# Supporting Information

### **Supramolecular Trap for a Transient Corannulene Trianion**

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#### Materials and Methods.

All manipulations were carried out using break-and-seal<sup>[1]</sup> and glove-box techniques under an atmosphere of argon. THF and hexanes were dried over Na/benzophenone and distilled prior to use. Diglyme was dried over NaK<sub>2</sub> alloy and vacuum-transferred. Lithium and dicyclohexano-18-crown-6 (99%) were purchased from Sigma-Aldrich. Cesium was purchased from Strem Chemicals. Crown ether was dried over P<sub>2</sub>O<sub>5</sub> in vacuo for 24 hours. Corannulene was prepared as described previously<sup>[2-4]</sup> and sublimed at 175 °C prior to use. The UV-vis spectra were recorded on a PerkinElmer Lambda 35 spectrometer. The ESR spectra were recorded on a Bruker ER-200 D-SRC X-band spectrometer that is interfaced to a Compag 386 PC equipped with the IBM analog-to-digital converter and Scientific Software Services Systems (Bloomington, IL). The trianion of corannulene was generated by the reaction of cesium metal or Li/Cs mixture (excess) with the solution of  $C_{20}H_{10}$  in THF ( $\approx$  $4 \times 10^{-4}$  M) in the sealed quartz capillary ( $\emptyset$  1.0 mm) at 25 °C. The probe for the ESR study was also prepared by dissolving crystals of **1** and transferring the resulting solution ( $\approx 2 \times 10^{-5}$ M) into the quartz capillary ( $\emptyset$  0.6 mm), which was then sealed. Magnetic measurements were performed on polycrystalline samples of 1 (between 10 and 20 mg). The samples were manipulated in a drybox under nitrogen atmosphere and sealed in a polyethylene bag  $(3 \times 0.5)$  $\times$  0.02 cm; between 20 and 35 mg) in order to collect data in the temperature range of 1.8 to 300 K at 1000 Oe. Magnetic measurements were obtained with the use of a Quantum Design SQUID magnetometer MPMS-XL functioning between 1.8 and 400 K for direct-current (dc) applied fields ranging from -7 to +7 T. Prior to the experiment, the field-dependent magnetization was measured at 100 K on the sample in order to prove the absence of any bulk ferromagnetic impurities. The magnetic data were corrected for the sample holder and diamagnetic contributions. Elemental analysis was performed by Complete Analysis Laboratories, Inc., Parsippany, NJ.

Crystallization of  $[Cs_{3}^{+}(diglyme)_{2}(C_{20}H_{10}^{-3-})]$  (1).

**Direct Cs reduction.** Diglyme (3 mL) was added to a flask containing Cs metal (28 mg, 0.21 mmol, 3.5 eq.), corannulene (15 mg, 0.06 mmol), and dicyclohexano-18-crown-6 (22 mg, 0.06 mmol). The resulting green mixture was stirred at room temperature for 60 hours to give a bright purple-red solution. This solution was filtered, layered with hexanes (3 mL), and kept at 10 °C. A few X-ray quality crystals of **1** were collected in 4 weeks. Yield: 5.5 mg, 10%.

**Cs/Li reduction.** Diglyme (3 mL) was added to a flask containing Cs metal (28 mg, 0.21 mmol, 3.5 eq.), Li (0.85 mg, 0.12 mmol), and corannulene (15 mg, 0.06 mmol). The resulting green solution was stirred at room temperature for 16 hours to give a bright purple-red solution. This solution was filtered, layered with hexanes (3 mL), and kept at 10 °C. The X-ray quality crystals (prisms) of 1 were deposited in 72 hours. Crystals of 1 were collected, washed with hexanes (2 x 3 mL), dried and used for characterization. Yield: 19.3 mg, 35%. UV-vis (diglyme, nm):  $\lambda_{max} = 388$ . UV-vis (THF, nm):  $\lambda_{max} = 386$ . Anal. Calcd for C<sub>32</sub>H<sub>38</sub>Cs<sub>3</sub>O<sub>6</sub>: C, 41.90; H, 4.18; Found: C, 41.78; H, 4.14.

**Magnetic Measurements.** Multiple samples of single crystals collected from the above reactions have been sent for magnetic measurements over the period of two years. All our attempts to collect good sets of magnetic data have failed likely due to extreme air- and moisture sensitivity of the title product. Our rough estimates point out to very weak interactions of corannulene trianions within the sandwich-type assemblies with an exchange coupling between -5 and -10 K, which makes a gap between the singlet ground state and the triplet state of about 10–20 K. This is consistent with our theoretical calculations showing degeneracy of the two states. Unfortunately, the absolute values of the susceptibility could not be obtained reliably.

**ESR Data.** Using probes prepared by dissolving the crystals of **1** in THF or diglyme, we were unable to detect any well-resolved ESR signal. Only in the presence of an excess of cesuim metal upon the *in situ* reduction of  $C_{20}H_{10}$  in THF the highly resolved ESR signal centered at g = 2.0038 could be observed in 24 h (Figure S1). These ESR data point out to the formation of trianion-radicals in solution, consistent with previous works of Scott and coworkers.<sup>[5]</sup> However, it has to be mentioned here that we could not isolate the sandwich type aggregates from the THF solutions, as the title product is formed only when diglyme is used as a solvent media.



**Figure S1.** Experimental ESR spectrum of  $C_{20}H_{10}^{3-}$  generated by *in situ* cesium reduction.

Crystal Structure Determinations and Refinement of 1. Data collection was performed on a Bruker SMART APEX CCD-based X-ray diffractometer with graphite-monochromated Mo-K $\alpha$  radiation ( $\lambda = 0.71073$  Å) at T = 100(2) K. Data were corrected for absorption effects using the empirical method SADABS.<sup>[6]</sup> The structure was solved by direct methods and refined using the Bruker SHELXTL (Version 6.14) software package.<sup>[7]</sup> Hydrogen atoms were included at idealized positions using the riding model. For further crystal and data collection details see Table S1.

**Table S1.** Crystallographic data for 1.

Parameter	1
Empirical formula	$C_{32}H_{38}Cs_{3}O_{6}$
$M_{ m r}$	917.35

Crystal system	monoclinic
Space group	C2/c
<i>a</i> (Å)	23.597(3)
<i>b</i> (Å)	14.073(2)
<i>c</i> (Å)	19.874(3)
$\alpha$ (°)	90
β(°)	93.283(2)
γ(°)	90
$V(\text{\AA}^3)$	6589.1(16)
Ζ	8
$\rho_{\text{calcd}} [g \cdot \text{cm}^{-3}]$	1.849
$\mu [\mathrm{mm}^{-1}]$	3.342
Reflections collected	27870
2 <i>θ</i> -range [deg]	3.38-56.54
independent reflections, R <sub>int</sub>	7687, 0.0465
data/restraints/parameters	7687/0/374
$R_1,^{[a]} w R_2^{[b]} [I \ge 2\sigma(I)]$	0.0449, 0.0978
$R_1$ , <sup>[a]</sup> $w R_2$ <sup>[b]</sup> [all data]	0.0598, 0.1052
quality of fit <sup>[c]</sup>	1.090
peak/hole [e·Å <sup>-3</sup> ]	1.834/-1.062
[a] $R_t = \Sigma  E _{-}  E   / \Sigma  E _{-}$ [b] $wR_t = 1$	$\int \Pi w(F^2 - F^2)^2  / \Pi w(F^2)^2   ^{\frac{1}{2}}$ [c] Quality-of-fit = $\int \Pi w(F^2 - F^2)^2  / (N + P^2)^2   ^{\frac{1}{2}}$

[a]  $R_1 = \Sigma ||F_0| - |F_c|| / \Sigma |F_0|$ . [b]  $wR_2 = [\Sigma [w(F_0^2 - F_c^2)^2] / \Sigma [w(F_0^2)^2]]^{1/2}$ . [c] Quality-of-fit =  $[\Sigma [w(F_0^2 - F_c^2)^2] / (N_{obs} - N_{params})]^{1/2}$ , based on all data.



Figure S2. UV-vis spectrum of 1 (in diglyme).



**Figure S3.** UV-vis spectra of *in-situ* generated products in diglyme using (a) excess Cs and (b) excess Li and Cs (3.5 eq.).

#### **Theoretical Calculations**

Geometry optimizations for systems 1-small,  $1^{4-}$ -small, and 1-full (Figures S3-S4) were performed at the PBE0/def2-TZVP(Cs)//cc-pVDZ(C,H,O) level of theory. Geometry optimizations of the structures of neutral C<sub>20</sub>H<sub>10</sub> and "naked" trianion C<sub>20</sub>H<sub>10</sub><sup>-3-</sup> species (Figure S6) were carried out at the PBE0/cc-pVDZ level of theory. All calculations were carried out with the Firefly program package (version 8.1.0).<sup>[8]</sup> The calculated structures correspond to the local minimum (no imaginary frequencies) on the corresponding potential energy surfaces, as determined by calculation of the full Hessian matrix followed by estimation of frequencies in the harmonic approximation. In the case of **1H**-small and **1H**-full models, only positions of hydrogen atoms were optimized, whereas positions of other atoms were taken from the crystal structure and kept frozen (Figures S4-S5). These calculations were described by relativistically re-contracted basis sets of triple- $\zeta$  quality (SARS-TZVP).<sup>[10]</sup> All calculations were carried out with RIJCOSX acceleration technique.<sup>[111]</sup> Scalar relativistic effects have been incorporated by applying the 0<sup>th</sup>-order regular approximation (ZORA). All optimized geometries were then used for subsequent analysis of the electronic structure of the

product in terms of natural bond orbitals (NBO) approach.<sup>[12]</sup> All NBO computations were performed with the NBO 6.0 program.<sup>[13]</sup> Broken-symmetry (BS-PBE0) calculations were performed with help of ORCA package using Yamaguchi formula<sup>[14]</sup> for calculating J coupling constant.



**Figure S4.** Equilibrium structures for models 1-*small*, 1H-*small*, and  $1^{4-}$ -*small*.



Figure S5. Equilibrium structures for models 1-full and 1H-full.



**Figure S6.** Equilibrium structures for (a) "naked" trianion  $C_{20}H_{10}$ , and (b) neutral corannulene (PBE0/cc-pVDZ).

Multireference calculations were performed at the level of multiconfigurational perturbation theory of the second in XMCQDPT2 variant.<sup>[15]</sup> The same basis sets were utilized as for the geometry optimization (def2-TZVP(Cs)//cc-pVDZ(C,H,O)). Two different active spaces, namely (6,4) and (14,8) were considered for reference CASSCF calculations. The first active space includes all doubly and singly occupied orbitals on the top of neutral corannulene and 6 cesium cations. This active space comes from the electronic structure of corannulene, which has two degenerate LUMOs of  $\pi$ -symmetry. These orbitals are populated when the system is reduced. Totally, this active space describes 6 electrons shared over 4 orbitals. The second active space (14 shared over 8 orbitals or 14/8 approach) was constructed by adding four occupied MOs, which represent two degenerate HOMOs of the neutral corannulene. These additional orbitals correspond to the bonding partners of LUMOs in C<sub>20</sub>H<sub>10</sub>. Both active spaces used in this study are depicted in Figures S7-S8 and Figures S9-S10 for systems 1-*small* and **1H**-*small*, respectively. An initial guess of the orbitals for CASSCF calculations were taken from the converged PBE0 calculations. CASSCF calculations were performed using a state-average approach. The lowest-lying one singlet and

one triplet states were considered (with ALDET keyword in Firefly terminology). The singlet state was found corresponding to an open-shell singlet electronic state. The converged CASSCF wavefunction was further used as a reference wavefunction for the calculations by multireference Møller-Plesset perturbation theory of the second order (MRMP2). The MRMP2 model is a special state-specific case of the XMCQDPT2 theory that was recently developed by Granovsky.<sup>[15]</sup> The conventional intruder state avoidance (ISA) technique<sup>[16]</sup> was used in MRPT2 calculations.



Figure S7. CASSCF(6,4) natural orbitals along with occupancies for 1-*small* model.



Figure S8. CASSCF(14,8) natural orbitals along with occupancies for 1-small model.



Figure S9. CASSCF(6,4) natural orbitals along with occupancies for 1H-small model.



Figure S10. CASSCF(14,8) natural orbitals along with occupancies for 1H-small model.

**Table S2.** Absolute energies of 1-*small*, 1H-*small*, 1-*full*, and 1H-*full* as well as of "naked"  $C_{20}H_{10}$ <sup>-3-</sup> anion and neutral corannulene (PBE0/def2-TZVP(Cs)//cc-pVDZ(C,H,O)).

Compound	Energy, a.u.
1-small	-1655.7565934532
1H-small	-1655.7403447424
1 <sup>4–</sup> -small	-1675.9241888309
<b>1</b> -full	-4428.9866489306
1H-full	-4428.9548977736
$C_{20}H_{10}^{\bullet 3-}$	-766.9410257367
$C_{20}H_{10}$	-767.3150125812

**Table S3.** Absolute energies of all systems as results of broken-symmetry calculations(PBE0/TZVP/ZORA).

	State	Energy, a.u.
<b>1</b> -small	Triplet (high-spin)	-49035.059958
	Broken-symmetry	-49035.059969

1H-small	Triplet (high-spin)	-49035.045014
	Broken-symmetry	-49035.044997
1-full	Triplet (high-spin)	-51811.568480
	Broken-symmetry	-51811.568467
<b>1H</b> -full	Triplet (high-spin)	-51811.530492
	Broken-symmetry	-51811.530490

**Table S4.** Absolute energies of 1-*small* and 1H-*small* systems as results of MRMP2 calculations based on different converged CASSCF wavefunctions (CAS(6,4) and CAS(14,8)).

		State	Energy, a.u.
	CAS(6.4)	Singlet state (OS)	-1650.579469309603
1-small	CA5(0,+)	Triplet state	-1650.579466511464
CAS(14,8)	Singlet state (OS)	-1650.568198642138	
	C/15(17,0)	Triplet state	-1650.568201337413
	CAS(6.4)	Singlet state (OS)	-1650.557621718485
1H-small	C/15(0,+)	Triplet state	-1650.557607114330
	CAS(14.8)	Singlet state (OS)	-1650.546739878118
	C/15(17,0)	Triplet state	-1650.546721943810



Figure S11. LUMO+1 for neutral  $C_{20}H_{10}$  molecule (PBE0/cc-pVDZ).

**Table S5.** Cartesian coordinates for 1-small system, optimized at the PBE0/def2-TZVP(Cs)//cc-pVDZ(C,H,O) level of theory.

Cs 5.29312240 0.04187413 -0.35440048 Cs -0.117419400 -2.762787425 -1.88312717 C 3.224904160 3.33568316 -0.19423199 H 3.656290767 4.310830343 -0.562730510 C 3.400349550 3.060869815 1.184146788 H 3.83969894 3.85632307 1.800219550 C 3.541138300 1.166011648 2.990473409 H 3.993396346 1.770470849 3.783182482 C 3.529761250 -0.239801482 3.189910002 H 3.97300320 -0.620255774 4.116050687 C 3.161312350 -1.169434765 2.149382482 C 3.429794986 -2.556000974 1.944137564 H 3.993032231 -3.142757626 2.746284072 C 3.02704532 -3.185531943 0.658327757 H 3.685391873 -4.20703747 0.564024887 C 2.891437194 -2.484779812 -0.505928392 C 3.122508581 -2.712128324 -1.912033927 H 3.490026222 -3.69050105 -2.242645193 C 3.008986573 -1.696940407 -2.896657424 H 3.315168090 -1.955100494 -3.916916653 C 2.710665419 -0.312085836 -2.575533368 C 2.02422488 0.8879744 -3.243613746 H 3.311003482 0.871283084 -4.281811191 C 3.104393847 2.174870837 -2.583860171 H 3.496757082 3.026551218 -3.121358835 C 2.664399742 2.30960053 -1.16064203 C 2.537793478 0.863550794 0.946764541 C 2.535795652 -0.535207763 1.028471413 C 2.645991742 3.026551218 -3.121358835 C 2.664399742 2.309600953 -1.160862203 C 2.330793478 0.863550794 0.946764541 C 2.535795478 0.86355794 0.946764541 C 2.535795478 0.86355794 0.946764541 C 2.53793478 0.86355794 0.946764541 C 2.53793478 0.86355794 0.946764541 C 2.415900585 -1.15722045 -0.240454758 C 2.325099468 -0.140977115 -1.209160726 C 3.122402945 -1.970148507 2.711431156 C 3.122492322 -3.335602499 0.193463727 H -3.85098725 -3.356022693 -1.800372701 C -3.22349218 -0.041380625 0.354227002 C -3.400379643 -3.06061677 -1.184162613 H -3.85098725 -3.35506284 0.194468921 H -3.85098725 -3.35506284 0.194468921 H -3.85098725 -3.355062849 0.194468921 H -3.85098733 4.20757295 -2.746282155 C -3.62244394 0.23755747 -3.190071348 H -3.8509873 -3.16079993 -1.165995733 H -3.8509873 -2.55060284 -1.94148921 C -3.6422703 2.255561264 0.3550993 -1.2653217 C -2.41599476 1.152717643 0.24543287 C -2.35561487 0.23557354 -2.				
cs         -0.117419400         -2.762787425         -1.88212717           cs         3.23404160         3.3568816         -0.19425198           H         3.562490767         4.310830343         -0.562730510           C         3.400349550         3.060868815         1.184146788           H         3.83696984         3.856323907         1.800219550           C         3.132829340         1.785066810         1.704845916           C         3.5276120         -0.239801462         3.189910002           H         3.93306330         -0.62025774         4.116050687           C         3.429734986         -2.556000974         1.944137564           H         3.80322831         -3.142757626         2.746284072           C         3.12508581         -2.112126324         -1.912033927           H         3.669391873         -4.69940407         -2.896657424           H         3.31103482         0.87128308         -2.57533368           C         3.02896573         -1.696940407         -2.896657424           H         3.31103482         0.87128308         -2.575353368           C         3.02896573         -1.696940407         -2.896657424           H         3.3	Cs	5.293312240	0.041387413	-0.354440048
C         3.22404160         3.3568316         -0.198425198           H         3.562490767         4.310830343         -0.562730510           C         3.400349550         3.060869815         1.184146788           H         3.835698984         3.855323007         1.800219550           C         3.541138300         1.165011648         2.990473409           H         3.983396364         1.760470849         3.783182482           C         3.52761250         -0.239801482         3.189910002           H         3.9973003320         -0.620255774         4.116050687           C         3.1613123150         -1.169434765         2.149382237           C         3.302704532         -3.185531943         0.658327757           H         3.685391873         -4.207703747         0.56024987           C         3.122508581         -2.712126324         -1.912033927           H         3.49026222         -3.690950105         -2.242645193           C         3.0028986573         -1.696940407         -2.896657424           H         3.31516800         -1.955100494         -3.912916653           C         2.70665419         -0.312085861         -2.1742645193           C	Cs	-0.117419400	-2.762787425	-1.883212717
H       3.562490767       4.310830343       -0.562730510         C       3.40034950       3.060869815       1.184146788         H       3.83696984       3.85623307       1.800219550         C       3.132829340       1.785066810       1.770845916         C       3.531123400       1.166011648       2.990473409         H       3.98396346       1.780470849       3.783182482         C       3.529761250       -0.239801482       3.189910002         H       3.973003320       -0.620255774       4.116050687         C       3.16312350       -1.169434765       2.149382237         C       3.02704532       -3.1185531943       0.65837757         H       3.65391873       -4.207703747       0.56028832         C       3.12250851       -2.112126324       -1.912033927         H       3.40026222       -3.690950105       -2.242665133         C       2.710655419       -0.31208586       -2.57953368         C       3.0103482       0.898879744       -3.243613746         H       3.315168090       -1.5028084       -2.89533585         C       2.308701913       1.113307263       -0.536023318         C       2.30870194	C	3 223404160	3 335688316	-0 198425198
C       3.400349550       3.660869815       1.14146788         H       3.836969894       3.856323007       1.800219550         C       3.541138300       1.165011648       2.990473409         H       3.983396364       1.780470849       3.783182482         C       3.529761250       -0.239801482       3.189910002         H       3.97300320       -0.620255774       4.116050687         C       3.161312350       -1.169434765       2.149382237         C       3.32704532       -3.185531943       0.658327757         H       3.685391873       -4.207703747       0.564024987         C       2.891437194       -2.484779812       -0.505928332         C       3.12508581       -2.712126324       -1.912033927         H       3.49002622       -3.690950105       -2.242645133         C       2.710665419       -0.312085836       -2.57953368         C       3.02422488       0.988879744       -3.243613746         H       3.315166009       -1.9351060953       -1.160862203         C       2.530793478       0.86356794       0.846764541         C       2.530793478       0.663565794       0.846746541         C	н	3 562490767	4 310830343	-0 562730510
C         3.83696994         3.85632907         1.800219550           C         3.132829340         1.785066810         1.770845916           C         3.5396346         1.780470849         3.783182482           C         3.93303320         -0.620255774         4.116050687           C         3.429734986         -2.556000974         1.944137564           H         3.80322831         -3.142757626         2.746284072           C         3.429734986         -2.556000974         1.944137564           H         3.80322831         -3.142757626         2.746284072           C         3.891373         -4.207703747         0.564024987           C         3.89143714         -2.444779812         -0.50528332           C         3.102508581         -2.712126324         -1.912033927           H         3.4506909407         -2.896657424           H         3.31508090         -1.955300494         -3.916916653           C         7.10665419         -0.312085836         -2.57533368           C         3.04393847         2.174870837         -2.553860171           H         3.496737082         3.022651218         -3.121535835           C         2.86439744         2.3	C	3 400349550	3 060869815	1 18/1/6788
1.30262940         1.785066810         1.70845916           C         3.59138636         1.785066810         1.770845916           C         3.59761250         -0.239801482         3.189910002           H         3.99336636         1.780470849         3.78182482           C         3.529761250         -0.239801482         3.189910002           H         3.9933063320         -0.620255774         4.116050687           C         3.161312350         -1.169434765         2.149382237           C         3.429794986         -2.55600974         1.944137564           H         3.685391873         -4.207703747         0.566024987           C         3.02704532         -3.185531943         0.658327757           H         3.685391873         -4.207703747         0.566024987           C         3.008986573         -1.69930007         -2.896657424           H         3.315168009         -1.953100494         -3.24613746           H         3.315168009         -9.5300953         -1.15082535           C         2.70665419         -0.312085836         -2.57953368           C         3.0439347         2.74470837         -2.53860171           H         3.49675474	с ц	3 836969897	3 856323907	1 800219550
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C 3.19136300 1.11000 1.1000 2.19007300 H 3.98339346 1.780470849 3.783182482 C 3.529761250 -0.239801482 3.189910002 H 3.973003320 -0.620255774 4.116050687 C 3.161312350 -1.169434765 2.149382237 C 3.429794986 -2.556000974 1.944137564 H 3.890322831 -3.142757626 2.746284072 C 3.302704532 -3.185531943 0.658327757 H 3.685391873 -4.207703747 0.564024987 C 2.891437194 -2.484779812 -0.505928392 C 3.12250581 -2.712126324 -1.912033927 H 3.490026222 -3.690950105 -2.242645193 C 3.008986573 -1.696940407 -2.896657424 H 3.31516609 -1.953100494 -3.916916653 C 2.710665419 -0.312085836 -2.579533368 C 3.02242248 0.898879744 -3.243613746 H 3.371003482 0.871283084 -4.28181191 C 3.104393847 2.174870837 -2.553860171 H 3.496757082 3.025651218 -3.121535835 C 2.864399742 2.30960953 -1.160862203 C 2.55575656 -0.535207763 1.028471413 C 2.415900585 -1.157222045 -0.240454758 C 2.325099468 -0.140977115 -1.209160726 Cs 0.114231952 -1.970148507 2.711431156 Cs 0.214254922 -3.335604249 0.198463727 H -3.562723309 -4.310643339 0.562751499 C -3.223492322 -3.335604249 0.198463727 H -3.562723309 -4.310643339 0.562751499 C -3.122349232 -3.355604249 0.198463727 H -3.562723309 -4.310643339 0.562751499 C -3.122349232 -3.355604249 0.198463727 H -3.562723309 -4.310643339 0.562751499 C -3.400379643 -3.060861677 -1.184152613 H -3.836998725 -3.855226093 -1.970814615 C -3.52961469 -1.16595743 -2.990566457 H -3.98347408 -1.16595743 -2.990566457 H -3.98347408 -1.16595743 -2.990566457 H -3.98347408 -1.16595743 -2.990566457 H -3.98929734 3.142756374 -2.746428355 C -3.624394035 2.555960284 -1.944148291 H -3.685637303 4.207572795 -0.563807123 C -3.62433415 -0.89990292 3.243577757 H -3.61515021 1.169412957 -2.149428192 C -3.42994035 2.555960284 -1.94428353 C -3.10243511 3.142756374 -2.746428355 C -3.022433415 -0.899902951 2.242530104 C -3.00901201 1.696874093 2.69668510 H -3.49612700 -3.022551255 3.1215077757 C -2.86442703 -2.309557334 1.160798087 C -2.39755746 -0.113281900 0.53599430 C -2.555614623 0.53520961 -1.02853	C	2 541120200	1 166011649	2 000472400
H       3.783398340       1.780470649       3.78318422         C       3.523761250       -0.233801482       3.189910002         H       3.973003320       -0.620255774       4.116050687         C       3.16311230       -1.169434765       2.149382237         C       3.429794986       -2.55600974       1.944137564         H       3.680322831       -3.142757626       2.746284072         C       3.302704532       -3.185531943       0.658327757         H       3.685391873       -4.207703747       0.564024987         C       2.891437194       -2.484779812       -0.505928392         C       3.122508581       -2.71216624       -1.912033927         H       3.49002622       -3.690950105       -2.242645193         C       2.71066549       -0.312085866       -2.579533368         C       2.71066549       -0.312085864       -2.579533368         C       3.022422488       0.871283084       -4.28181191         C       3.04393847       2.174870837       -2.553860171         H       3.496757082       3.025651218       -3.121358353         C       2.364399742       2.30960953       -1.16086250         C <td< td=""><td>C II</td><td>2.002206246</td><td>1 700470040</td><td>2.990473409</td></td<>	C II	2.002206246	1 700470040	2.990473409
C 3.323761230 -0.23001482 3.189910002 A 3.62704532 -0.20255774 4.116050687 C 3.429794986 -2.556000974 1.94137564 H 3.890322831 -3.142757626 2.746284072 C 3.302704532 -3.185531943 0.658327757 C 3.685391873 -4.207703747 0.564024987 C 2.891437194 -2.484779812 -0.505928392 C 3.12250581 -2.712126324 -1.912033927 H 3.490026222 -3.690950105 -2.242645193 C 3.002986573 -1.696940407 -2.896657424 H 3.315166090 -1.953100494 -3.916916653 C 2.710665419 -0.312085836 -2.579533368 C 3.022422488 0.898879744 -3.243613746 H 3.371003482 0.871283084 -4.281811191 C 3.104393847 2.174870837 -2.553860171 H 3.496757082 3.025651218 -3.121535835 C 2.864399742 2.30960953 -1.160862203 C 2.530793478 0.863656794 0.846764541 C 2.555756562 -0.535207763 1.028471413 C 2.555756562 -0.535207763 1.028471413 C 2.555756562 -0.535207763 1.028471413 C 2.555756562 -0.413907265 -0.240454758 C 2.325099468 -0.140977115 -1.209160726 C 2.325099468 -0.140977115 -1.209160726 C 2.325099468 -0.140977115 -1.209160726 C 3.122349232 -3.335604249 0.198463727 H -3.562723309 -4.310643339 0.562751499 C -3.400379643 -3.060861677 -1.184162613 H -3.836998725 -3.85622603 -1.800319618 C -3.52409873 -1.16595743 -2.990566457 H -3.54209873 -1.16595743 -2.990566457 H -3.983347408 -1.785039590 -1.770814615 C -3.52294284 0.420757279 -0.563297123 C -3.42994035 2.55596284 -1.944168921 H -3.983347408 -1.7850379942 -3.783274131 C -3.522614879 0.239755747 -3.190071348 H -3.90232734 3.142756374 -2.746428355 C -3.102435415 -0.89890292 3.243377757 H -3.42994033 2.555960284 -1.944168921 H -3.489029734 3.142756374 -2.746428355 C -3.022433415 -0.89809292 3.243377757 H -3.122472697 2.712100682 1.912091291 H -3.4901830 3.69025951 2.2422530104 C -2.89415303 3.05925951 2.2422530104 C -2.89415303 3.26555960284 -1.944168921 H -3.31510309 1.95319724 3.91688308 C -2.710560297 0.312017996 2.579626926 C -3.022433415 -0.89899292 3.243377757 C -2.864427033 -2.09557334 1.160798087 C -2.397212866 -1.113281900 0.555994330 C -2.5555414623 0.535290561 -0.84679	H C	3.983398348	1.780470849	3.783182482
H       3.97300320       -0.820257/4       4.11605087         C       3.16131230       -1.169434765       2.149382237         C       3.429794986       -2.55600974       1.944137564         H       3.680322831       -3.142557626       2.746284072         C       3.302704532       -3.185531943       0.658327757         H       3.685391873       -4.207703747       0.564024987         C       2.91437194       -2.484779812       -0.505928392         C       3.122508581       -2.712126324       -1.912033927         H       3.490026222       -3.690950105       -2.242645193         C       2.710665419       -0.312085836       -2.579533368         C       3.022422488       0.898879744       -3.243613746         H       3.3104393847       2.174870837       -2.553860171         H       3.496757082       3.025651218       -3.121535835         C       2.864399742       2.309600953       -1.160862203         C       2.55575652       -0.53520763       1.028471413         C       2.55575652       -0.53520763       1.028471413         C       2.35099468       -0.14977115       -1.209160726         Cs       <	C	3.529/61250	-0.239801482	3.189910002
C 3.161312350 -1.169434765 2.149382237 H 3.890322831 -3.142757626 2.746284072 C 3.302704532 -3.185531943 0.658327757 H 3.685391873 -4.207703747 0.564024987 C 2.891437194 -2.484779812 -0.505928392 C 3.122508581 -2.712126324 -1.912033927 H 3.490026222 -3.690950105 -2.242645193 C 3.008986573 -1.696940407 -2.896657424 H 3.315168090 -1.953100494 -3.916916653 C 2.710665419 -0.312085836 -2.579533368 C 3.02242248 0.891879744 -3.243613746 H 3.371003482 0.871283084 -4.28181191 C 3.104393847 2.174870837 -2.553860171 H 3.496757082 3.025651218 -3.121535835 C 2.864399742 2.30960953 -1.160862203 C 2.530793478 0.863656794 0.846764541 C 2.555755562 -0.535207763 1.028471413 C 2.328099468 -0.140977115 -1.209160726 C 2.325099468 -0.141380625 0.354227002 C 2.325099468 -0.141380625 0.354227002 C -3.223492322 -3.335604249 0.198467727 H -3.562723309 -4.316643339 0.562751499 C -3.400379643 -3.060861677 -1.180837277 H -3.562723309 -4.31664339 0.562751499 C -3.40379643 -3.060861677 -1.180319618 C -3.52294222 -3.335504249 0.198463727 H -3.562723309 -4.31664339 0.562751499 C -3.40379643 -3.060861677 -1.180319618 C -3.5220614879 0.23975743 -2.990566457 H -3.983347408 -1.780379942 -3.783274131 C -3.5220614879 0.23975747 -2.149242192 H -3.962347408 -1.785039590 -1.770814615 C -3.5220614879 0.23975747 -2.746428355 C -3.122472697 2.712100682 1.912091291 H -3.890292734 3.142756374 -2.746428355 C -3.102658531 3.18550090 -0.658299108 H -3.890292734 3.142756374 -2.746428355 C -3.102658531 3.18550090 -0.658299108 H -3.890292734 3.142756374 -2.746428355 C -3.022433415 -0.89809292 3.243577757 H -3.902565531 3.18550090 -0.558299108 H -3.4901730 3.690929251 2.242230104 C -2.891501788 2.484694479 0.505942037 C -2.864427033 -2.30955734 1.160798087 C -2.864427033 -2.30955734 1.160798087 C -2.864427033 -2.30955734 1.160798087 C -2.864427033 -2.30955734 1.160798087 C -2.93721866 -1.113281900 0.35599330 C -2.555614623 0.53520961 -0.284353217 C -2.41599476 1.157176439 0.240478050 C -2.325051614 0.140911779 1.20	Н	3.9/3003320	-0.620255774	4.116050687
C 3.429/94986 -2.55600974 1.94413/564 H 3.89032281 -3.142757626 2.746284072 C 3.302704532 -3.185531943 0.658327757 H 3.685391873 -4.207703747 0.564024987 C 2.891437194 -2.484779812 -0.505928392 C 3.122508581 -2.712126324 -1.912033927 H 3.49002622 -3.690950105 -2.242645193 C 3.008986573 -1.696940407 -2.896657424 H 3.315168090 -1.953100494 -3.916916653 C 3.022422488 0.898879744 -3.243613746 H 3.371003482 0.871283084 -4.281811191 C 3.104393847 2.174870837 -2.553860171 H 3.496757082 3.025651218 -3.121535835 C 2.864399742 2.30960953 -1.160862203 C 2.530793478 0.863656794 0.846764541 C 2.55575562 -0.535207763 1.028471413 C 2.415900585 -1.157222045 -0.240454758 C 2.455079562 -0.535207763 1.028471413 C 2.415900585 -1.157222045 0.354277002 C 2.325099468 -0.140977115 -1.209160726 Cs 0.11744803 2.762492176 1.883772701 C -3.223492322 -3.355604249 0.198463727 H -3.562723309 -4.316643339 0.562751499 C -3.1228474803 2.762492176 1.883772701 C -3.223492322 -3.355604249 0.198463727 H -3.562723309 -4.316643339 0.562751499 C -3.400379643 -3.060861677 -1.184162613 H -3.836998725 -3.856226093 -1.770814615 C -3.5241098973 -1.165995743 -2.990566457 H -3.52614879 0.239755747 -3.190071348 H -3.972932894 0.620244591 -4.116221538 C -3.161315622 1.169412957 -2.149428192 C -3.161315622 1.169412957 -2.149428192 H -3.99292734 3.142756374 -2.990566457 H -3.9026733 4.207572795 -0.563907123 C -2.891501788 2.484694479 0.505542037 C -3.00291201 1.69874093 2.896689510 H -3.49018730 3.69982951 2.242530104 C -3.009012021 1.69874093 2.89568510 H -3.49018730 3.69982951 2.242530104 C -2.3972186 -0.83890292 3.24357757 H -3.370654484 -0.871364818 4.281853238 C -2.112047779 -2.864427033 -2.39557334 1.160798087 C -2.864427033 -2.39557334 1.160798087 C -2.855164623 0.535209661 -1.028533217 C -2.855164623 0.535209	C	3.161312350	-1.169434765	2.149382237
H       3.89322831       -3.142757626       2.746284072         C       3.302704532       -3.185531943       0.658327757         H       3.665391873       -4.207703747       0.564024987         C       2.891437194       -2.484779812       -0.505928392         C       3.122506851       -2.112126324       -1.912033927         H       3.490026222       -3.690950105       -2.242645193         C       3.00898673       -1.953100494       -3.916916653         C       2.710665419       -0.312085836       -2.579533368         C       3.022422488       0.898879744       -3.243613746         H       3.371003482       0.871283084       -4.281811191         C       3.104339847       2.174870837       -2.553860171         H       3.397003478       0.86356794       0.846764541         C       2.530793478       0.863566794       0.846764541         C       2.530793478       0.863565074       0.846764541         C       2.32509468       -0.140977115       -1.209160726         Cs       0.114231952       -1.970148507       2.711431156         Cs       -5.293326816       -0.041380625       0.562751499         C	C	3.429794986	-2.556000974	1.944137564
C 3.302704532 -3.185531943 0.658327757 H 3.685391873 -4.207703747 0.564024987 C 2.891437194 -2.484779812 -0.505928392 C 3.122508581 -2.712126324 -1.912033927 H 3.490026222 -3.690950105 -2.242645193 C 3.008986573 -1.696940407 -2.896657424 H 3.315168090 -1.953100494 -3.916916653 C 2.710665419 -0.312085836 -2.579533368 C 3.022422488 0.898879744 -3.243613746 H 3.371003482 0.871283084 -4.28181191 C 3.104393847 2.174870837 -2.553860171 H 3.496757082 3.025651218 -3.121535835 C 2.864399742 2.309600953 -1.160862203 C 2.398701913 1.113307263 -0.536023918 C 2.555756562 -0.535207763 1.028471413 C 2.555756562 -0.535207763 1.028471413 C 2.415900585 -1.15722045 -0.240454758 C 2.325099468 -0.140977115 -1.209160726 Cs 0.117448903 2.762492176 1.883772701 C -3.223492322 -3.335604249 0.198463727 H -3.56272309 -4.31064339 0.562751499 C -3.400379643 -3.060861677 -1.184162613 H -3.836998725 -3.856226093 -1.800319618 C -3.5241098973 -1.16595743 -2.990566457 H -3.826987460 -1.785039590 -1.770814615 C -3.5241098973 -1.16595743 -2.990566457 H -3.82698347408 -1.785037942 -2.773274131 C -3.529614879 0.239755747 -3.190071348 H -3.92932894 0.620244591 -4.116221538 C -3.161315622 1.169412957 -2.149428192 C -3.1621879 0.239755747 -3.190071348 H -3.92932894 0.620244591 -4.116221538 C -3.161315622 1.169412957 -2.149428192 C -3.162472697 2.711201062 1.91291291 H -3.890292734 3.142756374 -2.746428355 C -3.10245531 3.185500990 -0.563907123 C -2.891501788 2.484694479 0.505942037 C -3.122472677 0.31201795 -0.563907123 C -2.891501788 2.484694479 0.505942037 C -3.122472677 0.31201795 -0.563907123 C -2.891501788 2.484694479 0.505942037 C -3.02243315 0.0898092951 2.242530104 C -3.009012021 1.696874093 2.896689510 H -3.490187303 3.690929951 2.242530104 C -2.89672166 -1.113281900 0.53594303 C -2.710560297 0.312017996 2.579626926 C -2.255051614 0.40911779 1.209149478 C -2.389721866 -1.113281900 0.53594330 C -2.239051614 0.140911779 1.209149478 C -2.45505161462 0.9535200961 -1.028533217 C -2.85614623 0.535200	Н	3.890322831	-3.142/5/626	2.746284072
H       3.685391873       -4.207703747       0.564024987         C       2.891437194       -2.484779812       -0.505928392         C       3.122508581       -2.712126324       -1.912033927         H       3.490026222       -3.690950105       -2.242645193         C       3.008986573       -1.6965940407       -2.896657424         H       3.315168090       -1.953100494       -3.916916653         C       2.710665419       -0.312085836       -2.579533368         C       3.022422488       0.898879744       -3.243613746         H       3.0103482       0.871283084       -4.281811191         C       3.104393847       2.174870837       -2.553860171         H       3.496757082       3.025651218       -3.121535835         C       2.398701913       1.113307263       -0.536023918         C       2.530793478       0.863656794       0.846764541         C       2.352099468       -0.140977115       -1.209160726         Cs       0.114231952       -1.970148507       2.711431156         Cs       0.3224922       -3.35604249       0.19846377         H       -3.622492320       -3.35604249       0.198463727         H	С	3.302704532	-3.185531943	0.658327757
C 2.891437194 -2.484779812 -0.505928392 H 3.49002622 -3.690950105 -2.242645193 C 3.008986573 -1.696940407 -2.896657424 H 3.315168090 -1.953100494 -3.916916653 C 2.710665419 -0.312085836 -2.579533368 C 3.022422488 0.898879744 -3.243613746 H 3.371003482 0.871283084 -4.281811191 C 3.104393847 2.174870837 -2.553860171 H 3.496757082 3.025651218 -3.121535835 C 2.864399742 2.309600953 -1.160862203 C 2.398701913 1.113307263 -0.536023918 C 2.55575652 -0.535207763 1.028471413 C 2.55575652 -0.535207763 1.028471413 C 2.415900585 -1.157222045 -0.240454758 C 2.325099468 -0.140977115 -1.209160726 Cs 0.114231952 -1.970148507 2.711431156 Cs -5.293326816 -0.041380625 0.354227002 Cs 0.117448903 2.762492176 1.883772701 C -3.223492322 -3.335604249 0.198463727 H -3.562723309 -4.310643339 0.562751499 C -3.400379643 -3.060861677 -1.184162613 H -3.86998725 -3.856226093 -1.770814615 C -3.541098973 -1.165995743 -2.9905664577 H -3.58209448 0.23755747 -3.190071348 H -3.983347408 -1.780379942 -3.783274131 C -3.529614879 0.23755747 -3.190071348 H -3.982347408 -1.780379942 -3.783274131 C -3.52994035 2.55960284 -1.944168921 H -3.89029734 3.142756374 -2.149428192 C -3.161315622 1.169412957 -2.149428192 C -3.42994035 2.559560284 -1.944168921 H -3.88026733 4.207572795 -0.563907123 C -2.891501788 2.484694479 0.505942037 C -3.102433415 -0.89890392 1.2242530104 C -3.02941330 3.69092951 2.242530104 C -3.022658531 3.1185500990 -0.658299108 H -3.685637303 4.207572795 -0.563907123 C -2.891501788 2.484694479 0.55942037 C -3.1022472697 2.712100682 1.912091291 H -3.490187330 3.69092951 2.242530104 C -3.002912021 1.696874093 2.895689510 H -3.0104236712 -2.17480589 2.55386500 H -3.496712700 -3.025551255 3.121507779 C -2.864427033 -2.309557334 1.160798087 C -2.39724297 -0.863661485 -0.846792296 C -2.350724297 -0.863661485 -0.846792296 C -2.550516142 0.140911779 1.209149478 C -2.325051614 0.140911779 1.209149478 C -2.325051614 0.140911779 1.209149478	H	3.685391873	-4.207703747	0.564024987
C 3.122508581 -2.712126324 -1.912033927 H 3.490026222 -3.690550105 -2.242645193 C 3.008986573 -1.696940407 -2.896657424 H 3.315168090 -1.953100494 -3.916916653 C 2.710665419 -0.312085836 -2.579533368 C 3.022422488 0.898879744 -3.243613746 H 3.371003482 0.871283084 -4.281811191 C 3.104393847 2.174870837 -2.553860171 H 3.496757082 3.025651218 -3.121535835 C 2.864399742 2.309600953 -1.160862203 C 2.3398701913 1.113307263 -0.536023918 C 2.555756562 -0.535207763 1.028471413 C 2.415900585 -1.15722045 -0.240454758 C 2.325099468 -0.140977115 -1.209160726 CS 0.114231952 -1.970148507 2.711431156 CS 0.114243952 -1.970148507 2.711431156 CS 0.1142439232 -3.335604249 0.198463727 H -3.562723309 -4.310643339 0.562751499 C -3.400379643 -3.060861677 -1.184162613 H -3.836998725 -3.85522609 -1.770814615 C -3.541098973 -1.16595743 -2.990566457 H -3.983347408 -1.78037942 -3.990566457 H -3.92342940 0.620244591 -4.116221538 C -3.541098973 -1.16595747 -3.190071348 H -3.972932894 0.620244591 -4.116221538 C -3.161315622 1.169412957 -2.149428192 C -3.42940335 2.555960284 -1.941468921 H -3.865637303 4.207572795 -0.563907123 C -3.422472697 2.712100682 1.912091291 H -3.89134730 3.69092951 2.242530104 C -3.122472697 2.712100682 1.912091291 H -3.490187330 3.69092951 2.242530104 C -3.02243315 -0.89899292 3.243577757 H -3.370854484 -0.871364818 4.281853238 C -2.710560297 0.312017996 2.579626926 C -3.02243315 -0.89899292 3.243577757 H -3.370854484 -0.871364818 4.281853238 C -2.114227366 -1.913264199 -2.5435610 H -3.496712700 -3.02551255 3.121507779 C -2.86427033 -2.309557334 1.160798087 C -2.38972486 -1.113281900 0.53599430 C -2.350724297 -0.863661485 -0.846792296 C -2.55051614 0.140911779 1.209149478 C -2.325051614 0.140911779 1.209149478	С	2.891437194	-2.484779812	-0.505928392
H       3.490026222       -3.690950105       -2.242645193         C       3.008986573       -1.953100494       -3.916916653         C       2.710665419       -0.312085836       -2.579533368         C       3.02242488       0.89887744       -3.243613746         H       3.371003482       0.871283084       -4.281811191         C       3.104393847       2.174870837       -2.553860171         H       3.496757082       3.025651218       -3.121535835         C       2.864399742       2.309600953       -1.160862203         C       2.530793478       0.863656794       0.846764541         C       2.555756562       -0.535207763       1.028471413         C       2.415900585       -1.15722045       -0.240454758         C       2.325099468       -0.140977115       -1.209160726         Cs       0.1112418033       2.762492176       1.883772701         C       -3.223492322       -3.335604249       0.198463727         H       -3.56272309       -4.310643339       0.562751499         C       -3.40379643       -3.060861677       -1.184162613         H       -3.8698725       -3.856226093       -1.800319618        C       <	С	3.122508581	-2.712126324	-1.912033927
C       3.008986573       -1.696940407       -2.896657424         H       3.315168090       -1.953100494       -3.916916653         C       3.022422488       0.898879744       -3.243613746         H       3.371003482       0.871283084       -4.28181191         C       3.104393847       2.174870837       -2.553860171         H       3.496757082       3.025651218       -3.121535835         C       2.864399742       2.309600953       -1.160862203         C       2.530793478       0.863556794       0.846764541         C       2.55575652       -0.535207763       1.028471413         C       2.415900585       -1.15722045       -0.240454758         C       2.325099468       -0.140977115       -1.209160726         Cs       0.114231952       -1.970148507       2.711431156         Cs       0.117448903       2.762492176       1.883772701         C       -3.22349232       -3.35602499       0.198463727         H       -3.562723309       -4.310643339       0.562751499         C       -3.40379643       -3.060861677       -1.184162613         H       -3.86998725       -3.856226093       -1.800319618         C	H	3.490026222	-3.690950105	-2.242645193
H       3.315168090       -1.953100494       -3.916916653         C       2.710665419       -0.312085836       -2.579533368         C       3.022422488       0.89879744       -3.243613746         H       3.371003482       0.871283084       -4.281811191         C       3.104393847       2.174870837       -2.553860171         H       3.496757082       3.025651218       -3.121535835         C       2.864399742       2.309600953       -1.160862203         C       2.530793478       0.863656794       0.846764541         C       2.555756562       -0.535207763       1.028471413         C       2.415900585       -1.157222045       -0.240454758         C       2.325099468       -0.140977115       -1.209160726         Cs       0.114231952       -1.970148507       2.711431156         Cs       0.1117448033       2.76242176       1.883772701         C       -3.22349232       -3.335604249       0.198463727         H       -3.562723309       -4.310643339       0.562751499         C       -3.400379643       -3.60861677       -1.184162613         H       -3.83694725       -3.856226093       -1.70814615         C <td>С</td> <td>3.008986573</td> <td>-1.696940407</td> <td>-2.896657424</td>	С	3.008986573	-1.696940407	-2.896657424
C       2.710665419       -0.312085836       -2.579533368         C       3.022422488       0.898879744       -3.243613746         H       3.371003482       0.871283084       -4.281811191         C       3.104393847       2.174870837       -2.553860171         H       3.496757082       3.025651218       -3.121535835         C       2.864399742       2.309600953       -1.160862203         C       2.530793478       0.863656794       0.846764541         C       2.555756562       -0.535207763       1.028471413         C       2.415900585       -1.157222045       -0.240454758         C       2.325099468       -0.140977115       -1.209160726         Cs       0.114231952       -1.970148507       2.711431156         Cs       0.114243952       -3.35604249       0.198467377         H       -3.562723309       -4.310643339       0.562751499         C       -3.40379643       -3.060861677       -1.184162613         C       -3.132867460       -1.785039590       -1.770814615         C       -3.529614879       0.239755747       -3.190071348         H       -3.9232894       0.620244591       -4.116221538         C<	Н	3.315168090	-1.953100494	-3.916916653
C       3.022422488       0.898879744       -3.243613746         H       3.371003482       0.871283084       -4.281811191         C       3.104339847       2.174870837       -2.553860171         H       3.496757082       3.025651218       -3.121535835         C       2.898701913       1.113307263       -0.536023918         C       2.530793478       0.863656794       0.846764541         C       2.555755656       -0.535207763       1.028471413         C       2.415900585       -1.15722045       -0.240454758         C       2.325099468       -0.140977115       -1.209160726         Cs       0.1114231952       -1.970148507       2.711431156         Cs       0.11148903       2.762492176       1.883772701         C       -3.223492322       -3.335604249       0.198463727         H       -3.562723309       -4.310643339       0.562751499         C       -3.40379643       -3.060861677       -1.184162613         H       -3.836998725       -3.856226093       -1.800319618         C       -3.54109873       -1.6595743       -2.90566457         H       -3.983347408       -1.785737952       -2.65492178         H <td>С</td> <td>2.710665419</td> <td>-0.312085836</td> <td>-2.579533368</td>	С	2.710665419	-0.312085836	-2.579533368
H       3.371003482       0.871283084       -4.281811191         C       3.104393847       2.174870837       -2.553860171         H       3.496757082       3.025561218       -3.121535835         C       2.864399742       2.309600953       -1.160862203         C       2.330793478       0.863656794       0.846764541         C       2.555756562       -0.535207763       1.028471413         C       2.415900585       -1.157222045       -0.240454758         C       2.0325099468       -0.140977115       -1.209160726         Cs       0.114231952       -1.970148507       2.711431156         Cs       0.117448903       2.762492176       1.883772701         C       -3.223492322       -3.35604249       0.198463727         H       -3.562723309       -4.310643339       0.562751499         C       -3.400379643       -3.060861677       -1.84162613         H       -3.36369875       -3.865226093       -1.800319618         C       -3.3400379643       -1.785039590       -1.770814615         C       -3.52614879       0.23975747       -3.180274131         H       -3.89347408       -1.7850379542       -2.746428355 <td< td=""><td>С</td><td>3.022422488</td><td>0.898879744</td><td>-3.243613746</td></td<>	С	3.022422488	0.898879744	-3.243613746
C       3.104393847       2.174870837       -2.553860171         H       3.496757082       3.025651218       -3.121535835         C       2.898701913       1.113307263       -0.536023918         C       2.3398701913       1.113307263       -0.536023918         C       2.55575652       -0.535207763       1.028471413         C       2.415900585       -1.157222045       -0.240454758         C       2.325099468       -0.140977115       -1.209160726         Cs       0.114231952       -1.970148507       2.711431156         Cs       -5.293326816       -0.041380625       0.354227002         Cs       0.117448903       2.762492176       1.883772701         C       -3.232492322       -3.335604249       0.198463727         H       -3.56273309       -4.3106861677       -1.184162613         H       -3.362098725       -3.856226093       -1.800319618         C       -3.3400379643       -1.76595743       -2.990566457         H       -3.92932894       0.620244591       -4.116221538         C       -3.12867460       -1.785037990       -7.70814615         C       -3.40037961       2.1694912957       -2.149428192	Н	3.371003482	0.871283084	-4.281811191
H       3.496757082       3.025651218       -3.121535835         C       2.864399742       2.309600953       -1.160862203         C       2.338701913       1.113307263       -0.536023918         C       2.530793478       0.863556794       0.846764541         C       2.555756562       -0.535207763       1.028471413         C       2.415900585       -1.157222045       -0.240454758         C       2.325099468       -0.140977115       -1.209160726         Cs       0.114231952       -1.970148507       2.711431156         Cs       -5.293326816       -0.041380625       0.354227002         Cs       0.114748903       2.762492176       1.883772701         C       -3.223492322       -3.335604249       0.198463727         H       -3.562723309       -4.310643339       0.562751499         C       -3.400379643       -3.060861677       -1.184162613         H       -3.32867460       -1.785039590       -1.770814615         C       -3.132867460       -1.785039590       -1.770814615         C       -3.529614879       0.239755747       -3.190071348         H       -3.9322894       0.620244591       -4.116221538 <t< td=""><td>С</td><td>3.104393847</td><td>2.174870837</td><td>-2.553860171</td></t<>	С	3.104393847	2.174870837	-2.553860171
C       2.864399742       2.309600953       -1.160862203         C       2.398701913       1.113307263       -0.536023918         C       2.555756562       -0.535207763       1.028471413         C       2.415900585       -1.157222045       -0.240454758         C       2.325099468       -0.140977115       -1.209160726         Cs       0.114231952       -1.970148507       2.711431156         Cs       0.117448903       2.762492176       1.883772701         C       -3.223492322       -3.335604249       0.198463727         H       -3.66273309       -4.310643339       0.562751499         C       -3.400379643       -3.060861677       -1.184162613         H       -3.83698725       -3.856226093       -1.70814615         C       -3.32867460       -1.785039590       -1.70814615         C       -3.541098973       -1.16595743       -2.990566457         H       -3.983347408       -1.780379942       -3.783274131         C       -3.541098973       2.555960284       -1.944168921         H       -3.92056531       3.18550990       -0.563907123         C       -3.322658531       3.182550992       2.746428355	Н	3.496757082	3.025651218	-3.121535835
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	С	2.864399742	2.309600953	-1.160862203
C       2.530793478       0.863656794       0.846764541         C       2.555756562       -0.535207763       1.028471413         C       2.415900585       -1.157222045       -0.240454758         C       2.325099468       -0.140977115       -1.209160726         Cs       0.114231952       -1.970148507       2.711431156         Cs       0.117448903       2.762492176       1.883772701         C       -3.223492322       -3.335604249       0.198463727         H       -3.562723309       -4.310643339       0.562751499         C       -3.400379643       -3.060861677       -1.184162613         H       -3.836998725       -3.856226093       -1.70814615         C       -3.132867460       -1.785039590       -1.770814615         C       -3.541098973       -1.165995743       -2.990566457         H       -3.983347408       -1.780379942       -3.783274131         C       -3.529614879       0.239755747       -3.190071348         H       -3.9022734       3.142756374       -2.746428355         C       -3.1326678671       -1.780379942       -3.783274131         C       -3.302658531       3.185500990       -0.658299108	С	2.398701913	1.113307263	-0.536023918
$\begin{array}{llllllllllllllllllllllllllllllllllll$	С	2.530793478	0.863656794	0.846764541
C       2.415900585       -1.157222045       -0.240454758         C       2.325099468       -0.140977115       -1.209160726         Cs       0.114231952       -1.970148507       2.711431156         Cs       -5.293326816       -0.041380625       0.354227002         Cs       0.117448903       2.762492176       1.883772701         C       -3.223492322       -3.335604249       0.198463727         H       -3.562723309       -4.310643339       0.562751499         C       -3.400379643       -3.060861677       -1.184162613         H       -3.836998725       -3.856226093       -1.800319618         C       -3.132867460       -1.785039590       -1.770814615         C       -3.529614879       0.239755747       -3.190071348         H       -3.972932894       0.620244591       -4.116221538         C       -3.161315622       1.169412957       -2.149428192         C       -3.302658531       3.185500990       -0.658299108         H       -3.890292734       3.142756374       -2.746428355         C       -3.302658531       3.185500990       -0.658299108         H       -3.890292734       3.142756374       -2.4242530104 <tr< td=""><td>C</td><td>2.555756562</td><td>-0.535207763</td><td>1.028471413</td></tr<>	C	2.555756562	-0.535207763	1.028471413
C       2.325099468       -0.140977115       -1.209160726         Cs       0.114231952       -1.970148507       2.711431156         Cs       -5.293326816       -0.041380625       0.354227002         Cs       0.117448903       2.762492176       1.883772701         C       -3.223492322       -3.335604249       0.198463727         H       -3.562723309       -4.310643339       0.562751499         C       -3.400379643       -3.060861677       -1.184162613         H       -3.836998725       -3.856226093       -1.800319618         C       -3.132867460       -1.785039590       -1.770814615         C       -3.541098973       -1.165995743       -2.990566457         H       -3.983347408       -1.780379942       -3.783274131         C       -3.529614879       0.239755747       -3.190071348         H       -3.972932894       0.620244591       -4.116221538         C       -3.132655531       3.18550090       -0.658299108         H       -3.685637303       4.207572795       -0.638907123         C       -3.122472697       2.712100682       1.912091291         H       -3.490187330       3.690292951       2.42530104	C	2.415900585	-1.157222045	-0.240454758
Cs       0.114231952       -1.970148507       2.711431156         Cs       -5.293326816       -0.041380625       0.354227002         Cs       0.117448903       2.762492176       1.883772701         C       -3.223492322       -3.35604249       0.198463727         H       -3.562723309       -4.310643339       0.562751499         C       -3.400379643       -3.060861677       -1.184162613         H       -3.836998725       -3.856226093       -1.800319618         C       -3.132867460       -1.785039590       -1.770814615         C       -3.541098973       -1.165995743       -2.990566457         H       -3.983347408       -1.780379942       -3.783274131         C       -3.529614879       0.239755747       -3.190071348         H       -3.972932894       0.620244591       -4.116221538         C       -3.429940335       2.555960284       -1.944168921         H       -3.890292734       3.142766374       -2.746428355         C       -3.122472697       2.712100682       1.912091291         H       -3.685637303       4.207572795       -0.563907123         C       -2.891501788       2.484694479       0.505942037	C	2 325099468	-0 140977115	-1 209160726
Cs       -5.293326816       -0.041380625       0.354227002         Cs       0.117448903       2.762492176       1.883772701         C       -3.223492322       -3.335604249       0.198463727         H       -3.562723309       -4.310643339       0.562751499         C       -3.400379643       -3.060861677       -1.184162613         H       -3.836998725       -3.856226093       -1.800319618         C       -3.132867460       -1.785039590       -1.770814615         C       -3.541098973       -1.165995743       -2.990566457         H       -3.983347408       -1.780379942       -3.783274131         C       -3.529614879       0.239755747       -3.190071348         H       -3.972932894       0.620244591       -4.116221538         C       -3.161315622       1.169412957       -2.149428192         C       -3.429940335       2.555960284       -1.944168921         H       -3.890292734       3.182550990       -0.658299108         H       -3.685637303       4.207572795       -0.563907123         C       -2.891501788       2.484694479       0.505942037         C       -3.102472697       2.712100682       1.912091291	Cs	0 114231952	-1 970148507	2 711431156
Cs       0.117448903       2.762492176       1.883772701         C       -3.223492322       -3.335604249       0.198463727         H       -3.562723309       -4.310643339       0.562751499         C       -3.400379643       -3.060861677       -1.184162613         H       -3.836998725       -3.856226093       -1.800319618         C       -3.132867460       -1.785033590       -1.770814615         C       -3.541098973       -1.165995743       -2.990566457         H       -3.983347408       -1.780379942       -3.783274131         C       -3.529614879       0.239755747       -3.190071348         H       -3.972932894       0.620244591       -4.116221538         C       -3.161315622       1.169412957       -2.149428192         C       -3.463940335       2.555960284       -1.944168921         H       -3.890292734       3.142756374       -2.746428355         C       -3.302658531       3.18550990       -0.658299108         H       -3.685637303       4.207572795       -0.563907123         C       -2.891501788       2.484694479       0.505942037         C       -3.102472667       2.712100682       1.912091291	C s	-5 293326816	-0 041380625	0 354227002
C       -3.223492322       -3.335604249       0.198463727         H       -3.562723309       -4.310643339       0.562751499         C       -3.400379643       -3.060861677       -1.184162613         H       -3.836998725       -3.856226093       -1.800319618         C       -3.132867460       -1.785039590       -1.770814615         C       -3.541098973       -1.165995743       -2.990566457         H       -3.983347408       -1.780379942       -3.783274131         C       -3.529614879       0.239755747       -3.190071348         H       -3.972932894       0.620244591       -4.116221538         C       -3.161315622       1.169412957       -2.746428355         C       -3.429940335       2.555960284       -1.944168921         H       -3.890292734       3.142756374       -2.746428355         C       -3.02658531       3.185500990       -0.658299108         H       -3.685637303       4.207572795       -0.565942037         C       -3.122472697       2.712100682       1.912091291         H       -3.49018730       3.690929951       2.242530104         C       -3.009012021       1.696874093       2.896689510	Ca	0 117//8903	2 762492176	1 883772701
C       3.522372322       3.33304249       0.562751499         H       -3.562723309       -4.310643339       0.562751499         C       -3.400379643       -3.060861677       -1.184162613         H       -3.836998725       -3.856226093       -1.800319618         C       -3.132867460       -1.785039590       -1.770814615         C       -3.541098973       -1.165995743       -2.990566457         H       -3.983347408       -1.780379942       -3.783274131         C       -3.529614879       0.239755747       -3.190071348         H       -3.972932894       0.620244591       -4.116221538         C       -3.161315622       1.169412957       -2.149428192         C       -3.429940335       2.555960284       -1.944168921         H       -3.890292734       3.142756374       -2.746428355         C       -3.02658531       3.185500900       -0.658299108         H       -3.685637303       4.207572795       -0.563907123         C       -2.891501788       2.484694479       0.505942037         C       -3.122472697       2.712100682       1.912091291         H       -3.490187330       3.690929951       2.242530104	C	-3 223/02322	-3 33560/2/9	0 198/63727
11       -3.400379643       -3.060861677       -1.184162613         12       -3.836998725       -3.856226093       -1.800319618         13       -3.132867460       -1.785039590       -1.770814615         14       -3.83699873       -1.165995743       -2.990566457         15       -3.529614879       0.239755747       -3.190071348         16       -3.529614879       0.239755747       -3.190071348         16       -3.79932894       0.620244591       -4.116221538         17       -3.429940335       2.555960284       -1.944168921         18       -3.890292734       3.142756374       -2.746428355         19       -3.685637303       4.207572795       -0.563907123         10       -3.890292734       3.185500990       -0.658299108         19       -3.685637303       4.207572795       -0.563907123         10       -2.891501788       2.484694479       0.505942037         11       -3.122472697       2.712100682       1.912091291         14       -3.490187300       3.690929951       2.242530104         11       -3.15103809       1.953197244       3.916888308         11       -2.710560297       0.312017996       2.57386500	с ц	-3 562723309	-1 3106/3339	0.562751/09
C       -3.000000000000000000000000000000000000		2 1002725505	2 060961677	1 104162612
H       -3.03099723       -3.030220933       -1.000319016         C       -3.132867460       -1.785039590       -1.770814615         C       -3.541098973       -1.165995743       -2.990566457         H       -3.983347408       -1.7850379942       -3.783274131         C       -3.529614879       0.239755747       -3.190071348         H       -3.972932894       0.620244591       -4.116221538         C       -3.161315622       1.169412957       -2.149428192         C       -3.429940335       2.555960284       -1.944168921         H       -3.890292734       3.142756374       -2.746428355         C       -3.302658531       3.185500990       -0.658299108         H       -3.685637303       4.207572795       -0.563907123         C       -2.891501788       2.484694479       0.505942037         C       -3.122472697       2.712100682       1.912091291         H       -3.490187330       3.690929951       2.242530104         C       -3.009012021       1.696874093       2.896689510         H       -3.315103809       1.953197244       3.916888308         C       -2.710560297       0.312017996       2.579626926		-3.4003/9043	-3.0000010//	1 000210610
C       -3.132807460       -1.763039390       -1.76814813         C       -3.541098973       -1.165995743       -2.990566457         H       -3.983347408       -1.780379942       -3.783274131         C       -3.529614879       0.239755747       -3.190071348         H       -3.972932894       0.620244591       -4.116221538         C       -3.161315622       1.169412957       -2.149428192         C       -3.429940335       2.555960284       -1.944168921         H       -3.890292734       3.142756374       -2.746428355         C       -3.302658531       3.185500990       -0.658299108         H       -3.685637303       4.207572795       -0.563907123         C       -2.891501788       2.484694479       0.505942037         C       -3.1022472697       2.712100682       1.912091291         H       -3.490187330       3.690929951       2.242530104         C       -3.009012021       1.696874093       2.896689510         H       -3.315103809       1.953197244       3.916888308         C       -2.710560297       0.312017996       2.579626926         C       -3.022433415       -0.898909292       3.243577757	п С	2 122067460	-3.630220093	1 770014615
C       -3.941098973       -1.163993743       -2.990386437         H       -3.983347408       -1.780379942       -3.783274131         C       -3.529614879       0.239755747       -3.190071348         H       -3.972932894       0.620244591       -4.116221538         C       -3.161315622       1.169412957       -2.149428192         C       -3.429940335       2.555960284       -1.944168921         H       -3.890292734       3.142756374       -2.746428355         C       -3.302658531       3.185500990       -0.658299108         H       -3.685637303       4.207572795       -0.563907123         C       -2.891501788       2.484694479       0.505942037         C       -3.122472697       2.712100682       1.912091291         H       -3.490187330       3.690929951       2.242530104         C       -3.009012021       1.696874093       2.896689510         H       -3.315103809       1.953197244       3.916888308         C       -2.710560297       0.312017996       2.579626926         C       -3.022433415       -0.871364818       4.281853238         C       -3.104236712       -2.174805809       2.553886500	C	-3.132007400	-1.765059590	-1.//0014013
H       -3.383347408       -1.780379342       -3.783274131         C       -3.529614879       0.239755747       -3.190071348         H       -3.972932894       0.620244591       -4.116221538         C       -3.161315622       1.169412957       -2.149428192         C       -3.429940335       2.555960284       -1.944168921         H       -3.890292734       3.142756374       -2.746428355         C       -3.302658531       3.185500990       -0.658299108         H       -3.685637303       4.207572795       -0.563907123         C       -2.891501788       2.484694479       0.505942037         C       -3.122472697       2.712100682       1.912091291         H       -3.490187330       3.690929951       2.242530104         C       -3.009012021       1.696874093       2.896689510         H       -3.315103809       1.953197244       3.916888308         C       -2.710560297       0.312017996       2.579626926         C       -3.104236712       -2.174805809       2.55386500         H       -3.30085484       -0.871364818       4.281853238         C       -3.104236712       -2.174805809       2.553886500 <td< td=""><td>C II</td><td>-3.541098973</td><td>-1.165995743</td><td>-2.990506457</td></td<>	C II	-3.541098973	-1.165995743	-2.990506457
$\begin{array}{llllllllllllllllllllllllllllllllllll$	H	-3.98334/408	-1.780379942	-3./832/4131
H-3.9729328940.620244991-4.116221538C-3.1613156221.169412957-2.149428192C-3.4299403352.555960284-1.944168921H-3.8902927343.142756374-2.746428355C-3.3026585313.185500990-0.658299108H-3.6856373034.207572795-0.563907123C-2.8915017882.4846944790.505942037C-3.1224726972.7121006821.912091291H-3.4901873303.6909299512.242530104C-3.0090120211.6968740932.896689510H-3.3151038091.9531972443.916888308C-2.7105602970.3120179962.579626926C-3.022433415-0.8989092923.243577757H-3.370854484-0.8713648184.281853238C-3.104236712-2.1748058092.553886500H-3.496712700-3.0255512553.121507779C-2.864427033-2.3095573341.160798087C-2.398721866-1.1132819000.535994330C-2.556146230.535200961-1.028533217C-2.4159949761.1571764390.240478050C-2.3250516140.1409117791.209149478Cs-0.1142273061.970376764-2.711047376	C	-3.529614879	0.239/55/4/	-3.1900/1348
C       -3.161315622       1.169412957       -2.149428192         C       -3.429940335       2.555960284       -1.944168921         H       -3.890292734       3.142756374       -2.746428355         C       -3.302658531       3.185500990       -0.658299108         H       -3.685637303       4.207572795       -0.563907123         C       -2.891501788       2.484694479       0.505942037         C       -3.122472697       2.712100682       1.912091291         H       -3.490187330       3.690929951       2.242530104         C       -3.009012021       1.696874093       2.896689510         H       -3.315103809       1.953197244       3916888308         C       -2.710560297       0.312017996       2.579626926         C       -3.002433415       -0.898909292       3.243577757         H       -3.370854484       -0.871364818       4.281853238         C       -3.104236712       -2.174805809       2.553886500         H       -3.496712700       -3.025551255       3.121507779         C       -2.864427033       -2.309557334       1.160798087         C       -2.30724297       -0.863661485       -0.846792296 <td< td=""><td>H</td><td>-3.972932894</td><td>0.620244591</td><td>-4.116221538</td></td<>	H	-3.972932894	0.620244591	-4.116221538
C       -3.429940335       2.555960284       -1.944168921         H       -3.890292734       3.142756374       -2.746428355         C       -3.302658531       3.185500990       -0.658299108         H       -3.685637303       4.207572795       -0.563907123         C       -2.891501788       2.484694479       0.505942037         C       -3.122472697       2.712100682       1.912091291         H       -3.490187330       3.690929951       2.242530104         C       -3.009012021       1.696874093       2.896689510         H       -3.315103809       1.953197244       3.916888308         C       -2.710560297       0.312017996       2.579626926         C       -3.022433415       -0.898909292       3.243577757         H       -3.370854484       -0.871364818       4.281853238         C       -3.104236712       -2.174805809       2.553886500         H       -3.496712700       -3.025551255       3.121507779         C       -2.864427033       -2.309557334       1.160798087         C       -2.398721866       -1.113281900       0.535994330         C       -2.555614623       0.535200961       -1.028533217 <t< td=""><td>C</td><td>-3.161315622</td><td>1.169412957</td><td>-2.149428192</td></t<>	C	-3.161315622	1.169412957	-2.149428192
H       -3.890292734       3.142756374       -2.746428355         C       -3.302658531       3.185500990       -0.658299108         H       -3.685637303       4.207572795       -0.563907123         C       -2.891501788       2.484694479       0.505942037         C       -3.122472697       2.712100682       1.912091291         H       -3.490187330       3.690929951       2.242530104         C       -3.009012021       1.696874093       2.896689510         H       -3.315103809       1.953197244       3.916888308         C       -2.710560297       0.312017996       2.579626926         C       -3.022433415       -0.898909292       3.243577757         H       -3.370854484       -0.871364818       4.281853238         C       -3.104236712       -2.174805809       2.553886500         H       -3.496712700       -3.025551255       3.121507779         C       -2.864427033       -2.309557334       1.160798087         C       -2.398721866       -1.113281900       0.535994330         C       -2.555614623       0.535200961       -1.028533217         C       -2.555614623       0.535200961       -1.028533217 <t< td=""><td>С</td><td>-3.429940335</td><td>2.555960284</td><td>-1.944168921</td></t<>	С	-3.429940335	2.555960284	-1.944168921
C       -3.302658531       3.185500990       -0.658299108         H       -3.685637303       4.207572795       -0.563907123         C       -2.891501788       2.484694479       0.505942037         C       -3.122472697       2.712100682       1.912091291         H       -3.490187330       3.690929951       2.242530104         C       -3.009012021       1.696874093       2.896689510         H       -3.315103809       1.953197244       3.916888308         C       -2.710560297       0.312017996       2.579626926         C       -3.022433415       -0.898909292       3.243577757         H       -3.370854484       -0.871364818       4.281853238         C       -3.104236712       -2.174805809       2.553886500         H       -3.496712700       -3.025551255       3.121507779         C       -2.864427033       -2.309557334       1.160798087         C       -2.398721866       -1.113281900       0.535994330         C       -2.555614623       0.535200961       -1.028533217         C       -2.555614623       0.535200961       -1.028533217         C       -2.325051614       0.140911779       1.209149478 <td< td=""><td>Н</td><td>-3.890292734</td><td>3.142/563/4</td><td>-2.746428355</td></td<>	Н	-3.890292734	3.142/563/4	-2.746428355
H-3.6856373034.207572795-0.563907123C-2.8915017882.4846944790.505942037C-3.1224726972.7121006821.912091291H-3.4901873303.6909299512.242530104C-3.0090120211.6968740932.896689510H-3.3151038091.9531972443.916888308C-2.7105602970.3120179962.579626926C-3.022433415-0.8989092923.243577757H-3.370854484-0.8713648184.281853238C-3.104236712-2.1748058092.553886500H-3.496712700-3.0255512553.121507779C-2.864427033-2.3095573341.160798087C-2.398721866-1.1132819000.535994330C-2.556146230.535200961-1.02853217C-2.3250516140.1409117791.209149478Cs-0.1142273061.970376764-2.711047376	C	-3.302658531	3.185500990	-0.658299108
C-2.8915017882.4846944790.505942037C-3.1224726972.7121006821.912091291H-3.4901873303.6909299512.242530104C-3.0090120211.6968740932.896689510H-3.3151038091.9531972443.916888308C-2.7105602970.3120179962.579626926C-3.002433415-0.8989092923.243577757H-3.370854484-0.8713648184.281853238C-3.104236712-2.1748058092.553886500H-3.496712700-3.0255512553.121507779C-2.864427033-2.3095573341.160798087C-2.398721866-1.1132819000.535994330C-2.5556146230.535200961-1.028533217C-2.5556146230.535200961-1.028533217C-2.3250516140.1409117791.209149478Cs-0.1142273061.970376764-2.711047376	H	-3.685637303	4.20/5/2/95	-0.563907123
C-3.1224726972.7121006821.912091291H-3.4901873303.6909299512.242530104C-3.0090120211.6968740932.896689510H-3.3151038091.9531972443.916888308C-2.7105602970.3120179962.579626926C-3.022433415-0.8989092923.243577757H-3.370854484-0.8713648184.281853238C-3.104236712-2.1748058092.553886500H-3.496712700-3.0255512553.121507779C-2.864427033-2.3095573341.160798087C-2.398721866-1.1132819000.535994330C-2.5556146230.535200961-1.02853217C-2.5556146230.535200961-1.02853217C-2.3250516140.1409117791.209149478Cs-0.114227061.970376764-2.711047376	С	-2.891501788	2.484694479	0.505942037
H-3.4901873303.6909299512.242530104C-3.0090120211.6968740932.896689510H-3.3151038091.9531972443.916888308C-2.7105602970.3120179962.579626926C-3.022433415-0.8989092923.243577757H-3.370854484-0.8713648184.281853238C-3.104236712-2.1748058092.553886500H-3.496712700-3.0255512553.121507779C-2.864427033-2.3095573341.160798087C-2.398721866-1.1132819000.535994330C-2.5556146230.535200961-1.028533217C-2.3250516140.1409117791.209149478C-2.3250516140.1409117791.209149478	С	-3.122472697	2.712100682	1.912091291
C       -3.009012021       1.696874093       2.896689510         H       -3.315103809       1.953197244       3.916888308         C       -2.710560297       0.312017996       2.579626926         C       -3.022433415       -0.898909292       3.243577757         H       -3.370854484       -0.871364818       4.281853238         C       -3.104236712       -2.174805809       2.553886500         H       -3.496712700       -3.025551255       3.121507779         C       -2.864427033       -2.309557334       1.160798087         C       -2.398721866       -1.113281900       0.535994330         C       -2.555614623       0.535200961       -1.028533217         C       -2.55551614       0.140911779       1.209149478         C       -2.325051614       0.140911779       1.209149478	H	-3.490187330	3.690929951	2.242530104
H-3.3151038091.9531972443.916888308C-2.7105602970.3120179962.579626926C-3.022433415-0.8989092923.243577757H-3.370854484-0.8713648184.281853238C-3.104236712-2.1748058092.553886500H-3.496712700-3.0255512553.121507779C-2.864427033-2.3095573341.160798087C-2.398721866-1.1132819000.535994330C-2.5556146230.535200961-1.028533217C-2.4159949761.1571764390.240478050C-2.3250516140.1409117791.209149478Cs-0.1142273061.970376764-2.711047376	С	-3.009012021	1.696874093	2.896689510
C-2.7105602970.3120179962.579626926C-3.022433415-0.8989092923.243577757H-3.370854484-0.8713648184.281853238C-3.104236712-2.1748058092.553886500H-3.496712700-3.0255512553.121507779C-2.864427033-2.3095573341.160798087C-2.398721866-1.1132819000.535994330C-2.530724297-0.863661485-0.846792296C-2.5556146230.535200961-1.02853217C-2.3250516140.1409117791.209149478Cs-0.1142273061.970376764-2.711047376	Н	-3.315103809	1.953197244	3.916888308
C       -3.022433415       -0.898909292       3.243577757         H       -3.370854484       -0.871364818       4.281853238         C       -3.104236712       -2.174805809       2.553886500         H       -3.496712700       -3.025551255       3.121507779         C       -2.864427033       -2.309557334       1.160798087         C       -2.3098721866       -1.113281900       0.535994330         C       -2.530724297       -0.863661485       -0.846792296         C       -2.555614623       0.535200961       -1.028533217         C       -2.325051614       0.140911779       1.209149478         C       -2.325051614       0.140911779       1.209149478	С	-2.710560297	0.312017996	2.579626926
H-3.370854484-0.8713648184.281853238C-3.104236712-2.1748058092.553886500H-3.496712700-3.0255512553.121507779C-2.864427033-2.3095573341.160798087C-2.398721866-1.1132819000.535994330C-2.530724297-0.863661485-0.846792296C-2.5556146230.535200961-1.028533217C-2.3250516140.1409117791.209149478Cs-0.1142273061.970376764-2.711047376	С	-3.022433415	-0.898909292	3.243577757
C       -3.104236712       -2.174805809       2.553886500         H       -3.496712700       -3.025551255       3.121507779         C       -2.864427033       -2.309557334       1.160798087         C       -2.398721866       -1.113281900       0.535994330         C       -2.530724297       -0.863661485       -0.846792296         C       -2.555614623       0.535200961       -1.028533217         C       -2.325051614       0.140911779       1.209149478         C       -0.114227306       1.970376764       -2.711047376	H	-3.370854484	-0.871364818	4.281853238
H       -3.496712700       -3.025551255       3.121507779         C       -2.864427033       -2.309557334       1.160798087         C       -2.398721866       -1.113281900       0.535994330         C       -2.530724297       -0.863661485       -0.846792296         C       -2.555614623       0.535200961       -1.028533217         C       -2.415994976       1.157176439       0.240478050         C       -2.325051614       0.140911779       1.209149478         Cs       -0.114227306       1.970376764       -2.711047376	С	-3.104236712	-2.174805809	2.553886500
C       -2.864427033       -2.309557334       1.160798087         C       -2.398721866       -1.113281900       0.535994330         C       -2.530724297       -0.863661485       -0.846792296         C       -2.555614623       0.535200961       -1.028533217         C       -2.415994976       1.157176439       0.240478050         C       -2.325051614       0.140911779       1.209149478         Cs       -0.114227306       1.970376764       -2.711047376	Н	-3.496712700	-3.025551255	3.121507779
C-2.398721866-1.1132819000.535994330C-2.530724297-0.863661485-0.846792296C-2.5556146230.535200961-1.028533217C-2.4159949761.1571764390.240478050C-2.3250516140.1409117791.209149478Cs-0.1142273061.970376764-2.711047376	С	-2.864427033	-2.309557334	1.160798087
C       -2.530724297       -0.863661485       -0.846792296         C       -2.555614623       0.535200961       -1.028533217         C       -2.415994976       1.157176439       0.240478050         C       -2.325051614       0.140911779       1.209149478         Cs       -0.114227306       1.970376764       -2.711047376	С	-2.398721866	-1.113281900	0.535994330
C         -2.555614623         0.535200961         -1.028533217           C         -2.415994976         1.157176439         0.240478050           C         -2.325051614         0.140911779         1.209149478           Cs         -0.114227306         1.970376764         -2.711047376	С	-2.530724297	-0.863661485	-0.846792296
C         -2.415994976         1.157176439         0.240478050           C         -2.325051614         0.140911779         1.209149478           Cs         -0.114227306         1.970376764         -2.711047376	С	-2.555614623	0.535200961	-1.028533217
C -2.325051614 0.140911779 1.209149478 Cs -0.114227306 1.970376764 -2.711047376	С	-2.415994976	1.157176439	0.240478050
Cs -0.114227306 1.970376764 -2.711047376	С	-2.325051614	0.140911779	1.209149478
	Cs	-0.114227306	1.970376764	-2.711047376

**Table S6.** Cartesian coordinates for  $1^{4-}$ -*small* system, optimized at the PBE0/def2-TZVP(Cs)//cc-pVDZ(C,H,O) level of theory.

Cs	-1 038500000	3 098199999	-0 679900000
Ca	1 5/6899999	-2 881299999	-1 332/00000
C	1 662200000	2.00120000	1.3324999999
C	-1.0022999999	-2.0491999999	-0.331900000
C	-2.2870999999	-1.161599999	0.561400000
C	-2.568299999	0.04/300000	-0.125200000
С	-2.117699999	-0.093100000	-1.462799999
С	-1.557899999	-1.388899999	-1.602999999
С	-1.481699999	-2.089099999	-2.866899999
С	-1.349399999	-3.505999998	-2.713999999
Н	-1.323099999	-4.138299998	-3.610499998
С	-1.454099999	-4.175899998	-1.444899999
н	-1.501199999	-5.271999998	-1,462499999
C	-1 702999999	-3 488799998	-0 213900000
C	-2 28/399999	-3 915999998	1 022300000
	2.204333333	4 000100000	1 212100000
п	-2.4007999999	-4.9901999990	1 040400000
	-2.916299999	-3.015399999	1.9494999999
Н	-3.4/0499998	-3.4659999998	2.782499999
С	-3.025699999	-1.606399999	1.722999999
С	-3.947399998	-0.625000000	2.208799999
H	-4.588199998	-0.873000000	3.064299999
С	-4.233699998	0.600700000	1.511799999
Н	-5.072699998	1.201599999	1.884699999
С	-3.622999998	0.956500000	0.267300000
С	-4.043199998	1.817799999	-0.796100000
Н	-4.866499998	2.521099999	-0.618700000
C	-3.586699998	1.674999999	-2.153099999
н	-4 094199998	2 279199999	-2 915599999
C	-2 668699999	0 658900000	-2 569499999
C	-2 /35599999	0.037900000	_3 838100008
	2.4555555555	0.037900000	4 742900009
п	1 0 0 7 0 0 0 0 0	1.276400000	-4./42099990
C	-1.867699999	-1.2764999999	-3.980299998
Н	-1.885199999	-1.720799999	-4.983499998
Cs	0.265900000	-2.4819999999	2.480699999
C	2.488399999	-0.383800000	0.868000000
С	2.591899999	0.278600000	-0.382100000
С	2.034099999	1.574599999	-0.238800000
С	1.585499999	1.713599999	1.099600000
С	1.866299999	0.503400000	1.783699999
С	2.051799999	0.425900000	3.216499999
С	2.782999999	-0.735300000	3.623499998
Н	3.015399999	-0.873100000	4.687099998
С	3,414999998	-1.634499999	2.694899999
H	4.085199998	-2.394799999	3.115299999
C	3 371999998	-1 454199999	1 275599999
C	4 2425999998	-1 890499999	0 226300000
с ц	1 982599999	-2 672/99999	0.438400000
	4.24600000	1 210100000	1 042200000
	4.3409999990 5 150200000	1 526200000	1 709100000
п	3.139299990	-1.3303999999	1 27(000000
C	3.5904999998	-0.030900000	-1.376099999
C	3.826199998	1.012400000	-2.304999999
Н	4.593699998	0.883800000	-3.0/8599999
С	3.258399999	2.326599999	-2.160699999
H	3.632199998	3.107799999	-2.834399999
С	2.403999999	2.696599999	-1.073300000
С	2.108899999	3.961699998	-0.472200000
H	2.385899999	4.881299998	-1.002900000
С	1.654099999	4.102799998	0.885400000
Н	1.615899999	5.119999998	1.294999999
С	1.453899999	2.991499999	1.764999999
С	1.466299999	2.881999999	3.192199999
Н	1.412399999	3.795899998	3.797099998
С	1.7522999999	1.654799999	3.886499998
н	1 897399999	1 718899999	4 972199998
 	-1 5/0600000	-1 026800000	-1 3/2599999
Co Co	1 620300000	1 720600000	1 362600000
05	4.0ZUJJJJJ0 0.741100000	1./23033333 0.560100000	T.307033333
05	U./41100000	U.JUUUUUUUUU	- 3.200333333
CS .	-1.35/033333	1.211499999	2.000333333

**Table S7.** Cartesian coordinates for 1H-small system, optimized at the PBE0/def2-TZVP(Cs)//cc-pVDZ(C,H,O) level of theory.

Cs	5 293300000	0 041400000	-0 354400000
Cs	-0 117400000	-2 762800000	-1 883200000
C	3 223400000	3 335700000	-0 198400000
с ц	3 562500000	4 310800000	-0 562700000
	3.400300000	3.060000000	1 184100000
C II	3.400300000	3.080900000	1.184100000
H	3.837000000	1.705100000	1.800200000
C	3.132800000	1.785100000	1.770800000
С	3.541100000	1.166000000	2.990500000
H	3.983400000	1.780500000	3.783200000
С	3.529800000	-0.239800000	3.189900000
H	3.973000000	-0.620300000	4.116100000
С	3.161300000	-1.169400000	2.149400000
С	3.429800000	-2.556000000	1.944100000
H	3.890300000	-3.142800000	2.746300000
С	3.302700000	-3.185500000	0.658300000
Н	3.685400000	-4.207700000	0.564000000
С	2.891400000	-2.484800000	-0.505900000
С	3.122500000	-2.712100000	-1.912000000
Н	3.490000000	-3.691000000	-2.242600000
С	3.009000000	-1.696900000	-2.896700000
Н	3.315200000	-1.953100000	-3.916900000
С	2.710700000	-0.312100000	-2.579500000
C	3.022400000	0.898900000	-3.243600000
н	3 371000000	0 871300000	-4 281800000
C	3 104400000	2 174900000	-2 553900000
н	3 496800000	3 025700000	-3 121500000
C	2 864400000	2 309600000	-1 160900000
C	2.209700000	1 112200000	0.53600000
C	2.398700000	1.113300000	-0.536000000
C	2.530800000	0.863700000	1.020500000
C	2.555800000	-0.535200000	1.028500000
C	2.415900000	-1.157200000	-0.240500000
C	2.325100000	-0.141000000	-1.209200000
Cs	0.114200000	-1.970100000	2.711400000
Cs	-5.293300000	-0.041400000	0.354200000
Cs	0.117400000	2.762500000	1.883800000
С	-3.223500000	-3.335600000	0.198500000
H	-3.562700000	-4.310600000	0.562800000
С	-3.400400000	-3.060900000	-1.184200000
H	-3.837000000	-3.856200000	-1.800300000
С	-3.132900000	-1.785000000	-1.770800000
С	-3.541100000	-1.166000000	-2.990600000
H	-3.983300000	-1.780400000	-3.783300000
С	-3.529600000	0.239800000	-3.190100000
Н	-3.972900000	0.620200000	-4.116200000
С	-3.161300000	1.169400000	-2.149400000
С	-3.429900000	2.556000000	-1.944200000
Н	-3.890300000	3.142800000	-2.746400000
С	-3.302700000	3.185500000	-0.658300000
Н	-3.685600000	4.207600000	-0.563900000
С	-2.891500000	2.484700000	0.505900000
С	-3.122500000	2.712100000	1.912100000
H	-3.490200000	3.690900000	2.242500000
C	-3.009000000	1.696900000	2.896700000
н	-3,315100000	1,953200000	3,916900000
C	-2 710600000	0 312000000	2 579600000
C	-3 022400000	-0.898900000	3 243600000
с ц	-3 370900000	-0.871400000	4 291900000
n C	-3.104200000	-0.871400000	2 553900000
с ц	-3 196700000	-3 025600000	2.333900000
C	-2 964400000	-2 300600000	1 160900000
	-2.0044UUUUU	-2.309000000	1.100000000
C	-2.398/00000	-1.113300000	0.536000000
C	-2.530/00000	-0.863/00000	-0.846800000
C	-2.555600000	0.535200000	-1.028500000
C	-2.416000000	1.157200000	0.240500000
С	-2.325100000	0.140900000	1.209100000
Cs	-0.114200000	1.970400000	-2.711000000

**Table S8.** Cartesian coordinates for 1-full system, optimized at the PBE0/def2-TZVP(Cs)//cc-pVDZ(C,H,O) level of theory.

Cs	-5.296100000	0.191800000	-1.545500000
Cs	5.296000000	-0.191800000	1.545500000
Cs	-0.492800000	2,422200000	1,986800000
Cs	0 492800000	-2 422200000	-1 986800000
0	-7 537600000	2 554100000	-0 933200000
0	7.537600000	-2 554100000	0.933200000
0	7.900100000	-2.554100000	0.955200000
0	7.899100000	-0.079800000	0.093400000
0	7.899100000	0.079800000	1 77000000
0	-7.539500000	-2.195200000	-1.778800000
0	7.539500000	2.195200000	1.778800000
0	-1.793900000	4.015800000	4.858/00000
0	1.793800000	-4.015800000	-4.858700000
0	-0.498800000	5.501200000	2.759400000
0	0.498800000	-5.501200000	-2.759400000
0	0.252700000	5.077800000	0.100800000
0	-0.252700000	-5.077800000	-0.100800000
С	-3.228900000	3.261700000	-0.153800000
С	3.228900000	-3.261600000	0.153800000
Н	-3.424800000	4.286800000	-0.489200000
Н	3.424800000	-4.286900000	0.489200000
С	-3.782600000	2.873500000	1.128200000
С	3.782600000	-2.873500000	-1.128200000
Н	-4.355300000	3.632200000	1.674900000
Н	4.355300000	-3,632200000	-1,675000000
С	-3.767500000	1.531000000	1,587200000
C	3.767500000	-1.531000000	-1.587200000
C	-4 525500000	0 809800000	2 591500000
C	1 525500000	-0.809800000	-2 591600000
U U	-5 136500000	1 372900000	3 307400000
и П	5 136500000	-1 372900000	-3 307400000
п С	-4 652900000	-1.572900000	2 60300000
C	4.652900000	-0.398700000	2.803000000
C	4.652900000	1.020400000	-2.603100000
H	-5.340900000	-1.032400000	3.337200000
H	5.340900000	1.032300000	-3.33/100000
С	-4.031000000	-1.453600000	1.629800000
С	4.031000000	1.453600000	-1.629900000
С	-4.285700000	-2.776400000	1.186100000
С	4.285700000	2.776400000	-1.186100000
Н	-4.947700000	-3.427400000	1.770500000
Н	4.947700000	3.427300000	-1.770500000
С	-3.806600000	-3.283100000	-0.071800000
С	3.806600000	3.283100000	0.071800000
Н	-4.166600000	-4.272200000	-0.380200000
Н	4.166600000	4.272200000	0.380200000
С	-3.075000000	-2.474200000	-1.013700000
С	3.074900000	2.474200000	1.013700000
С	2.875400000	2.559300000	2.432300000
С	-2.875400000	-2.559300000	-2.432300000
Н	3.202900000	3.453600000	2.975200000
Н	-3.203000000	-3,453600000	-2.975100000
C	2.478000000	1,422200000	3.228100000
C	-2.478100000	-1,422200000	-3.228200000
н	2 517400000	1 540700000	4 317900000
н	-2 517500000	-1 540800000	-4 317900000
	2 191100000	0 149100000	2 675000000
C	2.101100000	0.149100000	2.675000000
C	-2.101100000	1 174600000	-2.873000000
C	2.205100000	-1.174600000	3.243700000
C	-2.205100000	1.1/4600000	-3.243700000
H	2.198/00000	-1.2/9600000	4.335500000
Н	-2.198/00000	1.2/9600000	-4.335500000
С	2.401300000	-2.355200000	2.477000000
С	-2.401300000	2.355100000	-2.477000000
H	2.554100000	-3.291800000	3.029200000
Н	-2.554100000	3.291800000	-3.029200000
С	-2.618900000	2.339300000	-1.043600000
С	2.618900000	-2.339300000	1.043600000
С	-2.426700000	1.038900000	-0.484400000
С	2.426700000	-1.039000000	0.484400000
С	-3.008500000	0.657000000	0.757900000
С	3.008500000	-0.657000000	-0.757900000
С	-3.138300000	-0.737100000	0.770400000

С	3.138300000	0.737100000	-0.770400000
C	2 657100000	1 229400000	0 466200000
C	-2.03/100000	-1.228400000	-0.400300000
С	2.657100000	1.228400000	0.466300000
С	2.202000000	0.127600000	1,238100000
о С	2.202000000	0 107 000000	1 020100000
C	-2.202000000	-0.12/600000	-1.238100000
С	-6.888200000	3.791300000	-1.123700000
C	6 999200000	-3 701300000	1 123700000
C	0.000200000	-3.791300000	1.123/00000
H	-5.888500000	3.803700000	-0.652400000
TT	E 000E00000	2 002700000	0 652400000
п	5.0000000	-3.803700000	0.052400000
H	-6.777500000	3.938100000	-2.207300000
ч	6 777500000	-3 938000000	2 207400000
11	0.777500000	5.95000000	2.207400000
H	-7.492700000	4.624600000	-0.713900000
н	7 492700000	-4 624600000	0 71400000
~	7.752700000	1.021000000	0.12000000
C	-7.752800000	2.2/4300000	0.432/00000
С	7,752800000	-2.274300000	-0.432700000
	6 70050000	0 101400000	0 0 0 1 2 0 0 0 0 0
н	-6./90500000	2.131400000	0.964300000
Н	6.790400000	-2.131400000	-0.964300000
	0 20000000	2 11020000	0 01000000
п	-0.200000000	3.110200000	0.91000000
H	8.286000000	-3.118200000	-0.916600000
C	-9 609900000	1 0/1700000	0 557100000
C	-0.009000000	1.041/00000	0.33/100000
С	8.609800000	-1.041700000	-0.557200000
ч	-9 539400000	1 176700000	-0 031300000
п	-9.559400000	1.170700000	-0.031300000
H	9.539400000	-1.176700000	0.031300000
н	-8 893400000	0 907800000	1 620500000
11	0.000400000	0.007000000	1.020500000
H	8.893300000	-0.907800000	-1.620500000
C	-8 666400000	-1 258000000	0 098600000
~	0.000100000	1.250000000	0.00000000
C	8.666400000	1.258000000	-0.098600000
Н	-9.003500000	-1,496300000	1,127700000
		1.406000000	1 107700000
н	9.003400000	1.496300000	-1.12//00000
Н	-9.566700000	-1.132000000	-0.535600000
	0 5 6 6 7 0 0 0 0	1 122000000	0 525500000
н	9.566700000	1.132000000	0.535500000
С	-7.837100000	-2.405300000	-0.415800000
- -	7 0 0 7 1 0 0 0 0 0	0 40500000	0 415700000
C	/.83/100000	2.405300000	0.415/00000
Н	-8.421700000	-3.340100000	-0.291600000
	0 401700000	2 24010000	0 201 00000
н	8.421/00000	3.340100000	0.291600000
H	-6.906400000	-2.502600000	0.178300000
	C 00C10000	2 50260000	0 170200000
н	6.906400000	2.502600000	-0.1/8300000
С	-6.884100000	-3.305900000	-2.350200000
C	6 994200000	2 20500000	2 25010000
C	0.004200000	3.303900000	2.330100000
H	-7.527300000	-4.207500000	-2.315100000
ч	7 527300000	1 207500000	2 31500000
11	1.527500000	4.207500000	2.313000000
H	-6.677200000	-3.060500000	-3.400900000
н	6 677300000	3 060500000	3 400900000
11	0.077500000	5.000500000	5.400500000
H	-5.931200000	-3.522500000	-1.834200000
н	5 931200000	3 522500000	1 834200000
~	0.7000000	3.14600000	1.001200000
C	-2.793300000	3.146900000	5.339300000
С	2.793300000	-3.146800000	-5.339300000
	2 40400000	2 67760000	C 01200000
н	-3.494900000	3.6//600000	6.012800000
Н	3.494900000	-3.677600000	-6.012800000
	2 20050000	2 25 600000	E 01000000
п	-2.290300000	2.336900000	3.912200000
H	2.290400000	-2.356900000	-5.912200000
TT	2 267400000	2 695200000	4 514100000
п	-3.387400000	2.003300000	4.314100000
H	3.367400000	-2.685400000	-4.514200000
С	-2.347700000	5,139100000	4,219200000
0	2.547700000	5.155100000	4.219200000
C	2.347600000	-2.139100000	-4.219200000
Н	-3.025700000	5.679200000	4,912500000
	2 005 00000	E C7000000	1.010500000
н	3.025600000	-5.6/9200000	-4.912500000
Н	-2.938300000	4.831700000	3.332700000
TT	2 020200000	4 021700000	2 22270000
н	2.938300000	-4.831/00000	-3.332700000
С	-1.250900000	6.080500000	3.797600000
- -	1 250000000	C 000E00000	2 707(00000
C	T.50900000	-0.000000000	-3./9/600000
Н	-1.715000000	7.026000000	3.450200000
ц	1 715000000	-7 02600000	_3 /50200000
п	T. / TOOOOOO	-7.02000000	-3.430200000
Н	-0.602300000	6.318100000	4.664000000
ц	0 602200000	-6 319100000	-1 664000000
11	0.002200000	0.310100000	00400000
С	0.407600000	6.397400000	2.169200000
C	-0 407600000	-6 397400000	-2 169100000
~	1 1 5 6 5 6 5 5 5	0.00/100000	2.109100000
Н	1.172700000	6.737200000	2.896900000
Н	-1.172700000	-6.737300000	-2.896800000
	1 1 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		1.000000000
н	-0.132800000	1.302300000	T.823000000
Н	0.132900000	-7.302300000	-1.823000000
-	1 110000000	E 705400000	1 000500000
C	T'TT8500000	5./05400000	1.022500000
С	1 110200000	-5.705400000	-1.022500000
	-1.110200000		
U	-1.76000000	-6 452500000	_0 513300000
Н	-1.760000000	-6.452500000	-0.513200000
H H	-1.76000000	-6.452500000 6.452500000	-0.513200000 0.513300000
H H	-1.76000000 1.76000000	-6.452500000	-0.513200000 0.513300000
H H H	-1.76000000 1.764500000 1.764500000	-6.452500000 6.452500000 4.899500000	-0.513200000 0.513300000 1.403400000

С	0.644100000	-5.948700000	0.547200000
С	-0.644100000	5.948700000	-0.547200000
Н	-1.386500000	6.372100000	0.151400000
н	1.386500000	-6.372100000	-0.151400000
н	1 187200000	-5 349100000	1 290100000
и П	-1 187200000	5 349200000	-1 290100000
и П	0 105200000	-6 765700000	1 062500000
п	0.105200000	-0.705700000	1.002500000
н	-0.105200000	6.765800000	-1.062500000
Cs	-1.005000000	-2.783500000	2.137000000
Cs	1.005000000	2.783500000	-2.137000000
0	-1.719800000	-5.801900000	2.987200000
0	1.719900000	5.801900000	-2.987100000
0	-0.837100000	-4.399600000	5.264400000
0	0.837100000	4.399700000	-5.264300000
0	-1.174100000	-1,654700000	5,015400000
0	1 174100000	1 654700000	-5 015400000
C	-2 868100000	-6 358600000	2 396400000
C	2.000100000	6.358600000	2.330400000
	2.000100000	6.338800000	-2.390400000
н	-3.726700000	-6.340800000	3.093900000
Н	3.726700000	6.340800000	-3.093900000
H	-3.112000000	-5.743000000	1.519200000
Н	3.112000000	5.743000000	-1.519100000
Н	-2.694600000	-7.406400000	2.080100000
Н	2.694700000	7.406400000	-2.080100000
С	-1.354500000	-6.435000000	4.187000000
С	1.354600000	6,435000000	-4.187000000
н	-2 228800000	-6 515900000	4 862500000
и П	2 228800000	6 515900000	-1.862500000
11	2.220000000	7 460400000	2 002700000
п	-0.977300000	-7.480400000	3.993700000
н	0.977600000	7.460500000	-3.993/00000
C	-0.2/9000000	-5.622800000	4.862000000
С	0.279000000	5.622800000	-4.862000000
H	0.564300000	-5.459600000	4.159800000
Н	-0.564200000	5.459600000	-4.159800000
Н	0.115300000	-6.188100000	5.731500000
Н	-0.115300000	6.188100000	-5.731500000
С	0.104300000	-3.497400000	5.795000000
C	-0.104300000	3,497500000	-5.795000000
н	0 588100000	-3 916400000	6 701100000
н	-0 588100000	3 916500000	-6 701100000
и П	0.898300000	-3 284100000	5 052300000
11	0.00000000	2 204100000	5.052300000
п	-0.898300000	3.284100000	-5.052500000
C	-0.605100000	-2.220100000	6.166000000
С	0.605100000	2.220100000	-6.166000000
H	0.128900000	-1.527700000	6.626200000
Н	-0.128900000	1.527800000	-6.626100000
Н	-1.391600000	-2.432400000	6.918400000
Н	1.391500000	2.432400000	-6.918400000
С	-1.825800000	-0.434700000	5.269400000
С	1.825700000	0.434700000	-5.269300000
Н	-1.100900000	0.346700000	5.569500000
н	1 100800000	-0 346700000	-5 569500000
11 11	-2 344800000	_0 131000000	1 348000000
11	2.344000000	-0.131000000	4.340000000
п	2.344800000	0.131000000	-4.34/900000
Н	-2.583100000	-0.543400000	6.069900000
н	2.583000000	0.543300000	-0.009800000

**Table S9.** Cartesian coordinates for 1H-full system, optimized at the PBE0/def2-TZVP(Cs)//cc-pVDZ(C,H,O) level of theory.

Cs	5.229041342	-0.077637756	1.649744011
Cs	-0.617790374	2.486193422	2.107884411
0	7.624645400	-2.318698620	0.908430134
0	7.611308755	0.133960601	-0.277981528
0	7.748973801	2.105305785	1.542894653
0	-2.140112765	3.892351450	4.762827726
0	-0.493534002	5.436745582	2.941294647
0	0.309239866	4.967563509	0.319014051
С	3.406490518	-3.458906122	0.045315138
Н	3.643070826	-4.495868702	0.330365659
С	3.934989695	-2.985821201	-1.196844868
H	4.542354415	-3.691800226	-1.786196082

С	3.849828287	-1.624241291	-1.595714081
С	4.620329719	-0.825642969	-2.493791601
Н	5.299921385	-1.323303690	-3.205643558
C	1 673396876	0 589597597	-2 446384620
	E 270212220	1 000320450	2.110240660
н	5.3/9312230	1.099328456	-3.119248668
C	3.950121941	1.35/35244/	-1.46/4/3589
С	4.107910390	2.684883887	-0.968936351
Н	4.761575380	3.387399522	-1.508758443
С	3,601893861	3.094125700	0.313073406
н	3 942451869	4 068018182	0 702482429
	2 047122052	2 226265960	1 159624015
C a	2.04/132932	2.230303009	1.130024013
C	2.652022637	2.23283/585	2.583102378
H	2.917848641	3.128684341	3.168550321
С	2.301626478	1.060507095	3.318901365
Н	2.322731162	1.128333233	4.417941939
С	2.129305089	-0.220979303	2.700560363
C	2 227107/20	-1 529050757	3 230163432
	2.337107433	1 (20412705	4 201017447
н	2.440888466	-1.638412785	4.32121/44/
С	2.620897778	-2.6/91/39/3	2.424433651
Н	2.911591294	-3.606888340	2.942513897
С	2.762281316	-2.600064300	0.997198015
С	2.472524520	-1.302052128	0.482756956
C	3 020875973	-0.826880976	-0 724218547
C	2 042640164	0.522715420	0 600529672
0	3.042049104	0.373713420	-0.099528075
C	2.48/126502	0.988602394	0.541/54426
С	2.137285106	-0.182760792	1.282259046
С	6.962513681	-3.455279687	1.463015062
Н	5.874808345	-3.454465242	1.233163444
н	7 110853082	-3 419705954	2 555320920
11	7 206166505	4 405229619	1 070041505
п	7.390100303	-4.405228818	1.078841383
С	7.431696274	-2.206359311	-0.492592449
Н	6.349394719	-2.150887299	-0.743255935
Н	7.844940072	-3.097293785	-1.022966898
С	8.141830223	-0.983223975	-0.969755469
Н	9.235769958	-1.066288149	-0.773497694
п	7 99/719173	-0.881090805	-2 068720206
11	0.004510670	1.250052404	2.000720200
C	8.224518678	1.358953484	-0.664537313
Н	8.054114437	1.5/45/9345	-1.743166540
Н	9.322899675	1.302661074	-0.488991360
С	7.609755021	2.451922689	0.168674320
Н	8.125247576	3.415576447	-0.052043970
Н	6.534091955	2.575414995	-0.094558946
C	7 257506710	3 110000756	2 406231907
	7.237300710	3.110000730	2.400231007
Н	7.835403064	4.064445662	2.303740012
H	7.365692433	2.754466739	3.441720161
Н	6.186604119	3.345409292	2.208827225
С	-3.353960481	3.238341594	5.108231835
Н	-3.905103717	3.806861692	5.889680550
н	-3 102016620	2 246294492	5 510602206
11	1 000242500	2 104672509	4 224254696
п Я	-4.000242500	5.104072500	4.224334000
C	-2.411/326/0	5.219258123	4.324124214
H	-2.998758865	5.761315098	5.102213127
H	-3.021568591	5.202597748	3.392689617
С	-1.146525185	5.951526008	4.089053574
Н	-1.391610217	7.027262081	3.935424644
н	-0 482313746	5 885633383	4 979752808
C	0 113995767	6 323579720	2 276931110
	1 0071000707	0.323370723	2.3/0034449
Н	1.20/1339/5	6.64/632116	3.121638004
H	-0.071327618	7.247417288	2.023736456
С	1.165541514	5.613467478	1.248353777
Н	1.824458811	6.350221282	0.735999722
н	1 808323076	4 808946017	1 647312986
C	-0 500502704	5 952020903	_0 3/29//211
	1 2244104		0 200514277
п	-1.334416409	0.200928628	0.3605143//
Н	-1.150595305	5.249295269	-1.082007012
H	-0.053166024	6.667487574	-0.863091565
Cs	0.670043342	2.503344322	-1.870518542
Cs	-0.669983986	-2.503342506	1.870515488
Cs	0.617849729	-2.486191605	-2.107887467
C	-3 106131163	3 150007030	-0 0/5310100
C	2 021020240	J.4JUJU/JJJ J.00E002010	U.UHJJLOLYZ 1 10/041015
C G	-3.934930342	2.905023010	1.190841815
C	-3.849768933	1.624243114	1.595711031
С	-2.472465163	1.302053945	-0.482760011
С	-3.020816842	0.826883084	0.724214564
0	1.674327647	5.295559265	-2.841238122
0	0.869156993	3.898137363	-5.037188949
0	1 2503////11	1 257076502	-1 713000007
$\cup$	1.2JUJ44411	T.201010000	7.113302331

С	2.650051903	6.027850074	-2.099947537
Н	3.515514789	6.303750299	-2.739198902
Н	2,998232987	5.366708124	-1.290278364
н	2 220599786	6 961513037	-1 672756372
C	1 246427370	5 983632424	-1 005785434
	2 116547740	6 100651601	1.0007009994
п	2.11034/740	0.109031091	-4.009009004
Н	0./82208698	6.964425940	-3./4/210955
С	0.248675538	5.131300262	-4.717161582
Н	-0.643249098	4.958794581	-4.069966424
Н	-0.104259402	5.662370881	-5.632382365
С	-0.003796055	3.008010949	-5.723983828
Н	-0.336220518	3,434004738	-6.699047954
н	-0 904040799	2 803932513	-5 106268022
C	0.754776362	1 729641025	-5 062025535
	0.734770302	1.729041025	-3.902923333
н	0.0//3143/4	0.982387714	-0.435/51880
Н	1.604613082	1.908/89938	-6.660509045
С	1.921097549	0.013153876	-4.836446200
H	1.211458585	-0.806975556	-5.086119235
H	2.436324806	-0.192623734	-3.881864037
Н	2.699761603	0.057160818	-5.629104129
С	-2.129245732	0.220981119	-2.700563417
C	-2 337128082	1 529052571	-3 230166485
C	-2 620939422	2 670175707	-2 424436704
C	-2.020030422	2.079175787	-2.424430704
C	-2.762221958	2.600066115	-0.99/2010/1
С	-2.137225749	0.182/62608	-1.282262100
Cs	-5.228981985	0.077639572	-1.649747066
0	-7.624586029	2.318700422	-0.908433190
0	-7.611249395	-0.133958787	0.277978471
0	-7.748914651	-2.105303663	-1.542898639
0	2.140172125	-3.892349635	-4.762830798
0	0 493593355	-5 436743767	-2 941297704
0	0.200100511	4 067561600	0 210017105
0	-0.309100311	-4.987381890	-0.31901/103
H	-3.643696612	4.495676299	-0.330501253
Н	-4.543101016	3.691582993	1./85630958
С	-4.620270355	0.825644805	2.493788550
H	-5.300048584	1.323374856	3.205407630
С	-4.673337507	-0.589595798	2.446381562
Н	-5.379801180	-1.099325277	3.118675149
С	-3.950062583	-1.357350632	1.467470537
C	-4 107851034	-2 684882071	0 968933297
U U	-1 761723781	-3 387305119	1 508628075
	2 601024506	2 004122005	0 212076450
	-3.001034300	-3.094123003	-0.313076439
Н	-3.943150324	-4.06/5465/8	-0./02992840
С	-2.847073597	-2.236364051	-1.158627069
С	-2.651963282	-2.232835768	-2.583105433
H	-2.918111393	-3.128580766	-3.168567582
С	-2.301567121	-1.060505278	-3.318904419
Н	-2.322367890	-1.128311568	-4.417950776
н	-2 440485049	1 638540735	-4 321234729
и и	-2 01203/268	3 606408967	-2 9/2587152
	2.012500006	0 572712604	0 600525620
C	-3.042369606	-0.3/3/13004	0.099525020
C	-2.48/06/145	-0.988600577	-0.541/5/4/9
С	-6.962454325	3.455281508	-1.463018116
H	-5.873257497	3.450032677	-1.240396524
H	-7.118902181	3.425491415	-2.554314380
Н	-7.390179928	4.404651088	-1.070842996
С	-7.431636924	2.206361124	0.492589401
н	-6 349336506	2 150595568	0 743292723
и и	-7 844572097	3 097593751	1 022691708
п	0 141770050	0.000005701	1.022091/00
C	-8.141//0859	0.983225771	0.969/52405
H	-9.235/09/18	1.066282113	0.//3466106
Н	-7.994705058	0.8810/6464	2.068718313
С	-8.224459317	-1.358951639	0.664534252
Н	-8.054265162	-1.574524625	1.743204761
Н	-9.322840154	-1.302643866	0.488915069
С	-7.609695670	-2.451920873	-0.168677375
н	-8.125184324	-3.415630142	0.051751409
н	-6.534080441	-2.575477990	0.094735802
Ċ	-7 257//726/	_3 11000C017	-2 106221060
	7 000001501	-3.11000094/	-2.400234000
п	-7.829021521	-4.06/492385	-2.2965220/2
Н	-1.3/5243406	-2./58689692	-3.442143491
Н	-6.183998322	-3.338999604	-2.215440548
С	3.354019846	-3.238339763	-5.108234883
Н	3.909094003	-3.810853248	-5.883930664
Н	3.101587335	-2.249490059	-5.518263686
Н	4.004910535	-3.097076830	-4.223024142
~	2 111702022	5 010056000	_1 30/107070

Н	2.998995127	-5.761241637	-5.102095289
Н	3.021290918	-5.202687326	-3.392461313
С	1.146584539	-5.951524186	-4.089056636
Н	1.391593121	-7.027286941	-3.935549482
Н	0.482336050	-5.885486533	-4.979731160
С	-0.443826412	-6.323576912	-2.376837510
Н	-1.207091995	-6.647621988	-3.121630252
Н	0.071390484	-7.247434396	-2.023787153
С	-1.165482159	-5.613465664	-1.248356834
Н	-1.824231782	-6.350392925	-0.736039501
Н	-1.808341504	-4.809044152	-1.647386576
С	0.598562060	-5.852028075	0.342841152
Н	1.334354432	-6.287339612	-0.360375670
Н	1.150548028	-5.249177756	1.081974849
Н	0.053137336	-6.667353930	0.863237822
0	-1.674268292	-5.295557449	2.841235064
0	-0.869097638	-3.898135552	5.037185896
0	-1.250285054	-1.257874688	4.713979946
С	-2.649992548	-6.027848262	2.099944482
Н	-3.515346191	-6.303526458	2.739442688
Н	-2.998420244	-5.366588676	1.290466792
Н	-2.220659051	-6.961463010	1.672573595
С	-1.246368012	-5.983630605	4.005782376
Н	-2.116494456	-6.189644101	4.669663924
Н	-0.782147095	-6.964425202	3.747224087
С	-0.248616181	-5.131298450	4.717158527
Н	0.643309952	-4.958805579	4.069964114
Н	0.104333010	-5.662366227	5.632377095
С	0.003855411	-3.008009136	5.723980769
Н	0.336117937	-3.434061583	6.699079990
Н	0.904190858	-2.803990385	5.106378239
С	-0.754717004	-1.729639211	5.962922488
Н	-0.077154517	-0.982469951	6.435743348
Н	-1.604364280	-1.908865898	6.660707599
С	-1.921038197	-0.013152058	4.836443147
Н	-1.210548519	0.808003131	5.080265187
Н	-2.441345114	0.189548400	3.883914953
Н	-2.695349768	-0.055266861	5.633459395

**Table S10.** Cartesian coordinates for "naked" trianion  $C_{20}H_{10}$ <sup>-3-</sup>, optimized at the PBE0/cc-

pVDZ level of theory.

С	-3.265015562	0.235658907	0.720595975
С	-1.702839165	0.239717050	-2.869905617
С	2.225304702	0.227635818	-2.493165641
С	3.066918203	0.243604498	1.322069513
С	-0.325119872	0.230639008	3.321121380
Н	-4.214864304	0.508394695	1.215960021
Н	-2.466743225	0.547506396	-3.606190104
Н	2.699121969	0.505222477	-3.451713977
Н	4.122522033	0.533658823	1.475711385
Н	-0.140462667	0.530425700	4.367842704
С	-2.073693736	0.017338442	-1.515605622
С	0.786318393	0.019107786	-2.441776288
С	2.583438882	0.009444633	0.003397766
С	0.789490813	0.021649954	2.432666782
С	-2.085616106	0.010385502	1.521130559
С	-0.973298443	-0.344393466	-0.694682545
С	0.377699884	-0.341837798	-1.132940328
С	1.201337094	-0.352061348	-0.005224989
С	0.368825595	-0.337452829	1.131483121
С	-0.975809337	-0.352078037	0.699905312
С	-3.266469277	0.228211803	-0.710013059
С	-0.311371997	0.238063347	-3.322343825
С	3.065827335	0.237776284	-1.333238275
С	2.217904604	0.228999260	2.494108845
С	-1.704874197	0.244219829	2.870841615
Н	-4.214523117	0.502915166	-1.206513780
H	-0.125689077	0.546673114	-4.366559076
Н	4.125056646	0.512314509	-1.490582498
H	2.685181410	0.524348416	3.450073961
Н	-2.468557480	0.538825057	3.613544678

Table S11. Cartesian coordinates for neutral  $C_{20}H_{10}$ , optimized at the PBE0/cc-pVDZ level

of theory.

С	-3.209723411	0.253124867	0.698625151
С	-1.661468844	0.291317307	-2.808774635
С	2.191967488	0.254550867	-2.441317888
С	3.004107163	0.275987225	1.300290667
С	-0.325275676	0.277394691	3.251477159
Н	-4.120810974	0.586604390	1.209142910
Н	-2.422914522	0.677201734	-3.494695670
Н	2.624557273	0.592031173	-3.389403051
Н	4.030824922	0.641626936	1.415412809
Н	-0.112461853	0.648111131	4.259378665
С	-2.021240707	-0.052249624	-1.477159524
С	0.766283172	-0.049102069	-2.378785023
С	2.521536553	-0.068714640	0.003582705
С	0.768637037	-0.043425260	2.368487576
С	-2.034810038	-0.066015912	1.484737381
С	-0.976033088	-0.550202178	-0.697129172
С	0.378453573	-0.547538675	-1.136147411
С	1.206915877	-0.561492273	-0.004717277
С	0.369911900	-0.542120630	1.134238199
С	-0.979628587	-0.559959318	0.703197836
С	-3.210290204	0.251922050	-0.687653835
С	-0.309637393	0.290756977	-3.248277504
С	3.007712036	0.256589923	-1.316904656
С	2.179184907	0.271906005	2.438640987
С	-1.666394046	0.281168357	2.814071481
Н	-4.119841223	0.584873643	-1.199809496
H	-0.096155622	0.676265746	-4.250641498
H	4.043344352	0.595258350	-1.438469412
H	2.601796470	0.635551153	3.380889950
Н	-2.428546536	0.653491052	3.507710570

<b>Table S12.</b> NBO charges for 1- <i>small</i> model (PB	'BE0/det2-TZVP(Cs)//cc-pvDZ(C,H,O)).
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	Natural		Natural P	opulation		Natural
Atom No	Charge	Core	Valence	Rydberg	Total	Density
Cs 1	0.96110	53.99240	0.01210	0.03440	54.03890	0.00173
Cs 2	0.92064	53.98568	0.03767	0.05601	54.07936	0.01347
C 3	-0.36674	1.99900	4.34522	0.02253	6.36674	0.03629
Н 4	0.22893	0.00000	0.76784	0.00323	0.77107	0.00020
C 5	-0.31241	1.99898	4.29228	0.02114	6.31241	0.09691
Н 6	0.22853	0.00000	0.76810	0.00336	0.77147	0.00014
C 7	-0.21280	1.99879	4.19095	0.02306	6.21280	0.00295
C 8	-0.27897	1.99898	4.26030	0.01969	6.27897	0.09089
н 9	0.22641	0.00000	0.77028	0.00331	0.77359	0.00006
C 10	-0.35623	1.99899	4.33585	0.02139	6.35623	0.01911
H 11	0.22703	0.00000	0.76972	0.00325	0.77297	0.00015
C 12	-0.14253	1.99878	4.12185	0.02190	6.14253	0.07686
C 13	-0.38724	1.99899	4.36545	0.02280	6.38724	0.00272
Н 14	0.22756	0.00000	0.76910	0.00333	0.77244	0.00009
C 15	-0.31320	1.99898	4.29364	0.02058	6.31320	0.06730
Н 16	0.22685	0.00000	0.76988	0.00327	0.77315	0.00003
C 17	-0.17848	1.99878	4.15739	0.02231	6.17848	0.02482
C 18	-0.34941	1.99900	4.32781	0.02260	6.34941	0.12171
н 19	0.22998	0.00000	0.76656	0.00345	0.77002	0.00019
C 20	-0.35265	1.99900	4.33077	0.02289	6.35265	0.11664
H 21	0.22993	0.00000	0.76671	0.00336	0.77007	0.00017
C 22	-0.14703	1.99877	4.12694	0.02131	6.14703	0.03392
C 23	-0.37640	1.99898	4.35432	0.02310	6.37640	0.05215
Н 24	0.22944	0.00000	0.76727	0.00330	0.77056	0.00008
C 25	-0.41714	1.99899	4.39390	0.02424	6.41714	0.00663
Н 26	0.22987	0.00000	0.76673	0.00340	0.77013	0.00004
C 27	-0.13245	1.99877	4.11223	0.02144	6.13245	0.06488
C 28	-0.14343	1.99874	4.12353	0.02116	6.14343	0.05358

C 29	-0.17325	1.99873	4.15201	0.02251	6.17325	0.00216
C 30	-0.13338	1.99874	4.11367	0.02096	6.13338	0.05287
C 31	-0.16042	1.99873	4.13991	0.02177	6.16042	0.01987
C 32	-0.15830	1.99873	4.13819	0.02138	6.15830	0.02736
Cs 33	0.92618	53.98663	0.03178	0.05542	54.07382	0.01403
Cs 34	0.96110	53.99240	0.01211	0.03439	54.03890	0.00172
Cs 35	0.92063	53.98568	0.03767	0.05602	54.07937	0.01348
C 36	-0.36686	1.99900	4.34534	0.02253	6.36686	0.03605
Н 37	0.22892	0.00000	0.76785	0.00323	0.77108	0.00020
C 38	-0.31242	1.99898	4.29230	0.02114	6.31242	0.09683
Н 39	0.22853	0.00000	0.76810	0.00336	0.77147	0.00014
C 40	-0.21277	1.99879	4.19092	0.02306	6.21277	0.00293
C 41	-0.27892	1.99898	4.26025	0.01969	6.27892	0.09098
Н 42	0.22641	0.00000	0.77028	0.00331	0.77359	0.00006
C 43	-0.35614	1.99899	4.33576	0.02138	6.35614	0.01927
Н 44	0.22704	0.00000	0.76971	0.00325	0.77296	0.00015
C 45	-0.14256	1.99878	4.12188	0.02190	6.14256	0.07679
C 46	-0.38720	1.99899	4.36541	0.02280	6.38720	0.00274
Н 47	0.22757	0.00000	0.76909	0.00333	0.77243	0.00009
C 48	-0.31337	1.99898	4.29381	0.02058	6.31337	0.06709
Н 49	0.22685	0.00000	0.76988	0.00327	0.77315	0.00003
C 50	-0.17833	1.99878	4.15725	0.02230	6.17833	0.02495
C 51	-0.34957	1.99900	4.32796	0.02261	6.34957	0.12161
Н 52	0.22999	0.00000	0.76655	0.00345	0.77001	0.00019
C 53	-0.35249	1.99900	4.33061	0.02288	6.35249	0.11686
Н 54	0.22992	0.00000	0.76672	0.00336	0.77008	0.00017
C 55	-0.14720	1.99877	4.12711	0.02132	6.14720	0.03379
C 56	-0.37618	1.99898	4.35410	0.02310	6.37618	0.05238
Н 57	0.22944	0.00000	0.76726	0.00330	0.77056	0.00008
C 58	-0.41729	1.99899	4.39404	0.02425	6.41729	0.00656
Н 59	0.22987	0.00000	0.76673	0.00340	0.77013	0.00004
C 60	-0.13233	1.99877	4.11212	0.02144	6.13233	0.06499
C 61	-0.14335	1.99874	4.12346	0.02116	6.14335	0.05366
C 62	-0.17328	1.99873	4.15203	0.02251	6.17328	0.00214
C 63	-0.13343	1.99874	4.11372	0.02097	6.13343	0.05282
C 64	-0.16033	1.99873	4.13983	0.02177	6.16033	0.01998
C 65	-0.15840	1.99873	4.13828	0.02138	6.15840	0.02723
Cs 66	0.92617	53.98663	0.03179	0.05541	54.07383	0.01402
======================================	* 0 00000	403 88436	184 87989	1 23575	590 00000	2 00000
IUCAL	0.00000	-00-00-00		I.200/J	500.00000	2.00000

Table S13. NBO	charges for	<b>1</b> - <i>small</i> model	(PBE0/def2-	-TZVP(Cs)//cc-j	pvDZ(C,H,O)).
	0				

	Networl		Natural F	opulation		Natural
Atom No	Charge	Core	Valence	Rydberg	Total	Density
Cs 1	0.96110	53.99240	0.01210	0.03440	54.03890	0.00173
Cs 2	0.92064	53.98568	0.03767	0.05601	54.07936	0.01347
С 3	-0.36674	1.99900	4.34522	0.02253	6.36674	0.03629
Н 4	0.22893	0.00000	0.76784	0.00323	0.77107	0.00020
C 5	-0.31241	1.99898	4.29228	0.02114	6.31241	0.09691
Н б	0.22853	0.00000	0.76810	0.00336	0.77147	0.00014
C 7	-0.21280	1.99879	4.19095	0.02306	6.21280	0.00295
C 8	-0.27897	1.99898	4.26030	0.01969	6.27897	0.09089
н 9	0.22641	0.00000	0.77028	0.00331	0.77359	0.00006
C 10	-0.35623	1.99899	4.33585	0.02139	6.35623	0.01911
H 11	0.22703	0.00000	0.76972	0.00325	0.77297	0.00015
C 12	-0.14253	1.99878	4.12185	0.02190	6.14253	0.07686
C 13	-0.38724	1.99899	4.36545	0.02280	6.38724	0.00272
Н 14	0.22756	0.00000	0.76910	0.00333	0.77244	0.00009
C 15	-0.31320	1.99898	4.29364	0.02058	6.31320	0.06730
Н 16	0.22685	0.00000	0.76988	0.00327	0.77315	0.00003
C 17	-0.17848	1.99878	4.15739	0.02231	6.17848	0.02482
C 18	-0.34941	1.99900	4.32781	0.02260	6.34941	0.12171
Н 19	0.22998	0.00000	0.76656	0.00345	0.77002	0.00019
C 20	-0.35265	1.99900	4.33077	0.02289	6.35265	0.11664
Н 21	0.22993	0.00000	0.76671	0.00336	0.77007	0.00017
C 22	-0.14703	1.99877	4.12694	0.02131	6.14703	0.03392
C 23	-0.37640	1.99898	4.35432	0.02310	6.37640	0.05215
Н 24	0.22944	0.00000	0.76727	0.00330	0.77056	0.00008
C 25	-0.41714	1.99899	4.39390	0.02424	6.41714	0.00663
н 26	0.22987	0.00000	0.76673	0.00340	0.77013	0.00004

С	27	-0.13245	1.99877	4.11223	0.02144	6.13245	0.06488
С	28	-0.14343	1.99874	4.12353	0.02116	6.14343	0.05358
С	29	-0.17325	1.99873	4.15201	0.02251	6.17325	0.00216
С	30	-0.13338	1.99874	4.11367	0.02096	6.13338	0.05287
С	31	-0.16042	1.99873	4.13991	0.02177	6.16042	0.01987
С	32	-0.15830	1.99873	4.13819	0.02138	6.15830	0.02736
Cs	33	0.92618	53.98663	0.03178	0.05542	54.07382	0.01403
Cs	34	0.96110	53.99240	0.01211	0.03439	54.03890	0.00172
Cs	35	0.92063	53.98568	0.03767	0.05602	54.07937	0.01348
С	36	-0.36686	1.99900	4.34534	0.02253	6.36686	0.03605
Н	37	0.22892	0.00000	0.76785	0.00323	0.77108	0.00020
С	38	-0.31242	1.99898	4.29230	0.02114	6.31242	0.09683
Н	39	0.22853	0.00000	0.76810	0.00336	0.77147	0.00014
С	40	-0.21277	1.99879	4.19092	0.02306	6.21277	0.00293
С	41	-0.27892	1.99898	4.26025	0.01969	6.27892	0.09098
Н	42	0.22641	0.00000	0.77028	0.00331	0.77359	0.00006
С	43	-0.35614	1.99899	4.33576	0.02138	6.35614	0.01927
Н	44	0.22704	0.00000	0.76971	0.00325	0.77296	0.00015
С	45	-0.14256	1.99878	4.12188	0.02190	6.14256	0.07679
С	46	-0.38720	1.99899	4.36541	0.02280	6.38720	0.00274
Н	47	0.22757	0.00000	0.76909	0.00333	0.77243	0.00009
С	48	-0.31337	1.99898	4.29381	0.02058	6.31337	0.06709
Н	49	0.22685	0.00000	0.76988	0.00327	0.77315	0.00003
С	50	-0.17833	1.99878	4.15725	0.02230	6.17833	0.02495
С	51	-0.34957	1.99900	4.32796	0.02261	6.34957	0.12161
Н	52	0.22999	0.00000	0.76655	0.00345	0.77001	0.00019
С	53	-0.35249	1.99900	4.33061	0.02288	6.35249	0.11686
Н	54	0.22992	0.00000	0.76672	0.00336	0.77008	0.00017
С	55	-0.14720	1.99877	4.12711	0.02132	6.14720	0.03379
С	56	-0.37618	1.99898	4.35410	0.02310	6.37618	0.05238
Н	57	0.22944	0.00000	0.76726	0.00330	0.77056	0.00008
С	58	-0.41729	1.99899	4.39404	0.02425	6.41729	0.00656
Н	59	0.22987	0.00000	0.76673	0.00340	0.77013	0.00004
С	60	-0.13233	1.99877	4.11212	0.02144	6.13233	0.06499
С	61	-0.14335	1.99874	4.12346	0.02116	6.14335	0.05366
С	62	-0.17328	1.99873	4.15203	0.02251	6.17328	0.00214
С	63	-0.13343	1.99874	4.11372	0.02097	6.13343	0.05282
С	64	-0.16033	1.99873	4.13983	0.02177	6.16033	0.01998
С	65	-0.15840	1.99873	4.13828	0.02138	6.15840	0.02723
Cs	66	0.92617	53.98663	0.03179	0.05541	54.07383	0.01402
* Tot	cal	* 0.00000	403.88436	184.87989	1.23575	590.00000	2.00000

<b>Table S14.</b> NBO charges for $1^4$	-small model (PBE0/def2-7	ΓΖVP(Cs)//cc-pvDZ(C,H,O))

Natural			Natural P	opulation		
Ator	n No	Charge	Core	Valence	Rydberg	Total
Cs	1	0.92541	53.97776	0.02874	0.06808	54.07459
Cs	2	0.92547	53.97779	0.02870	0.06805	54.07453
С	3	-0.17938	1.99889	4.15166	0.02883	6.17938
С	4	-0.17896	1.99889	4.15126	0.02881	6.17896
С	5	-0.17945	1.99889	4.15171	0.02885	6.17945
С	6	-0.17985	1.99889	4.15208	0.02888	6.17985
С	7	-0.17966	1.99889	4.15190	0.02887	6.17966
С	8	-0.18333	1.99899	4.15528	0.02905	6.18333
С	9	-0.38684	1.99919	4.36100	0.02665	6.38684
Η	10	0.19085	0.0000	0.80644	0.00270	0.80915
С	11	-0.38738	1.99919	4.36153	0.02666	6.38738
Н	12	0.19090	0.00000	0.80640	0.00270	0.80910
С	13	-0.18262	1.99899	4.15459	0.02903	6.18262
С	14	-0.38654	1.99919	4.36074	0.02662	6.38654
Η	15	0.19084	0.00000	0.80646	0.00270	0.80916
С	16	-0.38677	1.99919	4.36096	0.02663	6.38677
Н	17	0.19087	0.00000	0.80643	0.00270	0.80913
С	18	-0.18220	1.99899	4.15421	0.02900	6.18220
С	19	-0.38677	1.99919	4.36097	0.02662	6.38677
Н	20	0.19086	0.00000	0.80644	0.00270	0.80914
С	21	-0.38648	1.99919	4.36068	0.02661	6.38648
Н	22	0.19086	0.00000	0.80644	0.00270	0.80914
С	23	-0.18272	1.99899	4.15469	0.02904	6.18272
С	24	-0.38768	1.99919	4.36182	0.02668	6.38768
Н	25	0.19091	0.00000	0.80639	0.00270	0.80909

 Table S15. NBO charges for 1-full model (PBE0/def2-TZVP(Cs)//cc-pvDZ(C,H,O)).

				Natural	Population		Natural
Atom	No	Natural Charge	Core	Valence	Rydberg	Total	- Spin Density
Cs	1	0.91631	53.98815	0.04846	0.04708	54.08369	-0.00039
Cs	2	0.91631	53.98815	0.04846	0.04708	54.08369	-0.00039
Cs	3	0.90420	53.98003	0.05847	0.05729	54.09580	0.00365
Cs	4	0.90420	53.98003	0.05847	0.05729	54.09580	0.00365
0	5	-0.61726	1.99979	6.60658	0.01089	8.61726	-0.00004
0	6	-0.61726	1.99979	6.60658	0.01089	8.61726	-0.00004
0	7	-0.62234	1.99976	6.61091	0.01167	8.62234	0.00000
0	8	-0.62234	1.99976	6.61091	0.01167	8.62234	0.00000
0	9	-0.61801	1.99979	6.60739	0.01084	8.61801	-0.00004
01	0	-0.61801	1.99979	6.60738	0.01084	8.61801	-0.00004
01	1	-0.60815	1.99978	6.59735	0.01102	8.60815	-0.00002
01	2	-0.60816	1.99978	6.59736	0.01102	8.60816	-0.00002
01	3	-0.62064	1.99976	6.60846	0.01242	8.62064	0.00006
01	4	-0.62065	1.99976	6.60847	0.01242	8.62065	0.00006
01	5	-0.61749	1.99979	6.60677	0.01092	8.61749	0.00000
01	6	-0.61751	1.99979	6.60679	0.01092	8.61751	0.00000
C 1	7	-0.37628	1.99899	4.35522	0.02207	6.37628	0.01695
C 1	8	-0.37628	1.99899	4.35522	0.02207	6.37628	0.01701
Н 1	9	0.21410	0.00000	0.78250	0.00340	0.78590	-0.00057
Н 2	0	0.21411	0.00000	0.78249	0.00340	0.78589	-0.00057
C 2	1	-0.39060	1.99899	4.36992	0.02170	6.39060	-0.00579
C 2	2	-0.39062	1.99899	4.36993	0.02170	6.39062	-0.00584
Н 2	3	0.21485	0.00000	0.78188	0.00327	0.78515	0.00010

н 24	0.21487	0.0000	0.78187	0.00327	0.78513	0.00011
0 25	0 12660	1 00076	1 10722	0.02051	6 12660	0 06060
C 25	-0.12000	1.99070	4.10733	0.02031	0.12000	0.06960
C 26	-0.12658	1.99876	4.10732	0.02051	6.12658	0.06962
C 27	-0.34275	1.99900	4.32379	0.01997	6.34275	0.03626
C 28	-0.34276	1,99900	4.32379	0.01997	6.34276	0.03626
11 20	0 01516	0.00000	0 70141	0 00242	0 70/0/	0.00000
п 29	0.21510	0.00000	0.70141	0.00343	0.70404	-0.00099
H 30	0.21516	0.00000	0.78141	0.00343	0.78484	-0.00099
C 31	-0.26960	1.99898	4.25102	0.01959	6.26960	0.15336
C 32	-0.26956	1.99898	4.25099	0.01959	6.26956	0.15330
11 22	0.20000	1.00000	0 77767	0.00242	0.20000	0.10000
пээ	0.21090	0.00000	0.77707	0.00343	0.70110	-0.00473
H 34	0.21889	0.00000	0.77768	0.00343	0.78111	-0.00473
C 35	-0.16667	1.99876	4.14654	0.02137	6.16667	-0.03045
C 36	-0.16669	1,99876	4.14657	0.02137	6.16669	-0.03043
C 37	-0 32665	1 00000	1 30651	0 02115	6 32665	0 13160
C 37	-0.32003	1.99090	4.30031	0.02115	0.32003	0.13109
C 38	-0.32662	1.99898	4.30649	0.02115	6.32662	0.13169
н 39	0.21986	0.00000	0.77691	0.00324	0.78014	-0.00413
Н 40	0.21985	0.00000	0.77691	0.00324	0.78015	-0.00413
C 41	-0 41904	1 99901	4 39743	0 02260	6 41904	-0 02881
0 10	0.41002	1 00001	4 20740	0.02200	C 41000	0.02001
C 42	-0.41903	1.99901	4.39/42	0.02260	6.41903	-0.02881
н 43	0.21369	0.00000	0.78314	0.00317	0.78631	0.00095
H 44	0.21369	0.00000	0.78314	0.00317	0.78631	0.00095
C 45	-0 10875	1 99877	4 08979	0 02019	6 10875	0 10544
0 10	0.10075	1 00077	4 00001	0.02010	C 10075	0.10544
C 40	-0.108/6	1.998//	4.08981	0.02019	0.108/0	0.10546
C 4'/	-0.43002	1.99900	4.40814	0.02288	6.43002	-0.03079
C 48	-0.43004	1.99900	4.40817	0.02288	6.43004	-0.03076
н 49	0 21972	0 00000	0 77708	0 00320	0 78028	0 00081
TT EO	0.01070	0.00000	0.77700	0.00320	0.70020	0.00001
H 30	0.21972	0.00000	0.77708	0.00320	0.78028	0.00081
C 51	-0.34138	1.99898	4.32080	0.02160	6.34138	0.15222
C 52	-0.34135	1.99898	4.32077	0.02160	6.34135	0.15221
H 53	0.22318	0.0000	0.77356	0.00326	0.77682	-0.00472
TT E /	0 00010	0.00000	0 77250	0.00020	0 77(00	0.00472
H 34	0.22318	0.00000	0.77356	0.00326	0.77682	-0.00472
C 55	-0.16665	1.99876	4.14613	0.02177	6.16665	-0.04190
C 56	-0.16667	1.99876	4.14614	0.02177	6.16667	-0.04189
C 57	-0.30809	1.99898	4.28792	0.02119	6.30809	0.19275
C 50	_0 30907	1 00000	1 29700	0 02110	6 30907	0 10271
C J0	-0.30807	1.99090	9.20790	0.02119	0.30007	0.19271
H 59	0.21461	0.00000	0.78166	0.003/3	0.78539	-0.00586
Н 60	0.21461	0.00000	0.78165	0.00373	0.78539	-0.00586
C 61	-0.38801	1,99900	4.36644	0.02257	6.38801	0.07694
C 62	_0 30700	1 00000	1 36613	0 02257	6 39700	0 07696
0 02	-0.30799	1.99900	4.30043	0.02237	0.30799	0.07000
H 63	0.21316	0.00000	0./8338	0.00346	0./8684	-0.00229
н 64	0.21316	0.00000	0.78338	0.00346	0.78684	-0.00229
C 65	-0.13203	1.99876	4.11245	0.02082	6.13203	0.04827
C 66	-0 13203	1 99876	1 11246	0 02082	6 13203	0 04820
0 00	0.1000	1 00070	4 11400	0.02002	C 1000	0.04020
0 07	-0.13333	1.998/3	4.11422	0.02037	0.13333	0.04634
C 68	-0.13333	1.99873	4.11423	0.02037	6.13333	0.04633
C 69	-0.12867	1.99874	4.10997	0.01996	6.12867	0.03399
C 70	-0.12867	1.99874	4.10997	0.01996	6.12867	0.03400
C 71	-0 15321	1 00073	1 13/15	0 02033	6 15321	-0 00367
C /1	-0.13321	1.99073	4.13413	0.02033	0.13321	-0.00307
C 72	-0.15320	1.99873	4.13414	0.02033	6.15320	-0.00368
C 73	-0.12566	1.99874	4.10699	0.01993	6.12566	0.08056
C 74	-0.12567	1.99874	4.10700	0.01993	6.12567	0.08055
C 75	-0 1/529	1 00871	1 12/85	0 02173	6 1/529	0 00000
0 70	0.14520	1.00071	1.12405	0.02175	0.14520	0.00000
C /6	-0.14530	1.998/1	4.12486	0.021/3	6.14530	0.00098
C 77	-0.27482	1.99935	4.25999	0.01547	6.27482	0.00033
C 78	-0.27482	1.99935	4.25999	0.01547	6.27482	0.00033
н 79	0.20751	0.0000	0.78824	0.00425	0.79249	0.00007
U 00	0 20751	0 00000	0 70024	0 00425	0 70240	0 00006
11 00	0.20751	0.00000	0.70024	0.00425	0.75245	0.00000
н ят	0.20704	0.00000	0./905/	0.00239	0./9296	0.00001
н 82	0.20704	0.00000	0.79057	0.00239	0.79296	0.00001
H 83	0.17660	0.0000	0.81941	0.00399	0.82340	-0.00003
ц 8/	0 17660	0 00000	0 81 9/1	0 00300	0 82340	-0 00003
0 05	0.17000	1 00010	4 07760	0.000000	0.02340	0.00003
000	-0.09055	T.222T0	4.0//08	0.019/1	0.09000	0.0001/
C 86	-0.09655	1.99916	4.07768	0.01970	6.09655	υ.00017
H 87	0.22044	0.00000	0.77352	0.00604	0.77956	0.00033
H 88	0.22044	0.0000	0.77352	0.00604	0.77956	0.00033
ц оо	0 10501	0 00000	0 00015	0 00161	0 00176	_0_000000
п оу	0.19524	0.00000	0.00015	0.00401	0.004/0	-0.00002
н 90	U.19524	0.00000	0.80015	0.00461	0.80476	-0.00002
C 91	-0.08482	1.99917	4.06609	0.01956	6.08482	0.00000
C 92	-0.08482	1.99917	4.06610	0.01956	6.08482	0.00000
H Q2	0 19493	0 00000	0 79873	0 00644	0 80517	0 00000
11 01	0.10404	0.00000	0.70070	0.00044	0.00017	0.00000
н 94	0.19484	0.00000	0./98/2	0.00644	0.80516	0.00000
Н 95	0.19900	0.00000	0.79624	0.00476	0.80100	-0.00002
Н 96	0.19901	0.00000	0.79623	0.00476	0.80099	-0.00002
C 97	-0.08488	1.99917	4.06617	0.01954	6.08488	0.00001
C 00	0.00100	1 00017	1.00017	0 01054	6 00400	0 00001
U 98	-0.08488	1.9991/	4.0661/	0.01954	0.08488	0.00001
Н 99	0.19828	0.0000	0.79698	0.00474	0.80172	0.00001
H100	0.19828	0.00000	0.79698	0.00474	0.80172	0.00001

H1(	0.1	9509	0.00000	0.79856	0.00636	0.80491	0.00005
H1(	0.1	9509	0.00000	0.79856	0.00636	0.80491	0.00005
C1 (		0670	1 00016	1 07707	0 01057	6 00670	0 00026
CIU	-0.0	9070	1.99910	4.0//9/	0.01937	0.09070	0.00020
C1(	04 -0.0	9670	1.99916	4.07797	0.01957	6.09670	0.00026
H1(	0.1	9461	0.00000	0.80073	0.00466	0.80539	-0.00002
1111		04.01	0.00000	0.00070	0.00100	0.00530	0.00000
HIU	0.1	9461	0.00000	0.80073	0.00466	0.80539	-0.00002
H1(	0.2	2163	0.00000	0.77224	0.00613	0.77837	0.00005
<b>ц</b> 1(	18 0 2	2163	0 00000	0 77224	0 00613	0 77837	0 00005
1110	0.2	2105	0.00000	0.77224	0.00013	0.77037	0.00005
C1(	)9 -0.2	7407	1.99935	4.25924	0.01548	6.27407	0.00022
C11	10 -0.2	7407	1.99935	4.25924	0.01548	6.27407	0.00022
u1 1	11 0 1	7663	0 00000	0 01030	0 00300	0 02337	0 00000
п1.		7005	0.00000	0.01939	0.00390	0.02337	0.00000
H11	L2 0.1	7663	0.00000	0.81939	0.00398	0.82337	0.00000
Н11	13 0.2	0935	0.00000	0.78821	0.00244	0.79065	-0.00004
111		0025	0 00000	0 70001	0 00244	0 700/5	0 00004
HI.	14 0.2	0935	0.00000	0./8821	0.00244	0.79065	-0.00004
H11	L5 0.2	0525	0.00000	0.79028	0.00447	0.79475	0.00031
Н11	16 0.2	0525	0.00000	0.79028	0.00447	0.79475	0.00031
C1 -	17 0.2	7124	1 00025	1 25501	0 01616	6 07124	0 00000
CI.	-0.2	7134	1.999933	4.23304	0.01010	0.2/154	0.00090
C11	L8 -0.2	7134	1.99935	4.25583	0.01616	6.27134	0.00090
H11	19 0.1	7833	0.00000	0.81774	0.00393	0.82167	0.00017
111		7022	0 00000	0 01774	0 00202	0 001 07	0 00017
піа	20 0.1	1033	0.00000	0.01//4	0.00393	0.0210/	0.0001/
H12	21 0.2	0514	0.00000	0.79210	0.00276	0.79486	0.00000
н1:	2 0.2	0.514	0.00000	0.79211	0.00276	0.79486	0.00000
1111		01.00	0.00000	0 70225	0.00407	0 70022	0.00115
H12	23 0.2	0108	0.00000	0./9335	0.00497	0.79832	0.00115
H12	24 0.2	0168	0.00000	0.79335	0.00497	0.79832	0.00115
C12	25 -0 0	9277	1 99916	4 07368	0 01992	6 09277	0 00005
012		0077	1 00010	1.07000	0.01000	0.00277	0.00005
CL	26 -0.0	9211	1.99910	4.0/368	0.01992	6.09277	0.00005
H12	27 0.1	9437	0.00000	0.80099	0.00464	0.80563	-0.00001
н13	28 0 1	9437	0 00000	0 80099	0 00464	0 80563	-0 00001
1112		0000	0.00000	0.000000	0.00711	0.00000	0.00001
H12	29 0.2	0932	0.00000	0./8356	0.00/11	0./9068	0.00008
H13	30 0.2	0932	0.00000	0.78356	0.00711	0.79068	0.00008
C11	31 -0 0	8469	1 99917	4 06579	0 01973	6 08469	0 00007
010		0400	1 00017	4.00575	0.01070	0.00100	0.00007
CL	32 -0.0	8468	1.99917	4.06579	0.01973	6.08468	0.00007
H13	33 0.1	9583	0.00000	0.79964	0.00453	0.80417	0.00001
н11	34 0 1	9582	0 00000	0 79964	0 00453	0 80418	0 00001
		0010	0.00000	0.75504	0.00433	0.00110	0.00001
HI.	35 0.1	9940	0.00000	0./9441	0.00619	0.80060	0.00000
H13	36 0.1	9940	0.00000	0.79441	0.00619	0.80060	0.00000
C1 3	37 _0 1	0104	1 00010	1 08/19	0 01766	6 10104	0 00004
C1.	0.1	0104	1.00010	4.00410	0.01700	0.10104	0.00004
CI.	38 -0.1	0104	1.99919	4.08419	0.01/66	6.10104	0.00004
H13	39 0.2	0463	0.00000	0.79056	0.00481	0.79537	0.00007
<b>ц</b> 1,	10 0 2	0463	0 00000	0 79056	0 00/81	0 79537	0 00007
	10 0.2	0105	0.00000	0.75050	0.00401	0.75557	0.00007
H14	41 0.1	8544	0.00000	0.80953	0.00502	0.81456	0.00015
H14	42 0.1	8545	0.00000	0.80953	0.00502	0.81455	0.00015
C1/	13 _0 0	0313	1 00013	1 06055	0 02445	6 00313	0 00172
CT.	13 -0.0	9313	1.99913	4.00955	0.02445	0.09313	0.001/2
C14	44 -0.0	9313	1.99913	4.06955	0.02444	6.09313	0.00172
H14	45 0.1	9385	0.00000	0.80142	0.00473	0.80615	-0.00002
<b>ш</b> 1,	16 0 1	0301	0 00000	0 90143	0 00473	0 90616	-0 00002
п1.	10 0.1	9504	0.00000	0.00143	0.00475	0.00010	-0.00002
H14	17 0.2	3877	0.00000	0.75420	0.00704	0.76123	0.00127
H14	48 0.2	3877	0.00000	0.75419	0.00704	0.76123	0.00127
C1/	10 _0 2	7174	1 00035	1 25152	0 01797	6 27174	0 00034
CI	-0.2	1114	1.999933	4.23432	0.01707	0.2/1/4	0.00034
C15	50 -0.2	7176	1.99935	4.25453	0.01788	6.27176	0.00034
H15	51 0.1	8682	0.00000	0.80833	0.00485	0.81318	0.00006
TT 1 [	50 0 1	0600	0 00000	0 00001	0 00495	0 01210	0 00006
п1.	JZ 0.1	0002	0.00000	0.00034	0.00405	0.01310	0.00000
H1;	53 0.2	1517	0.00000	0.78089	0.00394	0.78483	0.00107
H15	54 0.2	1518	0.00000	0.78089	0.00394	0.78482	0.00107
U1 0	55 0 1	7020	0 00000	0 01575	0 00106	0 92071	_0 00002
111.		7525	0.00000	0.01575	0.00490	0.02071	0.00002
HI:	of 0.1	7929	0.00000	0.81575	0.00496	0.82071	-0.00002
Cs15	57 0.8	9709	53.97911	0.06376	0.06003	54.10291	0.00393
Cal		0700	53 07011	0 06376	0 06003	5/ 10201	0 00303
0310		5705	33.37311	0.00070	0.00005	J4.102J1	0.00555
015	og -0.6	1448	1.99978	6.60349	0.01121	8.61448	0.00002
016	50 -0.6	1447	1.99978	6.60348	0.01121	8.61447	0.00002
014	s1 _0 6	1034	1 00076	6 50023	0 01235	9 61034	0 00000
010	JI 0.0	1004	1.00070	0.55025	0.01233	0.01004	0.00000
016	o∠ -0.6	1034	T.999/6	6.59823	0.01235	8.61034	0.00000
016	53 -0.6	1479	1.99978	6.60385	0.01116	8.61479	0.00032
014	54 _0 6	1479	1 99978	6 60385	0 01116	8 61479	0 00033
010			1 00000	0.00000	0.01505	0.011/2	0.000002
C16	-0.2	1018	T. AAA30	4.25498	0.01282	0.2/018	0.00005
C16	56 -0.2	7019	1.99936	4.25498	0.01585	6.27019	0.00005
ц14	57 ∩ 1	8814	0.00000	0.80803	0.00383	0.81186	0.00003
п1 (		0014	0.00000	0.00000	0.00000	0.01100	0.00003
Hle	oo 0.1	8814	0.00000	0.80803	0.00383	0.81180	0.00003
H1(	59 0.2	2297	0.00000	0.77219	0.00484	0.77703	0.00007
<b>U</b> 1 <sup>-</sup>	70 0 2	2297	0 00000	0 77219	0 00484	0 77703	0 00007
п⊥ / -	70 0.2	2271	0.00000	0.11210	0.00704	0.00410	0.00007
H1.	/1 0.1	1288	0.00000	0.82013	0.00399	0.82412	0.00005
Н1	72 0.1	7588	0.00000	0.82013	0.00399	0.82412	0.00005
C17	73 _0 0	8541	1,99918	4.06702	0.01921	6.08541	0.00002
C1	74 0.0	0 5 4 0	1 00010	1.00702	0 01001	C 00540	0.00002
C1.	-0.0	0042	т.ааатя	4.06/02	0.01921	6.08542	0.00002
Н17	75 0.2	0061	0.00000	0.79328	0.00611	0.79939	0.00001
ц1-	76 0 2	0061	0.0000	0.79328	0.00611	0.79939	0.00001
п⊥ / -	, , , , , , , , , , , , , , , , , , , ,	0461	0.00000	0.19920	0.00011	0.10000	0.00001
HL	// U.L	7461	0.00000	0.800/2	0.00466	0.80539	0.00000

*	Total	* 0.00000	511.81754	519.66021	2.52224	*******	2.00000
_	H204	0.18280	0.00000	0.81322	0.00398	0.81720	0.00001
	H203	0.18279	0.00000	0.81323	0.00398	0.81721	0.00001
	H202	0.23165	0.00000	0.76439	0.00397	0.76835	-0.00006
	H201	0.23165	0.00000	0.76439	0.00397	0.76835	-0.00006
	H200	0.17878	0.00000	0.81709	0.00414	0.82122	0.00005
	H199	0.17878	0.00000	0.81709	0.00414	0.82122	0.00005
	C198	-0.27426	1.99936	4.25847	0.01642	6.27426	0.00038
	C197	-0.27425	1.99936	4.25847	0.01642	6.27425	0.00038
	H196	0.19512	0.00000	0.79892	0.00597	0.80488	-0.00001
	H195	0.19512	0.00000	0.79892	0.00597	0.80488	-0.00001
	H194	0.20050	0.00000	0.79487	0.00463	0.79950	0.00004
	H193	0.20050	0.00000	0.79487	0.00463	0.79950	0.00004
	C192	-0.08333	1.99918	4.06481	0.01934	6.08333	0.00020
	C191	-0.08334	1.99918	4.06482	0.01934	6.08334	0.00020
	H190	0.20389	0.0000	0.78968	0.00643	0.79611	-0.00007
	H189	0.20389	0.0000	0.78968	0.00643	0.79611	-0.00007
	H188	0.19633	0.0000	0.79920	0.00448	0.80367	-0.00001
	H187	0.19633	0.00000	0.79920	0.00448	0.80367	-0.00001
	C186	-0.08966	1.99916	4.07050	0.02001	6.08966	-0.00007
	C185	-0.08967	1.99916	4.07050	0.02001	6.08967	-0.00007
	H184	0.19729	0.00000	0.79808	0.00462	0.80271	0.00001
	H183	0.19729	0.00000	0.79808	0.00462	0.80271	0.00001
	H182	0.19608	0.00000	0.79784	0.00608	0.80392	0.00040
	H181	0.19608	0.00000	0.79784	0.00608	0.80392	0.00040
	C180	-0.08684	1,99918	4.06773	0.01993	6.08684	0.00016
	C179	-0 08684	1 99918	4 06773	0 01993	6 08684	0 00016
	н178	0 19461	0 00000	0 80073	0 00466	0 80539	0 00000

 Table S16. NBO charges for 1H-full model (PBE0/def2-TZVP(Cs)//cc-pvDZ(C,H,O)).

	Natural		Natural	Population		Natural
Atom No	Charge	Core	Valence	Rydberg	Total	Density
Cs 1	0.91673	53.98673	0.05097	0.04557	54.08327	-0.00057
Cs 2	0.89976	53.97487	0.06803	0.05733	54.10024	0.00380
о З	-0.61493	1.99980	6.60454	0.01059	8.61493	0.00003
O 4	-0.62049	1.99977	6.60918	0.01154	8.62049	-0.00002
Ο 5	-0.61135	1.99979	6.60085	0.01071	8.61135	-0.00002
06	-0.61285	1.99980	6.60263	0.01042	8.61285	0.00004
07	-0.62875	1.99977	6.61679	0.01220	8.62875	0.00005
08	-0.61955	1.99981	6.60936	0.01039	8.61955	0.00005
C 9	-0.39737	1.99898	4.37463	0.02376	6.39737	-0.02454
H 10	0.21901	0.00000	0.77775	0.00324	0.78099	0.00101
C 11	-0.32532	1.99897	4.30564	0.02071	6.32532	0.14582
Н 12	0.21693	0.00000	0.77978	0.00328	0.78307	-0.00458
C 13	-0.17561	1.99878	4.15591	0.02091	6.17561	-0.03641
C 14	-0.29052	1.99898	4.27230	0.01924	6.29052	0.14547
н 15	0.21316	0.00000	0.78329	0.00354	0.78684	-0.00460
C 16	-0.31855	1.99897	4.29859	0.02099	6.31855	0.02273
Н 17	0.22053	0.00000	0.77616	0.00330	0.77947	-0.00066
C 18	-0.10543	1.99875	4.08639	0.02030	6.10543	0.08583
C 19	-0.38741	1.99899	4.36608	0.02235	6.38741	-0.02357
н 20	0.22106	0.00000	0.77581	0.00312	0.77894	0.00065
C 21	-0.37375	1.99897	4.35396	0.02082	6.37375	0.03837
н 22	0.21326	0.00000	0.78344	0.00331	0.78674	-0.00139
C 23	-0.15205	1.99876	4.13212	0.02117	6.15205	0.02855
C 24	-0.38809	1.99898	4.36654	0.02258	6.38809	0.10162
Н 25	0.22130	0.00000	0.77537	0.00332	0.77870	-0.00310
C 26	-0.33206	1.99897	4.31063	0.02246	6.33206	0.18704
Н 27	0.22519	0.00000	0.77163	0.00318	0.77481	-0.00558
C 28	-0.16340	1.99872	4.14226	0.02242	6.16340	-0.03396
C 29	-0.34350	1.99897	4.32250	0.02203	6.34350	0.13369
н 30	0.21537	0.00000	0.78120	0.00343	0.78463	-0.00420
C 31	-0.42904	1.99897	4.40665	0.02342	6.42904	-0.03514
н 32	0.21990	0.00000	0.77666	0.00344	0.78010	0.00093
C 33	-0.10848	1.99876	4.08894	0.02079	6.10848	0.11325
C 34	-0.12623	1.99871	4.10757	0.01995	6.12623	0.07066
C 35	-0.15098	1.99873	4.13130	0.02094	6.15098	-0.00377
C 36	-0.12712	1.99870	4.10893	0.01949	6.12712	0.03113
C 37	-0.14669	1.99875	4.12677	0.02117	6.14669	0.04804
C 38	-0.14353	1.99872	4.12317	0.02164	6.14353	0.00931
0 00	3.11000	1.0000	1.1001/	0.02101	0.11000	0.0000

C 39	-0.28431	1.99935	4.26988	0.01508	6.28431	-0.00010
н 40	0.20694	0.00000	0.78896	0.00410	0.79306	0.00019
ц /1	0 20657	0 00000	0 70100	0 00234	0 79343	-0 00001
11 11	0.20037	0.00000	0.75105	0.00234	0.75545	0.00001
H 42	0.18212	0.00000	0.81390	0.00398	0.81/88	0.00001
C 43	-0.10017	1.99911	4.08097	0.02009	6.10017	0.00000
Н 44	0.22275	0.0000	0.77046	0.00679	0.77725	0.00007
11 11	0 10501	0,00000	0 00016	0.00452	0 00400	0.00000
H 45	0.19501	0.00000	0.80046	0.00455	0.80499	0.00000
C 46	-0.08830	1.99915	4.06979	0.01936	6.08830	-0.00001
Н 47	0.19371	0.0000	0.80003	0.00626	0.80629	0.00014
TT / O	0 20451	0 00000	0 70072	0 00477	0 70540	0 00004
П 40	0.20451	0.00000	0.79073	0.004//	0.79549	-0.00004
C 49	-0.08857	1.99917	4.07048	0.01892	6.08857	0.00005
Н 50	0.20579	0.00000	0.78942	0.00479	0.79421	0.00005
H 51	0 19394	0 00000	0 79999	0 00607	0 80606	0 00007
n 01	0.10000	1 00010	4 00400	0.00007	C 10000	0.00007
C 52	-0.10282	1.99913	4.08429	0.01939	0.10282	-0.00015
Н 53	0.19594	0.00000	0.79958	0.00448	0.80406	0.00000
Н 54	0.22293	0.00000	0.77091	0.00616	0.77707	0.00005
C 55	-0 28099	1 99938	1 26618	0 01513	6 28099	-0 00004
0.55	0.20000	1.99990	9.20090	0.01313	0.20000	0.00004
H 56	0.18306	0.00000	0.81290	0.00404	0.81694	0.00001
Н 57	0.20900	0.00000	0.78868	0.00231	0.79100	0.00000
н 58	0 19535	0 00000	0 80004	0 00461	0 80465	-0 00003
11 50 0 50	0.17100	1 00000	4 000001	0.00101	0.00100	0.00000
C 59	-0.2/126	1.99933	4.25581	0.01613	6.2/126	0.00020
Н 60	0.17947	0.00000	0.81661	0.00392	0.82053	0.00009
Н 61	0.20969	0.00000	0.78732	0.00299	0.79031	0.00004
н 62	0 20081	0 00000	0 79/01	0 00518	0 79919	0 00002
11 02	0.20001	0.00000	0.75401	0.00010	0.75515	0.00002
C 63	-0.10115	1.99913	4.08233	0.01970	6.10115	0.00042
Н 64	0.20115	0.00000	0.79424	0.00462	0.79885	0.00002
н 65	0 21310	0 00000	0 78045	0 00646	0 78690	0 00048
	0.00101	1 00010	4 07215	0.00010	C 00101	0.00010
0 66	-0.09191	1.99912	4.0/315	0.01964	0.09191	-0.00001
н 67	0.20280	0.00000	0.79283	0.00437	0.79720	0.00002
Н 68	0.20675	0.00000	0.78735	0.00590	0.79325	0.00006
C 60	0 10449	1 00010	1 00000	0 01720	6 10440	0 00001
09	-0.10440	1.99910	4.00002	0.01/20	0.10440	0.00001
н 70	0.20683	0.00000	0.78854	0.00463	0.79317	0.00009
Н 71	0.19032	0.00000	0.80479	0.00489	0.80968	-0.00001
C 72	-0 09576	1 99913	4 07284	0 02379	6 09576	0 00099
U 72	0.00070	1.00010	1.07201	0.02375	0.00170	0.00007
H /3	0.19838	0.00000	0./9683	0.004/9	0.80162	0.0000/
Н 74	0.23579	0.00000	0.75715	0.00706	0.76421	0.00129
C 75	-0 27965	1 99934	4 26263	0 01768	6 27965	0 00101
U 70	0.27505	1.00000	1.20203	0.01/00	0.27903	0.00101
H /0	0.19130	0.00000	0.803/4	0.00490	0.80864	-0.00004
Н 77	0.22296	0.00000	0.77218	0.00486	0.77704	0.00106
Н 78	0.17937	0.00000	0.81649	0.00414	0.82063	0.00006
Ce 79	0 80300	53 97/16	0 07509	0 05774	54 10700	0 00342
CS 79	0.09300	53.97410	0.07509	0.03774	54.10700	0.00342
Cs 80	0.89300	53.97416	0.07509	0.05774	54.10700	0.00342
Cs 81	0.89977	53.97487	0.06803	0.05733	54.10023	0.00380
C 82	-0 39730	1 99898	4 37456	0 02376	6 39730	-0 02459
0 02	0.00700	1 00007	4 20504	0.02070	6.30530	0.02400
C 83	-0.32532	1.99897	4.30564	0.02072	6.32332	0.14582
C 84	-0.17551	1.99878	4.15581	0.02092	6.17551	-0.03642
C 85	-0.12624	1.99871	4.10757	0.01995	6.12624	0.07064
C 86	-0 15095	1 99873	/ 13127	0 02094	6 15095	-0 00376
000	0.13035	1.00075	4.13127	0.02004	0.13035	0.00370
0 87	-0.61285	1.99979	6.60234	0.01073	8.61285	0.00001
O 88	-0.60775	1.99977	6.59599	0.01199	8.60775	0.00000
0 89	-0 60891	1 99979	6 59829	0 01083	8 60891	0 00028
0 00	0.00000	1 00024	4 05050	0.01000	0.00001	0.00020
C 90	-0.2/45/	1.99934	4.25953	0.015/0	6.2/45/	0.00063
Н 91	0.18906	0.00000	0.80717	0.00376	0.81094	-0.00003
Н 92	0.22858	0.00000	0.76683	0.00459	0.77142	0.00047
п 03	0 17263	0 00000	0 82334	0 00404	0 82737	0 00000
11 55	0.17203	1 00015	0.02004	0.00404	6.02737	0.00000
C 94	-0.09034	1.99915	4.0/218	0.01901	6.09034	0.00001
Н 95	0.20012	0.00000	0.79381	0.00608	0.79988	0.00001
Н 96	0.19635	0.0000	0.79914	0.00451	0.80365	0.00001
C 07	0 00400	1 00015	1 07575	0 01000	6 00400	0 00012
0 97	-0.09400	1.99913	4.0/5/5	0.01999	0.09400	0.00013
Н 98	0.19960	0.00000	0.79308	0.00732	0.80040	0.00019
Н 99	0.19929	0.00000	0.79614	0.00457	0.80071	0.00001
C100	-0 09/79	1 99917	1 07626	0 01939	6 09/79	0 00064
C100	0.00470	1.00014	9.07020	0.01000	0.00470	0.00004
HIUI	0.19628	0.00000	0./9929	0.00442	0.803/2	0.00005
H102	0.21192	0.00000	0.78210	0.00598	0.78808	0.00021
C103	-0.08890	1,99917	4.07078	0.01895	6.08890	0.00020
U1 ∩ A	0 20100	0 00000	0 70211	0 00150	0 70000	0 00000
n104	0.20190	0.00000	0./9344	0.00438	0./9002	0.00000
H105	0.19584	0.00000	0.79837	0.00579	0.80416	0.00004
C106	-0.28576	1.99935	4.26977	0.01664	6.28576	0.00096
H107	0.17885	0.0000	0.81687	0.00428	0.82115	0.00032
1110/	0.00400	0.00000	0 7 4 1 0 1	0.00420	0.02110	0.000002
HT08	0.23460	0.00000	U./6104	0.00436	U./6540	0.00024
H109	0.18455	0.00000	0.81169	0.00376	0.81545	0.00011
C110	-0.16343	1,99872	4.14229	0.02242	6.16343	-0.03398
0111	-0 34344	1 00007	1 30011	0 000000	6 21211	0 10070
CIII	-0.34344	1.9989/	4.32244	0.02203	0.34344	0.133/2
C112	-0.42915	1.99897	4.40676	0.02342	6.42915	-0.03513
C113	-0.10848	1.99876	4.08893	0.02079	6.10848	0.11324
C117	-0 1/356	1 00872	4 12320	0 02164	6 1/356	0 00031
CTT4 C 11-	0.01/0	1.00012	I Z J Z U	0.02104	0.1300	0.00901
CS115	U.916/4	53.986/2	0.05098	0.04555	54.08326	-0.00058

0116	-0.61493	1,99980	6.60455	0.01059	8.61493	0.00003
0117	-0 62048	1 99977	6 60916	0 01154	8 62048	-0 00002
0110	0.02040	1 00070	6 600920	0.01070	0 61122	0.00002
0110	-0.01133	1.99979	0.00005	0.010/0	0.01133	-0.00002
0119	-0.6128/	1.99980	6.60265	0.01042	8.6128/	0.00004
0120	-0.62876	1.99977	6.61680	0.01220	8.62876	0.00005
0121	-0.61954	1.99981	6.60935	0.01039	8.61954	0.00005
H122	0.21900	0.00000	0.77777	0.00324	0.78100	0.00101
н123	0 21689	0 00000	0 77982	0 00328	0 78311	-0 00458
C124	-0.20053	1 00000	1 27230	0.01025	6 20053	0 1/553
U121	0.20000	1.00000	0 70200	0.01020	0.20000	0.14333
HIZD	0.21317	0.00000	0.78328	0.00354	0./8683	-0.00460
C126	-0.31863	I.99897	4.29867	0.02098	6.31863	0.02280
H127	0.22054	0.00000	0.77616	0.00330	0.77946	-0.00067
C128	-0.10543	1.99875	4.08638	0.02029	6.10543	0.08578
C129	-0.38743	1.99899	4.36609	0.02235	6.38743	-0.02351
H130	0.22106	0.0000	0.77582	0.00312	0.77894	0.00064
C131	-0 37373	1 99897	4 35395	0 02082	6 37373	0 03830
1122	0.01007	1.00000	0 70242	0.02002	0.37373	0.00000
G1 2 2	0.21327	1.00070	4 12011	0.00331	0.70073	-0.00130
CI33	-0.15203	1.998/6	4.13211	0.02117	6.15203	0.02859
C134	-0.38817	1.99898	4.36661	0.02258	6.38817	0.10155
H135	0.22130	0.00000	0.77537	0.00332	0.77870	-0.00309
C136	-0.33201	1.99897	4.31058	0.02246	6.33201	0.18707
H137	0.22519	0.00000	0.77163	0.00318	0.77481	-0.00558
H138	0 21536	0 00000	0 78120	0 00343	0 78464	-0 00420
u130	0.21002	0.00000	0.77664	0.00344	0 70000	0.000120
01 4 0	0.21002	1 00070	4 10004	0.000344	6.10714	0.000000
C140	-0.12/14	1.998/0	4.10894	0.01949	6.12/14	0.03111
C141	-0.14668	1.99875	4.12676	0.02117	6.14668	0.04805
C142	-0.28421	1.99935	4.26978	0.01508	6.28421	-0.00010
H143	0.20681	0.00000	0.78909	0.00410	0.79319	0.00020
H144	0.20664	0.00000	0.79102	0.00234	0.79336	-0.00001
H145	0.18210	0.00000	0.81391	0.00399	0.81790	0.00001
C146	-0 10018	1 00011	1 08099	0 02009	6 10018	0 00000
11147	0.10010	1.00000	9.000000	0.02000	0.10010	0.00000
H14/	0.222/4	0.00000	0.//04/	0.00679	0.///20	0.00007
HI48	0.19504	0.00000	0.80043	0.00453	0.80496	0.00000
C149	-0.08830	1.99915	4.06979	0.01936	6.08830	-0.00001
H150	0.19371	0.00000	0.80003	0.00626	0.80629	0.00014
H151	0.20451	0.00000	0.79072	0.00477	0.79549	-0.00004
C152	-0.08857	1.99917	4.07049	0.01891	6.08857	0.00005
H153	0 20580	0 00000	0 78942	0 00479	0 79420	0 00005
11155	0.20000	0.00000	0.70042	0.00475	0.75420	0.00003
R154	0.19393	0.00000	0.79999	0.00000	0.00007	0.00007
CISS	-0.10281	1.99913	4.08429	0.01939	6.10281	-0.00015
HI56	0.19595	0.00000	0.79957	0.00448	0.80405	0.00000
H157	0.22292	0.00000	0.77092	0.00616	0.77708	0.00005
C158	-0.28099	1.99938	4.26648	0.01513	6.28099	-0.00004
H159	0.18303	0.00000	0.81293	0.00404	0.81697	0.00001
H160	0.20907	0.00000	0.78862	0.00231	0.79093	0.00000
н161	0 19529	0 00000	0 80010	0 00461	0 80471	-0 00003
0160	0.27140	1 00022	4 25504	0.00401	6 27140	0.00000
C102	-0.27140	1.99933	4.23394	0.01013	0.2/140	0.00020
HI03	0.1/94/	0.00000	0.81001	0.00392	0.82053	0.00009
H164	0.20965	0.00000	0.78737	0.00298	0.79035	0.00003
H165	0.20096	0.00000	0.79385	0.00520	0.79904	0.00002
C166	-0.10113	1.99913	4.08231	0.01970	6.10113	0.00042
H167	0.20116	0.00000	0.79423	0.00461	0.79884	0.00002
H168	0 21308	0 00000	0 78046	0 00646	0 78692	0 00048
C169	_0 09191	1 99912	4 07315	0 01964	6 00101	-0.00001
U170	0 20290	0 00000	0 70203	0 00437	0 70720	0.00001
111 / U 11 7 1	0.20200	0.00000	0.70200	0.00437	0.79720	0.00002
HI/I	0.20673	0.00000	0.78736	0.00590	0.19321	0.00006
C172	-0.10448	1.99918	4.08802	0.01728	6.10448	0.00001
H173	0.20683	0.00000	0.78854	0.00463	0.79317	0.00009
H174	0.19031	0.00000	0.80480	0.00489	0.80969	-0.00001
C175	-0.09574	1.99913	4.07283	0.02379	6.09574	0.00099
H176	0.19837	0.0000	0.79684	0.00479	0.80163	0.00007
H177	0 23580	0 00000	0 75714	0 00706	0 76420	0 00129
C178	-0 27964	1 99934	1 26261	0.01768	6 27964	0 00101
U170	0 10126	1.00000		0.01100	0 00001	_0 000101
пт / У 11.00	0.12130	0.00000	0.003/4	0.00490	0.00004	-0.00004
нт80	0.22295	0.00000	0.//219	0.00486	0.///05	0.00106
н181	0.17936	0.00000	0.81649	0.00414	0.82064	0.00006
0182	-0.61286	1.99979	6.60235	0.01073	8.61286	0.00001
0183	-0.60776	1.99977	6.59600	0.01199	8.60776	0.00000
0184	-0.60891	1.99979	6.59828	0.01084	8.60891	0.00028
C185	-0.27458	1,99934	4,25954	0.01570	6.27458	0.00063
H186	0 18906	0 00000	0 20712	0 00376	0 8100/	-0 00003
u107	0 220500	0 00000	0 76601	0 00150	0 771/0	0 00047
11100	0.22000	0.00000	0./0001	0.00409	0.11140	0.0004/
UT Q Q	U.1/203	0.00000	0.02333	0.00404	0.02/3/	0.00000
CT88	-0.09034	T.99912	4.07218	0.01901	6.09034	0.00001
H190	0.20011	0.00000	0.79381	0.00608	0.79989	0.00001
H191	0.19635	0.00000	0.79914	0.00451	0.80365	0.00001
C192	-0.09488	1.99915	4.07574	0.01999	6.09488	0.00013

H193 H194 C195 H197 C198 H197 H200 C201 H202 H202 H202 H202 H202	3       0.1         4       0.1         5       -0.0         5       0.1         7       0.2         8       -0.0         9       0.2         0       0.1         -       -0.2         0       0.1         -       0.2         0       0.1         -       0.2         0       0.1         -       0.2         0       0.1         -       0.2         0       0.1	9959       0.00         9929       0.00         9479       1.99         9628       0.00         1191       0.00         8890       1.99         0198       0.00         9584       0.00         8593       1.99         7885       0.00         3481       0.00         8447       0.00	000         0.7931           000         0.7961           914         4.0762           000         0.7993           000         0.7821           917         4.0707           000         0.7934           000         0.7983           935         4.2699           000         0.8168           000         0.7608	0 0.00731 4 0.00457 5 0.01939 0 0.00442 0 0.00598 8 0.01895 4 0.00458 7 0.00579 5 0.01663 7 0.00428 4 0.00435 8 0.00376	0.80041 0.80071 6.09479 0.80372 0.78809 6.08890 0.79802 0.80416 6.28593 0.82115 0.76519 0.81553	0.00019 0.00001 0.00064 0.00021 0.00020 0.00000 0.00004 0.00096 0.00032 0.00024 0.00011
H204 ====================================	· · 0.0	3447 0.00 ======= 0000 511.79	000 0.8117 ===================================	8 0.00376 ====== 0 2.50843	0.81553 ===================================	2.00000

**Table S17.** NBO charges for "naked"  $C_{20}H_{10}$ . (PBE0/cc-pvDZ).

	Natural		Natural P	opulation		Natural
Atom No	Charge	Core	Valence	Rydberg	Total	Density
C 1	-0.32044	1.99902	4.30368	0.01774	6.32044	0.17076
C 2	-0.38095	1.99902	4.36365	0.01827	6.38095	0.01351
С З	-0.36522	1.99904	4.34758	0.01860	6.36522	0.09059
C 4	-0.32889	1.99901	4.31233	0.01755	6.32889	0.12764
C 5	-0.39981	1.99904	4.38194	0.01882	6.39981	-0.03376
Н б	0.15712	0.0000	0.83801	0.00487	0.84288	-0.00546
Н 7	0.15497	0.0000	0.84034	0.00469	0.84503	-0.00057
Н 8	0.15760	0.00000	0.83767	0.00473	0.84240	-0.00294
н 9	0.15570	0.00000	0.83945	0.00486	0.84430	-0.00413
H 10	0.15619	0.00000	0.83917	0.00464	0.84381	0.00090
C 11	-0.09902	1.99879	4.08199	0.01823	6.09902	0.02270
C 12	-0.09352	1.99879	4.07655	0.01818	6.09352	0.03692
C 13	-0.13115	1.99880	4.11376	0.01860	6.13115	-0.04444
C 14	-0.08229	1.99879	4.06540	0.01810	6.08229	0.07544
C 15	-0.12627	1.99880	4.10893	0.01854	6.12627	-0.03519
C 16	-0.08227	1.99878	4.06487	0.01862	6.08227	0.05644
C 17	-0.07440	1.99879	4.05703	0.01858	6.07440	0.07100
C 18	-0.11739	1.99877	4.09981	0.01881	6.11739	-0.00708
C 19	-0.05284	1.99880	4.03556	0.01849	6.05284	0.11087
C 20	-0.11325	1.99877	4.09569	0.01879	6.11325	0.00038
C 21	-0.35546	1.99903	4.33796	0.01846	6.35546	0.11473
C 22	-0.38907	1.99903	4.37163	0.01842	6.38907	-0.00554
C 23	-0.31659	1.99902	4.29996	0.01761	6.31659	0.17278
C 24	-0.39663	1.99904	4.37874	0.01885	6.39663	-0.02047
C 25	-0.33770	1.99901	4.32103	0.01765	6.33770	0.10712
Н 26	0.15762	0.00000	0.83762	0.00476	0.84238	-0.00369
Н 27	0.15506	0.00000	0.84027	0.00467	0.84494	0.00002
Н 28	0.15688	0.00000	0.83824	0.00489	0.84312	-0.00553
Н 29	0.15657	0.00000	0.83878	0.00465	0.84343	0.00050
Н 30	0.15546	0.00000	0.83971	0.00483	0.84454	-0.00349
Total *	-3.00000	39.97814	92.60736	0.41450	133.00000	1.00000

## Table S18. NBO charges for neutral $C_{20}H_{10}$ (PBE0/cc-pvDZ).

		Noturol	Natural Population			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.20947	1.99897	4.19404	0.01646	6.20947
С	2	-0.20682	1.99898	4.19155	0.01628	6.20682
С	3	-0.20223	1.99899	4.18686	0.01638	6.20223
С	4	-0.21196	1.99897	4.19660	0.01638	6.21196
С	5	-0.20067	1.99900	4.18541	0.01626	6.20067
Н	6	0.23997	0.00000	0.75680	0.00323	0.76003
Н	7	0.24035	0.00000	0.75651	0.00314	0.75965
Н	8	0.23958	0.00000	0.75724	0.00318	0.76042
Н	9	0.24042	0.00000	0.75638	0.00321	0.75958
н 1	0	0.23978	0.00000	0.75709	0.00313	0.76022
C 1	.1	-0.05453	1.99875	4.03892	0.01686	6.05453

 н 29 н 30	0.23968 0.24046	0.00000 0.00000	0.75718 0.75635	0.00313 0.00319	0.76032 0.75954
Н 28	0.24008	0.00000	0.75669	0.00323	0.75992
Н 27	0.24025	0.0000	0.75662	0.00313	0.75975
Н 26	0.23962	0.00000	0.75718	0.00319	0.76038
C 25	-0.21139	1.99897	4.19606	0.01636	6.21139
C 24	-0.20019	1.99900	4.18492	0.01627	6.20019
C 23	-0.21068	1,99897	4.19525	0.01645	6.21068
C 22	-0 20523	1 99899	4 18998	0.01627	6 20523
C 20	-0.01417	1 99870	J 1882A	0.01/01	6 20364
C 19	-0.01390	1 00070	3 99757	0.01700	6 01417
C 10	-0.01419	1 00070	2 00727	0.01781	6 01206
C 10	-0.01400	1 00070	3 00760	0.01703	6.01400
C 10	-0.01400	1.998/1	3.99/44	0.01784	6.01400
0 10	-0.04997	1.998/6	4.03431	0.01589	6.04997
0 14	-0.05820	1.998/5	4.04267	0.01678	6.05820
C 13	-0.04915	1.99876	4.03349	0.01690	6.04915
C 12	-0.05573	1.99875	4.04014	0.01684	6.05573

#### **EDA Analysis of Sandwich-Type Aggregates**

The bonding between bowl-shaped fragments and positively charged alkali metal belt (see Figures S12 and S13 for details) was further investigated by the energy decomposition analysis (EDA) developed by Morokuma and by Ziegler and Rauk.<sup>[17]</sup> For this purpose, single-point calculations were performed by the ADF program package<sup>[18]</sup> with the same functional. All atoms were described by uncontracted Slater-type orbitals (STOs) with TZ2P quality as basis functions.<sup>[19]</sup> An auxiliary set of s, p, d, and f STOs was used to fit the molecular densities and to represent the Coulomb and exchange potentials accurately in each SCF cycle.<sup>[20]</sup> Scalar relativistic effects have been taken into account by ZORA. Further details on the EDA can be found in literature.<sup>[21]</sup>



Figure S12. EDA Fragmentation scheme in 1-*small* and 1H-*small* models (*left*) as well as for  $1^{4-}$ -*small* (*right*).





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