Electronic Supporting Information

Stabilization of a 12-π Electrons Diamino-Benzoquinonediimine Tautomer

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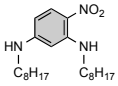
I. GENERAL REMARKS AND ANALYSIS CONDITIONS

Reagents. Reagents were purchased from Sigma Aldrich and Alfa Aesar. Column chromatography were performed using Silica gel 60 (0.040-0.063 mm) from Merck. Optical properties were recorded in spectroscopic grade solvents.

Analytical methods and apparatus. NMR spectra were recorded JEOL ECS400 NMR spectrometers at room temperature. NMR chemical shifts are given in ppm (δ) relative to Me_4Si with solvent resonances used as internal standards ($CDCl_3$: 7.26 ppm for ^1H and 77.2 for ^{13}C). IR spectra were recorded on an Agilent Cary 630 FTIR equipped with an attenuated total reflectance (ATR) sampling. UV-Vis absorption spectra were recorded on a VARIAN CARY 50 SCAN spectrophotometer at room temperature with a 300 nm/min scan rate. HRMS analyses were performed on a QStar Elite (Applied Biosystems SCIEX) or a SYNAPT G2 HDMS (Waters) spectrometers by the “Spectropole” of the Aix-Marseille University. These two instruments were equipped with an ESI or MALDI source. Electrochemical data were extracted from the cyclic voltamogramme performed on a potentiostat BAS 100 (Bioanalytical Systems) equipped with a computer with the BAS100W(v2.3) software. Working electrode : Pt (1.6 mm diameter) ; counter electrode : Pt and a Ag/AgCl electrode. The electrochemical study was performed in a $(nBu)_4NPF_6$ (c=0,1 M) dichloromethane solution. The reference electrode was calibrated with a ferrocene solution ($E°(Fc/Fc^+)$ = 0,46V/SCE). Scan rate: 100 mV.

II. SYNTHETICS PROTOCOLS AND CHARACTERIZATION

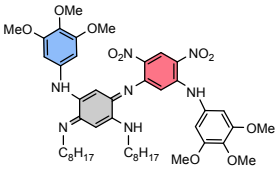
Compound 4



2,4-difluoronitrobenzene (4 mL, 36.5 mmol, 1.0 equiv.), **DIPEA** (12.7 mL, 72 mmol, 2.0 equiv.) and octylamine (24 mL, 146 mmol, 4.0 equiv.) were introduced into a glass pressure bomb equipped with a Teflon screwcap. The mixture was heated at 140 °C for 3 h under vigorous stirring. After that, the orange mixture was allowed to cool to room temperature and 10 mL of EtOH were added; a precipitate formed and the mixture was stirred for additional 2 h. The solid residue was isolated by filtration on a sintered glass and wash with hot water (30 mL at 60 °C). It was then dried under vacuum to quantitatively afford compound **4** as an orange solid.

R*f* = 0.53 (SiO_2, CH_2Cl_2). **^{1}H NMR** (**400 MHz, $CDCl_3$):** δ = 8.53 (bs, 1H), 8.00 (dd, 1H, $^3J_{H\text{-}H}$ = 9.4 Hz, $^5J_{H\text{-}H}$ = 1.1 Hz), 5.88 (dd, 1H, $^3J_{H\text{-}H}$ = 9.4 Hz, $^4J_{H\text{-}H}$ = 2.4 Hz), 5.61 (d, 1H, $^5J_{H\text{-}H}$ = 1.1 Hz), 4.4 (bs, 1H), 3.23 (q, 2H, $^3J_{H\text{-}H}$ = 7.2 Hz), 3.17 (q, 2H, $^3J_{H\text{-}H}$ = 7.2 Hz), 1.80-1.55 (m, 4H), 1.48-1.18 (m, 20H), 0.93-0.82 (m, 6H).). **^{13}C[^{1}H] NMR** (**101 MHz, $CDCl_3$):** δ = 154.4, 148.6, 129.2, 123.6, 104.7, 89.8, 43.3, 42.9, 31.8, 31.7, 29.3, 29.2, 29.1, 28.8, 27.1, 27.0, 22.6, 14.0. **IR-ATR (neat, cm^{-1}):** ν = 3320, 2925, 2851, 1613, 1577, 1541, 1514, 1459, 1401, 1380, 1312, 1259, 1219, 1187, 1090, 818, 789, 753, 540. **HRMS (ESI-TOF)** calculated for [M+H$^+$]: 378.3042 ($C_{22}H_{40}N_3O_2^+$), found 378.3075 .

Compound 9



A solution of compound **4** (628 mg, 1.66 mmol, 1.0 equiv.) in a THF/MeOH mixture (25 mL) was hydrogenated (40 bars) in the presence of activated (vacuum + heat) Pd/C (5% wt, 36 mg, 0.017 mmol, 1 mol%) overnight. After reducing the pressure, the solution was degassed with argon and cooled to 0 °C with an ice-bath. Then, **DFDNB** (320 mg, 1.57 mmol, 0.95 equiv.) was added (the mixture turned brown) and the mixture stirred for 10 mins at 0°C. Then, **DIPEA** (300 µL, 1,5 mmol, 1 equiv.) was added and the solution was stirred for another 10 mins at room temperature (25 °C). After that, **3,4,5-trimethoxylaniline** (637 mg, 3.48 mmol, 2.1 equiv.) and **DIPEA** (602 µL, 3.46 mmol, 2.1 equiv.) were added. The mixture was stirred under reflux for 12h under aerobic conditions then, MnO_2 (3 g, 34.8 mmol, 10 equiv) was added and the mixture stirred for another 12h at room temperature. Then, Pd/C was removed by filtration through a standard Celite pad and the solvent was evaporated. The crude was taken up with AcOEt and washed 2 times with water. The organic layer was dried other Na_2SO_4 and the solvent evaporated. The crude product was purified by silica gel column chromatography

(CH_2Cl_2 to CH_2Cl_2/MeOH 98.5/1.5) to afford the desired compound **9** as a shiny-brown solid in 28% yield.

R*f* = 0.45 (SiO_2, CH_2Cl_2/MeOH, 97:3). **^{1}H NMR** (**400 MHz, $CDCl_3$):** δ = 9.71 (br s, 1H), 9.10 (s, 1H), 6.52 (s, 1H), 6.41 (s, 2H), 6.22 (s, 2H), 5.72 (s, 1H), 5.40 (s, 1H), 3.84 (s, 3H), 3.79 (s, 3H), 3.74 (s, 6H), 3.71 (s, 6H), 3.45 (t, 2H, $^3J_{H\text{-}H}$ = 7.1 Hz), 3.17 (t, 2H, $^3J_{H\text{-}H}$ = 7.1 Hz), 1.77-1.66 (m, 4H), 1.46-1.27 (m, 20H), 0.90-0.86 (m, 6H). **^{13}C[^{1}H] NMR** (**101 MHz, $CDCl_3$**)**:** δ = 154.0, 153.6, 153.5, 151.9, 151.8, 146.4, 146.4, 146.2, 136.8, 136.5, 134.5, 132.6, 130.9, 127.1, 126.8, 105.9, 105.8, 102.6, 102.5, 98.9, 98.9, 90.8, 86.1, 61.0, 60.9, 56.2, 56.2, 56.0, 55.9, 49.5, 43.9, 31.9, 31.8, 30.6, 29.5, 29.3, 29.2, 28.8, 27.7, 27.2, 22.7, 22.6, 14.1, 14.1. **UV-Vis:** λ_{max} (CH_2Cl_2) = 366 nm (ε = 31300 $L.mol^{-1}.cm^{-1}$). **IR-ATR (neat, cm^{-1}):** ν = 3333, 2923, 2852, 2124, 1592, 1561, 1499, 1451, 1416, 1320, 1279, 1225, 1122, 1052, 997, 921, 830, 797, 744, 718. **HRMS (ESI-TOF+)** calculated for [M+H$^+$]: 874.4709 ($C_{46}H_{64}N_7O_{10}^+$), found 874.4707.

III. NMR SPECTRA

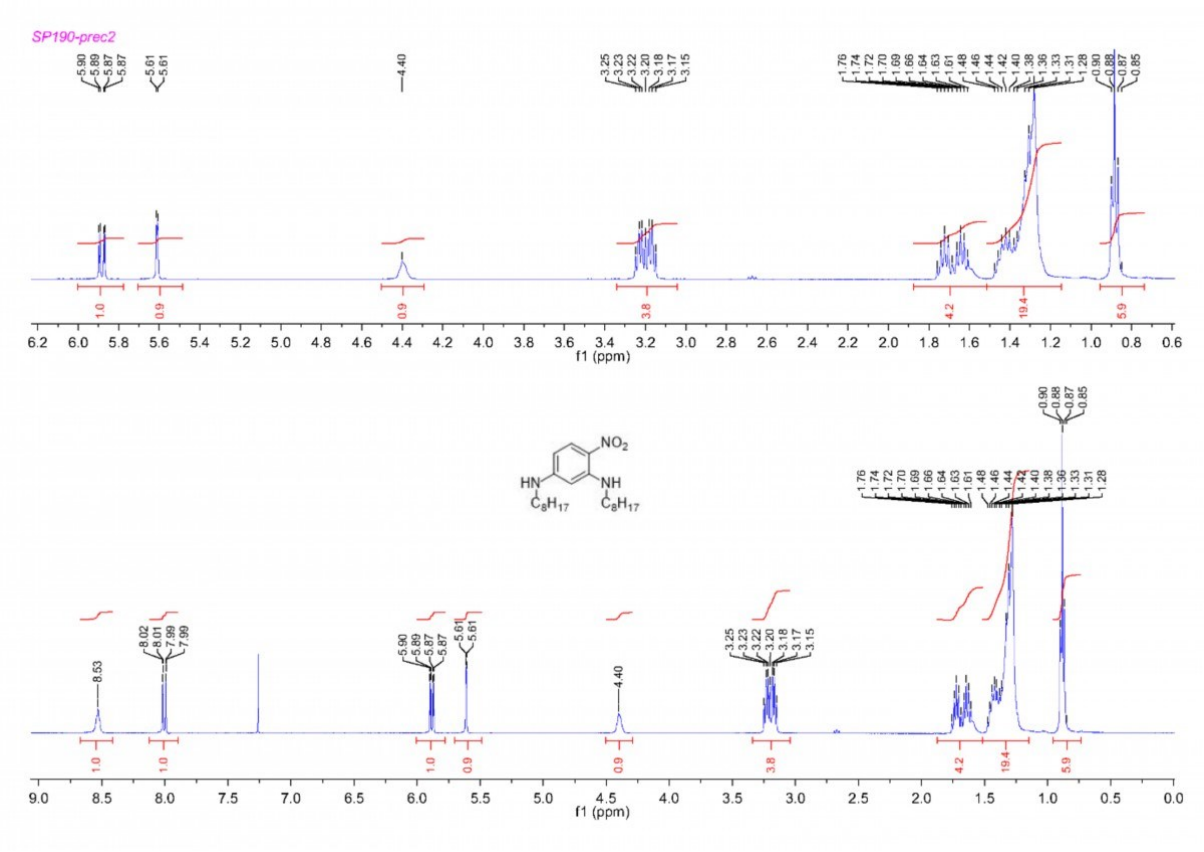


Figure S 1. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **4**.

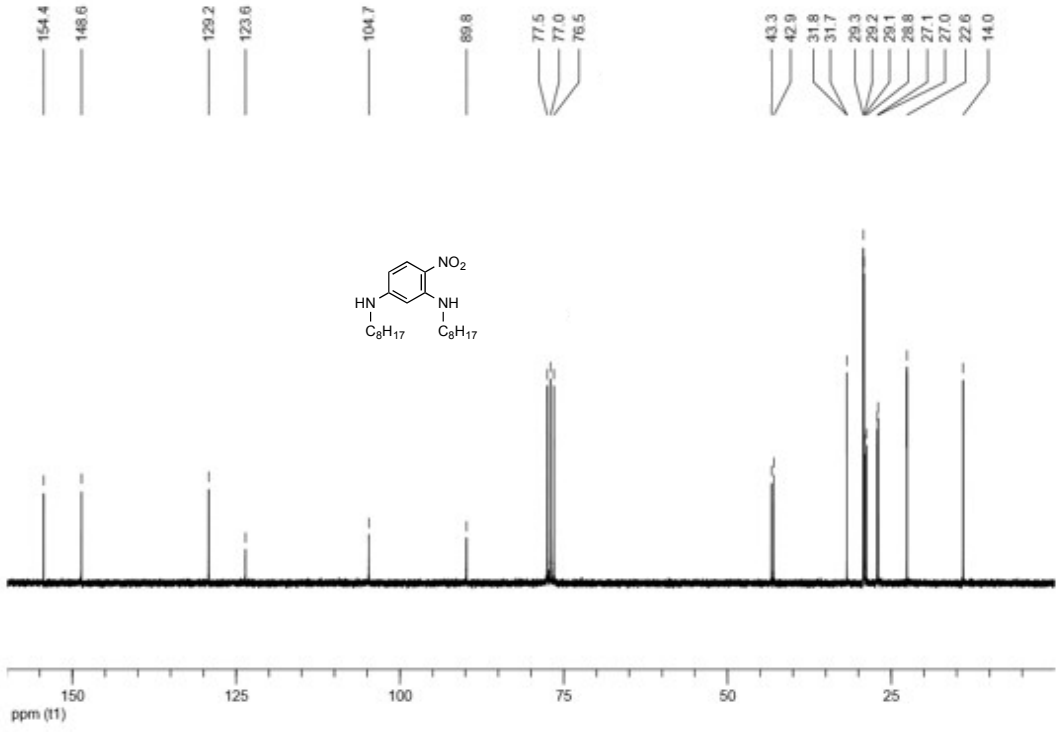


Figure S 2. ^{13}C NMR (101 MHz, $CDCl_3$) of compound **4**.

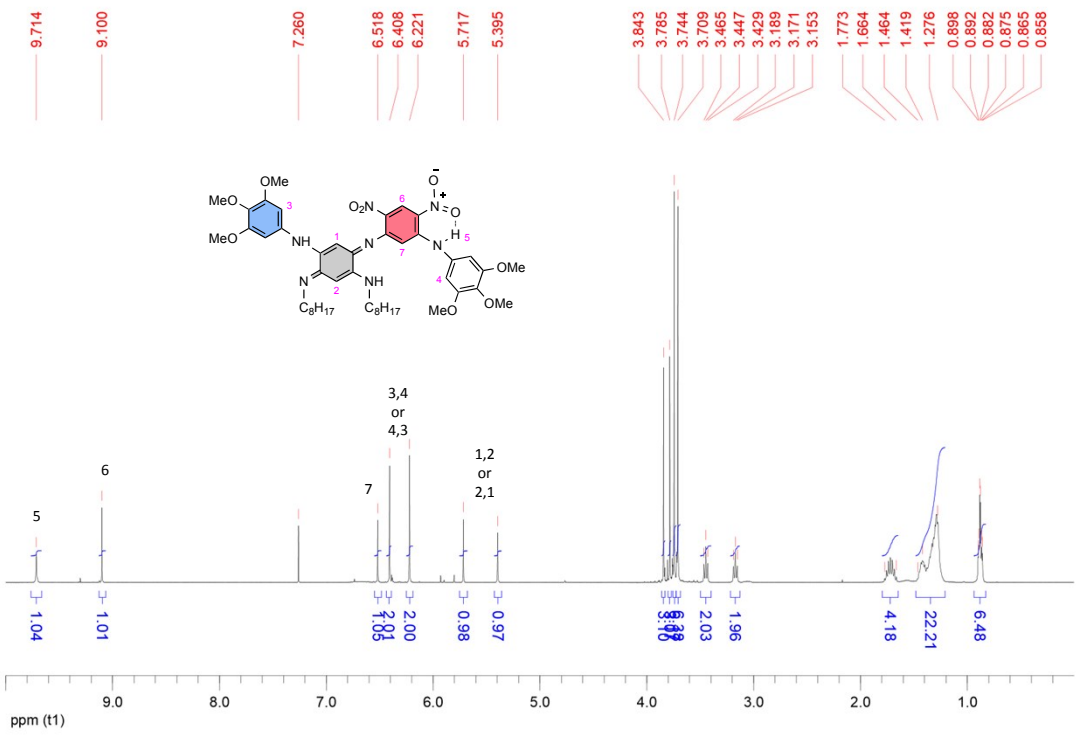


Figure S 3. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **9**.

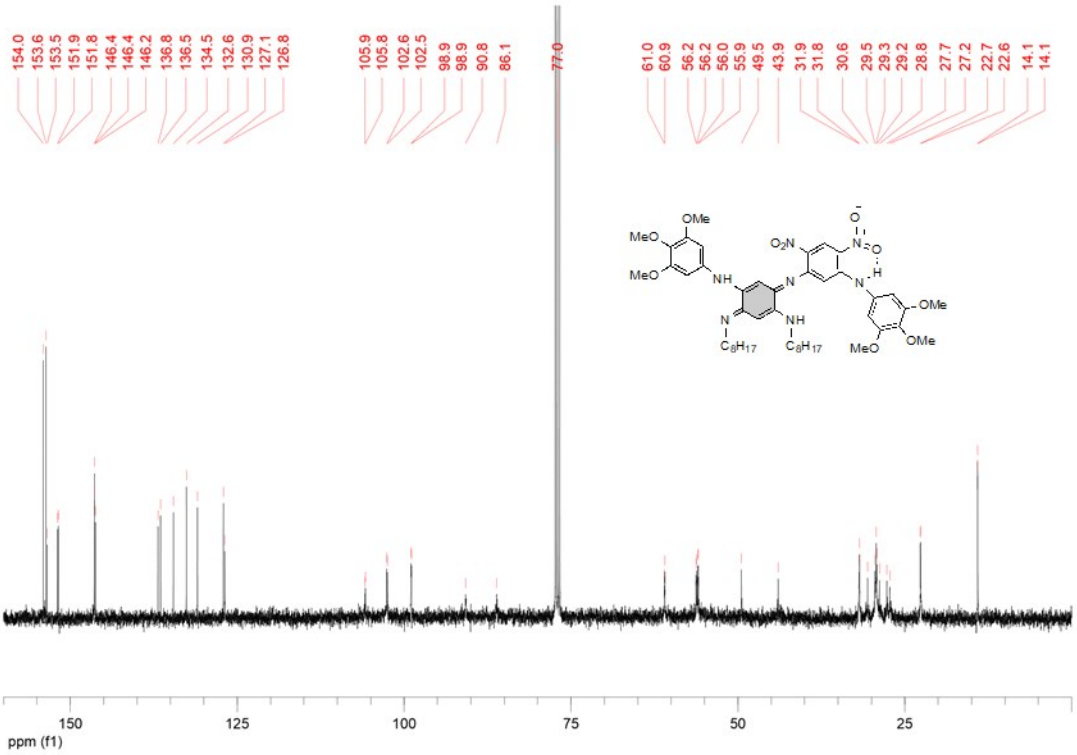


Figure S 4. $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) of compound **9**.

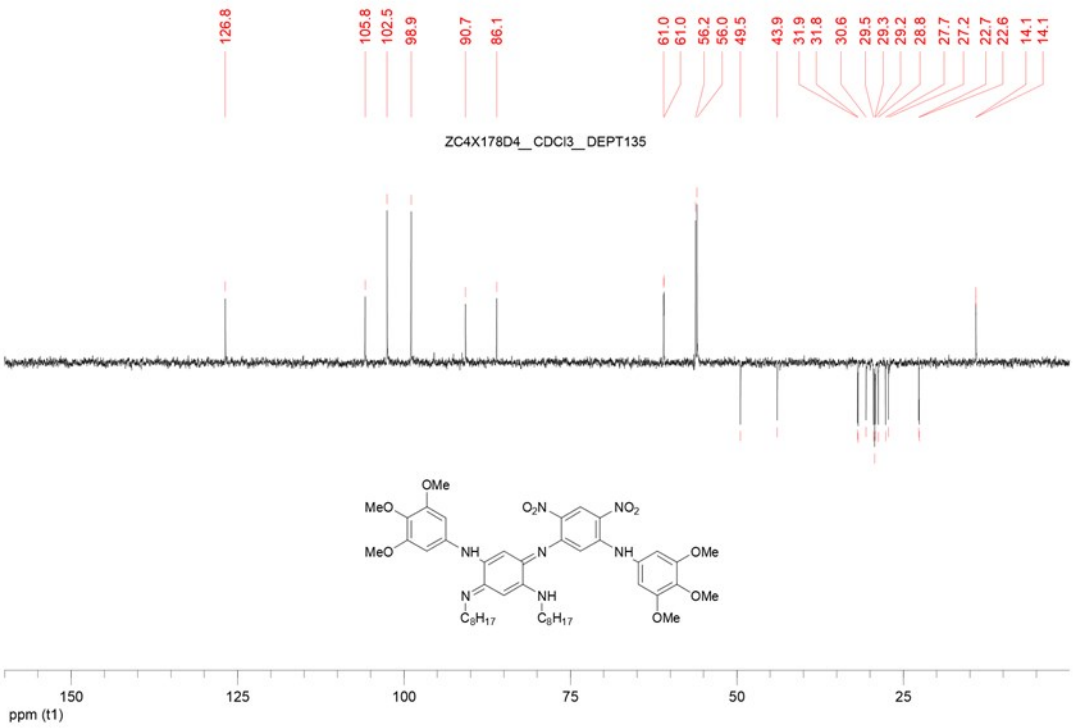


Figure S 5 ^{13}C DEPT NMR (101 MHz, $CDCl_3$) of compound **9**.

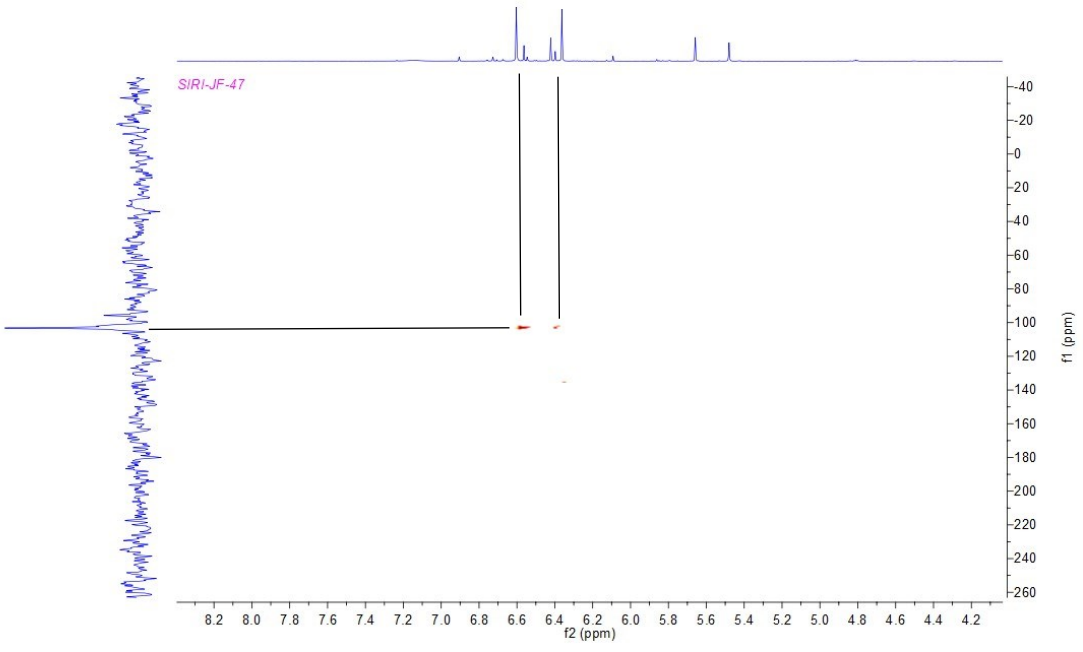


Figure S 6 ^{1}H-^{15}N HMBC NMR (500 MHz, DMSO-$[d]_6$) of compound **9**.

I. INFRARED ANALYSIS

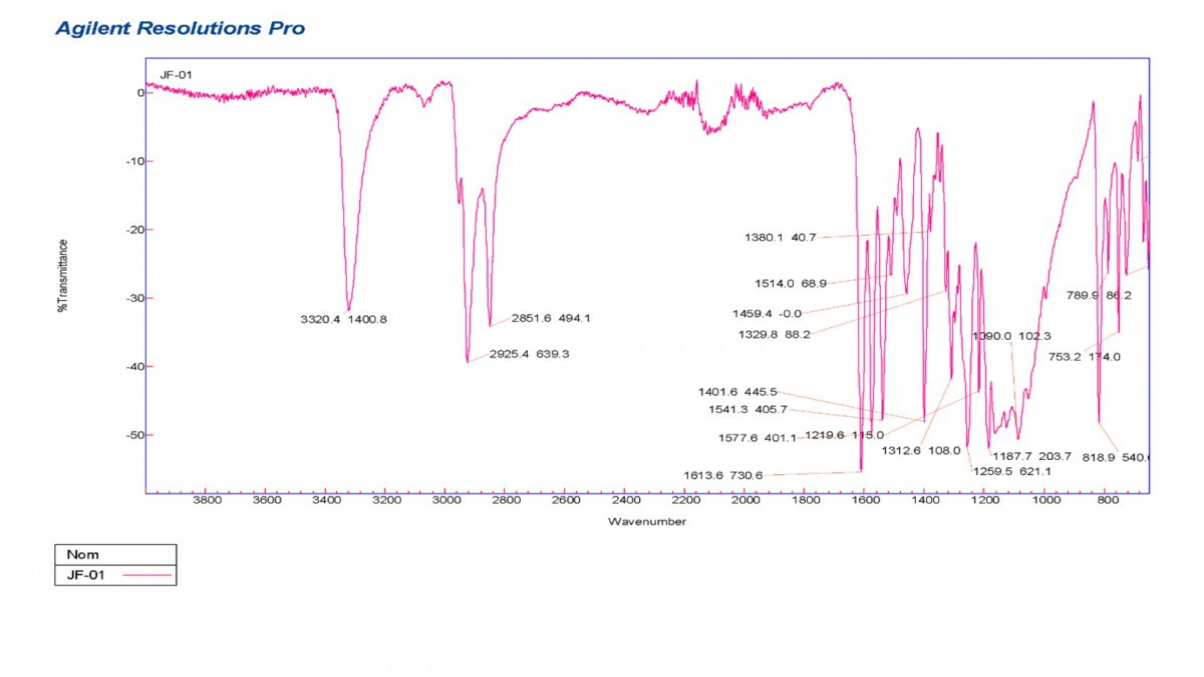


Figure S 7 IR-ATR spectrum of compound **4**.

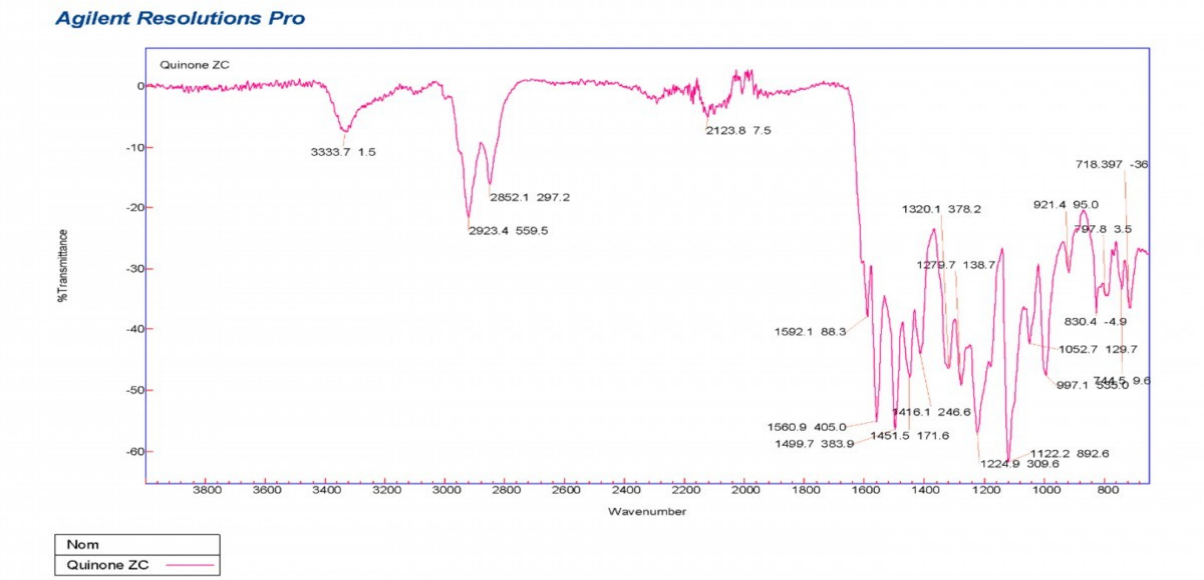


Figure S 8 IR-ATR spectrum of compound **9**.

II. MASS SPECTROMETRY

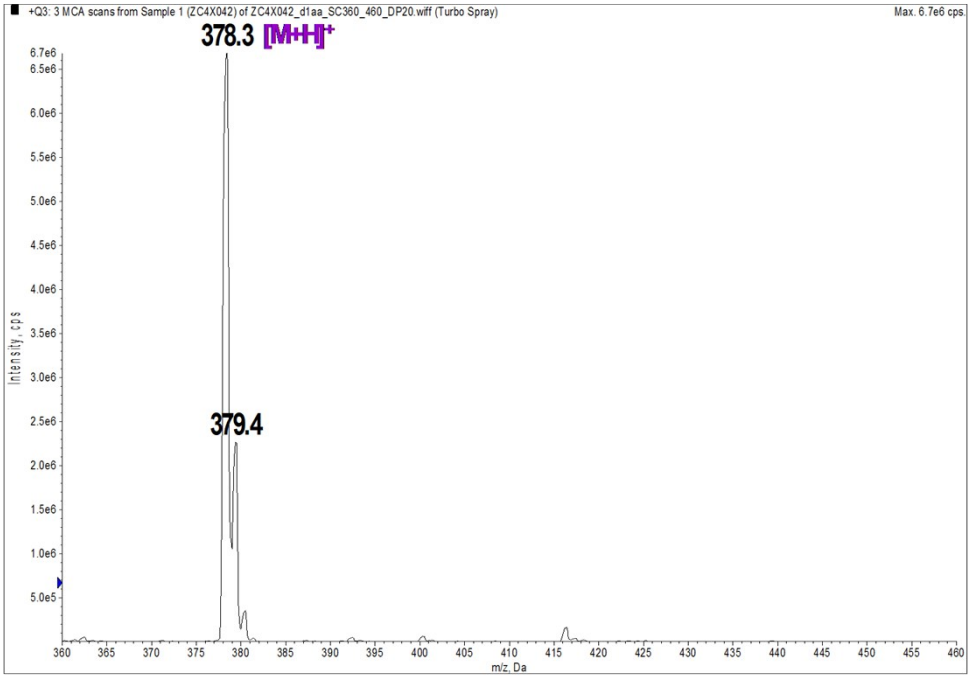


Figure S 9. ESI-MS$^+$ spectrum of compound **4**.

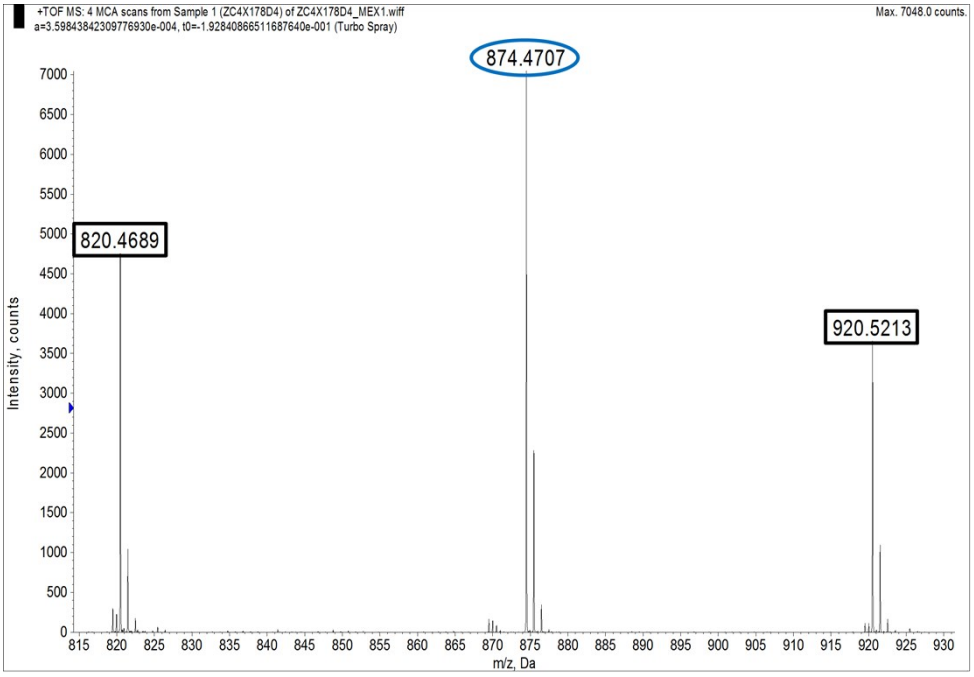
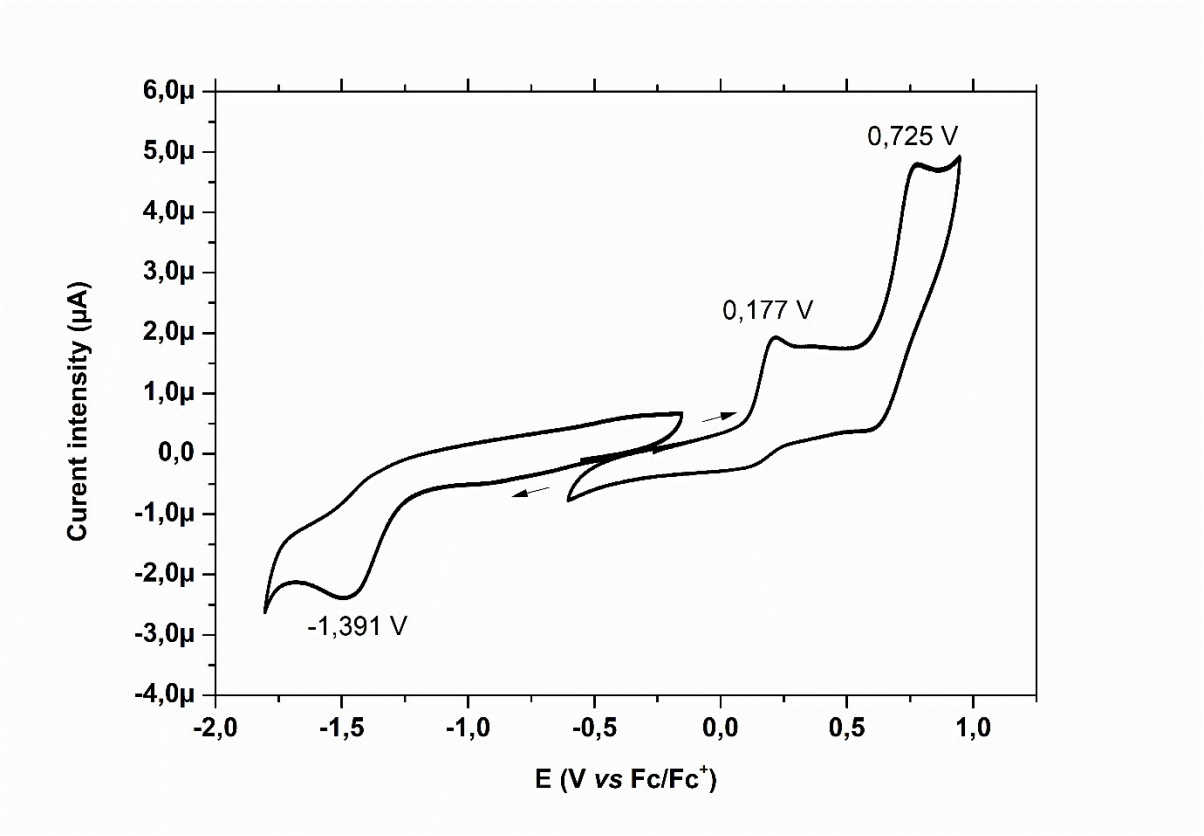


Figure S 10. ESI-HRMS$^+$ spectrum of compound **9**. Target ion is detected at m/z 874.4707 and calibration peaks are observed at m/z 820.4669 and m/z 920.5213.

III. ELECTROCHEMISTRY



	Ep_c (red_1)	$E_{1/2}$ red1	$E_{1/2}$ ox_1	Ep_a (ox_1)	$E_{1/2}$ ox_2	Ep_a (ox_2)
9 (DCM)	-1,47	-1,39 **1e**	0,18 **1e**	0,21	0,73 **2e**	0,77

Figure S 11. Voltamogramme of compound **9** in DCM, 0.1M $TBAPF_6$.

IV. ADDITIONAL OPTICAL INFORMATIONS

Solvent	Polarity index	λ_{max} (nm)	ε ($M^{-1}.cm^{-1}$)
DCM	3.1	374	31 800
MeOH	5.1	370	30 600
MeCN	5.8	373	31 100
DMF	6.4	373	31 700
DMSO	7.2	380, 657	32 600, 750

Table S 1. Spectral changes recorded during the solvatochromism study.

V. QUANTUM MECHANICAL CALCULATIONS

Methods

All calculations have been performed with Gaussian16.A.03,[1] using default procedures and algorithms except when noted below. The long alkyl chains were replaced by methyl groups in the calculations. We have used the PBE0[2] global hybrid functional for all our structural and vibrational calculations, and applied tighten thresholds for the energy (at least 10^{-9} au) and geometry convergences (so-called *tight* threshold in Gaussian, 10^{-5} au on rms residual forces), as well as used the largest DFT integration grid available in Gaussian (*superfine* grid). For all compounds, we have optimized the ground-state geometry with the 6-31++G(d,p) atomic basis set and subsequently verified the absence of imaginary frequencies by computing analytically the Hessian at the same level of theory. These calculations have been made starting with various conformers. Subsequent single-point calculations with the same functional and the larger 6-311++G(2d,p) basis set were next performed. The Gibbs energies use electronic energies determined with this larger basis set and thermodynamic/vibrational corrections obtained with the 6-31++G(d,p) basis. The excited-state calculations were performed with TD-DFT considering 15 states determined and the 6-311++G(2d,p) basis. Given the large number of strong accepting and donating groups in the compounds, CT states could be expected and the TD-DFT calculations have been performed with the range-separated CAM-B3LYP functional.[3] In all steps, the solvent effects were modelled through the well-known Polarizable Continuum Model (PCM, dichloromethane),[4] using the linear-response *non-equilibrium* model for the excited-state calculations.

Results

Theory was first used to screen the possible forms of the system. For **9**, as illustrated in the main text, one can draw one possible zwitterionic form, but two non-equivalent neutral quinoidal forms (***c*-9** and ***c'*-9**). After protonation, four possible isomers can be envisaged [**9+H$^+$(a-d)**], whereas only one doubly protonated isomer can be drawn (see **Figure S 12**). For each of these structures, we can build various conformers for these very flexible molecules and we have identified six non-equivalent chemically intuitive ones that were each optimized by DFT (see below for structures).

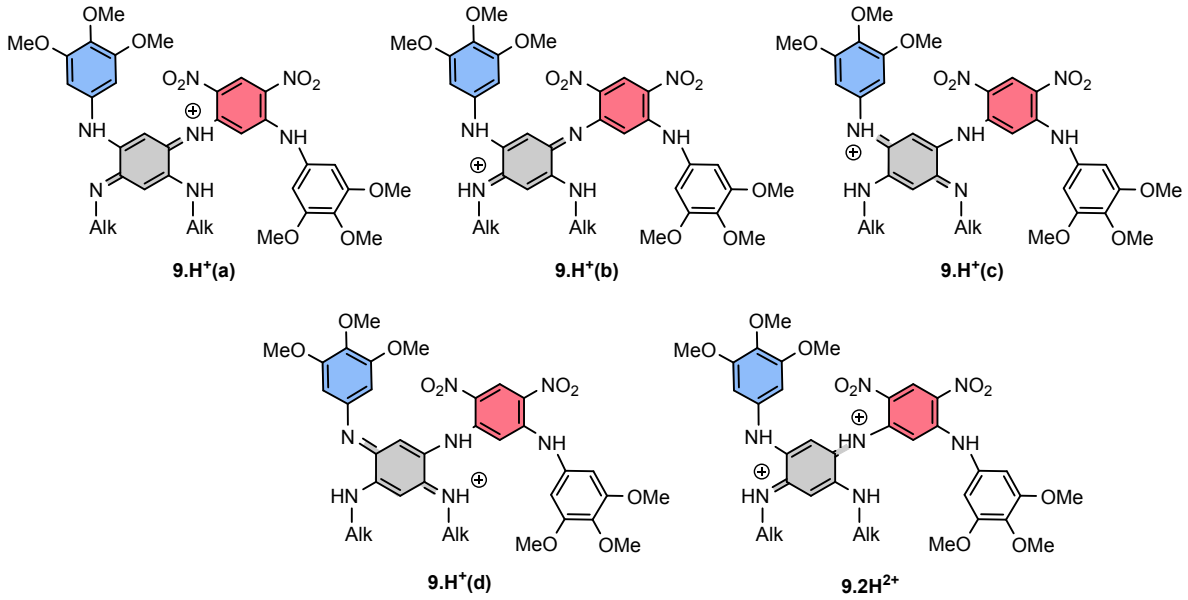


Figure S 12. Representation of possible mono-protonated and doubly-protonated structures

The various conformers obtained for the quinoidal neutral structures are displayed in **Figure S 13**, in which we also report the room temperature Boltzmann weight determined in the basis of the computed Gibbs energies. Although given the high flexibility of the decorating methoxy groups, it is not unlikely that we have missed some specific conformers, the results clearly indicate that the ***c*-9** form should be highly dominant in solution, the ***c'*-9** structure representing a significantly less stable tautomer. Indeed, the least stable ***c*-9** conformer found is nevertheless more stable that the most stable ***c'*-9** conformer. It is also noteworthy that the optical spectral features as given with TD-DFT are very similar for the various conformers of a given structure, *e.g.*, the vertical absorption energies differ by *ca*. 2 nm only between ***c*-9*f***, ***c*-9*e*** and ***c*-9*b***. We therefore discuss only the more stable structure in the following.

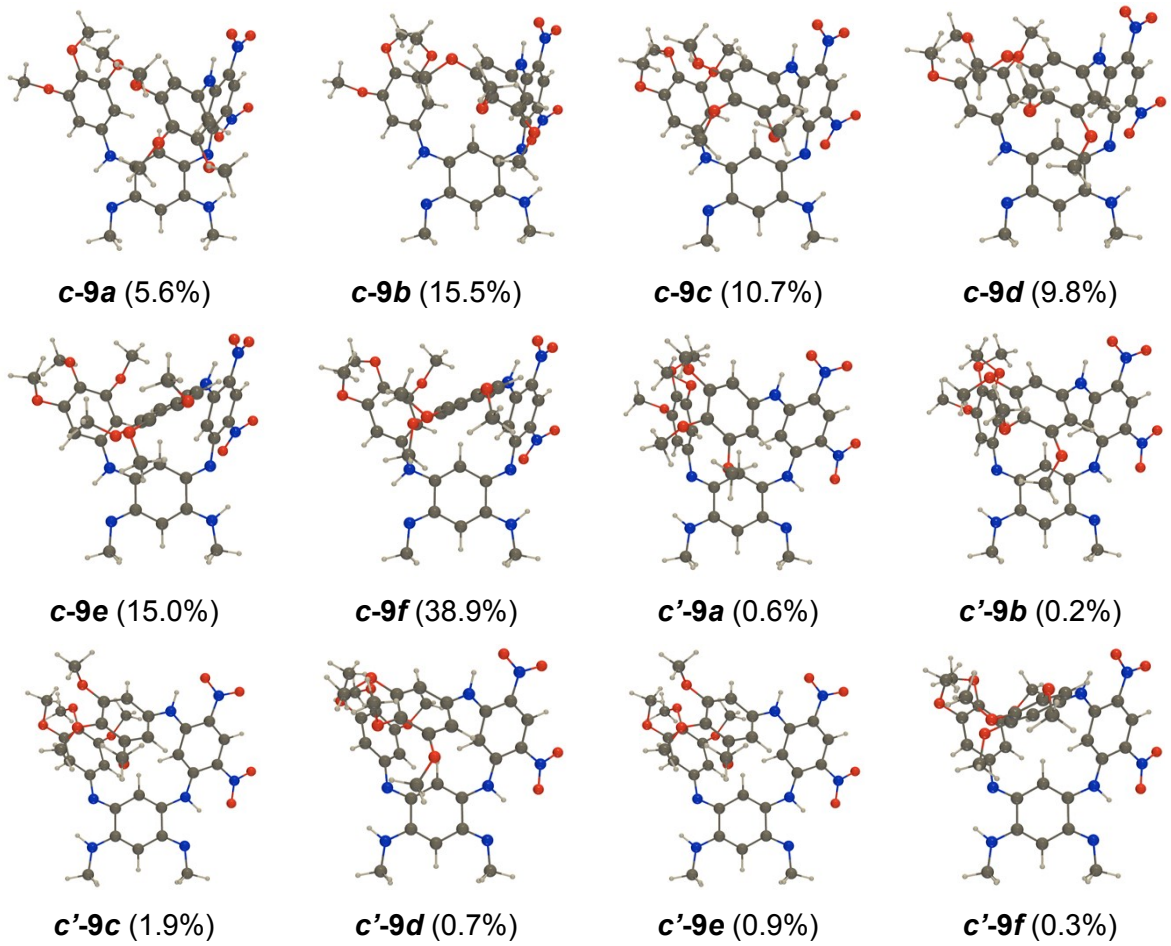


Figure S 13. Representation of the obtained (neutral) quinoidal structures and their relative computed percentage of presence at room temperature. Note that the given percentages do not account for the possible presence of ***z*-9** isomers.

We have also investigated the possible presence of zwitterionic isomers, considering the same six conformations depicted in **Figure S 12**. The most stable ***c*-9** structure has a conformation of type **e**. On the free energy scale this ***c*-9e** structure is found to be less stable by 1.3 kcal.mol^{-1} than ***c*-9*f***. The relative free energies determined for a zwitterionic and a canonical species are, of course, hard to evaluate with theory. In other words, this 1.3 kcal.mol^{-1} value should be interpreted as the fact that theory finds the ***z*-9** zwitterionic structures slightly (but only slightly) less stable than the ***c*-9** structures so that depending on the experimental conditions, such ***z*-9** zwitterion could be more or less accessible. Importantly, CAM-B3LYP predicts that the dipole moment of the zwitterionic structure is significantly larger than the one of the canonical form, which is already very polar (***z*-9e**: 17.7 D *versus* ***c*-9*f***: 12.8 D). The EDD of ***z*-9*d*** is represented in **Figure S 14** and is it logically located on the zwitterionic moiety with a clear CT character from the negatively charged cyanine to the single bonds and the positively charged cyanine, which is typical of such derivative.

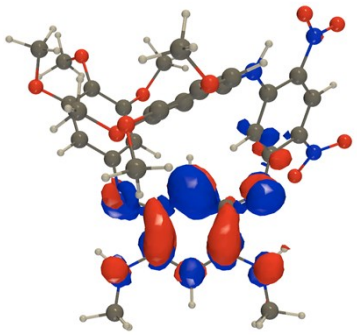
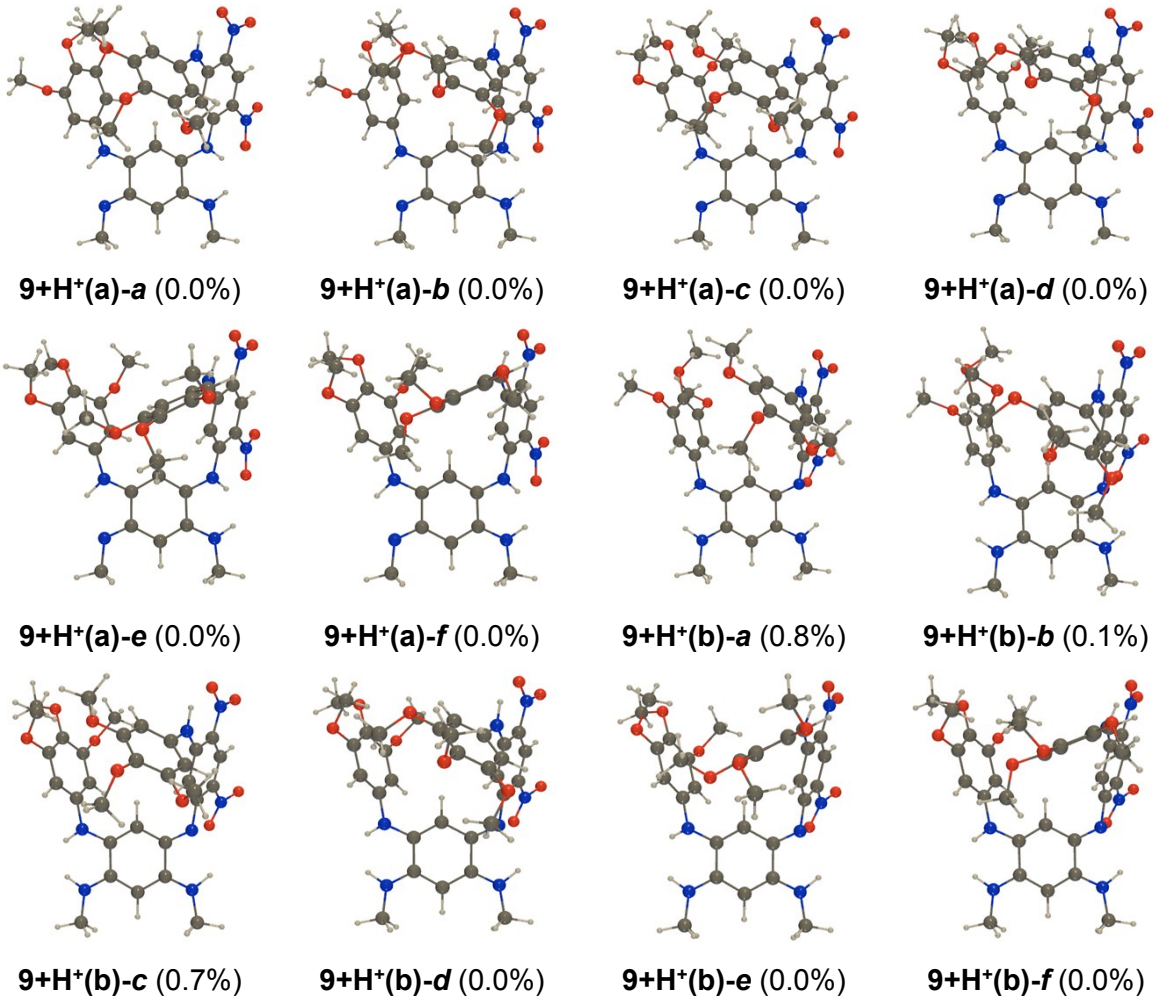


Figure S 14. Density difference plots (EDD) for the lowest vertical transitions in **9(z)-d**, located at 628 nm. The colour code and contour threshold are the same as for the Figure shown in the main text.

After mono-protonation, four possible tautomers can be envisaged (see **Figure S 12**). From our calculations, see **Figure S 15**, it is crystal-clear that the structures of form **9+H⁺(d)** are strongly favoured, all **9+H⁺(a)** and **9+H⁺(c)**conformers being less stable by more than 10 kcal.mol^{-1}, whereas the most stable **9+H⁺(b)** conformer, **9+H⁺(b)-a**, should still represent a tiny fraction of the mixture (< 1%).



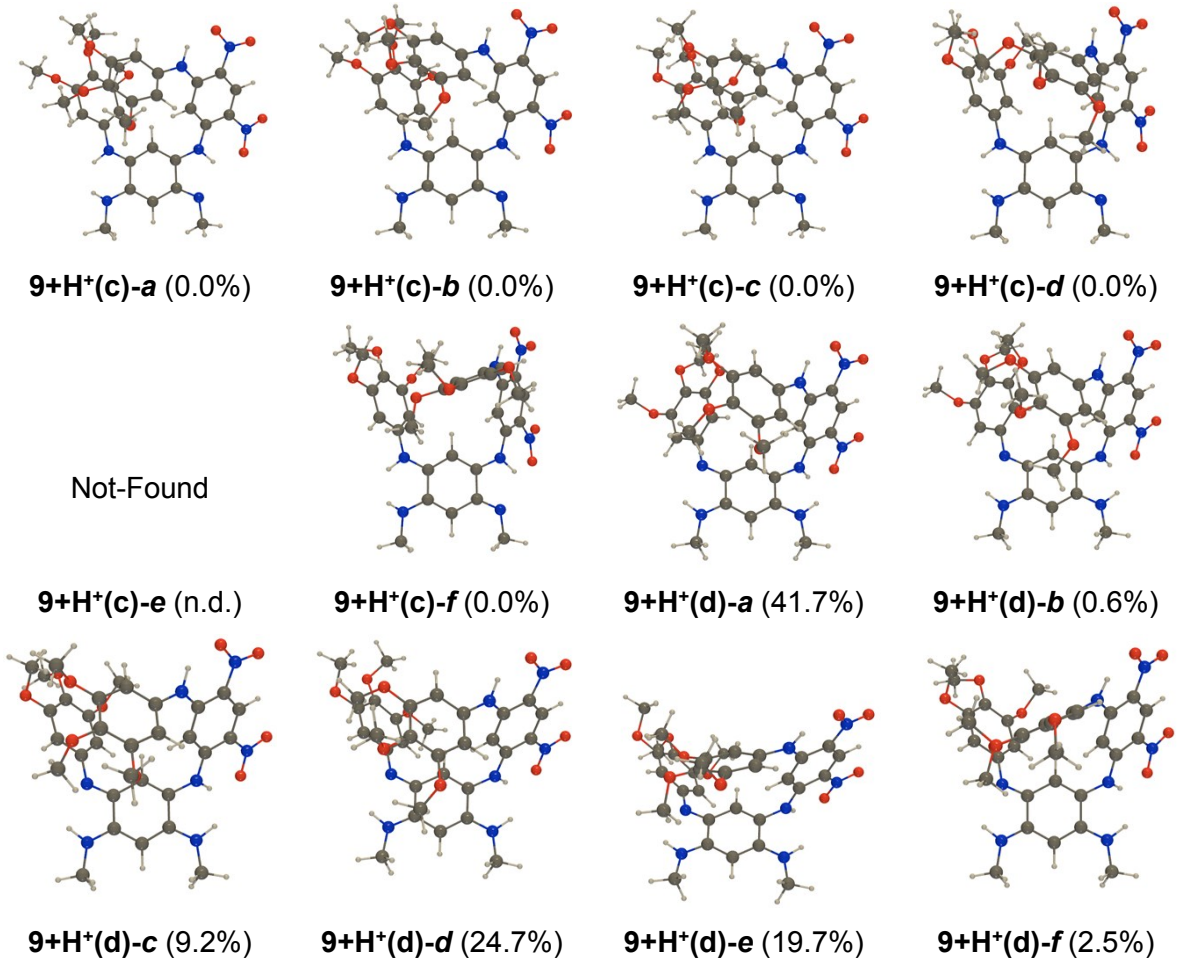


Figure S 15. Representation of the obtained mono-protonated species **9+H⁺**. See caption of Figure S 13 for more details.

For the most stable structure, namely, **9+H⁺(d)-*a***, TD-DFT returns ,for the lowest excited-state, a bright transition at 496 nm (*f* = 0.291). As compared to ***c*-9*f*** with 472 nm (*f* = 0.034) (*vide supra*), there is therefore a redshift, and more importantly a very large increase of intensity (hyperchromism). The density difference plots for the lowest transition of **9+H⁺(d)-*a***, is shown in **Figure S 16** and one can notice a CT character from the 3,4,5-trimethoxyphenyl towards the positively charged tetra-amino cycle.

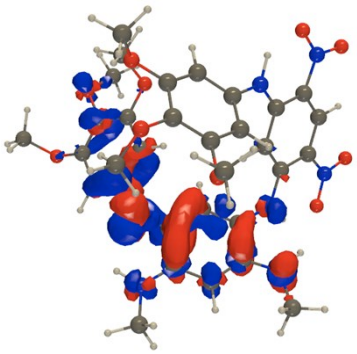


Figure S 16. Density difference plots (EDD) for the lowest vertical transitions in **9+H⁺(d)-a**, located at 496 nm. The colour code and contour threshold are the same as for the Figure shown in the main text.

Cartesian coordinates

c-9a

C	-1.6215100	2.9714610	-2.8013500
C	-0.5190900	3.8874800	-2.8363730
C	0.4094800	3.9319980	-1.8271010
C	0.2967620	3.0018040	-0.6641530
C	-0.8002990	2.0921970	-0.6155010
C	-1.7341380	2.0505370	-1.6203150
H	-0.4341050	4.5629420	-3.6785870
H	-0.9014550	1.4691460	0.2636340
N	-2.5609980	2.8518580	-3.6815460
N	1.4584240	4.7667800	-1.7955490
N	1.2109730	3.1403390	0.2485840
N	-2.8281650	1.2637600	-1.6662940
H	2.0334880	4.7110650	-0.9648010
H	-3.4159870	1.4978460	-2.4681840
C	-2.5482720	3.7038000	-4.8455370
H	-1.6334260	3.5723840	-5.4414660
H	-3.4034930	3.4625550	-5.4805020
H	-2.6140000	4.7679450	-4.5757850
C	1.7283100	5.7547900	-2.8055330
H	0.8986780	6.4675710	-2.8991540
H	2.6289420	6.3035980	-2.5301520
H	1.8904760	5.2863500	-3.7843060
C	-3.2654800	0.2628280	-0.7922430
C	-4.6458760	0.0927820	-0.6391570
C	-2.3864170	-0.6038060	-0.1348980
C	-5.1435780	-0.9036290	0.1939960
H	-5.3469440	0.7478680	-1.1473820
C	-2.8878650	-1.5992160	0.7004370
H	-1.3146290	-0.5554830	-0.2879870
C	-4.2694390	-1.7452580	0.8998080
C	1.4060270	2.2765820	1.2908670
C	1.7212200	0.9415560	1.0474730
C	1.4718590	2.7276440	2.6442700
C	2.0965030	0.0282680	2.0504440
H	1.6891150	0.6013490	0.0199390
C	1.8304160	1.8634300	3.6561160
C	2.1291370	0.5315070	3.3947320
H	1.8640100	2.2192680	4.6780330
O	-1.9971690	-2.3921470	1.3677650
O	-4.7696920	-2.6955670	1.7453310
O	-6.4939970	-0.9816040	0.3778490
C	-2.0209790	-3.7738650	1.0023020
H	-1.2934520	-4.2710770	1.6454620
H	-3.0116410	-4.2078840	1.1629600
H	-1.7228350	-3.8937080	-0.0454670
C	-7.1075370	-2.1709430	-0.1211690
H	-8.1715830	-2.0802460	0.1017500
H	-6.9674530	-2.2439060	-1.2060330
H	-6.7009330	-3.0592570	0.3698470
C	-4.6671360	-2.3519810	3.1293650
H	-5.0981840	-3.1859480	3.6853120
H	-3.6203330	-2.2165410	3.4199910
H	-5.2336660	-1.4382920	3.3399320
N	1.1307820	4.0768360	3.0180290
O	1.5355030	4.4943120	4.1022890
O	0.4464090	4.7416340	2.2493870
N	2.4591890	-0.2797160	4.5252730
O	2.5535520	0.2466210	5.6291520
O	2.6396410	-1.4947890	4.3575360
N	2.4015860	-1.2556180	1.7585910
H	2.5167060	-1.8567940	2.5685920
C	2.5259920	-1.8377380	0.4783990
C	3.3155490	-1.2556120	-0.5153200
C	1.9089310	-3.0676020	0.2489440
C	3.4451700	-1.8808470	-1.7522800
H	3.8562310	-0.3314480	-0.3403120
C	2.0437030	-3.6965810	-0.9868200
H	1.3021300	-3.5380690	1.0159700
C	2.7881560	-3.0950120	-2.0133890
O	4.1778260	-1.2552440	-2.7198730
O	2.8818940	-3.7058840	-3.2307000
O	1.3608930	-4.8577410	-1.2013560
C	5.3687660	-1.9371390	-3.1217670
H	5.1391060	-2.9224760	-3.5365440
H	5.8316270	-1.3119120	-3.8862460
H	6.0516650	-2.0391510	-2.2708070
C	2.1733080	-6.0160740	-1.4021460
H	1.4832940	-6.8472160	-1.5539220
H	2.8126730	-5.9002900	-2.2813550
H	2.7858910	-6.2082530	-0.5136880
C	2.0943640	-3.0921250	-4.2550120
H	2.4076660	-2.0562490	-4.4191770
H	2.2628000	-3.6761070	-5.1608540
H	1.0319850	-3.1234130	-3.9898950

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C	-1.3269570	2.9130160	-2.9473920
C	-0.2172690	3.8201040	-2.8944790
C	0.6189910	3.8699560	-1.8076060
C	0.3967840	2.9530990	-0.6503460
C	-0.7097550	2.0535530	-0.6891260
C	-1.5517660	2.0071450	-1.7710450
H	-0.0533930	4.4864280	-3.7323180
H	-0.8926960	1.4417130	0.1844610
N	-2.1862360	2.7913410	-3.9057380
N	1.6682070	4.6971740	-1.6925280
N	1.2293540	3.0882490	0.3374420
N	-2.6450680	1.2279990	-1.9031190
H	2.1658370	4.6488490	-0.8128070
H	-3.1609320	1.4576710	-2.7540080
C	-2.0630600	3.6301170	-5.0729660
H	-1.0992080	3.4871660	-5.5827270
H	-2.8592470	3.3866880	-5.7797900
H	-2.1460430	4.6975090	-4.8214560
C	2.0338700	5.6722130	-2.6849240
H	1.2238610	6.3934730	-2.8545980
H	2.9149260	6.2132040	-2.3397010
H	2.2719770	5.1922060	-3.6423570
C	-3.1725290	0.2530760	-1.0497530
C	-4.5634690	0.1049520	-1.0144980
C	-2.3681740	-0.6090500	-0.2978430
C	-5.1467630	-0.8617440	-0.2023080
H	-5.2073250	0.7562510	-1.5976690
C	-2.9550970	-1.5749990	0.5168560
H	-1.2865260	-0.5794140	-0.3575450
C	-4.3510430	-1.6949960	0.6001830
C	1.3064940	2.2263440	1.3985900
C	1.6496770	0.8933400	1.1890080
C	1.2088620	2.6717640	2.7516050
C	1.8925540	-0.0278330	2.2252660
H	1.7454760	0.5579140	0.1636800
C	1.4332030	1.7991820	3.7952010
C	1.7543820	0.4669240	3.5653330
H	1.3411160	2.1494620	4.8154480
O	-2.1318510	-2.3560340	1.2777210
O	-4.9408250	-2.6078930	1.4293410
O	-6.5089060	-0.9156780	-0.1339420
C	-2.1793360	-3.7570100	0.9996530
H	-1.4738710	-4.2260640	1.6869980
H	-3.1814450	-4.1611300	1.1653360
H	-1.8652570	-3.9491650	-0.0327590
C	-7.0966870	-2.1128570	-0.6451330
H	-8.1743540	-1.9997420	-0.5190060
H	-6.8643440	-2.2247260	-1.7106810
H	-6.7492570	-2.9893230	-0.0914440
C	-4.9519030	-2.2177150	2.8048500
H	-5.4499040	-3.0222120	3.3480990
H	-3.9317010	-2.0938100	3.1825530
H	-5.5123430	-1.2853560	2.9336060
N	0.8347230	4.0218940	3.0885310
O	1.0899850	4.4244350	4.2227590
O	0.2726830	4.7029990	2.2391840
N	1.9332610	-0.3546450	4.7225560
O	1.8872840	0.1627570	5.8335380
O	2.1279850	-1.5689030	4.5682230
N	2.2282290	-1.3093040	1.9603640
H	2.2409250	-1.9232970	2.7686950
C	2.5309910	-1.8624380	0.6951240
C	1.8882530	-3.0386290	0.3105080
C	3.4898870	-1.2828800	-0.1374640
C	2.2080110	-3.6436290	-0.9030190
H	1.1283040	-3.4895260	0.9404050
C	3.8061080	-1.8844500	-1.3527320
H	4.0240260	-0.3849660	0.1554620
C	3.1856790	-3.0830770	-1.7407470
O	1.5935440	-4.8203810	-1.2210960
O	3.5322800	-3.6697640	-2.9235500
O	4.8002810	-1.3377150	-2.1107300
C	0.7544750	-4.7819070	-2.3782360
H	1.3275010	-4.5313270	-3.2750460
H	0.3296720	-5.7816400	-2.4762700
H	-0.0527760	-4.0542190	-2.2365670
C	4.3743880	-0.7755760	-3.3531500
H	5.2733240	-0.3905850	-3.8364740
H	3.9089370	-1.5343740	-3.9882180
H	3.6733870	0.0487640	-3.1768370
C	4.3632700	-4.8256410	-2.7821360
H	3.8519700	-5.6053000	-2.2086530
H	4.5637250	-5.1830660	-3.7930540
H	5.3062770	-4.5597040	-2.2925540

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C	-1.6227350	-4.0209520	0.3947750
C	-2.9080900	-3.9066270	-0.2304530
C	-3.5176490	-2.6885790	-0.4015300
C	-2.8276830	-1.4368900	0.0340470
C	-1.5832140	-1.5471500	0.7168280
C	-0.9771140	-2.7650160	0.9019720
H	-3.4013240	-4.8093620	-0.5688540
H	-1.1045930	-0.6376570	1.0552590
N	-0.9388260	-5.1025290	0.5798830
N	-4.7206060	-2.5137030	-0.9669000
N	-3.4652150	-0.3327580	-0.2295800
N	0.2178180	-2.9744460	1.4891450
H	-5.0435780	-1.5556330	-1.0123950
H	0.5117750	-3.9484580	1.4053330
C	-1.4769410	-6.3607900	0.1235250
H	-1.6661710	-6.3592190	-0.9599030
H	-0.7657720	-7.1601360	0.3427770
H	-2.4264610	-6.6048220	0.6216830
C	-5.5408210	-3.5880340	-1.4586410
H	-5.7905650	-4.2963510	-0.6582900
H	-6.4668480	-3.1718990	-1.8554470
H	-5.0340770	-4.1406560	-2.2600530
C	1.1012820	-2.0473860	2.0604940
C	2.4694150	-2.2045880	1.8208790
C	0.6554280	-1.0037790	2.8761940
C	3.3893220	-1.3327310	2.3969360
H	2.8334900	-3.0019470	1.1802250
C	1.5755960	-0.1219450	3.4365340
H	-0.3936330	-0.8795530	3.1193890
C	2.9529830	-0.2843150	3.2224950
C	-2.9403250	0.9204630	-0.0788030
C	-1.7371340	1.2746370	-0.6858440
C	-3.6776820	1.9639310	0.5616230
C	-1.2057530	2.5778790	-0.6771540
H	-1.1855480	0.4955700	-1.1970750
C	-3.2025710	3.2568540	0.5745660
C	-1.9847570	3.5833540	-0.0120290
H	-3.7719410	4.0327520	1.0705070
O	1.1153170	0.8547690	4.2749730
O	3.8585120	0.5646980	3.7942840
O	4.7178550	-1.5607490	2.1866950
C	1.2375470	2.1849570	3.7684440
H	0.8424260	2.8439780	4.5427420
H	2.2835250	2.4346020	3.5676420
H	0.6431030	2.2997950	2.8541730
C	5.4037340	-0.5483810	1.4439810
H	6.4306540	-0.9004160	1.3343350
H	4.9493690	-0.4254530	0.4542850
H	5.3946280	0.4042340	1.9806260
C	4.1376680	0.2748650	5.1662150
H	4.8653180	1.0182630	5.4953570
H	3.2292460	0.3541480	5.7720330
H	4.5666790	-0.7282080	5.2663800
N	-4.9178550	1.7118410	1.2517050
O	-5.6819250	2.6601770	1.4264480
O	-5.1492050	0.5744670	1.6436420
N	-1.5681960	4.9459100	0.1013680
O	-2.3262790	5.7602720	0.6181510
O	-0.4486200	5.2666350	-0.3246190
N	-0.0160700	2.8544640	-1.2554910
H	0.3337190	3.7918590	-1.0837240
C	0.8018710	1.9510090	-1.9744250
C	0.3160330	1.2741140	-3.0939500
C	2.1326740	1.8003180	-1.5863860
C	1.1512680	0.4115220	-3.7986830
H	-0.7016760	1.4183550	-3.4419180
C	2.9710970	0.9423860	-2.2955780
H	2.5254190	2.3253240	-0.7212950
C	2.4817760	0.2152900	-3.3917290
O	0.6286840	-0.2806700	-4.8529380
O	3.3063120	-0.6465530	-4.0554840
O	4.2445170	0.7557600	-1.8430060
C	1.1770280	0.0474290	-6.1322890
H	2.2505610	-0.1576120	-6.1662990
H	0.6563150	-0.5822790	-6.8546930
H	0.9896070	1.1017600	-6.3649180
C	5.2752000	1.2368100	-2.7080970
H	6.2190640	1.0119930	-2.2093330
H	5.2404590	0.7340240	-3.6783480
H	5.1827700	2.3207550	-2.8422080
C	3.0581000	-2.0266170	-3.7724350
H	2.0394660	-2.3058180	-4.0597950
H	3.7769220	-2.5939930	-4.3651300
H	3.2156590	-2.2320710	-2.7080260

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C	1.2970120	-1.8090800	3.6967670
C	2.6554540	-1.3549670	3.7677120
C	3.3270040	-0.9215550	2.6518950
C	2.6294390	-0.8693820	1.3322350
C	1.2971240	-1.3686130	1.2420850
C	0.6350070	-1.8359560	2.3494090
H	3.1554040	-1.3669000	4.7283330
H	0.8124590	-1.3446120	0.2750310
N	0.5587790	-2.2124850	4.6785170
N	4.6009250	-0.5037390	2.6452030
N	3.3339820	-0.3923960	0.3495770
N	-0.6251260	-2.3150080	2.3859420
H	4.9632580	-0.2274570	1.7416710
H	-0.9255300	-2.4918670	3.3460080
C	1.1055960	-2.2211730	6.0133800
H	1.4403190	-1.2222560	6.3290850
H	0.3415970	-2.5612270	6.7158070
H	1.9684760	-2.8977570	6.0968090
C	5.4433660	-0.4756090	3.8107950
H	5.5536690	-1.4770820	4.2461010
H	6.4297890	-0.1106660	3.5243450
H	5.0345210	0.1904310	4.5812090
C	-1.5367830	-2.5447840	1.3492940
C	-2.8955970	-2.3485520	1.6190360
C	-1.1425610	-2.9991000	0.0870430
C	-3.8528720	-2.6130830	0.6444250
H	-3.2232900	-1.9901890	2.5901930
C	-2.1015460	-3.2437060	-0.8924790
H	-0.1063590	-3.2134770	-0.1456740
C	-3.4680800	-3.0723760	-0.6252080
C	2.8359240	-0.1067580	-0.8925170
C	1.8108560	0.8230060	-1.0472460

C	3.4448400	-0.6120130	-2.0817900
C	1.3393830	1.2719280	-2.2956480
H	1.3612660	1.2262940	-0.1482690
C	3.0160640	-0.1941240	-3.3229690
C	1.9746710	0.7168300	-3.4569120
H	3.4817070	-0.5955700	-4.2141380
O	-1.6892410	-3.7436990	-2.0960340
O	-4.4112780	-3.3355360	-1.5784060
O	-5.1703610	-2.4775220	0.9752340
C	-1.8298910	-2.8451900	-3.1977120
H	-1.4819780	-3.3858390	-4.0789580
H	-2.8743740	-2.5495620	-3.3331770
H	-1.2057340	-1.9565040	-3.0457460
C	-5.8722480	-1.4429240	0.2846350
H	-6.8969970	-1.4703620	0.6577190
H	-5.4282530	-0.4665060	0.5118290
H	-5.8659770	-1.6151750	-0.7949150
C	-4.7217560	-4.7242000	-1.7190530
H	-5.4762520	-4.7921530	-2.5042400
H	-3.8328750	-5.2925450	-2.0111340
H	-5.1287370	-5.1227200	-0.7832510
N	4.4931560	-1.6003660	-2.0446210
O	5.2076070	-1.7194620	-3.0389860
O	4.6186380	-2.2827780	-1.0348180
N	1.5875040	1.0496180	-4.7928170
O	2.2335450	0.5952290	-5.7310760
O	0.6057280	1.7868980	-4.9645080
N	0.3323910	2.1679570	-2.3850140
H	-0.0161950	2.3256350	-3.3254730
C	-0.2868520	2.8563810	-1.3157350
C	-1.6773620	2.8209840	-1.2157880
C	0.4636800	3.5999110	-0.4038390
C	-2.3210760	3.5347020	-0.2076030
H	-2.2721810	2.2338490	-1.9083050
C	-0.1794030	4.3086240	0.6078530
H	1.5439090	3.6655740	-0.4828540
C	-1.5801720	4.3012440	0.7062220
O	-3.6857690	3.5177800	-0.1676690
O	-2.1916370	5.0200860	1.6919780
O	0.5736110	5.0848930	1.4396700
C	-4.2523570	2.8734360	0.9758310
H	-3.9494190	3.3716060	1.9010500
H	-5.3344220	2.9402180	0.8561050
H	-3.9516680	1.8197180	1.0034560
C	0.6240320	4.6445220	2.7978480
H	1.2512630	5.3631120	3.3270710
H	-0.3749360	4.6274770	3.2422680
H	1.0792920	3.6489610	2.8579070
C	-2.8192880	6.2228760	1.2378800
H	-3.6039390	6.0009100	0.5078400
H	-3.2581250	6.6899800	2.1205460
H	-2.0773610	6.8967100	0.7960930

c-9e

C	-2.1583820	1.7704450	3.3173490
C	-3.0394490	0.7100490	3.7121440
C	-3.3461370	-0.3230650	2.8625170
C	-2.7184950	-0.3885600	1.5094200
C	-1.8762240	0.6833490	1.0917120
C	-1.6024570	1.7405060	1.9225410
H	-3.4722750	0.7400980	4.7043780
H	-1.4462080	0.6288660	0.1004970
N	-1.7832340	2.7778350	4.0354520
N	-4.1758140	-1.3331850	3.1608570
N	-3.0329790	-1.4291990	0.7973760
N	-0.8278130	2.8070720	1.6382720
H	-4.3101090	-2.0176910	2.4279020
H	-0.6938110	3.3931850	2.4643480
C	-2.2635130	2.8946420	5.3906270
H	-1.9873330	2.0236700	6.0026480
H	-1.8316020	3.7849940	5.8526850
H	-3.3584780	2.9890080	5.4294250
C	-4.8729120	-1.4565510	4.4130190
H	-5.5269890	-0.5933470	4.5908310
H	-5.4857970	-2.3576050	4.3885130
H	-4.1709850	-1.5342090	5.2529750
C	-0.2121530	3.1959040	0.4444780
C	0.9846870	3.9159100	0.5344270
C	-0.7678530	2.9386500	-0.8129270
C	1.6132060	4.3870830	-0.6139440
H	1.4378610	4.1213000	1.4995650
C	-0.1251710	3.3937760	-1.9613460
H	-1.7193010	2.4336200	-0.9267990
C	1.0609870	4.1381580	-1.8806450
C	-2.4325980	-1.7537030	-0.3894140
C	-1.0771220	-2.0707160	-0.4253130
C	-3.1845760	-1.9611620	-1.5853380
C	-0.4191310	-2.5736400	-1.5639420
H	-0.5163380	-1.9684380	0.4957660
C	-2.5850210	-2.4808300	-2.7119080
C	-1.2297460	-2.7888830	-2.7293350
H	-3.1728440	-2.6403870	-3.6069980
O	-0.7266660	3.1796030	-3.1702800
O	1.6758090	4.6094380	-3.0068310
O	2.7342010	5.1528550	-0.4703040
C	-0.0453880	2.2584180	-4.0232830
H	-0.6284900	2.2059510	-4.9437340
H	0.9681150	2.6045270	-4.2462320
H	-0.0083240	1.2658160	-3.5587360
C	3.9364500	4.5946450	-1.0021120
H	4.7212450	5.3276110	-0.8099070
H	4.1798950	3.6581310	-0.4870330
H	3.8481230	4.4190610	-2.0773980
C	1.0840480	5.7987690	-3.5355110
H	1.6645590	6.0634940	-4.4206140
H	0.0414430	5.6205260	-3.8176740
H	1.1387410	6.6121860	-2.8036880
N	-4.5824410	-1.6227960	-1.6758440
O	-5.2476570	-2.1514820	-2.5651490
O	-5.0405580	-0.8173980	-0.8743220
N	-0.7119390	-3.3090300	-3.9569970
O	-1.4488050	-3.3720480	-4.9353690
O	0.4692260	-3.6837590	-3.9968330
N	0.9018280	-2.8582380	-1.5481240
H	1.2380950	-3.3478960	-2.3716440
C	1.8259420	-2.5946880	-0.5146420
C	2.7279990	-3.6018740	-0.1685390
C	1.9101610	-1.3414580	0.0949100
C	3.6935030	-3.3670850	0.8065930
H	2.6859460	-4.5768610	-0.6438170
C	2.8582990	-1.1158210	1.0901740
H	1.2590170	-0.5234100	-0.1944910
C	3.7470100	-2.1327970	1.4744720
O	4.5228430	-4.3924410	1.1596600
O	4.6567640	-1.9024960	2.4661220
O	2.8567630	0.0950220	1.7174200
C	5.9053230	-4.1879610	0.8573510
H	6.2980340	-3.3111450	1.3797250
H	6.4251170	-5.0848140	1.1965070
H	6.0433860	-4.0728120	-0.2236860
C	4.0285900	0.8891270	1.5251230
H	3.8513670	1.8235330	2.0594940
H	4.9135590	0.3912900	1.9300500
H	4.1715630	1.0999100	0.4588090
C	4.3329560	-2.5250810	3.7127370
H	4.2846070	-3.6130660	3.6034170
H	5.1339780	-2.2592220	4.4038590
H	3.3786080	-2.1447620	4.0928330

c-9f

C	-1.1652060	-2.9129420	-2.9605830
C	-2.4173010	-2.3962980	-3.4319870
C	-3.1471310	-1.4974570	-2.6947010
C	-2.6190750	-0.9965670	-1.3906570
C	-1.4010730	-1.5424340	-0.8908550
C	-0.6899990	-2.4733320	-1.6059550
H	-2.7890530	-2.7361250	-4.3906750
H	-1.0471570	-1.1929790	0.0700680
N	-0.3807770	-3.7360160	-3.5760920
N	-4.3310370	-0.9909460	-3.0677940
N	-3.3579600	-0.1099340	-0.7924500
N	0.4681290	-3.0539140	-1.2328570
H	-4.7549150	-0.3466020	-2.4127120
H	0.8569280	-3.6234740	-1.9861330
C	-0.7510740	-4.2158460	-4.8852090
H	-0.8809520	-3.3941320	-5.6045860
H	0.0310960	-4.8776660	-5.2632990
H	-1.6930410	-4.7827720	-4.8612430
C	-5.0065980	-1.3426010	-4.2881250
H	-5.2170600	-2.4189250	-4.3302650
H	-5.9516330	-0.8016150	-4.3365740
H	-4.4056750	-1.0755430	-5.1667050
C	1.1935450	-2.9325060	-0.0410870
C	2.5898240	-2.9629870	-0.1176160
C	0.5725700	-2.8219510	1.2064260
C	3.3583540	-2.8798450	1.0383030
H	3.0936590	-3.0352530	-1.0766370
C	1.3452190	-2.7357300	2.3624820
H	-0.5054720	-2.8527530	1.3117760
C	2.7454910	-2.7754390	2.2973730
C	-2.9656730	0.5887740	0.3177180
C	-1.8595090	1.4326980	0.2645520
C	-3.7632120	0.6309510	1.5016230
C	-1.4909420	2.3097700	1.3028950
H	-1.2824520	1.4441960	-0.6522550
C	-3.4568780	1.5000670	2.5259710
C	-2.3476190	2.3348410	2.4544660
H	-4.0793360	1.5262560	3.4114690
O	0.7057620	-2.7024780	3.5690430
O	3.4873890	-2.6992930	3.4423170
O	4.7177940	-2.9589220	0.9263440
C	0.8121540	-1.4644120	4.2726050
H	0.2662320	-1.5968850	5.2077770
H	1.8572650	-1.2222060	4.4852420
H	0.3500780	-0.6561870	3.6928710
C	5.4208730	-1.7581490	1.2537150
H	6.4802660	-1.9801960	1.1181840
H	5.1266490	-0.9495800	0.5747000
H	5.2335810	-1.4624540	2.2899070
C	3.9802790	-3.9611490	3.8988570
H	4.5489230	-3.7583010	4.8076500
H	3.1492760	-4.6369230	4.1288700
H	4.6345080	-4.4167380	3.1483800
N	-4.8988270	-0.2366230	1.6872810
O	-5.7465020	0.0920060	2.5157330
O	-4.9617720	-1.2650730	1.0242830
N	-2.1179250	3.1864000	3.5804440
O	-2.8413710	3.0802810	4.5651220
O	-1.1934770	4.0106970	3.5277860
N	-0.3990710	3.0989990	1.2023610
H	-0.3056120	3.7917570	1.9387980
C	0.5799990	3.0754650	0.1846090
C	1.1983110	1.8860810	-0.2066010
C	0.9638590	4.2869840	-0.3907310
C	2.1917870	1.9135350	-1.1814100
H	0.9409770	0.9355980	0.2492920
C	1.9756120	4.3164570	-1.3480890
H	0.4853030	5.2171050	-0.1009020
C	2.6069390	3.1289880	-1.7489850
O	2.8209210	0.7472350	-1.5122310
O	3.5975700	3.1633460	-2.6875020
O	2.3762810	5.5260840	-1.8340530
C	2.5273370	0.2621520	-2.8240720
H	2.8095550	0.9948640	-3.5859160
H	3.1156540	-0.6475190	-2.9518310
H	1.4612420	0.0218160	-2.9105370
C	2.1033580	5.7513260	-3.2186610
H	2.4816630	6.7494810	-3.4430950
H	2.6112230	5.0129060	-3.8447230
H	1.0230330	5.7210700	-3.4016910
C	4.9175130	3.0632190	-2.1457470
H	5.0467860	2.1159360	-1.6127220
H	5.6008390	3.1042650	-2.9951110
H	5.1187050	3.9027560	-1.4715010

c'-9a

C	1.6866830	3.6245270	-1.8344800
C	2.9678490	3.2266300	-2.1228640
C	3.5786390	2.1171090	-1.4497460
C	2.7452140	1.3514680	-0.4760570
C	1.4846590	1.7518030	-0.1627620
C	0.9049340	2.9282700	-0.7693880
H	3.5464030	3.7635190	-2.8645370
H	0.9191500	1.2546110	0.6161930
N	1.0524410	4.6420180	-2.4372660
N	4.7953000	1.6965660	-1.5809440
N	3.4253830	0.3097690	0.1110630
N	-0.2073970	3.4984310	-0.4388640
C	1.6592040	5.4906780	-3.4275270
H	1.9713810	4.9107160	-4.3046170
H	0.9303230	6.2352210	-3.7485340
H	2.5405990	6.0111610	-3.0294230
C	5.6831900	2.3930160	-2.4796260
H	5.7997600	3.4520170	-2.2066040
H	6.6690310	1.9241130	-2.4494000
H	5.3227740	2.3600340	-3.5181940
C	-1.0852500	2.9938210	0.5233670
C	-1.4888440	3.8594170	1.5486180
C	-1.6590460	1.7179740	0.4393460
C	-2.3956360	3.4371620	2.5146190
H	-1.0780920	4.8620590	1.6086900
C	-2.5959880	1.3104640	1.3867620
H	-1.4147470	1.0446080	-0.3766650
C	-2.9521450	2.1495020	2.4535370
C	2.9588530	-0.8392190	0.6781560
C	1.6779460	-1.3237800	0.4142720
C	3.7847620	-1.6158910	1.5598250
C	1.1708230	-2.5218360	0.9429940
H	1.0554030	-0.7673780	-0.2723840
C	3.2717600	-2.7402660	2.1753900
C	1.9925110	-3.1990690	1.9098910
H	3.8910730	-3.2867410	2.8750410
O	-3.1146510	0.0495050	1.2936680
O	-3.8490170	1.7450910	3.4029800
O	-2.6867610	4.2782210	3.5516410
C	-4.5024580	-0.0022550	0.9579010
H	-4.7522390	-1.0584040	0.8522820
H	-5.1137760	0.4558440	1.7412670
H	-4.6803780	0.5046960	0.0021330
C	-4.0248530	4.7757400	3.5710040
H	-4.0961230	5.4243110	4.4454560
H	-4.2259520	5.3612590	2.6660660
H	-4.7471260	3.9591030	3.6564330
C	-3.3011300	0.8520190	4.3746540
H	-4.1130120	0.6098380	5.0622610
H	-2.9355520	-0.0635090	3.8984290
H	-2.4870260	1.3369070	4.9247970
N	5.1425990	-1.2769840	1.8759360
O	5.6812740	-1.8300550	2.8295260
O	5.7252560	-0.4511990	1.1675600
N	1.5826480	-4.3796250	2.6061820
O	2.3826040	-4.9438960	3.3443930
O	0.4251510	-4.7950170	2.4483240
N	-0.0247630	-3.0256750	0.5635090
H	-0.3425910	-3.8023870	1.1364400
C	-0.8249780	-2.6842560	-0.5424650
C	-0.2896170	-2.2855860	-1.7701630
C	-2.2038200	-2.8662950	-0.4140660
C	-1.1374000	-2.0174990	-2.8416770
H	0.7793730	-2.2116920	-1.9341200
C	-3.0483860	-2.6105100	-1.4895040
H	-2.6376770	-3.1871490	0.5276510
C	-2.5288870	-2.1474870	-2.7085240
O	-0.5810920	-1.5717460	-4.0065940
O	-3.3716770	-1.8586030	-3.7439070
O	-4.3941100	-2.7327200	-1.3003380
C	-0.7150710	-2.4533780	-5.1242610
H	-1.7671980	-2.6303460	-5.3637700
H	-0.2225980	-1.9571760	-5.9614930
H	-0.2127790	-3.4052290	-4.9175940
C	-5.0244680	-3.7657960	-2.0601330
H	-6.0825800	-3.7329140	-1.7966910
H	-4.9045620	-3.5939860	-3.1331680

H	-4.6110440	-4.7435960	-1.7870670
C	-3.5803990	-0.4590710	-3.9498920
H	-2.6370840	0.0448540	-4.1840220
H	-4.2636430	-0.3724610	-4.7959960
H	-4.0353640	-0.0055120	-3.0623590
H	0.1476500	4.8717780	-2.0451700
H	4.4369900	0.3792520	-0.0198840

c'-9b

C	0.4418320	-2.8687810	3.0090430
C	1.8066070	-2.9183980	3.1485570
C	2.6872080	-2.4822210	2.1015990
C	2.0673000	-1.8853760	0.8845800
C	0.7190080	-1.8726480	0.7168400
C	-0.1647930	-2.4104960	1.7234950
H	2.2417540	-3.3073580	4.0610230
H	0.2793500	-1.5264650	-0.2108910
N	-0.4343670	-3.2388330	3.9562580
N	3.9792440	-2.5496630	2.0842330
N	2.9804490	-1.4583080	-0.0525500
N	-1.4376790	-2.6060530	1.6054790
C	-0.0517990	-3.8015420	5.2237620
H	0.5711250	-3.1004380	5.7923440
H	-0.9513040	-4.0105590	5.8030920
H	0.5109920	-4.7364870	5.0990310
C	4.6626800	-3.1375790	3.2107580
H	4.3439930	-4.1744030	3.3922850
H	5.7379430	-3.1410500	3.0198280
H	4.4841320	-2.5728320	4.1374890
C	-2.1639730	-2.2716100	0.4573710
C	-2.9056370	-3.2927710	-0.1506920
C	-2.2596710	-0.9657660	-0.0418120
C	-3.6642680	-3.0337920	-1.2865470
H	-2.8699580	-4.3025190	0.2450030
C	-3.0500120	-0.7003320	-1.1603310
H	-1.7472010	-0.1395460	0.4416050
C	-3.7296310	-1.7365060	-1.8198200
C	2.8410480	-0.4782010	-0.9941120
C	1.8816950	0.5207670	-0.8567880
C	3.6815180	-0.4228120	-2.1557400
C	1.6911390	1.5590830	-1.7813920
H	1.2719690	0.5234030	0.0369420
C	3.4528170	0.5313190	-3.1286460
C	2.4715010	1.4992560	-2.9853010
H	4.0639110	0.5304900	-4.0223610
O	-3.0792090	0.5784740	-1.6424640
O	-4.4647740	-1.5011760	-2.9490730
O	-4.2873680	-4.0783310	-1.9089260
C	-4.3622590	1.2072960	-1.6466260
H	-4.2014100	2.2223050	-2.0129280
H	-5.0603410	0.6815060	-2.3032240
H	-4.7683940	1.2487180	-0.6295950
C	-5.7141110	-4.0468100	-1.8652120
H	-6.0547120	-4.9375300	-2.3952600
H	-6.0635440	-4.0852620	-0.8266790
H	-6.1034740	-3.1517880	-2.3582840
C	-3.6762360	-1.3601150	-4.1327020
H	-4.3772240	-1.1839110	-4.9500720
H	-2.9907650	-0.5106310	-4.0452110
H	-3.1089900	-2.2770520	-4.3268620
N	4.7590490	-1.3395970	-2.3893540
O	5.2543030	-1.3951370	-3.5105160
O	5.1572690	-2.0302940	-1.4474340
N	2.3286630	2.4363580	-4.0558490
O	3.1010130	2.3778760	-5.0065120
O	1.4204150	3.2764100	-3.9913520
N	0.8208870	2.5610260	-1.5285670
H	0.6368160	3.1801130	-2.3113540
C	0.2638330	2.8853170	-0.2691830
C	-1.0989560	3.1642980	-0.1872210
C	1.0700220	2.9823340	0.8672380
C	-1.6588080	3.5550890	1.0280220
H	-1.7417500	3.0590260	-1.0545060
C	0.5107490	3.3681430	2.0814380
H	2.1376130	2.7941900	0.8208220
C	-0.8551000	3.6830470	2.1724010
O	-2.9879470	3.8646970	1.0526540
O	-1.3713020	4.0930890	3.3679030
O	1.3348590	3.5305320	3.1571000
C	-3.7981300	3.0565250	1.9098540
H	-3.5171940	3.1828340	2.9586860
H	-4.8247630	3.3913250	1.7563710
H	-3.7118720	2.0010890	1.6279020
C	1.1405080	2.5895050	4.2140600
H	1.8617450	2.8501460	4.9898510
H	0.1254330	2.6548000	4.6157870
H	1.3396780	1.5715970	3.8584610
C	-1.6459260	5.4953650	3.4356290
H	-2.3883180	5.7842480	2.6847210
H	-2.0410030	5.6812810	4.4352650
H	-0.7257820	6.0715630	3.2909310
H	-1.4026240	-3.2493850	3.6602190
H	3.9114550	-1.8545860	0.0758480

c'-9c

C	-1.2680230	4.1291890	0.6526190
C	-2.5986550	4.0308810	0.9751460
C	-3.3509080	2.8384810	0.7111350
C	-2.6176330	1.6631960	0.1516950
C	-1.3167010	1.7727830	-0.2276390
C	-0.5881390	3.0084640	-0.0604480
H	-3.1066630	4.8701030	1.4341400
H	-0.7939630	0.9462690	-0.6911340
N	-0.5050340	5.2060470	0.8939810
N	-4.6148160	2.6514460	0.9140260
N	-3.4212910	0.5555240	0.0108120
N	0.6216650	3.2527530	-0.4509920
C	-0.9915110	6.4141680	1.5039340
H	-1.3898480	6.2179790	2.5071800
H	-0.1668890	7.1219030	1.5921420
H	-1.7867120	6.8764710	0.9041020
C	-5.4068200	3.7307520	1.4510110
H	-5.3700260	4.6269320	0.8144810
H	-6.4483620	3.4114320	1.5278670
H	-5.0673730	4.0271280	2.4542770
C	1.3662940	2.4049630	-1.2700230
C	2.7198870	2.2169510	-0.9595950
C	0.8502360	1.8339270	-2.4437230
C	3.5417460	1.4626460	-1.7912950
H	3.1419830	2.6715230	-0.0690110
C	1.6743730	1.0890350	-3.2813880
H	-0.1803100	1.9972300	-2.7419700
C	3.0321350	0.9050170	-2.9764630
C	-3.1029210	-0.7610760	-0.1388720
C	-1.8484630	-1.2593920	0.2100640
C	-4.0585550	-1.7021430	-0.6565210
C	-1.4707680	-2.6046140	0.0700250
H	-1.1333690	-0.5801560	0.6512040
C	-3.6891830	-3.0151520	-0.8706560
C	-2.4268850	-3.4834020	-0.5451230
H	-4.4089270	-3.7009330	-1.2989370
O	1.1548740	0.6095140	-4.4527720
O	3.8527620	0.2063300	-3.8176050
O	4.8686660	1.3742330	-1.4843460
C	1.0403890	-0.8124950	-4.5205910
H	0.6245810	-1.0387440	-5.5034950
H	2.0176690	-1.2919850	-4.4127040
H	0.3574950	-1.1766010	-3.7438510
C	5.3588020	0.0589610	-1.2099890
H	6.4203400	0.1758880	-0.9853100
H	4.8481370	-0.3691400	-0.3407470
H	5.2359710	-0.5942610	-2.0780400
C	4.2940910	0.9562640	-4.9517470
H	4.9333470	0.2888810	-5.5318660
H	3.4425070	1.2741180	-5.5619900
H	4.8710500	1.8309700	-4.6318880
N	-5.4075660	-1.3552030	-1.0012750
O	-6.0717700	-2.1511120	-1.6576320
O	-5.8565840	-0.2730360	-0.6135550
N	-2.1672020	-4.8630060	-0.8173960
O	-3.0724110	-5.5649900	-1.2547370
O	-1.0290520	-5.3082460	-0.6088750
N	-0.2676910	-3.0509240	0.4927150
H	-0.0486460	-4.0001040	0.2049840
C	0.6758020	-2.3766170	1.2951430
C	0.2966390	-1.6475510	2.4244650
C	2.0282200	-2.5399530	0.9917920
C	1.2674240	-1.0421550	3.2174950
H	-0.7422960	-1.5613970	2.7238710
C	2.9991380	-1.9453790	1.7937730
H	2.3408050	-3.1158110	0.1262810
C	2.6298910	-1.1603320	2.8970140
O	0.8555280	-0.2878890	4.2778990
O	3.5921660	-0.5518880	3.6503400
O	4.3073560	-2.0682660	1.4278210
C	1.2328180	-0.7817780	5.5658910
H	2.3203630	-0.8303630	5.6675620
H	0.8234860	-0.0772910	6.2909350
H	0.7963480	-1.7728890	5.7334000
C	5.1274210	-2.8126620	2.3312060
H	6.1292380	-2.8138020	1.8994850
H	5.1500830	-2.3439830	3.3186010
H	4.7636440	-3.8434890	2.4114160
C	3.7100700	0.8549610	3.4203740
H	2.7715970	1.3677030	3.6543330
H	4.4989220	1.2083360	4.0858570
H	3.9923760	1.0493010	2.3798700
H	0.4381160	5.1519790	0.5303200
H	-4.4146760	0.7875170	0.1009570

c'-9d

C	1.0098060	3.9816340	-1.0190930
C	2.3277310	3.8866310	-1.3929070
C	3.1373130	2.7582610	-1.0260930
C	2.4712350	1.6379540	-0.3006190
C	1.1911770	1.7574920	0.1380490
C	0.4104140	2.9395060	-0.1359360
H	2.7828700	4.6808280	-1.9720090
H	0.7238760	0.9757700	0.7240460
N	0.1930730	4.9929120	-1.3522410
N	4.3973370	2.5876020	-1.2642170
N	3.2979150	0.5612050	-0.0756700
N	-0.7834540	3.1839190	0.3001160
C	0.6016480	6.1314510	-2.1305140
H	0.9669640	5.8233830	-3.1179980
H	-0.2559270	6.7900600	-2.2697860
H	1.3997200	6.6965190	-1.6308680
C	5.1250470	3.6222500	-1.9581600
H	5.0830850	4.5841880	-1.4267150
H	6.1732170	3.3291610	-2.0478070
H	4.7313060	3.7899400	-2.9712920
C	-1.4019990	2.4012470	1.2783100
C	-2.7123160	1.9582250	1.0636230
C	-0.7827330	2.1379280	2.5092110
C	-3.3929510	1.2551650	2.0552500
H	-3.2121000	2.1629590	0.1221860
C	-1.4693660	1.4533530	3.5064790
H	0.2215230	2.4938980	2.7162010
C	-2.7889970	1.0203100	3.3022030
C	2.9737250	-0.7397200	0.1804440
C	1.7296070	-1.2586850	-0.1699120
C	3.8998390	-1.6352940	0.8143000
C	1.3303840	-2.5810460	0.0789400
H	1.0382840	-0.6164440	-0.6980700
C	3.5055580	-2.9181400	1.1418100
C	2.2483650	-3.4021800	0.8173850
H	4.2004820	-3.5667160	1.6599720
O	-0.8615910	1.2829710	4.7197690
O	-3.4814960	0.3896670	4.2991050
O	-4.6870170	0.8952920	1.8108190
C	-0.5473860	-0.0703670	5.0516110
H	-0.0776010	-0.0416540	6.0357600
H	-1.4502090	-0.6866990	5.0900430
H	0.1588650	-0.4860800	4.3233060
C	-4.9799420	-0.5007550	1.8938190
H	-6.0283970	-0.6048670	1.6106030
H	-4.3573050	-1.0627820	1.1884800
H	-4.8278690	-0.8779920	2.9076480
C	-4.0088550	1.2779030	5.2873110
H	-4.5328490	0.6540660	6.0131460
H	-3.2028270	1.8260250	5.7858140
H	-4.7134400	1.9829580	4.8325070
N	5.2397280	-1.2637440	1.1660720
O	5.8755890	-1.9926320	1.9208450
O	5.7087160	-0.2286640	0.6847940
N	1.9547220	-4.7450910	1.2114800
O	2.8310010	-5.4140120	1.7482280
O	0.8167980	-5.1894180	1.0038750
N	0.1407330	-3.0453550	-0.3628350
H	-0.1202570	-3.9597950	-0.0075450
C	-0.6959580	-2.4416380	-1.3291140
C	-2.0696680	-2.4041060	-1.0951920
C	-0.1748410	-1.9451800	-2.5258050
C	-2.9312870	-1.8873500	-2.0627570
H	-2.4859040	-2.7694970	-0.1617890
C	-1.0327830	-1.4244640	-3.4893750
H	0.8870260	-1.9891570	-2.7433860
C	-2.4222390	-1.4133770	-3.2831710
O	-4.2695010	-1.9271390	-1.8049900
O	-3.2408510	-0.9430580	-4.2696980
O	-0.5039500	-1.0217900	-4.6807220
C	-4.9688480	-0.6801440	-1.8562340
H	-4.9868720	-0.2719020	-2.8694050
H	-5.9842220	-0.8949880	-1.5213280
H	-4.5067550	0.0422260	-1.1748210
C	-0.5874310	0.3812140	-4.9373780
H	-0.1316380	0.5384860	-5.9158620
H	-1.6283630	0.7156250	-4.9559690
H	-0.0260580	0.9401650	-4.1794100
C	-3.9341250	-1.9672330	-4.9885680
H	-4.5900740	-2.5370230	-4.3221020
H	-4.5312840	-1.4580800	-5.7462360
H	-3.2212200	-2.6420880	-5.4741860
H	-0.7258830	4.9596240	-0.9292160
H	4.2871420	0.7849500	-0.1965330

c'-9e

C	-1.4599600	2.1806130	3.4060480
C	-2.4629880	1.3635710	3.8668910
C	-3.0458250	0.3437740	3.0401170
C	-2.4485640	0.1269520	1.6911710
C	-1.4966860	0.9663090	1.2074020
C	-1.0088850	2.0766900	1.9877240
H	-2.8407860	1.4891460	4.8741750
H	-1.1070320	0.8472170	0.2038220
N	-0.8593000	3.1351850	4.1328890
N	-4.0398860	-0.4306670	3.3327730
N	-3.0169190	-0.9155800	0.9972660
N	-0.2024240	3.0028680	1.5791450
C	-1.2089960	3.4470970	5.4927250
H	-1.0712150	2.5759560	6.1451080
H	-0.5629380	4.2500490	5.8481420
H	-2.2536630	3.7754580	5.5753500
C	-4.6828250	-0.2884880	4.6165630
H	-5.0745400	0.7272490	4.7729570
H	-5.5182890	-0.9888290	4.6821810
H	-3.9928430	-0.5049460	5.4451800
C	0.1587670	3.1435510	0.2366920
C	1.5126740	3.2898630	-0.0868960
C	-0.8022990	3.2425770	-0.7806300
C	1.9040190	3.5098650	-1.4044680
H	2.2694900	3.2254420	0.6873470
C	-0.4119290	3.4837400	-2.0941500
H	-1.8616360	3.1661740	-0.5565710
C	0.9442400	3.6351760	-2.4226380
C	-2.5362650	-1.5793680	-0.0953290
C	-1.1648690	-1.7111520	-0.3051280
C	-3.4114570	-2.1771790	-1.0598770
C	-0.6018590	-2.3724830	-1.4084040
H	-0.4992850	-1.3397520	0.4625380
C	-2.8872520	-2.7720150	-2.1904320
C	-1.5204980	-2.8687520	-2.3974340
H	-3.5612130	-3.1863510	-2.9294180

O	-1.3810950	3.6465380	-3.0459780
O	1.3327010	3.9012440	-3.7067120
O	3.2334800	3.6908130	-1.6636140
C	-1.4363370	2.6136370	-4.0307460
H	-2.2452400	2.8834870	-4.7111700
H	-0.4948600	2.5451970	-4.5834890
H	-1.6640990	1.6502660	-3.5592420
C	3.8291840	2.7192510	-2.5236430
H	4.8858350	2.9822720	-2.5925220
H	3.7314770	1.7163330	-2.0909180
H	3.3754890	2.7405720	-3.5178950
C	1.1749130	5.2699940	-4.0871990
H	1.5189460	5.3437470	-5.1200650
H	0.1240610	5.5710350	-4.0260270
H	1.7861630	5.9181670	-3.4495250
N	-4.8402930	-2.1767610	-0.9315990
O	-5.5199960	-2.4551750	-1.9143260
O	-5.3309300	-1.9101100	0.1682770
N	-1.1063680	-3.5299340	-3.5980030
O	-1.9579340	-3.8843930	-4.4054010
O	0.1031480	-3.7209040	-3.7888220
N	0.7319930	-2.5638650	-1.5189530
H	1.0002940	-3.1413570	-2.3102310
C	1.7130240	-2.3358280	-0.5228730
C	2.4899040	-3.4237090	-0.1218620
C	1.9590210	-1.0673510	0.0026260
C	3.4882960	-3.2530280	0.8325440
H	2.3196590	-4.4131420	-0.5344920
C	2.9407210	-0.9010900	0.9806790
H	1.4140000	-0.1939820	-0.3401580
C	3.6977200	-1.9970780	1.4246860
O	4.1864540	-4.3500230	1.2463110
O	4.6320550	-1.8281950	2.4058870
O	3.0916580	0.3331060	1.5377350
C	5.5835890	-4.3345860	0.9417260
H	6.0815630	-3.4846270	1.4163480
H	5.9887700	-5.2679670	1.3342930
H	5.7337750	-4.2990690	-0.1431840
C	4.3661230	0.9525760	1.3527290
H	4.3108480	1.9146840	1.8639470
H	5.1664410	0.3488210	1.7871020
H	4.5557590	1.1183310	0.2861470
C	4.2260460	-2.3181530	3.6873840
H	4.0310730	-3.3944730	3.6480640
H	5.0554140	-2.1183360	4.3671810
H	3.3316930	-1.7884690	4.0328630
H	-0.1978690	3.7090430	3.6253190
H	-3.9236810	-1.1991410	1.3693860

c'-9f

C	-1.3565330	-3.7289590	-1.9063650
C	-2.5789810	-3.3769480	-2.4227310
C	-3.2698540	-2.1970050	-1.9864510
C	-2.5668790	-1.3005670	-1.0212990
C	-1.3712900	-1.6583070	-0.4818480
C	-0.7429600	-2.9131050	-0.8175250
H	-3.0519650	-4.0059910	-3.1668650
H	-0.8860350	-1.0349690	0.2583380
N	-0.6549060	-4.8094640	-2.2821840
N	-4.4507880	-1.8057600	-2.3409050
N	-3.2958090	-0.1811780	-0.6994830
N	0.3205300	-3.4158110	-0.2756210
C	-1.1150720	-5.7660740	-3.2526820
H	-1.2893430	-5.2889400	-4.2249860
H	-0.3535870	-6.5360400	-3.3780640
H	-2.0499900	-6.2463320	-2.9343780
C	-5.2068730	-2.6110210	-3.2686940
H	-5.3712680	-3.6307260	-2.8908200
H	-6.1824710	-2.1497230	-3.4363110
H	-4.7010860	-2.6993400	-4.2412500
C	0.9414930	-2.8708570	0.8490480
C	2.3389420	-2.7751480	0.8451970
C	0.2373860	-2.5073450	2.0075820
C	3.0149710	-2.2780860	1.9525550
H	2.9037810	-3.0653610	-0.0341330
C	0.9183560	-2.0438930	3.1298600
H	-0.8404070	-2.6207420	2.0659010
C	2.3163800	-1.9234870	3.1186940
C	-2.9134870	0.9473870	-0.0319750
C	-1.6084740	1.4289680	-0.1173880
C	-3.8408540	1.6907850	0.7705560
C	-1.1558760	2.5816160	0.5480950
H	-0.9272180	0.9284390	-0.7925120
C	-3.4068660	2.7868240	1.4886600
C	-2.0993990	3.2383710	1.4122390
H	-4.1095340	3.3164960	2.1192230
O	0.2040960	-1.7768630	4.2649700
O	2.9716450	-1.4594820	4.2241090
O	4.3814620	-2.2123340	1.9205170
C	0.1323350	-0.3961300	4.6197120
H	-0.4617360	-0.3455290	5.5334550
H	1.1291060	0.0149130	4.8037210
H	-0.3684510	0.1753820	3.8286800
C	4.9066150	-0.8848540	1.8523060
H	5.9930180	-0.9862310	1.8438660
H	4.5758920	-0.3938040	0.9299790
H	4.5987720	-0.2968120	2.7225170
C	3.6213800	-2.4775490	4.9887750
H	4.0986380	-1.9721740	5.8298120
H	2.8886780	-3.2008210	5.3634950
H	4.3788450	-2.9904860	4.3876860
N	-5.2283190	1.3462840	0.8975600
O	-5.8803660	1.8550550	1.8036430
O	-5.7172630	0.5624750	0.0802010
N	-1.7847170	4.3999200	2.1884850
O	-2.6377990	4.8630880	2.9369380
O	-0.6563070	4.9018970	2.0847060
N	0.0882830	3.0731870	0.3623760
H	0.2511130	3.9636710	0.8239280
C	1.0568720	2.6512840	-0.5792750
C	1.5629920	1.3511470	-0.5977590
C	1.5420120	3.6063000	-1.4740930
C	2.5482060	1.0107650	-1.5240180
H	1.2354950	0.6009110	0.1146190
C	2.5442120	3.2723330	-2.3811100
H	1.1490310	4.6180920	-1.4738210
C	3.0660020	1.9701420	-2.4082240
O	3.0715170	-0.2490550	-1.4950300
O	4.0530630	1.6477540	-3.2940490
O	3.0454160	4.2505570	-3.1873400
C	2.7533990	-1.0573380	-2.6299810
H	3.1026080	-0.5906350	-3.5555310
H	3.2670930	-2.0080060	-2.4808890
H	1.6724300	-1.2315670	-2.6807790
C	2.7907340	4.0854510	-4.5841670
H	3.2546880	4.9396130	-5.0789760
H	3.2306880	3.1568020	-4.9570460
H	1.7116060	4.0946930	-4.7757970
C	5.3602720	1.5929820	-2.7157880
H	5.4050180	0.8319520	-1.9302610
H	6.0418060	1.3275840	-3.5251080
H	5.6383850	2.5703700	-2.3068080
H	-4.2784240	-0.2649580	-0.9677450
H	0.1862320	-4.9808020	-1.7455050

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C	-1.5301190	-1.5828450	3.5982900
C	-0.4497690	-2.3171160	4.0828630
C	0.5537430	-2.7249450	3.2036850
C	0.5388230	-2.3153880	1.7640370
C	-0.5633680	-1.6089380	1.2990750
C	-1.6519910	-1.2610810	2.1357400
H	-0.3960930	-2.5837750	5.1311230
H	-0.6045920	-1.3345440	0.2519870
N	-2.5213670	-1.1572420	4.3610310
N	1.5878870	-3.4597200	3.5704620
N	1.5775590	-2.7659370	1.0714080
N	-2.7683380	-0.6565810	1.8264390
C	-2.6340670	-1.3707810	5.7831010
H	-1.7808070	-0.9340000	6.3133910
H	-3.5471420	-0.8931570	6.1364900
H	-2.6830150	-2.4402670	6.0167950
C	1.8313250	-3.9607470	4.9017780
H	1.0084750	-4.6029510	5.2340980
H	2.7501600	-4.5455210	4.8908230
H	1.9459750	-3.1369360	5.6143870
C	-3.1824180	-0.4259600	0.5200150
C	-3.8305790	0.7872270	0.2414160
C	-3.0808760	-1.3851030	-0.5032890
C	-4.3518640	1.0459530	-1.0220540
H	-3.9343590	1.5361500	1.0200120
C	-3.6182630	-1.1334120	-1.7603290
H	-2.6217430	-2.3512490	-0.3221770
C	-4.2718610	0.0781870	-2.0365830
C	1.9854640	-2.2605800	-0.1099020
C	2.0617520	-0.8777780	-0.3473750
C	2.5358470	-3.1103790	-1.1290580
C	2.6565710	-0.3025320	-1.4761990
H	1.7085560	-0.2234310	0.4397150
C	3.1279960	-2.5817090	-2.2530100
C	3.1971760	-1.2069260	-2.4594290
H	3.5365510	-3.2442910	-3.0052750
O	-3.5686860	-2.1215500	-2.7073130
O	-4.8233460	0.3164440	-3.2656930
O	-5.0244230	2.2202830	-1.2198680
C	-2.6898530	-1.8546770	-3.8002700
H	-2.7593550	-2.7157330	-4.4667660
H	-2.9903820	-0.9484360	-4.3347520
H	-1.6578530	-1.7530840	-3.4439280
C	-4.4517270	3.1015040	-2.1854440
H	-5.0868850	3.9886210	-2.2015890
H	-3.4367470	3.3870940	-1.8853520
H	-4.4309040	2.6418530	-3.1770860
C	-6.0957350	-0.3044220	-3.4586960
H	-6.4179960	-0.0399850	-4.4672060
H	-6.0136710	-1.3926920	-3.3715040
H	-6.8219440	0.0738740	-2.7305620
N	2.4667890	-4.5471440	-1.0475910
O	3.2970660	-5.2011010	-1.6811420
O	1.5808750	-5.0594680	-0.3735520
N	3.8282740	-0.7794250	-3.6599920
O	4.1960770	-1.6206780	-4.4785910
O	3.9977490	0.4368970	-3.8558510
N	2.7584670	1.0417760	-1.6311270
H	3.3335340	1.3238300	-2.4191510
C	2.3197620	2.0513620	-0.7520650
C	3.2101710	3.0867610	-0.4562190
C	1.0190650	2.0872180	-0.2444160
C	2.8149240	4.1342660	0.3699830
H	4.2209510	3.0826960	-0.8524550
C	0.6312230	3.1252650	0.6014770
H	0.2858780	1.3315620	-0.5055150
C	1.5315780	4.1478550	0.9388650
O	3.7323180	5.0944320	0.6894260
O	1.1504580	5.1443960	1.7930470
O	-0.6235610	3.0846770	1.1349280
C	3.4384790	6.4023420	0.1932110
H	2.4875710	6.7695850	0.5893120
H	4.2528340	7.0447690	0.5307000
H	3.4100860	6.3945180	-0.9023610
C	-1.4867310	4.1594970	0.7612280
H	-2.4498290	3.9508170	1.2289310
H	-1.1004220	5.1185410	1.1155750
H	-1.6088670	4.1852550	-0.3277750
C	1.6514070	4.9895360	3.1231130
H	2.7461510	4.9929940	3.1288840
H	1.2779410	5.8418480	3.6926850
H	1.2788690	4.0597030	3.5668780
H	-3.2458920	-0.6611830	3.8448340
H	2.2273180	-3.6771590	2.8080810

9+H+(a)-a

C	-0.6293890	-3.4575480	-2.5462710
C	-2.0574010	-3.4253580	-2.6653270
C	-2.8306780	-2.7107660	-1.7907850
C	-2.1857040	-2.0153530	-0.6537120
C	-0.8141640	-1.9636020	-0.5286660
C	-0.0070780	-2.6856830	-1.4227190
H	-2.5149610	-3.9238310	-3.5097860
H	-0.3722000	-1.4957150	0.3409840
N	0.2111560	-4.0624170	-3.3143260
N	-4.1789480	-2.6108980	-1.8825290
N	-3.0403670	-1.4895630	0.2691870
N	1.3001260	-2.8422080	-1.3183910
C	-0.2626290	-4.8622470	-4.4148310
H	-0.7234090	-4.2302950	-5.1870560
H	0.5792910	-5.3880690	-4.8673580
H	-1.0115340	-5.6011130	-4.0996860
C	-4.9186820	-3.2490060	-2.9479170
H	-4.7634530	-4.3316760	-2.9173470
H	-5.9795110	-3.0470770	-2.8030040
H	-4.6171240	-2.8766920	-3.9360890
C	2.2362320	-2.3293250	-0.4034100
C	3.2979800	-3.1693430	-0.0583430
C	2.1666340	-1.0301090	0.1031700
C	4.2583580	-2.7379260	0.8491770
H	3.3721740	-4.1745240	-0.4608110
C	3.1346920	-0.5960480	1.0060830
H	1.4154830	-0.3206440	-0.2242970
C	4.1663490	-1.4574310	1.4230740
C	-2.7697220	-0.5131370	1.2180590
C	-1.9447650	0.5510830	0.9081910
C	-3.3704600	-0.5548610	2.5117150
C	-1.6487360	1.5935360	1.8150080
H	-1.5206600	0.6072730	-0.0864960
C	-3.0552640	0.4196870	3.4406350
C	-2.2055100	1.4668730	3.1302570
H	-3.4881950	0.3685130	4.4319770
O	3.0183040	0.6599530	1.5193080
O	5.0972970	-1.0725280	2.3357240
O	5.2227030	-3.6153750	1.2346820
C	4.0886460	1.5592600	1.2037810
H	3.8874090	2.4741870	1.7621690
H	5.0542170	1.1479900	1.5084960
H	4.0900610	1.7789140	0.1310730
C	6.5618700	-3.2630150	0.8740020
H	7.1955150	-4.0651820	1.2534520
H	6.6563500	-3.2067270	-0.2162280
H	6.8542610	-2.3128880	1.3277720
C	4.6070070	-0.9198950	3.6737920
H	5.4657240	-0.6222840	4.2759910
H	3.8331820	-0.1484060	3.7219080
H	4.2116850	-1.8723970	4.0412000
N	-4.2968610	-1.5732980	2.9173730
O	-4.6004740	-1.6566790	4.0972220
O	-4.7667230	-2.3221730	2.0497620
N	-1.9521700	2.4182050	4.1800280
O	-2.5375670	2.2897360	5.2454870
O	-1.1452310	3.3293410	3.9653460
N	-0.8868550	2.6373990	1.4444380
H	-0.6231000	3.2634400	2.2000270
C	-0.4475280	2.9460720	0.1346710
C	-1.3434900	2.9936270	-0.9344850
C	0.8902450	3.2883690	-0.0524910
C	-0.8867850	3.3368320	-2.2043080
H	-2.4017760	2.7969190	-0.7974210
C	1.3471580	3.6368600	-1.3217850
H	1.5924330	3.2657160	0.7737740
C	0.4703060	3.6333490	-2.4189980
O	-1.7781690	3.3192810	-3.2368900
O	0.9430520	3.9454830	-3.6589530
O	2.6765730	3.8843970	-1.4855600
C	-2.0334700	4.5873900	-3.8501710
H	-1.1210210	5.0093410	-4.2797170
H	-2.7626450	4.3990320	-4.6387840
H	-2.4582120	5.2817990	-3.1170120
C	3.0116870	5.2231760	-1.8610550
H	4.0985350	5.2487400	-1.9484270
H	2.5563190	5.4885320	-2.8185910
H	2.6912920	5.9253670	-1.0830820
C	1.0523830	2.8304260	-4.5487560
H	0.0745870	2.3686300	-4.7173610
H	1.4393730	3.2276170	-5.4878290

H	1.7526880	2.0902480	-4.1468650
H	-3.8931700	-2.0157700	0.4706600
H	1.6407680	-3.5006030	-2.0304580
H	-4.6096340	-1.7956870	-1.4707650

9+H+(a)-b

C	-0.4695640	-3.0442990	-3.0077740
C	-1.8991700	-3.1474310	-3.0245490
C	-2.6627030	-2.6647260	-1.9954660
C	-1.9946870	-2.0866750	-0.8071000
C	-0.6290200	-1.9047830	-0.7695110
C	0.1663280	-2.3927730	-1.8184800
H	-2.3750170	-3.5586760	-3.9050730
H	-0.1625430	-1.5278270	0.1313420
N	0.3588750	-3.4320720	-3.9166250
N	-4.0163980	-2.6947670	-1.9807020
N	-2.8123050	-1.8031560	0.2463110
N	1.4866560	-2.4242010	-1.8185200
C	-0.1278810	-4.1037210	-5.0947420
H	-0.7471650	-3.4316440	-5.7053820
H	0.7187940	-4.4288300	-5.7008690
H	-0.7389830	-4.9816370	-4.8449790
C	-4.7810290	-3.2320340	-3.0830910
H	-4.5205270	-4.2823300	-3.2451340
H	-5.8398400	-3.1719910	-2.8334280
H	-4.6025160	-2.6769780	-4.0136300
C	2.4229330	-1.9567070	-0.8767910
C	3.5512150	-2.7506020	-0.6608840
C	2.2790080	-0.7321020	-0.2226960
C	4.5071390	-2.3562310	0.2686140
H	3.6802440	-3.6960960	-1.1777700
C	3.2447480	-0.3311790	0.6989840
H	1.4633040	-0.0532580	-0.4459620
C	4.3435600	-1.1604670	0.9909180
C	-2.5409700	-0.9600810	1.3166250
C	-1.8697800	0.2286010	1.1081750
C	-2.9814080	-1.2713690	2.6372290
C	-1.5713540	1.1433960	2.1430540
H	-1.5741180	0.4892520	0.0994670
C	-2.6541240	-0.4252210	3.6810080
C	-1.9497890	0.7469720	3.4673950
H	-2.9619920	-0.6788660	4.6879530
O	3.0551680	0.8511540	1.3475570
O	5.2680930	-0.8239810	1.9296280
O	5.5396620	-3.2010690	0.5284510
C	4.0840980	1.8333840	1.1750260
H	3.7736910	2.6991500	1.7608400
H	5.0484800	1.4690040	1.5366750
H	4.1621620	2.1143010	0.1194130
C	6.8442270	-2.7100800	0.2046650
H	7.5389760	-3.5063050	0.4734670
H	6.9152940	-2.5103240	-0.8703050
H	7.0770840	-1.8065740	0.7732910
C	4.7981710	-0.8745670	3.2826690
H	5.6487340	-0.5994070	3.9066940
H	3.9777500	-0.1680600	3.4398380
H	4.4717870	-1.8896650	3.5305580
N	-3.7547230	-2.4382130	2.9528520
O	-3.9119690	-2.7411330	4.1253050
O	-4.2485590	-3.0868420	2.0203700
N	-1.6650820	1.5461460	4.6298050
O	-2.1032310	1.1871560	5.7131560
O	-0.9804520	2.5648360	4.4880050
N	-0.9686200	2.3128270	1.8703070
H	-0.6779310	2.8507530	2.6813450
C	-0.7559980	2.8638600	0.5809410
C	0.5291490	3.2671940	0.2277760
C	-1.8222110	3.0440870	-0.3006970
C	0.7512870	3.8675910	-1.0098320
H	1.3669260	3.1058890	0.8969330
C	-1.6012910	3.6421500	-1.5393450
H	-2.8345020	2.7626530	-0.0288650
C	-0.3163990	4.0847090	-1.8974480
O	2.0125200	4.2962340	-1.3013460
O	-0.1298920	4.7021240	-3.0982790
O	-2.6768420	3.8795550	-2.3414870
C	2.6419010	3.6546490	-2.4137080
H	2.0800820	3.8190460	-3.3371030
H	3.6330360	4.1015810	-2.4979890
H	2.7410500	2.5797400	-2.2229650
C	-2.6831450	3.1852110	-3.5904630
H	-3.6008690	3.4849930	-4.0977590
H	-1.8171380	3.4593340	-4.1981770
H	-2.6975720	2.1019250	-3.4214560
C	0.0900850	6.1146460	-3.0100740
H	0.9925350	6.3331890	-2.4311840
H	0.2136050	6.4666570	-4.0348160
H	-0.7756890	6.6058370	-2.5538670
H	-3.5840320	-2.4473640	0.4302580
H	1.8409870	-2.9264250	-2.6413410
H	-4.4888530	-2.0196720	-1.3974690

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C	1.7306080	-4.0973220	-0.3356570
C	3.0277180	-3.9194070	0.2505550
C	3.5562460	-2.6750060	0.4599210
C	2.8033820	-1.4799760	0.0081540
C	1.5315150	-1.5965160	-0.5118570
C	0.9698860	-2.8660200	-0.7178740
H	3.5596660	-4.7960100	0.5956820
H	0.9948430	-0.7155870	-0.8323270
N	1.1102730	-5.2051210	-0.5561400
N	4.7570550	-2.4563310	1.0538210
N	3.4728910	-0.2999780	0.1138360
N	-0.2121850	-3.0890740	-1.2616860
C	1.7438470	-6.4619140	-0.2479310
H	1.8967010	-6.5728700	0.8347910
H	1.1064900	-7.2798620	-0.5865010
H	2.7245280	-6.5569300	-0.7330660
C	5.5711350	-3.5484640	1.5400390
H	5.8281730	-4.2202340	0.7159250
H	6.4926720	-3.1367220	1.9508070
H	5.0597960	-4.1265760	2.3215120
C	-1.1474410	-2.1832920	-1.8073470
C	-2.4960080	-2.3922520	-1.5206980
C	-0.7492200	-1.1372650	-2.6401720
C	-3.4627140	-1.5563490	-2.0759360
H	-2.8133210	-3.2006070	-0.8697610
C	-1.7133870	-0.2899700	-3.1785550
H	0.2867500	-0.9869350	-2.9224800
C	-3.0803240	-0.5056000	-2.9296350
C	2.9753140	0.9905390	-0.0063700
C	1.7146420	1.3134670	0.4578880
C	3.7726000	2.0258800	-0.5843520
C	1.1529760	2.6062440	0.3454480
H	1.1264970	0.5490200	0.9486950
C	3.2371070	3.2907990	-0.7413480
C	1.9555410	3.5924120	-0.3158940
H	3.8340620	4.0661320	-1.2053060
O	-1.3048210	0.6929640	-4.0301210
O	-4.0310990	0.2864480	-3.4961880
O	-4.7662220	-1.8485500	-1.8336150
C	-1.5071510	2.0286880	-3.5582690
H	-1.1401730	2.6864360	-4.3466800
H	-2.5666960	2.2257830	-3.3731630
H	-0.9284240	2.1969350	-2.6423610
C	-5.5509050	-0.8290530	-1.2008170
H	-6.5226320	-1.2850170	-1.0075450
H	-5.0895730	-0.5261920	-0.2549320
H	-5.6692800	0.0374450	-1.8551680
C	-4.2484870	0.0518180	-4.8932750
H	-5.0302470	0.7482380	-5.1980060
H	-3.3366170	0.2429280	-5.4664940
H	-4.5870500	-0.9765760	-5.0564110
N	5.1246550	1.8313190	-1.0262050
O	5.6687330	2.7174540	-1.6656060
O	5.6981600	0.7737600	-0.7281400
N	1.5047840	4.9398380	-0.5461920
O	2.2851350	5.7478640	-1.0276050
O	0.3388900	5.2275500	-0.2532780
N	-0.0710010	2.8731100	0.8323680
H	-0.4337140	3.7924360	0.5959080
C	-0.8678260	2.0242910	1.6385470
C	-0.3536660	1.4475990	2.8003570
C	-2.2063380	1.8438670	1.2942030
C	-1.1702090	0.6479800	3.5958430
H	0.6667030	1.6316020	3.1207450
C	-3.0255150	1.0490930	2.0936330
H	-2.6223480	2.2999370	0.4013790
C	-2.5085560	0.4145200	3.2351940
O	-0.6201000	0.0572150	4.6951780
O	-3.3206690	-0.3836410	3.9839410
O	-4.3076520	0.8283900	1.6897520
C	-1.1538370	0.4813440	5.9541720
H	-2.2216110	0.2581050	6.0264440
H	-0.6059010	-0.0744080	6.7157140
H	-0.9856100	1.5549700	6.0923540
C	-5.3230750	1.3672230	2.5411740
H	-6.2752120	1.1031010	2.0791170
H	-5.2649260	0.9352740	3.5434750
H	-5.2324520	2.4579600	2.5936130
C	-3.0370420	-1.7825130	3.8825450
H	-2.0211980	-2.0008820	4.2259290
H	-3.7600110	-2.2861330	4.5251660
H	-3.1652210	-2.1223800	2.8491190
H	4.4899280	-0.3332160	0.0045510
H	-0.4403060	-4.0897430	-1.2671470
H	4.8726680	-1.5804580	1.5431160

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C	-1.7063050	-2.6431140	3.0609000
C	-2.9902470	-2.9312200	2.4878980
C	-3.5038720	-2.1862410	1.4608050
C	-2.7412640	-1.0178060	0.9612780
C	-1.4828860	-0.7309580	1.4470650
C	-0.9450930	-1.4843260	2.4997870
H	-3.5269260	-3.8010480	2.8430150
H	-0.9407760	0.1260110	1.0731290
N	-1.1017520	-3.2800220	4.0041490
N	-4.6953300	-2.4440190	0.8652100
N	-3.3786870	-0.2502870	0.0352330
N	0.2146790	-1.2339170	3.0800920
C	-1.7411590	-4.4033350	4.6409040
H	-1.8770470	-5.2343900	3.9346390
H	-1.1172340	-4.7549730	5.4636440
H	-2.7308080	-4.1405690	5.0381370
C	-5.5187730	-3.5611560	1.2715820
H	-5.7926440	-3.4614020	2.3260660
H	-6.4305450	-3.5543310	0.6751740
H	-5.0068940	-4.5223620	1.1288320
C	1.1066490	-0.1592620	2.8600560
C	2.4683670	-0.4400460	2.7632840
C	0.6407870	1.1528240	2.7749540
C	3.3805780	0.6001580	2.5903850
H	2.8390610	-1.4583580	2.8216570
C	1.5492410	2.1900340	2.5839660
H	-0.4089390	1.3974850	2.8939430
C	2.9305400	1.9316670	2.5259900
C	-2.8204350	0.7593550	-0.7423920
C	-1.5686750	0.5956700	-1.3001740
C	-3.5242810	1.9748510	-0.9941740
C	-0.9164840	1.5988350	-2.0538680
H	-1.0526700	-0.3458620	-1.1596680
C	-2.9003830	2.9890850	-1.6970770
C	-1.6190760	2.8385450	-2.1992630
H	-3.4237370	3.9233140	-1.8596450
O	1.0700410	3.4652090	2.5553750
O	3.8319500	2.9442900	2.4048400
O	4.7006720	0.2824140	2.5737010
C	1.2583420	4.1663990	1.3217460
H	0.8183340	5.1533200	1.4668000
H	2.3199780	4.2642780	1.0797960
H	0.7351320	3.6489310	0.5090380
C	5.4534700	0.6904320	1.4254290
H	6.4415290	0.2456830	1.5480190
H	4.9897700	0.3029900	0.5119270
H	5.5354020	1.7776560	1.3722980
C	4.0057530	3.7351240	3.5878140
H	4.7544730	4.4878000	3.3393310
H	3.0686070	4.2224350	3.8721710
H	4.3694050	3.1107890	4.4103560
N	-4.8646650	2.2167650	-0.5407020
O	-5.3216550	3.3453670	-0.6294570
O	-5.5142340	1.2636750	-0.0895270
N	-1.0626100	3.9699030	-2.8934650
O	-1.7606490	4.9587440	-3.0627570
O	0.1072300	3.8993270	-3.2845420
N	0.2979330	1.3717100	-2.5810920
H	0.7447140	2.1755150	-3.0123410
C	0.9454950	0.1092270	-2.6518480
C	2.2063690	-0.0411010	-2.0803130
C	0.3378510	-0.9517610	-3.3226120
C	2.8778000	-1.2582340	-2.1966570
H	2.6767420	0.7726600	-1.5377600
C	1.0077270	-2.1668670	-3.4423660
H	-0.6351460	-0.8398010	-3.7899830
C	2.2979070	-2.3236730	-2.9075630
O	4.1295230	-1.3513470	-1.6659480
O	2.9525010	-3.5063400	-3.0832570
O	0.4274650	-3.1535180	-4.1804380
C	4.3156540	-2.3606160	-0.6686510
H	4.1318810	-3.3592920	-1.0719180
H	5.3537260	-2.2753030	-0.3459690
H	3.6517430	-2.1741660	0.1829850
C	0.0896680	-4.3455150	-3.4678050
H	-0.3580310	-5.0179000	-4.2004800
H	0.9782010	-4.8099660	-3.0328920
H	-0.6425660	-4.1224540	-2.6829560
C	4.0296370	-3.4517180	-4.0258320
H	4.8010720	-2.7483440	-3.6974000
H	4.4434970	-4.4595810	-4.0716630
H	3.6553820	-3.1617290	-5.0130460
H	-4.3939940	-0.1685570	0.1183100
H	0.4473990	-1.9346660	3.7914500
H	-4.8052440	-2.1488390	-0.0943840

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C	0.8154480	-2.6678290	3.2916100
C	2.1342360	-2.2571310	3.6786420
C	2.9204670	-1.4979330	2.8544210
C	2.4119060	-1.1164890	1.5164470
C	1.1342260	-1.4463100	1.1176980
C	0.3293540	-2.2520650	1.9371670
H	2.4794040	-2.5081520	4.6731420
H	0.7858490	-1.1523230	0.1376640
N	-0.0309140	-3.3532400	3.9808600
N	4.1610990	-1.0620190	3.1847090
N	3.2994950	-0.4629300	0.7147990
N	-0.8566010	-2.7298080	1.6062750
C	0.3242060	-3.8328170	5.2921170
H	0.4857440	-2.9988400	5.9893900
H	-0.4859360	-4.4503110	5.6823370
H	1.2442490	-4.4323650	5.2733030
C	4.7554980	-1.3565790	4.4692570
H	4.8402730	-2.4389090	4.6043350
H	5.7557810	-0.9248380	4.4953960
H	4.1672620	-0.9416940	5.2986030
C	-1.5667950	-2.6799800	0.3906830
C	-2.9575750	-2.5879540	0.4597850
C	-0.9230830	-2.7805100	-0.8437240
C	-3.7139780	-2.6010580	-0.7089170
H	-3.4683470	-2.5093880	1.4143100
C	-1.6787710	-2.7771490	-2.0126980
H	0.1483600	-2.9194060	-0.9277220
C	-3.0824950	-2.7166910	-1.9606740
C	3.0140220	0.2328060	-0.4542920
C	1.9165540	1.0700900	-0.5087730
C	3.8603650	0.1388510	-1.5977570
C	1.5712540	1.8211040	-1.6560160
H	1.3179080	1.1977650	0.3845970
C	3.5339920	0.8370730	-2.7455230
C	2.4194850	1.6559230	-2.8004630
H	4.1681210	0.7506090	-3.6191900

O	-1.0264990	-2.9383430	-3.1983590
O	-3.8353700	-2.7655130	-3.0928540
O	-5.0682500	-2.5951270	-0.5920380
C	-1.1001130	-1.8259640	-4.0957130
H	-0.5464060	-2.1211090	-4.9873830
H	-2.1363540	-1.5983970	-4.3597050
H	-0.6262220	-0.9460020	-3.6456270
C	-5.7583310	-1.4983760	-1.1985830
H	-6.8165480	-1.6624720	-0.9931270
H	-5.4410350	-0.5544880	-0.7418540
H	-5.5876990	-1.4714450	-2.2769780
C	-3.8986490	-4.0549860	-3.7160310
H	-4.5360700	-3.9348220	-4.5924360
H	-2.9031610	-4.3886990	-4.0227370
H	-4.3455780	-4.7837350	-3.0320930
N	5.0599500	-0.6501030	-1.6271360
O	5.6073030	-0.8471900	-2.7006210
O	5.5035510	-1.0873570	-0.5572450
N	2.1943710	2.3430960	-4.0458670
O	2.9289130	2.1007650	-4.9922350
O	1.2619860	3.1513090	-4.1125660
N	0.5213760	2.6594940	-1.6440670
H	0.4190510	3.2289110	-2.4793500
C	-0.3365500	2.9177040	-0.5433260
C	-0.4310220	4.2251580	-0.0707490
C	-1.1178170	1.9056970	0.0126200
C	-1.2889090	4.5177520	0.9868270
H	0.1591670	5.0240340	-0.5080390
C	-1.9547440	2.1914880	1.0908050
H	-1.0992670	0.8950820	-0.3832310
C	-2.0283420	3.4960890	1.6073340
O	-1.3198180	5.7957730	1.4600160
O	-2.8314740	3.7517620	2.6787400
O	-2.6371310	1.1606310	1.6619580
C	-2.5711960	6.4746710	1.3120110
H	-3.3683520	5.9566260	1.8520700
H	-2.4248230	7.4703020	1.7318020
H	-2.8309260	6.5595050	0.2511200
C	-4.0635380	1.2558380	1.6245060
H	-4.4376900	0.3292440	2.0615960
H	-4.4178170	2.1117700	2.2034530
H	-4.4086320	1.3365700	0.5874750
C	-2.1302410	4.0144710	3.8987610
H	-1.4919970	4.8976320	3.8001970
H	-2.8951500	4.1938440	4.6551030
H	-1.5272360	3.1460540	4.1848970
H	4.2763690	-0.7560190	0.7740480
H	-1.2804000	-3.2391820	2.3907030
H	4.4878170	-0.2198570	2.7338280

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C	1.7820040	3.9052920	-1.2497340
C	2.9825450	3.4672860	-1.9013600
C	3.4622540	2.1959020	-1.7421860
C	2.7595080	1.2644260	-0.8278100
C	1.5652830	1.6153410	-0.2333440
C	1.0649600	2.9173990	-0.3822200
H	3.4748500	4.1487000	-2.5825370
H	1.0680970	0.9189260	0.4258670
N	1.2140520	5.0586500	-1.3377180
N	4.5742530	1.7264220	-2.3619750
N	3.4001120	0.0871630	-0.5945780
N	-0.0140830	3.3880760	0.2164410
C	1.8156450	6.1016840	-2.1290850
H	1.8121920	5.8391970	-3.1962610
H	1.2457770	7.0234250	-2.0044120
H	2.8574170	6.2904670	-1.8371720
C	5.3415250	2.5521800	-3.2679950
H	5.7070860	3.4411110	-2.7455870
H	6.1995680	1.9787160	-3.6173990
H	4.7492500	2.8705600	-4.1362940
C	-0.8894090	2.7679520	1.1326850
C	-2.2564250	2.9895720	0.9716120
C	-0.4163190	1.9778700	2.1812190
C	-3.1618040	2.3978470	1.8463520
H	-2.6362460	3.5903230	0.1517190
C	-1.3223310	1.3944780	3.0631760
H	0.6432410	1.8475630	2.3701770
C	-2.7038210	1.6115010	2.9192360
C	2.9077410	-1.0255200	0.0816050
C	1.6349600	-1.4971040	-0.1760910
C	3.7209690	-1.7247490	1.0221340
C	1.0858080	-2.6303280	0.4713080
H	1.0435770	-1.0123630	-0.9435910
C	3.2000090	-2.8123620	1.6974360
C	1.9158550	-3.2655540	1.4530970
H	3.8112960	-3.3292930	2.4268080
O	-0.8295970	0.6903390	4.1191380
O	-3.5595360	1.0405600	3.8083430
O	-4.4879940	2.6472840	1.6650720
C	-1.1158540	-0.7107140	4.1071880
H	-0.6470630	-1.1225530	5.0015230
H	-2.1933220	-0.8920720	4.1356710
H	-0.6792060	-1.1784230	3.2164220
C	-5.2848160	1.5056240	1.3218520
H	-6.2923150	1.8861530	1.1513530
H	-4.9009570	1.0428850	0.4065630
H	-5.2966620	0.7746440	2.1351650
C	-4.2259210	1.9589690	4.6836590
H	-4.8581270	1.3513750	5.3316420
H	-3.4930270	2.5024950	5.2886560
H	-4.8411810	2.6636980	4.1169720
N	5.0801940	-1.3630840	1.3148710
O	5.6278000	-1.8709900	2.2804660
O	5.6528750	-0.5616790	0.5643630
N	1.4928330	-4.4156210	2.2106400
O	2.2358010	-4.8542610	3.0761540
O	0.3906600	-4.9146760	1.9596360
N	-0.1346290	-3.0893180	0.1529990
H	-0.3936570	-3.9607240	0.6072930
C	-1.0125680	-2.5643980	-0.8325720
C	-1.5700020	-1.2939210	-0.6966180
C	-1.3474490	-3.3751360	-1.9148390
C	-2.4793240	-0.8373450	-1.6500830
H	-1.3475020	-0.6694010	0.1629820
C	-2.2565140	-2.9200760	-2.8673500
H	-0.9064280	-4.3595750	-2.0329030
C	-2.8497210	-1.6535510	-2.7317600
O	-3.0795390	0.3702540	-1.4541000
O	-3.7648640	-1.1958230	-3.6318570
O	-2.6029530	-3.7600590	-3.8828420
C	-2.7558470	1.3776370	-2.4137370
H	-3.0040520	1.0511210	-3.4269540
H	-3.3563390	2.2497990	-2.1522780
H	-1.6916560	1.6342480	-2.3491500
C	-2.2442250	-3.3239950	-5.1974380
H	-2.5829760	-4.1068650	-5.8765940
H	-2.7310790	-2.3776710	-5.4478450
H	-1.1564810	-3.2180110	-5.2755580
C	-5.0529860	-1.8139940	-3.5339980
H	-5.4907080	-1.6248890	-2.5481700
H	-5.6705990	-1.3510740	-4.3043600
H	-4.9831380	-2.8913420	-3.7120140
H	4.4221210	0.1210280	-0.5934890
H	-0.2172370	4.3491700	-0.0812080
H	4.6227500	0.7317740	-2.5308020

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C	3.0227330	1.9828600	-2.7429090
C	3.8738450	0.9082700	-2.9966130
C	3.9061980	-0.1751960	-2.1210190
C	3.0021670	-0.2003610	-0.9281250
C	2.0751070	0.8789390	-0.7615380
C	2.0066180	1.8997680	-1.6616890
H	4.5852870	0.9675490	-3.8092870
H	1.3644210	0.8253170	0.0532770
N	3.0954160	3.1176110	-3.4295180
N	4.7267780	-1.1982280	-2.2488220
N	3.1364180	-1.2286400	-0.1613680
N	1.0690120	2.8987150	-1.6380250
H	4.6739020	-1.8841890	-1.5003260
H	0.7628700	3.2298240	-2.5442390
C	4.0305760	3.3628290	-4.5091810
H	3.8860850	2.6353740	-5.3126630
H	3.8475480	4.3616030	-4.9015870
H	5.0637630	3.3040640	-4.1503360
C	5.6831920	-1.3735690	-3.3183050
H	6.4419560	-0.5839590	-3.2948910
H	6.1736610	-2.3369300	-3.1892400
H	5.1809520	-1.3583460	-4.2904540
C	0.1099760	3.0765230	-0.6153470
C	0.5007750	3.1578900	0.7216510
C	-1.2299090	3.2355850	-0.9678440
C	-0.4604440	3.3405000	1.7123800
H	1.5428970	3.0845690	1.0140430
C	-2.1883200	3.4450850	0.0214120
H	-1.5517510	3.1900320	-2.0042820
C	-1.8200860	3.4605180	1.3769720
C	2.3418130	-1.4906560	0.9348720
C	0.9878090	-1.7401740	0.7687680
C	2.9022750	-1.6652560	2.2323730
C	0.1352050	-2.1342000	1.8244610
H	0.5681510	-1.6341560	-0.2240750
C	2.1026890	-2.0527150	3.2870740
C	0.7438480	-2.2762180	3.1145850
H	2.5359830	-2.1689800	4.2725530
O	-3.4940370	3.5363290	-0.3585150
O	-2.7504430	3.6064480	2.3636870
O	-0.0525640	3.3248030	3.0118220
C	-4.1341440	4.7844490	-0.0760660
H	-5.1561800	4.6878090	-0.4437920
H	-4.1426000	4.9911140	0.9973200
H	-3.6288140	5.5969430	-0.6100470
C	-0.2411410	4.5423810	3.7380590
H	0.1396590	4.3552230	4.7427350
H	0.3347360	5.3513840	3.2743750
H	-1.2989020	4.8125310	3.7859860
C	-3.5279300	2.4314710	2.6156370
H	-4.2231270	2.6919110	3.4146670
H	-4.0851440	2.1336410	1.7218060
H	-2.8811520	1.6108180	2.9447090
N	4.2928800	-1.4083240	2.5064360
O	4.7594110	-1.8277220	3.5619620
O	4.9431550	-0.7782220	1.6789430
N	0.0053470	-2.6446580	4.2893290
O	0.6130200	-2.8343900	5.3347470
O	-1.2246790	-2.7554780	4.2066960
N	-1.1800250	-2.3421580	1.6202390
H	-1.7214860	-2.4949960	2.4660550
C	-1.8680510	-2.3149230	0.3840820
C	-1.4567870	-3.1037130	-0.6910740
C	-3.0244720	-1.5421650	0.2878360
C	-2.1823430	-3.0846040	-1.8794240
H	-0.5947590	-3.7585410	-0.6157870
C	-3.7548610	-1.5280900	-0.8987570
H	-3.3596710	-0.9316990	1.1204510
C	-3.3255270	-2.2771820	-2.0059230
O	-1.7231160	-3.8237720	-2.9308620
O	-4.0372830	-2.2320210	-3.1688800
O	-4.8358300	-0.7029050	-0.9857380
C	-2.5680580	-4.9064640	-3.3329760
H	-3.5496830	-4.5441300	-3.6500210
H	-2.0624820	-5.3890460	-4.1701320
H	-2.6803130	-5.6227250	-2.5115240
C	-6.0983360	-1.3602750	-1.1203030
H	-6.8464660	-0.5686770	-1.1779690
H	-6.1304020	-1.9675050	-2.0287680
H	-6.2951980	-1.9854400	-0.2418670
C	-3.4180810	-1.4705330	-4.2089580
H	-2.4443680	-1.8940090	-4.4749110
H	-4.0893810	-1.5237770	-5.0669840
H	-3.3010810	-0.4264040	-3.8988420
H	2.5812290	3.9143810	-3.0794340

9+H+(b)-b

C	-3.3162640	-1.8794730	-2.4916080
C	-3.8529100	-0.7377570	-3.0856210
C	-3.6315970	0.5127930	-2.5126110
C	-2.7849420	0.6331700	-1.2839010
C	-2.1547100	-0.5506380	-0.7802150
C	-2.3380790	-1.7615580	-1.3777220
H	-4.5344660	-0.8357520	-3.9200450
H	-1.4747300	-0.4536750	0.0568060
N	-3.6655660	-3.1029480	-2.8705990
N	-4.1615560	1.6315630	-2.9642190
N	-2.6931090	1.8209210	-0.7929420
N	-1.7031730	-2.9176030	-1.0082430
H	-3.9580030	2.4570660	-2.4070100
H	-1.4655050	-3.5490740	-1.7630490
C	-4.6123340	-3.3964330	-3.9278720
H	-4.2650960	-2.9834450	-4.8789430
H	-4.6959220	-4.4778070	-4.0225740
H	-5.5980890	-2.9813750	-3.6922250
C	-5.0181540	1.7415960	-4.1235020
H	-5.9469000	1.1801310	-3.9754650
H	-5.2619850	2.7917890	-4.2750570
H	-4.5095620	1.3625720	-5.0151450
C	-0.8821380	-3.0601790	0.1330630
C	0.3757120	-3.6437480	-0.0122720
C	-1.3314640	-2.6600520	1.3923340
C	1.1885800	-3.8316050	1.1027680
H	0.7511640	-3.9416740	-0.9866050
C	-0.5176330	-2.8464660	2.5068300
H	-2.3178520	-2.2311920	1.5339450
C	0.7448890	-3.4507120	2.3794850
C	-1.9044980	2.1531600	0.2902940
C	-0.5238560	2.1621790	0.1626910
C	-2.4715140	2.6615760	1.4937420
C	0.3444600	2.6526480	1.1648050
H	-0.0955690	1.8285810	-0.7749900
C	-1.6571760	3.1613190	2.4881310
C	-0.2765390	3.1694010	2.3492890
H	-2.0990650	3.5479100	3.3979760
O	-1.0151390	-2.5155120	3.7315810
O	1.5189570	-3.6378480	3.4858940
O	2.3944080	-4.4444660	0.9315610
C	-0.3527760	-1.4346780	4.3921960
H	-0.8614690	-1.3072090	5.3484580
H	0.7024140	-1.6644590	4.5611860
H	-0.4491310	-0.5145850	3.8034640
C	3.5367690	-3.6122100	1.1650660
H	4.4090310	-4.2446740	0.9956960
H	3.5433910	-2.7770150	0.4561180
H	3.5454580	-3.2377540	2.1925640
C	1.5826720	-4.9938450	3.9399660
H	2.2244490	-4.9893600	4.8217790
H	0.5840700	-5.3506910	4.2137990
H	2.0143920	-5.6415310	3.1707780
N	-3.8926420	2.6603560	1.7294900
O	-4.3259430	3.3520420	2.6464710
O	-4.6007500	1.9632000	1.0102670
N	0.4705360	3.7071130	3.4514800
O	-0.1269490	4.0250080	4.4713440
O	1.6959860	3.8323840	3.3331540
N	1.6804290	2.6483870	0.9962230
H	2.2011140	3.1408910	1.7162830
C	2.4115490	2.0570490	-0.0607210
C	2.2303440	0.7176840	-0.4086640
C	3.3752890	2.8291660	-0.7079430
C	3.0204220	0.1526840	-1.4069180
H	1.5092110	0.0904450	0.1052350
C	4.1775200	2.2587960	-1.6942560
H	3.5190230	3.8733240	-0.4491180
C	4.0171400	0.9089470	-2.0449670
O	2.8755250	-1.1777270	-1.6761250
O	4.8182370	0.3488160	-2.9972060
O	5.1624100	3.0190590	-2.2487100
C	2.3849590	-1.4874100	-2.9817640
H	3.0456350	-1.0896140	-3.7567930
H	2.3574430	-2.5762170	-3.0445170
H	1.3723360	-1.0870610	-3.1112400
C	5.0169820	3.3004470	-3.6428840
H	5.8804090	3.9064920	-3.9196610

H	5.0061730	2.3793620	-4.2312280
H	4.0987500	3.8723020	-3.8190840
C	5.9118040	-0.4061020	-2.4658620
H	5.5468970	-1.2414390	-1.8595160
H	6.4651890	-0.7884660	-3.3244930
H	6.5636810	0.2363140	-1.8644280
H	-3.3802850	-3.8758000	-2.2852310

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C	2.7731340	1.1611920	-3.3226220
C	3.6956540	0.1174690	-3.2651190
C	3.8301160	-0.6289090	-2.0963070
C	2.9542410	-0.3382510	-0.9179410
C	1.9590740	0.6833350	-1.0527710
C	1.7970130	1.3661290	-2.2208480
H	4.3812250	-0.0379900	-4.0873590
H	1.2742470	0.8459420	-0.2303370
N	2.7405590	2.0188300	-4.3361930
N	4.7234850	-1.5838580	-1.9333370
N	3.1723420	-1.0718100	0.1204880
N	0.7964650	2.2700480	-2.4654000
H	4.7366440	-2.0029480	-1.0071930
H	0.4293820	2.2669570	-3.4091500
C	3.6139860	1.9563070	-5.4910180
H	3.4912030	1.0022970	-6.0113360
H	3.3444890	2.7642620	-6.1689500
H	4.6618720	2.0740380	-5.1947960
C	5.6654830	-2.0256980	-2.9366080
H	6.3536620	-1.2176130	-3.2064740
H	6.2406270	-2.8558710	-2.5301600
H	5.1410700	-2.3637270	-3.8357710
C	-0.1142710	2.7586800	-1.5035990
C	-1.4721530	2.7911280	-1.8209170
C	0.3315550	3.2443450	-0.2732260
C	-2.3886540	3.3281930	-0.9187940
H	-1.8386920	2.4104330	-2.7695620
C	-0.5871270	3.7576250	0.6377690
H	1.3838880	3.2535400	-0.0103660
C	-1.9540850	3.8312490	0.3180950
C	2.4096910	-1.0402850	1.2684110
C	1.0712930	-1.4001830	1.2219920
C	2.9941430	-0.7950230	2.5436940
C	0.2554420	-1.5118790	2.3701450
H	0.6358510	-1.6178170	0.2545850
C	2.2315260	-0.8995610	3.6880390
C	0.8864300	-1.2373600	3.6274970
H	2.6824750	-0.6989680	4.6518900
O	-0.1149710	4.2720350	1.8098320
O	-2.8556430	4.3684670	1.1889800
O	-3.6915650	3.4168210	-1.3024320
C	-0.5122190	3.5669050	2.9890210
H	-0.0608240	4.0996160	3.8266520
H	-1.6003460	3.5591440	3.0966870
H	-0.1306860	2.5394560	2.9621210
C	-4.6224340	2.6409470	-0.5396790
H	-5.6028020	2.8388250	-0.9751780
H	-4.3926850	1.5733710	-0.6295130
H	-4.6169900	2.9443460	0.5102910
C	-2.8311960	5.7983150	1.2545800
H	-3.5944680	6.0828260	1.9798580
H	-1.8520360	6.1555020	1.5881570
H	-3.0742560	6.2283420	0.2771060
N	4.3698510	-0.3934960	2.6898540
O	4.8732280	-0.4565430	3.8079160
O	4.9701190	-0.0005330	1.6949680
N	0.1839640	-1.2851740	4.8787200
O	0.8106370	-1.1128630	5.9159000
O	-1.0353100	-1.4969930	4.8663920
N	-1.0468000	-1.8400570	2.2673840
H	-1.5736310	-1.7783130	3.1336010
C	-1.7361130	-2.1939290	1.0814420
C	-1.3140370	-3.2696530	0.2999150
C	-2.8926180	-1.4915500	0.7472360
C	-2.0303240	-3.6177160	-0.8423710
H	-0.4475690	-3.8621610	0.5757720
C	-3.6123540	-1.8417250	-0.3936640
H	-3.2358450	-0.6587320	1.3527720
C	-3.1730410	-2.8903110	-1.2177440
O	-1.5620210	-4.6411670	-1.6142480
O	-3.8788840	-3.2014100	-2.3422700
O	-4.6923780	-1.0845040	-0.7374190
C	-2.4022190	-5.7983850	-1.6711770
H	-3.3833980	-5.5541170	-2.0873550
H	-1.8911410	-6.5107320	-2.3196870
H	-2.5168590	-6.2309260	-0.6711720
C	-5.9548790	-1.7530750	-0.6729490
H	-6.7019570	-1.0179920	-0.9750420
H	-5.9810400	-2.6088920	-1.3525370
H	-6.1580220	-2.0799760	0.3531570
C	-3.2346270	-2.8413620	-3.5673940
H	-2.2770500	-3.3606710	-3.6724270
H	-3.9098740	-3.1473830	-4.3673420
H	-3.0807130	-1.7576520	-3.6120700
H	2.1809280	2.8539380	-4.2289710

9+H+(b)-d

C	2.8863230	0.6677040	3.3326670
C	3.4291930	1.8871910	2.9282070
C	3.3517740	2.2751290	1.5925240
C	2.6336950	1.4109670	0.6040700
C	2.0192970	0.2069210	1.0795760
C	2.0639940	-0.1414210	2.3954030
H	4.0059610	2.4761390	3.6286670
H	1.4479500	-0.3897470	0.3792200
N	3.0987790	0.1678800	4.5440240
N	3.9058030	3.3694280	1.1101140
N	2.6161270	1.8547130	-0.6061980
N	1.4199080	-1.2261100	2.9336490
H	3.8039520	3.4920700	0.1063400
H	1.0245650	-1.0913070	3.8561980
C	3.8771140	0.8207600	5.5773560
H	3.4474290	1.7964990	5.8201890
H	3.8568140	0.1955440	6.4683270
H	4.9164550	0.9528970	5.2577840
C	4.6477120	4.3422410	1.8801330
H	5.5414050	3.8882680	2.3215940
H	4.9541860	5.1483230	1.2152620
H	4.0263100	4.7578760	2.6794940
C	0.7761170	-2.2308680	2.1758150
C	-0.5354090	-2.5837990	2.4904250
C	1.4559280	-2.8904240	1.1508050
C	-1.1657730	-3.6168300	1.7979370
H	-1.0847100	-2.0718380	3.2747120
C	0.8185090	-3.9053370	0.4435940
H	2.4820640	-2.6439100	0.8991210
C	-0.4887730	-4.3024180	0.7769280
C	1.9094540	1.2614510	-1.6321550
C	0.5236380	1.2490640	-1.5908450
C	2.5507610	0.7868780	-2.8112890
C	-0.2818410	0.7729280	-2.6495310
H	0.0364970	1.6346130	-0.7034520
C	1.7978560	0.3112470	-3.8651040
C	0.4117570	0.2833320	-3.8044510
H	2.2952010	-0.0613500	-4.7518980
O	1.5278980	-4.5682860	-0.5141740
O	-1.1044790	-5.3265650	0.1196420
O	-2.4175480	-3.9796410	2.1924000
C	1.0442550	-4.4128760	-1.8513720
H	1.7119040	-4.9985140	-2.4841000
H	0.0205060	-4.7847330	-1.9467510
H	1.0901810	-3.3591380	-2.1499690
C	-3.4531980	-3.8230380	1.2182930
H	-4.3757620	-4.1360230	1.7085480
H	-3.5374780	-2.7711800	0.9217410
H	-3.2675120	-4.4473570	0.3411990
C	-0.6542520	-6.6292660	0.5069620
H	-1.2297360	-7.3393300	-0.0881000
H	0.4130350	-6.7497590	0.2972610
H	-0.8487690	-6.7984430	1.5713970
N	3.9849660	0.7405380	-2.9378730
O	4.4594020	0.5335660	-4.0511090
O	4.6641490	0.9021670	-1.9291780
N	-0.2661700	-0.2571660	-4.9492080
O	0.3915110	-0.5697920	-5.9329080
O	-1.4952340	-0.3914940	-4.9007670
N	-1.6249280	0.7685320	-2.5524670
H	-2.1082400	0.2933230	-3.3089220
C	-2.4010060	1.3318980	-1.5099800
C	-3.3412260	0.5264150	-0.8700880
C	-2.2691710	2.6762990	-1.1618180
C	-4.1658040	1.0680680	0.1142490
H	-3.4420400	-0.5239640	-1.1240500
C	-3.0902210	3.2179740	-0.1754410
H	-1.5644240	3.3254740	-1.6712380
C	-4.0641370	2.4268980	0.4567370
O	-5.1118770	0.2619060	0.6749920
O	-4.8850590	2.9886250	1.3903770
O	-2.9963750	4.5532910	0.0817700
C	-4.9904640	0.0440150	2.0828710
H	-5.0873850	0.9797390	2.6395600
H	-5.8000660	-0.6348030	2.3529280
H	-4.0278390	-0.4282050	2.3108120
C	-2.5446140	4.8984570	1.3923000
H	-2.5286930	5.9883960	1.4292040
H	-3.2231760	4.5118430	2.1571660
H	-1.5312500	4.5136820	1.5576210
C	-6.2168640	3.2360170	0.9264630
H	-6.7076270	2.3018920	0.6357760
H	-6.7511710	3.6891850	1.7623000
H	-6.2018390	3.9297870	0.0793450
H	2.8350450	-0.7943500	4.7066070

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C	-2.5838110	-1.3084630	3.3149230
C	-2.6157340	-2.6866650	3.0996750
C	-2.3197800	-3.2036800	1.8406740
C	-1.8994540	-2.2855920	0.7371570
C	-1.8183860	-0.8826320	1.0193710
C	-2.0826610	-0.3896160	2.2598000
H	-2.9705740	-3.3427140	3.8831930
H	-1.4774900	-0.2194400	0.2340170
N	-3.0243860	-0.7609330	4.4407830
N	-2.4012500	-4.4827190	1.5320290
N	-1.6190390	-2.8555590	-0.3843990
N	-1.9548310	0.9305880	2.6143180
H	-2.1888870	-4.7050920	0.5634250
H	-1.5517680	1.0997960	3.5277750
C	-3.5474590	-1.5078300	5.5668400
H	-2.8013340	-2.2182730	5.9331590
H	-3.7863150	-0.8056030	6.3636030
H	-4.4560850	-2.0513930	5.2859860
C	-2.7813040	-5.5387510	2.4429410
H	-3.8035690	-5.3884720	2.8058420
H	-2.7326540	-6.4879510	1.9119540
H	-2.0998470	-5.5750100	3.2986870
C	-1.7806440	1.9949990	1.7031430
C	-0.7950630	2.9490680	1.9532490
C	-2.6156520	2.1227750	0.5912830
C	-0.6570270	4.0496890	1.1083530
H	-0.1262030	2.8594930	2.8039200
C	-2.4622610	3.2089580	-0.2643260
H	-3.4006160	1.4035350	0.3829780
C	-1.5021660	4.2022880	-0.0019910
C	-1.0778870	-2.1822910	-1.4618660
C	0.2220110	-1.7074420	-1.3771670
C	-1.7435650	-2.0985200	-2.7165920
C	0.9144740	-1.1369130	-2.4684350
H	0.7453370	-1.8270170	-0.4362770
C	-1.0948840	-1.5627930	-3.8101520
C	0.2048920	-1.0862290	-3.7134770
H	-1.6098860	-1.5030470	-4.7608250
O	-3.3306790	3.3359470	-1.3087000
O	-1.3775720	5.2937520	-0.8107840
O	0.2670150	4.9943620	1.4376100
C	-2.7431320	3.2269350	-2.6081250
H	-3.5587410	3.3551430	-3.3205280
H	-1.9869650	4.0008470	-2.7656910
H	-2.2972030	2.2342010	-2.7396950
C	1.3154070	5.2039710	0.4879010
H	1.9719320	5.9560180	0.9270260
H	1.8766720	4.2750960	0.3340120
H	0.9193850	5.5646430	-0.4641950
C	-2.3954990	6.2827970	-0.6238250
H	-2.1699850	7.0878780	-1.3242320
H	-3.3846170	5.8684960	-0.8420700
H	-2.3683370	6.6683970	0.4009280
N	-3.1043560	-2.5370970	-2.8898620
O	-3.5323300	-2.6542500	-4.0343920
O	-3.7726620	-2.7656680	-1.8868050
N	0.7754140	-0.5447980	-4.9151080
O	0.0736550	-0.4521620	-5.9135820
O	1.9605950	-0.1894940	-4.9005920
N	2.1767820	-0.6856960	-2.3349160
H	2.6245560	-0.4111830	-3.2043410
C	2.9360360	-0.6140300	-1.1432150
C	4.2308730	-1.1312110	-1.1536080
C	2.4459660	0.0286810	-0.0056250
C	5.0270100	-1.0334980	-0.0150510
H	4.6328080	-1.6172870	-2.0369290
C	3.2306610	0.1000640	1.1433770
H	1.4638040	0.4893790	0.0066860
C	4.5218740	-0.4529330	1.1607820
O	6.2696450	-1.5951500	-0.0442570
O	5.2660410	-0.3925290	2.3022650
O	2.6842250	0.6609700	2.2599990
C	7.3587900	-0.6761430	0.0837650
H	7.3142900	-0.1407190	1.0361630
H	8.2674620	-1.2772930	0.0384300
H	7.3505010	0.0373320	-0.7476500
C	3.3249970	1.8469750	2.7370900
H	2.7517180	2.1703740	3.6070520
H	4.3592410	1.6468830	3.0272790
H	3.2943800	2.6287800	1.9697710
C	5.4322210	-1.6475640	2.9696520
H	5.9495500	-2.3662490	2.3270070
H	6.0352240	-1.4429130	3.8551010
H	4.4590890	-2.0491160	3.2724300
H	-3.1397720	0.2433260	4.4608830

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C	-3.3162630	-1.8794810	-2.4916040
C	-3.8529110	-0.7377670	-3.0856180
C	-3.6316000	0.5127840	-2.5126100
C	-2.7849440	0.6331640	-1.2839010
C	-2.1547100	-0.5506420	-0.7802130
C	-2.3380780	-1.7615630	-1.3777180
H	-4.5344670	-0.8357650	-3.9200410
H	-1.4747290	-0.4536770	0.0568080
N	-3.6655640	-3.1029580	-2.8705920
N	-4.1615600	1.6315520	-2.9642190
N	-2.6931120	1.8209160	-0.7929440
N	-1.7031700	-2.9176060	-1.0082370
H	-3.9580080	2.4570560	-2.4070120
H	-1.4655010	-3.5490780	-1.7630420
C	-4.6123310	-3.3964460	-3.9278630
H	-4.2650960	-2.9834590	-4.8789350
H	-4.6959170	-4.4778210	-4.0225650
H	-5.5980880	-2.9813900	-3.6922160
C	-5.0181580	1.7415830	-4.1235030
H	-5.9469040	1.1801160	-3.9754650
H	-5.2619920	2.7917740	-4.2750600
H	-4.5095660	1.3625570	-5.0151460
C	-0.8821340	-3.0601800	0.1330690
C	0.3757180	-3.6437470	-0.0122660
C	-1.3314600	-2.6600510	1.3923390
C	1.1885870	-3.8316010	1.1027730
H	0.7511690	-3.9416740	-0.9866000
C	-0.5176270	-2.8464630	2.5068340
H	-2.3178470	-2.2311920	1.5339500
C	0.7448950	-3.4507070	2.3794900
C	-1.9045010	2.1531580	0.2902910
C	-0.5238590	2.1621800	0.1626880
C	-2.4715170	2.6615760	1.4937380

C	0.3444570	2.6526520	1.1648000
H	-0.0955720	1.8285800	-0.7749940
C	-1.6571800	3.1613230	2.4881250
C	-0.2765420	3.1694070	2.3492830
H	-2.0990680	3.5479140	3.3979700
O	-1.0151330	-2.5155080	3.7315860
O	1.5189640	-3.6378390	3.4858990
O	2.3944160	-4.4444600	0.9315670
C	-0.3527710	-1.4346710	4.3921980
H	-0.8614630	-1.3072020	5.3484610
H	0.7024200	-1.6644510	4.5611880
H	-0.4491270	-0.5145790	3.8034650
C	3.5367750	-3.6122010	1.1650680
H	4.4090380	-4.2446630	0.9956990
H	3.5433940	-2.7770070	0.4561180
H	3.5454640	-3.2377420	2.1925650
C	1.5826820	-4.9938360	3.9399730
H	2.2244590	-4.9893470	4.8217850
H	0.5840810	-5.3506830	4.2138070
H	2.0144020	-5.6415220	3.1707860
N	-3.8926460	2.6603540	1.7294870
O	-4.3259470	3.3520420	2.6464670
O	-4.6007520	1.9631950	1.0102660
N	0.4705320	3.7071210	3.4514720
O	-0.1269530	4.0250180	4.4713360
O	1.6959810	3.8323950	3.3331450
N	1.6804250	2.6483920	0.9962170
H	2.2011100	3.1408990	1.7162760
C	2.4115460	2.0570520	-0.0607250
C	2.2303440	0.7176860	-0.4086640
C	3.3752840	2.8291700	-0.7079500
C	3.0204210	0.1526850	-1.4069170
H	1.5092120	0.0904480	0.1052370
C	4.1775160	2.2587980	-1.6942620
H	3.5190170	3.8733280	-0.4491280
C	4.0171380	0.9089470	-2.0449690
O	2.8755260	-1.1777280	-1.6761210
O	4.8182350	0.3488160	-2.9972070
O	5.1624050	3.0190610	-2.2487180
C	2.3849590	-1.4874150	-2.9817580
H	3.0456340	-1.0896200	-3.7567890
H	2.3574460	-2.5762220	-3.0445080
H	1.3723360	-1.0870680	-3.1112330
C	5.0169750	3.3004440	-3.6428940
H	5.8804010	3.9064890	-3.9196720
H	5.0061680	2.3793570	-4.2312340
H	4.0987420	3.8722970	-3.8190950
C	5.9118020	-0.4061040	-2.4658620
H	5.5468940	-1.2414400	-1.8595150
H	6.4651870	-0.7884680	-3.3244920
H	6.5636790	0.2363130	-1.8644280
H	-3.3802800	-3.8758090	-2.2852230

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C	-1.5522890	4.1184890	0.3058840
C	-2.8888740	4.0289860	0.5439880
C	-3.5976400	2.7770010	0.4196860
C	-2.7914220	1.5493620	0.1281770
C	-1.4627490	1.6695350	-0.2230570
C	-0.8644130	2.9396440	-0.2657390
H	-3.4326740	4.8894180	0.9115180
H	-0.8942910	0.8163510	-0.5669510
N	-0.8055720	5.2555720	0.4618310
N	-4.8543570	2.5735140	0.5946280
N	-3.5109750	0.4127370	0.1640990
N	0.3257730	3.1560020	-0.8158170
H	0.6460300	4.1190740	-0.8265940
C	-1.4307480	6.4797160	0.9228480
H	-1.8845470	6.3695470	1.9170150
H	-0.6704970	7.2597550	0.9670680
H	-2.2029190	6.7897490	0.2136070
C	-5.7613150	3.6539670	0.8740490
H	-6.7603260	3.3705600	0.5357350
H	-5.8190970	3.8028600	1.9609170
H	-5.4826400	4.6071500	0.4100010
C	1.1741140	2.2232410	-1.4737500
C	0.6883400	1.3934770	-2.4820560
C	2.5243780	2.2253960	-1.1321880
C	1.5589800	0.5091350	-3.1164920
H	-0.3473370	1.4272500	-2.8020060
C	3.3974120	1.3537130	-1.7783230
H	2.9111800	2.8865980	-0.3633760
C	2.9156140	0.4606920	-2.7522870
C	-3.1184860	-0.9106740	0.0834720
C	-1.8581880	-1.3152390	0.4899030
C	-4.0210490	-1.9081110	-0.4030280
C	-1.4062740	-2.6524300	0.4178280
H	-1.1876120	-0.5834180	0.9167680
C	-3.5958260	-3.2167560	-0.5174660
C	-2.3222020	-3.6042680	-0.1372750
H	-4.2758490	-3.9612030	-0.9120320
O	4.6977850	1.3318210	-1.3797000
O	3.7504910	-0.4241240	-3.3622910
O	1.0420680	-0.3476340	-4.0373700
C	5.6592610	1.7116220	-2.3709130
H	6.6329390	1.6397980	-1.8855010
H	5.6225750	1.0422000	-3.2338320
H	5.4838260	2.7452770	-2.6886900
C	1.5225640	-0.1934680	-5.3771300
H	1.0017090	-0.9459260	-5.9699660
H	1.2741000	0.8050210	-5.7535030
H	2.6011500	-0.3590870	-5.4293860
C	4.0477750	-1.5880720	-2.5799160
H	4.7789190	-2.1591690	-3.1530950
H	4.4676560	-1.3107880	-1.6083050
H	3.1423300	-2.1881260	-2.4384490
N	-5.3765770	-1.6341690	-0.8003190
O	-5.9892310	-2.4945960	-1.4174570
O	-5.8736570	-0.5480610	-0.4906730
N	-2.0000550	-4.9942660	-0.3118710
O	-2.8673270	-5.7543950	-0.7189420
O	-0.8524510	-5.3731590	-0.0475860
N	-0.1787350	-3.0023770	0.8429730
H	0.0793420	-3.9625420	0.6315310
C	0.7850960	-2.1886810	1.4810600
C	0.4667190	-1.4059580	2.5915720
C	2.1013400	-2.2585150	1.0248830
C	1.4572350	-0.6422220	3.2055720
H	-0.5351130	-1.3897130	3.0077330
C	3.0975100	-1.5200930	1.6582160
H	2.3672000	-2.8842940	0.1786630
C	2.7793800	-0.6713030	2.7324050
O	1.0965620	0.1767630	4.2340770
O	3.7301980	0.0917730	3.3427300
O	4.3633870	-1.5776380	1.1553120
C	1.6381270	-0.1674860	5.5124950
H	2.7305730	-0.1354900	5.4977620
H	1.2552730	0.5758530	6.2128330
H	1.2938310	-1.1635640	5.8127020
C	5.3451730	-2.1450010	2.0285240
H	6.2877650	-2.1156890	1.4808520
H	5.4338710	-1.5672470	2.9525170
H	5.0885670	-3.1846520	2.2600380
C	4.1704420	1.2170390	2.5760490
H	3.3388940	1.9115730	2.4123700
H	4.9425750	1.7062920	3.1711690
H	4.5861280	0.8999500	1.6149160
H	0.1210420	5.1107660	0.8431310
H	-4.5215880	0.5843420	0.2274300

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C	-1.8106400	3.9964590	0.3841920
C	-3.1023620	3.7790420	0.7552040
C	-3.6980440	2.4652560	0.6928990
C	-2.8131580	1.3206800	0.3101060
C	-1.5382700	1.5644480	-0.1583410
C	-1.0729010	2.8847550	-0.2567220
H	-3.6887810	4.5862100	1.1744710
H	-0.9278180	0.7670830	-0.5607940
N	-1.1688940	5.2019510	0.4652810
N	-4.9064700	2.1438530	0.9900920
N	-3.4138060	0.1204490	0.3872140
N	0.0269440	3.2043220	-0.9310420
H	0.2570560	4.1908970	-0.9832150
C	-1.8612120	6.3634400	0.9878990
H	-2.2002930	6.2187360	2.0225930
H	-1.1808830	7.2143570	0.9558890
H	-2.7274640	6.5900660	0.3603500
C	-5.8716740	3.1415390	1.3704630
H	-6.8749890	2.7377600	1.2227330
H	-5.7634450	3.3676850	2.4401700
H	-5.7783800	4.0805970	0.8118170
C	0.8555000	2.3312050	-1.6923050
C	0.3094990	1.5252970	-2.6889370
C	2.2281810	2.3608530	-1.4630260
C	1.1447590	0.6881780	-3.4256960
H	-0.7515480	1.5372510	-2.9140910
C	3.0656290	1.5388260	-2.2138140
H	2.6607440	3.0063130	-0.7054890
C	2.5279420	0.6632190	-3.1743870
C	-2.8906420	-1.1499290	0.2100800
C	-1.5845580	-1.4370320	0.5645340
C	-3.6897650	-2.2018280	-0.3332800
C	-0.9868660	-2.7047000	0.3781930
H	-0.9906040	-0.6637070	1.0320390
C	-3.1211580	-3.4372300	-0.5713130
C	-1.7997690	-3.7020150	-0.2515740
H	-3.7224770	-4.2210060	-1.0147600
O	4.3967230	1.5456590	-1.9278080
O	3.3201260	-0.1836690	-3.8856030
O	0.5749980	-0.1507090	-4.3311970
C	5.2579150	1.9879280	-2.9838330
H	6.2710910	1.9364150	-2.5844930
H	5.1700290	1.3434820	-3.8621960
H	5.0216220	3.0231160	-3.2525090
C	0.9329730	0.0686450	-5.6998270
H	0.3895250	-0.6814310	-6.2750970
H	0.6190390	1.0699420	-6.0150360
H	2.0081520	-0.0550820	-5.8496470
C	3.8331080	-1.2930000	-3.1377490
H	4.4426840	-1.8698630	-3.8336620
H	4.4487700	-0.9495800	-2.3010100
H	3.0092510	-1.9131020	-2.7691610
N	-5.0803050	-2.0501100	-0.6701800
O	-5.6105790	-2.9099270	-1.3600210
O	-5.6855010	-1.0669830	-0.2358630
N	-1.3226130	-5.0242890	-0.5543890
O	-2.1101800	-5.8489180	-0.9958500
O	-0.1275030	-5.2785820	-0.3625080
N	0.2785880	-2.9468190	0.7670520
H	0.6462320	-3.8446620	0.4633960
C	1.1188120	-2.1266820	1.5538690
C	2.4531250	-1.9954120	1.1688680
C	0.6613380	-1.5184700	2.7238180
C	3.3394710	-1.2665360	1.9591790
H	2.8203920	-2.4573340	0.2577980
C	1.5440010	-0.7790930	3.5078940
H	-0.3574990	-1.6474300	3.0734600
C	2.8969970	-0.6632650	3.1493400
O	4.6495690	-1.2309450	1.5880020
O	3.7494110	0.0278330	3.9594330
O	1.0851330	-0.2671030	4.6848870
C	5.1895380	0.0618870	1.2925610
H	5.1015970	0.7329360	2.1509650
H	6.2423140	-0.1018110	1.0591140
H	4.6882630	0.4923110	0.4191760
C	1.0650140	1.1586450	4.7675890
H	0.6728270	1.3990620	5.7565150
H	2.0703580	1.5734970	4.6570420
H	0.3991410	1.5732100	4.0011360
C	4.6269860	-0.7992690	4.7317080
H	5.2720930	-1.3970600	4.0804090
H	5.2345810	-0.1208550	5.3317370
H	4.0489890	-1.4559890	5.3902970
H	-0.1940450	5.1572100	0.7344760
H	-4.4268070	0.1869710	0.5340780

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C	1.4924720	4.0992190	-0.1572290
C	2.8172760	4.0012340	-0.4546020
C	3.5146630	2.7384000	-0.3992700
C	2.7055620	1.5121460	-0.1177790
C	1.3939390	1.6356900	0.2907680
C	0.8174800	2.9106970	0.4108960
H	3.3590610	4.8675610	-0.8114610
H	0.8274190	0.7770430	0.6247050
N	0.7565080	5.2492190	-0.2434030
N	4.7621990	2.5299030	-0.6280690
N	3.4044250	0.3662780	-0.2173910
N	-0.3335630	3.1210360	1.0408500
H	-0.6452020	4.0851920	1.0997080
C	1.3783030	6.4804860	-0.6893750
H	1.7880600	6.3986190	-1.7052470
H	0.6282220	7.2712770	-0.6743330
H	2.1843920	6.7555300	-0.0037480
C	5.6566090	3.6238710	-0.9057390
H	5.4787420	4.5015460	-0.2722360
H	6.6849060	3.2867320	-0.7649180
H	5.5503470	3.9344340	-1.9542790
C	-1.1265480	2.1814950	1.7570010
C	-2.4995750	2.1765870	1.5261860
C	-0.5537260	1.3344290	2.7038140
C	-3.3212980	1.3242970	2.2625130
H	-2.9499470	2.8325570	0.7882230
C	-1.3713220	0.4675260	3.4246820
H	0.5083750	1.3518220	2.9220540
C	-2.7651930	0.4756250	3.2368620
C	2.9759190	-0.9477650	-0.1542230
C	1.7060110	-1.3033960	-0.5739890
C	3.8380960	-1.9792360	0.3308310
C	1.2032550	-2.6223460	-0.5099840
H	1.0678730	-0.5436050	-1.0034240
C	3.3603720	-3.2695520	0.4473910
C	2.0730280	-3.6059080	0.0621830
H	4.0084460	-4.0400110	0.8461020
O	-0.7944850	-0.3103230	4.3823830
O	-3.5811610	-0.3246950	3.9749690
O	-4.6624220	1.4133920	2.0726480
C	-0.8742770	-1.7223000	4.1607210
H	-0.3696860	-2.1882420	5.0074180
H	-1.9138360	-2.0575750	4.1160660
H	-0.3541540	-1.9883750	3.2335700
C	-5.3294420	0.2259610	1.6237130
H	-6.3768870	0.5053340	1.5040690
H	-4.9230920	-0.0965260	0.6593210
H	-5.2413410	-0.5749820	2.3611830
C	-3.7457130	0.0838210	5.3391760
H	-4.4222510	-0.6418820	5.7912980
H	-2.7872550	0.0776150	5.8663200
H	-4.1929460	1.0821480	5.3835000
N	5.2032770	-1.7543290	0.7259940
O	5.7823560	-2.6323860	1.3505350
O	5.7396830	-0.6909750	0.4051070
N	1.6897800	-4.9797810	0.2411400
O	2.5217210	-5.7758470	0.6527860
O	0.5262680	-5.3065250	-0.0224020
N	-0.0298760	-2.9201950	-0.9593190
H	-0.3383020	-3.8662280	-0.7529860
C	-0.9116080	-2.0741140	-1.6716490
C	-0.4871170	-1.3668810	-2.7975470
C	-2.2481850	-2.0307290	-1.2761850
C	-1.3931460	-0.5772560	-3.5010000
H	0.5317560	-1.4404220	-3.1633750
C	-3.1568500	-1.2491080	-1.9865770
H	-2.5950510	-2.5876860	-0.4114840
C	-2.7334830	-0.4889080	-3.0886580
O	-0.9323060	0.1474270	-4.5606800
O	-3.6315760	0.2906280	-3.7560140
O	-4.4384120	-1.1689330	-1.5307860
C	-1.4583390	-0.2283430	-5.8380820
H	-2.5443260	-0.1066530	-5.8689590
H	-0.9891720	0.4363920	-6.5641040
H	-1.1905570	-1.2659390	-6.0655790

C	-5.4347450	-1.7268940	-2.3927000
H	-6.3884830	-1.5827460	-1.8835080
H	-5.4486770	-1.2157180	-3.3586820
H	-5.2545220	-2.7983320	-2.5345660
C	-3.5008500	1.6917870	-3.5030170
H	-2.5109490	2.0513960	-3.8015600
H	-4.2671520	2.1829730	-4.1039030
H	-3.6743050	1.9050560	-2.4424140
H	-0.1907520	5.1309450	-0.5800910
H	4.4152450	0.5184910	-0.3044380

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C	-2.1159890	3.4740870	1.8574110
C	-3.2681840	2.8959450	2.3009270
C	-3.7163930	1.6191830	1.8060380
C	-2.8555790	0.9215570	0.8041760
C	-1.6745430	1.5002510	0.3786960
C	-1.2616260	2.7297680	0.9061000
H	-3.9190650	3.4387360	2.9739850
H	-1.0334670	0.9938110	-0.3292470
N	-1.6694950	4.7036520	2.2577990
N	-4.8125360	1.0126230	2.0997300
N	-3.3434210	-0.2551660	0.3830700
N	-0.0858790	3.2831080	0.5963910
H	0.2425620	4.0119850	1.2210810
C	-2.4166830	5.4724520	3.2331160
H	-2.4936820	4.9098230	4.1675350
H	-1.8751410	6.3977270	3.4304150
H	-3.4280340	5.7211500	2.8838400
C	-5.7242330	1.5715070	3.0649210
H	-6.2328540	2.4506860	2.6456560
H	-6.4857030	0.8296940	3.3096390
H	-5.2216900	1.8830640	3.9893720
C	0.8070780	2.9102950	-0.4373530
C	2.1722870	2.8799090	-0.1595540
C	0.3322410	2.6355880	-1.7198810
C	3.0811660	2.5907770	-1.1770830
H	2.5516360	3.0871050	0.8360510
C	1.2370860	2.3278570	-2.7313350
H	-0.7229570	2.6885780	-1.9645800
C	2.6219570	2.3382460	-2.4827750
C	-2.7349430	-1.1971740	-0.4416070
C	-1.4106100	-1.5309170	-0.2418470
C	-3.4427820	-1.8313130	-1.5026770
C	-0.7044530	-2.4387670	-1.0654460
H	-0.8843140	-1.0917790	0.5965960
C	-2.7693060	-2.6767220	-2.3617000
C	-1.4256880	-2.9689280	-2.1815280
H	-3.3006390	-3.1274560	-3.1909430
O	0.7489270	2.1223340	-3.9857720
O	3.5167090	2.1088780	-3.4820450
O	4.4027020	2.6567160	-0.8742460
C	0.9708150	0.8173970	-4.5313150
H	0.5128460	0.8242510	-5.5206350
H	2.0386210	0.5998330	-4.6163360
H	0.4822660	0.0600870	-3.9077770
C	5.1991410	1.4980400	-1.1490340
H	6.1907170	1.7237310	-0.7555260
H	4.7913640	0.6260680	-0.6270180
H	5.2568040	1.3021640	-2.2211070
C	3.6602380	3.1879280	-4.4149940
H	4.4067160	2.8619640	-5.1397760
H	2.7131920	3.3921720	-4.9229180
H	4.0133440	4.0878480	-3.9010800
N	-4.8462970	-1.6218160	-1.7429200
O	-5.3079510	-1.9557830	-2.8256730
O	-5.5225600	-1.1305510	-0.8384590
N	-0.8269820	-3.8590990	-3.1396230
O	-1.5347550	-4.3614810	-4.0006810
O	0.3872890	-4.0756020	-3.0593750
N	0.5731990	-2.7589070	-0.7907030
H	1.0425000	-3.3140440	-1.5003160
C	1.2489790	-2.5138290	0.4315710
C	2.5129440	-1.9297070	0.3996210
C	0.6797990	-2.9037400	1.6445300
C	3.2268890	-1.7528060	1.5850850
H	2.9563070	-1.6061030	-0.5365580
C	1.3909890	-2.7288020	2.8284710
H	-0.2920640	-3.3847910	1.6852340
C	2.6848820	-2.1802890	2.8096480
O	4.4803520	-1.2263110	1.4959200
O	3.3821910	-2.0780140	3.9772630
O	0.8478590	-3.2065870	3.9825740
C	4.7363860	-0.0492860	2.2679990
H	4.6769550	-0.2513340	3.3398090
H	5.7457440	0.2668460	2.0029170
H	4.0248510	0.7396530	2.0000100
C	0.5472530	-2.2273900	4.9790530
H	0.1273340	-2.7754640	5.8232460
H	1.4490180	-1.6960650	5.2938170
H	-0.1968650	-1.5172050	4.5997750
C	4.4408660	-3.0326190	4.1141930
H	5.1911300	-2.8996560	3.3281810
H	4.8915820	-2.8485240	5.0900110
H	4.0409670	-4.0512520	4.0790320
H	-1.2515230	5.2718490	1.5322830
H	-4.3145990	-0.4156820	0.6625220

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C	2.1623570	3.7727530	-1.1744930
C	3.2350080	3.2755290	-1.8522790
C	3.6478780	1.9013700	-1.7190710
C	2.8329960	1.0162830	-0.8334270
C	1.7163260	1.5136750	-0.1874290
C	1.3403730	2.8515100	-0.3574820
H	3.8570760	3.9401930	-2.4370820
H	1.1051200	0.8684370	0.4269540
N	1.7582750	5.0797560	-1.2308420
N	4.6810420	1.3433280	-2.2445520
N	3.2970990	-0.2371910	-0.7308140
N	0.2299330	3.3645740	0.1791260
H	-0.0807600	4.2473690	-0.2120350
C	2.4645670	6.0267280	-2.0708040
H	2.4277230	5.6960280	-3.1123540
H	1.9646500	6.9925660	-1.9967250
H	3.5150960	6.1482890	-1.7737320
C	5.5483440	2.0771040	-3.1293570
H	6.2001860	2.7433140	-2.5472710
H	6.1885510	1.3743310	-3.6650260
H	5.0034330	2.6896610	-3.8582400
C	-0.6524430	2.7753540	1.1147120
C	-2.0214050	2.9569100	0.9261310
C	-0.1730840	2.0700360	2.2191320
C	-2.9229000	2.4192070	1.8396910
H	-2.4083610	3.4908490	0.0642230
C	-1.0746950	1.5354290	3.1357830
H	0.8879820	1.9657670	2.4166370
C	-2.4590200	1.7217350	2.9698480
C	2.7389960	-1.3026430	-0.0251200
C	1.4060090	-1.6155530	-0.2013700
C	3.5114840	-2.0828600	0.8796900
C	0.7580270	-2.6631740	0.4978640
H	0.8364340	-1.0643450	-0.9399950
C	2.9001950	-3.0775040	1.6162860
C	1.5545580	-3.3695350	1.4552560
H	3.4832440	-3.6503700	2.3268330
O	-0.5748620	0.9238700	4.2435380
O	-3.3120870	1.2109060	3.8968350
O	-4.2507710	2.6426980	1.6417070
C	-0.8638510	-0.4716130	4.3690280
H	-0.3948680	-0.7928810	5.2995430
H	-1.9411830	-0.6478900	4.4159280
H	-0.4265470	-1.0262400	3.5302550
C	-5.0377590	1.4732990	1.3758570
H	-6.0575400	1.8288770	1.2254180
H	-4.6770360	0.9820530	0.4664080
H	-5.0082470	0.7788440	2.2200960
C	-3.9873420	2.1854030	4.7023970
H	-4.6128220	1.6211650	5.3945310
H	-3.2595100	2.7796740	5.2642150
H	-4.6100550	2.8393370	4.0853810
N	4.9237510	-1.8829630	1.0785420
O	5.4431660	-2.3635590	2.0767060
O	5.5466950	-1.2527090	0.2243510
N	1.0330360	-4.4389310	2.2663780
O	1.7693450	-4.9674450	3.0866580
O	-0.1441830	-4.7795370	2.1073510
N	-0.5248670	-2.9714590	0.2434270
H	-0.8773960	-3.7834570	0.7416890
C	-1.3237250	-2.4211340	-0.7985430
C	-1.8202840	-1.1218560	-0.7109640
C	-1.6284120	-3.2275700	-1.8927390
C	-2.6309790	-0.6296160	-1.7329000
H	-1.6072080	-0.4919480	0.1470650
C	-2.4561050	-2.7431030	-2.9042650
H	-1.2369960	-4.2369840	-1.9670830
C	-2.9785570	-1.4424360	-2.8245680
O	-3.1594280	0.6224710	-1.6092650
O	-3.7998350	-0.9787250	-3.8090690
O	-2.8000770	-3.5825910	-3.9190840
C	-2.6824710	1.5788410	-2.5582290
H	-2.8426980	1.2322650	-3.5827680
H	-3.2566500	2.4903420	-2.3864530
H	-1.6172770	1.7792130	-2.3908460
C	-2.3314250	-3.2112600	-5.2182040
H	-2.6887870	-3.9843760	-5.8992420
H	-2.7309000	-2.2390490	-5.5175910
H	-1.2357590	-3.1905500	-5.2324680
C	-5.1885080	-0.9728240	-3.4608730
H	-5.3688820	-0.3247480	-2.5975550
H	-5.7187090	-0.5843800	-4.3311570
H	-5.5315390	-1.9901320	-3.2449760
H	1.4491080	5.4771380	-0.3529330
H	4.2346440	-0.3521130	-1.1236320

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C	0.3010200	3.8837280	-1.0023500
C	-1.0379980	4.2338480	-0.8432280
C	-2.0423380	3.2788390	-1.0230750
C	-1.6993730	1.9138950	-1.4588980
C	-0.4075590	1.5491350	-1.5973300
C	0.6733140	2.4814030	-1.3447020
H	-1.3029410	5.2437130	-0.5584120
H	-0.1661280	0.5604270	-1.9710380
N	1.3030710	4.7312600	-0.8327180
N	-3.3279810	3.5403500	-0.8294030
N	-2.7700240	1.0519490	-1.7561300
N	1.9387260	2.2539060	-1.4732400
C	1.1632670	6.1286210	-0.4948290
H	0.6594770	6.2478460	0.4704240
H	2.1572960	6.5684700	-0.4275140
H	0.5922420	6.6627580	-1.2618270
C	-3.8633960	4.8241390	-0.4308510
H	-3.6366100	5.5877010	-1.1816280
H	-4.9441760	4.7325510	-0.3368450
H	-3.4480970	5.1352820	0.5332790
C	2.5158690	1.0117880	-1.6722010
C	3.6663960	0.9815540	-2.4773630
C	2.0802290	-0.1701440	-1.0470190
C	4.3015620	-0.2207360	-2.7522570
H	4.0350110	1.8956750	-2.9301910
C	2.7479730	-1.3663450	-1.2786730
H	1.2734560	-0.1656840	-0.3212280
C	3.8307370	-1.4194530	-2.1800510
C	-2.9551770	-0.1911580	-1.2165200
C	-2.2549210	-0.5965970	-0.0852480
C	-3.9061660	-1.1093600	-1.7737320
C	-2.4261370	-1.8447710	0.5349890
H	-1.5377520	0.0882100	0.3461230
C	-4.0768690	-2.3560310	-1.1961770
C	-3.3655180	-2.7459420	-0.0772850
H	-4.7856270	-3.0466960	-1.6352070
O	2.2888880	-2.4949910	-0.6670490
O	4.4731590	-2.5778450	-2.4702820
O	5.3359940	-0.2264370	-3.6369870
C	3.1883690	-3.0891220	0.2766900
H	2.7019520	-4.0024460	0.6213260
H	4.1457930	-3.3360210	-0.1906100
H	3.3438090	-2.4154110	1.1259340
C	6.6154820	-0.5581790	-3.0910150
H	7.3188680	-0.5116220	-3.9230650
H	6.9025740	0.1745210	-2.3282630
H	6.6130190	-1.5644840	-2.6644590
C	3.6960120	-3.5646740	-3.1621010
H	4.3653760	-4.4092860	-3.3258890
H	2.8358060	-3.8786560	-2.5653180
H	3.3610110	-3.1677240	-4.1256310
N	-4.6990820	-0.8199470	-2.9288040
O	-5.4548680	-1.6794680	-3.3616390
O	-4.5983480	0.2980970	-3.4581640
N	-3.6249330	-4.0675110	0.4164220
O	-4.4997150	-4.7381610	-0.1164770
O	-2.9516710	-4.4894260	1.3655970
N	-1.7372120	-2.1783940	1.6448920
H	-1.8388720	-3.1472830	1.9321660
C	-0.8503900	-1.3551940	2.3763340
C	-1.2350670	-0.0903640	2.8247630
C	0.4029410	-1.8661750	2.7111020
C	-0.3436250	0.6828000	3.5639210
H	-2.2281620	0.3010950	2.6306150
C	1.2924110	-1.0963590	3.4580220
H	0.7092450	-2.8530230	2.3796270
C	0.9404380	0.1996970	3.8665180
O	-0.7265580	1.9404350	3.9316730
O	1.8325700	0.9570360	4.5686020
O	2.5395080	-1.5927960	3.6945870
C	-0.8697690	2.1489080	5.3404180
H	0.0746520	1.9740880	5.8625190
H	-1.1739830	3.1891190	5.4624450
H	-1.6481870	1.4907420	5.7421270
C	2.8437270	-1.8603770	5.0662290
H	3.8641950	-2.2451870	5.0796460
H	2.7828910	-0.9491710	5.6669210
H	2.1615620	-2.6205770	5.4633270
C	2.4810350	1.9663620	3.7907970
H	1.7498390	2.6710400	3.3811750
H	3.1553060	2.4898680	4.4698270
H	3.0586770	1.5113480	2.9786670
H	2.2264390	4.3358060	-0.9800590
H	-3.3355280	1.2306870	-2.5873600
H	-3.9709450	2.7670610	-0.9469150

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C	-0.2443160	-1.8434520	-3.5463600
C	1.1241190	-2.0265600	-3.7366590
C	2.0400610	-1.1318610	-3.1754120
C	1.5642290	0.0527850	-2.4413060
C	0.2450240	0.2312530	-2.2216610
C	-0.7390020	-0.7142590	-2.7083420
H	1.4823440	-2.8724410	-4.3088760
H	-0.0986500	1.1317370	-1.7255510
N	-1.1659090	-2.6489520	-4.0490060
N	3.3533240	-1.2843390	-3.2773030
N	2.5346230	0.9821990	-2.0264680
N	-2.0215080	-0.6363050	-2.5696660
C	-0.8992970	-3.7903640	-4.8931560
H	-0.3043560	-4.5402180	-4.3609100
H	-1.8493020	-4.2379420	-5.1809350
H	-0.3622940	-3.4891700	-5.7989360
C	4.0116890	-2.3637410	-3.9811450
H	3.7440330	-2.3534320	-5.0424110
H	5.0881460	-2.2298860	-3.8877000
H	3.7367560	-3.3326500	-3.5515410
C	-2.6804390	0.2633450	-1.7487310
C	-3.9204420	0.7351770	-2.2094230
C	-2.2281050	0.6456390	-0.4733520
C	-4.6353840	1.6680540	-1.4722110
H	-4.3001490	0.4112360	-3.1724060
C	-2.9690430	1.5403300	0.2896230
H	-1.3409530	0.2063820	-0.0283610
C	-4.1497410	2.1128770	-0.2260700
C	2.6494360	1.4636840	-0.7492140
C	2.0983360	0.7741220	0.3248700

C	3.3675630	2.6716320	-0.4654990
C	2.1976680	1.1974980	1.6603760
H	1.5655760	-0.1462000	0.1249880
C	3.4499310	3.1311480	0.8381440
C	2.8791890	2.4424920	1.8918790
H	3.9740710	4.0572220	1.0378250
O	-2.4806520	1.8969120	1.5113480
O	-4.8639070	3.0405530	0.4590480
O	-5.7676350	2.1969420	-2.0110280
C	-3.3141800	1.5844850	2.6324910
H	-2.7680030	1.9203430	3.5143990
H	-4.2756710	2.1013650	2.5726710
H	-3.4772040	0.5030940	2.6918940
C	-6.9842900	1.8829380	-1.3278410
H	-7.7795110	2.3757480	-1.8881430
H	-7.1514070	0.7998570	-1.3321180
H	-6.9680590	2.2577640	-0.3013020
C	-4.2051410	4.2969190	0.6693550
H	-4.9203990	4.9224940	1.2034000
H	-3.2979600	4.1722480	1.2667530
H	-3.9600640	4.7562080	-0.2934410
N	3.9998350	3.4674620	-1.4725450
O	4.5334730	4.5201500	-1.1497350
O	3.9909170	3.0630320	-2.6455930
N	3.0217540	3.0295160	3.1930360
O	3.6914320	4.0472550	3.3138990
O	2.4573830	2.4882220	4.1521990
N	1.6741750	0.4682060	2.6659990
H	1.6820840	0.9237020	3.5736800
C	1.1198180	-0.8297250	2.5728370
C	-0.1205810	-1.0689430	3.1621250
C	1.8147670	-1.8690080	1.9520830
C	-0.6675280	-2.3509020	3.1410320
H	-0.6773290	-0.2673420	3.6364400
C	1.2658060	-3.1483390	1.9237100
H	2.7982390	-1.7136820	1.5209620
C	0.0300890	-3.4108570	2.5380390
O	-1.8556010	-2.5504180	3.7794010
O	-0.4675250	-4.6813250	2.5319610
O	2.0035740	-4.1574570	1.3775110
C	-2.9380960	-3.0047560	2.9629000
H	-2.7279380	-3.9878300	2.5339200
H	-3.8056830	-3.0634820	3.6208880
H	-3.1362130	-2.2836400	2.1616650
C	1.4568390	-4.7457070	0.1966730
H	2.1489180	-5.5361600	-0.0968340
H	0.4692080	-5.1726870	0.3900810
H	1.3944720	-4.0000390	-0.6057040
C	-0.3520750	-5.3613080	3.7866250
H	-0.9097990	-4.8349800	4.5676420
H	-0.7769380	-6.3543280	3.6352010
H	0.7004280	-5.4511480	4.0752570
H	-2.1233370	-2.3980470	-3.8222750
H	2.9922030	1.5636890	-2.7297160
H	3.9275900	-0.6007830	-2.7991950

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C	-0.2038580	-3.0028090	2.6952300
C	-1.5315590	-3.4088970	2.5853700
C	-2.4970960	-2.5386680	2.0733610
C	-2.1358540	-1.1550360	1.7062090
C	-0.8579020	-0.7354320	1.8339730
C	0.1848610	-1.6113470	2.3266440
H	-1.8099330	-4.4204030	2.8499320
H	-0.5878090	0.2712540	1.5384040
N	0.7675070	-3.7881550	3.1294430
N	-3.7519540	-2.9132890	1.8600600
N	-3.1765100	-0.3440120	1.2362790
N	1.4378300	-1.3285380	2.4595070
C	0.6035500	-5.1632880	3.5401220
H	0.2157700	-5.7739320	2.7176180
H	1.5750890	-5.5536720	3.8393430
H	-0.0823690	-5.2361210	4.3905300
C	-4.2820970	-4.2301980	2.1428340
H	-4.1760210	-4.4674420	3.2056320
H	-5.3397870	-4.2372700	1.8846450
H	-3.7662210	-4.9936510	1.5510040
C	1.9948850	-0.0672000	2.3073100
C	3.2481110	-0.0007640	1.6805370
C	1.4102440	1.1051690	2.8148190
C	3.8858520	1.2214240	1.5140790
H	3.7229630	-0.9043220	1.3129920
C	2.0628740	2.3248400	2.6764750
H	0.4808500	1.0801080	3.3741600
C	3.3128040	2.3985660	2.0343110
C	-3.1219030	0.5156200	0.1712100
C	-2.1293510	0.4119040	-0.7958790
C	-4.1165510	1.5354000	-0.0030900
C	-2.0379580	1.2567440	-1.9155550
H	-1.3813720	-0.3618750	-0.6882590
C	-4.0429800	2.3882440	-1.0912820
C	-3.0370120	2.2839470	-2.0327640
H	-4.7912320	3.1623440	-1.2053750
O	1.4984770	3.4298790	3.2439040
O	3.9796970	3.5751820	1.9031080
O	5.1217630	1.2443120	0.9451170
C	1.0586580	4.4316460	2.3218790
H	0.6380600	5.2351450	2.9272240
H	1.8915960	4.8134390	1.7249160
H	0.2826320	4.0250550	1.6635010
C	5.2007550	1.9002830	-0.3250580
H	6.2511890	1.8629150	-0.6168590
H	4.5949730	1.3663250	-1.0657640
H	4.8791250	2.9424660	-0.2465260
C	4.5283750	4.1015160	3.1182660
H	5.0231900	5.0340400	2.8456930
H	3.7398390	4.2977180	3.8503110
H	5.2618010	3.4027860	3.5335440
N	-5.2006840	1.7471310	0.9064080
O	-5.9751040	2.6719830	0.7037600
O	-5.3255020	0.9829650	1.8772780
N	-3.0603100	3.2396230	-3.1029850
O	-3.9957570	4.0259590	-3.1742160
O	-2.1293440	3.2392960	-3.9182060
N	-1.0535560	1.1079670	-2.8228830
H	-1.0033460	1.8398200	-3.5251980
C	-0.0666520	0.0924460	-2.8351620
C	-0.4237710	-1.2560020	-2.8602700
C	1.2745460	0.4663140	-2.8952270
C	0.5668700	-2.2336560	-2.9010660
H	-1.4642140	-1.5641850	-2.8721760
C	2.2668420	-0.5112920	-2.9417960
H	1.5637770	1.5123680	-2.8882300
C	1.9254270	-1.8731100	-2.9134860
O	0.1844330	-3.5435470	-2.8686650
O	2.9120480	-2.8147260	-2.9292110
O	3.5699760	-0.1130120	-2.9180480
C	0.4881050	-4.2998550	-4.0453630
H	1.5655590	-4.3301510	-4.2283340
H	0.1142620	-5.3076060	-3.8610860
H	-0.0266530	-3.8715350	-4.9124020
C	4.3230640	-0.4018520	-4.0990440
H	5.3285460	-0.0204940	-3.9164520
H	4.3630570	-1.4780760	-4.2858680
H	3.8873050	0.1150310	-4.9615080
C	3.1025830	-3.4938290	-1.6851820
H	2.1961120	-4.0325510	-1.3914960
H	3.9164120	-4.2018030	-1.8464000
H	3.3855050	-2.7818330	-0.9022190
H	1.6869590	-3.3577000	3.1513840
H	-3.9613300	-0.1524040	1.8629050
H	-4.3592070	-2.2501620	1.3966110

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C	0.5202710	-0.8843360	3.5127990
C	-0.8111190	-0.9036420	3.9250100
C	-1.7604210	-0.0948720	3.2925300
C	-1.3570440	0.7988420	2.1975560
C	-0.0633200	0.8673930	1.8172720
C	0.9566310	0.0500730	2.4420020
H	-1.1187590	-1.5660160	4.7236710
H	0.2118600	1.4995210	0.9805850
N	1.4592040	-1.6513350	4.0477140
N	-3.0487960	-0.1147440	3.6117340
N	-2.3701520	1.5533430	1.5697560
N	2.2130080	-0.0026180	2.1283690
C	1.2412120	-2.6193160	5.0971110
H	0.5149240	-3.3787550	4.7865770
H	2.1883110	-3.1098800	5.3174210
H	0.8770460	-2.1329330	6.0085600
C	-3.6342290	-0.9443430	4.6421900
H	-3.1983460	-0.7131710	5.6192020
H	-4.7040260	-0.7454740	4.6788740
H	-3.4778350	-2.0058600	4.4233350
C	2.8809960	0.8714280	1.3000410
C	3.9496060	0.3383070	0.5634910
C	2.6047390	2.2533690	1.2266430
C	4.6666680	1.1431580	-0.3090050
H	4.1938440	-0.7152580	0.6439950
C	3.3712090	3.0748340	0.4098900
H	1.8707930	2.6877340	1.8936840
C	4.3882320	2.5208690	-0.4091050
C	-2.7174740	1.4493910	0.2529170
C	-2.2568140	0.3960440	-0.5309490
C	-3.5902020	2.4064010	-0.3661200
C	-2.5885430	0.2269490	-1.8851040
H	-1.5981820	-0.3325870	-0.0776640
C	-3.9246970	2.2677630	-1.7025120
C	-3.4468920	1.2225600	-2.4700990
H	-4.5745630	3.0023290	-2.1610330
O	3.2544180	4.4184450	0.3654950
O	5.2018110	3.2550870	-1.1891560
O	5.7082960	0.5937160	-0.9928630
C	2.2644690	5.0382450	1.1723910
H	2.3394650	6.1050370	0.9642620
H	1.2616560	4.6843890	0.9082430
H	2.4552350	4.8606870	2.2364910
C	5.5533720	0.5230610	-2.4111520
H	6.4482950	0.0266040	-2.7878040
H	4.6697430	-0.0721540	-2.6683850
H	5.4748440	1.5199010	-2.8521880
C	4.6591780	4.2841230	-2.0271620
H	5.3837670	4.4124690	-2.8323800
H	3.6972540	3.9722790	-2.4444810
H	4.5388590	5.2168880	-1.4760280
N	-4.1364280	3.5351290	0.3208990
O	-4.8617580	4.3095420	-0.2894210
O	-3.8579480	3.6978970	1.5195680
N	-3.8529980	1.2005670	-3.8451000
O	-4.6496530	2.0419080	-4.2413780
O	-3.3812420	0.3316490	-4.5897970
N	-2.1125900	-0.8138030	-2.5962200
H	-2.3170570	-0.7842790	-3.5905410
C	-1.3253670	-1.8823840	-2.1006050
C	-0.0967460	-2.1443800	-2.7042730
C	-1.7845900	-2.6881800	-1.0585240
C	0.6734890	-3.2226580	-2.2728790
H	0.2773750	-1.5162290	-3.5064480
C	-1.0133210	-3.7633040	-0.6231630
H	-2.7524080	-2.5166530	-0.5987840
C	0.2140680	-4.0570080	-1.2402630
O	1.8445830	-3.4818930	-2.9224640
O	0.9391470	-5.1332030	-0.8198380
O	-1.5254030	-4.5786100	0.3428820
C	3.0294510	-3.3492090	-2.1331190
H	3.0229380	-4.0438630	-1.2887110
H	3.8625330	-3.5810070	-2.7975630
H	3.1277640	-2.3196670	-1.7699480
C	-0.8140940	-4.5847280	1.5813970
H	-1.3415050	-5.2853900	2.2301750
H	0.2181420	-4.9162660	1.4410750
H	-0.8313250	-3.5855180	2.0336040
C	0.9017620	-6.2524690	-1.7121340
H	1.3163720	-5.9853480	-2.6890220
H	1.5130820	-7.0293520	-1.2514250
H	-0.1258860	-6.6127980	-1.8274090
H	2.3866570	-1.5313090	3.6535840
H	-3.6628770	0.4689180	3.0574370
H	-2.7275960	2.3890460	2.0322940

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C	-0.5981890	1.2648020	2.9860480
C	0.5097210	0.6208250	3.5322400
C	0.8690110	-0.6576670	3.0935720
C	0.1184920	-1.3070610	2.0050230
C	-0.9846150	-0.7251500	1.4975630
C	-1.4400360	0.5721870	1.9696820
H	1.0876730	1.1033450	4.3098230
H	-1.5075370	-1.1943670	0.6717450
N	-0.9921800	2.4759310	3.3459390
N	1.8894090	-1.3342740	3.6000980
N	0.5938540	-2.5490340	1.5254920
N	-2.4641840	1.2290560	1.5415270
C	-0.3305110	3.3059220	4.3255850
H	0.7093420	3.4957520	4.0380850
H	-0.8575210	4.2570430	4.3865440
H	-0.3447220	2.8319130	5.3131260
C	2.7533090	-0.8638030	4.6609840
H	2.1762280	-0.6631070	5.5694770
H	3.4889200	-1.6373230	4.8745160
H	3.2758410	0.0494320	4.3588240
C	-3.4472870	0.7152290	0.7111070
C	-3.9704410	1.5802030	-0.2617120
C	-3.9811950	-0.5765580	0.8542290
C	-4.9779930	1.1476190	-1.1125000
H	-3.5801740	2.5874320	-0.3621250
C	-5.0162730	-0.9972050	0.0272160
H	-3.6486660	-1.2429710	1.6432520
C	-5.5384410	-0.1363620	-0.9566510
C	1.4805150	-2.6606330	0.4916730
C	2.0579950	-1.5257140	-0.0677450
C	1.8770480	-3.9362280	-0.0300160
C	3.0137000	-1.5625760	-1.0970260
H	1.7623990	-0.5561310	0.3118110
C	2.8354090	-4.0017060	-1.0261910
C	3.4169060	-2.8641790	-1.5562310
H	3.1376470	-4.9707090	-1.4030220
O	-5.5592190	-2.2287470	0.2461900
O	-6.5663970	-0.5093830	-1.7615030
O	-5.4902850	2.0249760	-2.0180300
C	-5.3815230	-3.1741340	-0.8135890
H	-5.8572720	-4.0957570	-0.4774100
H	-5.8533570	-2.8277280	-1.7372300
H	-4.3143480	-3.3540630	-0.9843380
C	-5.2754650	1.6866630	-3.3905530
H	-5.7513560	2.4755960	-3.9739030
H	-4.2020510	1.6655600	-3.6112280
H	-5.7289930	0.7222680	-3.6337970
C	-7.8384400	-0.6331130	-1.1111580
H	-8.5436870	-0.9322790	-1.8867740
H	-7.8039730	-1.3919890	-0.3245700
H	-8.1401010	0.3314640	-0.6904500
N	1.3321750	-5.1761710	0.4305320
O	1.7685100	-6.2236570	-0.0290030
O	0.4297730	-5.1502120	1.2801200
N	4.4054330	-3.0651820	-2.5749450
O	4.6310570	-4.2034170	-2.9660920
O	5.0037530	-2.0787700	-3.0236490
N	3.5243160	-0.4278800	-1.6143430
H	4.2970460	-0.5596090	-2.2598470
C	3.0934720	0.8918310	-1.3405430
C	4.0498290	1.8526880	-1.0159550
C	1.7509860	1.2517910	-1.4693590
C	3.6607020	3.1721330	-0.7936420
H	5.0994820	1.5903030	-0.9299740
C	1.3578230	2.5640670	-1.2202800
H	0.9995010	0.5297360	-1.7714020
C	2.3054800	3.5358550	-0.8586170
O	4.6132830	4.0767340	-0.4254380
O	1.8990710	4.8135640	-0.6063390
O	0.0281910	2.8630790	-1.2744240
C	4.8525880	5.1273280	-1.3671100
H	3.9491690	5.7201120	-1.5347090

H	5.6310920	5.7533180	-0.9297610
H	5.2085820	4.7102900	-2.3156300
C	-0.3588110	3.7541390	-2.3239280
H	-1.4375850	3.8844230	-2.2272270
H	0.1420150	4.7205690	-2.2238920
H	-0.1305340	3.3110290	-3.2999910
C	1.9082580	5.1725620	0.7777550
H	2.9181410	5.0991680	1.1932890
H	1.5635580	6.2062230	0.8271890
H	1.2230620	4.5297950	1.3419850
H	-1.8267020	2.8131830	2.8765460
H	0.0963020	-3.4037490	1.7643440
H	2.0467880	-2.2611670	3.2227360

9+H+(d)-f

C	-0.8427000	0.0261260	3.9155350
C	0.3953570	-0.3399480	4.4382830
C	1.3025160	-1.0688960	3.6641790
C	0.9431200	-1.4956730	2.2997710
C	-0.2601810	-1.1668550	1.7831080
C	-1.2323880	-0.4083880	2.5434540
H	0.6723120	-0.0319310	5.4377780
H	-0.5074570	-1.4576100	0.7686190
N	-1.7362910	0.7392310	4.5812230
N	2.5208700	-1.3755850	4.0886070
N	1.8985330	-2.2555090	1.6053110
N	-2.4092950	-0.0461620	2.1536560
C	-1.5671540	1.2391280	5.9258990
H	-0.6982220	1.9027240	5.9913800
H	-2.4587910	1.8007730	6.2005220
H	-1.4379480	0.4144370	6.6348560
C	3.0602380	-1.0219390	5.3841700
H	2.4589180	-1.4618000	6.1857470
H	4.0751690	-1.4102230	5.4514330
H	3.0857930	0.0655660	5.5112760
C	-3.0274000	-0.4737520	0.9883970
C	-3.7935790	0.4709730	0.2897210
C	-2.9855200	-1.8037840	0.5350790
C	-4.4541950	0.1121730	-0.8767130
H	-3.8418930	1.4981430	0.6343560
C	-3.6944700	-2.1763030	-0.6009240
H	-2.4764120	-2.5774190	1.1004790
C	-4.4448620	-1.2261600	-1.3183690
C	2.2340430	-2.0857690	0.2862570
C	2.1153050	-0.8444280	-0.3293040
C	2.7642770	-3.1687550	-0.4878760
C	2.4844900	-0.5986020	-1.6634700
H	1.7591570	-0.0117630	0.2629680
C	3.1268930	-2.9568180	-1.8067700
C	3.0016770	-1.7183440	-2.4058220
H	3.5222120	-3.7827100	-2.3844110
O	-3.7200890	-3.4934650	-0.9474600
O	-5.1338960	-1.6239810	-2.4185920
O	-5.1855650	1.0588440	-1.5315640
C	-3.0738530	-3.8179730	-2.1809020
H	-3.1810460	-4.8963450	-2.3030270
H	-3.5460780	-3.3013630	-3.0203940
H	-2.0094810	-3.5604350	-2.1305950
C	-4.6964280	1.4104540	-2.8295470
H	-5.3835420	2.1628860	-3.2177350
H	-3.6907630	1.8381650	-2.7510900
H	-4.6826650	0.5428220	-3.4955560
C	-6.5620990	-1.5876680	-2.2969260
H	-6.9527970	-1.9403790	-3.2516610
H	-6.8873860	-2.2585550	-1.4953260
H	-6.9129760	-0.5707200	-2.1019710
N	2.9418790	-4.4937400	0.0237310
O	3.3148470	-5.3777570	-0.7348310
O	2.7152470	-4.7062570	1.2254840
N	3.4295920	-1.6302110	-3.7741020
O	3.7797840	-2.6512070	-4.3509000
O	3.4307480	-0.5229910	-4.3271580
N	2.3885660	0.6267770	-2.2158200
H	2.8031740	0.6983390	-3.1409770
C	1.9032060	1.8192490	-1.6336560
C	0.6658080	1.8855620	-0.9917350
C	2.6805000	2.9693820	-1.7778000
C	0.2119060	3.1047860	-0.4903080
H	0.0197740	1.0185130	-0.9038700
C	2.2142180	4.1922700	-1.3027450
H	3.6477670	2.9305230	-2.2686120
C	0.9653020	4.2770460	-0.6664450
O	-1.0248500	3.1395910	0.0849160
O	0.5082250	5.4865930	-0.2302120
O	2.9628950	5.3054820	-1.5377160
C	-1.0567430	3.5421260	1.4560810
H	-0.6908420	4.5647650	1.5784190
H	-2.1012460	3.4818270	1.7642130
H	-0.4565800	2.8565180	2.0654560
C	3.4878200	5.9550570	-0.3775840
H	4.0535580	6.8130380	-0.7425480
H	2.6842810	6.2937630	0.2814230
H	4.1598900	5.2784150	0.1626830
C	-0.4982680	6.0668770	-1.0664370
H	-1.3842600	5.4255090	-1.1108070
H	-0.7577650	7.0238180	-0.6119970
H	-0.1063280	6.2330180	-2.0753670
H	-2.5972340	0.9249150	4.0761050
H	2.0712060	-3.2074680	1.9369540
H	3.1317440	-1.8391080	3.4277070

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