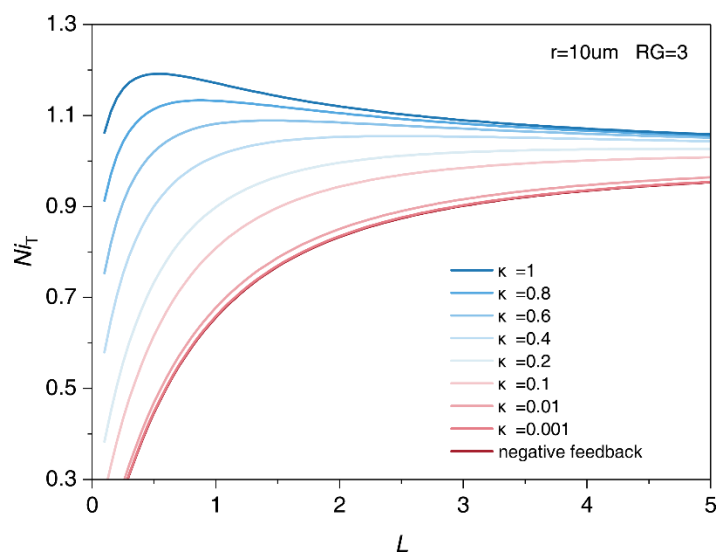
To a flame-dried Ar-filled Schlenk tube containing a magnetic stirring bar, (3,5-di-tert-butyl-4-hydroxyphenyl)boronic acid (2.2 mmol, 550 mg), 4-bromo-2-(tert-butyl)-6-methylphenol (2 mmol, 486 mg), $\text{Pd}(\text{PPh}_3)_4$ (5 mol%, 150 mg), K_2CO_3 (6 mmol, 828 mg) and toluene/ H_2O (6 mL/0.6 mL) were added subsequently. The reaction mixture was stirred at $120\text{ }^\circ\text{C}$ for 12 h. After being cooled to room temperature, the reaction mixture was concentrated under vacuum and directly purified by flash column chromatography (Petroleum Ether: Ethyl Acetate = 5:1) to afford analytically pure product BuMEBisPhenol (203 mg, Yield: 27%). ^1H NMR (600 MHz, CDCl_3): δ = 7.30 (s, 2H), 7.29 (d, J = 2.1 Hz, 1H), 7.14 (d, J = 1.9 Hz, 1H), 5.18 (s, 1H), 4.75 (s, 1H), 2.31 (s, 3H), 1.49 (s, 18H), 1.46 (s, 9H). To a flame-dried Schlenk tube containing a magnetic stirring bar, BuMEBisPhenol (0.27 mmol, 100 mg), Phenyliodine(III) diacetate (PIDA, 0.3 mmol, 78.2 mg) and MeOH (3.5 mL) were added subsequently. The reaction mixture was stirred for 12 h. The formed precipitates were washed with diethyl ether and ethanol to afford pure BuMeDPQ product as a red solid (82 mg, Yield: 81%). ^1H NMR (600 MHz, CDCl_3): δ = 7.77 (d, J = 2.6 Hz, 1H), 7.72 (d, J = 2.6 Hz, 1H), 7.67 (d, J = 2.6 Hz, 2H), 2.15 (s, 3H), 1.37 (s, 27H).

DiTEMPO

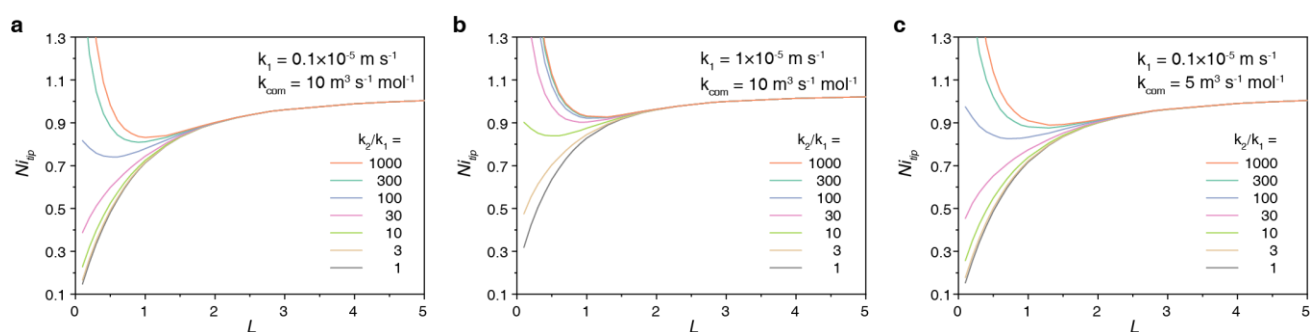


To a flame-dried Ar-filled Schlenk flask containing a magnetic stirring bar, 4-hydroxy-2,2,6,6-tetramethylpiperidine-1-oxyl (40 mmol, 6.4 g) and THF (50 mL) were added under N_2 atmosphere. The reaction mixture was cooled to $0\text{ }^\circ\text{C}$, then, Sodium hydride (60wt% in mineral oil, 60 mmol, 2.4 g) was added portionwise. The mixture was refluxed for 1 h, and cooled to room temperature. Under N_2 atmosphere, 1,2-dibromoethane (10 mmol, 0.86 mL) was injected via a syringe and the reaction mixture was refluxed overnight. After being cooled to room temperature, the reaction mixture was concentrated under vacuum and directly purified by flash column chromatography to afford analytically pure DiTEMPO as a red solid (1.4 g, Yield: 38%). HR-MS (ESI, m/z): calculated for $\text{C}_{20}\text{H}_{38}\text{N}_2\text{O}_4$ [M] $^{2+}$: 185.1416. found: 185.1418.

SUPPLEMENTARY FIGURES



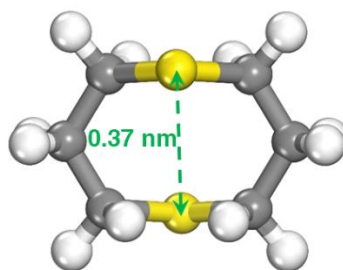
Supplementary Figure 1 | Theoretical SECM approach curves with various κ from negative approach curve to $\kappa = 1$.



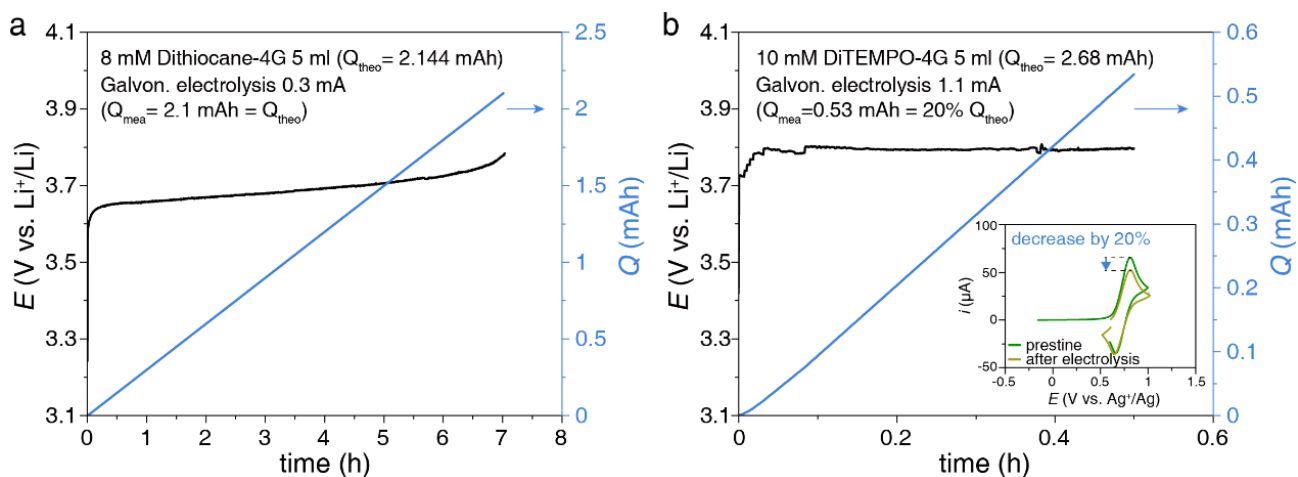
Supplementary Figure 2 | Fitting of approach curve with a bounced pattern. $D = 4 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$. **a**, $k_1 = 0.1 \times 10^{-5} \text{ m s}^{-1}$, $k_{\text{com}} = 10 \text{ m}^3 \text{ s}^{-1} \text{ mol}^{-1}$; **b**, $k_1 = 1 \times 10^{-5} \text{ m s}^{-1}$, $k_{\text{com}} = 10 \text{ m}^3 \text{ s}^{-1} \text{ mol}^{-1}$; **c**, $k_1 = 0.1 \times 10^{-5} \text{ m s}^{-1}$, $k_{\text{com}} = 5 \text{ m}^3 \text{ s}^{-1} \text{ mol}^{-1}$

Supplementary Table 1 | Summary of kinetics for each step in RMs oxidizing Li_2O_2 . k_1 and k_2 is the rate of constant of RM^+ and RM^{2+} reacting with Li_2O_2 , respectively. K_{COMP} is the rate constant of the comproportionation reaction of $\text{RM} + \text{RM}^{2+} \rightarrow 2\text{RM}^+$.

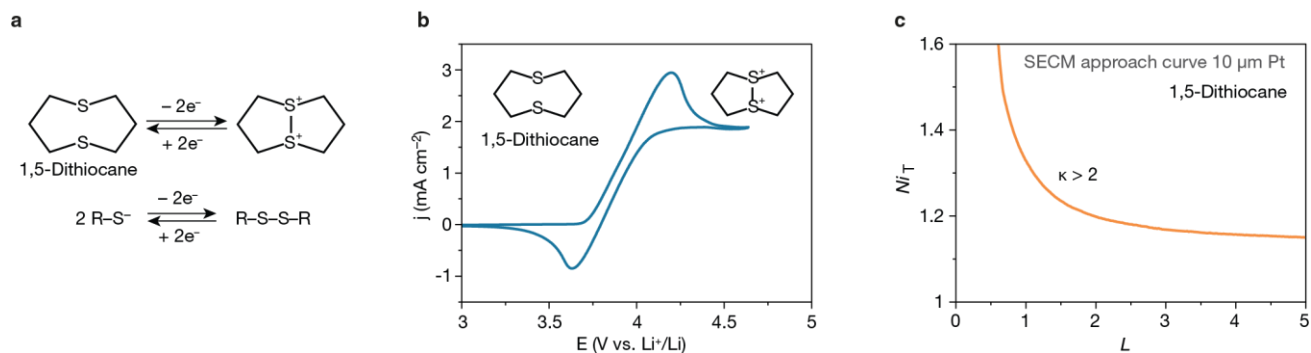
	$D (\times 10^{-10} \text{ m}^2 \text{ s}^{-1})$	$k_{\text{app},1} (\times 10^{-5} \text{ m s}^{-1})$	$k_{\text{app},2} (\times 10^{-5} \text{ m s}^{-1})$	$K_{\text{COMP}} (\text{m}^3 \text{ s}^{-1} \text{ mol}^{-1})$	$k_{\text{app},2}/k_{\text{app},1}$
DPAB	1.76	0.14	23.4	10	167
DMPZ	4.53	0.22	18.7	13	85
TMPD	3.89	0.078	10.5	9.2	135



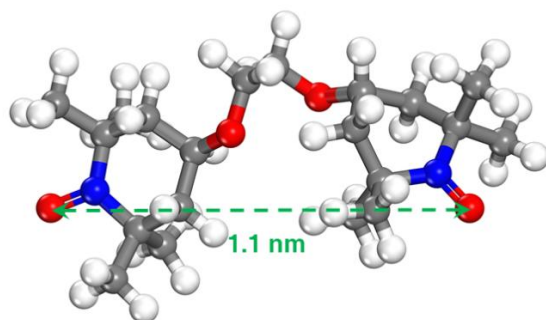
Supplementary Figure 3 | Molecular structure of 1,5-dithiocane.



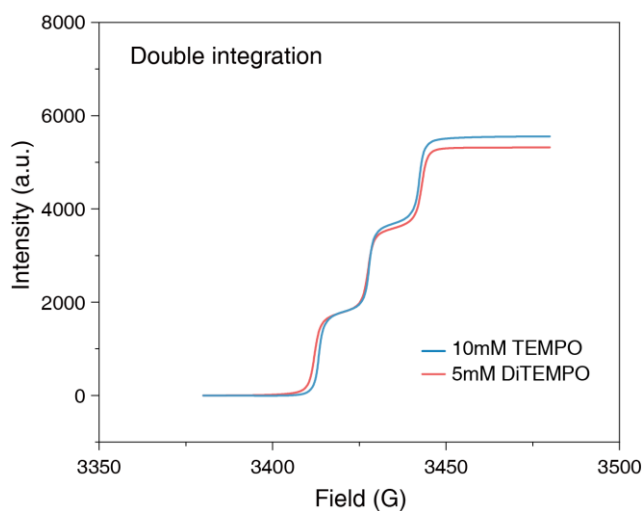
Supplementary Figure 4 | Coulombic titration of 1,5-dithiocane, which shows its redox peak being a $2e^-$ process.



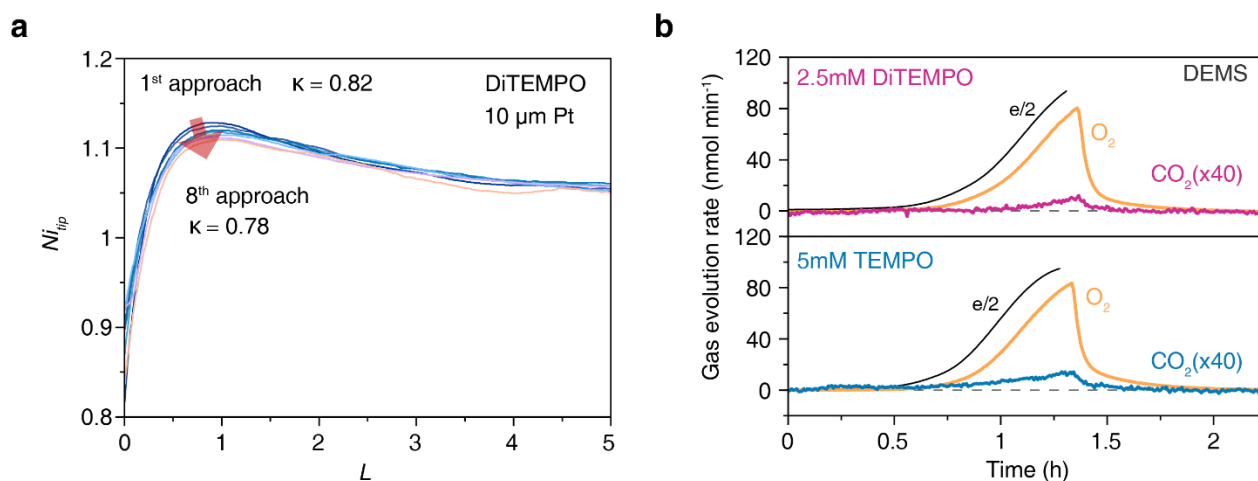
Supplementary Figure 5 | **a**, The structures of 1,5-dithiocane and its dication in comparison to dithiol/disulphide redox couples. **b**, CV curve of 1,5-dithiocane in $\text{LiClO}_4\text{-4G}$. Scan rate: 50 mV s^{-1} . **c**, SECM approach curve of 1,5-dithiocane towards an Li_2O_2 surface.



Supplementary Figure 6 | Molecular structure of DiTEMPO.



Supplementary Figure 7 | EPR signal of 5 mM DiTEMPO and 10 mM TEMPO in 4G.



Supplementary Figure 8 | **a**, Consecutive SECM approach curves of DiTEMPO towards Li_2O_2 at a single site, show almost identical kinetics. **b**, Gas evolution of Li_2O_2 electro-oxidation process in the electrolyte containing DiTEMPO and TEMPO.

SUPPLEMENTARY NOTES

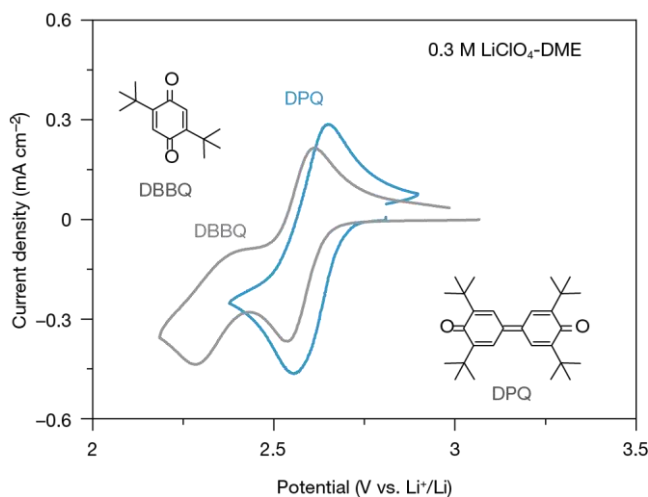
Supplementary Note 1: Characteristic times for reactions with one- and two-electron mediators

Let us consider the reduction of an O_2 molecule to Li_2O_2 . As illustrated in Fig. 1a, two one-electron mediators are required to encounter the specific O_2 moiety to reduce it to Li_2O_2 . Let us assume a RM concentration of 10 mM and that at a certain overpotential the steady state RM^- concentration is 1 mM. On average one RM^- is found per $1/NA = 1.66 \times 10^{-24} m^3$. Hence, the average distance between RM^- is $x_{RMS} = \sqrt[3]{1.66 \times 10^{-24} m^3} \approx 12 nm$. Diffusion coefficients of typical RMs⁵ range between $1.2 \times 10^{-6} cm^2 s^{-1}$ and $3.6 \times 10^{-6} cm^2 s^{-1}$, which gives typical diffusion times $\tau = x_{RMS}^2/2D$ between ~ 200 and 600 ns. Hence a $Li^+DBBQ^- \cdots O_2$ intermediate will only encounter another $Li^+DBBQ^- \cdots O_2$ or a Li^+DBBQ^- every ~ 200 and 600 ns, with which it could DISP or be reduced, respectively.

Let us further consider the reduction of O_2 to Li_2O_2 by a $2 e^-$ RM as illustrated in Fig. 1b. Only a single encounter between RM^{2-} and O_2 is required. For DPQ Fig. 1a shows a slight positive shift of the reduction wave under O_2 compared to an Ar atmosphere, which suggests coordination between $Li_2^+DPQ^{2-}$ and O_2 to form $Li_2^+DPQ^{2-} \cdots O_2$. Once encountered, the frequency of attempts for electron transfer between DPQ^{2-} and O_2 may be estimated from Marcus theory^{6,7}. Attempts are on the order of nuclear frequencies ν_n , for which values are reported between $\nu_n \approx 3 \times 10^{-10} s^{-1}$ (Ref. ⁸) and $\nu_n \approx 3500 cm^{-1} = 3 \times 10^{-14} s^{-1}$ (Ref. ⁶). This translates to attempts for electron transfer every 3.3 ps or less.

Supplementary Note 2: Ion-pairing controls one- or two-electron quinone reduction

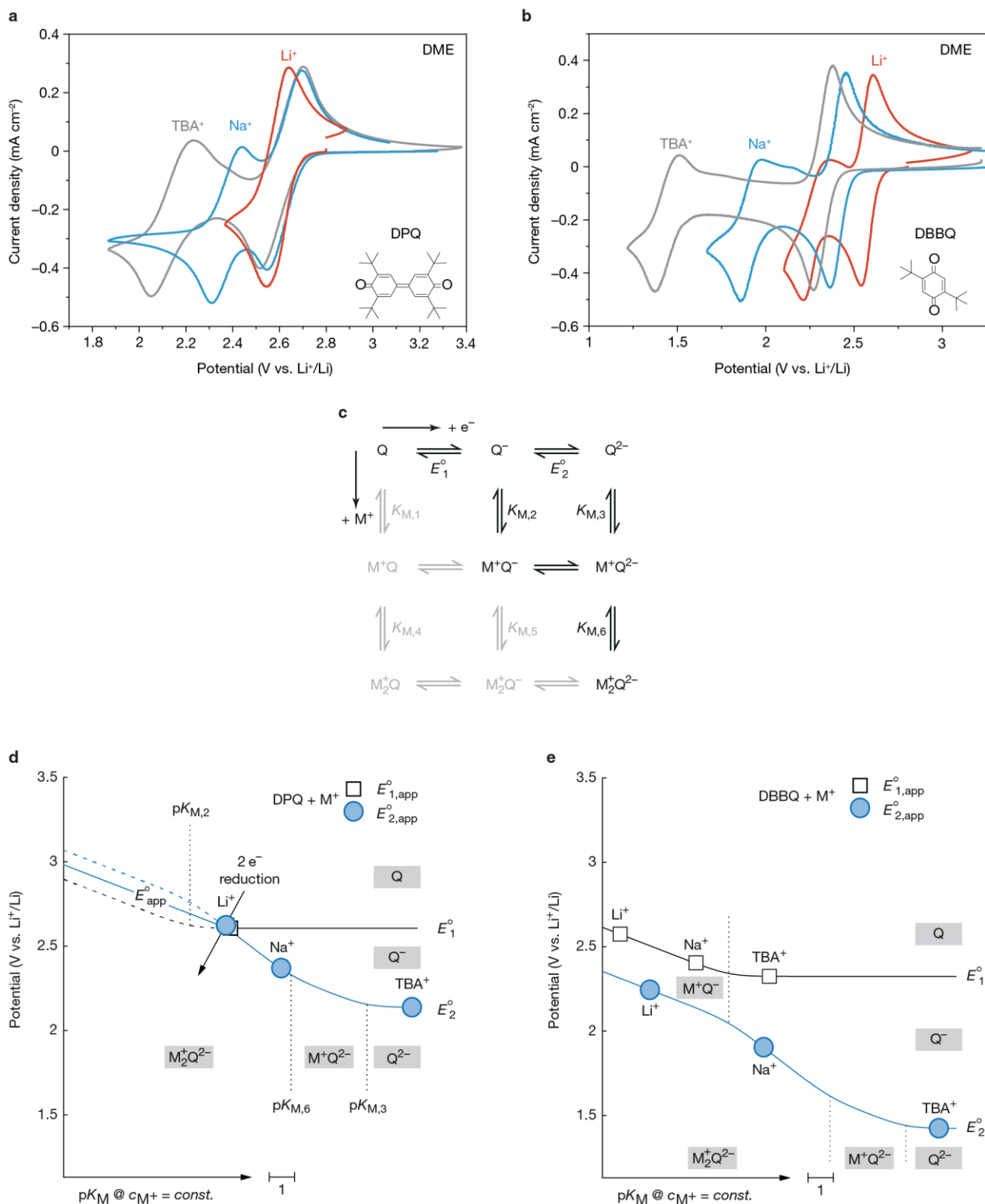
Quinones, which have in principle two $1 e^-$ reductions, have most widely been used as discharge mediators in Li-O₂ batteries, with DBBQ (2,5-di-tert-butyl-1,4-benzoquinone) having become a standard compound⁹. A typical CV curve for the reduction in ether-based electrolyte (0.3 M LiTFSI in DME) is shown in Supplementary Fig. 9, showing two well-separated reduction waves corresponding to DBBQ/DBBQ⁻ and DBBQ⁻/DBBQ²⁻, separated by ~250 mV. At the same conditions, DPQ shows a single $2 e^-$ reduction wave, corresponding to DPQ/DPQ²⁻. In the following, we examine how redox potentials with non-coordinating cations and ion-pairing give rise to separated or merged redox waves.



Supplementary Figure 9 | One- to two-electron quinone reduction in Li⁺ electrolyte. a, CVs of 1 mM DBBQ and DPQ reduction in Ar-saturated 0.3 M LiClO₄ in DME at 100 mV s⁻¹.

Supplementary Fig. 10a and b show CVs of DBBQ and DPQ reduction in TBA⁺, Na⁺, and Li⁺ electrolytes. Both quinones show in a weakly coordinating TBA⁺ electrolyte two well-separated reductions, separated by ~1 V and ~0.5 V for DBBQ and DPQ, respectively^A. As is typical for weakly solvating non-aqueous electrolytes, ion pairing strongly affects the reduction potentials¹². While the first reduction wave of DPQ shifts only slightly up, the second reduction wave shifts by ~300 mV each time as one changes the cation from TBA⁺ to Na⁺ and Li⁺. For the latter the waves merge into a single $2 e^-$ reduction wave. That the resulting wave represents a $2 e^-$ reduction wave is supported by observations in accord with established theory¹³: a) a higher peak current compared to the single electron wave, and b) a smaller peak-to-peak separation.

^A Similar CVs with TBA⁺ salt, but different solvents can be found in Refs. 10 Néron, S. et al. Diphenquinones Redux. *J. Org. Chem.* **87**, 7673-7695 (2022); 11 Yin, W. et al. Electrochemical Reduction of CO₂ Mediated by Quinone Derivatives: Implication for Li-CO₂ Battery. *J. Phys. Chem. C* **122**, 6546-6554 (2018).



Supplementary Figure 10 | Ion-pairing controlled shift from one- to two-electron quinone reduction. **a, b**, CVs of 2 mM DPQ and DBBQ showing their reduction in Ar-saturated DME at 100 mVs⁻¹. Salts were 0.3 M LiClO₄, NaTFSI and TBATFSI. **a** shows nearly unchanged first reduction with TBA⁺, Na⁺, and Li⁺ and strongly up-shifting second reduction, which merges for Li⁺ in a single wave. **c**, Nine-membered square scheme for quinone reduction with e⁻/M⁺ transfers in horizontal/vertical direction, respectively, and the numbering of the Lewis acid-base association equilibria. **d, e**, Pourbaix-type diagram for the quinone reduction potentials versus the Lewis acid-base dissociation equilibrium constant at constant M⁺ concentration. The lines are calculated using the Laviron model, wherein the pK_{M,n} are assumed (see text).

The peak-merging behaviour may be explained by a nine-membered square scheme (Supplementary Fig. 10c), in which horizontal and vertical processes correspond to electron and cation transfer, respectively. Laviron described a model to calculate the apparent redox potentials versus the pH (Pourbaix diagram) based on the measured equilibrium potentials of the non-coordinated species in the first row (resembling high pH) and the six acid dissociation constants $pK_{a,n}$ ^{14,15}. Savéant has shown that ion pairing in non-aqueous media has analogous effects on apparent potentials of 1 e⁻ redox couples^{12,16}. This is, below the pK_{IP} (K_{IP} being the ion-pairing equilibrium constant $K_{IP} = c_{MA}/(c_{M^+}c_{A^-})$), the apparent redox potentials are constant and above pK_{IP} , the redox potential increases with a slope of 59 mV/ pK_{IP} . We adapted the Laviron model using the formalism of Savéant for the case of quinones undergoing ion-pairing. To retain the typical Pourbaix-type style with more Lewis acidic conditions at the left, we used the Lewis acid-base dissociation constant $K_M = (c_{M^+}c_{A^-})/c_{MA}$. Rather than pH, the abscissa is given as pK_M at a constant M^+ concentration. $E_{Q^{0/-}}^\circ$ and $E_{Q^{-/2-}}^\circ$ are the potentials measured using the non-coordinating TBA⁺ salt. $E_{Q^{0/-}}^\circ = E_1^\circ$ and $E_{Q^{-/2-}}^\circ = E_2^\circ$ are used as a short hand in the plots. Apparent potentials are given by

$$E_{Q^{0/-},app}^\circ = E_3^\circ + \frac{RT}{F} \ln \left(\frac{K_{M,2}/c_{M^+}+1+c_{M^+}/K_{M,5}}{K_{M,1}/c_{M^+}+1+c_{M^+}/K_{M,4}} \right) \quad (S1)$$

$$E_{Q^{-/2-},app}^\circ = E_4^\circ + \frac{RT}{F} \ln \left(\frac{K_{M,3}/c_{M^+}+1+c_{M^+}/K_{M,6}}{K_{M,2}/c_{M^+}+1+c_{M^+}/K_{M,5}} \right) \quad (S2)$$

Where E_3° and E_4° are the potentials of the species in the middle row and given by

$$E_3^\circ = E_{Q^{0/-}}^\circ + \frac{2.3RT}{F} (pK_{M,2} - pK_{M,1}) \quad (S3)$$

$$E_4^\circ = E_{Q^{-/2-}}^\circ + \frac{2.3RT}{F} (pK_{M,3} - pK_{M,2}) \quad (S4)$$

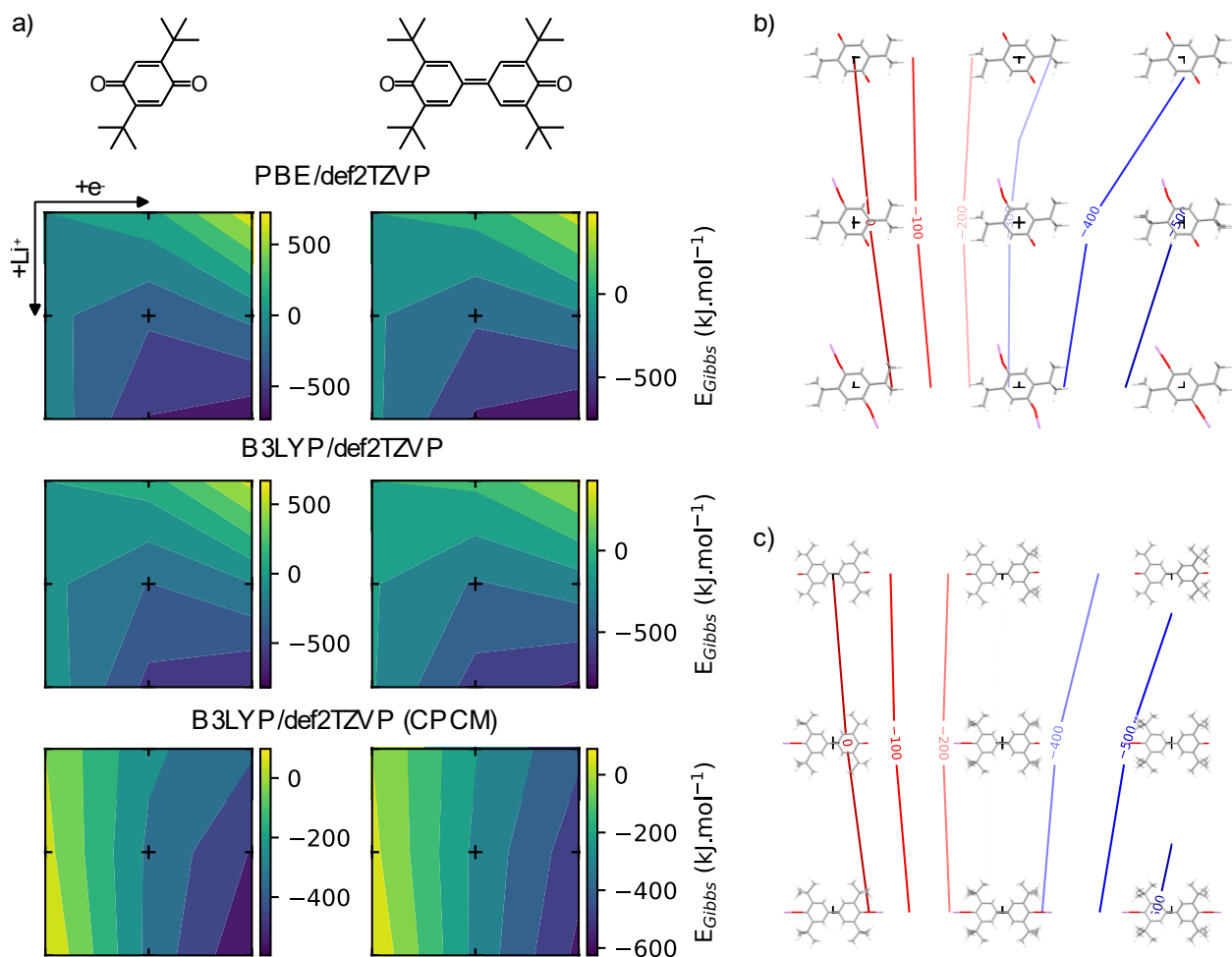
The apparent equilibrium potential for cases where $E_{Q^{-/2-},app}^\circ > E_{Q^{0/-},app}^\circ$ is given by $E_{app}^\circ = (E_{Q^{0/-},app}^\circ + E_{Q^{-/2-},app}^\circ)/2$.

While we do not know the $K_{M,n}$ for a particular quinone and cation, it is fair to assume, analogously to benzoquinone derivatives in aqueous solution¹⁷, that basicity follows the order $Q^{2-} > M^+Q^- > Q^-$ and hence $pK_{M,3} > pK_{M,6} > pK_{M,2}$. Association to form positively charged complexes ($pK_{M,1}$, $pK_{M,4}$, $pK_{M,5}$) is assumed negligible on the same acidity scale. Supplementary Fig. 10d and e show zones of thermodynamic stability of Q, Q⁻, Q²⁻, M⁺Q⁻, and M₂⁺Q²⁻ using assumed $pK_{M,3}$, $pK_{M,6}$, and $pK_{M,2}$ and the measured $E_{Q^{0/-}}^\circ$ and $E_{Q^{-/2-}}^\circ$ for DPQ and DBBQ with TBA⁺ electrolyte. $E_{Q^{-/2-},app}^\circ$ has a slope of 2×59 mV/ pK_{IP} between $pK_{M,3}$ and $pK_{M,6}$ and a slope of 59 mV/ pK_{IP} below $pK_{M,6}$. $E_{Q^{0/-},app}^\circ$ remains constant above $pK_{M,2}$ and has a slope of 59 mV/ pK_{IP} below. From Supplementary Fig. 10a we know that $E_{Q^{0/-},app}^\circ$ for DPQ remains nearly constant with TBA⁺, Na⁺ and Li⁺ electrolytes, while $E_{Q^{-/2-},app}^\circ$ increases and merges to a 2 e⁻ process with E_{app}° for Li⁺. By inserting the measured redox potentials of DPQ into the zone diagram, the relative Lewis acid-base dissociation constant K_M for TBA⁺, Na⁺, and Li⁺ can therefore be estimated as shown in Supplementary Fig. 10d. Analogously, Supplementary Fig. 10e shows the zone diagram for DBBQ. At large $pK_{M,1}$, measured $E_{Q^{0/-}}^\circ$ and $E_{Q^{-/2-}}^\circ$ with Li⁺ electrolyte show still two distinct reduction waves, which shows too little association between reduced DBBQ and Li⁺ to allow for a direct, concerted 2 e⁻, 2 Li⁺ reduction.

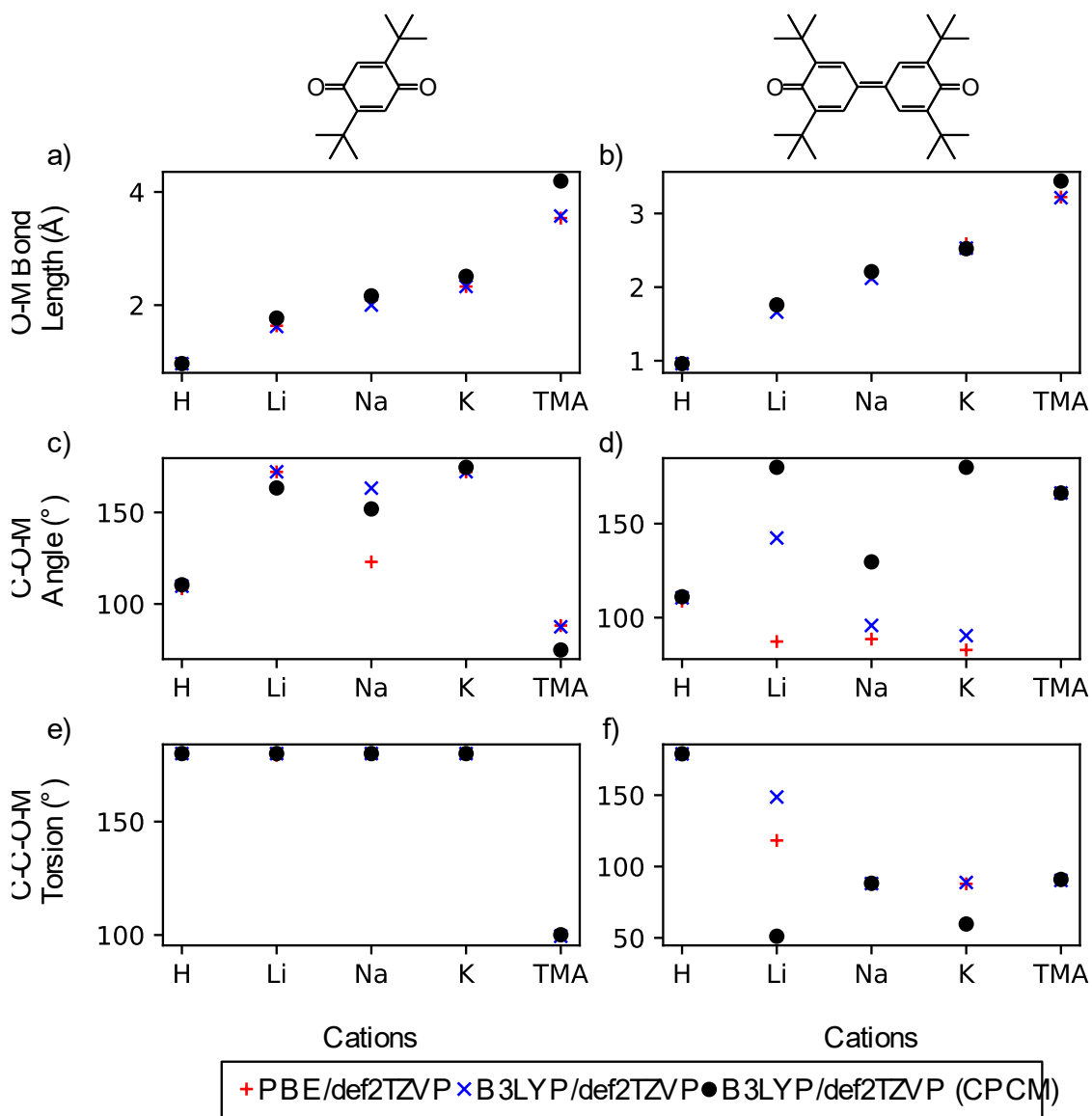
Supplementary Note 3: DFT study on ion-pairing of DBBQ and DPQ

To understand the difference in electrochemical behaviour between DBBQ and DPQ, we undertook a computational study. For lithium, each node of the square-scheme of the cation-coupled electron transfer was calculated with explicit cation inclusion. Supplementary Fig. 11a shows the free energy contour-maps for DBBQ and DPQ. For the gas-phase calculations, the results appear to favour lithium coordination first, followed by reduction, as the energies become more positive as one proceeds towards the top-right corner from the top-left. This is somewhat expected as charge is not screened in the gas-phase and so interactions that dissipate charge are favoured. For the implicit solvent calculations, movement from the top-left towards the bottom-left is disfavoured by an increase in free energy. Movement towards the bottom-right, in contrast, is greatly favoured with a greater driving force (more negative free energy) for DPQ than for DBBQ. This may be due to strain release once reduction facilitates rotation around the central C=C of DPQ as exemplified by the rotation around the central C-C bond in the relaxed structures of reduced DPQ (see Supplementary Fig. 11c).

The relaxed structures in Supplementary Fig. 11b and c also show linear coordination to lithium from the carbonyl groups as DBBQ and DPQ are reduced. This may be because of poor covalency between the oxygen lone-pairs in the carbonyl group and the associated lithium-ion, or because of a poor affinity between the carbonyl groups of the quinone compared to the interaction with the solvent. Supplementary Fig. 12 shows how the O-M distances, C-O-M bend angles and C-C-O-M dihedral angles vary with cation and level of theory. As expected, distance increases as the cation radius increases, the charge density decreases and the cation is unable to approach as closely to the carbonyl groups. Bend angles tend to be closer to 180° for DBBQ with the alkali metal cations, while DPQ appears to facilitate a less linear interaction with sodium cations. For torsional angles, with DBBQ, the cations (other than TMA⁺) are mostly able to occupy the less sterically hindered pocket near the quinoidal protons and away from the *t*-Butyl groups and hence are close to the plane of the aromatic ring in the relaxed structures. This is not possible in DPQ, where the cations (other than hydrogen) relax to positions above or below the ring-planes.

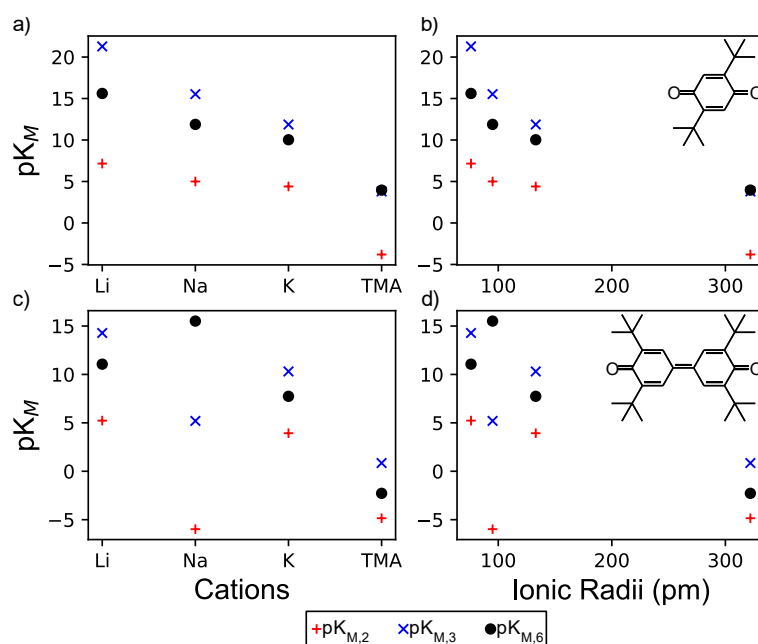


Supplementary Figure 11 | Gibbs free energy contour maps for the lithium-coupled electron transfer. The nodes are defined in Supplementary Fig. 10c. **a**, Gibbs free energy contour maps for the lithium-coupled electron transfer of DBBQ (left) and DPQ (right). The skeletal diagrams of DBBQ and DPQ have been included for clarity. As denoted in the figure, a horizontal step corresponds to an electron transfer step, while a vertical step corresponds to the association of a lithium cation. **a**, **b**, Renders of the relaxed structures and contour maps at the B3LYP/def2TZVP (CPCM) level of theory for DBBQ (**b**) and DPQ (**c**), respectively.



Supplementary Figure 12 | Comparison of the O-M bond length, C-O-M bond angle and C-C-O-M dihedral (torsional) angle as a function of cation.

The position and proximity of the cations to the compounds also contributes to the explanation of the observed pK_M 's. In the case of the calculated values, for both DBBQ and DPQ this broadly follows the expectation that as ionic radius decreases, the strength of the interaction decreases. There is a break in the trend for sodium for DPQ, which may be because of its less linear interaction in the relaxed structure (Supplementary Fig. 12d). Broadly speaking DBBQ appears to have a stronger interaction with all cations than DPQ does (except with sodium). A stronger interaction in the oxidised species would weaken the carbonyl bond and consequently make it easier to reduce (as experimentally observed).



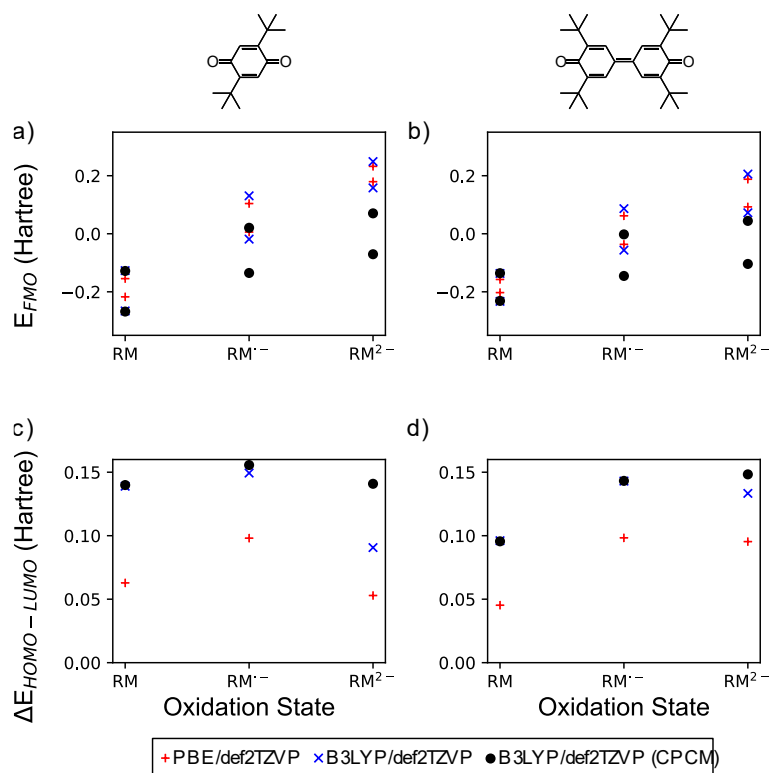
Supplementary Figure 13 | Calculated pK_M for DBBQ (a, b) and DPQ (c, d) as a function of cation (left) and ionic radius (right) at the B3LYP/def2TZVP level of theory with implicit solvent (DME via the CPCM model).

When comparing the calculated potentials in Supplementary Table 2, the DFT predicted potentials regrettably do not match the experimental values (see Supplementary Fig. 14) as DBBQ is predicted to undergo reduction at a lower voltage than DPQ, which is the opposite of what is experimentally observed. This may be due to the calculations' insufficiently capturing solvent-solute interactions. However, the trend that DPQ has a narrower potential separation between the first and second reductions is successfully predicted by the calculations, even though the magnitude of the separation is overestimated.

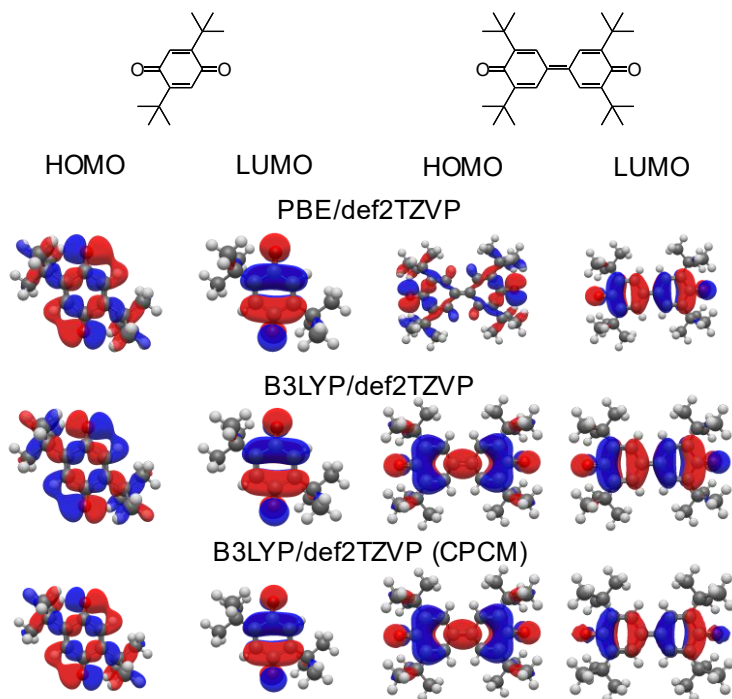
Supplementary Table 2 | Calculated potentials for the first and second reduction of DBBQ and DPQ using B3LYP/def2TZVP (CPCM, DME) as well as a combination of B3LYP/def2TZVP with single-point SMD solvation at the M062x/def2TZVP.¹⁸

	$Q + e^- \rightarrow Q^-$ (V/SHE)	$Q^- + e^- \rightarrow Q^{2-}$ (V/SHE)	ΔE (V)
DBBQ (SMD)	-1.03	-2.68	1.65
DBBQ (CPCM)	-0.73	-2.53	1.80
DPQ (SMD)	-0.63	-1.57	0.94
DPQ (CPCM)	-0.58	-1.69	1.11

When considering the frontier molecular orbitals of oxidised DBBQ and oxidised DPQ under implicit solvation (see Supplementary Figure 14a and b), DPQ has a higher energy HOMO and lower-lying LUMO than DPQ. This would suggest that DPQ is a better reductant than DBBQ (though this would require it to be further oxidised) and DPQ is harder to reduce (and consequently should have a lower reduction potential) than DBBQ, which matches up well with the experimental results. Considering the reduced species, DBBQ^{•-} has a higher HOMO and LUMO than DPQ^{•-}. This is also true for DBBQ²⁻ compared to DPQ²⁻. DBBQ^{•-} also has a greater energy separation between its frontier orbitals than DPQ^{•-} while this is reversed for DPQ²⁻ and DBBQ²⁻. The LUMOs of both DBBQ and DPQ (see Supplementary Figure 15) look similar, being localised to the quinoidal rings and containing π -antibonding character for the carbonyl groups.



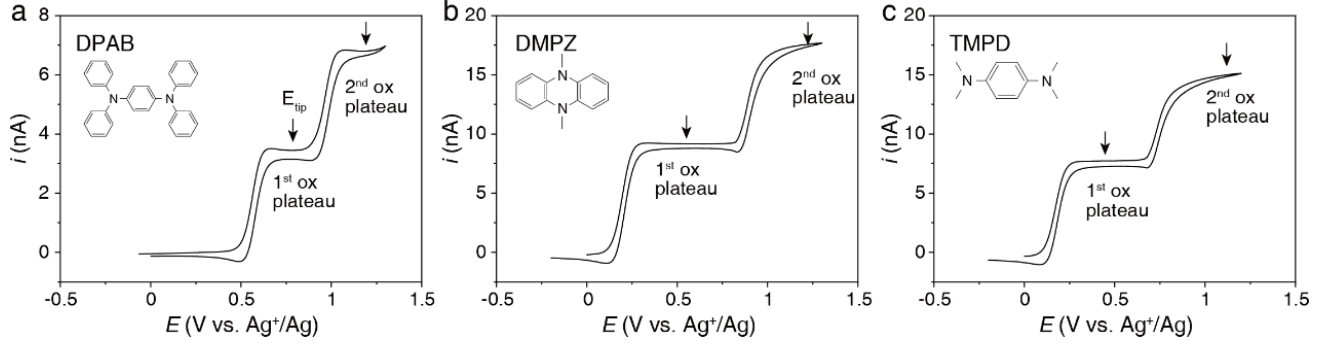
Supplementary Figure 14 | a, b, Comparison of the calculated energy levels of the FMO (frontier molecular orbitals), i.e., the HOMO and LUMO as a function of oxidation state of DBBQ (a) and DPQ (b) at various levels of theory as well as the change in energy between the two orbitals (c, d).



Supplementary Figure 15 | Rendered frontier molecular orbitals (FMOs) for DBBQ (left) and DPQ (right) at various levels of theory.

Supplementary Note 4: Concentration profiles in front of the SECM tip

We have selected three 1+1 e⁻ mediators and recorded approach curves with the SECM tip polarized to the first and second plateau respectively. The mediators, their CVs and the potentials used for the approach curves are shown in Supplementary Fig. 17.



Supplementary Figure 16 | Cyclic voltammogram of the MBT⁻/MBT₂ redox couple. CV of (a) DPAB, (b) DMPZ, and (c) TMPD at a SECM tip electrode (radius 10 μm).

To understand the feedback behaviour of the SECM approach curves with 1+1 e⁻ RMs, we calculate the concentration profiles of RM, RM⁺, and RM²⁺ as a function of distance from the tip based on the formalism described by Compton¹³. The reactions are



where

$$E_{\text{RM}^{0/+}}^{\circ} \ll E_{\text{RM}^{+/2+}}^{\circ} \quad (\text{S7})$$

hence



The equilibrium constant of these reactions is given by their relative standard potentials

$$K = \frac{C_{\text{RM}} C_{\text{RM}^{2+}}}{C_{\text{RM}^{+2}}} = \exp\left(\frac{F}{RT} (E_{\text{RM}^{+/2+}}^{\circ} - E_{\text{RM}^{0/+}}^{\circ})\right) = \frac{k_{\text{DISP}}}{k_{\text{COMP}}} \quad (\text{S10})$$

For brevity, we write in the following $C_{\text{RM}} = A$, $C_{\text{RM}^+} = B$, $C_{\text{RM}^{2+}} = C$. We consider the tip as a microsphere with the radius r_e . The coupled reaction-diffusion system in spherical coordinates is given by

$$\frac{\partial A}{\partial t} = D \left(\frac{\partial^2 A}{\partial r^2} + \frac{2}{r} \frac{\partial A}{\partial r} \right) + k_{\text{DISP}} B^2 - k_{\text{COMP}} AC \quad (\text{S11})$$

$$\frac{\partial B}{\partial t} = D \left(\frac{\partial^2 B}{\partial r^2} + \frac{2}{r} \frac{\partial B}{\partial r} \right) - 2k_{\text{DISP}} B^2 + 2k_{\text{COMP}} AC \quad (\text{S12})$$

$$\frac{\partial C}{\partial t} = D \left(\frac{\partial^2 C}{\partial r^2} + \frac{2}{r} \frac{\partial C}{\partial r} \right) + k_{\text{DISP}} B^2 - k_{\text{COMP}} AC \quad (\text{S13})$$

The boundary conditions are with A^* being the RM bulk concentration

$$t = 0, \text{ all } r: A = A^*, B = C = 0 \quad (\text{S14})$$

$$t > 0, r \rightarrow \infty: A = A^*, B = C = 0 \quad (\text{S15})$$

$$t > 0, r \rightarrow r_e: A = 0, C = A^*, \frac{\partial A}{\partial r} + \frac{\partial B}{\partial r} + \frac{\partial C}{\partial r} = 0 \quad (\text{S16})$$

u transformation with $u = rA, v = rB, w = rC$ simplifies the system to

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial r^2} + \frac{k_{\text{DISP}}}{r} v^2 - \frac{k_{\text{COMP}}}{r} u w \quad (\text{S17})$$

$$\frac{\partial v}{\partial t} = D \frac{\partial^2 v}{\partial r^2} - \frac{2k_{\text{DISP}}}{r} v^2 + \frac{2k_{\text{COMP}}}{r} u w \quad (\text{S18})$$

$$\frac{\partial w}{\partial t} = D \frac{\partial^2 w}{\partial r^2} + \frac{k_{\text{DISP}}}{r} v^2 - \frac{k_{\text{COMP}}}{r} u w \quad (\text{S19})$$

The boundary conditions become

$$t = 0, \text{all } r: u = rA^*, v = w = 0 \quad (\text{S20})$$

$$t > 0, r \rightarrow \infty: u = rA^*, v = w = 0 \quad (\text{S21})$$

$$t > 0, r \rightarrow r_e: u = 0, w = r_e, \frac{\partial u}{\partial r} + \frac{\partial v}{\partial r} + \frac{\partial w}{\partial r} = \frac{u+v+w}{r} \quad (\text{S22})$$

The solution has been implemented in Matlab using the PDE solver ode15s.

For polarization to the first plateau, only Eq. S5 applies. The governing equation is given by

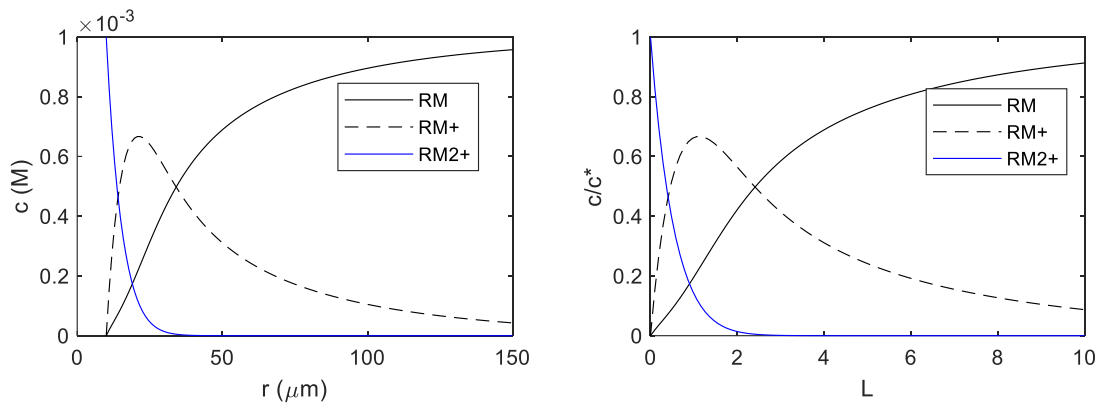
$$\frac{\partial A}{\partial t} = D \left(\frac{\partial^2 A}{\partial r^2} + \frac{2}{r} \frac{\partial A}{\partial r} \right) \quad (\text{S22})$$

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial r^2} \quad (\text{S23})$$

The latter has for analogous boundary conditions the analytical solution¹³

$$A(r, t) = A^* \left(1 - \frac{r_e}{r} \operatorname{erfc} \left(\frac{r-r_e}{2\sqrt{Dt}} \right) \right) \quad (\text{S24})$$

For the plots in Fig. 4, we used $D = 10^{-5} \text{ cm}^2\text{s}^{-1}$, $k_{\text{COMP}} = 10^5$, $r_e = 10 \text{ } \mu\text{m}$, $A^* = 10^{-3} \text{ M}$. Results for Eq. S11-S13 with $\Delta E^\circ = 0.4$ are shown in Supplementary Fig. 18.



Supplementary Figure 17 | Normalized concentrations of RM, RM⁺, and RM²⁺ as a function of the radius from the dip centre and the normalized distance L .

SUPPLEMENTARY REFERENCES

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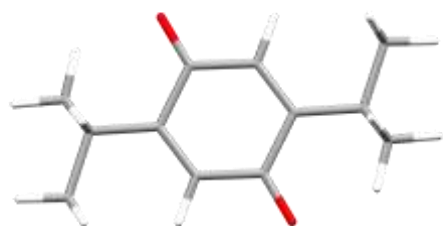
Supporting Information – DFT Coordinates

DBBQ

Cation-Free

Oxidised

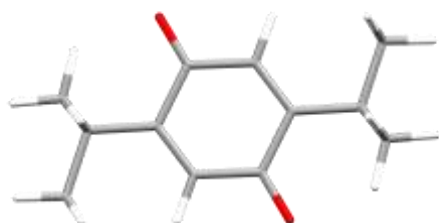
PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
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C	7.422635	6.437469	6.779379
C	6.089107	8.908684	6.779259
C	5.945342	6.490799	6.779437
C	7.5664	8.855354	6.779204
C	3.189583	7.232138	5.513872
C	3.18968	7.232313	8.045107
C	10.23705	5.960632	6.779277
C	10.32217	8.114007	8.04475
C	5.271293	7.831161	6.779368
C	8.240449	7.514992	6.779264
C	3.749381	7.924357	6.779421
C	9.762361	7.421793	6.779203
C	10.32205	8.113841	5.513514
H	3.578525	7.710227	4.602407
H	3.448344	6.167614	5.492432
H	3.448441	6.167792	8.066675
H	2.093291	7.326103	5.503598
H	11.41846	8.020038	8.055017
H	3.617495	9.930333	7.671718
H	2.093389	7.326281	8.055453
H	2.175642	9.406999	6.779384
H	3.617418	9.930208	5.886854
H	3.578691	7.710527	8.956478
H	7.808594	5.417058	6.779438
H	9.894316	5.415937	7.671757

H	9.894244	5.415823	5.886893
H	11.41835	8.019872	5.503161
H	9.933037	7.635629	4.602145
H	10.06329	9.178362	5.49195
H	10.06341	9.178532	8.066196
H	5.703148	9.929095	6.779204
H	9.933232	7.635916	8.956216
H	11.3361	5.939147	6.779234
O	5.315867	5.429195	6.779539
O	8.195874	9.916958	6.77911

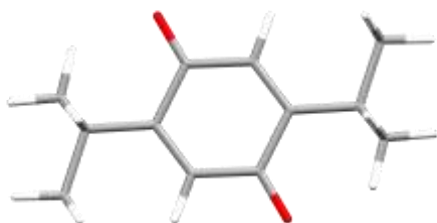
B3LYP/def2TZVP



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C	7.425609	6.441325	6.779369
C	6.086132	8.904825	6.779257
C	5.947653	6.497621	6.779428
C	7.564088	8.848529	6.779199
C	3.193401	7.234115	5.514987
C	3.193502	7.234279	8.043991
C	10.23962	5.962692	6.779287
C	10.31834	8.112042	8.043634
C	5.274409	7.83726	6.779365
C	8.237333	7.50889	6.779263
C	3.751736	7.924634	6.779422
C	9.760006	7.421516	6.779204
C	10.31824	8.111863	5.51463
H	3.580467	7.710535	4.611483
H	3.449634	6.178078	5.490412
H	3.449742	6.178247	8.068687
H	2.105289	7.325973	5.502806
H	11.40646	8.020196	8.055804
H	3.611092	9.924423	7.665095
H	2.10539	7.326133	8.056243
H	2.181394	9.402109	6.779387
H	3.611024	9.92431	5.893503
H	3.580634	7.710821	8.947402

H	7.801636	5.427858	6.779422
H	9.900729	5.421848	7.66514
H	9.900639	5.421718	5.893548
H	11.40635	8.019998	5.502368
H	9.93109	7.635325	4.611223
H	10.06201	9.167899	5.489935
H	10.0621	9.168077	8.068211
H	5.710106	9.918292	6.779203
H	9.931293	7.635619	8.947141
H	11.33035	5.944042	6.779233
O	5.324038	5.448752	6.779525
O	8.187704	9.897398	6.779098

B3LYP/def2TZVP (CPCM - DME)

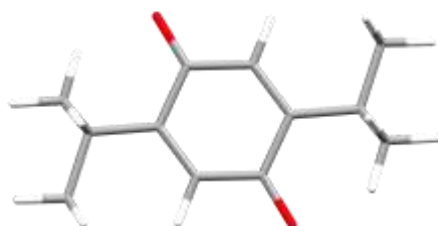


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
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C	7.427853823	6.443186396	6.779371289
C	6.083887842	8.902963618	6.779255217
C	5.951314369	6.498125805	6.779431684
C	7.560427297	8.84802421	6.779195988
C	3.191617337	7.235278933	5.514078518
C	3.191720455	7.235444965	8.044901298
C	10.23881517	5.963445346	6.779283504
C	10.32012567	8.110875207	8.044543706
C	5.273671488	7.83430519	6.779365171
C	8.238070178	7.511844823	6.779261224
C	3.751203644	7.923218537	6.779421991
C	9.760538022	7.422931466	6.779203061
C	10.32001989	8.110700883	5.513720925
H	3.579557195	7.71303374	4.611906953
H	3.446862234	6.178921947	5.486398232
H	3.446969663	6.179092203	8.072700762
H	2.10375728	7.328492707	5.504055532
H	11.40798587	8.017662902	8.054565015
H	3.613038059	9.922335974	7.665288969
H	2.103861049	7.328657751	8.054999198

H	2.182269265	9.400649393	6.779387407
H	3.612968477	9.92222082	5.893305889
H	3.579731503	7.713319763	8.946978693
H	7.808715487	5.431745054	6.779426021
H	9.898775056	5.423932386	7.665326118
H	9.898701697	5.423810825	5.893343039
H	11.40787915	8.017486599	5.503621349
H	9.932006597	7.632824182	4.611645502
H	10.06477203	9.167053908	5.48591908
H	10.06487945	9.167231935	8.072221616
H	5.703026177	9.91440496	6.779199424
H	9.932188045	7.63312231	8.946717241
H	11.32947239	5.945500594	6.77923968
O	5.329295804	5.445336287	6.779529013
O	8.182445859	9.900813728	6.779095864

Singly Reduced

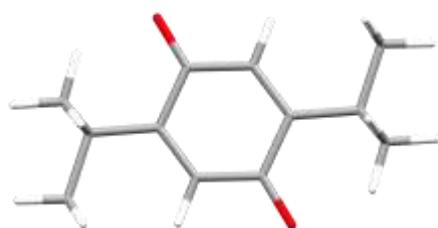
PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
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C	7.376386	6.4422	6.779372
C	6.135355	8.90395	6.779245
C	5.92775	6.47432	6.779427
C	7.583992	8.87183	6.779183
C	3.207441	7.232753	5.519652
C	3.207551	7.232913	8.039326
C	10.20949	5.962852	6.779286
C	10.3043	8.113404	8.038972
C	5.307766	7.80217	6.779361
C	8.203976	7.54398	6.779257
C	3.77835	7.922415	6.77942
C	9.733391	7.423735	6.779205
C	10.3042	8.113231	5.519297
H	3.580094	7.728777	4.609677
H	3.514952	6.179513	5.49905
H	3.515063	6.179676	8.060035

H	2.105011	7.291091	5.51675
H	11.40672	8.055066	8.04188
H	3.653533	9.927029	7.669603
H	2.105122	7.291252	8.042317
H	2.200319	9.408569	6.779395
H	3.653454	9.926916	5.888994
H	3.580283	7.729053	8.949205
H	7.783766	5.428358	6.779432
H	9.858283	5.419238	7.669642
H	9.858213	5.419116	5.889032
H	11.40663	8.054892	5.516312
H	9.931468	7.617086	4.60942
H	9.996684	9.166467	5.498582
H	9.996785	9.166643	8.059567
H	5.727976	9.917792	6.779191
H	9.931638	7.617384	8.948947
H	11.31142	5.937581	6.779244
O	5.264074	5.384845	6.779546
O	8.247667	9.961305	6.779077

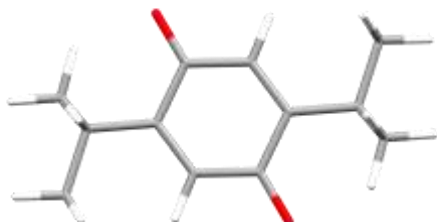
B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
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C	6.133969	8.897508	6.779251
C	5.933801	6.48152	6.779409
C	7.577941	8.864632	6.779184
C	3.210042	7.233158	5.520125
C	3.210158	7.233326	8.038862
C	10.20762	5.96808	6.779289
C	10.30169	8.112997	8.038503
C	5.312209	7.802276	6.779358
C	8.199533	7.543876	6.779252
C	3.783135	7.918411	6.779421
C	9.728607	7.42774	6.779204
C	10.3016	8.112818	5.519765
H	3.583665	7.724965	4.618004

H	3.503861	6.18603	5.493441
H	3.503977	6.186201	8.065658
H	2.116326	7.29949	5.515848
H	11.3954	8.046661	8.04279
H	3.651136	9.917919	7.663033
H	2.116443	7.299661	8.043231
H	2.210527	9.401879	6.779398
H	3.651049	9.9178	5.895552
H	3.583864	7.725253	8.940884
H	7.778229	5.443053	6.779412
H	9.860678	5.428353	7.663081
H	9.860613	5.428228	5.8956
H	11.39531	8.046483	5.515407
H	9.927898	7.620887	4.617743
H	10.00778	9.159943	5.492961
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H	5.733513	9.903099	6.779206
H	9.928056	7.621195	8.940623
H	11.30121	5.944269	6.779251
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O	8.234986	9.946547	6.779099

B3LYP/def2TZVP (CPCM – DME)

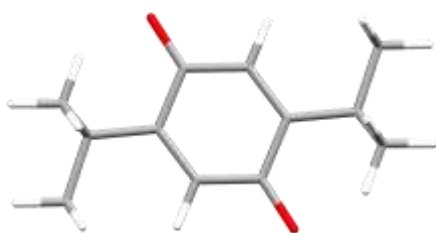


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
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C	6.126644	8.890609	6.779266
C	5.941947	6.481589	6.779426
C	7.569794	8.864561	6.779209
C	3.201039	7.235153	5.518545
C	3.201142	7.235327	8.040438
C	10.20863	5.970116	6.779285
C	10.31071	8.110999	8.040077
C	5.305797	7.794222	6.779368
C	8.205944	7.551928	6.779262
C	3.777163	7.914385	6.779421
C	9.734578	7.431765	6.779204

C	10.3106	8.110821	5.518184
H	3.576197	7.724574	4.616087
H	3.479519	6.184382	5.485504
H	3.479637	6.184564	8.073609
H	2.109873	7.311923	5.51487
H	11.40187	8.03423	8.043749
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H	2.109975	7.312084	8.044186
H	2.211015	9.401307	6.77938
H	3.647675	9.915682	5.894784
H	3.576364	7.724881	8.942798
H	7.797147	5.454972	6.779408
H	9.864072	5.430469	7.663844
H	9.863997	5.430346	5.894831
H	11.40176	8.034064	5.514433
H	9.935371	7.621267	4.615827
H	10.0321	9.161584	5.485014
H	10.03222	9.161769	8.073118
H	5.714595	9.891177	6.779219
H	9.935552	7.621578	8.942537
H	11.30073	5.944844	6.77924
O	5.295675	5.388683	6.779517
O	8.216067	9.957467	6.77911

Doubly Reduced

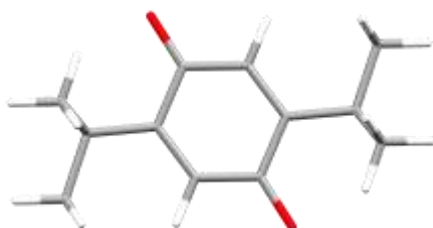
PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	3.319692	9.391844	6.779344
C	7.328489	6.431683	6.779376
C	6.183252	8.914467	6.779256
C	5.898235	6.456813	6.779437
C	7.613507	8.889336	6.7792
C	3.234636	7.233195	5.523949
C	3.234736	7.233357	8.035024
C	10.19205	5.954307	6.779289
C	10.27711	8.112964	8.034669
C	5.336029	7.790913	6.779367

C	8.175713	7.555237	6.779263
C	3.803985	7.934226	6.779418
C	9.707757	7.411924	6.779206
C	10.277	8.112784	5.523594
H	3.579973	7.751567	4.613721
H	3.613788	6.197137	5.521782
H	3.613887	6.197299	8.037294
H	2.12507	7.234524	5.528928
H	11.38668	8.111635	8.029686
H	3.676987	9.935771	7.668337
H	2.12517	7.234685	8.030133
H	2.213616	9.415122	6.779386
H	3.676916	9.935656	5.890252
H	3.580146	7.751846	8.945157
H	7.750047	5.419506	6.779425
H	9.83483	5.4105	7.668387
H	9.834751	5.410373	5.890302
H	11.38657	8.111457	5.528481
H	9.931588	7.594287	4.613465
H	9.897848	9.148842	5.521317
H	9.89796	9.149023	8.036829
H	5.761695	9.926644	6.779203
H	9.931775	7.594599	8.944901
H	11.29813	5.931029	6.779242
O	5.183272	5.352906	6.779539
O	8.32847	9.993244	6.779093

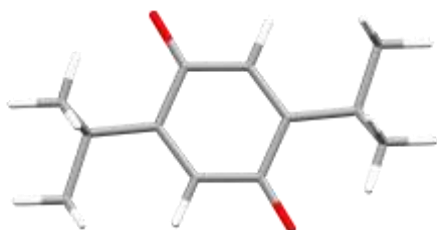
B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	3.323997	9.382255	6.77934
C	7.330661	6.440705	6.779372
C	6.181081	8.905445	6.779252
C	5.908428	6.462258	6.779431
C	7.603313	8.883892	6.779194
C	3.232131	7.232952	5.523495
C	3.232236	7.233122	8.035485
C	10.18774	5.963895	6.779285

C	10.27961	8.113198	8.03513
C	5.340614	7.783899	6.779364
C	8.171127	7.562251	6.77926
C	3.80882	7.924276	6.779419
C	9.702922	7.421874	6.779206
C	10.27951	8.113028	5.52314
H	3.579793	7.747505	4.621862
H	3.586232	6.200425	5.505683
H	3.586338	6.200597	8.053407
H	2.131135	7.252282	5.529072
H	11.38061	8.093869	8.029553
H	3.676674	9.922125	7.661695
H	2.131239	7.252451	8.029997
H	2.226341	9.405492	6.779385
H	3.6766	9.922005	5.896883
H	3.579973	7.747797	8.937019
H	7.748529	5.438352	6.779423
H	9.835142	5.424145	7.661742
H	9.835067	5.424025	5.896931
H	11.3805	8.093699	5.528628
H	9.931769	7.598353	4.621606
H	9.925403	9.145552	5.505218
H	9.925509	9.145725	8.052942
H	5.763212	9.907798	6.779201
H	9.931948	7.598646	8.936763
H	11.2854	5.940659	6.77924
O	5.202625	5.359231	6.779536
O	8.309117	9.986919	6.779089

B3LYP/def2TZVP (CPCM – DME)



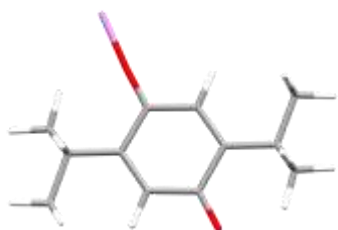
<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	3.321674	9.376295	6.779343
C	7.345289	6.455838	6.779367
C	6.166452	8.890312	6.779258
C	5.924129	6.460821	6.779437
C	7.587612	8.885329	6.779188
C	3.213691	7.238719	5.520951

C	3.213787	7.23889	8.038032
C	10.19007	5.969855	6.779282
C	10.29805	8.107431	8.037674
C	5.329162	7.76687	6.779373
C	8.18258	7.57928	6.779252
C	3.798016	7.914995	6.779424
C	9.713726	7.431155	6.779201
C	10.29796	8.10726	5.520593
H	3.558044	7.755074	4.619994
H	3.542288	6.20159	5.478181
H	3.54239	6.201769	8.080918
H	2.118029	7.272653	5.530875
H	11.39371	8.073497	8.02775
H	3.667797	9.917806	7.662552
H	2.118124	7.272821	8.028186
H	2.227763	9.402697	6.779386
H	3.667727	9.917686	5.896034
H	3.558206	7.755368	8.938893
H	7.783596	5.463598	6.779413
H	9.844015	5.428464	7.662591
H	9.843944	5.428344	5.896073
H	11.39362	8.073329	5.530439
H	9.953535	7.590782	4.619732
H	9.969352	9.144381	5.477707
H	9.969453	9.14456	8.080444
H	5.728146	9.882552	6.779212
H	9.953698	7.591076	8.938631
H	11.28398	5.943452	6.779239
O	5.243855	5.334991	6.779549
O	8.267886	10.01116	6.779076

Lithium

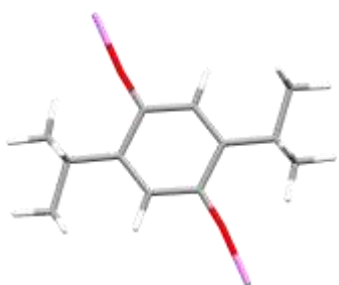
Oxidised

PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.3791	-1.79262	0.002996

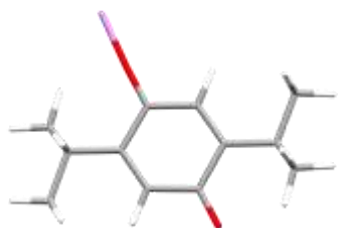
C	0.769699	1.144185	2.16E-05
C	-0.57826	-1.32013	-0.00034
C	-0.6827	1.072814	0.001908
C	0.903737	-1.27792	-0.00229
C	-3.48138	0.34216	1.277349
C	-3.48478	0.3444	-1.26732
C	3.584845	1.613614	-0.00335
C	3.656061	-0.54538	-1.2743
C	-1.38717	-0.23334	0.0017
C	1.593369	0.063357	-0.00203
C	-2.91352	-0.32682	0.003662
C	3.103912	0.155051	-0.00398
C	3.659464	-0.54761	1.263626
H	-3.10093	-0.14985	2.183669
H	-3.22751	1.407884	1.340689
H	-3.23105	1.410223	-1.32949
H	-4.57681	0.252016	1.280379
H	4.750293	-0.44189	-1.28271
H	-3.03733	-2.33412	-0.89099
H	-4.58022	0.254292	-1.26756
H	-4.47712	-1.82128	0.004437
H	-3.03494	-2.33569	0.895116
H	-3.10679	-0.14604	-2.17552
H	1.168914	2.159217	0.000383
H	3.249964	2.160951	-0.89759
H	3.252366	2.15938	0.892754
H	4.753716	-0.44413	1.269278
H	3.271461	-0.07703	2.178782
H	3.412198	-1.61437	1.277628
H	3.408755	-1.61212	-1.28951
H	-0.97478	-2.33551	-0.0007
H	3.265604	-0.0732	-2.18759
H	4.682779	1.628309	-0.00481
O	-1.31988	2.163314	0.003725
O	1.518653	-2.33966	-0.00404
Li	-2.08763	3.707886	0.006133



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	3.435388	1.791509	-0.000003
C	-0.648496	-1.246588	0.000013
C	0.648496	1.246593	-0.000002
C	0.811795	-1.157361	0.000015
C	-0.811795	1.157366	-0.000003
C	3.584878	-0.348495	1.275478
C	3.584881	-0.348511	-1.275456
C	-3.435388	-1.791504	0.000013
C	-3.584878	0.348500	-1.275468
C	1.490447	0.180593	0.000006
C	-1.490447	-0.180588	0.000005
C	3.002997	0.316630	0.000006
C	-3.002997	-0.316625	0.000004
C	-3.584882	0.348515	1.275466
H	3.194709	0.127633	2.185800
H	3.367337	-1.421703	1.328449
H	3.367339	-1.421720	-1.328415
H	4.676144	-0.222613	1.272553
H	-4.676145	0.222617	-1.272543
H	3.086979	2.326670	-0.895923
H	4.676147	-0.222630	-1.272530
H	4.531859	1.842931	0.000000
H	3.086974	2.326683	0.895909
H	3.194714	0.127607	-2.185785
H	-1.037197	-2.264948	0.000019
H	-3.086975	-2.326678	-0.895899
H	-3.086978	-2.326666	0.895933
H	-4.676148	0.222632	1.272540
H	-3.194714	-0.127602	2.185795
H	-3.367342	1.421724	1.328425
H	-3.367338	1.421708	-1.328439
H	1.037197	2.264953	-0.000008
H	-3.194709	-0.127629	-2.185789
H	-4.531860	-1.842927	0.000011
O	1.463240	-2.225340	0.000021

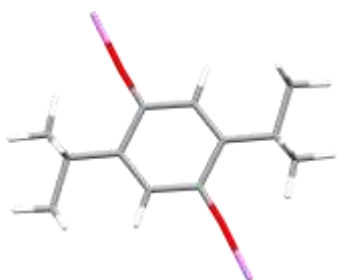
O	-1.463240	2.225346	-0.000011
Li	2.200684	-3.857904	0.000041
Li	-2.200684	3.857910	-0.000023

B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.38324	-1.78915	0.003007
C	0.771724	1.139483	1.28E-05
C	-0.58035	-1.31728	-0.00034
C	-0.6804	1.064213	0.001893
C	0.902719	-1.27179	-0.00228
C	-3.47547	0.343486	1.275494
C	-3.47888	0.34572	-1.26548
C	3.5865	1.611999	-0.00334
C	3.652398	-0.54233	-1.27326
C	-1.38316	-0.24037	0.001688
C	1.589833	0.069029	-0.00203
C	-2.91074	-0.32626	0.00366
C	3.102777	0.154924	-0.00398
C	3.655797	-0.54456	1.262603
H	-3.09789	-0.14639	2.174324
H	-3.21996	1.399842	1.339031
H	-3.22353	1.402187	-1.32784
H	-4.56292	0.258905	1.280637
H	4.738431	-0.44207	-1.28565
H	-3.04573	-2.32712	-0.88428
H	-4.56633	0.261147	-1.26785
H	-4.47297	-1.81326	0.004446
H	-3.04335	-2.32868	0.888441
H	-3.10371	-0.14257	-2.16618
H	1.158264	2.148594	0.000382
H	3.253949	2.154817	-0.8908
H	3.256331	2.153254	0.885953
H	4.74186	-0.44432	1.272253
H	3.268635	-0.0752	2.169254
H	3.410252	-1.6028	1.280269
H	3.406803	-1.60054	-1.29213

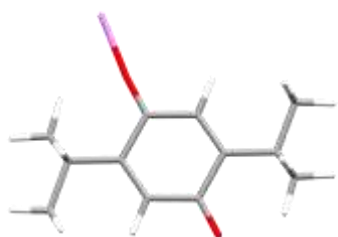
H	-0.9662	-2.32629	-0.00071
H	3.262808	-0.07138	-2.17805
H	4.676025	1.625279	-0.00479
O	-1.31218	2.143341	0.003689
O	1.512305	-2.32026	-0.00402
Li	-2.0965	3.666742	0.00608



Element	X	Y	Z
C	3.442302	1.785554	-0.000004
C	-0.652287	-1.242548	0.000011
C	0.652287	1.242553	-0.000005
C	0.810030	-1.149397	0.000010
C	-0.810031	1.149402	-0.000007
C	3.580160	-0.351648	1.273708
C	3.580167	-0.351670	-1.273679
C	-3.442302	-1.785549	0.000009
C	-3.580165	0.351659	-1.273692
C	1.487134	0.186913	0.000004
C	-1.487135	-0.186908	0.000003
C	3.003514	0.312788	0.000007
C	-3.003514	-0.312783	0.000004
C	-3.580164	0.351668	1.273696
H	3.192448	0.123323	2.175979
H	3.358789	-1.415388	1.328973
H	3.358796	-1.415410	-1.328928
H	4.663793	-0.234135	1.275511
H	-4.663798	0.234146	-1.275491
H	3.097329	2.316722	-0.889088
H	4.663800	-0.234157	-1.275477
H	4.530508	1.832462	0.000000
H	3.097322	2.316738	0.889069
H	3.192461	0.123287	-2.175960
H	-1.026671	-2.255701	0.000018
H	-3.097327	-2.316728	-0.889068
H	-3.097324	-2.316723	0.889089
H	-4.663797	0.234154	1.275497
H	-3.192454	-0.123293	2.175973

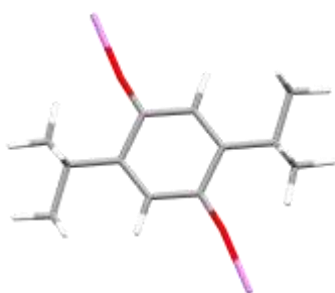
H	-3.358794	1.415408	1.328949
H	-3.358794	1.415399	-1.328952
H	1.026671	2.255706	-0.000011
H	-3.192456	-0.123308	-2.175966
H	-4.530508	-1.832458	0.000011
O	1.453921	-2.205913	0.000019
O	-1.453922	2.205918	-0.000015
Li	2.248048	-3.796084	0.000034
Li	-2.248048	3.796090	-0.000026

B3LYP/def2TZVP (CPCM – DME)



Element	X	Y	Z
C	-3.38779	-1.81006	0.002994
C	0.763758	1.129692	1.49E-05
C	-0.581	-1.3325	-0.00035
C	-0.70276	1.060358	0.00192
C	0.897399	-1.27749	-0.00228
C	-3.47406	0.331633	1.272376
C	-3.47745	0.333862	-1.26238
C	3.573011	1.612028	-0.00333
C	3.652323	-0.53568	-1.27184
C	-1.38942	-0.26228	0.001677
C	1.576723	0.061682	-0.00201
C	-2.91341	-0.34897	0.003643
C	3.095965	0.152307	-0.00397
C	3.655718	-0.5379	1.261187
H	-3.08447	-0.14885	2.171947
H	-3.22634	1.389482	1.310616
H	-3.22984	1.391777	-1.29943
H	-4.56115	0.234284	1.282027
H	4.739346	-0.43775	-1.28293
H	-3.04842	-2.3478	-0.88411
H	-4.56457	0.236528	-1.26929
H	-4.4781	-1.82967	0.004439
H	-3.04605	-2.34936	0.888242
H	-3.09028	-0.14504	-2.16384
H	1.143624	2.141232	0.000395

H	3.232865	2.152065	-0.88908
H	3.235242	2.150506	0.88428
H	4.742767	-0.44	1.269536
H	3.267044	-0.06327	2.164489
H	3.40527	-1.59526	1.286555
H	3.401805	-1.59299	-1.29839
H	-0.96334	-2.34287	-0.00072
H	3.261229	-0.05946	-2.17326
H	4.663289	1.629381	-0.00477
O	-1.3346	2.117414	0.003696
O	1.517828	-2.3274	-0.00404
Li	-1.92827	3.93072	0.006087

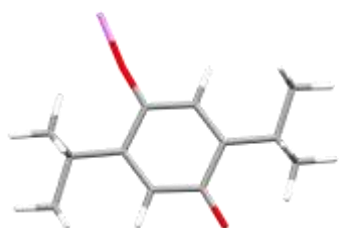


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	3.438924	1.791194	-0.000201
C	-0.645458	-1.246722	0.000101
C	0.645458	1.246726	-0.000074
C	0.822425	-1.146614	0.000062
C	-0.822425	1.146618	-0.000013
C	3.575286	-0.349993	1.268557
C	3.575191	-0.350131	-1.268736
C	-3.438925	-1.791189	0.000188
C	-3.575270	0.350009	-1.268553
C	1.480358	0.196122	-0.000042
C	-1.480358	-0.196118	0.000066
C	2.998913	0.319498	-0.000104
C	-2.998914	-0.319494	0.000109
C	-3.575207	0.350125	1.268739
H	3.175552	0.119898	2.169079
H	3.354670	-1.413608	1.306341
H	3.354581	-1.413752	-1.306384
H	4.659280	-0.225602	1.275937
H	-4.659264	0.225617	-1.275948
H	3.087318	2.321418	-0.887118
H	4.659184	-0.225733	-1.276214
H	4.528185	1.835385	-0.000255
H	3.087403	2.321510	0.886695

H	3.175384	0.119656	-2.169279
H	-1.003676	-2.265674	0.000164
H	-3.087391	-2.321499	-0.886707
H	-3.087334	-2.321421	0.887107
H	-4.659200	0.225728	1.276203
H	-3.175413	-0.119672	2.169284
H	-3.354595	1.413745	1.306400
H	-3.354655	1.413624	-1.306324
H	1.003675	2.265678	-0.000144
H	-3.175524	-0.119873	-2.169074
H	-4.528186	-1.835380	0.000225
O	1.473338	-2.186978	0.000099
O	-1.473339	2.186982	-0.000047
Li	2.246567	-3.960270	0.000119
Li	-2.246568	3.960275	-0.000050

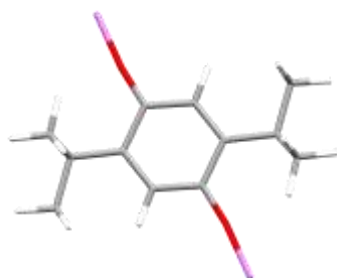
Singly Reduced

PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.348840	-1.818543	-0.000879
C	0.713139	1.136254	0.000154
C	-0.535950	-1.320413	-0.000182
C	-0.714541	1.072286	-0.000235
C	0.915639	-1.282936	0.000208
C	-3.478239	0.313093	1.266222
C	-3.477577	0.313012	-1.268165
C	3.536695	1.634044	0.000900
C	3.645410	-0.516283	-1.261638
C	-1.363119	-0.218770	-0.000400
C	1.549717	0.043043	0.000376
C	-2.893819	-0.349507	-0.000798
C	3.072941	0.169030	0.000785
C	3.644731	-0.516267	1.263524
H	-3.107220	-0.191961	2.170121
H	-3.193915	1.370954	1.331144
H	-3.193236	1.370877	-1.332985
H	-4.577525	0.241840	1.262055

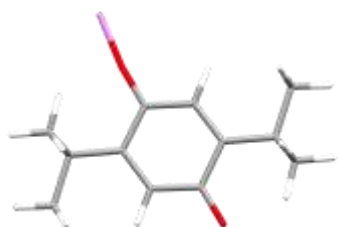
H	4.743726	-0.432015	-1.266619
H	-2.993647	-2.356861	-0.891498
H	-4.576863	0.241750	-1.264579
H	-4.448559	-1.858832	-0.001154
H	-2.994095	-2.356814	0.889947
H	-3.106068	-0.192075	-2.171843
H	1.121030	2.149265	0.000274
H	3.188643	2.175709	-0.892171
H	3.188168	2.175721	0.893777
H	4.743043	-0.431998	1.269096
H	3.260960	-0.032729	2.174949
H	3.369537	-1.577166	1.285109
H	3.370227	-1.577182	-1.283359
H	-0.941962	-2.332172	-0.000290
H	3.262132	-0.032754	-2.173276
H	4.636339	1.666166	0.001193
O	-1.383838	2.200596	-0.000419
O	1.567352	-2.364636	0.000388
Li	-2.018087	3.707775	-0.001404



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.397113	-1.810193	0.000013
C	0.603051	1.237954	-0.000010
C	-0.603029	-1.237943	0.000005
C	-0.829531	1.150066	-0.000009
C	0.829554	-1.150055	0.000003
C	-3.578651	0.319290	1.269517
C	-3.578656	0.319276	-1.269516
C	3.397128	1.810205	-0.000010
C	3.578676	-0.319281	-1.269516
C	-1.459165	-0.160917	-0.000001
C	1.459187	0.160928	-0.000004
C	-2.981331	-0.329674	0.000003
C	2.981352	0.329685	-0.000004
C	3.578672	-0.319271	1.269515
H	-3.190671	-0.167481	2.175922
H	-3.339400	1.387709	1.331752

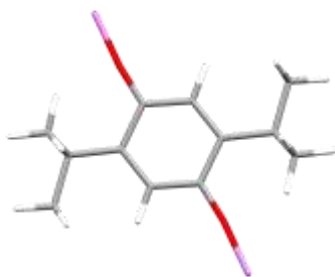
H	-3.339400	1.387692	-1.331767
H	-4.672877	0.207106	1.266603
H	4.672900	-0.207079	-1.266604
H	-3.035254	-2.339928	-0.893544
H	-4.672882	0.207095	-1.266594
H	-4.494048	-1.877567	0.000021
H	-3.035242	-2.339920	0.893571
H	-3.190683	-0.167509	-2.175916
H	0.995247	2.254975	-0.000016
H	3.035264	2.339931	-0.893570
H	3.035260	2.339939	0.893544
H	4.672896	-0.207071	1.266604
H	3.190683	0.167499	2.175916
H	3.339437	-1.387693	1.331744
H	3.339443	-1.387704	-1.331736
H	-0.995229	-2.254964	0.000014
H	3.190688	0.167480	-2.175923
H	4.494063	1.877581	-0.000008
O	-1.509869	2.249694	-0.000015
O	1.509901	-2.249679	0.000010
Li	-2.208584	3.774174	0.000014
Li	2.208207	-3.774355	-0.000092

B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.347985	-1.814564	-0.000898
C	0.711061	1.130151	0.000093
C	-0.536514	-1.316151	-0.000150
C	-0.711492	1.064296	-0.000292
C	0.910268	-1.275212	0.000241
C	-3.472506	0.314294	1.264758
C	-3.471821	0.314205	-1.266773
C	3.533374	1.630477	0.000839
C	3.641149	-0.515040	-1.260844
C	-1.358226	-0.220597	-0.000417
C	1.543989	0.044385	0.000362
C	-2.888505	-0.347554	-0.000826

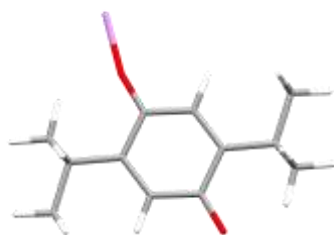
C	3.067495	0.166634	0.000772
C	3.640462	-0.514936	1.262756
H	-3.102009	-0.186059	2.161629
H	-3.195030	1.364332	1.329719
H	-3.194308	1.364237	-1.331661
H	-4.563341	0.240397	1.262132
H	4.730734	-0.425205	-1.268156
H	-2.997315	-2.349495	-0.884888
H	-4.562658	0.240309	-1.264731
H	-4.439463	-1.851938	-0.001191
H	-2.997790	-2.349433	0.883317
H	-3.100841	-0.186215	-2.163408
H	1.110051	2.135654	0.000162
H	3.188200	2.167799	-0.885457
H	3.187720	2.167871	0.886904
H	4.730043	-0.425102	1.270653
H	3.255478	-0.035636	2.166241
H	3.375809	-1.569051	1.288228
H	3.376511	-1.569156	-1.286374
H	-0.934041	-2.320519	-0.000218
H	3.256657	-0.035813	-2.164578
H	4.624641	1.661890	0.001134
O	-1.377027	2.187343	-0.000512
O	1.557047	-2.348049	0.000461
Li	-2.007490	3.682951	-0.000696



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.396190	-1.806356	0.000006
C	0.602058	1.233404	-0.000007
C	-0.602058	-1.233406	0.000003
C	-0.826299	1.142402	-0.000003
C	0.826299	-1.142404	0.000001
C	-3.572049	0.320708	1.267983
C	-3.572052	0.320702	-1.267980
C	3.396187	1.806355	-0.000010
C	3.572049	-0.320706	-1.267989
C	-1.453360	-0.164015	0.000001

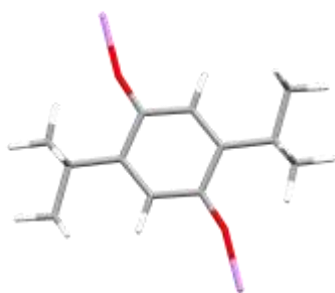
C	1.453360	0.164013	-0.000004
C	-2.976018	-0.327763	0.000002
C	2.976018	0.327763	-0.000007
C	3.572054	-0.320703	1.267975
H	-3.184349	-0.161639	2.167064
H	-3.337498	1.380938	1.329855
H	-3.337503	1.380932	-1.329856
H	-4.657830	0.207730	1.267508
H	4.657829	-0.207724	-1.267516
H	-3.037746	-2.332385	-0.886669
H	-4.657832	0.207721	-1.267504
H	-4.484878	-1.870921	0.000003
H	-3.037752	-2.332379	0.886687
H	-3.184350	-0.161646	-2.167059
H	0.983453	2.243789	-0.000012
H	3.037745	2.332380	-0.886689
H	3.037746	2.332383	0.886667
H	4.657834	-0.207724	1.267496
H	3.184356	0.161647	2.167055
H	3.337503	-1.380933	1.329852
H	3.337502	-1.380937	-1.329861
H	-0.983454	-2.243791	0.000008
H	3.184344	0.161639	-2.167069
H	4.484875	1.870923	-0.000010
O	-1.502687	2.233960	-0.000008
O	1.502686	-2.233962	0.000004
Li	-2.209741	3.741150	0.000009
Li	2.209740	-3.741152	-0.000014

B3LYP/def2TZVP (CPCM – DME)



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.352567	-1.830741	-0.000882
C	0.704824	1.120872	0.000093
C	-0.537630	-1.325510	-0.000134
C	-0.727847	1.066177	-0.000273
C	0.906791	-1.284090	0.000253
C	-3.476301	0.304896	1.262409

C	-3.475607	0.304804	-1.264400
C	3.522166	1.632187	0.000793
C	3.643088	-0.508463	-1.261126
C	-1.364906	-0.234710	-0.000399
C	1.537126	0.033998	0.000358
C	-2.893537	-0.364044	-0.000811
C	3.062633	0.166006	0.000753
C	3.642420	-0.508324	1.263013
H	-3.097825	-0.184897	2.162747
H	-3.212929	1.358952	1.307375
H	-3.212209	1.358856	-1.309299
H	-4.565979	0.216711	1.263828
H	4.732585	-0.417672	-1.265015
H	-3.003200	-2.366575	-0.885517
H	-4.565284	0.216620	-1.266409
H	-4.443918	-1.866106	-0.001189
H	-3.003700	-2.366505	0.883993
H	-3.096638	-0.185057	-2.164493
H	1.106055	2.125526	0.000158
H	3.173966	2.168297	-0.884593
H	3.173488	2.168398	0.885931
H	4.731915	-0.417534	1.267466
H	3.260308	-0.024436	2.165324
H	3.379005	-1.562735	1.296157
H	3.379692	-1.562878	-1.294293
H	-0.940346	-2.328928	-0.000202
H	3.261451	-0.024676	-2.163693
H	4.613461	1.667287	0.001086
O	-1.391858	2.165172	-0.000481
O	1.558580	-2.366131	0.000485
Li	-1.844946	3.876753	-0.000682

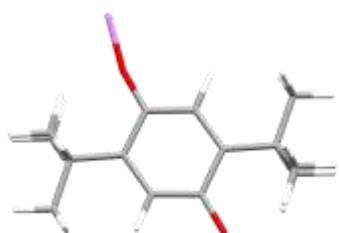


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.382863	-1.832885	-0.000812
C	0.586759	1.241245	0.000224
C	-0.586760	-1.241247	-0.000230
C	-0.846228	1.143445	-0.000059

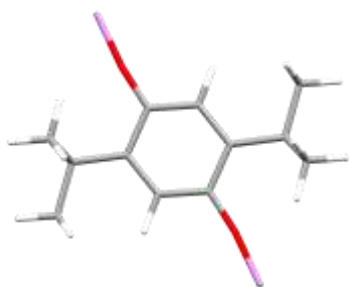
C	0.846228	-1.143448	0.000053
C	-3.570716	0.299344	1.263491
C	-3.570235	0.299571	-1.264806
C	3.382858	1.832885	0.000814
C	3.570717	-0.299340	-1.263498
C	-1.447920	-0.178348	-0.000296
C	1.447919	0.178345	0.000290
C	-2.969988	-0.352702	-0.000601
C	2.969987	0.352701	0.000597
C	3.570234	-0.299575	1.264801
H	-3.174299	-0.174959	2.164232
H	-3.345707	1.362190	1.306043
H	-3.345209	1.362424	-1.307080
H	-4.656097	0.172879	1.266159
H	4.656097	-0.172873	-1.266163
H	-3.018433	-2.357392	-0.886294
H	-4.655614	0.173106	-1.267910
H	-4.472153	-1.901536	-0.001025
H	-3.018769	-2.357551	0.884714
H	-3.173472	-0.174570	-2.165481
H	0.958610	2.256261	0.000389
H	3.018763	2.357554	-0.884710
H	3.018425	2.357388	0.886298
H	4.655613	-0.173108	1.267906
H	3.173470	0.174562	2.165477
H	3.345210	-1.362429	1.307072
H	3.345708	-1.362185	-1.306053
H	-0.958610	-2.256263	-0.000394
H	3.174299	0.174967	-2.164237
H	4.472147	1.901539	0.001028
O	-1.539469	2.214530	-0.000095
O	1.539471	-2.214532	0.000082
Li	-1.984242	3.951544	-0.000014
Li	1.984262	-3.951543	0.000005

Doubly Reduced

PBE/def2TZVP



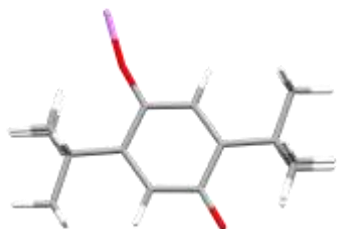
<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.420723	-1.714073	0.040486
C	0.667433	1.150947	-0.120159
C	-0.585663	-1.276553	0.055581
C	-0.751894	1.131089	-0.096693
C	0.855275	-1.281330	0.064347
C	-3.526896	0.492416	1.173048
C	-3.479651	0.347428	-1.349256
C	3.515741	1.578660	-0.193886
C	3.560023	-0.669913	-1.273625
C	-1.396595	-0.147403	-0.026287
C	1.484900	0.029392	-0.042276
C	-2.931216	-0.258441	-0.039108
C	3.014363	0.131707	-0.069894
C	3.587963	-0.465038	1.235669
H	-3.169298	0.043658	2.112651
H	-3.219350	1.545013	1.156852
H	-3.145123	1.387160	-1.462954
H	-4.629819	0.438763	1.160697
H	4.664270	-0.647344	-1.285268
H	-3.051057	-2.312623	-0.805175
H	-4.583473	0.322102	-1.359635
H	-4.522871	-1.731081	0.014414
H	-3.094658	-2.203995	0.970125
H	-3.114701	-0.229607	-2.212857
H	1.103840	2.149565	-0.213628
H	3.163570	2.055025	-1.122304
H	3.185287	2.199223	0.653679
H	4.692190	-0.444232	1.219171
H	3.245092	0.117865	2.105392
H	3.242322	-1.501890	1.344020
H	3.215884	-1.710503	-1.205084
H	-1.024049	-2.273782	0.127864
H	3.196230	-0.235486	-2.218279
H	4.618158	1.584745	-0.207668
O	-1.415251	2.285086	-0.146060
O	1.507771	-2.382943	0.150069
Li	-1.836412	3.865769	0.015107



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.366475	-1.828945	-0.001458
C	0.557640	1.240908	-0.000153
C	-0.557635	-1.240908	0.000001
C	-0.848896	1.150852	-0.000944
C	0.848902	-1.150851	0.000797
C	-3.565676	0.297072	1.263502
C	-3.564190	0.296256	-1.268021
C	3.366477	1.828948	0.001265
C	3.565677	-0.297094	-1.263656
C	-1.432345	-0.148515	-0.000865
C	1.432350	0.148514	0.000710
C	-2.957136	-0.346432	-0.001696
C	2.957141	0.346434	0.001531
C	3.564201	-0.296229	1.267866
H	-3.192907	-0.209757	2.166254
H	-3.285199	1.356086	1.331380
H	-3.283638	1.355227	-1.336250
H	-4.665464	0.215000	1.252488
H	4.665465	-0.215018	-1.252648
H	-2.993223	-2.355635	-0.892390
H	-4.663991	0.214187	-1.258247
H	-4.465175	-1.905148	-0.002084
H	-2.994279	-2.355058	0.890257
H	-3.190359	-0.211152	-2.170008
H	0.954279	2.257826	-0.000254
H	2.994272	2.355044	-0.890456
H	2.993232	2.355654	0.892191
H	4.664001	-0.214159	1.258088
H	3.190370	0.211192	2.169846
H	3.283651	-1.355200	1.336113
H	3.285203	-1.356110	-1.331514
H	-0.954272	-2.257826	0.000093
H	3.192903	0.209717	-2.166416
H	4.465176	1.905153	0.001879
O	-1.569056	2.279251	-0.001732
O	1.569062	-2.279251	0.001587
Li	-2.256180	3.732173	-0.002566

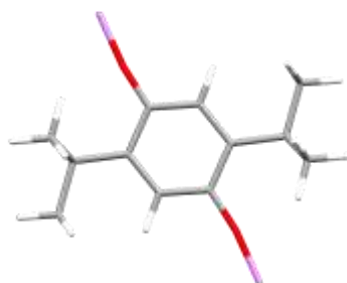
Li | 2.256187 -3.732172 0.002853

B3LYP/def2TZVP



Element	X	Y	Z
C	-3.418581	-1.706489	0.043495
C	0.662369	1.143334	-0.121846
C	-0.583395	-1.272341	0.051688
C	-0.746909	1.122343	-0.102422
C	0.850885	-1.278216	0.058736
C	-3.516126	0.496484	1.173652
C	-3.477070	0.348664	-1.346757
C	3.509929	1.573937	-0.187729
C	3.559465	-0.665650	-1.272850
C	-1.388961	-0.144785	-0.029359
C	1.477449	0.025866	-0.044647
C	-2.923392	-0.253253	-0.038788
C	3.006655	0.127307	-0.068407
C	3.582456	-0.467064	1.235624
H	-3.158119	0.049893	2.104556
H	-3.213677	1.540937	1.161036
H	-3.148313	1.379485	-1.466458
H	-4.611075	0.441775	1.165460
H	4.655751	-0.637121	-1.282220
H	-3.057192	-2.302147	-0.796456
H	-4.573037	0.320840	-1.353855
H	-4.512836	-1.720295	0.021640
H	-3.093489	-2.192642	0.965155
H	-3.116910	-0.226227	-2.203435
H	1.093712	2.133685	-0.211829
H	3.162816	2.048712	-1.108824
H	3.180775	2.187575	0.654487
H	4.678718	-0.439876	1.220556
H	3.238999	0.111112	2.098296
H	3.247956	-1.497032	1.347936
H	3.225847	-1.700324	-1.215839
H	-1.016979	-2.260810	0.122367
H	3.199025	-0.230075	-2.209050

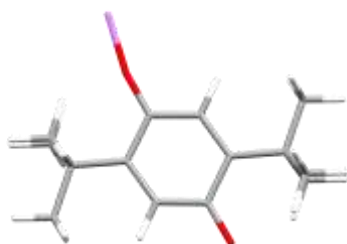
H	4.604222	1.580251	-0.199186
O	-1.408698	2.281038	-0.156226
O	1.500596	-2.372964	0.142386
Li	-1.851253	3.823448	-0.001811



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.361329	-1.825436	-0.001420
C	0.554444	1.235404	-0.000164
C	-0.554440	-1.235399	0.000024
C	-0.844428	1.142738	-0.000953
C	0.844432	-1.142733	0.000813
C	-3.561097	0.297027	1.262090
C	-3.559615	0.296167	-1.266606
C	3.361339	1.825437	0.001283
C	3.561099	-0.297025	-1.262231
C	-1.426265	-0.147935	-0.000856
C	1.426269	0.147941	0.000716
C	-2.950524	-0.343747	-0.001683
C	2.950529	0.343750	0.001543
C	3.559618	-0.296170	1.266465
H	-3.185165	-0.201752	2.158167
H	-3.295813	1.349987	1.329581
H	-3.294255	1.349082	-1.334500
H	-4.651834	0.204495	1.253445
H	4.651837	-0.204500	-1.253584
H	-2.991638	-2.348259	-0.885584
H	-4.650362	0.203637	-1.259179
H	-4.451729	-1.900745	-0.002034
H	-2.992675	-2.347656	0.883534
H	-3.182630	-0.203219	-2.161902
H	0.942604	2.244781	-0.000279
H	2.992687	2.347661	-0.883669
H	2.991651	2.348260	0.885449
H	4.650365	-0.203640	1.259038
H	3.182633	0.203212	2.161762
H	3.294257	-1.349085	1.334354
H	3.295807	-1.349982	-1.329726

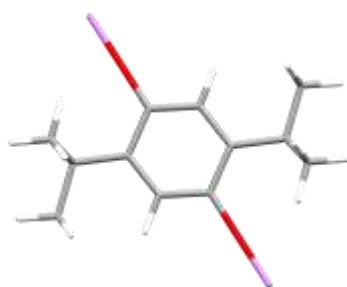
H	-0.942600	-2.244775	0.000140
H	3.185172	0.201760	-2.158306
H	4.451739	1.900743	0.001896
O	-1.561750	2.268275	-0.001755
O	1.561754	-2.268269	0.001615
Li	-2.224720	3.719851	-0.002638
Li	2.224727	-3.719845	0.002497

B3LYP/def2TZVP (CPCM – DME)



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.418083	-1.708274	0.049591
C	0.657535	1.130910	-0.127848
C	-0.572919	-1.274416	0.034766
C	-0.751357	1.129922	-0.123952
C	0.850623	-1.291991	0.040336
C	-3.499326	0.496545	1.180297
C	-3.496067	0.346031	-1.336872
C	3.504566	1.570474	-0.173103
C	3.577892	-0.656345	-1.269728
C	-1.386689	-0.138129	-0.042735
C	1.475469	0.000653	-0.051766
C	-2.921737	-0.255569	-0.037100
C	3.007429	0.120343	-0.063882
C	3.583099	-0.469484	1.241114
H	-3.152257	0.035805	2.109112
H	-3.179548	1.536491	1.171421
H	-3.173066	1.378548	-1.452817
H	-4.593972	0.460378	1.175005
H	4.673156	-0.633829	-1.263653
H	-3.076914	-2.306091	-0.797847
H	-4.590820	0.313144	-1.328700
H	-4.511592	-1.718823	0.046337
H	-3.083432	-2.199037	0.965625
H	-3.149385	-0.224611	-2.202699
H	1.107653	2.114841	-0.195366
H	3.164341	2.049921	-1.093911
H	3.170644	2.180847	0.669178

H	4.678313	-0.446925	1.228303
H	3.244520	0.113581	2.102468
H	3.246621	-1.497573	1.360330
H	3.240009	-1.690454	-1.235849
H	-1.027487	-2.255590	0.100096
H	3.237256	-0.205563	-2.206352
H	4.598109	1.580747	-0.177637
O	-1.412036	2.290428	-0.193396
O	1.504722	-2.416600	0.123901
Li	-1.903657	3.909072	-0.073591



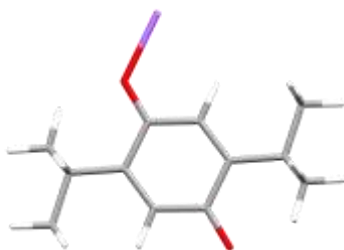
<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.372665	-1.811841	-0.001543
C	0.558434	1.232917	-0.000072
C	-0.558429	-1.232914	-0.000058
C	-0.849715	1.161813	-0.000865
C	0.849720	-1.161810	0.000740
C	-3.564271	0.313689	1.259794
C	-3.562802	0.313019	-1.264229
C	3.372671	1.811842	0.001389
C	3.564266	-0.313696	-1.259936
C	-1.427880	-0.138830	-0.000855
C	1.427886	0.138833	0.000723
C	-2.953874	-0.332412	-0.001691
C	2.953879	0.332414	0.001550
C	3.562815	-0.313009	1.264087
H	-3.193911	-0.186173	2.158608
H	-3.297896	1.366710	1.319614
H	-3.296358	1.366009	-1.324299
H	-4.655121	0.223929	1.249835
H	4.655116	-0.223938	-1.249986
H	-3.007234	-2.338835	-0.885255
H	-4.653662	0.223263	-1.255494
H	-4.463575	-1.879505	-0.002163
H	-3.008269	-2.338366	0.882876
H	-3.191394	-0.187320	-2.162346
H	0.959177	2.238737	-0.000109

H	3.008266	2.338362	-0.883029
H	3.007250	2.338842	0.885102
H	4.653676	-0.223257	1.255342
H	3.191417	0.187338	2.162204
H	3.296368	-1.365997	1.324168
H	3.297889	-1.366718	-1.319748
H	-0.959172	-2.238734	-0.000022
H	3.193900	0.186162	-2.158750
H	4.463582	1.879506	0.001997
O	-1.559537	2.281221	-0.001570
O	1.559541	-2.281219	0.001457
Li	-2.482305	3.712497	-0.002506
Li	2.482309	-3.712493	0.002381

Sodium

Singly Reduced

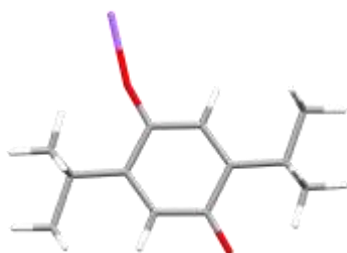
PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.445058	-1.773201	-0.000033
C	0.648872	1.118002	0.000275
C	-0.621007	-1.315378	-0.000246
C	-0.786849	1.089984	0.000179
C	0.830386	-1.299402	-0.000322
C	-3.537048	0.370880	1.263808
C	-3.537169	0.371070	-1.263529
C	3.488484	1.588164	0.000463
C	3.568077	-0.561210	-1.262722
C	-1.437131	-0.206588	0.000007
C	1.478515	0.019771	0.000006
C	-2.968036	-0.312140	0.000061
C	3.003839	0.129612	0.000089
C	3.567980	-0.561823	1.262610
H	-3.159683	-0.123073	2.171898
H	-3.252981	1.429722	1.297625
H	-3.253173	1.429939	-1.297153
H	-4.636395	0.299022	1.268948

H	4.667852	-0.496388	-1.266932
H	-3.099254	-2.317660	-0.891107
H	-4.636512	0.299153	-1.268615
H	-4.545232	-1.795484	0.000069
H	-3.099083	-2.317818	0.890877
H	-3.159830	-0.122692	-2.171735
H	1.100172	2.121058	0.000762
H	3.150051	2.134036	-0.895017
H	3.149974	2.133620	0.896162
H	4.667753	-0.497002	1.266939
H	3.192472	-0.072100	2.174303
H	3.273002	-1.617357	1.283877
H	3.273095	-1.616731	-1.284529
H	-1.041145	-2.321687	-0.000438
H	3.192647	-0.071041	-2.174210
H	4.588315	1.606224	0.000506
O	-1.457102	2.209892	0.000209
O	1.476213	-2.385627	-0.000627
Na	-0.538866	4.083384	-0.003065

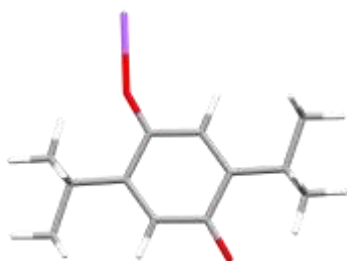
B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.429847	-1.725819	-0.000176
C	0.704842	1.109746	0.000042
C	-0.601752	-1.304098	-0.000080
C	-0.722895	1.087573	0.000001
C	0.845210	-1.300993	-0.000038
C	-3.492089	0.409738	1.263690
C	-3.492015	0.409828	-1.263895
C	3.541383	1.537107	0.000137
C	3.592602	-0.609790	-1.261336
C	-1.395471	-0.188670	-0.000063
C	1.509402	0.002912	0.000026
C	-2.928146	-0.273189	-0.000110
C	3.036423	0.086187	0.000072
C	3.592530	-0.609878	1.261464

H	-3.132502	-0.095653	2.162439
H	-3.184311	1.452147	1.315779
H	-3.184234	1.452240	-1.315891
H	-4.584873	0.363897	1.263911
H	4.684630	-0.551889	-1.268174
H	-3.093994	-2.270526	-0.884086
H	-4.584799	0.363987	-1.264182
H	-4.522175	-1.732620	-0.000209
H	-3.094046	-2.270588	0.883715
H	-3.132377	-0.095499	-2.162658
H	1.131944	2.104644	0.000089
H	3.209709	2.083203	-0.886155
H	3.209658	2.083142	0.886447
H	4.684559	-0.551977	1.268367
H	3.222077	-0.119062	2.164985
H	3.296250	-1.655575	1.287363
H	3.296323	-1.655486	-1.287325
H	-1.024895	-2.298339	-0.000126
H	3.222200	-0.118911	-2.164844
H	4.633301	1.540042	0.000168
O	-1.363832	2.215508	0.000023
O	1.467270	-2.390238	-0.000058
Na	-1.809917	4.166028	0.000084

B3LYP/def2TZVP (CPCM – DME)

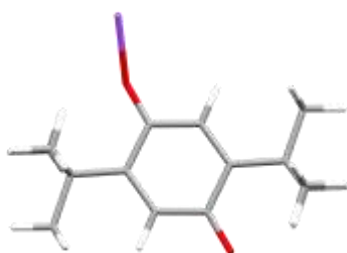


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.434868	-1.752235	-0.001482
C	0.690906	1.102745	0.000196
C	-0.605707	-1.313952	-0.000166
C	-0.745631	1.086492	-0.000497
C	0.838962	-1.306884	0.000527
C	-3.504486	0.388306	1.260561
C	-3.503267	0.388027	-1.264064
C	3.519811	1.549660	0.001522
C	3.591721	-0.592840	-1.260111
C	-1.408262	-0.204849	-0.000674
C	1.497662	-0.003370	0.000707

C	-2.939090	-0.297854	-0.001403
C	3.026307	0.094528	0.001436
C	3.590499	-0.592575	1.263674
H	-3.138925	-0.109339	2.162098
H	-3.211046	1.434833	1.299875
H	-3.209793	1.434547	-1.303321
H	-4.596294	0.329057	1.262454
H	4.683369	-0.530896	-1.262661
H	-3.098381	-2.296817	-0.885868
H	-4.595072	0.328773	-1.267000
H	-4.526880	-1.760802	-0.002020
H	-3.099255	-2.296616	0.883359
H	-3.136831	-0.109812	-2.165137
H	1.117598	2.097268	0.000293
H	3.184031	2.093700	-0.883891
H	3.183171	2.093886	0.886494
H	4.682144	-0.530626	1.267270
H	3.221960	-0.097634	2.165721
H	3.298683	-1.639454	1.298201
H	3.299934	-1.639724	-1.294703
H	-1.031969	-2.307866	-0.000264
H	3.224059	-0.098085	-2.162618
H	4.611729	1.559783	0.002052
O	-1.384208	2.196058	-0.000931
O	1.466907	-2.405076	0.000950
Na	-1.453349	4.358770	-0.001185

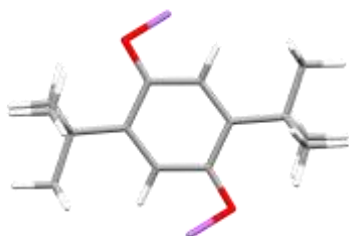
Doubly Reduced

PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.434603	-1.645531	0.023747
C	0.674009	1.209451	-0.089649
C	-0.598896	-1.217698	0.001981
C	-0.755151	1.200101	-0.099307
C	0.845183	-1.225391	-0.006538
C	-3.478078	0.513607	1.255983
C	-3.529135	0.478500	-1.267804

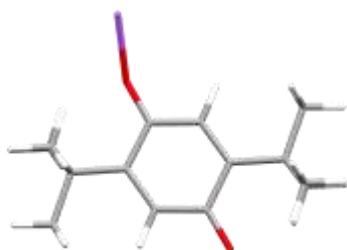
C	3.521046	1.635201	-0.066719
C	3.583395	-0.550632	-1.267486
C	-1.404097	-0.088771	-0.028024
C	1.485973	0.088336	-0.044769
C	-2.938277	-0.190582	-0.006630
C	3.015540	0.184817	-0.031974
C	3.562256	-0.482620	1.250577
H	-3.101450	0.014859	2.162336
H	-3.154776	1.563419	1.276649
H	-3.208415	1.525915	-1.326465
H	-4.580993	0.484808	1.278487
H	4.687116	-0.523654	-1.258281
H	-3.105448	-2.206205	-0.863923
H	-4.632101	0.433320	-1.246364
H	-4.536706	-1.654416	0.042005
H	-3.076520	-2.181082	0.915701
H	-3.181429	-0.042854	-2.173209
H	1.113885	2.210762	-0.117114
H	3.189662	2.161974	-0.974886
H	3.174288	2.210207	0.806280
H	4.665963	-0.454903	1.258007
H	3.198808	0.049827	2.143667
H	3.223797	-1.525758	1.297541
H	3.244002	-1.594678	-1.262513
H	-1.036634	-2.217533	0.028711
H	3.234876	-0.067737	-2.194048
H	4.623171	1.638927	-0.056957
O	-1.410142	2.335427	-0.186635
O	1.490246	-2.328869	0.027534
Na	-1.628137	4.200543	0.799709



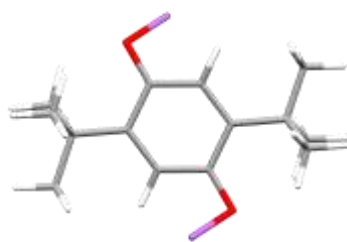
<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.456845	-1.667884	-0.136584
C	0.605997	1.198640	0.166605
C	-0.605997	-1.198640	-0.166611
C	-0.827478	1.194696	0.167808

C	0.827479	-1.194696	-0.167812
C	-3.535654	0.350858	1.324720
C	-3.556179	0.588844	-1.183907
C	3.456844	1.667885	0.136578
C	3.535655	-0.350859	-1.324724
C	-1.446257	-0.088080	0.007480
C	1.446257	0.088079	-0.007485
C	-2.975367	-0.215366	0.001434
C	2.975367	0.215366	-0.001439
C	3.556179	-0.588842	1.183903
H	-3.179217	-0.246264	2.179231
H	-3.204752	1.388742	1.459759
H	-3.271522	1.644935	-1.084922
H	-4.637622	0.318314	1.322614
H	4.637623	-0.318314	-1.322618
H	-3.132226	-2.127449	-1.082690
H	-4.656126	0.518830	-1.198973
H	-4.556933	-1.693209	-0.113706
H	-3.097199	-2.297515	0.693995
H	-3.176426	0.195062	-2.140025
H	1.062363	2.162990	0.432763
H	3.097199	2.297514	-0.694002
H	3.132225	2.127451	1.082682
H	4.656125	-0.518827	1.198970
H	3.176425	-0.195060	2.140021
H	3.271523	-1.644934	1.084919
H	3.204754	-1.388743	-1.459763
H	-1.062363	-2.162991	-0.432770
H	3.179219	0.246262	-2.179235
H	4.556933	1.693210	0.113699
O	-1.499185	2.336767	0.254700
O	1.499185	-2.336767	-0.254704
Na	-0.306797	3.064623	-1.350072
Na	0.306792	-3.064627	1.350064

B3LYP/def2TZVP



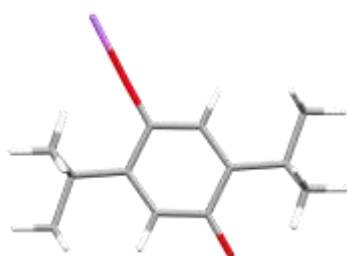
<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.433220	-1.639764	0.015760
C	0.671014	1.202045	-0.085916
C	-0.598465	-1.213818	0.006033
C	-0.750684	1.191362	-0.094115
C	0.840517	-1.221028	-0.000993
C	-3.472952	0.508547	1.258841
C	-3.523044	0.487209	-1.262803
C	3.516089	1.630229	-0.070573
C	3.578476	-0.552167	-1.266233
C	-1.398194	-0.088869	-0.025913
C	1.479845	0.086563	-0.041489
C	-2.931825	-0.186842	-0.006100
C	3.008906	0.180709	-0.031766
C	3.561841	-0.478856	1.250523
H	-3.099440	0.007292	2.155257
H	-3.155262	1.549556	1.289166
H	-3.213582	1.528350	-1.317385
H	-4.567758	0.477343	1.280564
H	4.673974	-0.517809	-1.259619
H	-3.106368	-2.192205	-0.867290
H	-4.617679	0.435211	-1.244545
H	-4.527177	-1.646142	0.031392
H	-3.082054	-2.176606	0.899021
H	-3.173316	-0.023439	-2.163708
H	1.103781	2.195344	-0.111759
H	3.185921	2.150977	-0.972328
H	3.174540	2.202387	0.795557
H	4.657325	-0.443968	1.255969
H	3.200234	0.052283	2.135304
H	3.235785	-1.515471	1.307188
H	3.251868	-1.590304	-1.265690
H	-1.029752	-2.205374	0.033644
H	3.228421	-0.074009	-2.185187
H	4.609972	1.633881	-0.063242
O	-1.401540	2.325275	-0.172418
O	1.481208	-2.316175	0.034784
Na	-1.635172	4.179375	0.759690



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.451039	-1.660087	-0.137791
C	0.605065	1.192088	0.167336
C	-0.605065	-1.192088	-0.167340
C	-0.818868	1.185849	0.167967
C	0.818868	-1.185849	-0.167970
C	-3.531277	0.353147	1.323111
C	-3.551826	0.593248	-1.183180
C	3.451039	1.660087	0.137787
C	3.531278	-0.353145	-1.323117
C	-1.439579	-0.085103	0.005657
C	1.439579	0.085103	-0.005663
C	-2.968288	-0.208203	0.000581
C	2.968288	0.208203	-0.000587
C	3.551825	-0.593250	1.183173
H	-3.173781	-0.239061	2.170264
H	-3.213205	1.384433	1.462180
H	-3.287233	1.644495	-1.084157
H	-4.624822	0.312023	1.320866
H	4.624823	-0.312019	-1.320871
H	-3.130372	-2.114211	-1.077818
H	-4.642361	0.508209	-1.205115
H	-4.542700	-1.685598	-0.113314
H	-3.092223	-2.285540	0.684794
H	-3.164530	0.210259	-2.131474
H	1.052981	2.151734	0.418702
H	3.092213	2.285542	-0.684792
H	3.130383	2.114207	1.077819
H	4.642361	-0.508214	1.205108
H	3.164530	-0.210261	2.131468
H	3.287229	-1.644496	1.084150
H	3.213207	-1.384431	-1.462188
H	-1.052981	-2.151735	-0.418707
H	3.173782	0.239064	-2.170270
H	4.542700	1.685599	0.113298
O	-1.482552	2.327168	0.252957
O	1.482552	-2.327169	-0.252958
Na	-0.344773	3.065662	-1.357672

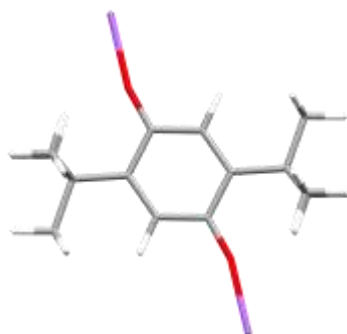
Na | 0.344771 -3.065661 1.357672

B3LYP/def2TZVP (CPCM – DME)



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.418149	-1.615851	0.021630
C	0.682659	1.192541	-0.000261
C	-0.567583	-1.206104	-0.002222
C	-0.729155	1.211159	0.012795
C	0.854747	-1.238181	-0.015450
C	-3.465411	0.511575	1.294444
C	-3.488547	0.525708	-1.226168
C	3.536259	1.604872	-0.024128
C	3.577861	-0.529742	-1.294189
C	-1.371862	-0.060331	0.011572
C	1.490249	0.051106	-0.014060
C	-2.907444	-0.165683	0.025074
C	3.023573	0.156230	-0.027536
C	3.600931	-0.543825	1.220975
H	-3.123767	-0.019077	2.187327
H	-3.120682	1.542114	1.353050
H	-3.144847	1.556876	-1.279531
H	-4.560847	0.498588	1.293707
H	4.673456	-0.517215	-1.296164
H	-3.093088	-2.159527	-0.867651
H	-4.583786	0.512599	-1.205470
H	-4.511876	-1.616484	0.031663
H	-3.076880	-2.169430	0.898645
H	-3.163403	0.005138	-2.131065
H	1.142499	2.174540	0.001019
H	3.196317	2.159614	-0.901721
H	3.212529	2.149718	0.865710
H	4.696380	-0.531210	1.202993
H	3.273307	-0.030488	2.129668
H	3.253560	-1.574935	1.255379
H	3.229813	-1.560438	-1.333758
H	-1.029570	-2.186319	-0.003472
H	3.233675	-0.006297	-2.190915

H	4.629952	1.604330	-0.034163
O	-1.379295	2.373294	0.025267
O	1.498585	-2.375407	-0.027725
Na	-2.327928	4.217632	0.044355



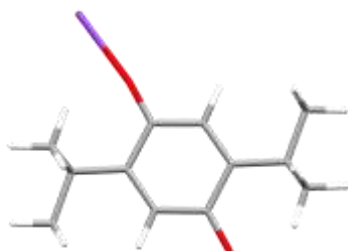
<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.482905	-1.594083	-0.023988
C	0.631521	1.196275	-0.018491
C	-0.631521	-1.196276	0.018487
C	-0.781188	1.218602	-0.045058
C	0.781189	-1.218602	0.045053
C	-3.554058	0.574441	1.180705
C	-3.507696	0.511041	-1.338020
C	3.482905	1.594083	0.023986
C	3.554058	-0.574438	-1.180711
C	-1.432130	-0.050367	-0.025097
C	1.432130	0.050366	0.025092
C	-2.966616	-0.146505	-0.050922
C	2.966616	0.146505	0.050917
C	3.507698	-0.511043	1.338013
H	-3.234829	0.076004	2.100082
H	-3.212142	1.607217	1.209699
H	-3.163991	1.541368	-1.406324
H	-4.648647	0.559745	1.152545
H	4.648647	-0.559740	-1.152553
H	-3.136713	-2.166008	-0.887564
H	-4.602594	0.496764	-1.349433
H	-4.575993	-1.590716	-0.044193
H	-3.169238	-2.121532	0.879408
H	-3.155331	-0.032707	-2.218802
H	1.095406	2.175277	-0.034596
H	3.169238	2.121534	-0.879409
H	3.136713	2.166007	0.887564
H	4.602595	-0.496766	1.349426
H	3.155332	0.032702	2.218797
H	3.163993	-1.541371	1.406315
H	3.212143	-1.607214	-1.209708

H	-1.095406	-2.175277	0.034591
H	3.234828	-0.076000	-2.100088
H	4.575993	1.590717	0.044191
O	-1.425629	2.373705	-0.085999
O	1.425629	-2.373706	0.085991
Na	-1.906926	4.406067	-0.146021
Na	1.906917	-4.406070	0.146021

Potassium

Singly Reduced

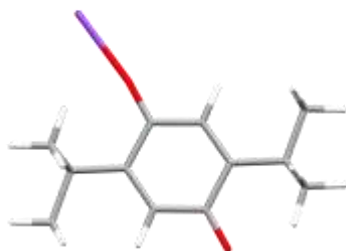
PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.426959	-1.658219	-0.000955
C	0.758235	1.125685	0.000115
C	-0.586167	-1.282443	-0.000133
C	-0.676162	1.129760	-0.000313
C	0.865143	-1.303494	0.000301
C	-3.455281	0.475628	1.266358
C	-3.454524	0.475466	-1.268559
C	3.601001	1.504785	0.000937
C	3.620171	-0.647841	-1.260824
C	-1.366183	-0.147180	-0.000437
C	1.547210	-0.002424	0.000422
C	-2.901313	-0.213440	-0.000891
C	3.075893	0.060716	0.000873
C	3.619420	-0.647681	1.262984
H	-3.138274	-0.068150	2.168200
H	-3.072889	1.502080	1.351335
H	-3.072080	1.501906	-1.353440
H	-4.557604	0.493595	1.248664
H	4.721573	-0.613693	-1.265039
H	-3.094899	-2.212048	-0.890811
H	-4.556858	0.493437	-1.251525
H	-4.527986	-1.649067	-0.001290
H	-3.095440	-2.211931	0.889175

H	-3.136980	-0.068428	-2.170142
H	1.206169	2.121718	0.000186
H	3.274385	2.060482	-0.891565
H	3.273855	2.060595	0.893175
H	4.720819	-0.613530	1.267851
H	3.258296	-0.146100	2.174091
H	3.294987	-1.694757	1.285053
H	3.295751	-1.694919	-1.282954
H	-1.032089	-2.277988	-0.000204
H	3.259591	-0.146376	-2.172210
H	4.701374	1.490998	0.001265
O	-1.303171	2.270338	-0.000573
O	1.475019	-2.412082	0.000552
K	-2.692490	4.139092	-0.001108

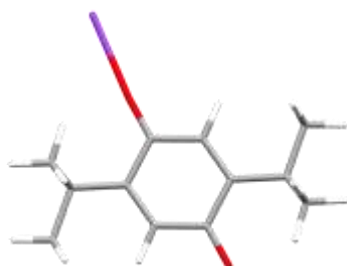
B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.425366	-1.654014	-0.000955
C	0.757059	1.119527	0.000113
C	-0.586515	-1.277735	-0.000134
C	-0.672718	1.121926	-0.000313
C	0.860076	-1.295829	0.000296
C	-3.450556	0.475848	1.265278
C	-3.449803	0.475687	-1.267473
C	3.598176	1.500916	0.000935
C	3.616512	-0.646688	-1.260084
C	-1.361315	-0.148957	-0.000437
C	1.542010	-0.001114	0.000419
C	-2.895774	-0.211173	-0.000889
C	3.070696	0.058152	0.000871
C	3.615760	-0.646526	1.262241
H	-3.134428	-0.064178	2.159695
H	-3.078618	1.495485	1.353232
H	-3.077812	1.495313	-1.355336
H	-4.544647	0.489563	1.247777
H	4.709442	-0.605938	-1.266610
H	-3.097902	-2.204321	-0.884198

H	-4.543903	0.489404	-1.250626
H	-4.518063	-1.642063	-0.001282
H	-3.098429	-2.204208	0.882554
H	-3.133142	-0.064452	-2.161634
H	1.196053	2.108356	0.000182
H	3.274587	2.052290	-0.884820
H	3.274058	2.052404	0.886427
H	4.708686	-0.605774	1.269414
H	3.253031	-0.149349	2.165449
H	3.302875	-1.687439	1.288316
H	3.303642	-1.687604	-1.286212
H	-1.024187	-2.265985	-0.000202
H	3.254322	-0.149626	-2.163572
H	4.690166	1.486521	0.001263
O	-1.295560	2.255201	-0.000570
O	1.465129	-2.395615	0.000548
K	-2.681999	4.126485	-0.001102

B3LYP/def2TZVP (CPCM – DME)

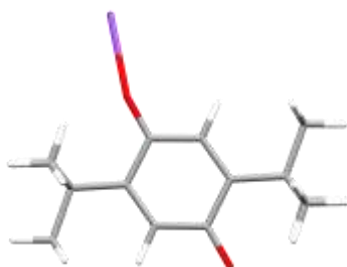


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.424863	-1.691131	-0.000957
C	0.742001	1.105892	0.000105
C	-0.590554	-1.291390	-0.000133
C	-0.695820	1.113344	-0.000331
C	0.853847	-1.306154	0.000303
C	-3.465752	0.447693	1.261943
C	-3.464996	0.447522	-1.264171
C	3.577725	1.508781	0.000939
C	3.616083	-0.634586	-1.260676
C	-1.376699	-0.170221	-0.000447
C	1.531389	-0.012647	0.000420
C	-2.908904	-0.243573	-0.000901
C	3.061577	0.061590	0.000878
C	3.615320	-0.634420	1.262858
H	-3.114029	-0.062018	2.162139
H	-3.149953	1.486981	1.310534
H	-3.149169	1.486805	-1.312712

H	-4.558627	0.411696	1.259687
H	4.708668	-0.590791	-1.263024
H	-3.095967	-2.240181	-0.885371
H	-4.557872	0.411524	-1.262565
H	-4.516989	-1.684863	-0.001284
H	-3.096496	-2.240062	0.883728
H	-3.112733	-0.062310	-2.164087
H	1.182567	2.094171	0.000171
H	3.250031	2.058060	-0.884211
H	3.249491	2.058178	0.885815
H	4.707904	-0.590620	1.265863
H	3.255607	-0.133138	2.164978
H	3.305938	-1.676276	1.297722
H	3.306717	-1.676445	-1.295592
H	-1.031649	-2.278974	-0.000198
H	3.256918	-0.133421	-2.163079
H	4.669751	1.502011	0.001272
O	-1.312257	2.233260	-0.000593
O	1.465833	-2.414004	0.000561
K	-2.312495	4.534208	-0.001026

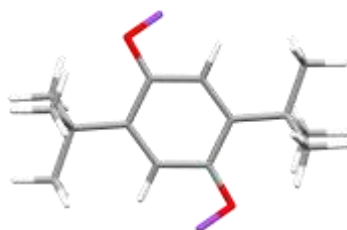
Doubly Reduced

PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.435686	-1.610847	-0.005382
C	0.700498	1.205703	0.073151
C	-0.592921	-1.211273	-0.009390
C	-0.729705	1.210610	0.087010
C	0.850813	-1.231500	-0.011223
C	-3.496944	0.516926	1.281728
C	-3.464270	0.546402	-1.242920
C	3.551692	1.604555	0.040867
C	3.570519	-0.514116	-1.275536
C	-1.388143	-0.074914	0.028280
C	1.501875	0.076177	0.024148
C	-2.923139	-0.161712	0.017433
C	3.032541	0.158948	0.007748

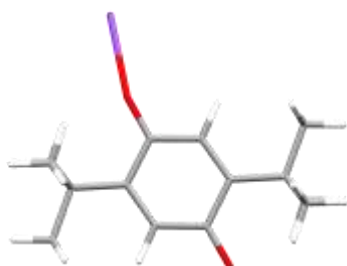
C	3.596167	-0.581424	1.242216
H	-3.154779	-0.010956	2.185422
H	-3.154239	1.557610	1.338867
H	-3.114190	1.587221	-1.271765
H	-4.600891	0.493832	1.265669
H	4.674587	-0.498209	-1.285000
H	-3.090753	-2.151714	-0.899289
H	-4.567869	0.540453	-1.253341
H	-4.538074	-1.608630	-0.013881
H	-3.103874	-2.173159	0.880294
H	-3.108022	0.034657	-2.150350
H	1.149205	2.203077	0.095771
H	3.206595	2.182666	-0.830801
H	3.228350	2.134115	0.950324
H	4.700187	-0.565168	1.231229
H	3.253744	-0.095199	2.169380
H	3.246263	-1.622116	1.237562
H	3.220385	-1.553523	-1.321149
H	-1.039626	-2.207383	-0.034650
H	3.210952	0.022020	-2.168036
H	4.653855	1.598252	0.027009
O	-1.371791	2.352367	0.154194
O	1.486464	-2.341846	-0.047636
K	-1.826692	4.623281	-0.518378



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.479669	-1.611277	-0.225304
C	0.622412	1.185973	0.232508
C	-0.622412	-1.185973	-0.232514
C	-0.809015	1.196000	0.250121
C	0.809015	-1.196000	-0.250125
C	-3.525877	0.319288	1.355259
C	-3.550947	0.705773	-1.130345
C	3.479669	1.611277	0.225295
C	3.525876	-0.319289	-1.355266
C	-1.442716	-0.072175	0.007683
C	1.442716	0.072175	-0.007689

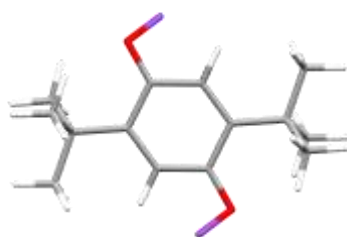
C	-2.975042	-0.178004	0.000729
C	2.975042	0.178004	-0.000736
C	3.550949	-0.705771	1.130339
H	-3.183806	-0.338029	2.170808
H	-3.168573	1.338874	1.551721
H	-3.266714	1.752069	-0.947761
H	-4.628685	0.312058	1.353810
H	4.628684	-0.312060	-1.353818
H	-3.158810	-2.017273	-1.196603
H	-4.651176	0.641467	-1.158952
H	-4.580435	-1.621688	-0.203024
H	-3.127048	-2.295951	0.562660
H	-3.168086	0.374333	-2.109864
H	1.082210	2.147092	0.492137
H	3.127047	2.295950	-0.562669
H	3.158812	2.017274	1.196594
H	4.651177	-0.641467	1.158944
H	3.168089	-0.374330	2.109857
H	3.266714	-1.752068	0.947757
H	3.168572	-1.338876	-1.551727
H	-1.082209	-2.147092	-0.492143
H	3.183805	0.338026	-2.170815
H	4.580435	1.621689	0.203013
O	-1.462657	2.337619	0.384608
O	1.462656	-2.337620	-0.384610
K	-0.555312	2.967996	-1.797207
K	0.555309	-2.967994	1.797204

B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.433910	-1.605084	-0.002008
C	0.697293	1.198312	0.065653
C	-0.592037	-1.207891	-0.008427
C	-0.725292	1.201811	0.079523
C	0.846346	-1.227616	-0.009955
C	-3.492856	0.524031	1.274059

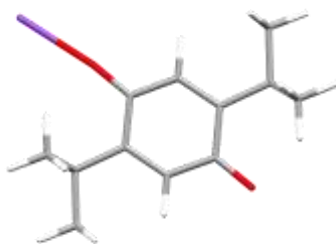
C	-3.457555	0.542283	-1.248454
C	3.546563	1.599519	0.035840
C	3.568979	-0.517063	-1.273722
C	-1.381983	-0.075210	0.026091
C	1.495680	0.073965	0.021593
C	-2.916392	-0.158023	0.014413
C	3.025812	0.154555	0.006492
C	3.592529	-0.576893	1.243099
H	-3.149308	0.006401	2.173306
H	-3.162797	1.558909	1.328630
H	-3.113622	1.574572	-1.286929
H	-4.588569	0.492843	1.259574
H	4.664918	-0.493820	-1.282315
H	-3.093033	-2.146659	-0.886382
H	-4.553141	0.533561	-1.259100
H	-4.528105	-1.600282	-0.011366
H	-3.107252	-2.159714	0.879787
H	-3.103781	0.028205	-2.145688
H	1.138706	2.187922	0.082631
H	3.205637	2.170429	-0.831399
H	3.225295	2.127462	0.936641
H	4.688421	-0.553227	1.233367
H	3.249580	-0.090573	2.160534
H	3.255414	-1.611745	1.248618
H	3.231326	-1.550370	-1.323680
H	-1.032388	-2.195802	-0.031594
H	3.210407	0.013354	-2.160211
H	4.640499	1.593239	0.023315
O	-1.363821	2.341630	0.138681
O	1.478062	-2.330049	-0.042401
K	-1.832540	4.612203	-0.428642



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.472872	-1.606179	-0.221464
C	0.620943	1.179153	0.230750
C	-0.620943	-1.179153	-0.230756
C	-0.801613	1.189334	0.238676

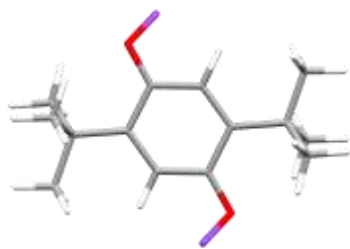
C	0.801613	-1.189334	-0.238682
C	-3.518843	0.323050	1.352299
C	-3.553329	0.703501	-1.132448
C	3.472872	1.606178	0.221459
C	3.518842	-0.323050	-1.352305
C	-1.436543	-0.068359	0.001726
C	1.436543	0.068359	-0.001733
C	-2.968382	-0.171866	-0.001789
C	2.968382	0.171866	0.001783
C	3.553329	-0.703501	1.132442
H	-3.171780	-0.326018	2.161535
H	-3.176292	1.337301	1.549126
H	-3.291544	1.746269	-0.957353
H	-4.613416	0.305022	1.353204
H	4.613415	-0.305022	-1.353211
H	-3.159647	-2.009722	-1.186558
H	-4.643960	0.620784	-1.164057
H	-4.565113	-1.618434	-0.193231
H	-3.117408	-2.283122	0.559941
H	-3.165210	0.380739	-2.103617
H	1.073466	2.132828	0.485719
H	3.117408	2.283122	-0.559947
H	3.159648	2.009721	1.186552
H	4.643960	-0.620784	1.164051
H	3.165210	-0.380741	2.103610
H	3.291544	-1.746270	0.957346
H	3.176292	-1.337301	-1.549133
H	-1.073466	-2.132828	-0.485725
H	3.171780	0.326019	-2.161541
H	4.565113	1.618434	0.193225
O	-1.449097	2.329351	0.367691
O	1.449097	-2.329351	-0.367699
K	-0.550200	3.032489	-1.787562
K	0.550200	-3.032489	1.787555

B3LYP/def2TZVP (CPCM – DME)



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
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C	-2.109561	-3.182026	0.001885
C	0.712902	0.911024	-0.002775
C	0.407811	-1.779194	0.001147
C	-0.612957	0.422395	-0.002767
C	1.746471	-1.297823	0.001156
C	-2.925507	-1.208665	1.260189
C	-2.924111	-1.212502	-1.263316
C	3.229967	2.317191	-0.003517
C	4.047490	0.335590	-1.258212
C	-0.753656	-0.996759	-0.000687
C	1.875934	0.133682	-0.000948
C	-2.149704	-1.645195	-0.000474
C	3.270180	0.781005	-0.001160
C	4.046095	0.339415	1.258102
H	-2.435024	-1.595003	2.157747
H	-2.953223	-0.122944	1.326734
H	-2.951751	-0.126989	-1.333192
H	-3.950258	-1.595680	1.243190
H	5.065857	0.739917	-1.250060
H	-1.601996	-3.576820	-0.880480
H	-3.948880	-1.599466	-1.246274
H	-3.131256	-3.572798	0.001914
H	-1.602974	-3.574135	0.886008
H	-2.432634	-1.601566	-2.159152
H	0.792292	1.992702	-0.004375
H	2.723581	2.710159	-0.888160
H	2.722601	2.712846	0.879365
H	5.064471	0.743716	1.249849
H	3.546066	0.705448	2.159546
H	4.091100	-0.747487	1.298682
H	4.092538	-0.751430	-1.295438
H	0.326174	-2.860158	0.002745
H	3.548461	0.698880	-2.161318
H	4.251424	2.708298	-0.003545
O	-1.639073	1.270209	-0.004625
O	2.757627	-2.126521	0.002976
K	-3.671057	2.575341	-0.007749

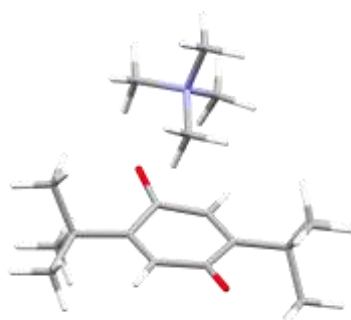


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.472010	-1.598634	-0.242963
C	0.626129	1.179204	0.207955
C	-0.626129	-1.179204	-0.207962
C	-0.793628	1.202205	0.211674
C	0.793628	-1.202205	-0.211680
C	-3.518869	0.306235	1.352827
C	-3.561693	0.719910	-1.126659
C	3.472011	1.598633	0.242957
C	3.518869	-0.306234	-1.352834
C	-1.435217	-0.056439	-0.007040
C	1.435216	0.056440	0.007034
C	-2.968781	-0.165217	-0.009756
C	2.968781	0.165217	0.009749
C	3.561693	-0.719911	1.126652
H	-3.167583	-0.351369	2.152909
H	-3.181301	1.320095	1.559958
H	-3.284684	1.759348	-0.962154
H	-4.613504	0.285099	1.356427
H	4.613503	-0.285099	-1.356434
H	-3.158449	-1.989188	-1.213568
H	-4.653637	0.644451	-1.140570
H	-4.564687	-1.608781	-0.218405
H	-3.117015	-2.285238	0.528770
H	-3.190429	0.402243	-2.105116
H	1.089108	2.140023	0.405337
H	3.117018	2.285238	-0.528776
H	3.158449	1.989188	1.213561
H	4.653637	-0.644451	1.140564
H	3.190427	-0.402246	2.105109
H	3.284685	-1.759349	0.962144
H	3.181300	-1.320094	-1.559965
H	-1.089108	-2.140023	-0.405343
H	3.167583	0.351370	-2.152915
H	4.564688	1.608780	0.218401
O	-1.435587	2.347457	0.362246
O	1.435587	-2.347457	-0.362252
K	-0.651221	3.177986	-1.956077
K	0.651220	-3.177985	1.956070

Tetramethylammonium

Singly Reduced

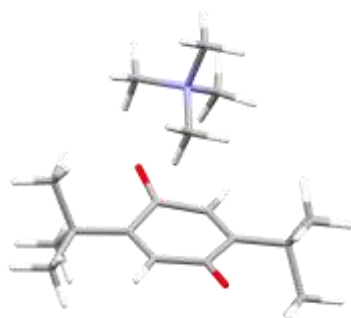
PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.448762	-0.451584	0.707190
C	0.892706	1.148675	-1.187028
C	-0.598552	-0.183682	0.704054
C	-0.528127	1.409067	-1.118548
C	0.848942	-0.280365	0.779322
C	-3.403874	1.974117	0.145195
C	-3.292858	0.252926	-1.682777
C	3.729237	0.931585	-1.588854
C	3.493702	-1.273910	-0.448655
C	-1.305522	0.585588	-0.196216
C	1.603690	0.377010	-0.294839
C	-2.840107	0.590249	-0.244614
C	3.125297	0.224498	-0.366074
C	3.755780	0.836916	0.905716
H	-3.051634	2.272020	1.146430
H	-3.097994	2.728833	-0.588777
H	-2.893840	0.984609	-2.396727
H	-4.504789	1.940807	0.173693
H	4.588314	-1.392988	-0.489187
H	-3.086476	-1.465743	0.484737
H	-4.392802	0.258780	-1.745999
H	-4.543557	-0.451734	0.595044
H	-3.221755	-0.231875	1.761398
H	-2.939887	-0.747959	-1.972286
H	1.400956	1.674442	-1.998901
H	3.320479	0.539689	-2.532112
H	3.554006	2.019334	-1.568059
H	4.850085	0.709175	0.890678
H	3.548512	1.920203	0.956001
H	3.350024	0.354051	1.803282
H	3.107464	-1.812055	0.425046

H	-1.111499	-0.784352	1.457058
H	3.067188	-1.724321	-1.357544
H	4.818119	0.773180	-1.602201
O	-1.023901	2.384936	-1.799312
O	1.394523	-0.920350	1.727588
N	0.302716	4.599614	0.619509
C	-1.115232	4.851401	0.180724
H	-1.756335	4.898787	1.068328
H	-1.144996	5.803912	-0.361975
H	-1.407599	4.021691	-0.483564
C	1.150208	4.433202	-0.615584
H	1.202337	5.403343	-1.124744
H	2.150702	4.102325	-0.315399
H	0.660966	3.687434	-1.261441
C	0.351211	3.345608	1.456150
H	1.393502	3.135662	1.719922
H	-0.248042	3.512784	2.358594
H	-0.056938	2.509491	0.878012
C	0.808041	5.748781	1.432991
H	1.842527	5.543833	1.732440
H	0.767353	6.661669	0.827740
H	0.177645	5.860813	2.322875

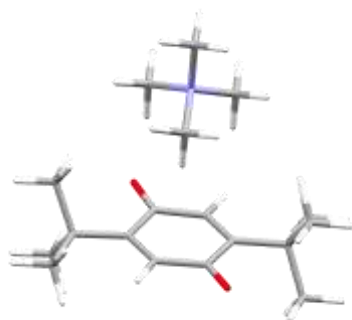
B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.456071	-0.426103	0.716872
C	0.885068	1.137816	-1.196501
C	-0.604741	-0.178726	0.693274
C	-0.532519	1.390613	-1.133405
C	0.838259	-0.271137	0.767177
C	-3.392149	1.986034	0.114872
C	-3.301700	0.233460	-1.681642
C	3.721067	0.937200	-1.587902
C	3.494908	-1.259605	-0.439703
C	-1.306869	0.578871	-0.206646
C	1.592094	0.380092	-0.302968

C	-2.840449	0.593185	-0.253471
C	3.114522	0.234334	-0.364431
C	3.738573	0.859911	0.902093
H	-3.030255	2.297450	1.099434
H	-3.092657	2.720671	-0.628000
H	-2.906145	0.942165	-2.406791
H	-4.484479	1.960249	0.155239
H	4.582222	-1.368989	-0.482735
H	-3.107308	-1.439433	0.511489
H	-4.393730	0.245009	-1.739459
H	-4.542986	-0.418281	0.610032
H	-3.224388	-0.191798	1.758036
H	-2.959400	-0.767837	-1.951368
H	1.384687	1.658836	-2.002751
H	3.322954	0.539162	-2.523138
H	3.539795	2.015301	-1.574590
H	4.826019	0.745949	0.885952
H	3.520498	1.932953	0.945222
H	3.346253	0.384742	1.798390
H	3.120809	-1.796615	0.428405
H	-1.108178	-0.770086	1.445578
H	3.073359	-1.713540	-1.339444
H	4.802740	0.787196	-1.594485
O	-1.027372	2.348563	-1.818408
O	1.380120	-0.898386	1.713268
N	0.313097	4.583817	0.627819
C	-1.108473	4.823630	0.197667
H	-1.739871	4.863220	1.082035
H	-1.150448	5.770085	-0.337631
H	-1.400531	4.004531	-0.459966
C	1.160090	4.435978	-0.608733
H	1.199638	5.401744	-1.108751
H	2.157536	4.119634	-0.314763
H	0.690421	3.697180	-1.255275
C	0.378435	3.326974	1.457548
H	1.415695	3.124514	1.709879
H	-0.208781	3.483240	2.359394
H	-0.026187	2.499715	0.886265
C	0.808237	5.732283	1.444990
H	1.837781	5.539150	1.738293
H	0.756932	6.642031	0.851289
H	0.185033	5.833167	2.330745

B3LYP/def2TZVP (CPCM – DME)

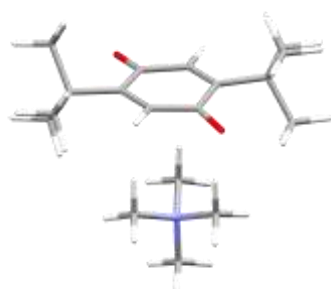


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.453653	-0.278344	0.949870
C	0.807090	1.080898	-1.322970
C	-0.608043	-0.177254	0.659103
C	-0.627428	1.231758	-1.299490
C	0.832658	-0.281887	0.670891
C	-3.363805	2.019874	0.006814
C	-3.463091	0.017402	-1.520277
C	3.646427	1.030078	-1.716971
C	3.492434	-1.201258	-0.630539
C	-1.352460	0.519798	-0.254577
C	1.553005	0.380357	-0.411828
C	-2.884257	0.567580	-0.199294
C	3.079539	0.280782	-0.501353
C	3.720243	0.886690	0.765888
H	-2.985461	2.417875	0.951777
H	-3.024528	2.658607	-0.804713
H	-3.116647	0.602722	-2.368990
H	-4.455942	2.051697	0.045069
H	4.581032	-1.283301	-0.691482
H	-3.175339	-1.329917	0.857008
H	-4.555669	0.049611	-1.493328
H	-4.544022	-0.220293	0.934255
H	-3.116914	0.079270	1.925125
H	-3.159981	-1.022168	-1.666423
H	1.280539	1.595106	-2.149374
H	3.255835	0.635481	-2.656953
H	3.427775	2.099403	-1.679412
H	4.808429	0.792649	0.716786
H	3.481595	1.949748	0.847879
H	3.363490	0.381005	1.659826
H	3.144661	-1.775786	0.224686
H	-1.084252	-0.712049	1.469776
H	3.070032	-1.637246	-1.539159
H	4.732456	0.918003	-1.735119
O	-1.189151	1.987524	-2.153837
O	1.404239	-0.932545	1.595224

N	0.394876	4.584747	0.732731
C	-0.789555	4.716228	-0.185106
H	-1.691038	4.777086	0.418049
H	-0.671039	5.623447	-0.771838
H	-0.833923	3.847861	-0.838601
C	1.641623	4.444223	-0.091463
H	1.737166	5.316297	-0.732525
H	2.496739	4.373393	0.574970
H	1.556870	3.541248	-0.688603
C	0.229887	3.366291	1.597845
H	1.097468	3.279406	2.246043
H	-0.671342	3.483141	2.192937
H	0.148657	2.490901	0.962098
C	0.500052	5.802629	1.601572
H	1.351663	5.686374	2.266550
H	0.636541	6.675570	0.969145
H	-0.414324	5.899411	2.180604

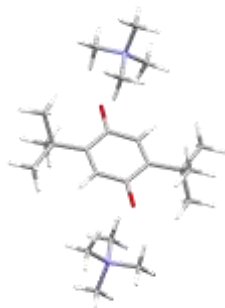
Doubly Reduced

PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.491541	0.210282	1.675216
C	0.512433	1.604613	-0.956133
C	-0.632975	0.369914	1.190955
C	-0.924788	1.512426	-0.971392
C	0.797706	0.365460	1.141196
C	-3.571211	2.301037	0.318180
C	-3.626535	0.062694	-0.816952
C	3.325462	2.168526	-1.230180
C	3.620601	-0.055271	-0.147022
C	-1.493564	0.903491	0.216511
C	1.366685	1.091383	0.030169
C	-3.021823	0.857086	0.363741
C	2.890451	1.301532	-0.038793
C	3.349316	2.001827	1.260089
H	-3.193559	2.876750	1.177880

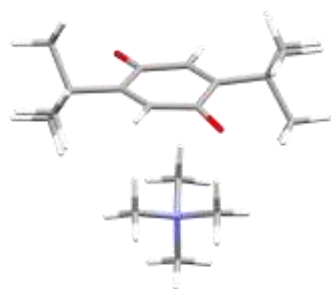
H	-3.229696	2.778341	-0.611982
H	-3.259228	0.504661	-1.755875
H	-4.676152	2.304797	0.354335
H	4.716204	0.088273	-0.172349
H	-3.175991	-0.843330	1.756216
H	-4.731155	0.094370	-0.792806
H	-4.593467	0.231679	1.723425
H	-3.100679	0.743989	2.555042
H	-3.320749	-0.997104	-0.768492
H	0.922653	2.130140	-1.822813
H	3.068349	1.700480	-2.193256
H	2.850663	3.160562	-1.202621
H	4.447568	2.126013	1.272760
H	2.887482	2.998598	1.334735
H	3.036900	1.399276	2.125165
H	3.352644	-0.670465	0.723070
H	-1.040522	-0.071843	2.108340
H	3.326894	-0.576548	-1.074279
H	4.419278	2.309976	-1.201899
O	-1.621443	1.964499	-1.964269
O	1.506638	-0.294762	2.043242
N	0.173891	-2.893433	-0.373885
C	0.220371	-4.202854	-1.097992
H	0.159284	-5.016399	-0.364020
H	-0.621963	-4.262505	-1.797704
H	1.168419	-4.260124	-1.647817
C	1.344380	-2.780067	0.579012
H	1.310788	-1.827289	1.195764
H	1.315976	-3.664658	1.231663
H	2.260955	-2.788745	-0.024689
C	-1.099047	-2.790396	0.411475
H	-1.111473	-1.782185	0.861292
H	-1.946668	-2.912524	-0.274995
H	-1.102250	-3.573780	1.179643
C	0.215072	-1.759787	-1.373595
H	1.122753	-1.872177	-1.978214
H	-0.684074	-1.819893	-1.999619
H	0.248914	-0.807915	-0.825491



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.763958	-0.470950	0.256888
C	0.945414	0.778135	-0.724958
C	-0.919951	-0.705130	0.566301
C	-0.412481	1.172114	-0.899157
C	0.438417	-1.086612	0.755729
C	-3.281398	1.965407	0.194006
C	-3.223342	0.606758	-1.921954
C	3.792921	0.487314	-0.485103
C	3.256937	-1.936165	-0.379001
C	-1.383314	0.350588	-0.231973
C	1.408038	-0.279617	0.070023
C	-2.889626	0.601640	-0.413722
C	2.912827	-0.556298	0.222051
C	3.284096	-0.548096	1.721402
H	-3.039840	1.993656	1.268673
H	-2.731725	2.762513	-0.318347
H	-2.598274	1.347000	-2.439272
H	-4.362614	2.152886	0.079385
H	4.333662	-2.154556	-0.277426
H	-3.544758	-1.475115	-0.139710
H	-4.288491	0.843956	-2.085940
H	-4.825892	-0.256002	0.057704
H	-3.625570	-0.498231	1.348535
H	-3.023148	-0.385030	-2.357846
H	1.669085	1.377995	-1.280969
H	3.623233	0.506718	-1.572302
H	3.610193	1.500844	-0.094092
H	4.347617	-0.806494	1.862471
H	3.117770	0.454537	2.147213
H	2.655571	-1.265920	2.265268
H	2.690131	-2.713296	0.145787
H	-1.645737	-1.310186	1.113936
H	2.999079	-1.964790	-1.449631
H	4.854724	0.248737	-0.313967
O	-0.704577	2.266489	-1.594455

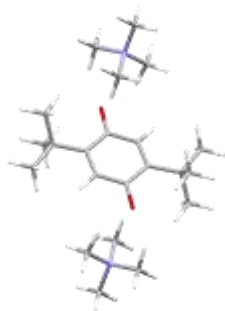
O	0.734195	-2.160872	1.482628
N	0.363826	4.669800	0.274473
N	-0.388644	-4.721302	-0.071143
C	-0.961173	4.939822	-0.390865
H	-1.695066	5.197282	0.382287
H	-0.829841	5.777347	-1.087354
H	-1.217577	3.996913	-0.923899
C	0.195146	3.547849	1.266046
H	1.163437	3.360056	1.744758
H	-0.549024	3.853782	2.011037
H	-0.131664	2.648262	0.726756
C	1.332790	4.237574	-0.797718
H	1.516702	5.097165	-1.454849
H	2.263954	3.914235	-0.317498
H	0.820978	3.403825	-1.339815
C	0.859935	5.889305	0.976755
H	1.830564	5.665794	1.435995
H	0.970751	6.701735	0.249220
H	0.137308	6.177321	1.750397
C	-0.906185	-5.996328	-0.647874
H	-0.971083	-6.748693	0.146723
H	-1.901116	-5.816986	-1.073150
H	-0.220456	-6.340113	-1.432272
C	0.972332	-4.928049	0.542682
H	1.251847	-3.940725	0.971838
H	0.884783	-5.700116	1.317277
H	1.664489	-5.252866	-0.243603
C	-1.307156	-4.210132	1.010998
H	-0.784021	-3.318744	1.440466
H	-2.270787	-3.950481	0.556322
H	-1.434962	-5.008465	1.753213
C	-0.282488	-3.678257	-1.153677
H	0.428257	-4.034050	-1.909151
H	-1.275304	-3.537445	-1.597081
H	0.060212	-2.739222	-0.698569

B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.491538	0.222279	1.665936
C	0.509825	1.617689	-0.941486
C	-0.638055	0.400570	1.196336
C	-0.918051	1.522163	-0.962656
C	0.780595	0.384402	1.144846
C	-3.590741	2.295923	0.294400
C	-3.611357	0.045024	-0.817564
C	3.323451	2.166327	-1.209855
C	3.596488	-0.066177	-0.151480
C	-1.490899	0.922234	0.216524
C	1.355116	1.101937	0.044856
C	-3.019097	0.862714	0.352028
C	2.880511	1.295095	-0.024584
C	3.356998	1.981590	1.273400
H	-3.225765	2.878403	1.144730
H	-3.264601	2.774801	-0.628495
H	-3.264551	0.471342	-1.759154
H	-4.687505	2.281729	0.332853
H	4.683851	0.068348	-0.204892
H	-3.167563	-0.818692	1.757358
H	-4.708127	0.054144	-0.788250
H	-4.585635	0.231409	1.706278
H	-3.116282	0.764088	2.536639
H	-3.287174	-1.000034	-0.755614
H	0.918141	2.137348	-1.799730
H	3.065078	1.710457	-2.168566
H	2.861196	3.154481	-1.175279
H	4.448371	2.095874	1.275224
H	2.909358	2.975288	1.356281
H	3.053293	1.386918	2.134580
H	3.352580	-0.680411	0.713146
H	-1.044190	-0.044483	2.100045
H	3.278154	-0.579399	-1.065393
H	4.410200	2.297913	-1.181524
O	-1.607894	1.960566	-1.960364
O	1.479683	-0.298743	2.033615

N	0.182614	-2.886438	-0.374973
C	0.201195	-4.192725	-1.092122
H	0.142069	-5.000696	-0.365059
H	-0.646663	-4.244693	-1.772721
H	1.129429	-4.270222	-1.654787
C	1.376114	-2.782066	0.547754
H	1.345201	-1.844323	1.163210
H	1.365721	-3.661840	1.192196
H	2.271493	-2.784184	-0.070652
C	-1.069712	-2.774068	0.439253
H	-1.076884	-1.779421	0.887079
H	-1.928376	-2.893823	-0.218333
H	-1.059012	-3.549552	1.203130
C	0.213975	-1.760715	-1.381505
H	1.096485	-1.889335	-2.004268
H	-0.692910	-1.806195	-1.980303
H	0.273575	-0.814202	-0.852103

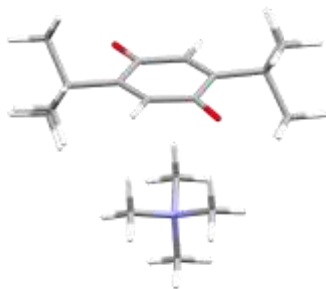


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.775314	-0.412610	0.431561
C	0.930327	0.736789	-0.644058
C	-0.930268	-0.736728	0.643809
C	-0.418651	1.134912	-0.806681
C	0.418711	-1.134841	0.806444
C	-3.216903	2.002589	0.346129
C	-3.274038	0.637085	-1.764974
C	3.775373	0.412617	-0.431877
C	3.216923	-2.002571	-0.346368
C	-1.386102	0.332045	-0.130766
C	1.386160	-0.331986	0.130514
C	-2.888011	0.627690	-0.270799
C	2.888067	-0.627649	0.270528
C	3.274121	-0.637011	1.764697
H	-2.956056	2.016157	1.408146
H	-2.653591	2.776214	-0.167211
H	-2.658791	1.353047	-2.306912
H	-4.284756	2.227786	0.255024

H	4.284777	-2.227774	-0.255296
H	-3.606824	-1.416301	0.033546
H	-4.331087	0.896293	-1.890131
H	-4.827810	-0.163723	0.270961
H	-3.600245	-0.442186	1.509016
H	-3.115696	-0.353924	-2.199532
H	1.645767	1.335490	-1.191950
H	3.600281	0.442167	-1.509329
H	3.606909	1.416322	-0.033886
H	4.331167	-0.896234	1.889842
H	3.115804	0.354012	2.199232
H	2.658871	-1.352949	2.306664
H	2.653623	-2.776174	0.167018
H	-1.645710	-1.335433	1.191694
H	2.956036	-2.016170	-1.408376
H	4.827868	0.163716	-0.271292
O	-0.708315	2.225029	-1.497548
O	0.708378	-2.224944	1.497336
N	0.322963	4.744485	0.169362
N	-0.323025	-4.744530	-0.169259
C	-0.961794	5.003712	-0.573124
H	-1.713983	5.332802	0.141115
H	-0.776821	5.782671	-1.310777
H	-1.231746	4.051387	-1.047689
C	0.083638	3.687367	1.215378
H	1.017208	3.509182	1.744154
H	-0.678049	4.050512	1.902137
H	-0.242782	2.777939	0.719440
C	1.338801	4.236781	-0.822198
H	1.567567	5.044856	-1.515336
H	2.232849	3.937199	-0.279908
H	0.860190	3.385412	-1.331010
C	0.808896	5.992149	0.822475
H	1.744835	5.782888	1.336591
H	0.968991	6.754384	0.063097
H	0.063744	6.335490	1.537654
C	-0.809038	-5.992228	-0.822246
H	-0.969080	-6.754410	-0.062803
H	-1.745018	-5.782985	-1.336293
H	-0.063955	-6.335631	-1.537468
C	0.961795	-5.003727	0.573125
H	1.231817	-4.051373	1.047587
H	0.776877	-5.782623	1.310858
H	1.713909	-5.332889	-0.141160
C	-1.338766	-4.236744	0.822361
H	-0.860097	-3.385336	1.331059
H	-2.232864	-3.937198	0.280133
H	-1.567471	-5.044767	1.515580

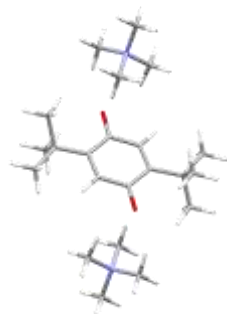
C	-0.083774	-3.687482	-1.215364
H	0.677834	-4.050693	-1.902176
H	-1.017391	-3.509301	-1.744058
H	0.242722	-2.778037	-0.719509

B3LYP/def2TZVP (CPCM – DME)



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.476782	0.217062	1.680515
C	0.513311	1.690790	-0.895917
C	-0.636649	0.480231	1.229968
C	-0.908566	1.617804	-0.908850
C	0.782855	0.506397	1.213492
C	-3.627076	2.313489	0.359897
C	-3.592739	0.080325	-0.798625
C	3.336201	2.115132	-1.266735
C	3.559539	-0.054023	-0.080951
C	-1.489967	0.993674	0.245439
C	1.364038	1.181766	0.091071
C	-3.018267	0.895201	0.379753
C	2.891185	1.334842	-0.019749
C	3.419260	2.093344	1.215930
H	-3.282608	2.885007	1.226472
H	-3.320588	2.832258	-0.546825
H	-3.270102	0.521276	-1.740147
H	-4.721089	2.268478	0.398744
H	4.649879	0.041857	-0.124610
H	-3.124665	-0.814288	1.755065
H	-4.687524	0.061563	-0.762642
H	-4.569695	0.193937	1.713112
H	-3.128415	0.755067	2.564743
H	-3.240302	-0.953618	-0.755568
H	0.935381	2.189061	-1.760932
H	3.035515	1.614743	-2.189889
H	2.924652	3.126454	-1.282269
H	4.511817	2.169545	1.188403
H	3.011333	3.107628	1.241087
H	3.119142	1.572342	2.123383

H	3.285421	-0.632870	0.798178
H	-1.058857	0.003530	2.108013
H	3.235291	-0.594018	-0.975016
H	4.426699	2.198350	-1.273531
O	-1.596139	2.102896	-1.911345
O	1.474552	-0.088106	2.165338
N	0.173006	-2.967355	-0.416306
C	0.273058	-4.279113	-1.129881
H	0.215373	-5.083229	-0.400765
H	-0.547473	-4.359517	-1.838276
H	1.223469	-4.320368	-1.655545
C	1.308058	-2.832326	0.563813
H	1.227983	-1.887675	1.110564
H	1.261852	-3.676114	1.248927
H	2.240834	-2.858300	0.006871
C	-1.127322	-2.894441	0.326153
H	-1.189964	-1.914500	0.791853
H	-1.941469	-3.028437	-0.381275
H	-1.147345	-3.682440	1.074658
C	0.231430	-1.843168	-1.414604
H	1.173852	-1.910896	-1.951497
H	-0.601441	-1.953456	-2.104415
H	0.168234	-0.897172	-0.885292



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.767904	-0.345795	0.563374
C	0.922859	0.714452	-0.677784
C	-0.922859	-0.714449	0.677691
C	-0.428091	1.111901	-0.843291
C	0.428091	-1.111899	0.843198
C	-3.197231	2.051739	0.276707
C	-3.323366	0.526964	-1.718005
C	3.767904	0.345796	-0.563468
C	3.197229	-2.051738	-0.276800
C	-1.388307	0.335177	-0.121312
C	1.388307	-0.335174	0.121219
C	-2.893402	0.630950	-0.239480

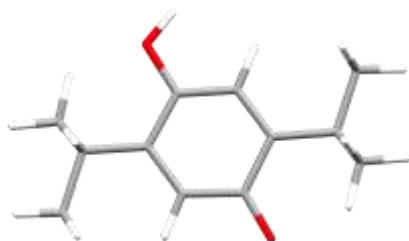
C	2.893402	-0.630948	0.239386
C	3.323366	-0.526962	1.717911
H	-2.924157	2.142735	1.331506
H	-2.630296	2.781766	-0.293626
H	-2.727520	1.203524	-2.327788
H	-4.264213	2.279305	0.182959
H	4.264212	-2.279304	-0.183053
H	-3.629717	-1.378481	0.235740
H	-4.383080	0.778650	-1.832584
H	-4.821547	-0.090137	0.422586
H	-3.555794	-0.299839	1.633737
H	-3.178711	-0.493577	-2.083673
H	1.634710	1.306936	-1.238117
H	3.555793	0.299840	-1.633831
H	3.629717	1.378482	-0.235835
H	4.383080	-0.778647	1.832489
H	3.178712	0.493579	2.083579
H	2.727521	-1.203521	2.327695
H	2.630295	-2.781764	0.293534
H	-1.634711	-1.306933	1.238024
H	2.924155	-2.142734	-1.331598
H	4.821547	0.090137	-0.422681
O	-0.722795	2.161440	-1.589167
O	0.722794	-2.161437	1.589075
N	0.320907	4.845724	0.213356
N	-0.320908	-4.845725	-0.213439
C	-0.910782	5.119317	-0.605262
H	-1.698744	5.465645	0.058910
H	-0.673570	5.889321	-1.335551
H	-1.178444	4.180078	-1.091689
C	0.005349	3.794454	1.240799
H	0.900716	3.606748	1.827933
H	-0.791228	4.164005	1.881456
H	-0.303752	2.892816	0.720971
C	1.393751	4.324928	-0.703084
H	1.656053	5.111838	-1.406436
H	2.259731	4.053795	-0.104560
H	0.973780	3.458894	-1.218137
C	0.779307	6.096567	0.892323
H	1.674769	5.877376	1.468406
H	0.998288	6.848111	0.138173
H	-0.009844	6.450516	1.551068
C	-0.779308	-6.096569	-0.892403
H	-0.998289	-6.848112	-0.138252
H	-1.674771	-5.877379	-1.468486
H	0.009843	-6.450519	-1.551148
C	0.910782	-5.119317	0.605179
H	1.178444	-4.180076	1.091603

H	0.673570	-5.889319	1.335470
H	1.698743	-5.465646	-0.058993
C	-1.393751	-4.324927	0.703001
H	-0.973780	-3.458892	1.218051
H	-2.259732	-4.053795	0.104476
H	-1.656053	-5.111835	1.406355
C	-0.005351	-3.794458	-1.240884
H	0.791226	-4.164010	-1.881541
H	-0.900717	-3.606752	-1.828018
H	0.303752	-2.892818	-0.721059

Hydrogen

Singly Reduced

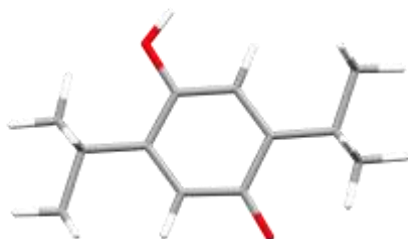
PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.447480	-1.765114	-0.000164
C	0.654166	1.128520	0.000152
C	-0.628683	-1.316083	-0.000123
C	-0.755648	1.045286	0.000144
C	0.824396	-1.291287	-0.000127
C	-3.548568	0.375301	1.267190
C	-3.548576	0.375588	-1.267034
C	3.478177	1.598979	0.000209
C	3.567339	-0.553788	-1.264146
C	-1.445346	-0.205434	0.000006
C	1.482686	0.025217	0.000022
C	-2.977909	-0.301085	0.000000
C	3.003549	0.137390	0.000032
C	3.567345	-0.554097	1.264038
H	-3.158406	-0.110255	2.173901
H	-3.300744	1.442231	1.312111
H	-3.300752	1.442528	-1.311714
H	-4.644887	0.278605	1.275778
H	4.665138	-0.472350	-1.269446
H	-3.102393	-2.308205	-0.892129

H	-4.644895	0.278894	-1.275636
H	-4.546736	-1.789321	-0.000161
H	-3.102382	-2.308408	0.891672
H	-3.158420	-0.109763	-2.173857
H	1.086212	2.134221	0.000270
H	3.138509	2.144264	-0.893972
H	3.138516	2.144046	0.894526
H	4.665144	-0.472662	1.269352
H	3.185784	-0.070820	2.176153
H	3.291006	-1.614398	1.284416
H	3.291001	-1.614084	-1.284780
H	-1.048982	-2.321075	-0.000237
H	3.185772	-0.070289	-2.176141
H	4.577356	1.621609	0.000208
O	-1.483629	2.198108	0.000281
O	1.462610	-2.377286	-0.000254
H	-0.864827	2.951924	0.000310

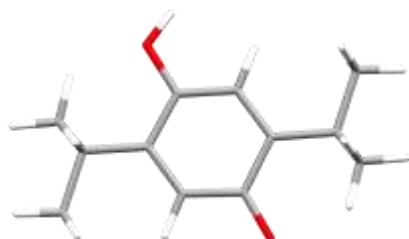
B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.446282	-1.762175	-0.000169
C	0.651494	1.122800	0.000152
C	-0.628251	-1.312649	-0.000125
C	-0.752884	1.038071	0.000147
C	0.819914	-1.283358	-0.000127
C	-3.540774	0.375837	1.265631
C	-3.540780	0.376129	-1.265477
C	3.475598	1.594644	0.000197
C	3.563152	-0.553260	-1.263269
C	-1.439220	-0.207871	0.000005
C	1.476915	0.026258	0.000022
C	-2.971756	-0.300612	-0.000002
C	2.998622	0.134379	0.000030
C	3.563159	-0.553551	1.263168
H	-3.153611	-0.107310	2.165188
H	-3.292021	1.433509	1.309632

H	-3.292025	1.433810	-1.309235
H	-4.629076	0.282557	1.275189
H	4.652261	-0.466959	-1.271495
H	-3.105403	-2.301719	-0.885503
H	-4.629082	0.282853	-1.275050
H	-4.537240	-1.783658	-0.000168
H	-3.105397	-2.301923	0.885039
H	-3.153622	-0.106812	-2.165147
H	1.074074	2.120868	0.000266
H	3.138316	2.135522	-0.887061
H	3.138322	2.135318	0.887581
H	4.652268	-0.467251	1.271409
H	3.180129	-0.074593	2.167307
H	3.296622	-1.607021	1.286878
H	3.296613	-1.606725	-1.287221
H	-1.039164	-2.310785	-0.000240
H	3.180118	-0.074093	-2.167296
H	4.566379	1.616372	0.000195
O	-1.479309	2.184963	0.000282
O	1.453513	-2.360637	-0.000252
H	-0.886129	2.945978	0.000368

B3LYP/def2TZVP (CPCM – DME)

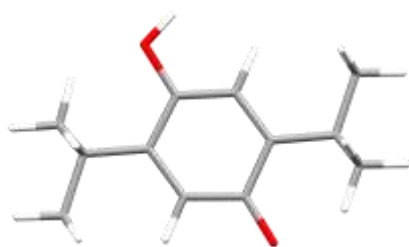


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.448295	-1.761537	-0.000166
C	0.655386	1.119820	0.000151
C	-0.630671	-1.313293	-0.000124
C	-0.751135	1.039745	0.000146
C	0.816492	-1.286020	-0.000125
C	-3.540484	0.376214	1.266022
C	-3.540490	0.376502	-1.265868
C	3.472880	1.593921	0.000202
C	3.566765	-0.551090	-1.263872
C	-1.439611	-0.208090	0.000005
C	1.476429	0.020916	0.000023
C	-2.971867	-0.300451	-0.000002
C	2.999057	0.132380	0.000031

C	3.566775	-0.551389	1.263768
H	-3.154846	-0.109012	2.165211
H	-3.289598	1.433362	1.311046
H	-3.289604	1.433660	-1.310654
H	-4.628756	0.283806	1.273043
H	4.655550	-0.461993	-1.270433
H	-3.108195	-2.301072	-0.885906
H	-4.628762	0.284095	-1.272906
H	-4.539193	-1.780011	-0.000165
H	-3.108190	-2.301273	0.885449
H	-3.154857	-0.108521	-2.165169
H	1.077740	2.116455	0.000264
H	3.132775	2.133553	-0.886153
H	3.132782	2.133343	0.886686
H	4.655560	-0.462291	1.270342
H	3.183205	-0.070414	2.166451
H	3.303318	-1.605762	1.292001
H	3.303306	-1.605456	-1.292354
H	-1.048231	-2.308902	-0.000237
H	3.183190	-0.069901	-2.166439
H	4.563740	1.616124	0.000200
O	-1.474214	2.179590	0.000276
O	1.448065	-2.370355	-0.000253
H	-0.890573	2.950250	0.000358

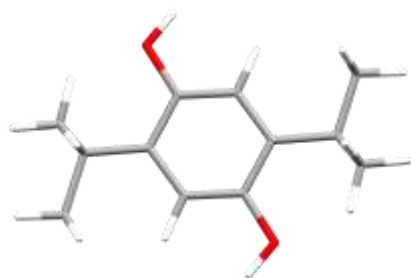
Doubly Reduced

PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.446962	-1.672377	-0.000041
C	0.608016	1.223780	-0.000067
C	-0.605615	-1.225237	0.000070
C	-0.787095	1.154152	-0.000121
C	0.835295	-1.220222	0.000131
C	-3.547719	0.466113	1.262939
C	-3.547613	0.465960	-1.263287
C	3.457270	1.687004	0.000026
C	3.536784	-0.467066	-1.258132

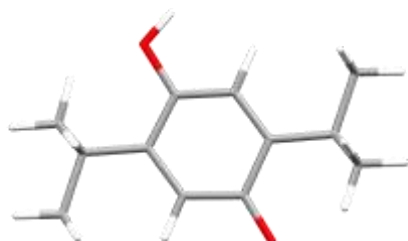
C	-1.433798	-0.097400	-0.000052
C	1.443731	0.103483	0.000054
C	-2.969205	-0.210781	-0.000109
C	2.970707	0.229908	0.000108
C	3.536682	-0.466891	1.258491
H	-3.165464	-0.032718	2.166699
H	-3.264106	1.524954	1.309881
H	-3.263995	1.524795	-1.310333
H	-4.649582	0.394957	1.269465
H	4.641508	-0.451707	-1.249673
H	-3.093140	-2.214455	-0.889149
H	-4.649476	0.394805	-1.269897
H	-4.549238	-1.696511	-0.000086
H	-3.093215	-2.214348	0.889163
H	-3.165283	-0.032980	-2.166956
H	1.051240	2.228689	-0.000124
H	3.112283	2.233584	-0.892551
H	3.112209	2.233709	0.892499
H	4.641406	-0.451533	1.250120
H	3.190223	0.048234	2.168851
H	3.182324	-1.507102	1.278937
H	3.182428	-1.507280	-1.278462
H	-1.041353	-2.225799	0.000130
H	3.190399	0.047931	-2.168591
H	4.559634	1.706751	0.000070
O	-1.541599	2.351391	-0.000246
O	1.506028	-2.314542	0.000244
H	-0.883923	3.067121	-0.000300



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.445246	-1.669035	-0.000030
C	0.618211	1.214046	-0.000058
C	-0.618211	-1.214047	0.000058
C	-0.777943	1.152550	-0.000113
C	0.777943	-1.152550	0.000113
C	-3.555653	0.470163	1.265768

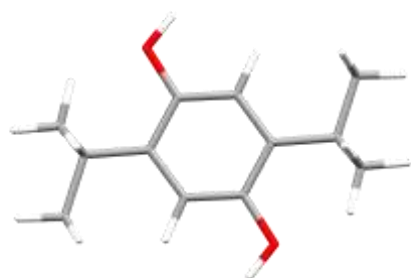
C	-3.555547	0.469990	-1.266129
C	3.445245	1.669035	0.000025
C	3.555651	-0.470166	-1.265769
C	-1.448374	-0.086569	-0.000054
C	1.448374	0.086568	0.000055
C	-2.979539	-0.203412	-0.000110
C	2.979539	0.203412	0.000109
C	3.555549	-0.469988	1.266128
H	-3.172032	-0.020897	2.172550
H	-3.294429	1.533713	1.312903
H	-3.294318	1.533535	-1.313387
H	-4.653314	0.383112	1.269305
H	4.653312	-0.383115	-1.269307
H	-3.101174	-2.211525	-0.893603
H	-4.653208	0.382939	-1.269745
H	-4.544575	-1.697734	-0.000077
H	-3.101254	-2.211403	0.893647
H	-3.171850	-0.021193	-2.172812
H	1.075190	2.206559	-0.000109
H	3.101250	2.211401	-0.893652
H	3.101177	2.211527	0.893598
H	4.653210	-0.382936	1.269743
H	3.171854	0.021197	2.172811
H	3.294322	-1.533532	1.313389
H	3.294427	-1.533716	-1.312901
H	-1.075190	-2.206559	0.000107
H	3.172028	0.020892	-2.172551
H	4.544575	1.697734	0.000068
O	-1.517120	2.321728	-0.000226
O	1.517120	-2.321729	0.000222
H	-0.892260	3.067297	-0.000261
H	0.892260	-3.067298	0.000247

B3LYP/def2TZVP



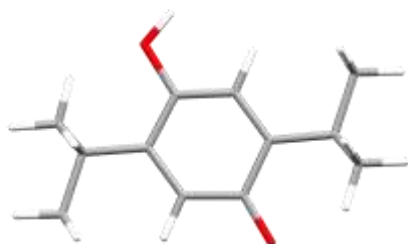
<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.446962	-1.672377	-0.000041

C	0.608016	1.223780	-0.000067
C	-0.605615	-1.225237	0.000070
C	-0.787095	1.154152	-0.000121
C	0.835295	-1.220222	0.000131
C	-3.547719	0.466113	1.262939
C	-3.547613	0.465960	-1.263287
C	3.457270	1.687004	0.000026
C	3.536784	-0.467066	-1.258132
C	-1.433798	-0.097400	-0.000052
C	1.443731	0.103483	0.000054
C	-2.969205	-0.210781	-0.000109
C	2.970707	0.229908	0.000108
C	3.536682	-0.466891	1.258491
H	-3.165464	-0.032718	2.166699
H	-3.264106	1.524954	1.309881
H	-3.263995	1.524795	-1.310333
H	-4.649582	0.394957	1.269465
H	4.641508	-0.451707	-1.249673
H	-3.093140	-2.214455	-0.889149
H	-4.649476	0.394805	-1.269897
H	-4.549238	-1.696511	-0.000086
H	-3.093215	-2.214348	0.889163
H	-3.165283	-0.032980	-2.166956
H	1.051240	2.228689	-0.000124
H	3.112283	2.233584	-0.892551
H	3.112209	2.233709	0.892499
H	4.641406	-0.451533	1.250120
H	3.190223	0.048234	2.168851
H	3.182324	-1.507102	1.278937
H	3.182428	-1.507280	-1.278462
H	-1.041353	-2.225799	0.000130
H	3.190399	0.047931	-2.168591
H	4.559634	1.706751	0.000070
O	-1.541599	2.351391	-0.000246
O	1.506028	-2.314542	0.000244
H	-0.883923	3.067121	-0.000300



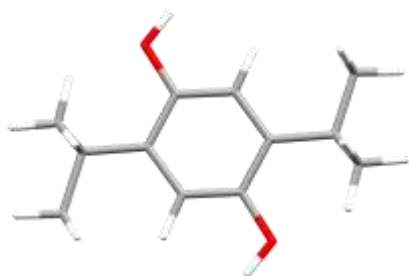
<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.441466	-1.665142	-0.000025
C	0.614473	1.209423	-0.000055
C	-0.614472	-1.209424	0.000053
C	-0.774557	1.145110	-0.000109
C	0.774557	-1.145111	0.000107
C	-3.548084	0.471489	1.264282
C	-3.547982	0.471305	-1.264651
C	3.441464	1.665142	0.000025
C	3.548086	-0.471486	-1.264286
C	-1.441388	-0.086988	-0.000057
C	1.441388	0.086987	0.000054
C	-2.972489	-0.201380	-0.000112
C	2.972489	0.201380	0.000109
C	3.547982	-0.471307	1.264647
H	-3.164739	-0.014670	2.164091
H	-3.291382	1.527037	1.309621
H	-3.291278	1.526847	-1.310122
H	-4.637321	0.382694	1.269835
H	4.637322	-0.382689	-1.269839
H	-3.100400	-2.203683	-0.886681
H	-4.637218	0.382509	-1.270279
H	-4.532442	-1.692423	-0.000070
H	-3.100475	-2.203554	0.886738
H	-3.164564	-0.014985	-2.164357
H	1.060951	2.195362	-0.000101
H	3.100472	2.203556	-0.886736
H	3.100398	2.203681	0.886682
H	4.637218	-0.382509	1.270276
H	3.164563	0.014981	2.164354
H	3.291279	-1.526849	1.310117
H	3.291386	-1.527035	-1.309627
H	-1.060951	-2.195364	0.000099
H	3.164739	0.014674	-2.164094
H	4.532440	1.692424	0.000069
O	-1.511777	2.309966	-0.000214
O	1.511777	-2.309967	0.000213
H	-0.910329	3.061890	-0.000239
H	0.910329	-3.061891	0.000237

B3LYP/def2TZVP (CPCM – DME)



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-3.450398	-1.665586	-0.000038
C	0.612190	1.204066	-0.000054
C	-0.610315	-1.219864	0.000050
C	-0.778000	1.145846	-0.000107
C	0.818366	-1.219340	0.000110
C	-3.546486	0.468396	1.262395
C	-3.546383	0.468235	-1.262751
C	3.445086	1.677847	0.000013
C	3.547148	-0.461455	-1.259858
C	-1.433363	-0.093087	-0.000056
C	1.440132	0.082791	0.000051
C	-2.968157	-0.205818	-0.000111
C	2.968437	0.216869	0.000106
C	3.547038	-0.461256	1.260229
H	-3.172178	-0.027139	2.161586
H	-3.273474	1.520191	1.313089
H	-3.273362	1.520022	-1.313560
H	-4.637914	0.393615	1.265624
H	4.641143	-0.420891	-1.250446
H	-3.108181	-2.206684	-0.883949
H	-4.637811	0.393458	-1.266057
H	-4.542856	-1.684009	-0.000080
H	-3.108252	-2.206572	0.883970
H	-3.172006	-0.027419	-2.161847
H	1.054402	2.194836	-0.000098
H	3.102491	2.219237	-0.885047
H	3.102418	2.219375	0.884959
H	4.641034	-0.420707	1.250900
H	3.198476	0.051236	2.161157
H	3.228847	-1.500810	1.304541
H	3.228973	-1.501020	-1.304027
H	-1.054036	-2.206182	0.000095
H	3.198654	0.050887	-2.160899
H	4.537695	1.703123	0.000056
O	-1.518296	2.335349	-0.000210
O	1.475174	-2.330258	0.000213

H -0.896448 3.071092 -0.000246



Element	X	Y	Z
C	-3.441532	-1.665331	-0.000026
C	0.616625	1.210305	-0.000058
C	-0.616625	-1.210305	0.000056
C	-0.773431	1.147827	-0.000110
C	0.773431	-1.147827	0.000108
C	-3.549897	0.470552	1.264267
C	-3.549789	0.470373	-1.264631
C	3.441532	1.665331	0.000025
C	3.549897	-0.470551	-1.264269
C	-1.441268	-0.085194	-0.000054
C	1.441268	0.085194	0.000052
C	-2.972865	-0.201302	-0.000110
C	2.972865	0.201302	0.000108
C	3.549790	-0.470374	1.264628
H	-3.169644	-0.019135	2.163666
H	-3.291169	1.525728	1.312520
H	-3.291050	1.525541	-1.313015
H	-4.639187	0.383122	1.267165
H	4.639187	-0.383122	-1.267168
H	-3.099220	-2.203848	-0.885948
H	-4.639080	0.382951	-1.267606
H	-4.532617	-1.691343	-0.000072
H	-3.099296	-2.203722	0.886002
H	-3.169466	-0.019446	-2.163929
H	1.062683	2.195734	-0.000107
H	3.099296	2.203723	-0.886003
H	3.099220	2.203847	0.885947
H	4.639080	-0.382951	1.267603
H	3.169466	0.019445	2.163926
H	3.291051	-1.525542	1.313012
H	3.291169	-1.525728	-1.312523
H	-1.062683	-2.195734	0.000105
H	3.169644	0.019136	-2.163669
H	4.532617	1.691343	0.000070

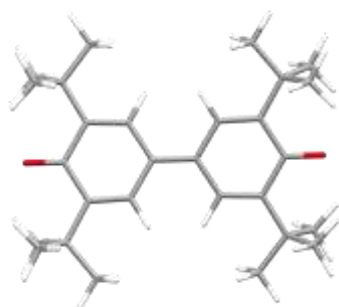
O	-1.507586	2.313862	-0.000219
O	1.507586	-2.313862	0.000216
H	-0.906950	3.068193	-0.000242
H	0.906950	-3.068193	0.000239

DPQ

Cation-Free

Oxidised

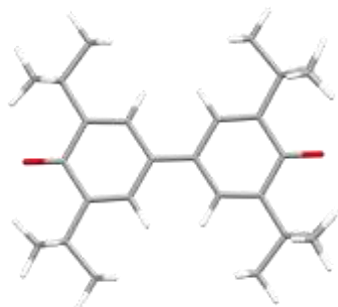
PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	1.418158	-4.082099	2.264601
C	1.901102	-2.852272	3.051613
C	1.252431	-2.906793	4.455521
C	3.440039	-2.948550	3.179547
C	1.519396	-1.543204	2.356382
C	0.831566	-1.527393	1.178719
C	0.467919	-0.321799	0.482404
C	-0.241169	-0.359255	-0.743409
C	-0.743391	-1.594169	-1.284991
C	-1.437029	-1.680458	-2.456175
C	-1.968857	-3.015184	-2.983782
C	-1.622016	-4.182698	-2.044787
C	-3.509714	-2.952679	-3.109548
C	-1.340546	-3.318786	-4.364997
C	-1.683299	-0.435429	-3.236408
O	-2.305224	-0.468277	-4.311503
C	-1.163220	0.850077	-2.691886
C	-1.390258	2.144718	-3.476146
C	-0.780760	3.362741	-2.761982
C	-0.728844	2.035745	-4.870642
C	-2.908243	2.401346	-3.632889
C	-0.492442	0.835858	-1.504407
C	0.857768	0.923596	1.088670
C	1.534337	1.011478	2.269679

C	1.911496	2.360631	2.886315
C	1.438148	3.539944	2.020140
C	3.449816	2.462140	3.020375
C	1.251976	2.503368	4.278660
C	1.910027	-0.245623	2.975416
O	2.531930	-0.212772	4.050523
H	1.866241	-4.134738	1.260422
H	0.322391	-4.104659	2.160725
H	1.715457	-4.992089	2.804913
H	1.606880	-2.087374	5.090033
H	0.156108	-2.847814	4.380139
H	1.507491	-3.861948	4.939328
H	3.841203	-2.129675	3.786373
H	3.708688	-3.903454	3.656407
H	3.915389	-2.920206	2.187421
H	0.563737	-2.478033	0.726090
H	-0.581215	-2.504350	-0.714386
H	-0.535062	-4.315391	-1.931082
H	-2.065977	-4.057654	-1.045194
H	-2.023869	-5.114100	-2.468353
H	-3.820338	-2.176742	-3.817475
H	-3.887717	-3.923590	-3.464309
H	-3.971717	-2.746258	-2.132296
H	-1.604892	-2.551068	-5.100128
H	-1.705123	-4.292352	-4.726519
H	-0.244051	-3.374768	-4.289826
H	-1.228042	3.529240	-1.769902
H	0.309944	3.271838	-2.643553
H	-0.971833	4.262821	-3.363439
H	-1.166602	1.220282	-5.456400
H	0.353662	1.862087	-4.775245
H	-0.873269	2.979060	-5.419011
H	-3.065291	3.347359	-4.173113
H	-3.391628	2.489724	-2.648200
H	-3.392872	1.594071	-4.192468
H	-0.103147	1.775167	-1.121695
H	0.574139	1.845106	0.587975
H	1.733783	4.481254	2.504846
H	1.894260	3.528712	1.018221
H	0.343333	3.558426	1.906290
H	3.844308	1.682285	3.680594
H	3.716383	3.444850	3.438310
H	3.933047	2.370769	2.035884
H	1.505755	3.485866	4.704927
H	0.156140	2.442256	4.198130
H	1.599161	1.724021	4.965542

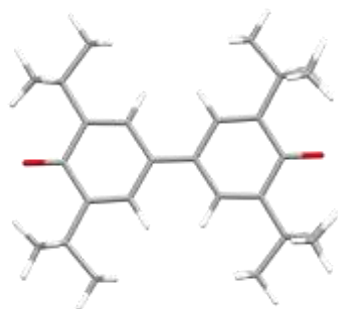
B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	1.274005	-4.076577	2.344637
C	1.798477	-2.845625	3.101632
C	1.143388	-2.843486	4.501220
C	3.330269	-2.997594	3.237003
C	1.467013	-1.541756	2.369861
C	0.791311	-1.525081	1.199593
C	0.463631	-0.322026	0.474967
C	-0.236890	-0.359027	-0.735967
C	-0.703315	-1.599056	-1.305680
C	-1.384938	-1.686638	-2.469338
C	-1.866542	-3.026504	-3.033473
C	-1.478825	-4.203579	-2.123788
C	-3.406629	-3.020597	-3.159583
C	-1.225414	-3.274484	-4.417472
C	-1.675761	-0.435026	-3.223229
O	-2.290160	-0.467478	-4.285295
C	-1.200893	0.857029	-2.653530
C	-1.484801	2.156461	-3.412676
C	-0.921337	3.383776	-2.678127
C	-0.825599	2.104028	-4.809282
C	-3.010126	2.357738	-3.557119
C	-0.530561	0.840855	-1.480170
C	0.896047	0.921175	1.064257
C	1.572300	1.009259	2.231006
C	2.006349	2.353561	2.822516
C	1.579639	3.534274	1.935278
C	3.545636	2.398125	2.951370
C	1.355442	2.552057	4.209861
C	1.902502	-0.246027	2.962229
O	2.516903	-0.213575	4.024294
H	1.719983	-4.169159	1.351824
H	0.187039	-4.060874	2.237800
H	1.533577	-4.976554	2.903775
H	1.521090	-2.031729	5.116539

H	0.058515	-2.744939	4.418056
H	1.356795	-3.788805	5.005321
H	3.760526	-2.189663	3.822129
H	3.560789	-3.944167	3.731106
H	3.804216	-3.008642	2.252712
H	0.484459	-2.464033	0.774950
H	-0.501272	-2.505637	-0.764015
H	-0.396286	-4.297223	-2.012008
H	-1.925288	-4.119536	-1.130433
H	-1.842221	-5.131735	-2.567005
H	-3.747207	-2.249441	-3.844835
H	-3.745947	-3.989766	-3.532213
H	-3.871750	-2.854116	-2.185147
H	-1.513557	-2.509284	-5.132783
H	-1.547660	-4.245604	-4.800055
H	-0.135782	-3.289222	-4.339621
H	-1.367022	3.511058	-1.689027
H	0.164132	3.333486	-2.566885
H	-1.148571	4.280736	-3.255881
H	-1.228904	1.293581	-5.409922
H	0.254969	1.970053	-4.719841
H	-1.004780	3.045811	-5.332941
H	-3.206498	3.301467	-4.071028
H	-3.486654	2.404859	-2.575142
H	-3.465785	1.553252	-4.127561
H	-0.186116	1.776301	-1.077167
H	0.656413	1.831263	0.544231
H	1.910694	4.465447	2.397112
H	2.029751	3.484934	0.941235
H	0.494655	3.593103	1.823493
H	3.911738	1.625652	3.621804
H	3.850844	3.370835	3.343761
H	4.017403	2.267197	1.974707
H	1.643422	3.526015	4.612045
H	0.266047	2.530600	4.130276
H	1.669069	1.783415	4.910628

B3LYP/def2TZVP (CPCM – DME)

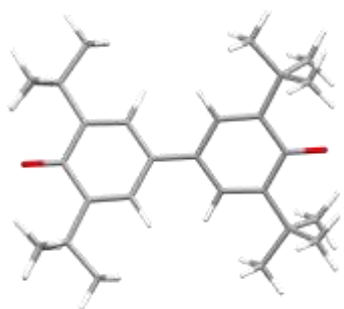


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	1.300552	-4.079086	2.318692
C	1.817397	-2.850158	3.084734
C	1.162619	-2.866026	4.484241
C	3.350174	-2.994844	3.215495
C	1.476102	-1.542161	2.363473
C	0.798374	-1.526101	1.193973
C	0.463689	-0.322023	0.475070
C	-0.236950	-0.359030	-0.736070
C	-0.710409	-1.598557	-1.300028
C	-1.393969	-1.685208	-2.463015
C	-1.885732	-3.026710	-3.016274
C	-1.505301	-4.199790	-2.097922
C	-3.425943	-3.012934	-3.138738
C	-1.246940	-3.292393	-4.397927
C	-1.674491	-0.434958	-3.221037
O	-2.290432	-0.467491	-4.285766
C	-1.190871	0.855652	-2.658143
C	-1.460333	2.156947	-3.420753
C	-0.885620	3.380477	-2.688024
C	-0.797703	2.096817	-4.815293
C	-2.982929	2.375948	-3.566862
C	-0.522111	0.840427	-1.483480
C	0.887626	0.922123	1.067535
C	1.562220	1.009612	2.235684
C	1.982151	2.357815	2.830293
C	1.543848	3.536295	1.945256
C	3.520736	2.420366	2.958547
C	1.326957	2.548851	4.216533
C	1.901233	-0.246094	2.960036
O	2.517176	-0.213561	4.024764
H	1.745536	-4.159642	1.324714
H	0.213776	-4.068807	2.212347
H	1.567773	-4.980508	2.872038
H	1.530454	-2.054878	5.106641
H	0.076993	-2.777886	4.400450
H	1.385986	-3.813264	4.980273
H	3.779262	-2.186866	3.801831
H	3.586415	-3.942420	3.704850
H	3.820131	-2.999001	2.229336
H	0.498991	-2.465087	0.764785
H	-0.515760	-2.503756	-0.753901
H	-0.423566	-4.298820	-1.985946
H	-1.949415	-4.103860	-1.104920
H	-1.876416	-5.127779	-2.535267
H	-3.765362	-2.242018	-3.825191

H	-3.771023	-3.981849	-3.506570
H	-3.886310	-2.839872	-2.163289
H	-1.525400	-2.529802	-5.120118
H	-1.579238	-4.263269	-4.772333
H	-0.157728	-3.317393	-4.318138
H	-1.330876	3.513125	-1.699769
H	0.198686	3.318362	-2.574377
H	-1.103911	4.277334	-3.269537
H	-1.202632	1.286584	-5.415535
H	0.281546	1.956445	-4.720930
H	-0.969847	3.038413	-5.341547
H	-3.167197	3.319538	-4.085402
H	-3.457838	2.433394	-2.584755
H	-3.449448	1.574007	-4.132456
H	-0.170078	1.774502	-1.084599
H	0.640327	1.832234	0.551716
H	1.866033	4.468848	2.410767
H	1.994142	3.492399	0.951372
H	0.458669	3.583036	1.832586
H	3.897882	1.648567	3.623929
H	3.813936	3.394889	3.355461
H	3.992058	2.299781	1.980442
H	1.607941	3.523746	4.621264
H	0.238115	2.520318	4.132881
H	1.642220	1.780187	4.916890

Singly Reduced

PBE/def2TZVP

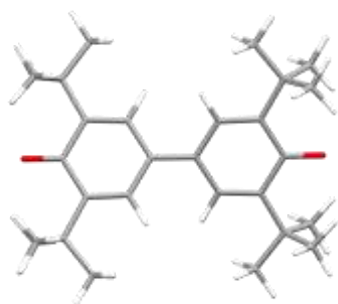


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	1.722975	-4.060290	2.124366
C	2.111378	-2.828409	2.959044
C	1.479897	-2.995547	4.360499
C	3.652118	-2.814972	3.084940
C	1.628204	-1.514581	2.326672
C	0.930836	-1.506555	1.136273

C	0.476301	-0.321356	0.496903
C	-0.249560	-0.359697	-0.757903
C	-0.839385	-1.557090	-1.246212
C	-1.541703	-1.636234	-2.431085
C	-2.174438	-2.956297	-2.896465
C	-1.921445	-4.109174	-1.910592
C	-3.704699	-2.785184	-3.034056
C	-1.575867	-3.368657	-4.261181
C	-1.698659	-0.436240	-3.262982
O	-2.334241	-0.469812	-4.361720
C	-1.088093	0.804297	-2.768052
C	-1.210496	2.084473	-3.608090
C	-0.513215	3.287543	-2.951205
C	-0.561700	1.866803	-4.994306
C	-2.702228	2.449657	-3.787400
C	-0.409986	0.798068	-1.566566
C	0.772019	0.903470	1.154505
C	1.455075	0.984411	2.350465
C	1.727038	2.338126	3.023510
C	1.165165	3.519813	2.215432
C	3.251676	2.552440	3.166071
C	1.067770	2.371248	4.421430
C	1.925401	-0.244814	3.001982
O	2.560981	-0.211243	4.100721
H	2.167370	-4.033745	1.117543
H	0.631790	-4.157847	2.015453
H	2.090783	-4.968024	2.627821
H	1.755757	-2.153316	5.005942
H	0.382304	-3.038540	4.283530
H	1.827761	-3.934674	4.822790
H	3.977433	-1.968228	3.700833
H	4.002596	-3.753219	3.546988
H	4.117077	-2.729333	2.090478
H	0.743247	-2.453906	0.632969
H	-0.756213	-2.448603	-0.626320
H	-0.847467	-4.314650	-1.782473
H	-2.352800	-3.906157	-0.918322
H	-2.392848	-5.025760	-2.298382
H	-3.936865	-1.991476	-3.753957
H	-4.162024	-3.728587	-3.376803
H	-4.149913	-2.523157	-2.061636
H	-1.759616	-2.588692	-5.009471
H	-2.030696	-4.313252	-4.604041
H	-0.489598	-3.525095	-4.171571
H	-0.943482	3.527017	-1.966529
H	0.566921	3.118795	-2.821917

H	-0.638215	4.172629	-3.594423
H	-1.048476	1.035119	-5.517259
H	0.509717	1.637855	-4.884198
H	-0.655415	2.781099	-5.604149
H	-2.797317	3.365206	-4.395193
H	-3.170689	2.638729	-2.808993
H	-3.238120	1.631681	-4.283165
H	0.061905	1.718900	-1.226910
H	0.404544	1.821503	0.698263
H	1.393759	4.459049	2.742984
H	1.612633	3.583369	1.211540
H	0.071994	3.459000	2.100705
H	3.695459	1.748221	3.764684
H	3.453730	3.520614	3.654432
H	3.731457	2.562801	2.175018
H	1.268333	3.338601	4.911973
H	-0.023388	2.252533	4.333370
H	1.461401	1.562479	5.048388

B3LYP/def2TZVP

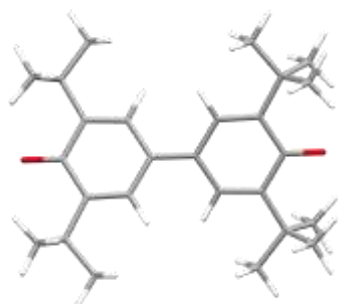


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	1.712578	-4.058210	2.122428
C	2.101745	-2.824858	2.953965
C	1.469886	-2.993036	4.353376
C	3.641072	-2.817507	3.078513
C	1.619688	-1.512589	2.317518
C	0.926991	-1.502945	1.134905
C	0.474595	-0.321447	0.493951
C	-0.247851	-0.359607	-0.754953
C	-0.835146	-1.553793	-1.245285
C	-1.532950	-1.634078	-2.422195
C	-2.164430	-2.953241	-2.891804
C	-1.910865	-4.108050	-1.908857
C	-3.693965	-2.788117	-3.027279
C	-1.565589	-3.366414	-4.254360
C	-1.690767	-0.435823	-3.249351

O	-2.320371	-0.469077	-4.337746
C	-1.084698	0.802783	-2.755950
C	-1.211368	2.081902	-3.596963
C	-0.516953	3.286782	-2.941129
C	-0.561268	1.870327	-4.981773
C	-2.701387	2.448003	-3.774993
C	-0.411207	0.794930	-1.562282
C	0.772850	0.899700	1.150658
C	1.451447	0.981777	2.338625
C	1.727537	2.334091	3.012801
C	1.168729	3.517371	2.205555
C	3.250565	2.549341	3.153975
C	1.067641	2.373192	4.408546
C	1.917515	-0.245231	2.988347
O	2.547112	-0.211976	4.076745
H	2.153700	-4.033785	1.123509
H	0.629768	-4.154026	2.015322
H	2.076520	-4.959045	2.622782
H	1.744561	-2.164158	5.000799
H	0.380210	-3.030690	4.275382
H	1.809442	-3.928750	4.809241
H	3.972930	-1.983765	3.692107
H	3.986332	-3.752333	3.531867
H	4.101019	-2.730631	2.090694
H	0.738165	-2.440633	0.637282
H	-0.749698	-2.436637	-0.632236
H	-0.845024	-4.311092	-1.782810
H	-2.339261	-3.908485	-0.924136
H	-2.377627	-5.017882	-2.294410
H	-3.934085	-2.006197	-3.743306
H	-4.145657	-3.727642	-3.361794
H	-4.134105	-2.526276	-2.061567
H	-1.749682	-2.599992	-5.002925
H	-2.011734	-4.307772	-4.591216
H	-0.486578	-3.516569	-4.164464
H	-0.944886	3.523515	-1.964420
H	0.555075	3.121213	-2.813201
H	-0.642157	4.165348	-3.578905
H	-1.041038	1.050382	-5.510227
H	0.501802	1.641389	-4.870623
H	-0.650562	2.781277	-5.582465
H	-2.795523	3.360826	-4.372125
H	-3.165807	2.630619	-2.802440
H	-3.237706	1.643531	-4.271811
H	0.053849	1.706852	-1.223661
H	0.411168	1.808311	0.696613
H	1.396745	4.449473	2.728534
H	1.613634	3.579494	1.209899

H	0.083982	3.458948	2.091824
H	3.696299	1.758514	3.751936
H	3.451287	3.513592	3.632099
H	3.725652	2.554533	2.169515
H	1.263365	3.336593	4.890401
H	-0.015229	2.253413	4.319504
H	1.455670	1.577475	5.039436

B3LYP/def2TZVP (CPCM – DME)

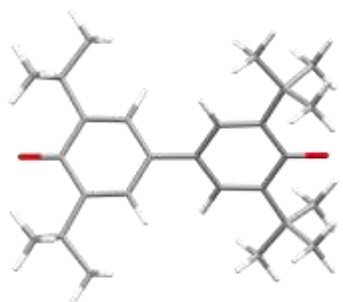


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	1.657398	-4.063555	2.135593
C	2.063501	-2.835065	2.966992
C	1.420920	-2.993532	4.362415
C	3.602201	-2.856694	3.095521
C	1.604946	-1.515372	2.326613
C	0.912954	-1.504427	1.142669
C	0.474779	-0.321437	0.494272
C	-0.248036	-0.359617	-0.755273
C	-0.821423	-1.557814	-1.252699
C	-1.518683	-1.639627	-2.430761
C	-2.127675	-2.969254	-2.903169
C	-1.856740	-4.121196	-1.920848
C	-3.659881	-2.833265	-3.038948
C	-1.517050	-3.373563	-4.262912
C	-1.689942	-0.435778	-3.247920
O	-2.320838	-0.469101	-4.338552
C	-1.099382	0.808311	-2.748107
C	-1.239973	2.098344	-3.571510
C	-0.554690	3.300793	-2.900811
C	-0.589573	1.915778	-4.960119
C	-2.733199	2.456037	-3.737529
C	-0.424583	0.798969	-1.554267
C	0.786536	0.901164	1.142295
C	1.466602	0.984582	2.330255
C	1.757629	2.343867	2.985687
C	1.207516	3.521850	2.164064

C	3.282811	2.548954	3.116026
C	1.100735	2.412074	4.381546
C	1.916682	-0.245276	2.986921
O	2.547578	-0.211951	4.077552
H	2.103300	-4.049396	1.138733
H	0.573836	-4.143791	2.024990
H	2.005292	-4.967800	2.639452
H	1.700490	-2.170115	5.014432
H	0.331393	-3.019234	4.279044
H	1.745613	-3.932278	4.820124
H	3.952917	-2.031711	3.710202
H	3.927071	-3.797352	3.549135
H	4.067734	-2.780653	2.109503
H	0.711441	-2.444473	0.655539
H	-0.723707	-2.445734	-0.649673
H	-0.788370	-4.308522	-1.793278
H	-2.291068	-3.931472	-0.936915
H	-2.307957	-5.036642	-2.309338
H	-3.919730	-2.057987	-3.755086
H	-4.091972	-3.780869	-3.372844
H	-4.106811	-2.581701	-2.073699
H	-1.706654	-2.612552	-5.015385
H	-1.948779	-4.319819	-4.601108
H	-0.436801	-3.511241	-4.169183
H	-0.982153	3.521974	-1.920437
H	0.519354	3.144857	-2.778857
H	-0.690336	4.185241	-3.526843
H	-1.059775	1.101941	-5.506023
H	0.476209	1.696900	-4.855550
H	-0.688322	2.835345	-5.543892
H	-2.835818	3.374068	-4.323067
H	-3.194587	2.626404	-2.761427
H	-3.270296	1.656641	-4.241310
H	0.025537	1.715826	-1.210238
H	0.440214	1.812273	0.682370
H	1.446492	4.457094	2.674723
H	1.650170	3.568230	1.166725
H	0.121895	3.473904	2.055039
H	3.729940	1.763923	3.720264
H	3.492466	3.515925	3.582050
H	3.753477	2.541966	2.129566
H	1.306705	3.380771	4.845600
H	0.016350	2.303347	4.297747
H	1.480066	1.625651	5.028908

Doubly Reduced

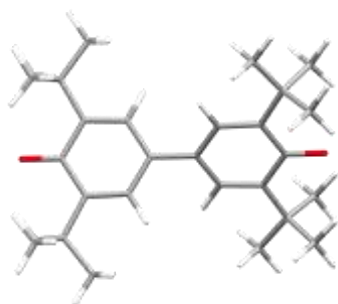
PBE/def2TZVP



Element	X	Y	Z
C	2.144733	-3.989698	1.927898
C	2.397077	-2.769459	2.828367
C	1.795146	-3.079608	4.218477
C	3.926932	-2.594797	2.966928
C	1.774700	-1.474193	2.276822
C	1.073547	-1.471340	1.068808
C	0.484242	-0.320934	0.510628
C	-0.257501	-0.360119	-0.771628
C	-0.976726	-1.497812	-1.184729
C	-1.682348	-1.573662	-2.387753
C	-2.450717	-2.849566	-2.776271
C	-2.331125	-3.967334	-1.727559
C	-3.952077	-2.522378	-2.946652
C	-1.897544	-3.398131	-4.111935
C	-1.716973	-0.437223	-3.294628
O	-2.365805	-0.471502	-4.416273
C	-0.978748	0.740045	-2.865469
C	-0.965741	1.976044	-3.782752
C	-0.146549	3.143410	-3.208570
C	-0.355638	1.601772	-5.153101
C	-2.413267	2.477358	-3.993168
C	-0.286649	0.738037	-1.652244
C	0.643310	0.869010	1.246165
C	1.339877	0.945703	2.454400
C	1.472863	2.280874	3.208656
C	0.786418	3.451517	2.486235
C	2.969147	2.638271	3.364617
C	0.834272	2.153297	4.610829
C	1.943714	-0.243830	3.033628
O	2.592549	-0.209553	4.155271
H	2.579546	-3.856210	0.925085
H	1.069387	-4.192205	1.804871
H	2.609086	-4.881368	2.383575

H	1.957145	-2.216951	4.879568
H	0.712748	-3.265817	4.129090
H	2.266560	-3.979147	4.657111
H	4.132128	-1.723861	3.604705
H	4.385428	-3.498144	3.411374
H	4.380137	-2.429277	1.976236
H	0.987545	-2.399137	0.498559
H	-0.991802	-2.350165	-0.501608
H	-1.284615	-4.272678	-1.572332
H	-2.740936	-3.660490	-0.752667
H	-2.896293	-4.851194	-2.070658
H	-4.062325	-1.721132	-3.690454
H	-4.512661	-3.416994	-3.277098
H	-4.376637	-2.183416	-1.987947
H	-1.965973	-2.612850	-4.877514
H	-2.470493	-4.286806	-4.437184
H	-0.842430	-3.692442	-3.992080
H	-0.542276	3.483136	-2.238776
H	0.910534	2.870763	-3.064511
H	-0.185193	3.995370	-3.909292
H	-0.923744	0.764688	-5.581982
H	0.695631	1.295920	-5.028405
H	-0.385894	2.465174	-5.844049
H	-2.432697	3.334737	-4.691970
H	-2.843635	2.804674	-3.033013
H	-3.021523	1.656326	-4.397386
H	0.290065	1.620061	-1.364457
H	0.167673	1.767135	0.845506
H	0.925881	4.375087	3.074376
H	1.210973	3.619644	1.484236
H	-0.295668	3.283834	2.370103
H	3.483836	1.811364	3.873321
H	3.090114	3.569105	3.950036
H	3.426793	2.791475	2.373991
H	0.966620	3.087858	5.187775
H	-0.245642	1.954669	4.518125
H	1.307435	1.318199	5.145732

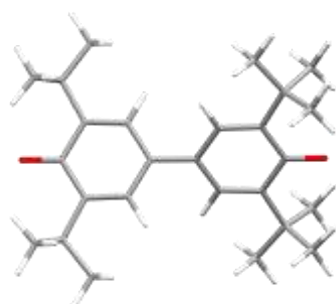
B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.251548	-3.956922	1.852117
C	2.467522	-2.746247	2.774810
C	1.876919	-3.107336	4.155975
C	3.991569	-2.535780	2.913369
C	1.805770	-1.461443	2.245842
C	1.106274	-1.457064	1.043821
C	0.484677	-0.320912	0.511377
C	-0.257934	-0.360143	-0.772380
C	-1.007453	-1.476906	-1.161976
C	-1.711557	-1.553692	-2.358850
C	-2.517709	-2.812003	-2.726568
C	-2.433013	-3.913445	-1.657273
C	-4.009262	-2.450181	-2.901407
C	-1.981476	-3.408373	-4.047027
C	-1.708289	-0.436765	-3.279618
O	-2.352739	-0.470809	-4.393675
C	-0.938607	0.720652	-2.875481
C	-0.888268	1.939035	-3.814338
C	-0.033395	3.090111	-3.259399
C	-0.286013	1.530235	-5.176830
C	-2.315436	2.488340	-4.034039
C	-0.251053	0.717386	-1.666586
C	0.605717	0.854474	1.262736
C	1.297879	0.932374	2.466484
C	1.391938	2.257108	3.244094
C	0.668350	3.418143	2.542555
C	2.873471	2.665267	3.403090
C	0.757186	2.093624	4.642871
C	1.935031	-0.244290	3.018616
O	2.579476	-0.210246	4.132675
H	2.678023	-3.793026	0.859761
H	1.191235	-4.188650	1.727833
H	2.739495	-4.836271	2.286373
H	2.013577	-2.271972	4.840652
H	0.807524	-3.317821	4.062685
H	2.366870	-4.000777	4.565246

H	4.184769	-1.686641	3.566760
H	4.470630	-3.433019	3.327206
H	4.432763	-2.335581	1.932607
H	1.044518	-2.366536	0.460619
H	-1.044461	-2.306833	-0.468486
H	-1.404724	-4.245736	-1.497231
H	-2.831181	-3.578888	-0.696521
H	-3.020083	-4.779806	-1.980839
H	-4.110165	-1.673738	-3.657870
H	-4.589374	-3.332606	-3.202399
H	-4.418046	-2.079641	-1.956831
H	-2.027977	-2.655819	-4.832387
H	-2.571947	-4.285252	-4.344045
H	-0.941990	-3.724651	-3.920341
H	-0.416564	3.456482	-2.304223
H	1.006364	2.789446	-3.111032
H	-0.043732	3.924913	-3.968572
H	-0.870411	0.717590	-5.605047
H	0.745982	1.192616	-5.044059
H	-0.280691	2.382295	-5.869480
H	-2.301358	3.334771	-4.733431
H	-2.732663	2.837489	-3.085025
H	-2.952639	1.699669	-4.430600
H	0.346178	1.576910	-1.391613
H	0.107250	1.734350	0.877475
H	0.777808	4.329055	3.141041
H	1.083546	3.615788	1.551618
H	-0.399712	3.220351	2.425791
H	3.420511	1.866026	3.900333
H	2.959912	3.589162	3.990235
H	3.320609	2.842875	2.420677
H	0.852915	3.021232	5.222681
H	-0.307215	1.860499	4.546287
H	1.249282	1.280692	5.174159

B3LYP/def2TZVP (CPCM – DME)



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
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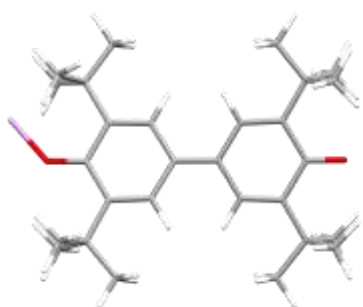
C	2.138410	-3.985647	1.885004
C	2.396275	-2.775915	2.799222
C	1.794410	-3.114556	4.180210
C	3.926640	-2.620108	2.928219
C	1.775517	-1.472573	2.262835
C	1.077455	-1.465188	1.059616
C	0.484430	-0.320924	0.510952
C	-0.257688	-0.360130	-0.771952
C	-0.979848	-1.490150	-1.176413
C	-1.682875	-1.570212	-2.374089
C	-2.450437	-2.852351	-2.746540
C	-2.324078	-3.958655	-1.685473
C	-3.954361	-2.542486	-2.905064
C	-1.900478	-3.427843	-4.069567
C	-1.706535	-0.436672	-3.276582
O	-2.351771	-0.470760	-4.392008
C	-0.966558	0.737212	-2.858970
C	-0.940201	1.980193	-3.767846
C	-0.113377	3.136854	-3.181130
C	-0.319009	1.623694	-5.135311
C	-2.375890	2.508892	-3.975989
C	-0.277686	0.730683	-1.650460
C	0.633561	0.862548	1.245257
C	1.327399	0.943467	2.448222
C	1.447847	2.285967	3.193164
C	0.752528	3.445343	2.459598
C	2.935440	2.671399	3.343346
C	0.800213	2.176795	4.590155
C	1.933277	-0.244381	3.015581
O	2.578513	-0.210294	4.131008
H	2.570886	-3.848341	0.891391
H	1.071633	-4.187655	1.765168
H	2.597012	-4.875036	2.325429
H	1.953543	-2.289061	4.870307
H	0.719611	-3.295870	4.090255
H	2.255255	-4.019917	4.589470
H	4.163707	-1.777885	3.574273
H	4.372819	-3.529548	3.344623
H	4.373504	-2.446260	1.945267
H	0.993981	-2.383725	0.495047
H	-0.996432	-2.333808	-0.500111
H	-1.286049	-4.262943	-1.533535
H	-2.731202	-3.649470	-0.720171
H	-2.883166	-4.838995	-2.013687
H	-4.099574	-1.766988	-3.653690
H	-4.503195	-3.440965	-3.206836
H	-4.371738	-2.197005	-1.955040
H	-1.970455	-2.683164	-4.859223

H	-2.463372	-4.319748	-4.364871
H	-0.852358	-3.716400	-3.949820
H	-0.507691	3.475149	-2.220269
H	0.934121	2.861501	-3.039412
H	-0.142069	3.986142	-3.869018
H	-0.874532	0.811175	-5.598056
H	0.721329	1.311124	-5.008414
H	-0.330391	2.492576	-5.801991
H	-2.374480	3.371134	-4.651329
H	-2.802706	2.830272	-3.021682
H	-3.005306	1.727263	-4.395383
H	0.294105	1.603672	-1.366975
H	0.161829	1.751754	0.850038
H	0.881707	4.365784	3.035276
H	1.175590	3.613344	1.466636
H	-0.320321	3.274208	2.346189
H	3.475700	1.882852	3.862299
H	3.036080	3.606422	3.904730
H	3.388936	2.819889	2.359247
H	0.914249	3.115830	5.142203
H	-0.269613	1.970036	4.496186
H	1.263881	1.371591	5.155473

Lithium

Oxidised

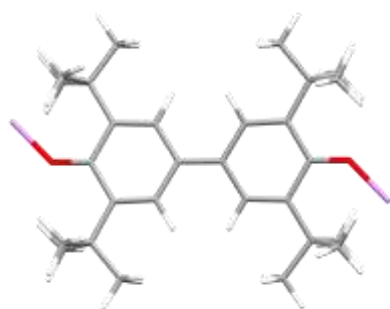
PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.623541	3.796514	0.373640
C	3.580620	2.599773	0.246045
C	4.458220	2.825438	-1.011636
C	4.472480	2.566342	1.512881
C	2.825377	1.282576	0.113309
C	1.463498	1.221801	0.114667
C	0.723872	-0.008383	0.017381
C	-0.700317	-0.014294	0.037720
C	-1.452887	1.200090	-0.057142

C	-2.822174	1.224757	-0.055870
C	-3.603865	2.540965	-0.186763
C	-2.686343	3.769681	-0.314531
C	-4.469925	2.520805	-1.481587
C	-4.458866	2.780773	1.093763
C	-3.556808	-0.038751	0.069406
C	-2.816066	-1.292385	0.181686
C	-3.556415	-2.627564	0.331544
C	-2.579749	-3.811147	0.438093
C	-4.413802	-2.613232	1.618649
C	-4.451703	-2.873107	-0.905931
C	-1.445015	-1.231177	0.151556
C	1.466447	-1.234170	-0.100700
C	2.828598	-1.288176	-0.133067
C	3.585365	-2.601857	-0.285103
C	2.630336	-3.802035	-0.393229
C	4.491955	-2.825175	0.952580
C	4.448921	-2.562217	-1.571465
C	3.591735	-0.001083	-0.018383
O	4.824470	0.002441	-0.032264
H	1.988240	3.727214	1.270240
H	1.978565	3.909114	-0.511755
H	3.214861	4.717667	0.464406
H	5.219590	2.045933	-1.117917
H	3.841390	2.847028	-1.922375
H	4.964717	3.797552	-0.924104
H	5.232505	1.780681	1.451221
H	4.981782	3.535245	1.617715
H	3.865626	2.404629	2.416147
H	0.907731	2.147867	0.233724
H	-0.914821	2.137340	-0.170208
H	-2.042240	3.891273	0.567950
H	-2.050923	3.713041	-1.209701
H	-3.298032	4.679165	-0.402630
H	-4.966971	1.557945	-1.693571
H	-5.204767	3.342796	-1.482373
H	-3.829407	2.674768	-2.360347
H	-4.947964	1.878858	1.501385
H	-5.198192	3.583261	0.934809
H	-3.811875	3.112491	1.916872
H	-1.952951	-3.916504	-0.460573
H	-1.924586	-3.732843	1.319011
H	-3.155630	-4.740705	0.543124
H	-5.179148	-1.829843	1.589999
H	-3.783564	-2.457019	2.506564
H	-4.919613	-3.583025	1.732220

H	-4.953950	-3.846287	-0.806130
H	-3.849013	-2.898769	-1.825778
H	-5.220778	-2.100319	-1.012523
H	-0.893853	-2.161129	0.254645
H	0.911292	-2.162066	-0.205485
H	3.223242	-4.720515	-0.499146
H	2.005664	-3.919490	0.505734
H	1.974239	-3.734211	-1.274664
H	5.252318	-2.042662	1.043410
H	5.000132	-3.795051	0.851602
H	3.895420	-2.851760	1.876534
H	4.958240	-3.529541	-1.689432
H	3.821398	-2.401178	-2.460596
H	5.208014	-1.774545	-1.525313
O	-4.834964	-0.034683	0.079502
Li	-6.002097	1.291686	-0.046572

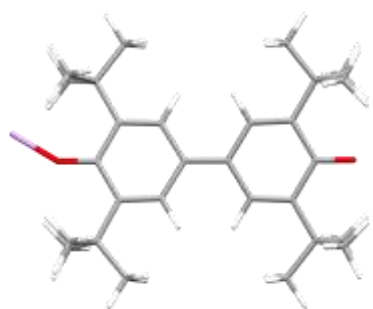


Element	X	Y	Z
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C	-3.559847	-2.635082	0.197500
C	-4.446916	-2.845600	-1.055269
C	-4.427893	-2.653047	1.480241
C	-2.819771	-1.301512	0.089654
C	-1.452509	-1.232462	0.074998
C	-0.710316	-0.005544	-0.003796
C	0.710322	0.007627	-0.002788
C	1.466264	-1.217591	-0.078180
C	2.829808	-1.246767	-0.084652
C	3.615752	-2.560323	-0.185778
C	2.697318	-3.791568	-0.278980
C	4.477752	-2.569134	-1.483037
C	4.478007	-2.764461	1.095729
C	3.565118	0.034435	0.006390
C	2.819641	1.303778	0.091163
C	3.559564	2.637557	0.197469
C	2.582104	3.822388	0.275586

C	4.425764	2.658029	1.481420
C	4.448434	2.845629	-1.054432
C	1.452402	1.234698	0.074677
C	-1.466148	1.219524	-0.082664
C	-2.829681	1.248684	-0.091151
C	-3.615477	2.562040	-0.195966
C	-2.696909	3.793103	-0.290245
C	-4.479570	2.768672	1.083903
C	-4.475615	2.568323	-1.494475
C	-3.565123	-0.032339	0.001331
H	-1.936767	-3.767175	1.169466
H	-1.950694	-3.901821	-0.618617
H	-3.158287	-4.751557	0.354050
H	-5.226980	-2.081869	-1.141715
H	-3.841776	-2.838152	-1.973514
H	-4.937844	-3.826347	-0.985679
H	-5.204673	-1.881120	1.463595
H	-4.922643	-3.630649	1.564996
H	-3.808580	-2.511932	2.377972
H	-0.902590	-2.164896	0.157781
H	0.928084	-2.157527	-0.161167
H	2.059537	-3.895182	0.610601
H	2.059591	-3.760252	-1.174031
H	3.309463	-4.701652	-0.347623
H	5.001479	-1.623874	-1.708147
H	5.192569	-3.406900	-1.469611
H	3.836137	-2.720204	-2.361727
H	4.992305	-1.860932	1.466510
H	5.199976	-3.584012	0.952945
H	3.838001	-3.056560	1.939294
H	1.951588	3.902698	-0.623434
H	1.935089	3.771545	1.164887
H	3.157783	4.754333	0.349307
H	5.202564	1.886069	1.467401
H	3.805159	2.518669	2.378533
H	4.920395	3.635794	1.564975
H	4.939266	3.826509	-0.986049
H	3.844614	2.836392	-1.973529
H	5.228618	2.081728	-1.138266
H	0.902365	2.167291	0.154849
H	-0.927848	2.159297	-0.166709
H	-3.308954	4.703050	-0.361545
H	-2.060409	3.898454	0.600049
H	-2.057894	3.760042	-1.184314
H	-4.994418	1.865872	1.455694
H	-5.201319	3.587956	0.938493

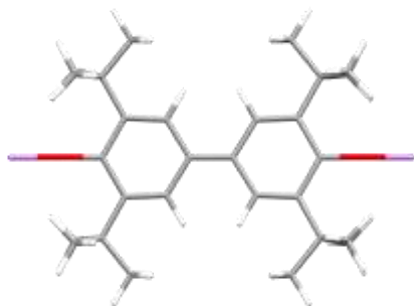
H	-3.840772	3.062395	1.927820
H	-5.190477	3.406090	-1.483691
H	-3.832744	2.717725	-2.372533
H	-4.998986	1.622612	-1.718515
O	4.827879	0.034143	0.010458
Li	6.086487	-1.263549	-0.079840
O	-4.827889	-0.032041	0.003579
Li	-6.086356	1.265480	-0.091078

B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.616345	3.807929	0.272836
C	3.570107	2.606239	0.178305
C	4.445714	2.796770	-1.083363
C	4.458363	2.606916	1.445163
C	2.809584	1.287248	0.081890
C	1.460293	1.224657	0.085552
C	0.716559	-0.007769	0.015562
C	-0.693795	-0.013700	0.034128
C	-1.450712	1.198286	-0.033003
C	-2.811128	1.233602	-0.027918
C	-3.577284	2.564878	-0.123292
C	-2.631861	3.775698	-0.220599
C	-4.449452	2.598024	-1.400305
C	-4.431389	2.789351	1.146832
C	-3.537866	-0.030825	0.067900
C	-2.802416	-1.285998	0.148058
C	-3.549396	-2.623890	0.262848
C	-2.577781	-3.813834	0.338027
C	-4.401776	-2.646873	1.550350
C	-4.441904	-2.840560	-0.978922
C	-1.441756	-1.229911	0.120441
C	1.465787	-1.235106	-0.074106
C	2.815423	-1.289355	-0.100681
C	3.580940	-2.603621	-0.216839
C	2.632027	-3.809946	-0.299252
C	4.480582	-2.794185	1.027930

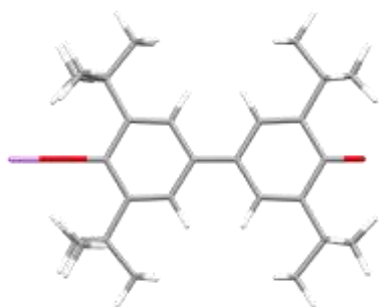
C	4.446011	-2.593640	-1.499706
C	3.577448	0.001038	-0.015747
O	4.795071	0.004973	-0.025651
H	1.985982	3.763882	1.163991
H	1.976431	3.895408	-0.608339
H	3.204178	4.723444	0.337641
H	5.201567	2.021840	-1.170711
H	3.831518	2.793251	-1.986511
H	4.949644	3.762981	-1.025461
H	5.213915	1.827596	1.408483
H	4.963406	3.570808	1.526909
H	3.853097	2.468929	2.343771
H	0.907291	2.142511	0.174190
H	-0.915984	2.126870	-0.118714
H	-1.990018	3.863329	0.657283
H	-2.002572	3.731016	-1.110683
H	-3.221239	4.691209	-0.284871
H	-5.106114	1.731608	-1.509855
H	-5.054040	3.506626	-1.426209
H	-3.821286	2.592694	-2.291795
H	-5.084940	1.949454	1.394214
H	-5.036752	3.692083	1.044927
H	-3.790738	2.917061	2.020120
H	-1.956436	-3.895476	-0.556260
H	-1.927557	-3.760086	1.213646
H	-3.151343	-4.737430	0.418020
H	-5.156788	-1.865236	1.552823
H	-3.771865	-2.519726	2.433003
H	-4.908620	-3.609478	1.637661
H	-4.946297	-3.805492	-0.903837
H	-3.840804	-2.847827	-1.890330
H	-5.200431	-2.068412	-1.075043
H	-0.897752	-2.153790	0.194478
H	0.915814	-2.155659	-0.151637
H	3.223558	-4.721778	-0.380101
H	2.009507	-3.905912	0.593261
H	1.984171	-3.765030	-1.177607
H	5.233485	-2.015257	1.105060
H	4.988720	-3.757238	0.956314
H	3.882770	-2.798648	1.941957
H	4.953730	-3.554815	-1.595181
H	3.823707	-2.454695	-2.386442
H	5.198702	-1.811090	-1.473266
O	-4.805075	-0.035062	0.081309
Li	-6.275151	0.839756	0.028223



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-2.594868	-3.811055	-0.124174
C	-3.563020	-2.615306	-0.087929
C	-4.425430	-2.697233	-1.367682
C	-4.433726	-2.781813	1.178087
C	-2.810666	-1.278219	-0.040756
C	-1.456488	-1.224849	-0.034319
C	-0.702032	0.000885	-0.000541
C	0.702038	0.001271	0.000505
C	1.457159	-1.223981	0.036806
C	2.811366	-1.276608	0.043354
C	3.564433	-2.613192	0.093286
C	2.596934	-3.809387	0.131971
C	4.435249	-2.781831	-1.172373
C	4.426869	-2.692030	1.373214
C	3.546668	0.002005	0.002592
C	2.810761	1.280241	-0.039223
C	3.563215	2.617213	-0.088004
C	2.595149	3.812909	-0.128057
C	4.432091	2.786252	1.178934
C	4.427478	2.696550	-1.366670
C	1.456575	1.226916	-0.034666
C	-1.457236	1.226191	0.032119
C	-2.811454	1.278795	0.036570
C	-3.564628	2.615457	0.082636
C	-2.597218	3.811759	0.120220
C	-4.428907	2.696934	1.361153
C	-4.433623	2.781431	-1.184627
C	-3.546664	0.000082	-0.002619
H	-1.964043	-3.856726	0.765768
H	-1.958106	-3.798086	-1.010941
H	-3.171246	-4.735202	-0.156630
H	-5.170522	-1.906597	-1.424394
H	-3.803276	-2.627930	-2.261320
H	-4.946179	-3.654957	-1.397294
H	-5.180060	-1.997194	1.281800
H	-4.953522	-3.739796	1.141020
H	-3.817616	-2.771069	2.078505

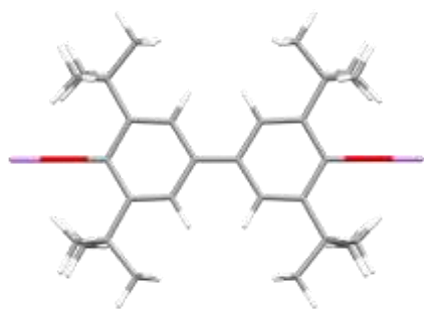
H	-0.915677	-2.152396	-0.070445
H	0.916849	-2.151743	0.074844
H	1.960142	-3.794942	1.018695
H	1.966151	-3.857236	-0.757886
H	3.173809	-4.733155	0.166340
H	5.181104	-1.996977	-1.277732
H	4.955632	-3.739413	-1.133287
H	3.819139	-2.773350	-2.072815
H	5.171532	-1.900876	1.428319
H	4.948146	-3.649402	1.404787
H	3.804667	-2.621230	2.266700
H	1.959702	3.798195	-1.015740
H	1.963005	3.860357	0.760855
H	3.171595	4.736977	-0.161493
H	5.178253	2.001828	1.285310
H	3.814676	2.777338	2.078477
H	4.951963	3.744148	1.140690
H	4.948296	3.654199	-1.397451
H	3.806617	2.625469	-2.261066
H	5.172629	1.905784	-1.420720
H	0.915848	2.154402	-0.073474
H	-0.917011	2.154047	0.069032
H	-3.174166	4.735579	0.151837
H	-1.961702	3.799178	1.007888
H	-1.965157	3.857772	-0.768826
H	-5.173602	1.905851	1.416855
H	-4.950284	3.654340	1.389964
H	-3.807985	2.628052	2.255679
H	-4.954069	3.739088	-1.148300
H	-3.816218	2.771064	-2.084161
H	-5.179322	1.996349	-1.289415
O	4.797391	0.002336	0.003493
Li	6.522499	0.002683	0.004748
O	-4.797389	-0.000285	-0.003498
Li	-6.522496	-0.000623	-0.004618

B3LYP/def2TZVP (CPCM – DME)



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.620753	3.818846	-0.008756
C	3.575358	2.613650	0.005537
C	4.471847	2.713473	-1.249622
C	4.438237	2.717041	1.283847
C	2.815224	1.285702	-0.002251
C	1.465984	1.231304	-0.015651
C	0.712579	0.001148	-0.019676
C	-0.689331	0.000324	-0.015195
C	-1.447028	1.221360	-0.012217
C	-2.800544	1.270703	0.040637
C	-3.552761	2.608691	0.036282
C	-2.594749	3.804130	-0.106440
C	-4.526912	2.666601	-1.161068
C	-4.312595	2.792184	1.368114
C	-3.544330	-0.001305	0.117785
C	-2.799064	-1.272481	0.041229
C	-3.549740	-2.611340	0.037515
C	-2.590333	-3.805730	-0.104624
C	-4.309393	-2.795083	1.369418
C	-4.523824	-2.670957	-1.159808
C	-1.445605	-1.221593	-0.011662
C	1.467436	-1.228117	-0.015355
C	2.816741	-1.280914	-0.001960
C	3.578449	-2.607957	0.006099
C	2.625273	-3.814287	-0.007928
C	4.441464	-2.710055	1.284422
C	4.475042	-2.706982	-1.249049
C	3.579439	0.002847	0.008026
O	4.805310	0.003574	0.024562
H	1.973185	3.839635	0.870273
H	1.994394	3.835258	-0.903106
H	3.209574	4.736892	-0.003806
H	5.220283	1.926194	-1.271842
H	3.869050	2.649357	-2.158229
H	4.983537	3.678146	-1.252522
H	5.186072	1.930103	1.328026
H	4.949289	3.681964	1.297851
H	3.811500	2.654991	2.176272
H	0.917595	2.155554	-0.020096
H	-0.906829	2.149107	-0.053732
H	-1.894337	3.872664	0.728052
H	-2.024699	3.763181	-1.036705
H	-3.178409	4.725533	-0.118511
H	-5.271687	1.876621	-1.125956
H	-5.046301	3.626998	-1.163950
H	-3.979734	2.577551	-2.101940
H	-5.028706	1.994864	1.544012

H	-4.850527	3.742446	1.356347
H	-3.612363	2.811596	2.205757
H	-2.020318	-3.764562	-1.034900
H	-1.889852	-3.873045	0.729911
H	-3.172915	-4.727819	-0.116261
H	-5.026556	-1.998602	1.544836
H	-3.609179	-2.813135	2.207105
H	-4.846090	-3.746050	1.358139
H	-5.042015	-3.632002	-1.162280
H	-3.976767	-2.581625	-2.100724
H	-5.269588	-1.881894	-1.125008
H	-0.904323	-2.148730	-0.052716
H	0.920139	-2.153015	-0.019616
H	3.215183	-4.731634	-0.002787
H	1.977737	-3.835656	0.871110
H	1.998928	-3.831633	-0.902271
H	5.188367	-1.922223	1.328425
H	4.953659	-3.674369	1.298624
H	3.814664	-2.648559	2.176841
H	4.987876	-3.671048	-1.251751
H	3.872159	-2.643772	-2.157662
H	5.222544	-1.918821	-1.271444
O	-4.784002	-0.002022	0.246785
Li	-6.622337	-0.002603	0.438107



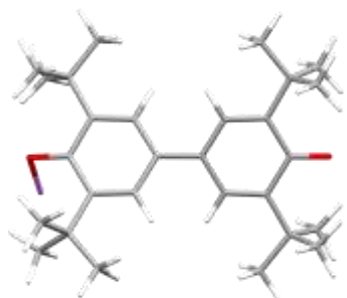
<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-2.596869	-3.812509	0.157841
C	-3.554660	-2.617830	0.009944
C	-4.294830	-2.789356	-1.335201
C	-4.546962	-2.683319	1.192249
C	-2.803951	-1.281265	0.023586
C	-1.453805	-1.227017	0.090982
C	-0.700401	-0.000020	0.099244
C	0.700269	0.002357	0.100177
C	1.457845	-1.222074	0.092910
C	2.808256	-1.271736	0.027319
C	3.563517	-2.605744	0.014669

C	2.609590	-3.803669	0.161273
C	4.306065	-2.774737	-1.329486
C	4.554452	-2.667881	1.198301
C	3.552097	0.007008	-0.053176
C	2.803923	1.283413	0.024222
C	3.554654	2.619942	0.008335
C	2.596667	3.814974	0.152042
C	4.545371	2.688310	1.191807
C	4.296624	2.788197	-1.336231
C	1.453688	1.229330	0.089940
C	-1.457967	1.224387	0.087988
C	-2.808290	1.273884	0.020466
C	-3.563533	2.607855	0.003561
C	-2.609805	3.806136	0.148535
C	-4.556056	2.672864	1.185709
C	-4.304275	2.773579	-1.341996
C	-3.552022	-0.005055	-0.057916
H	-2.040740	-3.777379	1.096732
H	-1.885037	-3.874625	-0.667445
H	-3.179481	-4.734362	0.155098
H	-5.009070	-1.991162	-1.515427
H	-3.582816	-2.802632	-2.162810
H	-4.832512	-3.739477	-1.337441
H	-5.298574	-1.900781	1.144695
H	-5.057087	-3.648302	1.185037
H	-4.016330	-2.590536	2.142041
H	-0.909674	-2.152215	0.135569
H	0.916800	-2.149115	0.136756
H	2.052089	-3.770439	1.099419
H	1.899077	-3.868189	-0.664965
H	3.195330	-4.723539	0.159301
H	5.017835	-1.974124	-1.508746
H	4.846966	-3.723031	-1.331018
H	3.595208	-2.790412	-2.158047
H	5.303468	-1.882797	1.151761
H	5.067858	-3.631127	1.191763
H	4.022237	-2.576913	2.147382
H	1.885942	3.875081	-0.674346
H	2.039280	3.782125	1.090270
H	3.179283	4.736819	0.147839
H	5.297048	1.905663	1.147164
H	4.013466	2.597835	2.141109
H	5.055503	3.653275	1.182931
H	4.834307	3.738313	-1.340063
H	3.585719	2.799455	-2.164822
H	5.011106	1.989571	-1.513558

H	0.909503	2.154634	0.131546
H	-0.916983	2.151534	0.130308
H	-3.195543	4.725996	0.143546
H	-2.053560	3.775186	1.087505
H	-1.898187	3.868654	-0.676906
H	-5.305009	1.887666	1.140072
H	-5.069453	3.636090	1.176140
H	-4.025116	2.584206	2.135721
H	-4.845178	3.721862	-1.346556
H	-3.592307	2.787248	-2.169637
H	-5.015801	1.972528	-1.520268
O	4.785065	0.008938	-0.185794
Li	6.646103	0.011786	-0.443996
O	-4.784810	-0.007312	-0.192183
Li	-6.645496	-0.010784	-0.452866

Singly Reduced

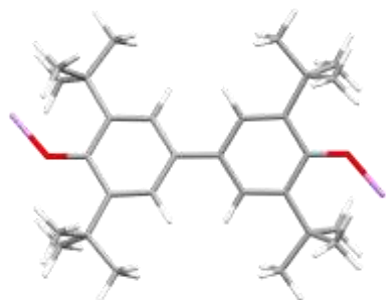
PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.623087	-3.718829	-0.859787
C	3.580056	-2.544664	-0.592484
C	4.458249	-2.923446	0.623539
C	4.470299	-2.368962	-1.844974
C	2.828610	-1.241899	-0.300603
C	1.453197	-1.186801	-0.296989
C	0.721514	0.005385	-0.048401
C	-0.734931	0.008864	-0.064042
C	-1.474063	-1.174754	0.135522
C	-2.866657	-1.213352	0.108813
C	-3.624356	-2.490611	0.558146
C	-2.656369	-3.623728	0.940112
C	-4.478073	-2.145349	1.798183
C	-4.563778	-3.073590	-0.533128
C	-3.594210	0.005939	-0.200506
C	-2.857004	1.245063	-0.318604
C	-3.605068	2.570545	-0.535737

C	-2.651009	3.777131	-0.540302
C	-4.342748	2.556077	-1.894329
C	-4.623189	2.781510	0.607411
C	-1.474329	1.202068	-0.251334
C	1.459388	1.190349	0.212986
C	2.835398	1.231702	0.240750
C	3.593050	2.527104	0.548438
C	2.641887	3.708689	0.803161
C	4.494996	2.901036	-0.651700
C	4.460583	2.339544	1.815191
C	3.592287	-0.008301	-0.024338
O	4.850465	-0.014472	-0.015471
H	1.985491	-3.541406	-1.739656
H	1.974208	-3.928658	0.004682
H	3.213602	-4.625449	-1.057220
H	5.198559	-2.142639	0.829483
H	3.836802	-3.066991	1.520645
H	4.985421	-3.868742	0.420064
H	5.210266	-1.575864	-1.690935
H	4.998827	-3.310967	-2.059847
H	3.857339	-2.115084	-2.723350
H	0.888354	-2.087647	-0.533137
H	-0.923623	-2.081048	0.379497
H	-2.039592	-3.952844	0.089748
H	-1.984665	-3.323487	1.755812
H	-3.233821	-4.491832	1.290334
H	-5.192483	-1.344360	1.569515
H	-5.035224	-3.031362	2.141301
H	-3.829422	-1.811229	2.619965
H	-5.479613	-2.467986	-0.653968
H	-4.919839	-4.072597	-0.243762
H	-4.032342	-3.224111	-1.495348
H	-2.086164	3.857912	0.400513
H	-1.932958	3.738628	-1.373517
H	-3.238578	4.699738	-0.654921
H	-5.115935	1.778374	-1.910441
H	-3.633908	2.383899	-2.719667
H	-4.830100	3.527953	-2.068863
H	-5.165832	3.727602	0.455840
H	-4.106230	2.839192	1.576986
H	-5.350382	1.962022	0.645023
H	-0.918002	2.126613	-0.393396
H	0.900582	2.096863	0.439488
H	3.237002	4.609262	1.013779
H	2.009731	3.927630	-0.071231
H	1.987450	3.534863	1.671035
H	5.232423	2.114870	-0.847548
H	5.026207	3.841403	-0.436485

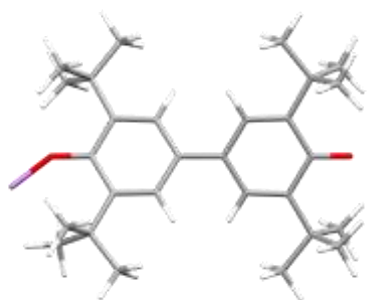
H	3.889869	3.052828	-1.558581
H	4.992718	3.276674	2.041802
H	3.830654	2.088619	2.682209
H	5.196902	1.541084	1.671471
O	-4.888079	-0.047951	-0.430985
Li	-4.522875	-1.169678	-1.742062



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.723152	-3.738422	-0.573351
C	3.635000	-2.518096	-0.356320
C	4.481189	-2.842514	0.911255
C	4.511163	-2.409374	-1.639708
C	2.853042	-1.212492	-0.141321
C	1.474309	-1.193146	-0.155190
C	0.724433	-0.000922	0.021182
C	-0.724785	-0.011151	-0.008216
C	-1.463736	-1.212165	0.155889
C	-2.843111	-1.274612	0.138888
C	-3.584017	-2.603397	0.344629
C	-2.613219	-3.777673	0.557561
C	-4.487089	-2.516162	1.596552
C	-4.435555	-2.927680	-0.904859
C	-3.581374	-0.042095	-0.071978
C	-2.845291	1.202232	-0.245785
C	-3.618142	2.509875	-0.480428
C	-2.698477	3.731950	-0.649290
C	-4.441601	2.412949	-1.799173
C	-4.515020	2.822948	0.754734
C	-1.467123	1.182760	-0.203993
C	1.455914	1.198420	0.225948
C	2.834835	1.260765	0.265379
C	3.566560	2.587495	0.512983
C	2.587720	3.759972	0.697065
C	4.467932	2.922931	-0.698011
C	4.418215	2.488753	1.799603
C	3.581256	0.030073	0.073417
H	2.094392	-3.622788	-1.467396

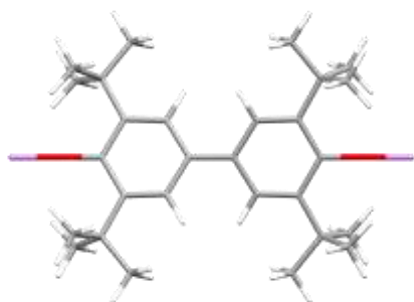
H	2.070532	-3.917319	0.292846
H	3.338428	-4.639117	-0.715777
H	5.229847	-3.626650	0.706422
H	4.956059	-1.963605	1.381356
H	3.827951	-3.234344	1.702380
H	4.994993	-1.427052	-1.780660
H	5.257054	-3.220790	-1.689164
H	3.877499	-2.513422	-2.530663
H	0.935059	-2.118820	-0.345093
H	-0.910566	-2.129384	0.343874
H	-1.953598	-3.933106	-0.309940
H	-1.989768	-3.643728	1.454609
H	-3.193186	-4.700771	0.696864
H	-5.242509	-1.729504	1.493046
H	-5.003760	-3.475629	1.748273
H	-3.886799	-2.310203	2.495247
H	-5.190196	-2.154961	-1.087904
H	-4.950229	-3.889664	-0.762417
H	-3.798575	-3.014391	-1.797774
H	-2.081498	3.902868	0.244207
H	-2.034012	3.624309	-1.518155
H	-3.307648	4.634012	-0.808342
H	-5.185030	3.224915	-1.871434
H	-4.919144	1.432033	-1.968500
H	-3.772401	2.524956	-2.662759
H	-5.254914	3.609046	0.526870
H	-3.894422	3.207471	1.575177
H	-5.008374	1.939902	1.197237
H	-0.920797	2.110018	-0.363510
H	0.895418	2.113999	0.399684
H	3.161402	4.681663	0.868096
H	1.963738	3.923380	-0.194989
H	1.928483	3.618018	1.566883
H	5.229507	2.151763	-0.857345
H	4.976240	3.883490	-0.526135
H	3.867613	3.017846	-1.615163
H	4.928144	3.446710	1.980809
H	3.782067	2.274769	2.671352
H	5.177351	1.702926	1.719646
O	-4.874646	-0.043582	-0.105932
Li	-6.002971	1.271121	-0.346763
O	4.874842	0.031631	0.091873
Li	6.012237	-1.281040	-0.114979

B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.657020	-3.716928	-0.801923
C	3.606164	-2.537238	-0.533707
C	4.476101	-2.909407	0.687866
C	4.501332	-2.366711	-1.781124
C	2.845225	-1.236844	-0.253385
C	1.478071	-1.184774	-0.259074
C	0.742693	0.002723	-0.023236
C	-0.712207	0.003757	-0.044738
C	-1.450744	-1.169701	0.181632
C	-2.831469	-1.197918	0.168481
C	-3.601585	-2.487390	0.504915
C	-2.672007	-3.701644	0.674296
C	-4.343067	-2.295758	1.847069
C	-4.616029	-2.852075	-0.630500
C	-3.554307	0.008825	-0.110961
C	-2.826940	1.222611	-0.330424
C	-3.568453	2.540408	-0.617418
C	-2.604769	3.726774	-0.790220
C	-4.379252	2.420764	-1.925107
C	-4.507204	2.884655	0.558678
C	-1.446418	1.179059	-0.286835
C	1.474057	1.187995	0.233768
C	2.841145	1.235458	0.269156
C	3.596986	2.533839	0.571404
C	2.643519	3.716423	0.809426
C	4.504895	2.901909	-0.623574
C	4.453314	2.361465	1.845594
C	3.599221	-0.001886	0.019646
O	4.846192	-0.004442	0.038791
H	2.028807	-3.546577	-1.679052
H	2.009075	-3.923443	0.052992
H	3.247412	-4.615382	-0.990603
H	5.211269	-2.136926	0.895691
H	3.852566	-3.046712	1.574706
H	4.999775	-3.849435	0.495298
H	5.237328	-1.581561	-1.631458

H	5.025449	-3.302889	-1.990440
H	3.895823	-2.116781	-2.655736
H	0.919632	-2.077763	-0.490463
H	-0.907594	-2.072062	0.411824
H	-2.100546	-3.904271	-0.233451
H	-1.970654	-3.562192	1.497132
H	-3.268676	-4.587947	0.901008
H	-4.998968	-1.425643	1.820650
H	-4.934345	-3.182238	2.094797
H	-3.623048	-2.136490	2.650593
H	-5.648322	-2.912405	-0.246503
H	-4.425677	-3.845740	-1.036515
H	-4.555689	-2.161169	-1.474413
H	-2.003200	3.897679	0.104677
H	-1.930167	3.588803	-1.637486
H	-3.182491	4.634350	-0.975801
H	-5.117495	1.625661	-1.858051
H	-3.716955	2.207330	-2.767130
H	-4.899119	3.359544	-2.133979
H	-5.037180	3.819005	0.354684
H	-3.931413	3.018394	1.477162
H	-5.238237	2.097692	0.724564
H	-0.893359	2.082699	-0.483872
H	0.911746	2.082935	0.446711
H	3.230576	4.613341	1.014890
H	2.022070	3.924031	-0.064512
H	1.988579	3.549321	1.667306
H	5.244201	2.127443	-0.808211
H	5.024789	3.840777	-0.415955
H	3.908987	3.040258	-1.529008
H	4.973274	3.296421	2.069959
H	3.820655	2.114375	2.701579
H	5.191466	1.574202	1.719223
O	-4.859607	-0.013220	-0.170552
Li	-6.142200	-0.991022	-0.566954

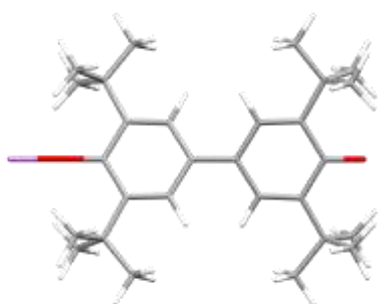


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
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C	2.622452	-3.748471	-0.582934
C	3.585102	-2.567132	-0.365613
C	4.432788	-2.911931	0.878154
C	4.471531	-2.481372	-1.626732
C	2.836523	-1.240516	-0.147396
C	1.465397	-1.196626	-0.160622
C	0.721079	-0.005766	0.012426
C	-0.721088	-0.006208	-0.016793
C	-1.464461	-1.199170	0.145495
C	-2.835548	-1.244037	0.131857
C	-3.583055	-2.573173	0.338064
C	-2.619445	-3.755633	0.544766
C	-4.469612	-2.499531	1.599857
C	-4.430423	-2.907403	-0.908794
C	-3.559419	-0.007074	-0.074294
C	-2.828546	1.230331	-0.250972
C	-3.567903	2.559016	-0.487277
C	-2.597443	3.742069	-0.654827
C	-4.402638	2.484863	-1.783915
C	-4.465227	2.892699	0.724280
C	-1.458004	1.186303	-0.209069
C	1.457049	1.185547	0.215465
C	2.827558	1.230289	0.257790
C	3.565861	2.557363	0.506131
C	2.594449	3.738078	0.684317
C	4.462992	2.902691	-0.702297
C	4.400589	2.472124	1.802081
C	3.559410	-0.004890	0.069943
H	1.999670	-3.612291	-1.468846
H	1.972321	-3.911081	0.278687
H	3.202302	-4.660720	-0.729747
H	4.973036	-3.847065	0.716427
H	5.154314	-2.132493	1.112126
H	3.793690	-3.040212	1.753574
H	5.193761	-1.670366	-1.566596
H	5.013953	-3.418434	-1.768826
H	3.859306	-2.309942	-2.513880
H	0.922158	-2.106592	-0.348749
H	-0.920495	-2.110360	0.325406
H	-1.969103	-3.909898	-0.318227
H	-1.996855	-3.626969	1.431938
H	-3.198551	-4.669654	0.683251
H	-5.192862	-1.688949	1.546786
H	-5.010903	-3.438459	1.733698
H	-3.857620	-2.335156	2.488497
H	-5.152451	-2.126381	-1.135781

H	-4.970038	-3.844319	-0.755485
H	-3.791187	-3.027405	-1.785284
H	-1.982666	3.896734	0.233783
H	-1.939368	3.613789	-1.516063
H	-3.171031	4.655733	-0.816665
H	-4.938787	3.423397	-1.939456
H	-5.126815	1.673714	-1.760249
H	-3.755062	2.321069	-2.647080
H	-4.998759	3.829295	0.549269
H	-3.862046	3.013057	1.625917
H	-5.195374	2.111234	0.921879
H	-0.907756	2.097829	-0.366810
H	0.906076	2.095175	0.381424
H	3.167303	4.650701	0.854416
H	1.979575	3.900267	-0.202885
H	1.936451	3.601504	1.544337
H	5.193801	2.123640	-0.906844
H	4.995747	3.838106	-0.518799
H	3.859775	3.030692	-1.602858
H	4.935810	3.409718	1.966258
H	3.753134	2.299780	2.663672
H	5.125579	1.661956	1.770971
O	-4.844902	-0.007461	-0.100345
Li	-6.501423	-0.007921	-0.133922
O	4.844900	-0.004501	0.096007
Li	6.501417	-0.005006	0.129409

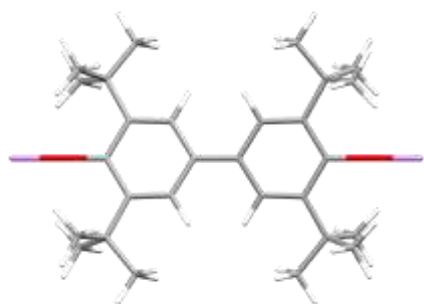
B3LYP/def2TZVP (CPCM – DME)



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.643143	-3.765133	-0.567667
C	3.598415	-2.575599	-0.373563
C	4.465582	-2.879896	0.868093
C	4.492790	-2.493189	-1.630048
C	2.846697	-1.252191	-0.173776
C	1.478681	-1.201827	-0.178846
C	0.735389	-0.004414	-0.015007

C	-0.711657	-0.002425	-0.032562
C	-1.459973	-1.187717	0.139578
C	-2.835929	-1.229276	0.134461
C	-3.579218	-2.561080	0.343999
C	-2.617165	-3.744273	0.551943
C	-4.470836	-2.484979	1.601838
C	-4.430898	-2.892264	-0.900407
C	-3.574118	0.001517	-0.067286
C	-2.827866	1.230264	-0.251036
C	-3.562181	2.564101	-0.478526
C	-2.592107	3.744630	-0.663042
C	-4.423221	2.490407	-1.757630
C	-4.442880	2.897694	0.744859
C	-1.452310	1.184917	-0.222772
C	1.477773	1.190958	0.166856
C	2.845643	1.237569	0.194966
C	3.595923	2.558914	0.412976
C	2.639494	3.751078	0.583858
C	4.493812	2.860770	-0.807255
C	4.459300	2.474104	1.690802
C	3.604455	-0.008350	0.019782
O	4.858474	-0.010077	0.035024
H	2.014970	-3.646123	-1.453015
H	1.993543	-3.914606	0.297396
H	3.229788	-4.676138	-0.700373
H	5.198633	-2.095416	1.036021
H	3.838758	-2.969078	1.758821
H	4.991322	-3.828404	0.730263
H	5.228738	-1.699003	-1.536515
H	5.016548	-3.441600	-1.775772
H	3.885760	-2.304313	-2.518946
H	0.927147	-2.112197	-0.347248
H	-0.918115	-2.102014	0.315171
H	-1.964075	-3.898666	-0.309244
H	-1.992636	-3.614348	1.438015
H	-3.199557	-4.657303	0.690920
H	-5.194848	-1.677933	1.531534
H	-5.009697	-3.426333	1.738343
H	-3.857862	-2.316946	2.490545
H	-4.978058	-3.825844	-0.744665
H	-3.788666	-3.020986	-1.774865
H	-5.145320	-2.103128	-1.117721
H	-1.959723	3.897304	0.213764
H	-1.946579	3.612912	-1.533665
H	-3.168432	4.659248	-0.816153
H	-5.150906	1.685324	-1.704965
H	-3.789319	2.320708	-2.631210
H	-4.956059	3.433216	-1.907116

H	-4.983529	3.832768	0.575897
H	-3.821691	3.024689	1.634635
H	-5.164537	2.110546	0.944774
H	-0.903837	2.097710	-0.385144
H	0.924816	2.102842	0.321875
H	3.225245	4.660464	0.730851
H	2.011543	3.902335	-0.296741
H	1.989646	3.633805	1.453657
H	5.228558	2.074267	-0.957359
H	5.018660	3.807833	-0.656678
H	3.889043	2.951641	-1.712935
H	4.981961	3.421084	1.849226
H	3.830354	2.286925	2.564695
H	5.195128	1.677905	1.615141
O	-4.856642	0.003277	-0.082846
Li	-6.615261	0.005688	-0.104183



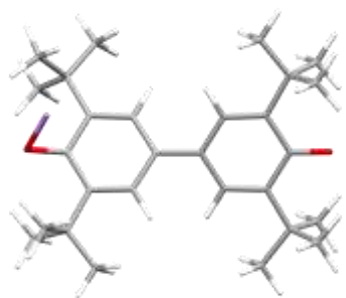
<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.623680	-3.755783	-0.540632
C	3.585805	-2.573303	-0.329808
C	4.426641	-2.898231	0.923908
C	4.487058	-2.500906	-1.581346
C	2.839975	-1.242993	-0.132136
C	1.468922	-1.197789	-0.147161
C	0.721460	-0.005773	0.012428
C	-0.721462	-0.006216	-0.016790
C	-1.467974	-1.200214	0.132063
C	-2.838991	-1.246371	0.116632
C	-3.583760	-2.578999	0.302325
C	-2.620691	-3.762561	0.502501
C	-4.485062	-2.518586	1.554464
C	-4.424345	-2.893301	-0.954264
C	-3.578774	-0.007094	-0.074643
C	-2.832616	1.232640	-0.235833
C	-3.570078	2.564812	-0.451541
C	-2.600424	3.748967	-0.612591
C	-4.419923	2.503855	-1.739134

C	-4.461028	2.878587	0.769990
C	-1.462070	1.187325	-0.195755
C	1.461120	1.186697	0.202134
C	2.831629	1.232740	0.242626
C	3.568031	2.563501	0.470325
C	2.597436	3.745389	0.642015
C	4.458739	2.888966	-0.748321
C	4.417917	2.491631	1.757327
C	3.578772	-0.004899	0.070287
H	2.006855	-3.628696	-1.432456
H	1.964337	-3.906503	0.316395
H	3.206273	-4.669444	-0.671469
H	4.968309	-3.835978	0.777510
H	5.145943	-2.113858	1.141586
H	3.778069	-3.016942	1.794878
H	5.217645	-1.700282	-1.507708
H	5.019746	-3.446005	-1.712400
H	3.882242	-2.329410	-2.474755
H	0.925255	-2.110761	-0.321661
H	-0.923580	-2.114287	0.298341
H	-1.961241	-3.905044	-0.355852
H	-2.003954	-3.643008	1.395426
H	-3.202555	-4.677825	0.625121
H	-5.216293	-1.717919	1.488029
H	-5.016987	-3.465253	1.677014
H	-3.880377	-2.354645	2.449379
H	-5.144282	-2.107581	-1.164868
H	-4.965254	-3.832766	-0.816317
H	-3.775685	-3.003639	-1.826270
H	-1.976339	3.891845	0.271745
H	-1.947982	3.629804	-1.479824
H	-3.177411	4.663875	-0.758671
H	-4.947042	3.450193	-1.883123
H	-5.152745	1.702732	-1.702341
H	-3.779410	2.340303	-2.608838
H	-4.996492	3.817718	0.610244
H	-3.848263	2.989322	1.667534
H	-5.188414	2.092421	0.951297
H	-0.911954	2.101735	-0.339873
H	0.910277	2.099334	0.354478
H	3.173697	4.659409	0.796288
H	1.973214	3.895700	-0.240990
H	1.945114	3.617926	1.508157
H	5.186757	2.105047	-0.936680
H	4.993446	3.827052	-0.580128
H	3.845892	3.007275	-1.644842
H	4.944286	3.437052	1.909834
H	3.777530	2.319751	2.625517

H	5.151374	1.691452	1.713334
O	-4.851450	-0.007484	-0.100407
Li	-6.631085	-0.008028	-0.136437
O	4.851448	-0.004511	0.096061
Li	6.631084	-0.003969	0.132101

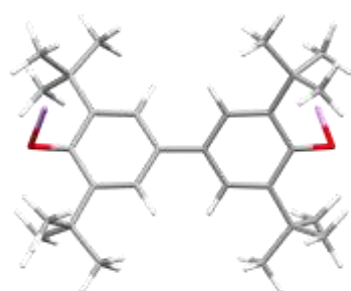
Doubly Reduced

PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.686847	-3.664756	-0.959481
C	3.621499	-2.485602	-0.642769
C	4.514523	-2.903649	0.547916
C	4.507482	-2.242581	-1.885750
C	2.858947	-1.198322	-0.288195
C	1.469918	-1.166674	-0.279279
C	0.721415	-0.010094	0.020739
C	-0.747534	-0.010335	0.021702
C	-1.498432	-1.182067	0.271780
C	-2.888827	-1.215511	0.346535
C	-3.639435	-2.528322	0.634256
C	-2.699049	-3.744598	0.672026
C	-4.352961	-2.447302	2.003178
C	-4.685451	-2.777140	-0.475006
C	-3.629137	0.006050	0.171966
C	-2.893394	1.199809	-0.179918
C	-3.651268	2.466476	-0.669594
C	-2.687920	3.565745	-1.148038
C	-4.561142	2.072037	-1.852723
C	-4.537715	3.117307	0.427679
C	-1.489865	1.153323	-0.236844
C	1.455537	1.154284	0.326797
C	2.843747	1.203035	0.343931
C	3.589403	2.498066	0.705728
C	2.639673	3.666762	1.017012
C	4.485908	2.927526	-0.478203
C	4.469487	2.263571	1.954469
C	3.621808	0.006779	0.029758

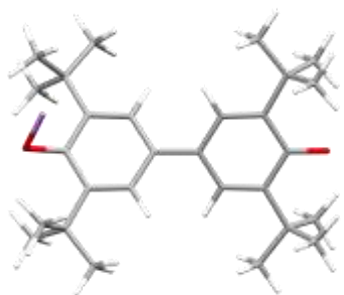
O	4.902939	0.014517	0.035070
H	2.039414	-3.455992	-1.825586
H	2.041711	-3.919261	-0.103765
H	3.292286	-4.553914	-1.199584
H	5.201352	-2.085262	0.798799
H	3.893206	-3.130864	1.428839
H	5.096924	-3.807108	0.294859
H	5.195739	-1.410143	-1.691390
H	5.088781	-3.149442	-2.128878
H	3.881402	-1.991785	-2.756754
H	0.919141	-2.068935	-0.553198
H	-0.938953	-2.099590	0.453138
H	-2.148101	-3.863902	-0.272653
H	-1.964043	-3.676217	1.487973
H	-3.294168	-4.657131	0.834127
H	-5.095043	-1.638385	1.995960
H	-4.869330	-3.396535	2.224396
H	-3.621383	-2.265543	2.806845
H	-5.390447	-1.938288	-0.531893
H	-5.245329	-3.705172	-0.270324
H	-4.187084	-2.887411	-1.450246
H	-2.033391	3.927454	-0.340545
H	-2.048118	3.210155	-1.966856
H	-3.270183	4.422795	-1.521779
H	-5.262585	1.285344	-1.544202
H	-3.947983	1.691812	-2.682184
H	-5.130426	2.944410	-2.216112
H	-4.940953	4.082520	0.084768
H	-3.947831	3.346626	1.338146
H	-5.418247	2.491750	0.659301
H	-0.934762	2.043760	-0.528246
H	0.890824	2.049007	0.598628
H	3.233494	4.562769	1.260922
H	1.997024	3.913511	0.157007
H	1.989465	3.449975	1.879383
H	5.182015	2.115816	-0.725240
H	5.057962	3.836228	-0.220101
H	3.868352	3.149380	-1.363098
H	5.040634	3.175742	2.202083
H	3.840334	2.005548	2.821285
H	5.166627	1.437713	1.763327
O	-4.940719	0.092523	0.437134
Li	-4.294862	1.210886	1.645790



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.639516	-3.669586	-0.961591
C	3.596240	-2.475250	-0.807124
C	4.611717	-2.827974	0.302624
C	4.339078	-2.297751	-2.151110
C	2.854995	-1.180814	-0.431939
C	1.466256	-1.141448	-0.356446
C	0.738787	0.015148	-0.015277
C	-0.738789	0.015158	0.015296
C	-1.466273	-1.141427	0.356475
C	-2.855012	-1.180774	0.431979
C	-3.596274	-2.475205	0.807146
C	-2.639559	-3.669548	0.961612
C	-4.339144	-2.297728	2.151117
C	-4.611734	-2.827903	-0.302627
C	-3.598880	0.024423	0.161194
C	-2.874839	1.201095	-0.272038
C	-3.638474	2.419067	-0.859827
C	-2.678223	3.506457	-1.371425
C	-4.497600	1.934946	-2.048247
C	-4.575004	3.118080	0.163236
C	-1.472613	1.159065	-0.314323
C	1.472627	1.159050	0.314327
C	2.874852	1.201060	0.272054
C	3.638499	2.419043	0.859798
C	2.678265	3.506479	1.371330
C	4.575053	3.117982	-0.163292
C	4.497602	1.934964	2.048252
C	3.598879	0.024369	-0.161140
H	1.921969	-3.525635	-1.783696
H	2.072316	-3.862604	-0.038612
H	3.224719	-4.573334	-1.188170
H	5.332728	-2.014051	0.443886
H	4.090956	-3.008162	1.255244
H	5.159163	-3.745973	0.035559
H	5.106800	-1.518638	-2.066972

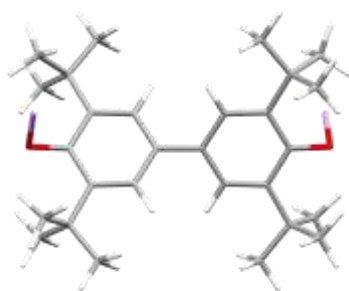
H	4.832338	-3.239453	-2.440207
H	3.631588	-2.029597	-2.951967
H	0.899501	-2.038295	-0.606171
H	-0.899529	-2.038280	0.606198
H	-2.072337	-3.862553	0.038644
H	-1.922032	-3.525615	1.783737
H	-3.224772	-4.573298	1.188161
H	-5.106966	-1.518719	2.066945
H	-4.832284	-3.239481	2.440253
H	-3.631694	-2.029452	2.951969
H	-5.332729	-2.013966	-0.443894
H	-5.159203	-3.745893	-0.035579
H	-4.090958	-3.008093	-1.255238
H	-2.055771	3.926399	-0.566133
H	-2.011152	3.119047	-2.153656
H	-3.261484	4.330261	-1.809542
H	-5.198461	1.155727	-1.722022
H	-3.850490	1.518552	-2.833158
H	-5.068324	2.772081	-2.481853
H	-4.959133	4.065031	-0.243534
H	-4.032138	3.395076	1.089963
H	-5.470795	2.509039	0.377821
H	-0.918808	2.031876	-0.659716
H	0.918830	2.031876	0.659699
H	3.261537	4.330293	1.809411
H	2.055829	3.926392	0.566011
H	2.011178	3.119123	2.153576
H	5.470851	2.508926	-0.377805
H	4.959171	4.064965	0.243415
H	4.032209	3.394905	-1.090054
H	5.068336	2.772111	2.481822
H	3.850474	1.518624	2.833177
H	5.198449	1.155715	1.722074
O	-4.905576	0.101321	0.375061
Li	-4.437031	1.328533	1.548569
O	4.905590	0.101230	-0.374952
Li	4.437193	1.328356	-1.548577

B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.677202	-3.632520	-1.062283
C	3.611669	-2.462784	-0.712158
C	4.500763	-2.919531	0.465337
C	4.497250	-2.192800	-1.948143
C	2.848249	-1.185913	-0.324088
C	1.465500	-1.152126	-0.314851
C	0.722493	-0.009247	0.015910
C	-0.748347	-0.009303	0.016171
C	-1.492404	-1.165936	0.309933
C	-2.876997	-1.197617	0.379913
C	-3.629150	-2.500118	0.707781
C	-2.687201	-3.711771	0.801925
C	-4.357779	-2.376984	2.063879
C	-4.659078	-2.797705	-0.402516
C	-3.610053	0.011655	0.157229
C	-2.882633	1.187210	-0.226290
C	-3.639182	2.443775	-0.736085
C	-2.678455	3.542039	-1.220127
C	-4.539491	2.039863	-1.921352
C	-4.529095	3.100199	0.351981
C	-1.484783	1.138324	-0.280148
C	1.452300	1.140352	0.353086
C	2.834363	1.189121	0.372148
C	3.581927	2.473057	0.767376
C	2.633297	3.634193	1.108806
C	4.477087	2.938631	-0.402000
C	4.458989	2.211797	2.011201
C	3.606235	0.005409	0.026917
O	4.878410	0.011808	0.033501
H	2.035878	-3.401037	-1.916175
H	2.036776	-3.908317	-0.220821
H	3.276724	-4.508950	-1.324834
H	5.191352	-2.125429	0.740594
H	3.881223	-3.164245	1.332794
H	5.070216	-3.814946	0.190290
H	5.189319	-1.379615	-1.740576

H	5.065490	-3.091175	-2.215902
H	3.875468	-1.916442	-2.804315
H	0.915310	-2.036211	-0.608104
H	-0.934221	-2.064185	0.526118
H	-2.130526	-3.864230	-0.124406
H	-1.967529	-3.611091	1.616661
H	-3.276655	-4.612767	0.990263
H	-5.114411	-1.596021	2.019933
H	-4.849631	-3.320760	2.319855
H	-3.643739	-2.145584	2.859611
H	-5.365054	-1.976179	-0.502149
H	-5.210447	-3.714888	-0.171352
H	-4.150972	-2.941253	-1.359143
H	-2.035683	3.910106	-0.417771
H	-2.038610	3.186111	-2.027228
H	-3.256712	4.387566	-1.601617
H	-5.240579	1.263760	-1.619010
H	-3.924966	1.656472	-2.737612
H	-5.100027	2.904080	-2.293146
H	-4.923968	4.058887	0.008802
H	-3.946535	3.321826	1.258427
H	-5.404327	2.482958	0.578637
H	-0.932088	2.010830	-0.591189
H	0.889868	2.018117	0.643130
H	3.222025	4.516896	1.374975
H	1.996847	3.902078	0.261659
H	1.987722	3.396961	1.958226
H	5.176411	2.150170	-0.671326
H	5.036792	3.838651	-0.121750
H	3.863138	3.178077	-1.274855
H	5.017363	3.115006	2.283730
H	3.832371	1.929668	2.862093
H	5.159439	1.404378	1.809239
O	-4.920807	0.096054	0.399100
Li	-4.363584	1.194772	1.630914

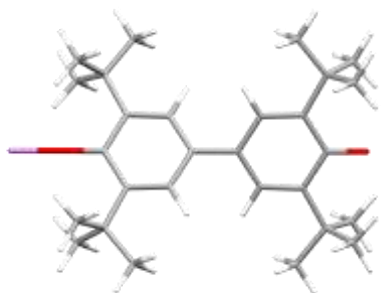


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
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C	2.624752	-3.630232	-1.092403
C	3.587807	-2.457849	-0.840306
C	4.547500	-2.880656	0.292037
C	4.389228	-2.240992	-2.142918
C	2.846386	-1.170245	-0.438037
C	1.461141	-1.129648	-0.385183
C	0.739629	0.009344	-0.011221
C	-0.739627	0.009352	0.011205
C	-1.461151	-1.129624	0.385189
C	-2.846397	-1.170205	0.438041
C	-3.587832	-2.457794	0.840334
C	-2.624789	-3.630181	1.092463
C	-4.389258	-2.240903	2.142937
C	-4.547523	-2.880617	-0.292005
C	-3.583513	0.014250	0.107752
C	-2.863557	1.178469	-0.321877
C	-3.623507	2.415535	-0.855058
C	-2.670085	3.543471	-1.283616
C	-4.461647	2.005396	-2.083656
C	-4.573914	3.031613	0.205218
C	-1.469470	1.138807	-0.348452
C	1.469485	1.138796	0.348415
C	2.863573	1.178444	0.321839
C	3.623536	2.415505	0.855014
C	2.670125	3.543449	1.283573
C	4.573946	3.031575	-0.205263
C	4.461675	2.005361	2.083611
C	3.583516	0.014209	-0.107775
H	1.946743	-3.435355	-1.926118
H	2.025022	-3.859569	-0.209670
H	3.202233	-4.523411	-1.339566
H	5.265314	-2.092892	0.507103
H	3.984653	-3.098867	1.202456
H	5.090808	-3.786032	0.006662
H	5.186744	-1.516733	-1.987787
H	4.846756	-3.178852	-2.468908
H	3.731329	-1.895315	-2.945636
H	0.896147	-2.004159	-0.670494
H	-0.896167	-2.004135	0.670519
H	-2.025057	-3.859543	0.209737
H	-1.946783	-3.435291	1.926176
H	-3.202280	-4.523348	1.339643
H	-5.186768	-1.516641	1.987784
H	-4.846796	-3.178751	2.468944
H	-3.731362	-1.895212	2.945651
H	-5.265326	-2.092850	-0.507096
H	-5.090843	-3.785980	-0.006613
H	-3.984671	-3.098857	-1.202415

H	-2.069299	3.913119	-0.449382
H	-1.993024	3.217830	-2.073494
H	-3.250870	4.381460	-1.674781
H	-5.150614	1.203128	-1.826420
H	-3.804955	1.657377	-2.882719
H	-5.033940	2.857806	-2.461809
H	-4.915675	4.021907	-0.101411
H	-4.056286	3.176166	1.164981
H	-5.480867	2.430659	0.318599
H	-0.916922	2.000817	-0.690706
H	0.916946	2.000818	0.690657
H	3.250918	4.381433	1.674737
H	2.069341	3.913103	0.449340
H	1.993061	3.217814	2.073451
H	5.480889	2.430607	-0.318658
H	4.915727	4.021860	0.101373
H	4.056313	3.176148	-1.165021
H	5.033974	2.857766	2.461764
H	3.804982	1.657346	2.882675
H	5.150637	1.203088	1.826374
O	-4.900510	0.059605	0.242848
Li	-4.744161	1.126565	1.585324
O	4.900510	0.059554	-0.242887
Li	4.744107	1.126531	-1.585348

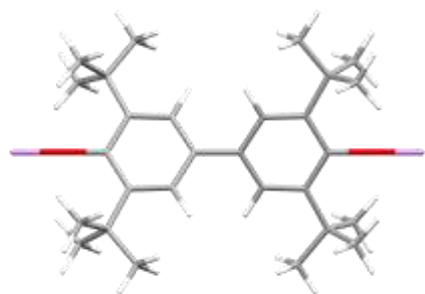
B3LYP/def2TZVP (CPCM – DME)



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.640665	-3.654018	-1.027927
C	3.600883	-2.493620	-0.716147
C	4.497341	-2.948610	0.455769
C	4.468904	-2.269696	-1.972843
C	2.868255	-1.192568	-0.340539
C	1.480070	-1.144162	-0.316596
C	0.749465	0.004037	0.014414
C	-0.731380	0.008986	0.031826
C	-1.469656	-1.129187	0.371392
C	-2.861747	-1.167230	0.390482

C	-3.594829	-2.470604	0.766645
C	-2.630399	-3.626545	1.088007
C	-4.462977	-2.255023	2.024328
C	-4.472268	-2.941930	-0.412827
C	-3.601064	0.018574	0.065560
C	-2.861683	1.199441	-0.276736
C	-3.594681	2.507718	-0.635649
C	-2.630372	3.657220	-0.979671
C	-4.493578	2.298056	-1.872559
C	-4.440977	2.984788	0.564095
C	-1.469813	1.152096	-0.290375
C	1.495308	1.147301	0.328064
C	2.883964	1.186429	0.319355
C	3.633899	2.482526	0.677531
C	2.689053	3.649291	1.011707
C	4.505577	2.931605	-0.515174
C	4.529711	2.252709	1.913489
C	3.638408	-0.005617	-0.019554
O	4.923300	-0.009911	-0.034661
H	1.991791	-3.432233	-1.878278
H	2.007290	-3.901837	-0.173072
H	3.221525	-4.545270	-1.279111
H	5.204015	-2.163632	0.714872
H	3.886346	-3.175579	1.333969
H	5.049983	-3.854922	0.187091
H	5.176654	-1.462012	-1.801331
H	5.019638	-3.181365	-2.226907
H	3.838176	-2.008970	-2.827373
H	0.919057	-2.028564	-0.585668
H	-0.916259	-2.014329	0.647801
H	-1.991407	-3.874984	0.238387
H	-1.988826	-3.399802	1.941810
H	-3.210209	-4.518443	1.338033
H	-5.174122	-1.446809	1.874872
H	-5.012245	-3.168607	2.271853
H	-3.831113	-2.001314	2.879345
H	-5.175528	-2.168808	-0.711353
H	-5.031254	-3.842097	-0.139138
H	-3.845460	-3.185337	-1.274527
H	-1.969941	3.901312	-0.145324
H	-2.010573	3.426270	-1.848302
H	-3.209928	4.552992	-1.216063
H	-5.206395	1.494597	-1.706372
H	-3.883699	2.040211	-2.742179
H	-5.042400	3.215311	-2.107162
H	-5.000209	3.888701	0.303568
H	-3.792470	3.223915	1.410806
H	-5.142182	2.216360	0.879121

H	-0.917165	2.033543	-0.579784
H	0.946699	2.035412	0.610182
H	3.281601	4.536620	1.249101
H	2.037429	3.901408	0.171958
H	2.058878	3.431778	1.877093
H	5.200699	2.141940	-0.790760
H	5.070430	3.834180	-0.259636
H	3.875633	3.162723	-1.378784
H	5.092347	3.160658	2.154461
H	3.917520	1.996137	2.782632
H	5.227819	1.440326	1.725448
O	-4.911057	0.022949	0.080958
Li	-6.630718	0.028688	0.101177



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.607501	-3.626811	-1.108196
C	3.580730	-2.475373	-0.797470
C	4.471732	-2.951949	0.369677
C	4.432671	-2.260066	-2.066178
C	2.856779	-1.170924	-0.409108
C	1.466387	-1.128170	-0.369353
C	0.740602	0.013412	-0.018707
C	-0.740600	0.013400	0.018709
C	-1.466375	-1.128289	0.369030
C	-2.856767	-1.171068	0.408768
C	-3.580706	-2.475634	0.796757
C	-2.607467	-3.627150	1.107163
C	-4.432657	-2.260693	2.065521
C	-4.471698	-2.951888	-0.370529
C	-3.604189	0.013377	0.091038
C	-2.873779	1.197834	-0.264017
C	-3.616405	2.502388	-0.614961
C	-2.660097	3.653922	-0.974102
C	-4.531317	2.287433	-1.839098
C	-4.447340	2.978624	0.595818
C	-1.483154	1.155077	-0.294523
C	1.483145	1.155007	0.294848

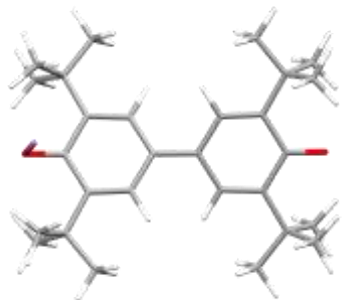
C	2.873770	1.197787	0.264349
C	3.616382	2.502250	0.615660
C	2.660061	3.653670	0.975130
C	4.447306	2.978841	-0.594987
C	4.531304	2.286961	1.839730
C	3.604191	0.013438	-0.091046
H	1.955353	-3.395791	-1.952896
H	1.979646	-3.875374	-0.250238
H	3.180360	-4.520085	-1.368246
H	5.182896	-2.183191	0.660265
H	3.855706	-3.194073	1.239435
H	5.022733	-3.853924	0.086792
H	5.150343	-1.456336	-1.924852
H	4.973728	-3.175663	-2.323181
H	3.790815	-2.000903	-2.912025
H	0.905572	-2.010899	-0.638588
H	-0.905551	-2.011088	0.638016
H	-1.979607	-3.875466	0.249137
H	-1.955325	-3.396361	1.951930
H	-3.180319	-4.520503	1.366960
H	-5.150338	-1.456933	1.924416
H	-4.973705	-3.176369	2.322264
H	-3.790809	-2.001760	2.911444
H	-5.182869	-2.183055	-0.660901
H	-5.022690	-3.853950	-0.087903
H	-3.855665	-3.193758	-1.240354
H	-1.989723	3.902245	-0.148868
H	-2.051432	3.423146	-1.850717
H	-3.245350	4.547265	-1.204642
H	-5.240945	1.483659	-1.661944
H	-3.932987	2.028513	-2.716346
H	-5.084653	3.203099	-2.068198
H	-5.011930	3.880664	0.341365
H	-3.788182	3.220525	1.433427
H	-5.142916	2.209769	0.921734
H	-0.936639	2.037885	-0.591480
H	0.936623	2.037726	0.592055
H	3.245303	4.546956	1.205920
H	1.989680	3.902217	0.149969
H	2.051403	3.422639	1.851683
H	5.142926	2.210106	-0.921092
H	5.011844	3.880847	-0.340296
H	3.788147	3.220919	-1.432544
H	5.084634	3.202567	2.069083
H	3.932982	2.027791	2.716910
H	5.240937	1.483242	1.662347
O	-4.910003	0.013366	0.124020
Li	-6.634711	0.013361	0.167581

O	4.910004	0.013451	-0.124035
Li	6.634712	0.013459	-0.167615

Sodium

Singly Reduced

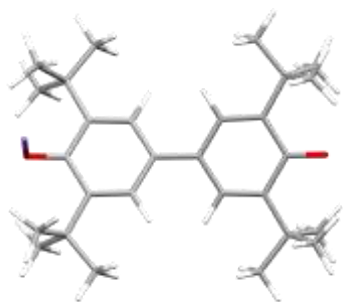
PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	4.219373	-1.978801	-1.481562
C	3.739145	-0.520918	-1.269151
C	4.388318	-0.020536	0.032289
C	4.260007	0.356123	-2.429320
C	2.201317	-0.449741	-1.220104
C	1.546528	0.022947	-0.092413
C	0.138811	0.112262	0.012129
C	-0.508377	0.586434	1.225687
C	-1.872424	0.293375	1.496111
C	-2.523464	0.705999	2.636854
C	-3.991131	0.349283	2.896723
C	-4.108480	-0.481397	4.195934
C	-4.826706	1.644516	3.028246
C	-4.598152	-0.482178	1.754012
C	-1.782816	1.502231	3.634633
O	-2.339387	1.897756	4.692684
C	-0.369461	1.820029	3.352786
C	0.426995	2.664659	4.353280
C	0.483640	1.939928	5.718792
C	1.874672	2.901316	3.890683
C	-0.243944	4.047586	4.524175
C	0.199577	1.355222	2.188500
C	-0.607801	-0.288290	-1.120475
C	-0.029451	-0.763332	-2.288417
C	-0.897935	-1.143108	-3.502864
C	-0.707378	-2.636311	-3.871415
C	-2.398291	-0.936945	-3.234378
C	-0.505124	-0.270692	-4.715424

C	1.418114	-0.880639	-2.366757
H	5.311815	-2.049682	-1.367165
H	3.978308	-2.315046	-2.500901
H	3.778063	-2.649912	-0.720781
H	5.482864	-0.066748	-0.067015
H	4.105956	-0.631956	0.903101
H	4.120449	1.024374	0.245117
H	3.988794	1.408109	-2.259262
H	3.829567	0.032957	-3.384793
H	5.358101	0.294293	-2.492063
H	2.138124	0.308840	0.775157
H	-2.411751	-0.320731	0.776444
H	-3.733555	0.083927	5.056297
H	-3.534683	-1.417014	4.110031
H	-5.162904	-0.744400	4.375484
H	-4.766766	2.239103	2.103870
H	-5.884114	1.388675	3.200375
H	-4.469613	2.256236	3.864040
H	-4.581350	0.058067	0.794836
H	-5.649283	-0.703971	1.990233
H	-4.078994	-1.443997	1.620940
H	1.067830	2.540420	6.433852
H	-0.523477	1.788637	6.122753
H	0.975036	0.960099	5.616814
H	2.432606	1.958733	3.778193
H	2.398221	3.506969	4.644951
H	1.920748	3.448836	2.936811
H	0.336431	4.656968	5.234727
H	-0.275444	4.583630	3.563346
H	-1.266836	3.941686	4.902292
H	1.232855	1.618043	1.967609
H	-1.690039	-0.182144	-1.077171
H	-1.433935	-2.943638	-4.639014
H	0.296170	-2.799985	-4.291307
H	-0.887032	-3.282106	-2.991095
H	-2.765687	-1.565412	-2.408437
H	-2.629261	0.111353	-2.997024
H	-2.968547	-1.204242	-4.136277
H	0.559228	-0.389564	-4.951675
H	-1.101053	-0.551793	-5.598240
H	-0.700806	0.789209	-4.497652
O	1.991957	-1.420808	-3.406867
Na	1.779315	-3.355742	-2.452504

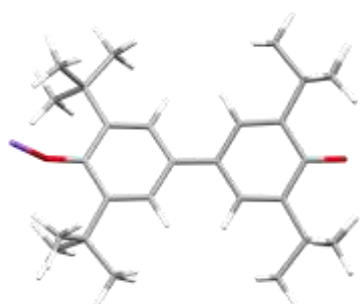
B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	4.211078	-2.014523	-1.451252
C	3.726931	-0.558594	-1.247774
C	4.378698	-0.053183	0.050124
C	4.250277	0.314151	-2.407814
C	2.189210	-0.482918	-1.197266
C	1.538595	-0.006735	-0.076705
C	0.138362	0.098838	0.021721
C	-0.508005	0.576479	1.231991
C	-1.863201	0.269654	1.510774
C	-2.512712	0.684009	2.641317
C	-3.974559	0.313375	2.915284
C	-4.076426	-0.503368	4.222542
C	-4.827299	1.596567	3.032452
C	-4.577165	-0.540289	1.787311
C	-1.777924	1.498829	3.622692
O	-2.330533	1.896665	4.667792
C	-0.372760	1.830481	3.335560
C	0.413637	2.696117	4.326332
C	0.485007	1.989177	5.698434
C	1.857142	2.945404	3.858935
C	-0.269805	4.072697	4.482173
C	0.192158	1.362290	2.180871
C	-0.604266	-0.280049	-1.112662
C	-0.029586	-0.756040	-2.274062
C	-0.893527	-1.098165	-3.502977
C	-0.749059	-2.589825	-3.890747
C	-2.390235	-0.851093	-3.250464
C	-0.465941	-0.222799	-4.699364
C	1.406653	-0.906649	-2.335625
H	5.293288	-2.083673	-1.321346
H	3.989944	-2.350765	-2.464887
H	3.757015	-2.681077	-0.707525
H	5.464937	-0.095954	-0.049934
H	4.101817	-0.659998	0.915172
H	4.110449	0.983263	0.259463
H	3.985508	1.359703	-2.239547

H	3.823192	-0.003705	-3.356178
H	5.340109	0.248372	-2.470608
H	2.122946	0.269942	0.785705
H	-2.388120	-0.353425	0.804363
H	-3.715974	0.069962	5.072201
H	-3.490057	-1.422475	4.146349
H	-5.117729	-0.782185	4.404244
H	-4.775684	2.176302	2.107657
H	-5.873375	1.330420	3.205461
H	-4.485700	2.220400	3.853757
H	-4.571851	-0.015879	0.829121
H	-5.616173	-0.771279	2.029207
H	-4.049833	-1.489161	1.665143
H	1.065091	2.597488	6.397336
H	-0.507740	1.834047	6.111801
H	0.980636	1.019725	5.604399
H	2.421016	2.015375	3.756674
H	2.371638	3.561025	4.598984
H	1.893684	3.478298	2.906292
H	0.305050	4.694439	5.173478
H	-0.312864	4.589733	3.520524
H	-1.280632	3.967532	4.866601
H	1.211190	1.629421	1.951495
H	-1.674052	-0.153883	-1.074480
H	-1.484326	-2.864538	-4.650154
H	0.236290	-2.777708	-4.318662
H	-0.931729	-3.235356	-3.022429
H	-2.782464	-1.478943	-2.447135
H	-2.590885	0.191122	-2.998882
H	-2.953229	-1.082958	-4.156590
H	0.588604	-0.363096	-4.925736
H	-1.054627	-0.476389	-5.585426
H	-0.636277	0.831270	-4.472528
O	1.974570	-1.452837	-3.367735
Na	1.845087	-3.446006	-2.655975

B3LYP/def2TZVP (CPCM – DME)

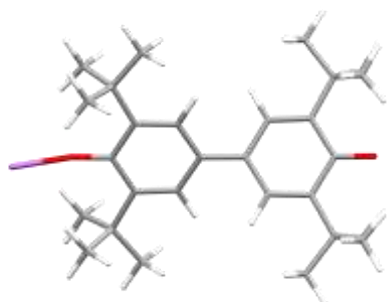


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	4.340204	-1.833626	-1.353951
C	3.725819	-0.419865	-1.290191
C	4.362254	0.292370	-0.083569
C	4.128938	0.368900	-2.554802
C	2.189858	-0.469952	-1.190810
C	1.542551	0.034026	-0.086897
C	0.135202	0.078273	0.045389
C	-0.507307	0.559345	1.247243
C	-1.880802	0.310370	1.503072
C	-2.533711	0.734391	2.629654
C	-4.018583	0.417087	2.858630
C	-4.190480	-0.414014	4.148901
C	-4.825736	1.729355	2.969855
C	-4.626455	-0.397403	1.704366
C	-1.791431	1.499911	3.638918
O	-2.352995	1.912477	4.683352
C	-0.369776	1.765874	3.385252
C	0.445312	2.571108	4.407611
C	0.456674	1.837277	5.766770
C	1.909704	2.753298	3.974333
C	-0.162775	3.980481	4.577913
C	0.200853	1.294008	2.233341
C	-0.610946	-0.348481	-1.078439
C	-0.043513	-0.857568	-2.222548
C	-0.915594	-1.207988	-3.442330
C	-0.868239	-2.718708	-3.750921
C	-2.393842	-0.840138	-3.224675
C	-0.421682	-0.418174	-4.673351
C	1.399175	-1.039532	-2.270478
H	5.428161	-1.775130	-1.268999
H	4.107647	-2.309408	-2.302162
H	3.970315	-2.460273	-0.539410
H	5.442654	0.347849	-0.229744
H	4.184246	-0.244224	0.850794
H	3.991676	1.312726	0.030671
H	3.766904	1.397830	-2.494691
H	3.716518	-0.092757	-3.449330
H	5.217907	0.399809	-2.647875
H	2.135574	0.394004	0.737221
H	-2.424561	-0.273563	0.778546
H	-3.821677	0.128153	5.015628
H	-3.646360	-1.358553	4.069757
H	-5.247428	-0.646762	4.303739
H	-4.736157	2.311464	2.049270
H	-5.884330	1.503167	3.123270
H	-4.473816	2.335708	3.800225
H	-4.576262	0.138140	0.753912

H	-5.679439	-0.590103	1.918786
H	-4.133250	-1.363947	1.580772
H	1.043919	2.406658	6.492193
H	-0.551517	1.713535	6.153033
H	0.914921	0.850460	5.663568
H	2.425922	1.797398	3.862320
H	2.439443	3.326348	4.737795
H	1.993901	3.301597	3.033636
H	0.423562	4.554122	5.300695
H	-0.146364	4.520141	3.627718
H	-1.190198	3.924209	4.927701
H	1.238584	1.513807	2.043811
H	-1.681340	-0.231725	-1.040612
H	-1.591793	-2.966074	-4.531882
H	0.116833	-3.006019	-4.105558
H	-1.112528	-3.307607	-2.864036
H	-2.844058	-1.412096	-2.410582
H	-2.523252	0.222385	-3.010372
H	-2.955635	-1.064702	-4.133375
H	0.618833	-0.647617	-4.892067
H	-1.026414	-0.669533	-5.548862
H	-0.512546	0.656474	-4.498956
O	1.953410	-1.678034	-3.229358
Na	2.458801	-3.823908	-3.389561

Doubly Reduced

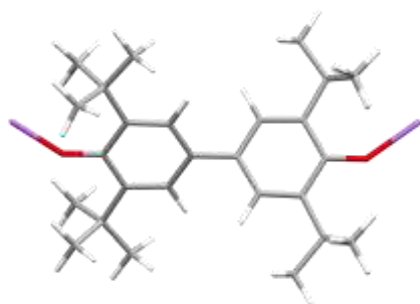
PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	1.961802	-0.873133	-4.808100
C	1.205314	-1.846943	-3.875829
C	2.253955	-2.616443	-3.055329
C	0.431292	-2.878038	-4.729244
C	0.221040	-1.064266	-2.992915
C	0.324564	-1.083552	-1.610587
C	-0.544077	-0.370989	-0.753556

C	-0.394893	-0.416371	0.704956
C	-0.867816	0.619851	1.534446
C	-0.745295	0.612776	2.921564
C	-1.275373	1.798955	3.750725
C	-1.969685	2.868338	2.887763
C	-0.100286	2.498711	4.467129
C	-2.320120	1.309422	4.779478
C	-0.105100	-0.505138	3.574279
O	0.000020	-0.559377	4.882487
Na	0.827253	-0.272465	6.760438
C	0.391969	-1.573598	2.739247
C	1.086885	-2.796031	3.370826
C	0.142825	-3.494960	4.375189
C	2.384362	-2.344663	4.075705
C	1.493667	-3.854978	2.329961
C	0.230349	-1.497162	1.358386
C	-1.562025	0.389220	-1.372248
C	-1.736712	0.459618	-2.745723
C	-2.873630	1.289509	-3.361934
C	-2.280637	2.379798	-4.284043
C	-3.805652	0.371668	-4.185630
C	-3.733535	1.995884	-2.300529
C	-0.834548	-0.276946	-3.632377
O	-0.962398	-0.235310	-4.902608
H	1.247825	-0.316376	-5.427420
H	2.654577	-1.430164	-5.462278
H	2.551687	-0.156970	-4.214664
H	2.923392	-3.159585	-3.741472
H	2.875005	-1.942832	-2.444695
H	1.789785	-3.356121	-2.384530
H	-0.317473	-2.366591	-5.346450
H	-0.080404	-3.604935	-4.079007
H	1.126637	-3.431934	-5.383384
H	1.135891	-1.647036	-1.147959
H	-1.328451	1.479040	1.048461
H	-2.333500	3.678927	3.539341
H	-1.285532	3.313736	2.150448
H	-2.835203	2.458090	2.346609
H	0.474581	1.780781	5.068179
H	0.585133	2.941614	3.728954
H	-0.463800	3.304146	5.127330
H	-2.665195	2.148925	5.407268
H	-1.897213	0.523474	5.416401
H	-3.194763	0.890252	4.259025
H	0.656909	-4.340901	4.862966
H	-0.741098	-3.889095	3.850836

H	-0.203777	-2.787115	5.137604
H	2.176593	-1.550204	4.805725
H	2.864010	-3.189824	4.597490
H	3.097729	-1.945221	3.339150
H	0.622344	-4.253089	1.789146
H	2.202563	-3.455786	1.589432
H	1.984304	-4.697332	2.843487
H	0.570691	-2.326258	0.739340
H	-2.261502	0.915838	-0.721749
H	-1.672971	1.915477	-5.070392
H	-1.645601	3.067270	-3.703383
H	-3.089942	2.969223	-4.748610
H	-3.232321	-0.137692	-4.969955
H	-4.612636	0.963856	-4.650651
H	-4.268240	-0.386447	-3.534283
H	-4.223112	1.279255	-1.623025
H	-4.524051	2.576398	-2.802554
H	-3.141197	2.694745	-1.689552

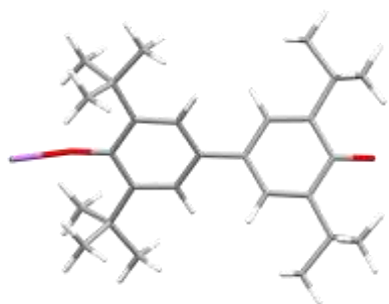


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.015071	-0.702720	-4.821103
C	1.317288	-1.718786	-3.889507
C	2.414759	-2.406056	-3.058784
C	0.626822	-2.815621	-4.731063
C	0.274737	-0.999916	-3.013437
C	0.385673	-1.009637	-1.622902
C	-0.528054	-0.372758	-0.766316
C	-0.370758	-0.416463	0.702621
C	-0.759530	0.656187	1.516505
C	-0.623679	0.638171	2.906401
C	-1.059946	1.850287	3.748086
C	-1.645535	3.001860	2.911783
C	0.171887	2.437022	4.487988
C	-2.181672	1.418678	4.730171
C	-0.055178	-0.514613	3.558249
O	0.092145	-0.559531	4.869466

Na	-0.176945	0.514900	6.596065
C	0.350347	-1.620041	2.732092
C	0.956808	-2.882216	3.372645
C	-0.057432	-3.518111	4.349434
C	2.254024	-2.514305	4.127547
C	1.324226	-3.954784	2.332701
C	0.177724	-1.536212	1.350368
C	-1.595370	0.303868	-1.372236
C	-1.764519	0.361884	-2.757377
C	-2.962135	1.112644	-3.365704
C	-2.443961	2.269336	-4.261592
C	-3.851975	0.115052	-4.154449
C	-3.878049	1.764912	-2.314950
C	-0.822819	-0.299619	-3.624918
O	-0.958773	-0.268370	-4.937758
Na	-2.156083	0.419114	-6.454917
H	1.276151	-0.186587	-5.446232
H	2.743475	-1.215136	-5.471407
H	2.557408	0.049279	-4.227833
H	3.123349	-2.905358	-3.737739
H	2.984762	-1.686240	-2.452384
H	2.002164	-3.171914	-2.384865
H	-0.165182	-2.379680	-5.352175
H	0.177243	-3.575225	-4.073447
H	1.360878	-3.318765	-5.382248
H	1.235382	-1.513733	-1.162244
H	-1.156794	1.546210	1.026476
H	-1.940845	3.829479	3.577059
H	-0.913498	3.394739	2.191925
H	-2.538136	2.684291	2.353931
H	0.835405	1.642792	4.863458
H	0.782967	3.024436	3.787909
H	-0.127418	3.122526	5.303988
H	-2.341215	2.171386	5.525854
H	-1.983368	0.425288	5.161117
H	-3.133861	1.321128	4.189267
H	0.380628	-4.407025	4.833142
H	-0.961676	-3.835332	3.807848
H	-0.349264	-2.795958	5.121774
H	2.049927	-1.753589	4.890928
H	2.682079	-3.407264	4.612753
H	3.003201	-2.114616	3.427146
H	0.444638	-4.302676	1.770514
H	2.070653	-3.589971	1.611107
H	1.756544	-4.826117	2.848707
H	0.456029	-2.387258	0.728603

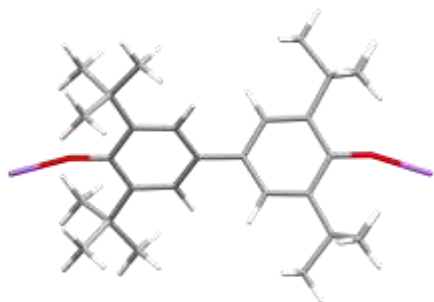
H	-2.331797	0.775809	-0.720289
H	-1.562362	1.965487	-4.846676
H	-2.107018	3.105935	-3.632841
H	-3.240248	2.664883	-4.920838
H	-3.245800	-0.616013	-4.711342
H	-4.558866	0.638280	-4.826677
H	-4.458616	-0.477669	-3.454985
H	-4.315529	1.018145	-1.637176
H	-4.706743	2.287652	-2.819690
H	-3.335665	2.503209	-1.707066

B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	1.977533	-0.791981	-4.798329
C	1.243623	-1.785311	-3.871081
C	2.313108	-2.528970	-3.054005
C	0.503934	-2.836824	-4.727382
C	0.238094	-1.033089	-2.985449
C	0.339865	-1.051837	-1.608647
C	-0.544688	-0.370511	-0.754750
C	-0.394989	-0.415510	0.705337
C	-0.832715	0.631753	1.527429
C	-0.709337	0.624901	2.909979
C	-1.206067	1.825164	3.739357
C	-1.872947	2.912370	2.877568
C	-0.015935	2.497616	4.454267
C	-2.263839	1.368247	4.767737
C	-0.100418	-0.500493	3.556775
O	0.018631	-0.546837	4.862704
Na	0.795745	-0.305646	6.719903
C	0.358912	-1.581286	2.734007
C	1.020114	-2.819031	3.371588
C	0.059753	-3.489457	4.377773
C	2.330794	-2.405957	4.072736
C	1.396408	-3.894793	2.336992
C	0.194573	-1.506996	1.357902
C	-1.577970	0.357838	-1.369376

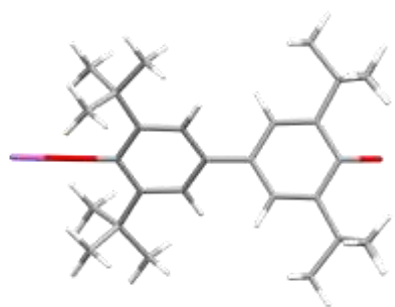
C	-1.753320	0.427874	-2.737083
C	-2.911900	1.226954	-3.353932
C	-2.353220	2.337774	-4.270498
C	-3.820356	0.289150	-4.178740
C	-3.793674	1.907128	-2.293655
C	-0.833854	-0.277320	-3.620671
O	-0.960591	-0.235714	-4.882690
H	1.261433	-0.255482	-5.416534
H	2.683453	-1.324854	-5.445361
H	2.541665	-0.067540	-4.204518
H	2.993174	-3.047416	-3.735750
H	2.910157	-1.845782	-2.445371
H	1.872107	-3.277686	-2.391646
H	-0.252786	-2.355537	-5.342567
H	0.016717	-3.573643	-4.082867
H	1.211512	-3.366569	-5.375184
H	1.157357	-1.588432	-1.148309
H	-1.264384	1.492599	1.040743
H	-2.211878	3.727478	3.523116
H	-1.183597	3.334916	2.144692
H	-2.742652	2.527483	2.342309
H	0.536688	1.776299	5.054469
H	0.676098	2.916382	3.720437
H	-0.357664	3.310237	5.103911
H	-2.585463	2.212515	5.387545
H	-1.872245	0.579543	5.404914
H	-3.142230	0.975198	4.250559
H	0.545993	-4.344016	4.861076
H	-0.828915	-3.855813	3.858530
H	-0.265532	-2.781913	5.136133
H	2.152829	-1.610622	4.795027
H	2.783287	-3.258422	4.590059
H	3.048711	-2.032799	3.339096
H	0.520514	-4.268134	1.803612
H	2.109096	-3.521885	1.599473
H	1.860865	-4.741896	2.849551
H	0.504916	-2.338294	0.744075
H	-2.284045	0.857974	-0.721744
H	-1.736807	1.903730	-5.054320
H	-1.743709	3.035533	-3.689675
H	-3.173458	2.902278	-4.728204
H	-3.244402	-0.200008	-4.960931
H	-4.638917	0.856437	-4.635965
H	-4.257721	-0.477026	-3.532744
H	-4.259717	1.181024	-1.623467
H	-4.594179	2.461932	-2.791074
H	-3.226349	2.615928	-1.685759



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.017730	-0.606530	-4.809620
C	1.343940	-1.643398	-3.885773
C	2.463671	-2.302387	-3.061705
C	0.692704	-2.760781	-4.728790
C	0.281728	-0.960182	-3.003907
C	0.397315	-0.973419	-1.618915
C	-0.530784	-0.371543	-0.766791
C	-0.371348	-0.413666	0.703570
C	-0.724104	0.670338	1.506760
C	-0.591321	0.662274	2.891491
C	-0.997313	1.896612	3.719218
C	-1.542757	3.048951	2.856802
C	0.228578	2.462582	4.470764
C	-2.127292	1.525154	4.705969
C	-0.061746	-0.500207	3.537372
O	0.081309	-0.540397	4.843428
Na	0.069430	-0.014862	6.767550
C	0.309263	-1.618765	2.727395
C	0.877960	-2.894810	3.376286
C	-0.152921	-3.502702	4.351138
C	2.188011	-2.568886	4.125198
C	1.214377	-3.985126	2.344209
C	0.139810	-1.540812	1.350098
C	-1.614738	0.270412	-1.364748
C	-1.792448	0.332442	-2.743061
C	-3.015847	1.055530	-3.338031
C	-2.555377	2.231275	-4.229155
C	-3.885660	0.061786	-4.140434
C	-3.937025	1.665096	-2.266109
C	-0.833279	-0.293551	-3.601609
O	-0.972467	-0.258016	-4.908216
Na	-1.705882	0.111783	-6.725885
H	1.278198	-0.099286	-5.424792
H	2.752024	-1.092550	-5.460045
H	2.539511	0.146494	-4.214611
H	3.181018	-2.773383	-3.738426
H	3.007973	-1.574353	-2.457343

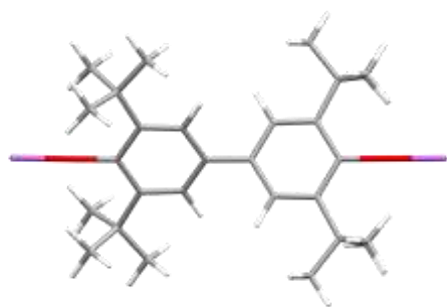
H	2.077844	-3.077358	-2.396726
H	-0.115607	-2.363412	-5.338138
H	0.278919	-3.533340	-4.076648
H	1.435525	-3.230792	-5.381277
H	1.252628	-1.448599	-1.161951
H	-1.092857	1.556299	1.010895
H	-1.816773	3.888252	3.501787
H	-0.800266	3.408006	2.142620
H	-2.433774	2.752359	2.301285
H	0.755540	1.680161	5.016531
H	0.943355	2.881880	3.760312
H	-0.066820	3.261040	5.160205
H	-2.342101	2.355087	5.388021
H	-1.876644	0.632261	5.278215
H	-3.043588	1.297050	4.158299
H	0.258326	-4.392855	4.837922
H	-1.054506	-3.799454	3.810379
H	-0.437117	-2.780119	5.112548
H	2.023239	-1.797271	4.873551
H	2.582279	-3.464896	4.615251
H	2.943700	-2.207060	3.424220
H	0.331841	-4.306829	1.788161
H	1.965668	-3.649192	1.627025
H	1.617212	-4.859836	2.860911
H	0.389292	-2.392853	0.735315
H	-2.351888	0.713005	-0.710906
H	-1.798104	1.913313	-4.945385
H	-2.096973	3.009466	-3.616082
H	-3.403458	2.678214	-4.759372
H	-3.285049	-0.510381	-4.847274
H	-4.688736	0.582949	-4.672958
H	-4.346697	-0.662328	-3.466222
H	-4.344095	0.903096	-1.599836
H	-4.778800	2.166222	-2.751704
H	-3.415675	2.405785	-1.657791

B3LYP/def2TZVP (CPCM – DME)



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	1.992625	-0.714393	-4.814257
C	1.284039	-1.723978	-3.886050
C	2.376089	-2.428557	-3.063366
C	0.587485	-2.807363	-4.737516
C	0.246297	-0.998094	-3.010305
C	0.357518	-1.010489	-1.625110
C	-0.546585	-0.370685	-0.767939
C	-0.388077	-0.411117	0.704502
C	-0.778453	0.656974	1.519507
C	-0.645690	0.657498	2.905520
C	-1.107027	1.875207	3.729992
C	-1.713368	2.991597	2.861344
C	0.090049	2.495309	4.481592
C	-2.200764	1.450579	4.733600
C	-0.061275	-0.481587	3.562343
O	0.094499	-0.510153	4.856132
Na	0.410497	-0.515309	6.932950
C	0.344901	-1.587975	2.736862
C	0.968012	-2.844124	3.376495
C	-0.025095	-3.488865	4.366962
C	2.276699	-2.470535	4.105370
C	1.329965	-3.925639	2.343171
C	0.163844	-1.518235	1.358154
C	-1.605231	0.312325	-1.379685
C	-1.783699	0.381937	-2.756233
C	-2.973930	1.154506	-3.354023
C	-2.458376	2.292522	-4.261332
C	-3.865216	0.201387	-4.178694
C	-3.869048	1.800328	-2.282863
C	-0.848155	-0.285454	-3.641243
O	-0.981876	-0.246837	-4.919662
H	1.262142	-0.191493	-5.427164
H	2.707112	-1.227341	-5.466552
H	2.545513	0.020563	-4.222466
H	3.072949	-2.927836	-3.741620
H	2.951687	-1.724795	-2.457810
H	1.960415	-3.188299	-2.397519
H	-0.194953	-2.360594	-5.346540
H	0.139137	-3.566822	-4.090747
H	1.310716	-3.306374	-5.390990
H	1.194849	-1.521309	-1.169748
H	-1.186647	1.529412	1.030109
H	-2.028194	3.817212	3.504625
H	-0.993603	3.388981	2.142915
H	-2.590745	2.648735	2.309204
H	0.579593	1.753728	5.107676
H	0.823840	2.880696	3.768922

H	-0.239538	3.329637	5.108855
H	-2.500235	2.298933	5.357159
H	-1.847357	0.646966	5.374655
H	-3.086625	1.098653	4.198452
H	0.430176	-4.354378	4.858734
H	-0.915422	-3.835222	3.835616
H	-0.335995	-2.774105	5.124695
H	2.100006	-1.690203	4.841128
H	2.700536	-3.345558	4.608270
H	3.016137	-2.104813	3.388150
H	0.453026	-4.281719	1.798745
H	2.060052	-3.567527	1.614579
H	1.769871	-4.783075	2.858781
H	0.445501	-2.363749	0.747353
H	-2.326057	0.791524	-0.731394
H	-1.820730	1.888509	-5.044278
H	-1.881364	3.012749	-3.674454
H	-3.296298	2.827292	-4.720701
H	-3.280515	-0.275317	-4.962000
H	-4.696018	0.750108	-4.634516
H	-4.288271	-0.574267	-3.534151
H	-4.312353	1.056919	-1.616419
H	-4.687154	2.335952	-2.771455
H	-3.320647	2.520368	-1.671210



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	4.442478	2.261023	-1.999891
C	3.592074	2.488718	-0.732088
C	2.626967	3.645798	-1.045542
C	4.489889	2.962352	0.431224
C	2.861799	1.189648	-0.340227
C	1.471289	1.144341	-0.319367
C	0.741091	0.003014	0.026746
C	-0.740573	-0.002746	0.028575
C	-1.471624	-1.143977	-0.316053
C	-2.862181	-1.189278	-0.333492
C	-3.593423	-2.488239	-0.723911

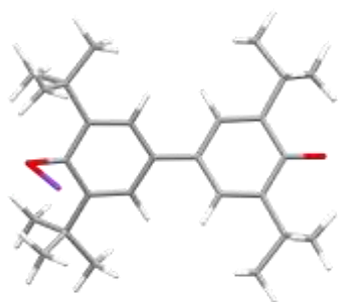
C	-2.629094	-3.645232	-1.040069
C	-4.446954	-2.260190	-1.989547
C	-4.488363	-2.962197	0.441481
C	-3.613714	-0.007706	0.002661
O	-4.914031	-0.006902	-0.019015
Na	-7.017882	0.009315	-0.120709
C	-2.872386	1.173187	0.363282
C	-3.615529	2.467418	0.746743
C	-4.513795	2.223859	1.978342
C	-4.467885	2.957992	-0.443311
C	-2.661898	3.618334	1.113227
C	-1.481544	1.133679	0.367950
C	1.482897	-1.133506	0.363974
C	2.873724	-1.173011	0.355861
C	3.617811	-2.467348	0.737125
C	4.467226	-2.957591	-0.455166
C	4.519116	-2.224131	1.966570
C	2.665088	-3.618367	1.105643
C	3.614160	0.007983	-0.006260
O	4.914419	0.007185	-0.031147
Na	7.018012	-0.009001	-0.138035
H	5.142499	1.442311	-1.855007
H	5.001839	3.166388	-2.255266
H	3.797574	2.014711	-2.847403
H	3.205067	4.536148	-1.304929
H	1.974701	3.418354	-1.891169
H	1.998476	3.897308	-0.188738
H	5.192303	2.185056	0.720793
H	3.877797	3.213403	1.301427
H	5.048686	3.858500	0.144056
H	0.911785	2.024071	-0.602995
H	-0.912822	-2.023627	-0.601307
H	-3.207833	-4.535509	-1.298276
H	-1.978917	-3.417552	-1.887240
H	-1.998489	-3.896980	-0.184889
H	-5.146613	-1.441518	-1.842707
H	-3.804143	-2.013644	-2.838580
H	-5.006945	-3.165484	-2.243793
H	-5.047869	-3.858264	0.155444
H	-5.190059	-2.184981	0.733001
H	-3.874125	-3.213491	1.310101
H	-5.077601	3.128450	2.226619
H	-3.901681	1.961921	2.845305
H	-5.212166	1.411229	1.795594
H	-5.155277	2.183143	-0.772478
H	-5.041022	3.847773	-0.164723

H	-3.822761	3.224155	-1.284652
H	-2.037902	3.374286	1.975459
H	-2.005502	3.886361	0.282821
H	-3.248699	4.503747	1.369962
H	-0.930849	2.015180	0.663282
H	0.932933	-2.015089	0.660419
H	5.153802	-2.182649	-0.785815
H	3.820026	-3.223522	-1.294985
H	5.041050	-3.847448	-0.178242
H	5.217033	-1.411450	1.782325
H	5.083535	-3.128791	2.213202
H	3.909145	-1.962437	2.835116
H	2.043223	-3.374560	1.969481
H	3.252522	-4.503851	1.360682
H	2.006643	-3.886164	0.276786

Potassium

Singly Reduced

PBE/def2TZVP

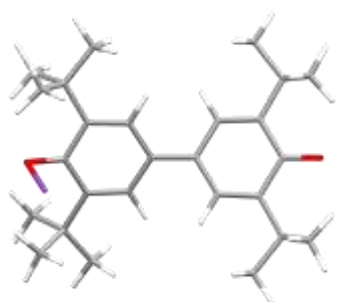


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-1.849143	-4.619370	-1.992670
C	-0.441296	-3.983641	-1.970725
C	0.598685	-5.075954	-1.624848
C	-0.124463	-3.487061	-3.391115
C	-0.414032	-2.843594	-0.935026
C	-0.037111	-1.558330	-1.295448
C	-0.059781	-0.457546	-0.403422
C	0.401579	0.861225	-0.804515
C	1.246831	1.032026	-1.934757
C	1.730690	2.254909	-2.342022
C	2.654793	2.387705	-3.557826
C	1.993965	3.301591	-4.616647
C	4.011838	2.989227	-3.124307
C	2.936388	1.031017	-4.225415
C	1.355701	3.462418	-1.581854

O	1.781202	4.599766	-1.916796
C	0.466205	3.293502	-0.417021
C	0.031631	4.526549	0.383318
C	-0.899560	4.162572	1.552110
C	-0.731245	5.507611	-0.537117
C	1.275912	5.228586	0.976343
C	0.039074	2.028855	-0.079529
C	-0.566843	-0.709082	0.894983
C	-0.954659	-1.965734	1.336299
C	-1.533250	-2.166660	2.749546
C	-1.724342	-0.834813	3.494283
C	-2.914335	-2.850663	2.639478
C	-0.602606	-3.047913	3.616033
C	-0.805036	-3.108908	0.444589
H	-2.599153	-3.871533	-2.288883
H	-2.115966	-5.011624	-1.003953
H	-1.882999	-5.443057	-2.723111
H	0.606644	-5.858802	-2.399036
H	0.346386	-5.553311	-0.667695
H	1.617870	-4.648498	-1.596113
H	-0.200878	-4.329073	-4.094908
H	0.894205	-3.077725	-3.475012
H	-0.833321	-2.713288	-3.719660
H	0.257218	-1.368971	-2.326351
H	1.550709	0.139761	-2.480286
H	1.034193	2.877260	-4.948838
H	1.814120	4.302785	-4.209686
H	2.651078	3.387291	-5.496507
H	4.504989	2.338629	-2.385511
H	4.676950	3.076868	-3.997966
H	3.874604	3.982521	-2.682658
H	3.445024	0.331790	-3.543492
H	2.015879	0.551336	-4.592375
H	3.596398	1.186585	-5.091526
H	-1.176327	5.081040	2.090375
H	-1.830981	3.687666	1.207583
H	-0.412945	3.489596	2.275161
H	-1.630990	5.028167	-0.951997
H	-1.051329	6.388297	0.041767
H	-0.095637	5.840469	-1.365209
H	1.955647	5.554856	0.181399
H	0.963169	6.108000	1.561244
H	1.819478	4.548334	1.650080
H	-0.641342	1.913865	0.762622
H	-0.624354	0.127688	1.588956
H	-2.187288	-1.029765	4.472974

H	-0.770891	-0.315751	3.677565
H	-2.386530	-0.151541	2.942900
H	-3.608865	-2.215492	2.070501
H	-3.341246	-3.007998	3.642557
H	-2.830363	-3.819967	2.133512
H	-0.531799	-4.059157	3.191588
H	0.398093	-2.586777	3.705863
H	-1.000950	-3.139977	4.638329
O	-0.914652	-4.320138	0.886125
K	1.616182	-4.033078	1.350362

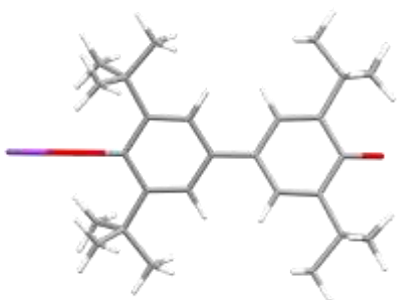
B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-1.887532	-4.564217	-1.979672
C	-0.467101	-3.960208	-1.974293
C	0.552553	-5.080029	-1.666310
C	-0.166762	-3.458375	-3.396264
C	-0.397978	-2.829067	-0.930295
C	-0.025121	-1.549760	-1.287805
C	-0.033651	-0.457444	-0.395379
C	0.418553	0.860682	-0.798884
C	1.271185	1.032726	-1.918623
C	1.742362	2.249471	-2.329591
C	2.677824	2.387955	-3.536297
C	2.019326	3.283517	-4.609500
C	4.022981	3.005379	-3.094312
C	2.983654	1.031279	-4.192134
C	1.345409	3.453615	-1.582672
O	1.756537	4.582595	-1.919280
C	0.449613	3.286141	-0.427185
C	-0.004576	4.522736	0.357055
C	-0.942094	4.159633	1.520439
C	-0.771673	5.486255	-0.575370
C	1.223307	5.243221	0.957431
C	0.037168	2.026668	-0.088179
C	-0.522268	-0.712071	0.902349
C	-0.904037	-1.963088	1.342327

C	-1.487537	-2.166461	2.753605
C	-1.665453	-0.837346	3.506131
C	-2.877060	-2.829153	2.638666
C	-0.575787	-3.060362	3.623875
C	-0.760347	-3.096048	0.448940
H	-2.619378	-3.802663	-2.255854
H	-2.147658	-4.956550	-0.999141
H	-1.951376	-5.374554	-2.711019
H	0.546504	-5.831998	-2.458896
H	0.295711	-5.580810	-0.733616
H	1.570247	-4.673249	-1.620601
H	-0.272161	-4.285271	-4.101276
H	0.850619	-3.072286	-3.492731
H	-0.860258	-2.673816	-3.702621
H	0.250673	-1.355683	-2.311906
H	1.585505	0.146136	-2.445816
H	1.073619	2.849122	-4.942574
H	1.827201	4.280585	-4.223024
H	2.677722	3.364576	-5.478487
H	4.507981	2.371545	-2.347531
H	4.693565	3.086755	-3.953925
H	3.878652	3.995077	-2.669735
H	3.488932	0.348588	-3.504919
H	2.079850	0.542427	-4.562622
H	3.646110	1.187159	-5.045586
H	-1.232102	5.072057	2.044696
H	-1.857512	3.675229	1.173714
H	-0.458007	3.503352	2.247350
H	-1.652482	4.993298	-0.993866
H	-1.110537	6.357672	-0.008916
H	-0.141229	5.825616	-1.392689
H	1.902393	5.575968	0.177271
H	0.896461	6.113189	1.533181
H	1.765494	4.576848	1.633067
H	-0.642695	1.906464	0.739765
H	-0.571487	0.115853	1.591040
H	-2.128382	-1.030020	4.475917
H	-0.713069	-0.335290	3.691087
H	-2.314328	-0.149214	2.962106
H	-3.556810	-2.183977	2.078686
H	-3.304021	-2.986961	3.632859
H	-2.810135	-3.788047	2.129814
H	-0.538015	-4.070950	3.218840
H	0.431751	-2.632409	3.692703
H	-0.963692	-3.126315	4.643127
O	-0.883450	-4.302645	0.880695
K	1.585121	-4.377480	1.429267

B3LYP/def2TZVP (CPCM – DME)

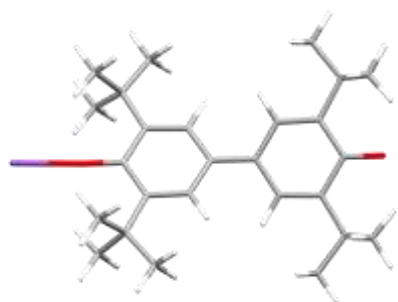


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-1.586010	-4.585325	-2.182253
C	-0.190500	-3.983640	-1.910674
C	0.760188	-5.066809	-1.356463
C	0.378486	-3.541090	-3.269873
C	-0.298918	-2.820352	-0.909865
C	0.094237	-1.551217	-1.260753
C	0.013418	-0.434588	-0.394866
C	0.436105	0.884250	-0.808144
C	1.224414	1.085136	-1.971026
C	1.650195	2.314389	-2.399226
C	2.513276	2.464545	-3.660626
C	1.778302	3.340798	-4.698857
C	3.871221	3.106408	-3.301380
C	2.808979	1.112421	-4.331138
C	1.276852	3.507510	-1.630185
O	1.644222	4.653766	-1.989384
C	0.459174	3.314233	-0.426692
C	0.034867	4.533116	0.405699
C	-0.819798	4.141179	1.622743
C	-0.808273	5.497533	-0.456900
C	1.285471	5.265707	0.939769
C	0.084378	2.045565	-0.072128
C	-0.504756	-0.682563	0.898638
C	-0.914966	-1.920006	1.333220
C	-1.458355	-2.113885	2.759318
C	-1.466428	-0.806387	3.570120
C	-2.917264	-2.616388	2.702006
C	-0.577318	-3.117395	3.533894
C	-0.826810	-3.056179	0.426645
H	-2.238141	-3.837885	-2.640513
H	-2.054384	-4.927605	-1.263862
H	-1.505061	-5.429417	-2.872506
H	0.813075	-5.912350	-2.047720
H	0.426731	-5.426635	-0.387180
H	1.768829	-4.662491	-1.242188
H	0.434780	-4.406821	-3.933037

H	1.385911	-3.130114	-3.178643
H	-0.253776	-2.794942	-3.755360
H	0.459952	-1.384867	-2.260406
H	1.524527	0.212863	-2.527949
H	0.830090	2.878690	-4.984840
H	1.576001	4.331602	-4.300827
H	2.388851	3.441573	-5.600241
H	4.413494	2.478483	-2.589957
H	4.486181	3.204645	-4.200036
H	3.734701	4.091102	-2.862138
H	3.364047	0.440967	-3.672541
H	1.896113	0.604339	-4.649382
H	3.419638	1.280473	-5.220422
H	-1.087551	5.043039	2.176754
H	-1.748461	3.646958	1.329433
H	-0.281051	3.481943	2.306784
H	-1.711932	4.997877	-0.814974
H	-1.115289	6.360126	0.140665
H	-0.242994	5.850644	-1.315366
H	1.915432	5.609281	0.123587
H	0.983923	6.129057	1.539028
H	1.872660	4.601360	1.578743
H	-0.536823	1.915992	0.798740
H	-0.551910	0.145021	1.586830
H	-1.864261	-1.006303	4.567221
H	-0.462855	-0.394031	3.692567
H	-2.097402	-0.042803	3.110836
H	-3.556653	-1.868614	2.226712
H	-3.296800	-2.790025	3.712638
H	-2.995048	-3.539642	2.134792
H	-0.525396	-4.074430	3.022661
H	0.438863	-2.728998	3.636211
H	-0.979504	-3.275608	4.538239
O	-1.199251	-4.218215	0.790782
K	-1.936824	-6.519399	1.511858

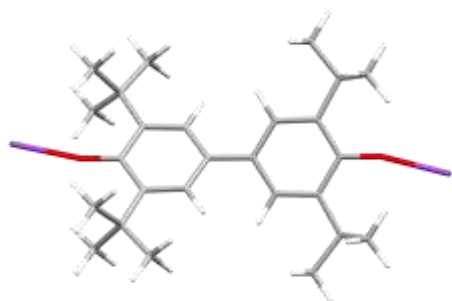
Doubly Reduced

PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	1.222334	-5.914137	-1.557155
C	1.601560	-4.945202	-0.413491
C	3.003725	-4.400381	-0.737770
C	1.714116	-5.710945	0.923469
C	0.539833	-3.835486	-0.288415
C	0.900579	-2.496424	-0.430972
C	-0.011141	-1.429540	-0.315054
C	0.407519	-0.029735	-0.476189
C	-0.289483	1.028756	0.145508
C	0.074668	2.362242	0.021357
C	-0.714355	3.471952	0.733905
C	-1.900110	2.927892	1.548099
C	0.214208	4.232180	1.708287
C	-1.279962	4.460426	-0.311808
C	1.235832	2.727617	-0.789442
O	1.601691	3.945906	-0.927740
C	1.957593	1.631372	-1.434463
C	3.176809	1.957268	-2.311469
C	2.752362	2.880058	-3.476718
C	4.253827	2.668608	-1.460251
C	3.821407	0.701491	-2.921735
C	1.528485	0.323313	-1.258292
C	-1.345532	-1.781316	-0.033993
C	-1.777626	-3.096863	0.126715
C	-3.257525	-3.399149	0.432280
C	-4.123775	-2.129755	0.511320
C	-3.369170	-4.105550	1.801698
C	-3.860769	-4.288173	-0.679028
C	-0.832334	-4.178259	-0.005121
O	-1.209115	-5.432922	0.121372
K	-1.743475	-7.654240	0.674180
H	1.246600	-5.387514	-2.523265
H	1.935473	-6.755558	-1.607445
H	0.205211	-6.298482	-1.409140
H	3.375221	-3.726334	0.048110
H	3.710688	-5.241764	-0.820677
H	3.019122	-3.852628	-1.691669
H	0.726210	-6.069711	1.242723
H	2.403098	-6.568228	0.830924
H	2.099864	-5.044997	1.710057
H	1.944485	-2.244314	-0.616123
H	-1.137058	0.766768	0.780745
H	-1.572902	2.239990	2.343172
H	-2.426824	3.768761	2.027529
H	-2.625448	2.395939	0.912852
H	1.067075	4.651339	1.160018
H	0.591865	3.549873	2.486104

H	-0.337418	5.049001	2.205459
H	-0.460454	4.883903	-0.905639
H	-1.978541	3.942528	-0.987795
H	-1.828132	5.276990	0.189622
H	2.016001	2.370649	-4.118141
H	3.626974	3.141411	-4.097532
H	2.301602	3.798236	-3.079920
H	3.836310	3.581708	-1.018098
H	5.125338	2.930411	-2.085267
H	4.598788	2.006647	-0.650296
H	3.123123	0.156358	-3.575640
H	4.689350	0.999565	-3.531792
H	4.178883	0.005137	-2.147156
H	2.055444	-0.482045	-1.772356
H	-2.073012	-0.972358	0.027758
H	-4.126087	-1.575248	-0.438782
H	-3.781489	-1.447276	1.303339
H	-5.164321	-2.413307	0.738028
H	-3.040271	-3.429100	2.605089
H	-4.412042	-4.402102	2.007726
H	-2.726445	-4.995882	1.825525
H	-4.901108	-4.564962	-0.434401
H	-3.258340	-5.196021	-0.809378
H	-3.867533	-3.745179	-1.636372

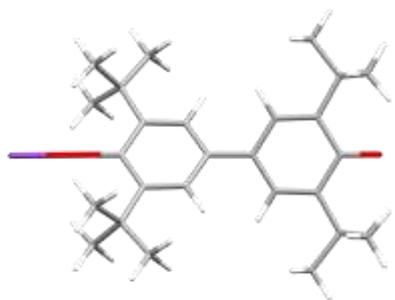


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	1.291736	-5.895349	-1.437238
C	1.607738	-4.938946	-0.263266
C	3.030057	-4.403409	-0.503415
C	1.644034	-5.706614	1.078911
C	0.543932	-3.826630	-0.201084
C	0.912058	-2.488098	-0.350001
C	-0.009215	-1.431494	-0.299970
C	0.414590	-0.025402	-0.468074
C	-0.234735	1.023148	0.200192
C	0.136654	2.361582	0.058690
C	-0.617417	3.464726	0.825012

C	-1.760764	2.920927	1.699370
C	0.354636	4.202525	1.775191
C	-1.259916	4.449519	-0.180050
C	1.239571	2.706634	-0.800926
O	1.612960	3.963277	-0.952240
K	1.830408	6.262548	-0.851469
C	1.918605	1.640119	-1.487457
C	3.100852	1.951579	-2.424895
C	2.634814	2.871216	-3.575726
C	4.235842	2.633277	-1.627785
C	3.699054	0.688803	-3.069091
C	1.486342	0.325589	-1.304436
C	-1.353293	-1.774420	-0.082701
C	-1.792928	-3.088732	0.083559
C	-3.285795	-3.390993	0.314846
C	-4.152722	-2.120259	0.348141
C	-3.471881	-4.100801	1.674936
C	-3.827863	-4.280767	-0.826117
C	-0.838290	-4.163409	0.023572
O	-1.214215	-5.419978	0.169115
K	-1.309014	-7.722883	0.347232
H	1.445206	-5.379743	-2.396684
H	1.953661	-6.779089	-1.419061
H	0.238886	-6.208867	-1.405344
H	3.355021	-3.729965	0.302985
H	3.737900	-5.246980	-0.541966
H	3.105945	-3.858346	-1.455648
H	0.629353	-6.001030	1.381418
H	2.294629	-6.596269	1.010464
H	2.042146	-5.059139	1.874030
H	1.963611	-2.233544	-0.486702
H	-1.048570	0.761553	0.877311
H	-1.392513	2.226946	2.468910
H	-2.259436	3.758301	2.213442
H	-2.519100	2.396083	1.100148
H	1.266161	4.499958	1.238139
H	0.665351	3.534069	2.591617
H	-0.126927	5.087201	2.227841
H	-0.521880	4.772362	-0.927632
H	-2.075711	3.953531	-0.726322
H	-1.685367	5.326254	0.339372
H	1.884586	2.356373	-4.194717
H	3.484978	3.143612	-4.223922
H	2.177691	3.783573	-3.171949
H	3.859747	3.532543	-1.123677
H	5.068327	2.909461	-2.297003

H	4.627316	1.948121	-0.860658
H	2.963812	0.156558	-3.690805
H	4.541115	0.975940	-3.718452
H	4.082794	-0.014059	-2.314486
H	1.978921	-0.478272	-1.852131
H	-2.082123	-0.963562	-0.072084
H	-4.108948	-1.567527	-0.602104
H	-3.849148	-1.437759	1.156061
H	-5.203138	-2.401227	0.523831
H	-3.164502	-3.436337	2.496628
H	-4.530351	-4.370320	1.830385
H	-2.854790	-5.007190	1.718658
H	-4.882761	-4.547082	-0.643355
H	-3.230119	-5.197298	-0.910175
H	-3.772103	-3.745359	-1.785953

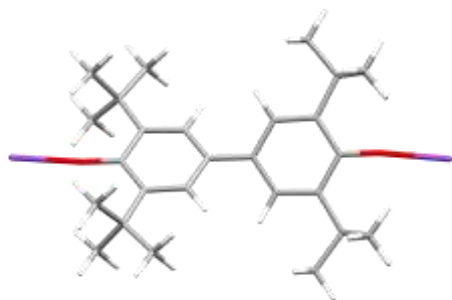
B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	1.273229	-5.910973	-1.469446
C	1.607704	-4.932853	-0.321259
C	3.019612	-4.390748	-0.603921
C	1.683321	-5.688062	1.023136
C	0.541637	-3.823085	-0.240981
C	0.902393	-2.488035	-0.383252
C	-0.011991	-1.430172	-0.312784
C	0.407535	-0.027804	-0.475515
C	-0.259308	1.021482	0.175643
C	0.103462	2.350286	0.051826
C	-0.656661	3.457709	0.799051
C	-1.817912	2.913549	1.647468
C	0.301409	4.205698	1.751788
C	-1.255564	4.457579	-0.214653
C	1.232632	2.716995	-0.789707
O	1.596881	3.928262	-0.928042
C	1.924180	1.629436	-1.465226
C	3.115602	1.960274	-2.378269

C	2.661235	2.892491	-3.522637
C	4.225337	2.656552	-1.559891
C	3.736607	0.709624	-3.022180
C	1.496076	0.326445	-1.287570
C	-1.346897	-1.781947	-0.077260
C	-1.777553	-3.093375	0.086543
C	-3.264869	-3.401674	0.346893
C	-4.139636	-2.136767	0.389563
C	-3.423448	-4.098313	1.715403
C	-3.831228	-4.298019	-0.775902
C	-0.828423	-4.161370	0.000323
O	-1.202834	-5.415476	0.135377
K	-1.669295	-7.632208	0.594881
H	1.336622	-5.395906	-2.430567
H	1.982073	-6.747042	-1.485831
H	0.259504	-6.291951	-1.366068
H	3.361285	-3.714790	0.181563
H	3.725152	-5.225254	-0.655899
H	3.065148	-3.855312	-1.553679
H	0.697399	-6.040939	1.321260
H	2.370815	-6.538993	0.957022
H	2.045827	-5.020655	1.807953
H	1.940424	-2.232226	-0.533645
H	-1.079175	0.756398	0.828971
H	-1.470514	2.222480	2.419167
H	-2.321305	3.745772	2.148084
H	-2.560369	2.394832	1.036253
H	1.132856	4.626695	1.190862
H	0.696915	3.518403	2.504851
H	-0.228586	5.012233	2.271659
H	-0.466188	4.883863	-0.829704
H	-1.973700	3.950529	-0.865128
H	-1.781213	5.264396	0.309184
H	1.908441	2.393404	-4.139153
H	3.510667	3.151444	-4.165344
H	2.230669	3.803790	-3.113560
H	3.836380	3.560480	-1.096481
H	5.071079	2.917145	-2.206809
H	4.591091	1.988146	-0.775391
H	3.020645	0.177281	-3.652861
H	4.578860	1.007822	-3.653296
H	4.114120	0.010508	-2.272066
H	1.996535	-0.471089	-1.819351
H	-2.069042	-0.979966	-0.050428
H	-4.114499	-1.593335	-0.556537
H	-3.827531	-1.452776	1.180569
H	-5.178070	-2.420543	0.583952
H	-3.120772	-3.422035	2.518081

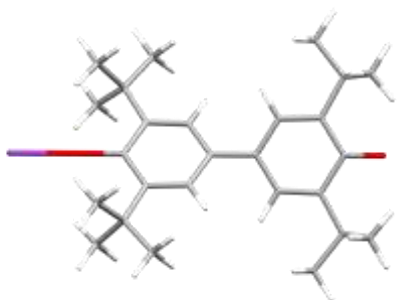
H	-4.466889	-4.384883	1.888120
H	-2.793347	-4.984157	1.769211
H	-4.872944	-4.567456	-0.567311
H	-3.236129	-5.202438	-0.880341
H	-3.803991	-3.766166	-1.729732



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	1.355895	-5.893033	-1.352784
C	1.625996	-4.920217	-0.183713
C	3.050179	-4.375092	-0.387830
C	1.633008	-5.679428	1.161261
C	0.555519	-3.812592	-0.162741
C	0.916760	-2.477988	-0.311333
C	-0.007838	-1.432659	-0.299458
C	0.414047	-0.024262	-0.466685
C	-0.209510	1.012149	0.229563
C	0.156948	2.346599	0.092832
C	-0.571300	3.444087	0.891812
C	-1.689436	2.889898	1.791681
C	0.422529	4.173652	1.822106
C	-1.241054	4.444744	-0.075746
C	1.228270	2.692367	-0.792220
O	1.600189	3.942670	-0.940990
K	2.063307	6.193835	-1.033427
C	1.881308	1.639819	-1.509345
C	3.034722	1.962334	-2.478268
C	2.538882	2.892968	-3.605914
C	4.198406	2.627566	-1.711724
C	3.611148	0.708192	-3.157760
C	1.454096	0.329152	-1.328593
C	-1.349342	-1.777144	-0.122866
C	-1.783857	-3.087595	0.041285
C	-3.280549	-3.399943	0.229811
C	-4.158855	-2.136860	0.223024
C	-3.508395	-4.092898	1.590761
C	-3.785497	-4.300931	-0.917695
C	-0.824104	-4.149227	0.021433

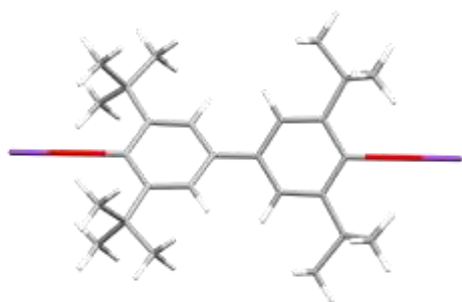
O	-1.197100	-5.399499	0.167751
K	-1.599811	-7.652455	0.397486
H	1.487328	-5.379401	-2.307369
H	2.052616	-6.738014	-1.325762
H	0.332050	-6.261095	-1.320003
H	3.345176	-3.697931	0.415479
H	3.759811	-5.206859	-0.398709
H	3.148829	-3.842235	-1.335093
H	0.633801	-6.031443	1.411280
H	2.324717	-6.528233	1.126343
H	1.955752	-5.015640	1.965941
H	1.959290	-2.216376	-0.419365
H	-0.996186	0.742959	0.919243
H	-1.303243	2.192555	2.536962
H	-2.169034	3.714850	2.325508
H	-2.459378	2.376929	1.212864
H	1.285442	4.529706	1.262244
H	0.791113	3.489384	2.589056
H	-0.062512	5.016333	2.326855
H	-0.521443	4.821819	-0.800163
H	-2.038359	3.950837	-0.634929
H	-1.683867	5.282204	0.474454
H	1.780851	2.385944	-4.207002
H	3.365297	3.171939	-4.268226
H	2.089725	3.792769	-3.191203
H	3.851684	3.509446	-1.177547
H	5.001534	2.912050	-2.399830
H	4.612840	1.932311	-0.978276
H	2.861367	0.189041	-3.757467
H	4.426349	0.999650	-3.825280
H	4.014573	0.001198	-2.430503
H	1.921974	-0.465443	-1.891159
H	-2.072528	-0.974987	-0.140706
H	-4.089163	-1.597560	-0.723356
H	-3.888700	-1.449821	1.027070
H	-5.204545	-2.421491	0.366558
H	-3.241226	-3.417834	2.406844
H	-4.561031	-4.369993	1.711646
H	-2.888848	-4.982859	1.676810
H	-4.834806	-4.573299	-0.762102
H	-3.184946	-5.205216	-0.988234
H	-3.711364	-3.773647	-1.871355

B3LYP/def2TZVP (CPCM – DME)



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	1.309291	-5.892299	-1.451229
C	1.627209	-4.929501	-0.286829
C	3.040738	-4.377174	-0.540624
C	1.683752	-5.710197	1.043609
C	0.555364	-3.824876	-0.210108
C	0.911455	-2.486805	-0.354750
C	-0.005823	-1.431123	-0.302207
C	0.414316	-0.020201	-0.469958
C	-0.237462	1.028675	0.190813
C	0.121177	2.364817	0.056946
C	-0.645771	3.461840	0.818012
C	-1.793741	2.905685	1.677441
C	0.310128	4.215949	1.766937
C	-1.269934	4.457398	-0.183637
C	1.234045	2.732630	-0.797251
O	1.598778	3.957485	-0.942878
C	1.914475	1.648227	-1.478790
C	3.101655	1.962438	-2.407641
C	2.645791	2.887563	-3.556213
C	4.227393	2.651285	-1.606255
C	3.709498	0.704725	-3.051417
C	1.485284	0.338659	-1.298100
C	-1.342323	-1.783289	-0.082277
C	-1.775382	-3.095372	0.088177
C	-3.266472	-3.398670	0.332292
C	-4.138124	-2.131245	0.369713
C	-3.444860	-4.102562	1.694861
C	-3.820942	-4.290158	-0.799327
C	-0.822295	-4.173027	0.023798
O	-1.191511	-5.412943	0.171224
K	-1.884773	-7.741100	0.448029
H	1.364454	-5.361221	-2.405140
H	2.033311	-6.712826	-1.481147
H	0.308860	-6.304488	-1.346835
H	3.370072	-3.711056	0.259430
H	3.748633	-5.208472	-0.591179

H	3.102996	-3.831338	-1.484265
H	0.705821	-6.113379	1.294064
H	2.403748	-6.532174	0.977817
H	2.001482	-5.050004	1.854907
H	1.951616	-2.232028	-0.499096
H	-1.050936	0.766918	0.853525
H	-1.434339	2.218357	2.446668
H	-2.299151	3.732635	2.183074
H	-2.538769	2.381092	1.074893
H	1.139540	4.639212	1.205119
H	0.709222	3.533914	2.522992
H	-0.219701	5.021289	2.286404
H	-0.496916	4.887055	-0.816587
H	-2.000966	3.948050	-0.817884
H	-1.788365	5.262661	0.347327
H	1.894009	2.385196	-4.171452
H	3.491977	3.144618	-4.201990
H	2.214406	3.800959	-3.153312
H	3.851350	3.554766	-1.131805
H	5.063233	2.911957	-2.263951
H	4.606526	1.978876	-0.831506
H	2.987320	0.173774	-3.675797
H	4.547747	0.995534	-3.689947
H	4.090112	0.005521	-2.303370
H	1.984035	-0.456491	-1.835154
H	-2.068363	-0.983169	-0.063356
H	-4.106136	-1.583988	-0.574610
H	-3.835016	-1.450080	1.167466
H	-5.177866	-2.414363	0.552764
H	-3.143098	-3.435022	2.506258
H	-4.493642	-4.372652	1.854453
H	-2.834611	-5.000680	1.746262
H	-4.864828	-4.555871	-0.604217
H	-3.234086	-5.200290	-0.893623
H	-3.783138	-3.756414	-1.752584



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
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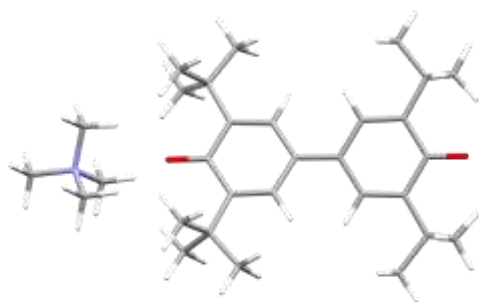
C	1.318662	-5.892050	-1.441750
C	1.630562	-4.928600	-0.276279
C	3.044650	-4.374885	-0.523804
C	1.681540	-5.708205	1.055001
C	0.558055	-3.824638	-0.205224
C	0.912887	-2.487146	-0.350020
C	-0.006778	-1.434117	-0.299865
C	0.413048	-0.022808	-0.466146
C	-0.235308	1.022183	0.200786
C	0.124050	2.359541	0.066280
C	-0.642513	3.454439	0.832853
C	-1.785901	2.892705	1.695774
C	0.311712	4.204261	1.786744
C	-1.281458	4.446060	-0.163277
C	1.227900	2.716444	-0.788887
O	1.596043	3.954020	-0.934700
K	2.290817	6.289858	-1.209956
C	1.907537	1.647288	-1.476033
C	3.093194	1.961259	-2.408606
C	2.636172	2.882890	-3.559438
C	4.228075	2.636818	-1.608916
C	3.694986	0.702315	-3.057004
C	1.478883	0.335621	-1.298428
C	-1.343921	-1.784507	-0.084359
C	-1.777102	-3.096040	0.082954
C	-3.268711	-3.400945	0.319997
C	-4.141194	-2.133982	0.353013
C	-3.452754	-4.104664	1.681888
C	-3.816903	-4.292804	-0.814358
C	-0.821631	-4.173369	0.022875
O	-1.189776	-5.410944	0.168686
K	-1.884612	-7.746774	0.443854
H	1.377417	-5.361437	-2.395687
H	2.043784	-6.711500	-1.467895
H	0.318543	-6.305912	-1.342089
H	3.369571	-3.707930	0.277447
H	3.753558	-5.205364	-0.570197
H	3.111000	-3.830129	-1.467870
H	0.703501	-6.113398	1.301321
H	2.403156	-6.528823	0.993003
H	1.994174	-5.047160	1.867563
H	1.953232	-2.231105	-0.491198
H	-1.044880	0.759304	0.866590
H	-1.421346	2.205322	2.461940
H	-2.291193	3.717152	2.205052
H	-2.531774	2.368083	1.095052
H	1.158104	4.613355	1.241145
H	0.692964	3.522659	2.551625

H	-0.213765	5.019068	2.294633
H	-0.528153	4.867230	-0.824033
H	-2.029340	3.935865	-0.775954
H	-1.782889	5.258886	0.371388
H	1.899633	2.370130	-4.183589
H	3.484732	3.154201	-4.195301
H	2.181138	3.789424	-3.168853
H	3.865029	3.527571	-1.102746
H	5.053682	2.913756	-2.271987
H	4.619499	1.948731	-0.855045
H	2.969264	0.175562	-3.680113
H	4.531718	0.992070	-3.697565
H	4.076182	0.001006	-2.311835
H	1.974271	-0.457676	-1.839794
H	-2.070084	-0.984373	-0.067621
H	-4.104942	-1.586810	-0.591283
H	-3.842860	-1.452799	1.152643
H	-5.181548	-2.417703	0.530675
H	-3.155048	-3.436986	2.494646
H	-4.502056	-4.374978	1.836425
H	-2.842901	-5.002725	1.736795
H	-4.861612	-4.558302	-0.624400
H	-3.230230	-5.203239	-0.905673
H	-3.774246	-3.759494	-1.767635

Tetramethylammonium

Singly Reduced

PBE/def2TZVP

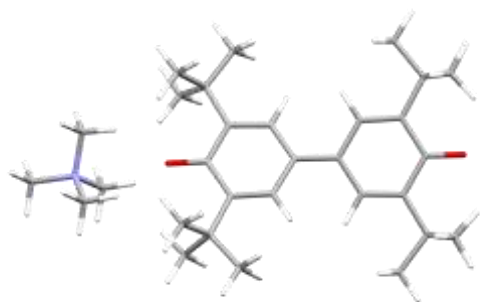


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	0.770350	-6.355537	-2.173037
C	1.334572	-5.525180	-0.996949
C	2.693097	-4.968624	-1.458769
C	1.616475	-6.422544	0.228859
C	0.330709	-4.419452	-0.624887
C	0.707763	-3.088957	-0.693035
C	-0.156021	-2.013082	-0.381954

C	0.286028	-0.630841	-0.442577
C	-0.434373	0.405140	0.212002
C	-0.051601	1.727669	0.188502
C	-0.851979	2.806832	0.927729
C	-2.079177	2.227941	1.651893
C	0.041235	3.488849	1.989856
C	-1.359433	3.863004	-0.081871
C	1.161111	2.110669	-0.556962
O	1.544659	3.311419	-0.606757
C	1.910205	1.041682	-1.241955
C	3.169082	1.399180	-2.041444
C	2.809393	2.390404	-3.172448
C	4.218861	2.038904	-1.102869
C	3.816456	0.164344	-2.690987
C	1.456983	-0.255694	-1.155799
C	-1.479885	-2.357687	-0.021482
C	-1.937359	-3.661789	0.060582
C	-3.410672	-3.942109	0.407122
C	-4.234836	-2.656385	0.597702
C	-3.501405	-4.727028	1.735065
C	-4.072114	-4.730341	-0.746646
C	-1.019128	-4.759774	-0.201756
O	-1.391962	-5.997977	-0.067232
H	0.725775	-5.737290	-3.081832
H	1.420744	-7.220474	-2.384390
H	-0.246186	-6.707494	-1.961905
H	3.197114	-4.395019	-0.666841
H	3.352747	-5.806709	-1.731736
H	2.594092	-4.322314	-2.343243
H	0.685239	-6.824965	0.639734
H	2.282040	-7.257413	-0.047187
H	2.112611	-5.839653	1.019137
H	1.732727	-2.851096	-0.969862
H	-1.312785	0.122769	0.790260
H	-1.797057	1.489315	2.417965
H	-2.615191	3.043840	2.159384
H	-2.784578	1.751428	0.953615
H	0.392048	2.752671	2.729406
H	-0.536282	4.260039	2.524366
H	0.912475	3.959705	1.520824
H	-2.013980	3.395332	-0.833384
H	-1.943344	4.633824	0.446206
H	-0.519807	4.343497	-0.596448
H	2.078312	1.940691	-3.861747
H	3.713076	2.641490	-3.750557
H	2.384144	3.312467	-2.760389

H	4.500716	1.336697	-0.303217
H	3.825030	2.953556	-0.645717
H	5.127726	2.287545	-1.673940
H	3.140847	-0.329087	-3.406546
H	4.713772	0.478311	-3.244873
H	4.131849	-0.579027	-1.942512
H	1.997104	-1.036226	-1.689134
H	-2.180444	-1.545734	0.162451
H	-4.244447	-2.034719	-0.309503
H	-3.860512	-2.044236	1.431715
H	-5.277299	-2.926364	0.826637
H	-3.117534	-4.114830	2.564725
H	-4.549248	-4.987043	1.959980
H	-2.905049	-5.643405	1.686348
H	-5.095119	-5.035990	-0.471414
H	-3.486260	-5.618560	-1.010822
H	-4.139193	-4.097511	-1.643931
N	-2.077164	-8.974883	0.960235
C	-1.087711	-9.032894	-0.173801
H	-1.527336	-9.618870	-0.989513
H	-0.894215	-7.994664	-0.483480
H	-0.169327	-9.511304	0.185902
C	-3.326666	-8.291451	0.469795
H	-4.041126	-8.229651	1.298908
H	-3.030432	-7.286966	0.131024
H	-3.747497	-8.883572	-0.351372
C	-2.395152	-10.353502	1.442375
H	-1.472750	-10.831633	1.792170
H	-3.116515	-10.287039	2.265174
H	-2.824460	-10.930810	0.615155
C	-1.484687	-8.157279	2.078647
H	-2.214658	-8.102045	2.894615
H	-0.566466	-8.648664	2.420919
H	-1.272504	-7.158205	1.665166

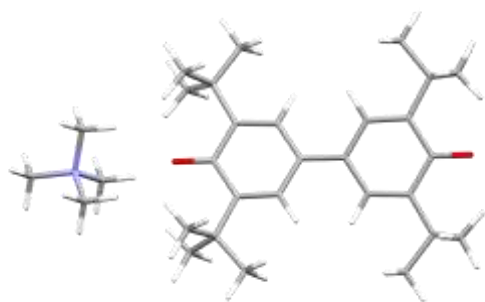
B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	0.786217	-6.353234	-2.161176
C	1.335793	-5.522407	-0.980461
C	2.700661	-4.970809	-1.427934
C	1.604827	-6.420350	0.245864
C	0.331741	-4.413468	-0.619741
C	0.706683	-3.089532	-0.684752
C	-0.156418	-2.017330	-0.384029
C	0.284546	-0.638516	-0.442022
C	-0.426547	0.392769	0.222736
C	-0.047811	1.707155	0.202330
C	-0.837529	2.786123	0.953442
C	-2.057265	2.206972	1.688987
C	0.064449	3.461995	2.009619
C	-1.357356	3.845418	-0.043846
C	1.154957	2.089784	-0.552256
O	1.534271	3.279145	-0.600469
C	1.897215	1.027946	-1.248006
C	3.147910	1.392716	-2.057198
C	2.778558	2.385340	-3.181498
C	4.207293	2.026706	-1.128414
C	3.790985	0.162509	-2.718631
C	1.445669	-0.260538	-1.163095
C	-1.478006	-2.361421	-0.036247
C	-1.934296	-3.658692	0.041352
C	-3.409656	-3.943843	0.373686
C	-4.239389	-2.661363	0.558491
C	-3.514475	-4.729439	1.698362
C	-4.061256	-4.730726	-0.784627
C	-1.016675	-4.751605	-0.211151
O	-1.387610	-5.980103	-0.080254
H	0.749050	-5.739076	-3.063214
H	1.437086	-7.209182	-2.365373
H	-0.221680	-6.708240	-1.964253
H	3.193081	-4.402156	-0.636979
H	3.356668	-5.803994	-1.691059
H	2.613586	-4.330213	-2.307151
H	0.681003	-6.829491	0.639792
H	2.275980	-7.243184	-0.020041
H	2.081587	-5.840156	1.038808
H	1.723971	-2.852335	-0.949358
H	-1.290422	0.107406	0.801280
H	-1.769359	1.470970	2.442990
H	-2.583239	3.014704	2.201807
H	-2.764913	1.737807	1.001702
H	0.423146	2.725591	2.733088
H	-0.505362	4.220040	2.554131
H	0.922539	3.938341	1.543166

H	-2.012231	3.382316	-0.786126
H	-1.935906	4.604705	0.489619
H	-0.534637	4.331754	-0.560805
H	2.043100	1.941130	-3.856799
H	3.668861	2.631227	-3.766864
H	2.365365	3.303103	-2.771876
H	4.490992	1.326653	-0.338591
H	3.829394	2.935750	-0.668514
H	5.105767	2.269869	-1.702370
H	3.114061	-0.324278	-3.424197
H	4.675905	0.476716	-3.275625
H	4.111591	-0.577591	-1.981921
H	1.972692	-1.033805	-1.698274
H	-2.172189	-1.556275	0.140284
H	-4.241428	-2.042999	-0.340635
H	-3.877256	-2.054913	1.390766
H	-5.275706	-2.931482	0.774951
H	-3.134280	-4.125300	2.524913
H	-4.557887	-4.979361	1.915199
H	-2.932300	-5.643231	1.655798
H	-5.080526	-5.030120	-0.521270
H	-3.483485	-5.614608	-1.041086
H	-4.117149	-4.103018	-1.676303
N	-2.070869	-8.940997	0.965901
C	-1.076333	-9.014305	-0.161669
H	-1.504461	-9.615660	-0.960812
H	-0.887344	-7.994571	-0.491779
H	-0.163843	-9.476278	0.208221
C	-3.321189	-8.271959	0.460492
H	-4.031687	-8.196947	1.280515
H	-3.036510	-7.283816	0.103610
H	-3.736394	-8.878060	-0.341878
C	-2.386576	-10.312488	1.463330
H	-1.472404	-10.780394	1.821956
H	-3.107040	-10.239747	2.275048
H	-2.806258	-10.898812	0.648836
C	-1.487591	-8.111442	2.079600
H	-2.216873	-8.052300	2.884385
H	-0.578404	-8.594708	2.430159
H	-1.274940	-7.124178	1.668851

B3LYP/def2TZVP (CPCM – DME)



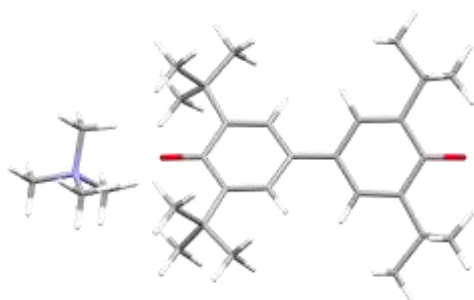
<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	0.739245	-6.293483	-2.239005
C	1.320098	-5.478026	-1.062915
C	2.678922	-4.927073	-1.528365
C	1.598067	-6.399230	0.143769
C	0.334793	-4.365557	-0.667334
C	0.707098	-3.044985	-0.727730
C	-0.146403	-1.968268	-0.385959
C	0.293541	-0.593679	-0.448698
C	-0.443541	0.454240	0.161626
C	-0.065224	1.770566	0.130640
C	-0.901857	2.856603	0.823482
C	-2.150354	2.282127	1.513804
C	-0.060467	3.563127	1.908619
C	-1.387416	3.889858	-0.216897
C	1.166488	2.144281	-0.573556
O	1.547051	3.341066	-0.629707
C	1.937820	1.070656	-1.210019
C	3.229640	1.411675	-1.967825
C	2.920944	2.376067	-3.133788
C	4.248067	2.061992	-1.005767
C	3.901544	0.166043	-2.569845
C	1.485253	-0.219339	-1.122064
C	-1.459920	-2.315836	0.012651
C	-1.917591	-3.607946	0.095196
C	-3.370492	-3.902113	0.504160
C	-4.183591	-2.622095	0.762986
C	-3.396120	-4.721687	1.812163
C	-4.088864	-4.669782	-0.626962
C	-1.011675	-4.708700	-0.219798
O	-1.382133	-5.919528	-0.110955
H	0.640930	-5.660384	-3.124143
H	1.406659	-7.122217	-2.490783
H	-0.241427	-6.693867	-1.998053
H	3.187024	-4.368067	-0.739930
H	3.325412	-5.761306	-1.808947
H	2.580998	-4.277761	-2.400693

H	0.680609	-6.834404	0.525015
H	2.276256	-7.206938	-0.144933
H	2.071215	-5.834089	0.950411
H	1.714785	-2.809530	-1.027527
H	-1.336571	0.187210	0.702450
H	-1.892675	1.564288	2.295505
H	-2.705282	3.096284	1.984240
H	-2.821494	1.792022	0.805205
H	0.262534	2.846175	2.667698
H	-0.660270	4.330977	2.404800
H	0.819569	4.032033	1.476327
H	-2.011913	3.405877	-0.972057
H	-1.989092	4.659377	0.274432
H	-0.547262	4.367073	-0.714429
H	2.227383	1.911322	-3.839122
H	3.840911	2.614663	-3.674424
H	2.479287	3.300164	-2.770204
H	4.499902	1.373518	-0.195139
H	3.848716	2.975845	-0.574013
H	5.169854	2.300006	-1.543559
H	3.258903	-0.335987	-3.296264
H	4.813032	0.467654	-3.089781
H	4.183795	-0.558388	-1.802811
H	2.046600	-0.996482	-1.613975
H	-2.144242	-1.513510	0.233913
H	-4.242468	-1.987634	-0.123635
H	-3.768387	-2.030439	1.581416
H	-5.203578	-2.896875	1.040081
H	-2.956036	-4.144252	2.628723
H	-4.426438	-4.963568	2.087224
H	-2.837038	-5.645354	1.708461
H	-5.104662	-4.933238	-0.319793
H	-3.555804	-5.578632	-0.891254
H	-4.159615	-4.044453	-1.520233
N	-2.109432	-9.110398	0.952800
C	-1.179806	-9.167190	-0.227204
H	-1.664838	-9.723992	-1.024650
H	-0.974815	-8.147094	-0.537536
H	-0.263713	-9.668324	0.074051
C	-3.373713	-8.407574	0.543470
H	-4.036309	-8.354429	1.403328
H	-3.105313	-7.412061	0.203498
H	-3.843260	-8.976252	-0.254908
C	-2.426994	-10.496849	1.422573
H	-1.504287	-10.988776	1.718630
H	-3.104209	-10.433370	2.270267
H	-2.897676	-11.043969	0.610032
C	-1.451288	-8.335219	2.059986

H	-2.129246	-8.297553	2.908476
H	-0.531291	-8.841846	2.339557
H	-1.242616	-7.335565	1.688964

Doubly Reduced

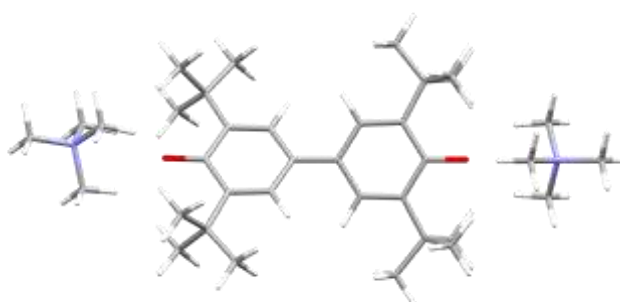
PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	0.874156	-6.420239	-2.096967
C	1.373008	-5.559490	-0.913057
C	2.743023	-4.993331	-1.327864
C	1.617527	-6.431182	0.338710
C	0.332523	-4.465678	-0.600362
C	0.711748	-3.120903	-0.647837
C	-0.170622	-2.052520	-0.413937
C	0.268748	-0.646179	-0.456222
C	-0.370238	0.350997	0.306494
C	0.014512	1.688354	0.299001
C	-0.715205	2.729178	1.164696
C	-1.867146	2.123924	1.983887
C	0.278976	3.372715	2.158111
C	-1.313449	3.828748	0.257533
C	1.134932	2.124220	-0.527899
O	1.518577	3.350479	-0.559386
C	1.795248	1.089507	-1.317085
C	2.974185	1.487569	-2.220910
C	2.507628	2.534625	-3.257875
C	4.106010	2.092718	-1.358977
C	3.564046	0.296440	-2.993849
C	1.350250	-0.227587	-1.255902
C	-1.503663	-2.411418	-0.148845
C	-1.950515	-3.733436	-0.069067
C	-3.443170	-4.016577	0.193476
C	-4.295450	-2.738656	0.292552
C	-3.606746	-4.758268	1.538918
C	-4.026815	-4.849587	-0.971130
C	-1.021930	-4.817697	-0.260680
O	-1.401686	-6.091554	-0.137357

H	0.877869	-5.818988	-3.018677
H	1.532626	-7.292689	-2.257248
H	-0.154851	-6.760175	-1.925473
H	3.207145	-4.403312	-0.524009
H	3.422592	-5.828075	-1.567422
H	2.667573	-4.352761	-2.218468
H	0.668210	-6.814265	0.725677
H	2.288242	-7.278705	0.108438
H	2.088012	-5.826967	1.129146
H	1.751212	-2.869062	-0.856878
H	-1.188688	0.036798	0.958099
H	-1.511674	1.352553	2.685073
H	-2.350714	2.919497	2.574666
H	-2.635297	1.669581	1.338322
H	1.114595	3.818230	1.602740
H	0.674675	2.610112	2.847859
H	-0.222443	4.153592	2.757608
H	-0.513632	4.283014	-0.341717
H	-2.065545	3.394795	-0.420587
H	-1.806049	4.608117	0.866232
H	1.737050	2.101462	-3.915408
H	3.354735	2.861250	-3.887360
H	2.083625	3.402624	-2.736456
H	3.717115	2.950181	-0.794419
H	4.945531	2.421815	-1.997305
H	4.487098	1.340935	-0.649387
H	2.821879	-0.167849	-3.662073
H	4.404831	0.646461	-3.615378
H	3.947534	-0.482943	-2.316547
H	1.835069	-0.981277	-1.880390
H	-2.219680	-1.599136	-0.026291
H	-4.250503	-2.144664	-0.631718
H	-3.978200	-2.094549	1.125756
H	-5.348344	-3.017822	0.464311
H	-3.303087	-4.100904	2.367702
H	-4.658166	-5.055941	1.703443
H	-2.969596	-5.647824	1.561752
H	-5.055519	-5.182074	-0.743807
H	-3.394743	-5.721264	-1.181903
H	-4.063110	-4.235263	-1.883472
N	-2.027396	-8.889384	1.041440
C	-1.001712	-8.990855	-0.058035
H	-1.403728	-9.641207	-0.844985
H	-0.838426	-7.955871	-0.417144
H	-0.081694	-9.417361	0.359169
C	-3.270409	-8.264423	0.462142
H	-4.014553	-8.159023	1.260596
H	-2.958839	-7.276655	0.069729

H	-3.648709	-8.921833	-0.330676
C	-2.329523	-10.236350	1.604896
H	-1.408283	-10.666900	2.015961
H	-3.078585	-10.132016	2.399264
H	-2.718844	-10.878004	0.803961
C	-1.488768	-7.975740	2.114243
H	-2.247585	-7.880316	2.900417
H	-0.569454	-8.418785	2.516228
H	-1.295090	-7.007338	1.603625

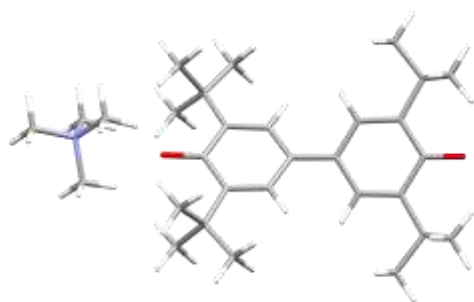


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-4.405126	3.015310	0.899901
C	-3.536004	2.622916	-0.317387
C	-2.540484	3.775707	-0.538886
C	-4.392175	2.527153	-1.599775
C	-2.847466	1.273989	-0.035938
C	-1.453493	1.193904	-0.037394
C	-0.746937	0.015772	0.244330
C	0.730105	-0.028854	0.226116
C	1.429280	-1.191703	-0.128172
C	2.822867	-1.270987	-0.162896
C	3.503941	-2.604458	-0.524694
C	2.502910	-3.745838	-0.778148
C	4.330190	-2.446745	-1.820518
C	4.400844	-3.054372	0.651859
C	3.613948	-0.103803	0.146876
O	4.933947	-0.124940	0.067453
C	2.903576	1.085115	0.555275
C	3.674465	2.343292	0.997870
C	4.573288	1.998115	2.207623
C	4.515646	2.887148	-0.178629
C	2.752740	3.492050	1.444620
C	1.507720	1.084591	0.576759
C	-1.516831	-1.113661	0.559037
C	-2.912810	-1.113929	0.569935
C	-3.673928	-2.392339	0.969355

C	-2.742731	-3.560714	1.338921
C	-4.542474	-2.879533	-0.212079
C	-4.544260	-2.106160	2.214810
C	-3.631800	0.092835	0.235691
O	-4.953275	0.117027	0.188016
H	-3.758538	3.254842	1.757421
H	-5.017426	3.906338	0.677151
H	-5.057909	2.185891	1.198037
H	-1.901052	3.606169	-1.418007
H	-3.099749	4.710087	-0.707324
H	-1.889125	3.927998	0.334301
H	-5.087509	1.684731	-1.531716
H	-4.960496	3.459190	-1.764786
H	-3.743738	2.363439	-2.473791
H	-0.870081	2.079818	-0.289237
H	0.839691	-2.064827	-0.408670
H	1.843354	-3.534634	-1.633046
H	3.057597	-4.670739	-1.004188
H	1.871894	-3.940248	0.101591
H	5.027385	-1.608175	-1.728229
H	3.661746	-2.241609	-2.670387
H	4.894011	-3.369465	-2.043234
H	5.060824	-2.239861	0.974265
H	3.774186	-3.335174	1.511651
H	5.007320	-3.933330	0.372433
H	3.947778	1.787037	3.087923
H	5.238853	2.842147	2.458755
H	5.174843	1.103518	2.005943
H	3.853010	3.239965	-0.983389
H	5.154126	2.097848	-0.587453
H	5.143065	3.735932	0.145094
H	2.122489	3.204161	2.298747
H	3.369002	4.350401	1.757096
H	2.093865	3.832022	0.631645
H	0.980441	1.979031	0.909210
H	-0.982482	-2.022741	0.835831
H	-2.092678	-3.313826	2.191040
H	-2.103080	-3.860883	0.495494
H	-3.352058	-4.433424	1.624024
H	-3.898877	-3.192921	-1.048008
H	-5.162687	-3.743236	0.084970
H	-5.189825	-2.071866	-0.567603
H	-5.204294	-2.961648	2.440484
H	-5.149828	-1.203243	2.070335
H	-3.898382	-1.937258	3.089487
N	7.941857	0.049826	-0.829759

N	-7.981276	-0.016130	-0.646569
C	9.368498	0.133232	-1.259079
H	9.530959	-0.554577	-2.097417
H	9.588916	1.160826	-1.571729
H	10.012404	-0.146668	-0.416670
C	7.602975	-1.350673	-0.390004
H	6.540231	-1.331635	-0.088961
H	7.763434	-2.031687	-1.234196
H	8.258265	-1.619345	0.447311
C	7.027811	0.429223	-1.966641
H	5.997184	0.342018	-1.570402
H	7.258864	1.457254	-2.269911
H	7.201516	-0.264198	-2.798031
C	7.682012	0.981622	0.325182
H	8.336479	0.693900	1.156788
H	7.900601	2.007048	0.004418
H	6.614650	0.863423	0.584013
C	-7.631513	1.361823	-0.148038
H	-8.267066	1.589604	0.716181
H	-6.562086	1.328944	0.127025
H	-7.811123	2.082505	-0.954601
C	-7.695238	-1.002171	0.455954
H	-7.921774	-2.011132	0.091469
H	-6.622096	-0.895942	0.695343
H	-8.330087	-0.755086	1.315370
C	-9.417535	-0.079621	-1.046205
H	-9.599009	0.647565	-1.846550
H	-9.645711	-1.091137	-1.402650
H	-10.041579	0.159138	-0.176622
C	-7.094048	-0.339979	-1.821248
H	-7.332642	-1.352388	-2.168101
H	-7.286596	0.392473	-2.614124
H	-6.054462	-0.271330	-1.445281

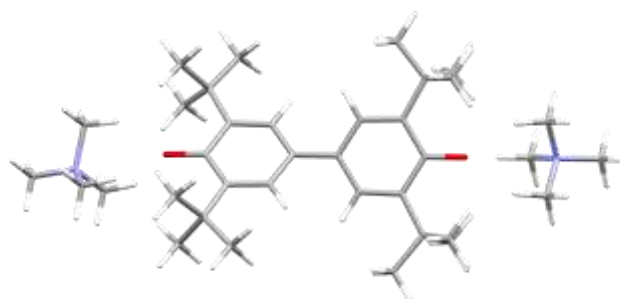
B3LYP/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
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C	0.955435	-6.425823	-2.004951
C	1.403035	-5.554287	-0.810098
C	2.788149	-4.991957	-1.175869
C	1.602333	-6.416631	0.454570
C	0.352269	-4.457821	-0.548632
C	0.726244	-3.117262	-0.599011
C	-0.164608	-2.057270	-0.411724
C	0.271704	-0.647447	-0.456504
C	-0.332872	0.333477	0.340309
C	0.047492	1.666236	0.333209
C	-0.646159	2.696953	1.239463
C	-1.763857	2.081566	2.097670
C	0.381843	3.328832	2.203330
C	-1.285945	3.806329	0.375925
C	1.127375	2.108707	-0.531070
O	1.506857	3.327692	-0.563096
C	1.752698	1.090779	-1.357054
C	2.892617	1.502081	-2.303763
C	2.386965	2.557858	-3.311144
C	4.062920	2.093934	-1.487666
C	3.450265	0.321536	-3.115874
C	1.312297	-0.221731	-1.292332
C	-1.497617	-2.413590	-0.189097
C	-1.941038	-3.731001	-0.107578
C	-3.439011	-4.021091	0.108565
C	-4.300845	-2.747680	0.171584
C	-3.648091	-4.754102	1.451152
C	-3.983664	-4.861860	-1.067682
C	-1.005524	-4.806872	-0.252588
O	-1.380979	-6.071571	-0.120765
H	0.993244	-5.836453	-2.923779
H	1.619702	-7.289207	-2.131296
H	-0.067817	-6.770039	-1.877155
H	3.215926	-4.398420	-0.366247
H	3.472550	-5.821651	-1.378415
H	2.748626	-4.365694	-2.068261
H	0.653198	-6.809094	0.801370
H	2.288780	-7.249404	0.258783
H	2.028239	-5.807866	1.255390
H	1.760846	-2.861493	-0.771867
H	-1.117373	0.009825	1.011812
H	-1.382836	1.308395	2.769372
H	-2.220534	2.862826	2.713034
H	-2.551289	1.638454	1.482986
H	1.188055	3.787952	1.634894
H	0.804517	2.561617	2.858408
H	-0.097012	4.088797	2.832696
H	-0.525386	4.277071	-0.243616

H	-2.056214	3.380555	-0.273498
H	-1.757390	4.565326	1.012013
H	1.593020	2.134588	-3.933059
H	3.201215	2.881176	-3.970957
H	1.992608	3.419928	-2.777112
H	3.713907	2.942478	-0.902812
H	4.870678	2.419693	-2.154242
H	4.467065	1.338792	-0.807315
H	2.686515	-0.131734	-3.752464
H	4.257430	0.676297	-3.764070
H	3.860167	-0.458973	-2.470083
H	1.765769	-0.964600	-1.935418
H	-2.209529	-1.606864	-0.099597
H	-4.229673	-2.163839	-0.747241
H	-4.016437	-2.102142	1.004103
H	-5.349708	-3.028207	0.309542
H	-3.368690	-4.098544	2.279080
H	-4.698711	-5.039997	1.583619
H	-3.026552	-5.640823	1.502101
H	-5.012112	-5.189053	-0.873012
H	-3.355236	-5.729318	-1.253173
H	-3.990479	-4.258430	-1.978101
N	-2.047994	-8.864213	1.029176
C	-0.985273	-8.974955	-0.032547
H	-1.352021	-9.634609	-0.816883
H	-0.812777	-7.959956	-0.402111
H	-0.084908	-9.386875	0.418201
C	-3.273500	-8.249529	0.405385
H	-4.034775	-8.134916	1.174044
H	-2.962999	-7.278294	0.009595
H	-3.626872	-8.913232	-0.381672
C	-2.366490	-10.206096	1.588022
H	-1.467570	-10.631450	2.029763
H	-3.136972	-10.102180	2.349390
H	-2.724186	-10.850881	0.787453
C	-1.549460	-7.950062	2.119911
H	-2.329199	-7.857259	2.872999
H	-0.652855	-8.389080	2.552462
H	-1.337276	-6.988697	1.634552

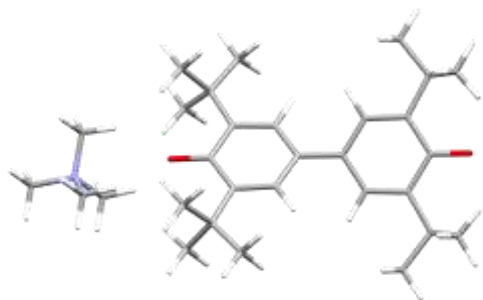


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
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C	-3.521933	2.601922	-0.411034
C	-2.526302	3.743356	-0.683112
C	-4.381306	2.458567	-1.685106
C	-2.833503	1.265657	-0.076641
C	-1.445532	1.181170	-0.076426
C	-0.747550	0.018263	0.249453
C	0.730836	-0.031588	0.231100
C	1.420425	-1.177114	-0.166351
C	2.807970	-1.260719	-0.202814
C	3.487715	-2.578999	-0.616870
C	2.485405	-3.706606	-0.920287
C	4.317387	-2.374145	-1.902175
C	4.380121	-3.083689	0.538904
C	3.597973	-0.114520	0.153313
O	4.908792	-0.137121	0.074064
C	2.896678	1.055669	0.605438
C	3.675161	2.290085	1.097147
C	4.570102	1.897457	2.293538
C	4.521156	2.877667	-0.052680
C	2.760391	3.426197	1.587508
C	1.506551	1.059572	0.623895
C	-1.514555	-1.090934	0.607278
C	-2.904733	-1.086924	0.621275
C	-3.672291	-2.343963	1.071057
C	-2.747027	-3.501803	1.484944
C	-4.545053	-2.876119	-0.085731
C	-4.539025	-2.009742	2.305357
C	-3.615673	0.103237	0.242256
O	-4.927965	0.128888	0.194605
H	-3.743285	3.316627	1.629113
H	-4.985501	3.930991	0.530490
H	-5.044307	2.249991	1.118329
H	-1.894641	3.537756	-1.549338
H	-3.080009	4.664049	-0.887400
H	-1.877533	3.929801	0.174340
H	-5.084384	1.639759	-1.582125

H	-4.931505	3.383640	-1.890989
H	-3.741432	2.247607	-2.545005
H	-0.861020	2.044493	-0.358845
H	0.829039	-2.026204	-0.476273
H	1.833939	-3.459995	-1.760756
H	3.033712	-4.616117	-1.181341
H	1.856593	-3.934375	-0.057963
H	5.023121	-1.560836	-1.776325
H	3.657860	-2.122489	-2.735879
H	4.862148	-3.287956	-2.164952
H	5.045344	-2.300073	0.891911
H	3.755924	-3.390733	1.380917
H	4.971984	-3.950936	0.225543
H	3.946775	1.650545	3.155703
H	5.226107	2.727115	2.579751
H	5.172723	1.022868	2.062892
H	3.866997	3.253723	-0.842638
H	5.162740	2.117116	-0.483041
H	5.136882	3.711587	0.302738
H	2.131495	3.111340	2.421823
H	3.376027	4.261617	1.932520
H	2.110625	3.799304	0.793616
H	0.982538	1.933410	0.982323
H	-0.982856	-1.980685	0.911078
H	-2.098776	-3.227026	2.318607
H	-2.116057	-3.835991	0.659194
H	-3.354962	-4.353171	1.803622
H	-3.909601	-3.213439	-0.907796
H	-5.152834	-3.726488	0.243413
H	-5.196022	-2.096135	-0.464075
H	-5.188678	-2.852553	2.566533
H	-5.146345	-1.125421	2.131016
H	-3.895733	-1.804173	3.163696
N	7.907687	0.070636	-0.835024
N	-7.947252	-0.036643	-0.653615
C	9.328085	0.170444	-1.274151
H	9.482144	-0.478463	-2.133741
H	9.545688	1.201041	-1.546616
H	9.976712	-0.139612	-0.457418
C	7.577425	-1.346573	-0.447858
H	6.533627	-1.348662	-0.128761
H	7.722417	-1.986859	-1.315216
H	8.243980	-1.647013	0.358129
C	6.988020	0.495746	-1.950405
H	5.968010	0.399065	-1.565540
H	7.219012	1.525890	-2.212970
H	7.155997	-0.158708	-2.803032
C	7.664942	0.956725	0.357995

H	8.330925	0.643977	1.159760
H	7.873425	1.986129	0.074903
H	6.616572	0.830427	0.633687
C	-7.607310	1.360521	-0.206599
H	-8.254826	1.621536	0.628128
H	-6.556391	1.347865	0.087936
H	-7.772022	2.041642	-1.038610
C	-7.677398	-0.978868	0.489522
H	-7.892964	-1.993605	0.162232
H	-6.622845	-0.865372	0.746573
H	-8.324432	-0.705356	1.320612
C	-9.377508	-0.116039	-1.063968
H	-9.551100	0.573315	-1.887598
H	-9.601946	-1.132483	-1.380492
H	-10.006846	0.154075	-0.218464
C	-7.053937	-0.407184	-1.809154
H	-7.291531	-1.423659	-2.115459
H	-7.241279	0.287368	-2.625242
H	-6.025223	-0.328530	-1.443849

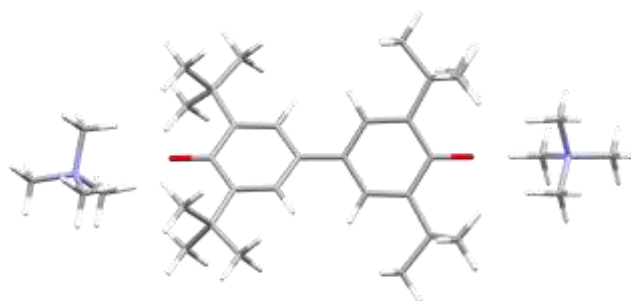
B3LYP/def2TZVP (CPCM – DME)



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	1.014364	-6.376806	-1.967948
C	1.433814	-5.505506	-0.763833
C	2.829849	-4.945614	-1.088285
C	1.586354	-6.378782	0.499186
C	0.381626	-4.405256	-0.526837
C	0.749450	-3.063816	-0.582420
C	-0.146449	-2.005161	-0.398618
C	0.287963	-0.589849	-0.458438
C	-0.312899	0.399909	0.329361
C	0.060224	1.738785	0.302028
C	-0.647375	2.767609	1.203013
C	-1.756990	2.145417	2.067612
C	0.369503	3.417201	2.166032
C	-1.307648	3.860591	0.335071
C	1.132797	2.172501	-0.572082

O	1.507570	3.402231	-0.623778
C	1.761662	1.148924	-1.384273
C	2.906108	1.535225	-2.339326
C	2.410423	2.570186	-3.371989
C	4.081773	2.131744	-1.535520
C	3.459532	0.336649	-3.128457
C	1.321915	-0.167443	-1.303310
C	-1.478609	-2.359954	-0.159766
C	-1.924186	-3.675936	-0.075887
C	-3.415742	-3.972337	0.171479
C	-4.273363	-2.699893	0.285384
C	-3.588493	-4.743866	1.496832
C	-3.990397	-4.793081	-1.003422
C	-0.987123	-4.762447	-0.237821
O	-1.359215	-6.004718	-0.131356
H	1.033192	-5.782060	-2.885019
H	1.705651	-7.215711	-2.097761
H	0.007810	-6.763570	-1.833201
H	3.233979	-4.349261	-0.267656
H	3.518495	-5.776448	-1.262907
H	2.823314	-4.326057	-1.987373
H	0.627978	-6.790362	0.797136
H	2.286579	-7.201017	0.319605
H	1.976292	-5.779400	1.326054
H	1.784861	-2.810072	-0.759837
H	-1.096276	0.085654	1.005460
H	-1.368328	1.384174	2.747860
H	-2.221309	2.926215	2.675686
H	-2.541444	1.688539	1.459994
H	1.176232	3.881701	1.603706
H	0.795355	2.661858	2.832530
H	-0.118822	4.176131	2.786316
H	-0.562826	4.339756	-0.296140
H	-2.079526	3.421601	-0.303359
H	-1.784105	4.617577	0.966867
H	1.618282	2.138648	-3.990339
H	3.227522	2.872910	-4.035248
H	2.018850	3.449002	-2.864992
H	3.744728	2.990024	-0.958727
H	4.887476	2.444857	-2.207831
H	4.488880	1.384239	-0.848772
H	2.697601	-0.124230	-3.761187
H	4.269225	0.676130	-3.779706
H	3.865609	-0.434645	-2.470031
H	1.781155	-0.915050	-1.935608
H	-2.192439	-1.555351	-0.055112
H	-4.237292	-2.098504	-0.625246
H	-3.962717	-2.069640	1.121236

H	-5.315658	-2.983094	0.453982
H	-3.270747	-4.122109	2.337954
H	-4.637849	-5.013409	1.654362
H	-2.988659	-5.647566	1.493817
H	-5.025355	-5.086799	-0.800754
H	-3.395808	-5.685654	-1.178922
H	-3.985076	-4.192840	-1.917075
N	-2.112165	-9.051087	0.981295
C	-1.037605	-9.134045	-0.067057
H	-1.400273	-9.752530	-0.884327
H	-0.832020	-8.119770	-0.401134
H	-0.153429	-9.584126	0.377203
C	-3.329086	-8.410632	0.373372
H	-4.102364	-8.342047	1.134332
H	-3.035822	-7.422684	0.026371
H	-3.670719	-9.031967	-0.450819
C	-2.446639	-10.419159	1.484751
H	-1.553952	-10.862818	1.918218
H	-3.224892	-10.336730	2.239186
H	-2.797028	-11.024908	0.653017
C	-1.622881	-8.191341	2.113927
H	-2.408609	-8.124800	2.862120
H	-0.737699	-8.654590	2.542288
H	-1.391853	-7.211818	1.698297



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	-4.402414	3.047453	0.857000
C	-3.534077	2.611074	-0.343166
C	-2.540567	3.755337	-0.610024
C	-4.405022	2.472608	-1.609384
C	-2.841366	1.272907	-0.023032
C	-1.452711	1.187191	-0.023854
C	-0.748402	0.016541	0.276020
C	0.732305	-0.031143	0.257692
C	1.428818	-1.185649	-0.114309
C	2.817070	-1.270532	-0.149811
C	3.501424	-2.591394	-0.549820

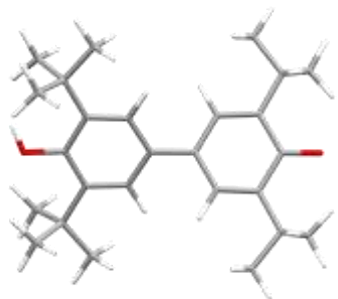
C	2.501354	-3.722075	-0.848209
C	4.342846	-2.391794	-1.827785
C	4.397118	-3.084422	0.607543
C	3.614788	-0.113579	0.185418
O	4.911803	-0.141380	0.124237
C	2.902484	1.074734	0.595626
C	3.681779	2.332046	1.025338
C	4.585106	2.002903	2.233595
C	4.532159	2.854328	-0.151991
C	2.766429	3.490670	1.457977
C	1.511556	1.073821	0.616266
C	-1.519743	-1.104803	0.599091
C	-2.910776	-1.105498	0.610696
C	-3.680596	-2.382430	0.997489
C	-2.756104	-3.559984	1.352641
C	-4.558343	-2.848043	-0.183525
C	-4.555474	-2.112196	2.240783
C	-3.631740	0.100746	0.274660
O	-4.929809	0.130731	0.244981
H	-3.766791	3.269237	1.718308
H	-4.968577	3.952631	0.615552
H	-5.095916	2.259930	1.139296
H	-1.908388	3.556162	-1.477929
H	-3.096848	4.674505	-0.811043
H	-1.891481	3.942249	0.247953
H	-5.121228	1.666096	-1.494611
H	-4.945954	3.402779	-1.810526
H	-3.776380	2.254667	-2.476774
H	-0.872540	2.060750	-0.285206
H	0.842254	-2.045972	-0.403786
H	1.849328	-3.481801	-1.690652
H	3.052312	-4.630218	-1.105986
H	1.872237	-3.950336	0.014625
H	5.061970	-1.591324	-1.691054
H	3.694377	-2.132798	-2.668894
H	4.878449	-3.310929	-2.085857
H	5.097420	-2.310979	0.911173
H	3.781519	-3.347668	1.471716
H	4.957025	-3.976645	0.309837
H	3.971088	1.758388	3.104368
H	5.210410	2.862601	2.494553
H	5.224818	1.151266	2.018424
H	3.883100	3.179588	-0.969289
H	5.188103	2.075388	-0.525594
H	5.138148	3.711393	0.158644
H	2.142206	3.222725	2.312895
H	3.382392	4.344102	1.752897
H	2.111599	3.819981	0.648465

H	0.990157	1.962018	0.943859
H	-0.991382	-2.007417	0.871472
H	-2.112072	-3.333058	2.204733
H	-2.120408	-3.849674	0.513279
H	-3.365537	-4.426938	1.620442
H	-3.928595	-3.133317	-1.030333
H	-5.157442	-3.719376	0.099563
H	-5.222341	-2.052426	-0.503975
H	-5.175036	-2.983784	2.474586
H	-5.199530	-1.251565	2.081654
H	-3.921290	-1.909440	3.107819
N	8.107737	0.053735	-0.827080
N	-8.147055	-0.020254	-0.640231
C	9.538599	0.137134	-1.255017
H	9.696429	-0.540517	-2.090089
H	9.756867	1.157987	-1.557924
H	10.173256	-0.147039	-0.419637
C	7.778911	-1.347168	-0.391258
H	6.733183	-1.357217	-0.093454
H	7.951850	-2.020531	-1.226975
H	8.427502	-1.611017	0.440443
C	7.206367	0.433624	-1.969098
H	6.181219	0.359349	-1.610433
H	7.442609	1.450152	-2.273049
H	7.383907	-0.253092	-2.792803
C	7.856980	0.988109	0.323650
H	8.509126	0.705473	1.146233
H	8.080130	2.002281	0.002148
H	6.810103	0.889301	0.599813
C	-7.807429	1.358286	-0.145378
H	-8.436409	1.581527	0.712852
H	-6.755070	1.354604	0.128232
H	-7.999328	2.070910	-0.943557
C	-7.870198	-1.008673	0.458173
H	-8.101309	-2.006359	0.093599
H	-6.817143	-0.922659	0.714409
H	-8.502933	-0.766231	1.308284
C	-9.587502	-0.083803	-1.038379
H	-9.764280	0.633082	-1.836059
H	-9.813306	-1.089053	-1.384819
H	-10.202457	0.159570	-0.175821
C	-7.272625	-0.344358	-1.819773
H	-7.516419	-1.345247	-2.166630
H	-7.468838	0.381024	-2.605208
H	-6.239393	-0.286822	-1.481827

Hydrogen

Singly Reduced

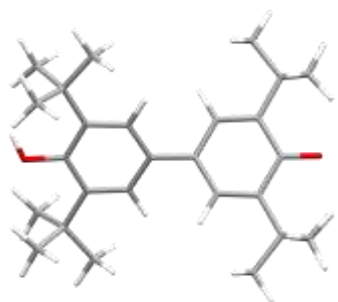
PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	0.183649	-4.316086	2.180970
C	1.419680	-3.509771	2.621832
C	1.266222	-3.285164	4.147075
C	2.647110	-4.402907	2.309766
C	1.519684	-2.161382	1.875054
C	0.558975	-1.800202	0.933380
C	0.590858	-0.577465	0.237099
C	-0.440506	-0.232695	-0.739515
C	-1.191230	-1.242735	-1.395489
C	-2.169544	-0.968271	-2.324704
C	-2.945880	-2.084389	-3.028553
C	-2.498663	-3.481131	-2.564811
C	-4.455110	-1.946633	-2.716042
C	-2.718247	-1.999774	-4.556366
C	-2.463436	0.443467	-2.650638
O	-3.351908	0.739957	-3.488632
C	-1.684944	1.496875	-1.965290
C	-1.973148	2.969301	-2.269437
C	-1.069294	3.914596	-1.459942
C	-1.722121	3.249998	-3.770359
C	-3.441634	3.301398	-1.913674
C	-0.719364	1.121687	-1.057952
C	1.655889	0.300074	0.521393
C	2.659137	0.008808	1.440471
C	3.810187	1.000463	1.698285
C	3.670764	2.269462	0.838075
C	5.167057	0.352735	1.339261
C	3.804428	1.450724	3.177378
C	2.573471	-1.238220	2.116149
H	0.156985	-5.265373	2.735175
H	-0.753247	-3.781690	2.393485

H	0.211801	-4.558638	1.108937
H	2.097399	-2.741209	4.619939
H	0.356214	-2.703902	4.352553
H	1.179071	-4.253666	4.661596
H	2.549623	-5.367670	2.829358
H	3.618666	-3.977084	2.602799
H	2.706807	-4.598327	1.229742
H	-0.275389	-2.472440	0.749954
H	-0.945904	-2.280596	-1.174977
H	-1.437655	-3.672144	-2.787285
H	-2.661907	-3.631182	-1.486357
H	-3.089119	-4.241396	-3.096383
H	-5.009066	-2.762499	-3.205803
H	-4.845173	-0.988607	-3.076609
H	-4.635133	-2.016729	-1.632459
H	-3.072554	-1.042539	-4.954234
H	-3.263550	-2.815104	-5.056576
H	-1.649620	-2.109082	-4.795991
H	-1.314420	4.954564	-1.719868
H	-1.217002	3.802073	-0.374978
H	-0.002531	3.761086	-1.684545
H	-2.382067	2.643033	-4.399698
H	-0.677292	3.029473	-4.036986
H	-1.909212	4.314098	-3.982496
H	-3.632647	3.118922	-0.845229
H	-4.136565	2.694902	-2.504767
H	-3.638802	4.365427	-2.116784
H	-0.164337	1.892159	-0.524976
H	1.712469	1.233911	-0.032431
H	4.509632	2.944329	1.061010
H	3.703717	2.047337	-0.238949
H	2.741039	2.817080	1.053613
H	5.377080	-0.531008	1.951625
H	5.977823	1.080296	1.497219
H	5.182658	0.053439	0.280655
H	2.848977	1.934854	3.428850
H	4.609099	2.183103	3.344026
H	3.958139	0.611720	3.864675
O	3.564575	-1.510361	3.020799
H	3.405847	-2.389422	3.404586

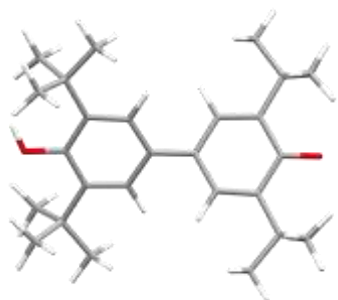
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<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	0.119402	-4.261709	2.253805
C	1.372739	-3.469550	2.667996
C	1.235818	-3.209557	4.187072
C	2.579751	-4.390322	2.367096
C	1.496220	-2.138588	1.894405
C	0.539582	-1.778631	0.954684
C	0.592025	-0.579054	0.237464
C	-0.440632	-0.233526	-0.740335
C	-1.161279	-1.241683	-1.420628
C	-2.134713	-0.970201	-2.344531
C	-2.886917	-2.083270	-3.079394
C	-2.417217	-3.481206	-2.644023
C	-4.398641	-1.983681	-2.773863
C	-2.650356	-1.963822	-4.601620
C	-2.451201	0.439091	-2.638943
O	-3.331817	0.733191	-3.469124
C	-1.702694	1.492258	-1.929522
C	-2.020962	2.963969	-2.207731
C	-1.142871	3.911254	-1.373536
C	-1.764321	3.282181	-3.698216
C	-3.495605	3.260594	-1.854290
C	-0.742822	1.117062	-1.027746
C	1.669447	0.278799	0.492617
C	2.668869	-0.012830	1.408011
C	3.841615	0.961038	1.638177
C	3.723942	2.214902	0.753954
C	5.181737	0.280708	1.284230
C	3.855512	1.442600	3.105448
C	2.563566	-1.236513	2.107174
H	0.078536	-5.191263	2.823850
H	-0.798548	-3.709568	2.459606
H	0.135405	-4.525776	1.195442
H	2.074662	-2.671864	4.630891
H	0.343585	-2.613829	4.385322
H	1.139489	-4.156829	4.721477
H	2.474392	-5.332988	2.907802

H	3.550117	-3.971576	2.638225
H	2.624547	-4.612035	1.299805
H	-0.301680	-2.430311	0.789128
H	-0.895058	-2.267055	-1.217937
H	-1.359615	-3.645311	-2.861592
H	-2.583424	-3.655766	-1.578607
H	-2.984871	-4.235298	-3.191566
H	-4.928665	-2.796435	-3.276479
H	-4.808502	-1.037434	-3.115727
H	-4.580556	-2.076689	-1.700479
H	-3.020929	-1.017261	-4.985148
H	-3.167040	-2.776338	-5.118297
H	-1.585219	-2.042301	-4.831975
H	-1.405008	4.943381	-1.611582
H	-1.294539	3.773952	-0.300753
H	-0.080326	3.784422	-1.592396
H	-2.403104	2.686697	-4.344469
H	-0.721604	3.085714	-3.958880
H	-1.964493	4.339724	-3.886885
H	-3.687792	3.048500	-0.799846
H	-4.173803	2.664837	-2.458905
H	-3.709173	4.317924	-2.028927
H	-0.208497	1.874891	-0.476961
H	1.735895	1.190708	-0.076659
H	4.571336	2.872035	0.955416
H	3.744588	1.971684	-0.310066
H	2.814248	2.781211	0.963008
H	5.376479	-0.586476	1.909179
H	6.002292	0.989353	1.419064
H	5.182468	-0.039506	0.240010
H	2.917831	1.946423	3.350217
H	4.668966	2.157248	3.251193
H	3.995956	0.621801	3.803204
O	3.555608	-1.502150	3.007721
H	3.414377	-2.356089	3.421945

B3LYP/def2TZVP (CPCM – DME)

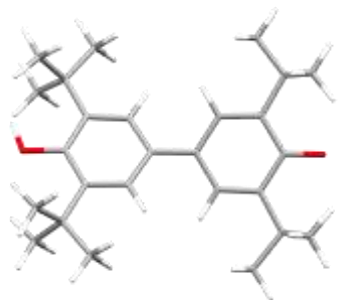


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	0.156566	-4.297140	2.192180
C	1.398125	-3.496743	2.625740
C	1.252363	-3.263897	4.148335
C	2.619321	-4.393825	2.311560
C	1.506460	-2.151309	1.875843
C	0.550554	-1.789628	0.937642
C	0.588917	-0.576787	0.237796
C	-0.441870	-0.232183	-0.738714
C	-1.181807	-1.239578	-1.401742
C	-2.154710	-0.968054	-2.325879
C	-2.923896	-2.087330	-3.035683
C	-2.466895	-3.482667	-2.578112
C	-4.432105	-1.968235	-2.720784
C	-2.695767	-2.001474	-4.561294
C	-2.452629	0.439987	-2.641570
O	-3.334440	0.734617	-3.475456
C	-1.686648	1.492441	-1.951222
C	-1.979968	2.967004	-2.247562
C	-1.084843	3.910500	-1.426761
C	-1.717693	3.263677	-3.741306
C	-3.447675	3.296116	-1.894765
C	-0.728247	1.118410	-1.047808
C	1.654124	0.293509	0.511462
C	2.652592	0.000888	1.426428
C	3.810084	0.988461	1.676376
C	3.679049	2.253077	0.809241
C	5.162206	0.333291	1.319976
C	3.809317	1.450027	3.150256
C	2.561472	-1.236543	2.107664
H	0.128700	-5.236509	2.746194
H	-0.769335	-3.761182	2.405711
H	0.179637	-4.541806	1.129231
H	2.084260	-2.728153	4.606794
H	0.351322	-2.683357	4.352706
H	1.165283	-4.222675	4.662591
H	2.524291	-5.345416	2.837519
H	3.582436	-3.967095	2.594449
H	2.667582	-4.597985	1.240762
H	-0.278285	-2.453217	0.759200
H	-0.933873	-2.265761	-1.183298
H	-1.412937	-3.662071	-2.800019
H	-2.625727	-3.635434	-1.508628
H	-3.047953	-4.238899	-3.108483
H	-4.974165	-2.781518	-3.209308
H	-4.835583	-1.021774	-3.070258
H	-4.605936	-2.046461	-1.644970
H	-3.054564	-1.057493	-4.962555

H	-3.226649	-2.816995	-5.058282
H	-1.633133	-2.099632	-4.795529
H	-1.330693	4.943227	-1.679424
H	-1.237814	3.789264	-0.352452
H	-0.025104	3.761652	-1.643814
H	-2.361377	2.667162	-4.382059
H	-0.676776	3.051648	-3.996699
H	-1.905223	4.320929	-3.943679
H	-3.639340	3.103665	-0.836499
H	-4.139565	2.703272	-2.486943
H	-3.642433	4.354312	-2.084997
H	-0.180750	1.878755	-0.514597
H	1.711678	1.215989	-0.041063
H	4.516175	2.918494	1.025989
H	3.708996	2.024644	-0.257812
H	2.759498	2.802291	1.020343
H	5.366117	-0.541308	1.931831
H	5.970532	1.052556	1.471156
H	5.173299	0.030720	0.270427
H	2.864130	1.939869	3.395017
H	4.613476	2.172197	3.309549
H	3.954858	0.621404	3.837930
O	3.551147	-1.499410	3.005432
H	3.428351	-2.360652	3.413693

Doubly Reduced

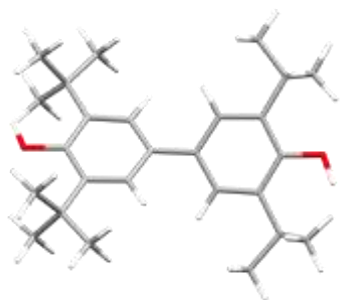
PBE/def2TZVP



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.857265	2.311698	-3.293188
C	2.714150	0.825548	-2.893384
C	1.739638	0.167531	-3.884261
C	4.081678	0.120746	-3.045354
C	2.240486	0.722715	-1.434266
C	1.044343	0.096689	-1.110734
C	0.553599	-0.009115	0.207547
C	-0.719707	-0.673284	0.506623
C	-1.265276	-1.662322	-0.336792
C	-2.475459	-2.313838	-0.086013

C	-3.007429	-3.389369	-1.055761
C	-2.070716	-3.594928	-2.260034
C	-3.125967	-4.752221	-0.336064
C	-4.382625	-2.965797	-1.620834
C	-3.177810	-1.962300	1.090809
O	-4.382269	-2.625283	1.329288
C	-2.683150	-0.976733	1.978782
C	-3.447740	-0.565642	3.257675
C	-4.841119	0.012927	2.906663
C	-2.713603	0.538465	4.042037
C	-3.572370	-1.762360	4.234665
C	-1.470722	-0.358355	1.655069
C	1.349500	0.558761	1.224440
C	2.559046	1.196189	0.984334
C	3.393413	1.778087	2.137195
C	4.779224	1.094823	2.176642
C	3.578294	3.298515	1.927316
C	2.734238	1.575690	3.511693
C	3.067216	1.310903	-0.381672
O	4.176240	1.894223	-0.641487
H	3.231430	2.398405	-4.328413
H	3.555703	2.812561	-2.610817
H	1.880133	2.817272	-3.237401
H	1.609758	-0.907150	-3.680623
H	0.746245	0.642580	-3.862250
H	2.137567	0.269467	-4.906955
H	4.451322	0.215997	-4.081475
H	4.807806	0.570779	-2.356601
H	3.985952	-0.951546	-2.811794
H	0.424672	-0.304755	-1.915087
H	-0.689342	-1.943849	-1.215792
H	-1.072650	-3.939558	-1.952475
H	-2.501219	-4.362357	-2.921981
H	-1.948320	-2.674020	-2.848734
H	-3.489467	-5.520213	-1.038685
H	-3.817347	-4.702643	0.512940
H	-2.141080	-5.070940	0.037412
H	-4.292573	-2.012616	-2.163448
H	-4.751018	-3.727403	-2.327845
H	-5.127120	-2.840571	-0.826331
H	-4.694723	-2.364746	2.209380
H	-5.483941	-0.674224	2.338095
H	-5.380872	0.295225	3.824935
H	-4.721141	0.913308	2.287167
H	-1.714889	0.214719	4.367113
H	-2.598641	1.454105	3.445457

H	-3.296466	0.792216	4.941189
H	-4.100679	-2.639412	3.828995
H	-4.107388	-1.456131	5.147812
H	-2.570471	-2.112965	4.520940
H	-1.088245	0.428151	2.301736
H	1.005712	0.451806	2.255357
H	5.401561	1.529972	2.978266
H	4.667416	0.016994	2.374798
H	5.284109	1.227798	1.211379
H	2.601567	3.807681	1.946765
H	4.054778	3.481570	0.955894
H	4.205479	3.725202	2.729750
H	2.601717	0.508999	3.751930
H	1.749147	2.065235	3.570736
H	3.375899	2.017977	4.291010

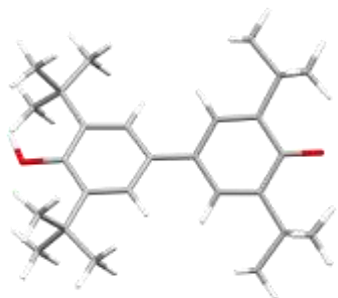


<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.711812	2.541293	-3.246336
C	2.597188	1.036060	-2.898110
C	1.551706	0.452113	-3.866818
C	3.921757	0.291212	-3.201929
C	2.185341	0.841976	-1.421827
C	0.981143	0.207474	-1.099349
C	0.558399	0.009881	0.220038
C	-0.722303	-0.667677	0.519507
C	-1.198303	-1.710805	-0.286175
C	-2.404121	-2.372113	-0.041916
C	-2.879674	-3.515793	-0.959551
C	-1.887642	-3.777700	-2.107219
C	-3.005696	-4.831398	-0.158008
C	-4.235461	-3.151493	-1.607023
C	-3.154634	-1.951942	1.083910
O	-4.340765	-2.615750	1.313084
C	-2.717245	-0.904972	1.933345
C	-3.537770	-0.438512	3.156395
C	-4.920572	0.106008	2.718807

C	-2.843556	0.713189	3.907445
C	-3.691174	-1.586617	4.185915
C	-1.502454	-0.287593	1.617431
C	1.390111	0.478072	1.246132
C	2.603139	1.127726	1.006341
C	3.481245	1.620758	2.173413
C	4.856927	0.916537	2.146206
C	3.663067	3.153938	2.093455
C	2.841639	1.313036	3.539456
C	2.987304	1.299684	-0.346488
O	4.187842	1.940206	-0.566735
H	2.997857	2.663747	-4.301982
H	3.444352	3.097598	-2.643258
H	1.742373	3.036383	-3.093032
H	1.416746	-0.629248	-3.721263
H	0.573654	0.942230	-3.759195
H	1.890948	0.609482	-4.901190
H	4.195180	0.425261	-4.259464
H	4.784394	0.616493	-2.601292
H	3.799802	-0.784560	-3.011469
H	0.324196	-0.126980	-1.900100
H	-0.580252	-2.031535	-1.122945
H	-0.897715	-4.084272	-1.737878
H	-2.274551	-4.594555	-2.733870
H	-1.760787	-2.896114	-2.753381
H	-3.321631	-5.646866	-0.827171
H	-3.738494	-4.748469	0.652089
H	-2.034952	-5.108554	0.279617
H	-4.140868	-2.232140	-2.204286
H	-4.556355	-3.961804	-2.280087
H	-5.019274	-2.996665	-0.857583
H	-4.747726	-2.253193	2.116624
H	-5.549480	-0.617799	2.179947
H	-5.489870	0.441384	3.598937
H	-4.789221	0.965518	2.046188
H	-1.856307	0.416995	4.290005
H	-2.718045	1.601035	3.271553
H	-3.461077	1.005600	4.769384
H	-4.198951	-2.485450	3.805158
H	-4.264137	-1.236527	5.057842
H	-2.701016	-1.914115	4.533430
H	-1.152056	0.542338	2.228233
H	1.081316	0.298950	2.274528
H	5.466862	1.256811	2.997544
H	4.731889	-0.173222	2.232611
H	5.407126	1.128745	1.222964

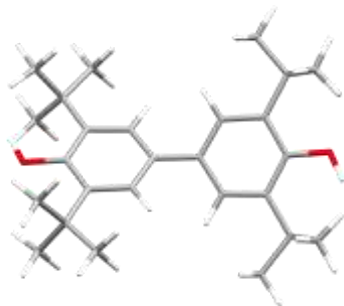
H	2.686954	3.659386	2.144495
H	4.161782	3.459915	1.167358
H	4.270098	3.501764	2.943821
H	2.709639	0.232943	3.701717
H	1.864793	1.805286	3.658932
H	3.501331	1.688988	4.335137
H	4.347042	1.978108	-1.523793

B3LYP/def2TZVP



Element	X	Y	Z
C	2.818760	2.382644	-3.258530
C	2.671255	0.889969	-2.891472
C	1.678537	0.266957	-3.886809
C	4.027623	0.177407	-3.086602
C	2.214861	0.750925	-1.430018
C	1.024007	0.129013	-1.106969
C	0.554138	-0.008389	0.208657
C	-0.720776	-0.671643	0.507444
C	-1.248024	-1.674413	-0.318301
C	-2.450767	-2.326478	-0.064755
C	-2.966395	-3.427265	-1.014722
C	-2.021602	-3.649906	-2.208892
C	-3.075575	-4.774706	-0.268775
C	-4.340410	-3.030711	-1.597401
C	-3.161550	-1.955694	1.091978
O	-4.365225	-2.613608	1.327072
C	-2.690653	-0.947760	1.955671
C	-3.479149	-0.500728	3.207126
C	-4.880388	0.021541	2.814354
C	-2.781614	0.652133	3.952635
C	-3.588665	-1.655268	4.232000
C	-1.481189	-0.335184	1.634072
C	1.363905	0.521883	1.225353
C	2.569728	1.153534	0.988559
C	3.425169	1.698868	2.143635
C	4.804473	1.004652	2.152433
C	3.618841	3.222232	1.978101

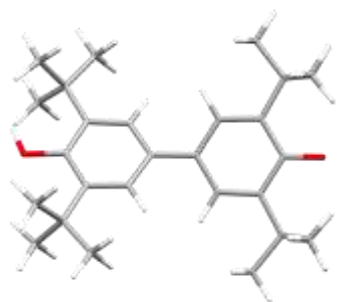
C	2.783506	1.465370	3.521424
C	3.055812	1.299948	-0.375944
O	4.157892	1.876980	-0.633325
H	3.167959	2.490041	-4.291943
H	3.528513	2.863500	-2.589056
H	1.853677	2.889643	-3.171658
H	1.544609	-0.803532	-3.712373
H	0.697205	0.745215	-3.838322
H	2.059225	0.392555	-4.904446
H	4.374227	0.291215	-4.120215
H	4.770121	0.596593	-2.411289
H	3.925742	-0.891357	-2.878292
H	0.394097	-0.244779	-1.902742
H	-0.664491	-1.965051	-1.176378
H	-1.030266	-3.976926	-1.891096
H	-2.437344	-4.428662	-2.852873
H	-1.905625	-2.747458	-2.811256
H	-3.417684	-5.556577	-0.953651
H	-3.773312	-4.716556	0.562597
H	-2.098577	-5.070168	0.120478
H	-4.257742	-2.093236	-2.152103
H	-4.691548	-3.802866	-2.288751
H	-5.087496	-2.901848	-0.818552
H	-4.594646	-2.532398	2.254244
H	-5.478752	-0.710408	2.274463
H	-5.436222	0.324582	3.706345
H	-4.778741	0.892717	2.164874
H	-1.792423	0.366592	4.312159
H	-2.672143	1.533071	3.319702
H	-3.383201	0.936435	4.819461
H	-4.120619	-2.540309	3.873168
H	-4.115862	-1.318170	5.128460
H	-2.592204	-1.990716	4.523303
H	-1.111462	0.461676	2.257818
H	1.031829	0.390671	2.246394
H	5.430227	1.406040	2.957909
H	4.685081	-0.069719	2.318068
H	5.305601	1.158410	1.199334
H	2.652363	3.732348	2.020763
H	4.085895	3.436794	1.019512
H	4.248489	3.617728	2.783479
H	2.646533	0.402050	3.733064
H	1.811466	1.957781	3.606373
H	3.433721	1.877661	4.298313



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.662897	2.635551	-3.183136
C	2.538051	1.121147	-2.891721
C	1.469010	0.585322	-3.861262
C	3.847421	0.376822	-3.247975
C	2.155064	0.878132	-1.415358
C	0.956973	0.243967	-1.092795
C	0.559215	0.009379	0.219942
C	-0.722334	-0.668444	0.520090
C	-1.172853	-1.734636	-0.256484
C	-2.371609	-2.395565	-0.009897
C	-2.822599	-3.574235	-0.895603
C	-1.811640	-3.866588	-2.018273
C	-2.948003	-4.862310	-0.053455
C	-4.169654	-3.247047	-1.576200
C	-3.139879	-1.946543	1.083838
O	-4.319512	-2.613755	1.309689
C	-2.729361	-0.872609	1.900607
C	-3.575072	-0.367724	3.090249
C	-4.952781	0.142874	2.605342
C	-2.908272	0.818243	3.810546
C	-3.737565	-1.477093	4.157152
C	-1.517866	-0.260109	1.586350
C	1.405880	0.435279	1.241982
C	2.615795	1.078171	1.002311
C	3.519836	1.524575	2.168743
C	4.885532	0.807965	2.095125
C	3.717042	3.055887	2.136854
C	2.903154	1.179655	3.535722
C	2.975543	1.289444	-0.344561
O	4.174559	1.925329	-0.558401
H	2.932586	2.796142	-4.229318
H	3.405029	3.150219	-2.572167
H	1.708311	3.130182	-2.997178
H	1.328006	-0.491373	-3.757186
H	0.505577	1.075460	-3.715675
H	1.785871	0.779110	-4.887628
H	4.101171	0.544927	-4.296837

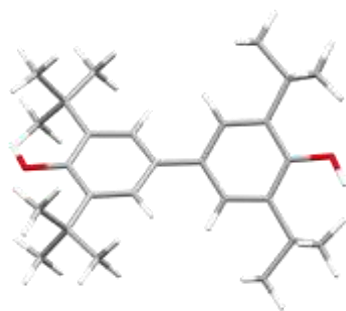
H	4.714843	0.673859	-2.656391
H	3.720595	-0.695912	-3.094498
H	0.288126	-0.061043	-1.881672
H	-0.542614	-2.067767	-1.065742
H	-0.832500	-4.147986	-1.626233
H	-2.177482	-4.702050	-2.617744
H	-1.684333	-3.013316	-2.687379
H	-3.240182	-5.697840	-0.694563
H	-3.689984	-4.761542	0.733758
H	-1.988956	-5.110427	0.406710
H	-4.075208	-2.352251	-2.195647
H	-4.468277	-4.075015	-2.224115
H	-4.961223	-3.079399	-0.851208
H	-4.749711	-2.272131	2.095427
H	-5.550355	-0.605443	2.083947
H	-5.541823	0.498455	3.453640
H	-4.818354	0.973865	1.911182
H	-1.934641	0.549162	4.222401
H	-2.778308	1.675243	3.148507
H	-3.541588	1.135941	4.640824
H	-4.227701	-2.383937	3.799350
H	-4.325555	-1.104966	4.998906
H	-2.758901	-1.781185	4.531506
H	-1.181658	0.582547	2.169111
H	1.109559	0.228697	2.258148
H	5.508527	1.108796	2.941220
H	4.749838	-0.274702	2.145139
H	5.418791	1.044556	1.178581
H	2.753986	3.565023	2.218080
H	4.201679	3.384332	1.221676
H	4.335029	3.367665	2.982659
H	2.763216	0.104648	3.663681
H	1.941873	1.674338	3.688068
H	3.575806	1.519219	4.325303
H	4.356785	1.984503	-1.497792

B3LYP/def2TZVP (CPCM – DME)



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.793074	2.410200	-3.268237
C	2.644148	0.917851	-2.902614
C	1.632175	0.307274	-3.886870
C	3.989564	0.194197	-3.126558
C	2.210210	0.773917	-1.432816
C	1.015277	0.151457	-1.105646
C	0.558888	-0.003623	0.210229
C	-0.721825	-0.672814	0.512472
C	-1.228762	-1.691299	-0.302173
C	-2.433779	-2.343008	-0.053275
C	-2.934938	-3.457647	-0.995252
C	-1.970080	-3.698590	-2.169964
C	-3.057489	-4.794303	-0.232028
C	-4.297618	-3.067145	-1.608161
C	-3.158644	-1.952283	1.091257
O	-4.349362	-2.612727	1.318637
C	-2.698262	-0.932910	1.950134
C	-3.491569	-0.480162	3.196707
C	-4.880939	0.066845	2.792738
C	-2.783907	0.660044	3.951790
C	-3.626384	-1.640778	4.211494
C	-1.488627	-0.319292	1.626075
C	1.378448	0.508679	1.225009
C	2.586996	1.144342	0.984949
C	3.441424	1.673552	2.150787
C	4.820387	0.979716	2.155484
C	3.631254	3.199644	2.012947
C	2.799729	1.419396	3.525307
C	3.059295	1.305043	-0.379902
O	4.169607	1.886031	-0.641833
H	3.128744	2.518785	-4.304579
H	3.512755	2.890342	-2.609469
H	1.831687	2.922170	-3.171001
H	1.492326	-0.763040	-3.718779
H	0.655228	0.792042	-3.824073
H	1.999669	0.436316	-4.907975
H	4.322279	0.316755	-4.162305
H	4.749165	0.594420	-2.459278
H	3.880831	-0.876582	-2.933006
H	0.380246	-0.215199	-1.900052
H	-0.637336	-1.993496	-1.151318
H	-0.984307	-4.022598	-1.831455
H	-2.375774	-4.487271	-2.806684
H	-1.845494	-2.806873	-2.786982
H	-3.391704	-5.582131	-0.912303

H	-3.766063	-4.727364	0.589284
H	-2.086681	-5.089533	0.173032
H	-4.204365	-2.140829	-2.180024
H	-4.636855	-3.850832	-2.290709
H	-5.059157	-2.924041	-0.846155
H	-4.704590	-2.373870	2.177364
H	-5.504118	-0.652632	2.262252
H	-5.430714	0.385091	3.681239
H	-4.763252	0.931634	2.137293
H	-1.798422	0.360892	4.311315
H	-2.668974	1.549039	3.330357
H	-3.383546	0.938482	4.820376
H	-4.146345	-2.522116	3.831822
H	-4.175591	-1.304598	5.093448
H	-2.637549	-1.974565	4.530403
H	-1.127493	0.484740	2.246377
H	1.051897	0.371412	2.246476
H	5.443808	1.372304	2.965238
H	4.703025	-0.096030	2.313021
H	5.327172	1.140600	1.206936
H	2.665293	3.708750	2.073051
H	4.092794	3.437855	1.057610
H	4.263493	3.581200	2.821149
H	2.665605	0.353720	3.724613
H	1.827339	1.908261	3.619683
H	3.449428	1.822068	4.306404



<i>Element</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
C	2.673955	2.599470	-3.201453
C	2.554608	1.087831	-2.894863
C	1.491084	0.535153	-3.861230
C	3.869077	0.346361	-3.237485
C	2.166520	0.860555	-1.416908
C	0.968551	0.226064	-1.092681
C	0.561790	0.006261	0.221105
C	-0.720740	-0.672070	0.521512

C	-1.180510	-1.726922	-0.266410
C	-2.380627	-2.386690	-0.019378
C	-2.840923	-3.550738	-0.920454
C	-1.837666	-3.831176	-2.053302
C	-2.967495	-4.851221	-0.097618
C	-4.189946	-3.207843	-1.589587
C	-3.140970	-1.949735	1.086367
O	-4.320498	-2.615050	1.309596
C	-2.721350	-0.886504	1.914222
C	-3.557370	-0.389783	3.114622
C	-4.934800	0.132024	2.641656
C	-2.878704	0.784947	3.842511
C	-3.720494	-1.509232	4.170663
C	-1.509136	-0.275036	1.598822
C	1.400384	0.448818	1.243761
C	2.610179	1.092944	1.002725
C	3.502275	1.559076	2.171358
C	4.872602	0.849275	2.119197
C	3.691319	3.091061	2.121718
C	2.876650	1.229156	3.538202
C	2.979452	1.288076	-0.345341
O	4.176066	1.925773	-0.557982
H	2.944099	2.746848	-4.249017
H	3.417067	3.121225	-2.598226
H	1.716846	3.092627	-3.023295
H	1.355072	-0.541090	-3.745413
H	0.524930	1.023054	-3.725552
H	1.812585	0.719460	-4.887578
H	4.117865	0.498518	-4.289499
H	4.736752	0.663984	-2.657325
H	3.750368	-0.724629	-3.065261
H	0.308930	-0.092083	-1.884015
H	-0.560178	-2.050852	-1.086947
H	-0.857779	-4.122945	-1.670858
H	-2.212010	-4.656005	-2.662174
H	-1.709191	-2.968620	-2.709941
H	-3.269627	-5.674187	-0.750116
H	-3.702070	-4.758609	0.697761
H	-2.005667	-5.112584	0.349675
H	-4.092638	-2.307453	-2.200662
H	-4.496753	-4.027101	-2.244571
H	-4.976464	-3.042594	-0.858246
H	-4.742331	-2.297856	2.111373
H	-5.541000	-0.611024	2.123269
H	-5.513808	0.483870	3.497835
H	-4.800337	0.968511	1.953753
H	-1.904292	0.506079	4.246200
H	-2.748642	1.648427	3.188754

H	-3.506661	1.095971	4.678966
H	-4.230953	-2.404226	3.811851
H	-4.294079	-1.136412	5.021419
H	-2.741482	-1.828751	4.531515
H	-1.167673	0.557349	2.193013
H	1.098071	0.258732	2.261355
H	5.486878	1.167729	2.965106
H	4.742241	-0.233263	2.187115
H	5.411288	1.073271	1.202438
H	2.724906	3.595409	2.194265
H	4.177340	3.411497	1.204178
H	4.304159	3.415682	2.966328
H	2.741753	0.155167	3.679348
H	1.911142	1.719501	3.676185
H	3.542034	1.583582	4.327409
H	4.378850	1.962630	-1.495491