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Is cannabidiolic acid an overlooked natural antioxidant? – insights from quantum chemistry calculations

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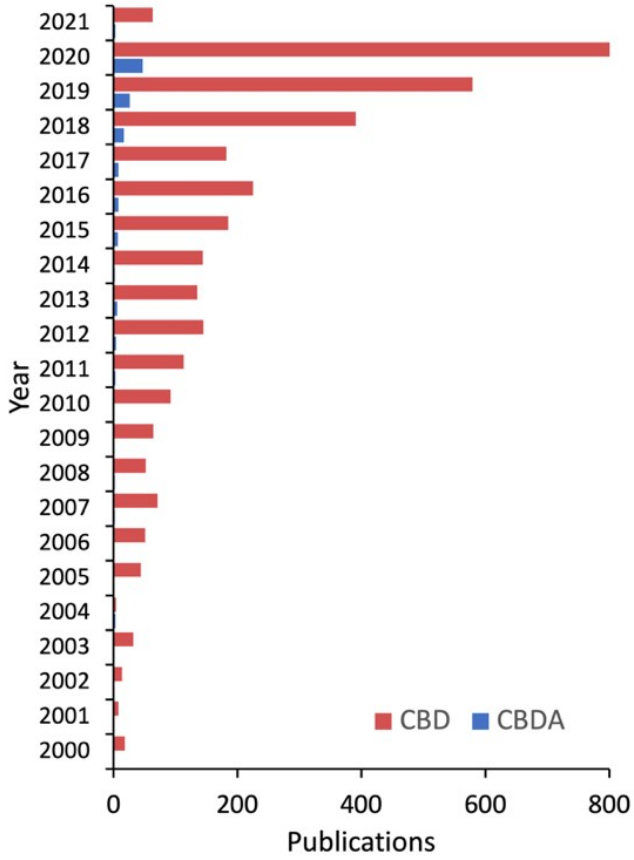

Figure S1. The number of publications published between 2000 and 2021 dealing with "cannabidiol" and "cannabidiolic acid" (PubMed, August 6, 2021).

Table S1. The method to calculate rate constant following the conventional transition state theory.

The antiradical action of phenolic compounds is well recognized to be directed by three distinct processes; HAT, SET, and RAF [1-5]. A hydrogen atom is transferred from the antioxidant to the free radical in a one-step process known as HAT. The BDE of the active OH/CH bonds of the antioxidant may be used to describe this mechanism, which may occur in both polar and lipid environments [6]. RAF is a one-step process that leads to the product [antioxidant–free radical]• by combining free radicals with antioxidants [7]. The Gibbs free energy of the reaction could be used to describe this mechanism. Unlike HAT and RAF, the SET process, which involves an electron transfer, could only occur in polar environments [8]. In these media, the phenolic OH bonds of the antioxidant could exist in both protonated and deprotonated forms and therefore electron transfer can occur from the neutral or anionic state of the antioxidant. However, SET from an undissociated phenol is often an infeasible chemical route, thus it is only significant for deprotonated phenols. The Gibbs free energy of electron transfer may be used to describe this pathway (dominant step). The following equations describe the mentioned mechanisms.

$$AntioxOH + R^{\cdot} \rightarrow AntioxO^{\cdot} + ROH \text{ (FHT)}$$

$$AntioxOH + R^{\cdot} \rightarrow [AntioxOH{-}R]^{\cdot} \text{ (RAF)}$$

$$AntioxOH \rightarrow AntioxO^{-} + H^{+}; AntioxO^{-} + R^{\cdot} \rightarrow AntioxO^{\cdot} + R^{-} \text{ (SET)}$$

PA (proton affinity) and BDE (bond dissociation enthalpy) values were calculated as follows.

$$BDE = H(ArO^{\cdot}) + H(H^{\cdot}) - H(ArOH)$$

$$PA = H(ArO^{-}) + H(H^{+}) - H(ArOH)$$

Where $H(ArOH)$, $H(ArO^{\cdot})$, $H(ArO^{-})$, $H(H^{\cdot})$, $and\ H(H^{+})$ are enthalpies of the neutral molecule, radical, anion, hydrogen atom, and proton respectively.

The pKa values of CBDA were computed according to the literature using the following equation [9]:

$$AH + OH^{-}(3H_2O) \rightarrow A^{-}(H_2O) + 3H_2O$$

$$pK_a = \frac{\Delta G_{sol}}{RTln(10)} + 14 + 3log[H_2O]$$

Where DG_{sol} is the Gibbs free energy of the reaction in solution, R is the gas constant, and T is the temperature (298.15 K).

The kinetic calculations were carried out following the methodology of the quantum mechanics-based test for overall free radical scavenging activity (QM-ORSA)[10, 11]. The rate constant (*k*) was calculated by using standard transition state theory (TST) and 1M standard state at 298.15 K according to the equation below: [12-19]

$$k = \sigma\kappa\frac{k_B T}{h} e^{-(\Delta G^{\neq})/RT}$$

Where σ is the reaction symmetry number,[20, 21] κ represents tunneling corrections computed using the Eckart barrier,[22] k_B is the Boltzmann constant, *h* is the Planck constant, $\Delta G^{\neq}$ is Gibbs free energy of activation.

The apparent rate constants (k_{app}, rate constants close to the diffusion limit) were corrected using the Collins−Kimball theory [23]. Branching ratios (Γ, %) were calculated as follows:

$$\Gamma_{path} = \frac{k}{k_{overall}} \times 100$$

Where *k* and $k_{overall}$ are the rate constants of a specific reaction path and the sum of the rate constants of all reaction paths, respectively.

Marcus theory has been used to predict the Gibbs free energy of activation of the single electron transfer mechanism [24]:

$$\Delta G_{SET}^{\neq} = \frac{\lambda}{4}(1 + \frac{\Delta G_{SET}^{0}}{\lambda})^2$$

$$\lambda \approx \Delta E_{SET} + \Delta G_{SET}^{0}$$

Where λ is the nuclear reorganization energy, ΔG_{SET}^{0} is the Gibbs free energy of reaction, and ΔE_{SET} is the nonadiabatic energy difference between reactants and vertical products. The computational kinetic study was performed with Eyringpy software[17].

Table S2. The cartesian coordinates and energies of the TSs of the CBDA+HOO$^{\bullet}$/NO_2 reaction at M06-2X/6-311++G(d,p) in water and pentyl ethanoate..

CBDA-1O…H…OOH (PE)				
Cartesian Coordinates				Frequency and Energy
C	0.92739200	-0.30522600	-0.01743900	Zero-point Energy Correction = 0.495776 Hartree
C	0.15875200	0.84474600	-0.27712100	Thermal Correction to Energy = 0.525422 Hartree
C	-1.20943000	0.75673700	-0.63386600	Thermal Correction to Enthalpy = 0.526367 Hartree
C	-1.85208700	-0.52278200	-0.69187900	Thermal Correction to Free Energy = 0.433578 Hartree
C	-1.09546000	-1.63995500	-0.44231400	
C	0.28605700	-1.56133900	-0.14341700	EE + Zero-point Energy = -1307.5606 Hartree
O	0.96338100	-2.67558800	-0.00393600	EE + Thermal Energy Correction = -1307.531 Hartree
O	0.80982100	2.01170500	-0.19840100	
C	-3.33194500	-0.72410100	-0.92583200	EE + Thermal Enthalpy Correction = -1307.53 Hartree
C	-4.17572200	-0.27762500	0.27610500	
C	-5.67112000	-0.41692300	0.00782500	EE + Thermal Free Energy Correction = -1307.6228 Hartree
C	-6.53251600	-0.00326000	1.19876500	
C	-8.02519100	-0.14906800	0.91777500	
C	2.39668300	-0.22545300	0.30898100	
C	2.70450500	0.73400100	1.44324300	
C	3.83550900	1.43247800	1.54999600	
C	4.91493700	1.36288700	0.49959700	
C	4.71575400	0.21955800	-0.49183900	
C	3.25307500	0.12173000	-0.94101300	
C	4.08684900	2.37932500	2.68776900	
C	3.04296200	-0.88324500	-2.05269800	
C	2.29340500	-0.57613300	-3.11195200	
C	3.69513800	-2.23158600	-1.90548000	
H	-1.53968700	-2.62743200	-0.48212000	
H	1.18635600	-2.87422900	1.10379200	
H	0.16378100	2.73439500	-0.34593100	
H	-3.66517500	-0.20580300	-1.82379000	
H	-3.49622900	-1.79192800	-1.08933000	
H	-3.89639200	-0.88150500	1.14703600	
H	-3.94822700	0.76268800	0.52981300	
H	-5.93980300	0.19368100	-0.86337300	
H	-5.89811700	-1.45652200	-0.25936900	
H	-6.25957600	-0.61070300	2.06867100	
H	-6.30625300	1.03612800	1.46190300	
H	-8.62726700	0.14882800	1.77954300	
H	-8.32521900	0.47157700	0.06837200	
H	-8.27649900	-1.18603500	0.67646900	

H	2.69939300	-1.23129600	0.62159200	
H	1.92954000	0.88459700	2.19521500	
H	4.93310700	2.32493400	-0.02940100	
H	5.89056100	1.27260200	0.98988800	
H	5.36353900	0.35984900	-1.36209800	
H	5.00872900	-0.72515100	-0.02037000	
H	2.92460600	1.10437800	-1.29402900	
H	4.27564200	3.38889900	2.30725700	
H	3.23907400	2.42150500	3.37387300	
H	4.97662900	2.08082700	3.25160000	
H	2.11437700	-1.29486000	-3.90586000	
H	1.83777100	0.40461600	-3.21686900	
H	3.46625400	-2.67912700	-0.93422600	
H	3.35422500	-2.91531700	-2.68436000	
H	4.78407400	-2.14520100	-1.97725400	
H	1.47540400	-1.05224600	2.74860300	
O	1.30005300	-2.85623800	2.31603300	
O	0.73023900	-1.67410800	2.67492400	
C	-1.88092300	2.03235300	-0.96138400	
O	-1.39147200	3.13275300	-0.75091000	
O	-3.07202100	1.94146600	-1.54815000	
H	-3.38437600	2.84521100	-1.71465000	

CBDA-7C…H…OOH (PE)				
Cartesian Coordinates				Frequency and Energy
C	-0.71707800	-0.30503900	-0.15057300	Zero-point Energy Correction = 0.495796 Hartree
C	-0.10327400	-1.32173200	-0.88430900	Thermal Correction to Energy = 0.525535 Hartree
C	1.26308200	-1.28154600	-1.18751700	Thermal Correction to Enthalpy = 0.526479 Hartree
C	2.06428800	-0.22516300	-0.80558200	Thermal Correction to Free Energy = 0.434176 Hartree
C	1.47196900	0.85150300	-0.08689000	
C	0.08613600	0.78440900	0.22839100	EE + Zero-point Energy = -1307.5652 Hartree
O	-0.53571000	1.75591300	0.89787900	EE + Thermal Energy Correction = -1307.5354 Hartree
O	-0.77398800	-2.38610100	-1.37280900	
C	3.53584700	-0.34191700	-1.13333400	EE + Thermal Enthalpy Correction = -1307.5345 Hartree
C	4.36938700	-0.75738700	0.08678300	
C	5.85810200	-0.84150500	-0.23708000	EE + Thermal Free Energy Correction = -1307.6268 Hartree
C	6.70663600	-1.25776400	0.96234100	
C	8.19045200	-1.36141900	0.62164000	
C	-2.19880700	-0.30549300	0.11259200	
C	-2.74925700	-1.60047800	0.55388900	
C	-3.98422600	-2.05211700	0.24707800	
C	-4.92595400	-1.24022400	-0.60107800	
C	-4.52018000	0.22829200	-0.68627100	
C	-3.02825900	0.36452800	-1.00658800	
C	-4.48583000	-3.37793600	0.72970900	
C	-2.61259500	1.79093000	-1.30090400	
C	-1.80835500	2.05669900	-2.33016100	
C	-3.14144000	2.87210800	-0.39925600	

H	1.68133300	-2.11150100	-1.74462500	
H	0.12715100	2.45087500	1.11091900	
H	-1.68889600	-2.38548000	-1.05579400	
H	3.64364500	-1.10926300	-1.90425900	
H	3.92577100	0.58712900	-1.54598800	
H	4.21274200	-0.04536300	0.90226200	
H	4.01339800	-1.73096500	0.44309400	
H	6.01337200	-1.55563300	-1.05555300	
H	6.20400300	0.13279700	-0.60446800	
H	6.56362500	-0.53279100	1.77128700	
H	6.34693900	-2.22096700	1.34081300	
H	8.78355000	-1.64886600	1.49320400	
H	8.35998300	-2.10804300	-0.15965200	
H	8.57478200	-0.40468000	0.25599100	
H	-2.38540400	0.38054200	1.18603600	
H	-2.11710300	-2.20396200	1.20294200	
H	-4.96018000	-1.68361900	-1.60569200	
H	-5.94002600	-1.33888900	-0.19924200	
H	-5.11170600	0.73897500	-1.45075100	
H	-4.73062000	0.72785800	0.26680300	
H	-2.82460600	-0.22184300	-1.91542300	
H	-4.83664600	-3.98322600	-0.11291800	
H	-3.71609500	-3.93333600	1.26720000	
H	-5.34459900	-3.23724700	1.39508600	
H	-1.48458300	3.07026700	-2.54621200	
H	-1.44185400	1.26867700	-2.98172400	
H	-2.97159900	2.62269900	0.65045000	
H	-2.65629300	3.82531400	-0.61542600	
H	-4.22047100	2.99915200	-0.53836700	
H	-4.44507800	0.05034800	2.54674200	
O	-2.77923500	0.86692300	2.30915700	
O	-3.55065400	-0.11062900	2.88539800	
C	2.18083000	2.06241800	0.33831400	
O	3.46243500	2.16960800	-0.02178600	
O	1.66863800	2.97152900	0.98354900	
H	3.78474100	3.01610300	0.32498200	
CBDA-1O…H…OOH (W)				
Cartesian Coordinates				Frequency and Energy
C	0.96445200	-0.21551100	0.34839500	Zero-point Energy Correction = 0.481584 Hartree
C	0.16009700	0.89856100	0.06899300	Thermal Correction to Energy = 0.510931 Hartree
C	-1.21784100	0.92241800	0.37949000	Thermal Correction to Enthalpy = 0.511876 Hartree
C	-1.84371300	-0.24356400	0.90004000	Thermal Correction to Free Energy = 0.420119
C	-1.06924200	-1.35910100	1.13578500	Hartree
C	0.31637900	-1.36390000	0.86761100	EE + Zero-point Energy = -1307.1218 Hartree
O	0.99386500	-2.48840400	1.06579100	EE + Thermal Energy Correction = -1307.0924
O	0.74887700	1.96811900	-0.51535800	Hartree
C	-3.33431000	-0.35211100	1.11859100	EE + Thermal Enthalpy Correction = -1307.0915

C	-4.11810500	-0.31338700	-0.19955300	Hartree
C	-5.62565100	-0.33308300	0.03015000	EE + Thermal Free Energy Correction = -1307.1832
C	-6.42804200	-0.33757500	-1.26818900	Hartree
C	-7.93360700	-0.34499300	-1.02165000	
C	2.44275700	-0.24269700	0.04616500	
C	3.17677700	0.95278600	0.61636900	
C	4.17360400	1.59173000	0.00216600	
C	4.66024400	1.17421400	-1.36296500	
C	4.19863900	-0.22896500	-1.74336300	
C	2.69934900	-0.39912100	-1.47832200	
C	4.85905000	2.78254300	0.60887600	
C	2.15428500	-1.71742700	-1.98213300	
C	0.99552500	-1.76907100	-2.64163000	
C	2.95344600	-2.95786000	-1.68591100	
H	-1.51354600	-2.27309400	1.51343100	
H	-0.01101700	2.57451600	-0.76572000	
H	-3.53351500	-1.30346300	1.61893200	
H	-3.68694700	0.44514500	1.77241100	
H	-3.85033600	0.58454200	-0.76704600	
H	-3.82571800	-1.17394700	-0.81249300	
H	-5.89254800	-1.21618300	0.62374300	
H	-5.90807000	0.54245800	0.62788700	
H	-6.15521700	0.54189800	-1.86170400	
H	-6.14680900	-1.21444700	-1.86161800	
H	-8.49503500	-0.34952200	-1.95872200	
H	-8.22889500	-1.22886100	-0.44905400	
H	-8.23788700	0.53774800	-0.45211800	
H	2.84705200	-1.13443900	0.53655100	
H	2.85141400	1.28983300	1.59841700	
H	4.30192600	1.90510900	-2.09996500	
H	5.75359200	1.23271100	-1.38696400	
H	4.41414700	-0.42740200	-2.79728400	
H	4.75529300	-0.96564800	-1.15346900	
H	2.16430900	0.40907400	-1.98740400	
H	4.79619100	3.64195300	-0.06722300	
H	4.41484800	3.06021600	1.56633000	
H	5.92361300	2.57905100	0.76271800	
H	0.57998300	-2.71256500	-2.98284700	
H	0.43154200	-0.86600000	-2.85842200	
H	3.22831900	-3.01016300	-0.62813800	
H	2.38950600	-3.85526000	-1.94453400	
H	3.88677100	-2.96067500	-2.25755800	
O	2.14509200	-1.98502800	3.07227100	
O	1.69524100	-0.70534000	3.16326100	
C	-1.97054700	2.22627000	0.16506200	
O	-1.50914700	2.99902300	-0.73741100	
O	-2.95059800	2.49448800	0.88045000	

H	1.62708500	-2.37897000	1.96865300	
H	0.85203200	-0.75741400	3.64730200	
CBDA-7C…H…OOH (W)				
Cartesian Coordinates				Frequency and Energy
C	-0.69677200	-0.29241100	-0.15186300	Zero-point Energy Correction = 0.480107 Hartree
C	-0.10467100	-1.31308900	-0.89795300	Thermal Correction to Energy = 0.509595 Hartree
C	1.25392200	-1.29189400	-1.21114500	Thermal Correction to Enthalpy = 0.510539 Hartree
C	2.07367500	-0.24543000	-0.81355100	Thermal Correction to Free Energy = 0.418775
C	1.51583400	0.82890800	-0.08062500	Hartree
C	0.13081100	0.78132800	0.22868900	EE + Zero-point Energy = -1307.1271 Hartree
O	-0.44756900	1.78582800	0.90562000	EE + Thermal Energy Correction = -1307.0976
O	-0.80896200	-2.37415300	-1.39746600	Hartree
C	3.53954300	-0.37011900	-1.15744200	EE + Thermal Enthalpy Correction = -1307.0967
C	4.37358700	-0.82646900	0.04704200	Hartree
C	5.87173900	-0.75808700	-0.23039700	EE + Thermal Free Energy Correction = -1307.1884
C	6.71984800	-1.24648900	0.94078300	Hartree
C	8.21595300	-1.14021400	0.66116500	
C	-2.17811000	-0.28636200	0.11996500	
C	-2.71471700	-1.56365300	0.62018100	
C	-3.95428300	-2.02910700	0.35027800	
C	-4.90889100	-1.25876200	-0.51733800	
C	-4.50820000	0.20335000	-0.68296800	
C	-3.02018300	0.32482800	-1.02477700	
C	-4.43941000	-3.34042600	0.88187500	
C	-2.60841300	1.73500800	-1.39172800	
C	-1.77869400	1.95091200	-2.41362200	
C	-3.17341900	2.86592000	-0.57611300	
H	1.66045700	-2.11587400	-1.78674500	
H	0.33210800	2.43899500	1.08737100	
H	-1.72546400	-2.35613200	-1.08417400	
H	3.64092700	-1.11232500	-1.95406500	
H	3.92982300	0.57480900	-1.53095900	
H	4.13523300	-0.20129500	0.91274300	
H	4.09094900	-1.85342800	0.30730200	
H	6.10798500	-1.35207800	-1.12224100	
H	6.14252200	0.27896100	-0.46557700	
H	6.46851600	-0.66143200	1.83231000	
H	6.45869400	-2.28630700	1.16606500	
H	8.81014400	-1.48478900	1.51073200	
H	8.49302500	-1.74217900	-0.20902400	
H	8.49804000	-0.10427100	0.45240600	
H	-2.37395900	0.44056400	1.13518400	
H	-2.06349900	-2.14976100	1.26605300	
H	-4.95293300	-1.75572600	-1.49602300	
H	-5.91541000	-1.34004600	-0.09463500	
H	-5.10881300	0.67045100	-1.46782100	
H	-4.71208900	0.74717100	0.24621500	

H	-2.81681200	-0.31110500	-1.89913500	
H	-4.79313100	-3.97289800	0.06116600	
H	-3.65991600	-3.87110300	1.42975300	
H	-5.29474000	-3.18035500	1.54678900	
H	-1.46125900	2.95432700	-2.68071600	
H	-1.39093100	1.12888700	-3.00878700	
H	-3.03087700	2.69036400	0.49267300	
H	-2.69872700	3.81065700	-0.84536800	
H	-4.25079400	2.96145700	-0.74456000	
H	-4.47236800	0.19506600	2.45981800	
O	-2.78600100	0.99820900	2.26602400	
O	-3.59815000	0.06476800	2.86184900	
C	2.31195700	2.03245600	0.36469400	
O	3.51763200	2.15170000	0.08385500	
O	1.67638300	2.92342500	1.04166300	

CBDA-7C…H…ONO (PE)

Cartesian Coordinates				Frequency and Energy
C	-0.55765300	-0.35402600	-0.29130100	Zero-point Energy Correction = 0.488369 Hartree
C	0.09503800	-1.37806100	-0.97818400	Thermal Correction to Energy = 0.518902 Hartree
C	1.47239400	-1.32912600	-1.21994200	Thermal Correction to Enthalpy = 0.519847 Hartree
C	2.24675600	-0.26362800	-0.80614000	Thermal Correction to Free Energy = 0.424799 Hartree
C	1.61674600	0.81028700	-0.11628100	
C	0.21840600	0.73920200	0.12638000	EE + Zero-point Energy = -1361.7131 Hartree
O	-0.44640400	1.70350200	0.76453200	EE + Thermal Energy Correction = -1361.6826 Hartree
O	-0.54644900	-2.45507200	-1.47939500	
C	3.73060800	-0.36035300	-1.07827100	EE + Thermal Enthalpy Correction = -1361.6817 Hartree
C	4.52005900	-0.79729300	0.16395700	
C	6.02670200	-0.76470500	-0.07391300	EE + Thermal Free Energy Correction = -1361.7767 Hartree
C	6.83207800	-1.24721100	1.13009800	
C	8.33766000	-1.18212200	0.89072100	
C	-2.05122100	-0.35225900	-0.11909500	
C	-2.61834100	-1.58746200	0.38918800	
C	-3.89702400	-2.00510400	0.13522400	
C	-4.78808700	-1.24169300	-0.79468500	
C	-4.33646300	0.19752200	-1.02679500	
C	-2.83151700	0.27910100	-1.30282600	
C	-4.45360800	-3.23742500	0.76043300	
C	-2.36953300	1.68500700	-1.62792500	
C	-1.49922200	1.89312200	-2.61565100	
C	-2.92487100	2.81259400	-0.80179700	
H	1.92315700	-2.15684400	-1.75446700	
H	0.19625600	2.40953900	1.00389300	
H	-1.48165900	-2.44259000	-1.23543800	
H	3.87677200	-1.10605700	-1.86386000	
H	4.12463400	0.58353500	-1.45185100	
H	4.27126600	-0.14831700	1.00862000	
H	4.20942900	-1.81130500	0.44131600	

H	6.27424400	-1.38236700	-0.94648100	
H	6.32712800	0.26051300	-0.32403300	
H	6.57102700	-0.63948400	2.00368100	
H	6.54101200	-2.27600800	1.36952600	
H	8.89830000	-1.52946900	1.76189100	
H	8.62493900	-1.80371500	0.03764600	
H	8.65431400	-0.15724300	0.67621700	
H	-2.31826200	0.36328400	0.88099500	
H	-2.01081400	-2.17103200	1.07909400	
H	-4.81269000	-1.79430400	-1.74541900	
H	-5.81190300	-1.27290100	-0.40892000	
H	-4.88582000	0.62703500	-1.86842300	
H	-4.57888700	0.79910300	-0.14607300	
H	-2.60404000	-0.34653200	-2.17812900	
H	-4.92054600	-3.87493400	0.00296500	
H	-3.69490100	-3.80606900	1.29833200	
H	-5.24483800	-2.95288500	1.46388300	
H	-1.14092500	2.89074800	-2.85002800	
H	-1.11271200	1.07332900	-3.21444000	
H	-2.83796900	2.59907100	0.26589500	
H	-2.39366000	3.74153500	-1.01470000	
H	-3.98633900	2.96870700	-1.02065900	
O	-2.92149400	0.92645000	2.03015400	
C	2.30002700	2.01892300	0.35852900	
O	3.60785000	2.11019900	0.10925700	
O	1.74274400	2.93374800	0.95540700	
N	-3.79339900	0.06700500	2.32648200	
O	-4.48954400	0.27118900	3.28937100	
H	3.91006300	2.95473800	0.47864400	

CBDA-7C…H…ONO (W)				
Cartesian Coordinates				Frequency and Energy
C	-0.66389700	-0.04270500	-0.36668500	Zero-point Energy Correction = 0.473117 Hartree
C	-0.10489100	-1.21098300	-0.88435800	Thermal Correction to Energy = 0.503405 Hartree
C	1.25324900	-1.28399800	-1.19200300	Thermal Correction to Enthalpy = 0.504349 Hartree
C	2.10049800	-0.19840700	-1.02008400	Thermal Correction to Free Energy = 0.408913
C	1.57387200	1.01438100	-0.51878500	Hartree
C	0.19993100	1.05704700	-0.17811400	EE + Zero-point Energy = -1361.2771 Hartree
O	-0.32929500	2.16586500	0.37273000	EE + Thermal Energy Correction = -1361.2468
O	-0.81676000	-2.35700600	-1.09399100	Hartree
C	3.56580400	-0.42284900	-1.31475200	EE + Thermal Enthalpy Correction = -1361.2459
C	4.40126300	-0.51124700	-0.03080400	Hartree
C	5.89690500	-0.58205000	-0.32068400	EE + Thermal Free Energy Correction = -1361.3413
C	6.74504500	-0.69146000	0.94337500	Hartree
C	8.23965400	-0.74024800	0.64091000	
C	-2.07414200	0.07665300	0.13696300	
C	-2.79942500	1.21318700	-0.33343200	
C	-3.86751800	1.78432000	0.34782700	

C	-4.27174500	1.27229200	1.68712200
C	-3.77702100	-0.14303500	1.96637000
C	-2.29020700	-0.27923800	1.63010600
C	-4.59936500	2.94954000	-0.20593800
C	-1.71923900	-1.63326000	1.99648500
C	-0.49798000	-1.72673700	2.52362600
C	-2.56952500	-2.84815100	1.74353200
H	1.63891900	-2.22082400	-1.57774500
H	0.48071900	2.79388400	0.48083900
H	-1.76928600	-2.19131200	-1.14985100
H	3.66297400	-1.36458000	-1.86152500
H	3.95886900	0.37098200	-1.94805200
H	4.19534100	0.35823900	0.60108400
H	4.09070700	-1.39712700	0.53577500
H	6.10479700	-1.43921000	-0.97313800
H	6.19358600	0.31476600	-0.87902400
H	6.52738800	0.16263000	1.59398100
H	6.45124100	-1.58917300	1.49834900
H	8.83310600	-0.80969700	1.55553800
H	8.48249800	-1.60486800	0.01663400
H	8.55598500	0.15801700	0.10304300
H	-2.80347600	-0.75278200	-0.48910000
H	-2.52047000	1.63307100	-1.29643000
H	-3.85147100	1.97412700	2.42397200
H	-5.35819000	1.34935800	1.78997300
H	-3.94498800	-0.39359300	3.01607400
H	-4.35240900	-0.85265100	1.36290400
H	-1.72883000	0.48118300	2.18947100
H	-4.68888300	3.73167700	0.55456100
H	-4.12374700	3.35273800	-1.09896900
H	-5.62266500	2.64162800	-0.45345500
H	-0.06372300	-2.69018600	2.77247900
H	0.10210400	-0.84215400	2.71789200
H	-2.96109400	-2.86009800	0.72318000
H	-1.99739900	-3.76175600	1.91089800
H	-3.43615000	-2.85801400	2.41222200
O	-3.59459100	-1.65800500	-1.24535900
C	2.39274200	2.27324800	-0.34893600
O	3.51625600	2.38093200	-0.86970900
O	1.85310000	3.21805100	0.33461400
N	-4.11762000	-0.88533000	-2.12147700
O	-4.88322900	-1.43168400	-2.88474700

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