Supporting Information

Superhelicenes in the gas phase: Experimental and computational evidence of stable radical cation dimers

Marina Kinzelmann, David Reger, Vera Warmbrunn, Dominik Lungerich,
Norbert Jux, Thomas Drewello

Contents

Mass Spectrometry

Material and Sample preparation

Both molecules (**A** and **B**) were synthesized following reported procedures.[1] Stock solutions of **A** and **B** were prepared in dichloromethane (0.2 g/L). The final concentration for the electrospray measurements was 10^{-5} M for **A** and **B**, diluted in acetonitrile (ACN) and dicholormethane (DCM) (1:1; v:v). All solvents were purchased from VWR Chemicals in HPLC grade purity.

Instrumentation and methods

The measurements were performed using a MS/MS capable electrospray ionization quadrupole/time-of-flight (ESI-Qq-ToF) instrument (micrOTOF-Q II, Bruker). Between the needle and the glass capillary, a voltage of - 4.5 kV (positive ion mode) was applied. The nebulizer nitrogen pressure was set to 400 hPa, the dry gas flowrate to 4.0 L/min and 453 K gas temperature. The instrumental parameters were optimized to obtain good intensities for the respective experiments. For the MS/MS experiments, the precursor ions were mass selected by the mass analyser quadrupole and accelerated into the collision cell quadrupole, which contained nitrogen as collision gas, generated by a Parker LCMS64 nitrogen generator with a purity of 99.999 % and a flow rate of 0.5 L/min.

The survival yield (SY) of the precursor ion was plotted as a function of the collision energy in the centre-of-mass frame (E_{com}).[2] E_{com} is expressed by equation (1) through conversion of the laboratory frame collision energy E_{lab}. M_{N2} represents the molecular mass of nitrogen used as the collision gas and M_{ion} is the molecular mass of the investigated precursor ion.

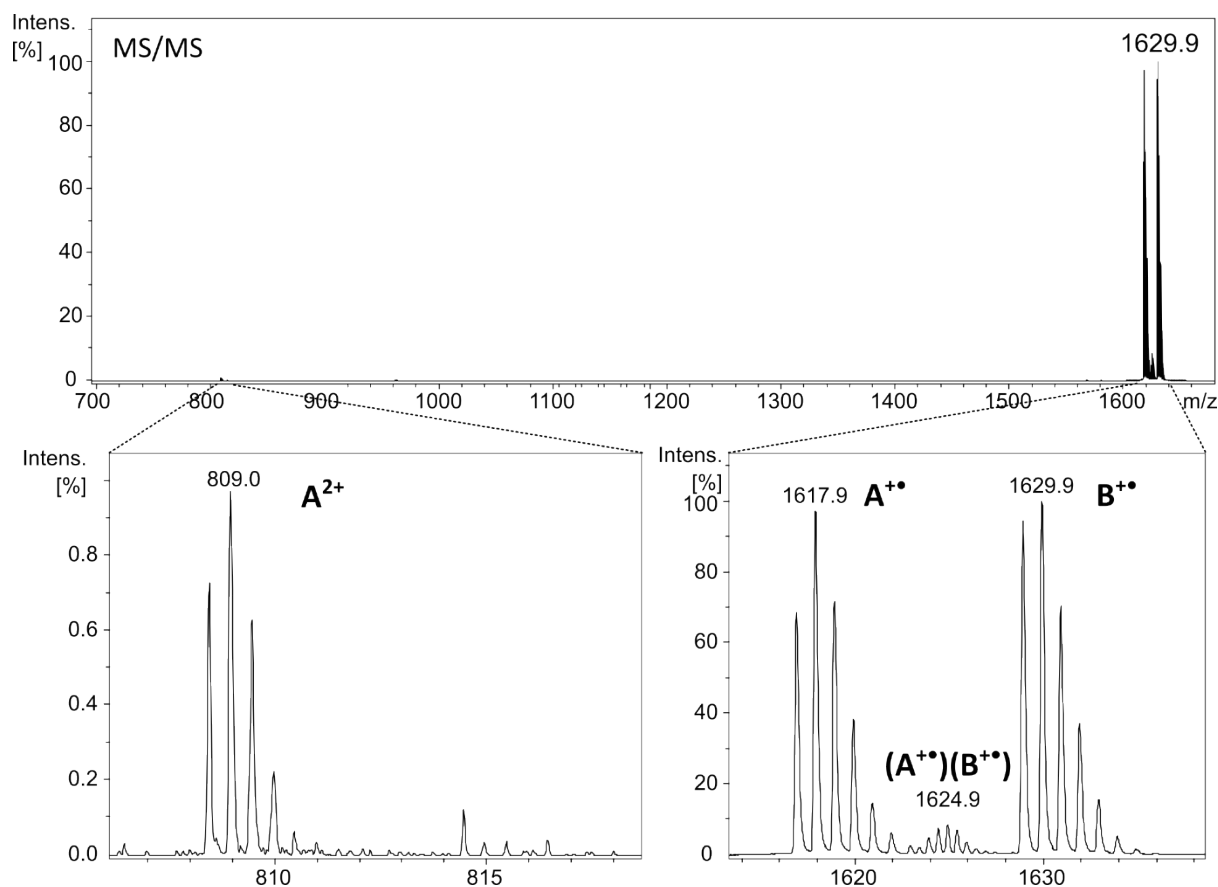$$E_{com} = E_{lab} \times \frac{M_{N2}}{M_{N2} + M_{ion}}$$

(1)

Breakdown graph of mono- and dicationic monomers A and B
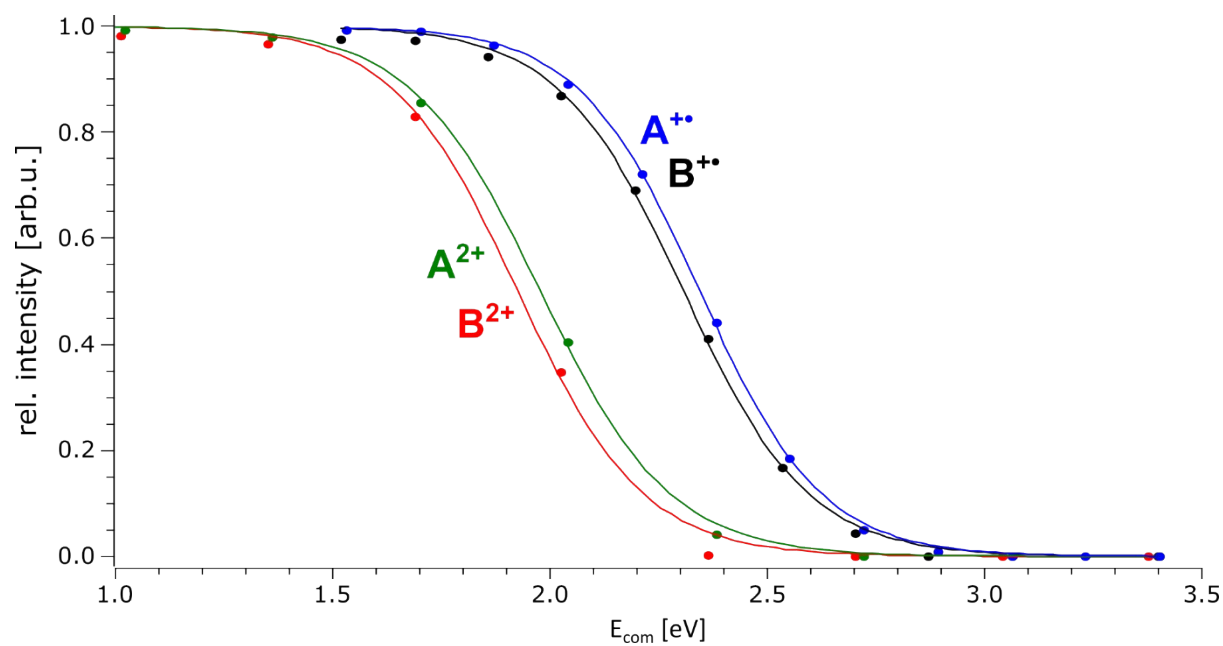
Figure S1: Breakdown graphs of the mono- and dicationic superhelicene monomers **A** and **B**.

CID mass spectrum of $(A^{+\bullet})(B^{+\bullet})$

Figure S2: The CID mass spectrum of **AB²⁺**

The CID spectra of AB^{2+} show a signal for A^{2+} of about 1% relative intensity to the signals of $A^{+\bullet}$ and $B^{+\bullet}$. The A^{2+} signal is, however, not very likely caused by fragmentation of AB^{2+} and, therefore, cannot be taken as evidence of a dication-neutral complex on the basis of the following points.

Firstly, the A^{2+} signal did not show any intensity variations and was observed in low abundance at various collision energies almost throughout the whole CID experiment.

Secondly, there is no clearly visible signal for B^{2+} in the CID spectra of AB^{2+}. A dication-neutral complex would not only have a composition of A^{2+}-B but also of B^{2+}-A and should also show the B^{2+} fragment ion in similar abundance as A^{2+}.

Thirdly, in the CID spectra of A_2^{2+} and B_2^{2+} a dication fragment signal (A^{2+} or B^{2+}) could not be established.

We assume that the A^{2+} signal in the CID spectrum of AB^{2+} is caused by the fragmentation of a higher charged isobaric interference.

DFT calculations

General Computational Methods

Geometry optimization and energy calculations were carried out using Q-Chem, implemented in the Spartan '20 work-package.[3, 4]

The structures of monomeric helicenes were first optimized at the semi-empirical level PM6, and then further refined at the density functional theory level, using the Grimme dispersion-corrected range-separated hybrid generalized gradient approximation (RSH-GGA) functional ωB97X-D by Head-Gordon with the Pople-type dual basis split-valance double-ζ quality basis set 6-31G(d).[5] All geometries were optimized in the respective charge state of interest (neutral, open-shell radical cation, open-shell dication, and closed-shell dication). Outer *tert*-butyl groups, which do not interact with the π-surfaces, were omitted to reduce the computational costs. Single-point calculations for the energy evaluation and display of surfaces were carried out using the triple-ζ quality basis set 6-311G(d,p).

Calculations of dimeric structures were generated from the crystal structure of **A** (CIF: 2062652).[1] The *tert*-butyl groups were replaced by H-atoms and the carbon skeleton was frozen to maintain the geometrical arrangement of the two molecules as obtained in the crystal structure. Derivatives of **A** and **AB** dimers were made from the parent crystal structure and modification at the appropriate position. Single point calculations of the neutral, open-shell radical cation, open-shell dication, and closed-shell dication were carried out using the generalized gradient approximation (GGA) PBE-D3,[6, 7] the global-hybrid generalized gradient approximation (GH-GGA) B3LYP-D3,[7-9] and the RSH-GGA CAM-B3LYP functional,[10] in combination with the Karlsruhe-type dual-basis double-ζ def2-SVPD[def2-SV(P)] basis set by Ahlrich and Weigend.[11]

Table 1: Summary of DFT calculations. Basis set for entries 1–8: 6-311G(d,p)[6-31G(d)], for 9-23: def2-SVPD[def2-SV(P)].

Entry	Functional	Species	E (a.u.)	ΔE (eV)	HOMO (eV)	LUMO (eV)	HLG (eV)
1	ωB97X-D	[**B**]	-3648.035473	0	-6.94	-1.12	-5.82
2		[**B**]$^{+\bullet}$	-3647.795282	6.53593338	-9.17	-3.89	-5.28
3		[os**B**]$^{2+}$	-3647.470186	15.3822507	-11.25	-8.3	-2.95
4		[cs**B**]$^{2+}$	-3647.478728	15.1498109	-11.31	-5.62	-5.69
5	ωB97X-D	[**A**]	-3609.931973	0	-6.86	-0.93	-5.93
6		[**A**]$^{+\bullet}$	-3609.69469	6.45680263	-9.09	-3.67	-5.42
7		[os**A**]$^{2+}$	-3609.371914	15.2399895	-11.16	-8.28	-2.88
8		[cs**A**]$^{2+}$	-3609.382105	14.9626781	-11.2	-5.4	-5.8
9	B3LYP-D3	[2**B**]	-6663.72539	0	-5.23	-2.66	2.57
10		[2**B**]$^{+\bullet}$	-6663.506755	5.94936444	-7.01	-4.45	2.56
11		[os-2**B**]$^{2+}$	-6663.224752	13.6230609	-8.51	-8.23	0.28
12		[cs-2**B**]$^{2+}$	-6663.230083	13.4779969	-8.66	-6.11	2.55
13	CAM-	[2**B**]	-6659.636864	0	-6.28	-1.66	4.62
14	B3LYP	[2**B**]$^{+\bullet}$	-6659.399816	6.45040795	-8.06	-3.57	4.49
15		[os-2**B**]$^{2+}$	-6659.093702	14.7801984	-9.27	-8.4	0.87
16		[cs-2**B**]$^{2+}$	-6659.114852	14.2046773	-9.69	-5.23	4.46
17	B3LYP-D3	[**AB**]	-6625.624393	0	-5.22	-2.64	2.58
18		[**AB**]$^{+\bullet}$	-6625.406322	5.93401721	-6.99	-4.43	2.56
19		[os-**AB**]$^{2+}$	-6625.12507	13.5872779	-8.49	-8.21	0.28
20		[cs-**AB**]$^{2+}$	-6625.130327	13.4442276	-8.63	-6.09	2.54
21	CAM-	[**AB**]	-6621.560839	0	-6.27	-1.65	4.62
22	B3LYP	[**AB**]$^{+\bullet}$	-6621.324355	6.43506072	-7.98	-3.45	4.53
23		[os-**AB**]$^{2+}$	-6621.018761	14.7507013	-9.25	-8.39	0.86
24		[cs-**AB**]$^{2+}$	-6621.039828	14.1774387	-9.64	-5.2	4.44
25	B3LYP-D3	[2**A**]	-6591.989552	0	-4.94	-2.09	2.85
26		[2**A**]$^{+\bullet}$	-6591.783819	5.59828296	-6.72	-3.88	2.84
27		[os-2**A**]$^{2+}$	N/A	--	--	--	--
28		[cs-2**A**]$^{2+}$	N/A	--	--	--	--
29	CAM-	[2**A**]	-6583.484891	0	-6.26	-1.45	4.81
30	B3LYP	[2**A**]$^{+\bullet}$	-6583.248788	6.42469317	-8.01	-3.34	4.67
31		[os-2**A**]$^{2+}$	-6582.94384	14.7227552	-9.23	-8.38	0.85
32		[cs-2**A**]$^{2+}$	-6582.964828	14.1516423	-9.62	-4.95	4.67
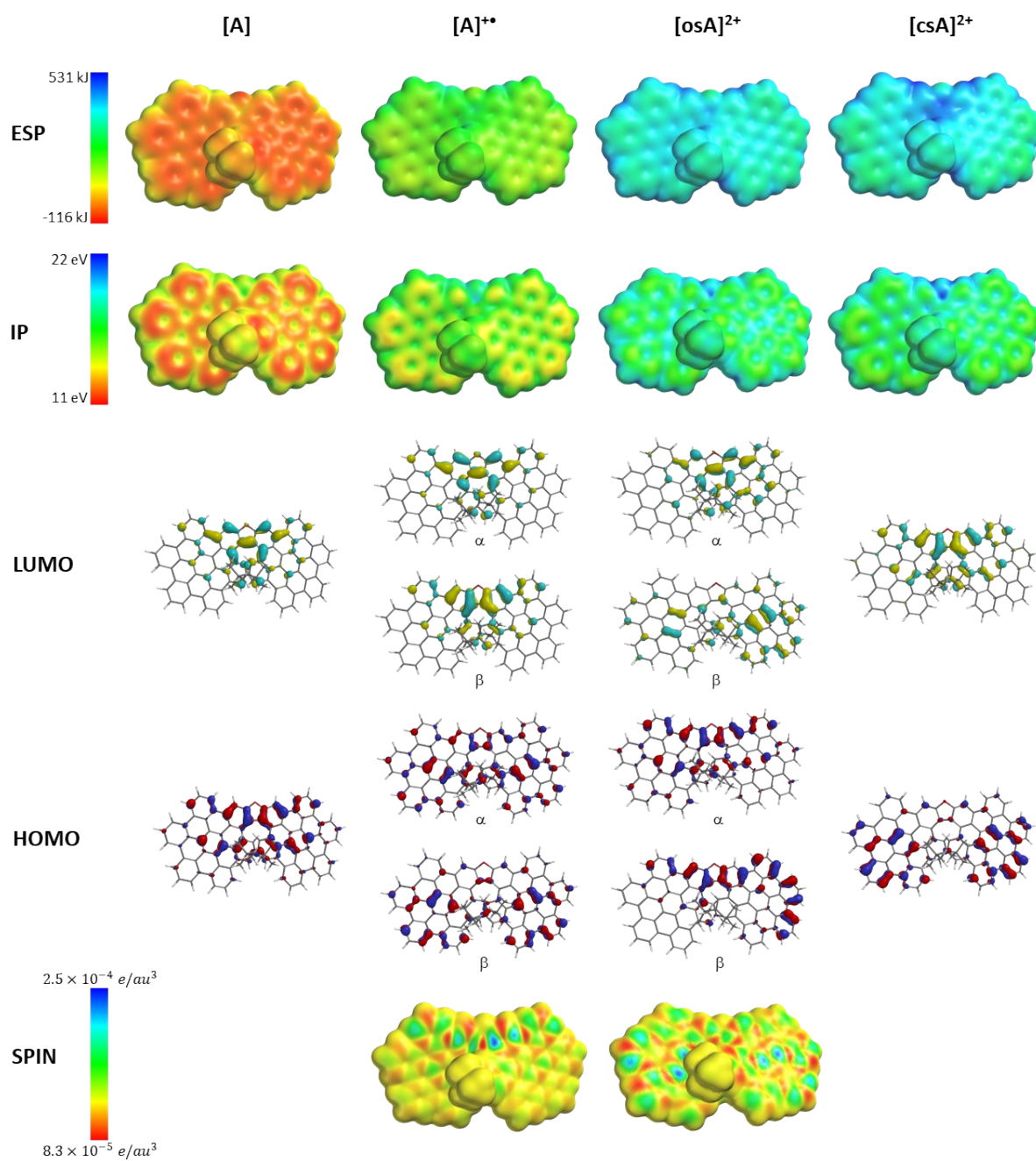
Figure S3: Visualization and comparison of different surfaces of each calculated molecule/ion of **A**; ESP = electrostatic potential map, IP = ionization potential map, LUMO = lowest unoccupied molecular orbital, HOMO = highest occupied molecular orbital, SPIN = spin density map; Isovalue for density maps: 0.002 e/au³, for orbitals: 0.032 (e/au³)$^{0.5}$.
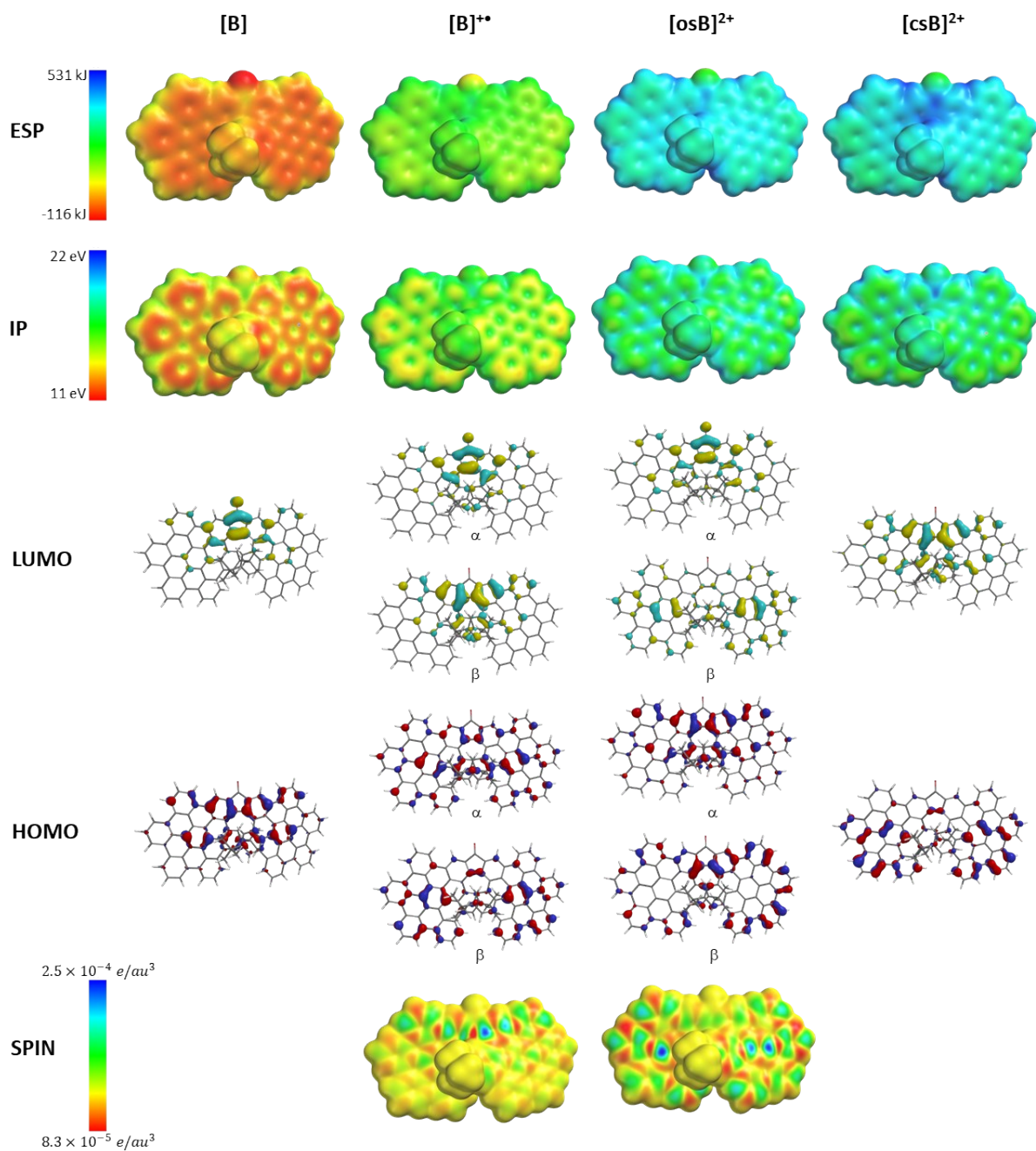
Figure S4: Visualization and comparison of different surfaces of each calculated molecule/ion of **B**; ESP = electrostatic potential map, IP = ionization potential map, LUMO = lowest unoccupied molecular orbital, HOMO = highest occupied molecular orbital, SPIN = spin density map; Isovalue for density maps: 0.002 e/au³, for orbitals: 0.032 (e/au³)$^{0.5}$.

Figure S5: Thermochemical analysis of gas-phase dimer ions of a) **B**, b) **A**, and c) **A** and **B**, calculated with different density functionals with the def2-SVPD[SV(P)] basis set; cs = closed shell, os = open shell.
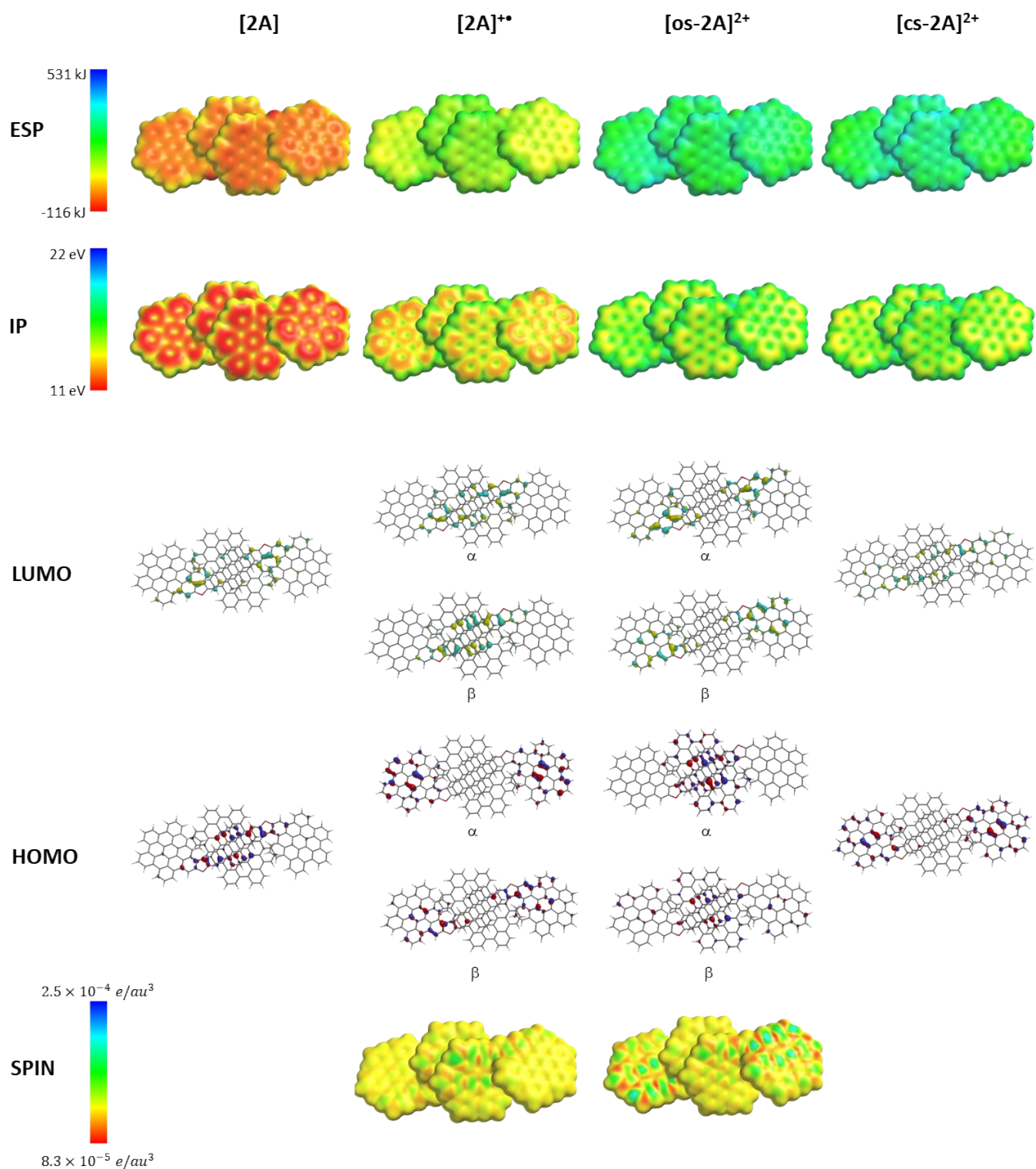
Figure S6: Visualization and comparison of different surfaces of each calculated molecule/ion dimer pair of **A**; ESP = electrostatic potential map, IP = ionization potential map, LUMO = lowest unoccupied molecular orbital, HOMO = highest occupied molecular orbital, SPIN = spin density map; Isovalue for density maps: 0.002 e/au^3, for orbitals: 0.032 (e/au^3)$^{0.5}$.
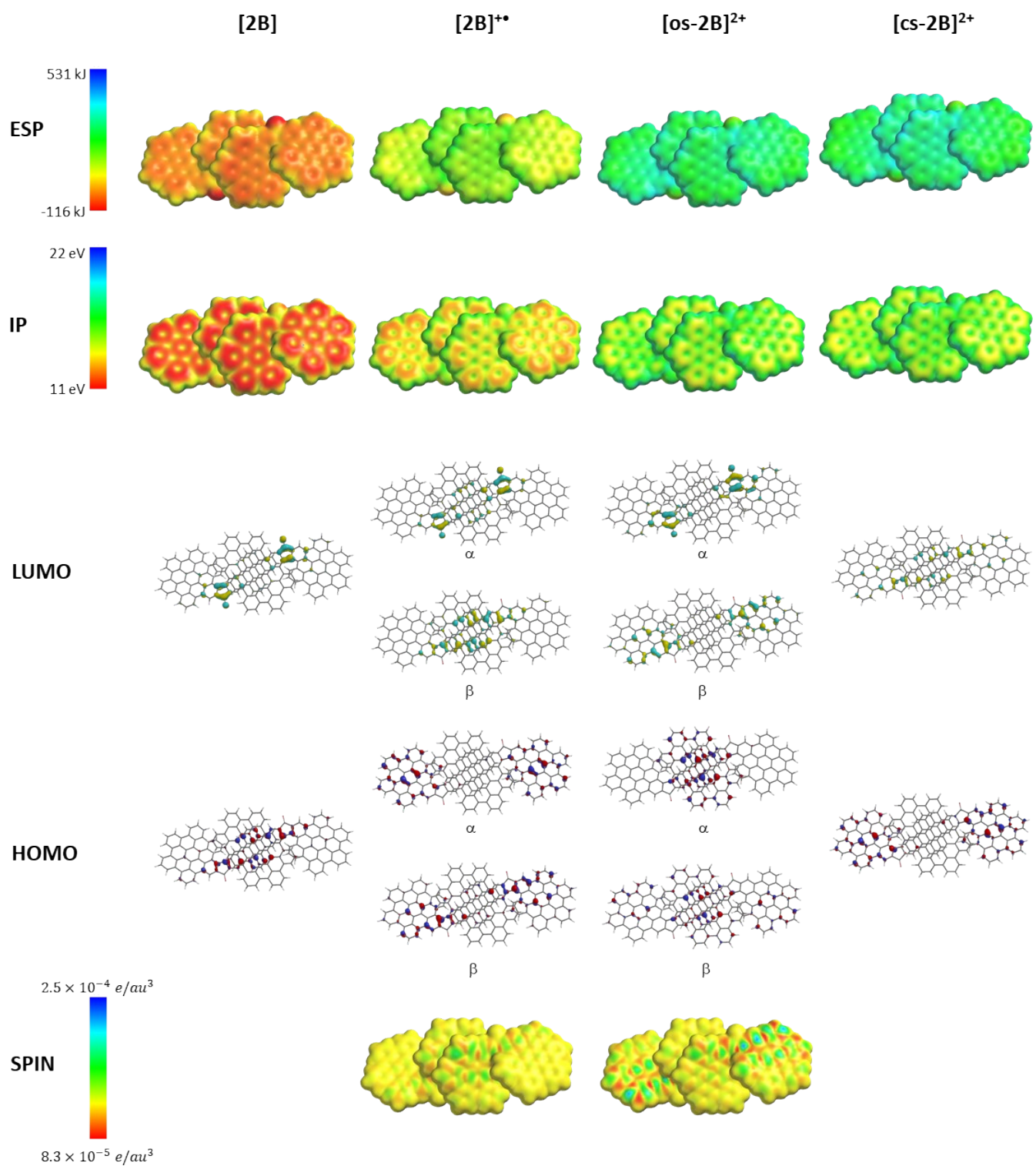
Figure S7: Visualization and comparison of different surfaces of each calculated molecule/ion dimer pair of **B**; ESP = electrostatic potential map, IP = ionization potential map, LUMO = lowest unoccupied molecular orbital, HOMO = highest occupied molecular orbital, SPIN = spin density map; Isovalue for density maps: 0.002 e/au³, for orbitals: 0.032 (e/au³)$^{0.5}$.
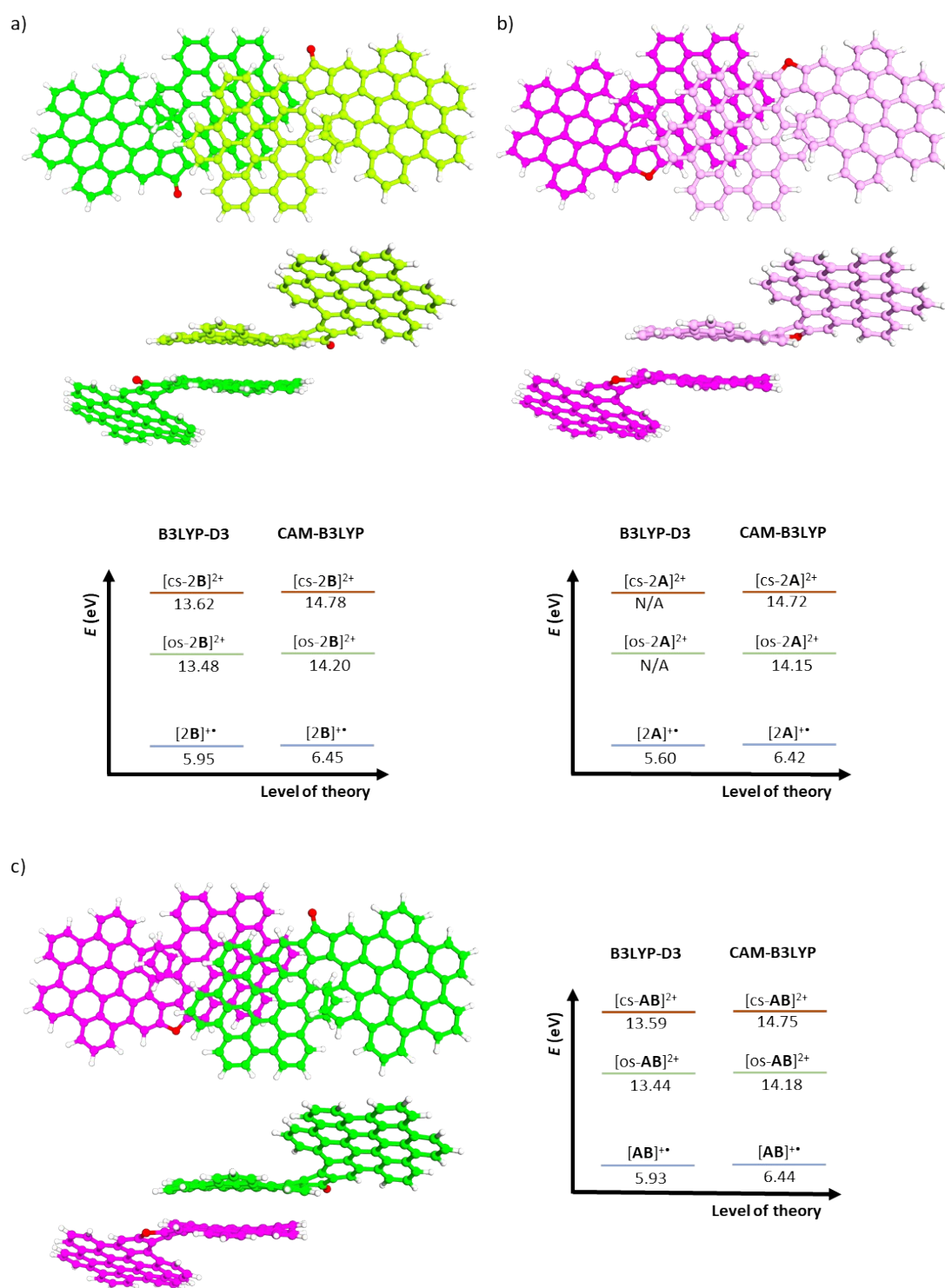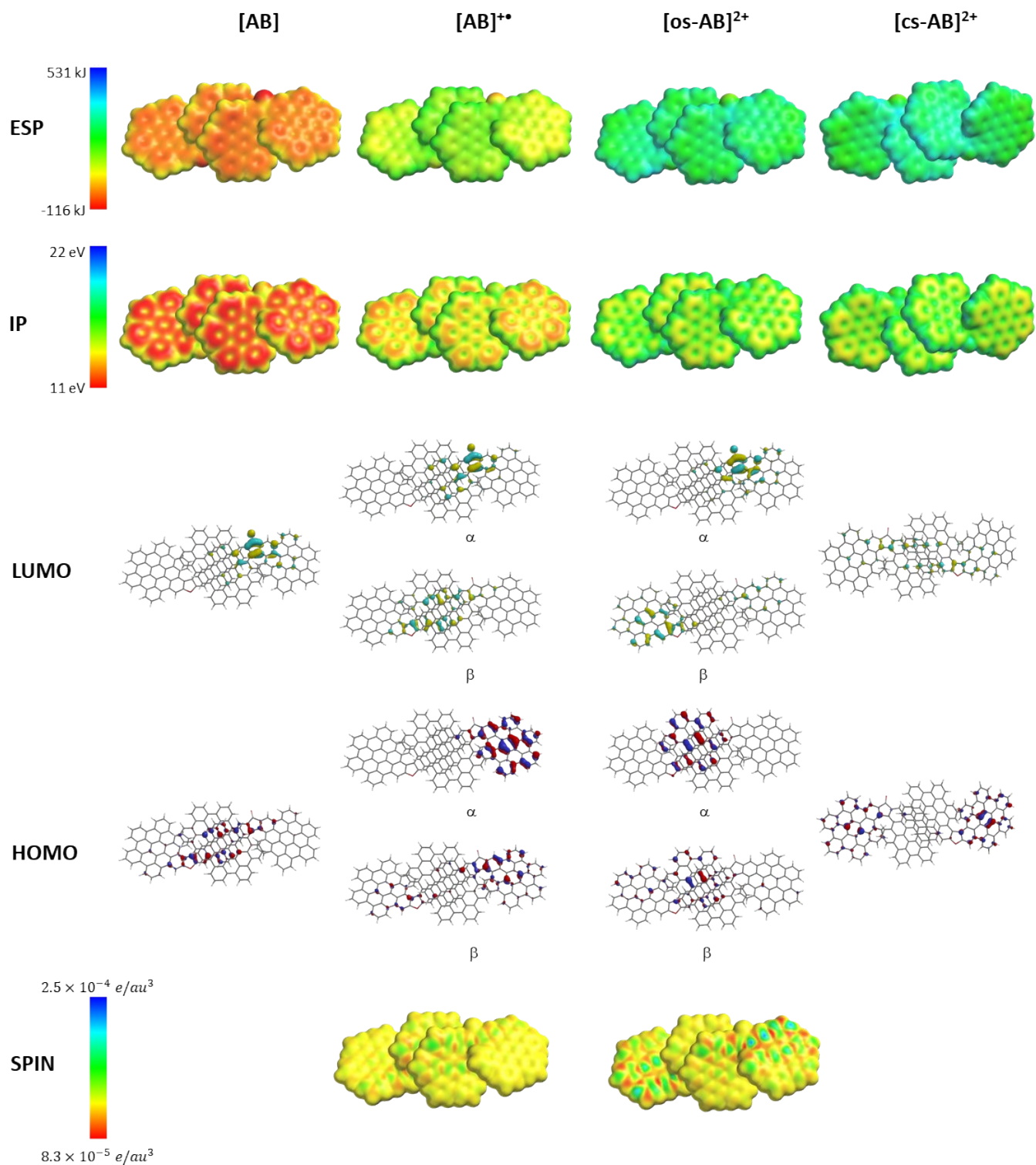
Figure S8: Visualization and comparison of different surfaces of each calculated molecule/ion dimer pair of **A** and **B**; ESP = electrostatic potential map, IP = ionization potential map, LUMO = lowest unoccupied molecular orbital, HOMO = highest occupied molecular orbital, SPIN = spin density map; Isovalue for density maps: 0.002 e/au³, for orbitals: 0.032 (e/au³)^0.5.

a)

b)

c)

	X-ray	Alternative 1	Alternative 2
$[cs\text{-}\mathbf{AB}]^{2+}$	14.75	14.97	14.88
$[os\text{-}\mathbf{AB}]^{2+}$	14.18	14.24	14.27
$[\mathbf{AB}]^{+\bullet}$	6.44	6.56	N/A
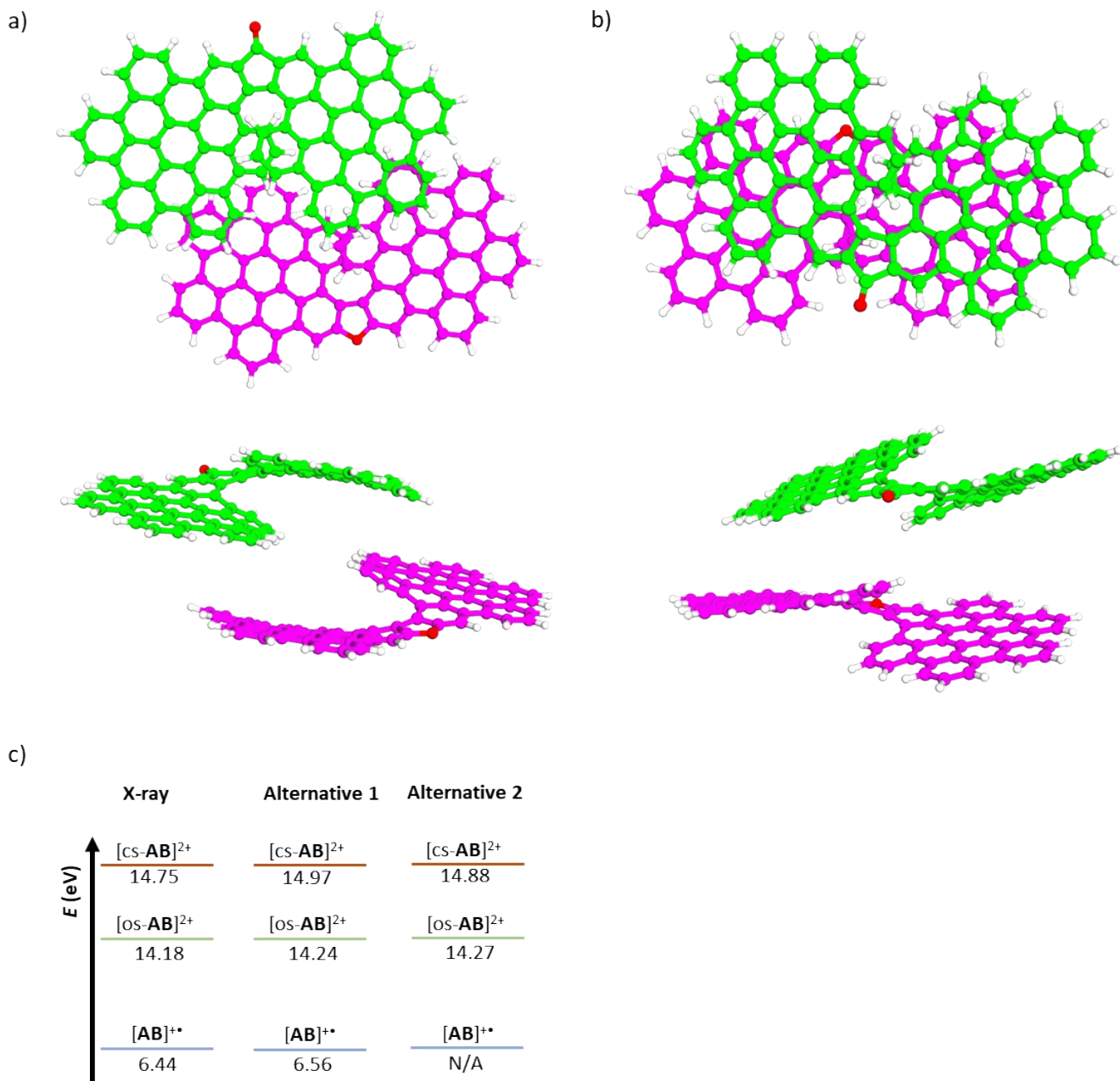
Figure S9: Thermochemical analysis of gas-phase dimer ions of **A** and **B** in alternative packing configurations. Alternatives are PM6 geometry optimized structures derived from t-butylated models (compare Figure S10). a) Alternative packing structure 1. b) Alternative packing structure 2. c) Thermochemical summary of gas phase dimer ions, calculated at the CAM-B3LYP/def2-SVPD[SV(P)] level of DFT; cs = closed shell, os = open shell.

Alternative Structure 1
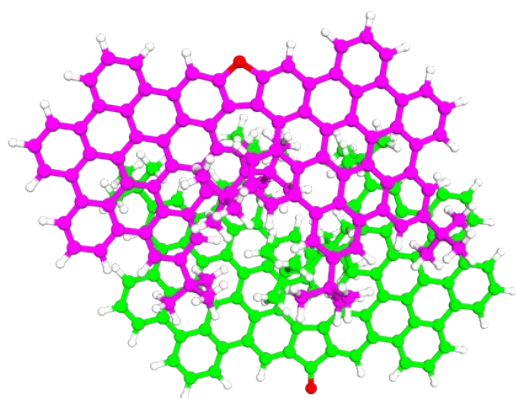
Alternative Structure 2
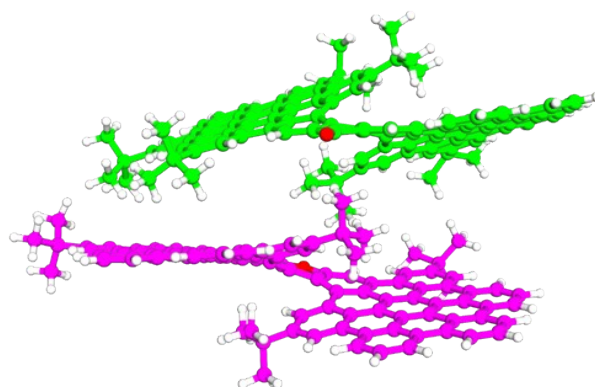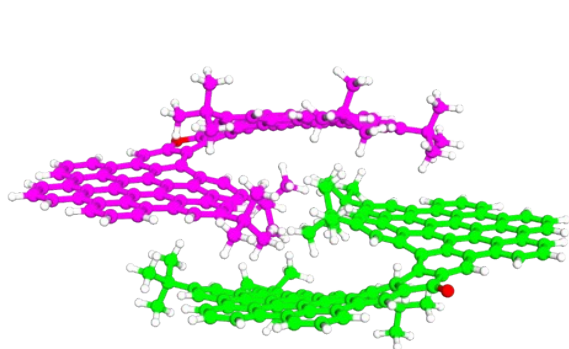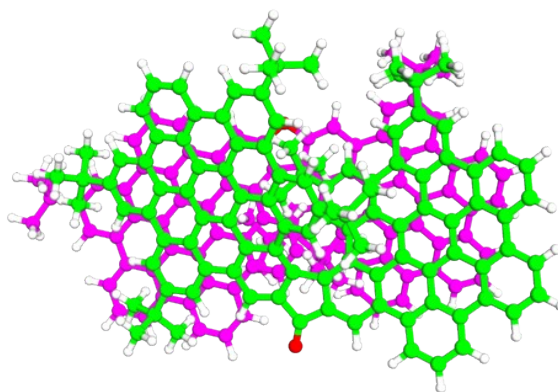
Figure S10: Alternative packing structures derived from PM6 geometry optimization, including *t*-Bu groups that are of relevance to the packing.

XYZ Coordinates

[A] C$_{92}$H$_{48}$O

	X	Y	Z
C	-1.703046	3.562863	1.795751
C	-1.019595	4.032410	4.498743
C	-1.239087	2.504344	2.608925
C	-1.885891	4.846067	2.355271
C	-1.530933	5.084364	3.702709
C	-0.912869	2.731684	3.961703
C	-1.938413	3.342498	0.383732
C	-2.191425	2.983985	-2.328424
C	-2.452584	4.389554	-0.428223
C	-1.610353	2.086287	-0.179894
C	-1.556199	1.985843	-1.583324
C	-2.647970	4.168282	-1.794941
H	-3.093491	4.901780	-2.453032
C	-1.172406	1.169527	2.069669
C	-1.461474	-1.461490	1.069714
C	-1.429911	0.946721	0.705418
C	-0.915786	0.060680	2.905603
C	-1.067390	-1.224379	2.387024
C	-1.613381	-0.358359	0.242022
H	-0.923073	-2.077646	3.039047
H	-1.913900	-0.500191	-0.785954
C	-0.478306	1.627494	4.791958
C	0.344982	-0.502409	6.408986
C	-0.493629	0.302084	4.287047
C	-0.045830	1.869382	6.117184
C	0.347780	0.787834	6.910286
C	-0.064619	-0.742077	5.108037
H	0.653501	0.940054	7.938040
H	-0.033245	-1.757894	4.733070
H	0.664938	-1.328158	7.037066
C	-0.578796	4.289120	5.852288
C	0.475243	4.831292	8.385809
C	-0.034760	3.240287	6.633932
C	-0.646590	5.599422	6.383080
C	-0.101742	5.848604	7.645505
C	0.498055	3.538829	7.890404
H	-0.101251	6.849938	8.058134
H	0.958178	2.764794	8.492066
H	0.909376	5.046841	9.357188
C	-1.698237	6.404285	4.272176
C	-2.080700	8.938619	5.397965
C	-1.281061	6.663151	5.601049
C	-2.292531	7.438677	3.508189
C	-2.466813	8.696841	4.091198
C	-1.494838	7.931766	6.145336
H	-2.909493	9.509605	3.529434
H	-1.217791	8.145837	7.170114
H	-2.237044	9.919016	5.836975
C	-2.450621	5.907515	1.549524
C	-3.677048	7.917748	0.036177
C	-2.698513	7.177463	2.124369
C	-2.781498	5.674931	0.190456
C	-3.400062	6.690996	-0.541482
C	-3.321231	8.161260	1.351286
H	-3.683218	6.531573	-1.574625
H	-3.544861	9.133907	1.770761
H	-4.169057	8.691756	-0.544384
C	-1.069880	1.033140	-2.577120
C	-0.912095	-0.494416	-4.934116
C	-1.643610	1.453019	-3.781327
C	-0.172341	-0.050852	-2.625926
C	-0.198715	-0.885194	-3.768877
C	-1.581059	0.733391	-4.953599
H	-2.086830	1.114597	-5.830428
C	-0.915879	-1.381462	-6.098831
C	-1.001056	-3.114169	-8.291184
C	-1.500338	-0.986888	-7.304541
C	-0.335556	-2.671674	-6.001949
C	-0.412099	-3.557620	-7.103493
C	-1.530682	-1.839600	-8.394461
H	-1.929733	0.001625	-7.411079
H	-1.974291	-1.510301	-9.328840
H	-1.043311	-3.757827	-9.160816
C	0.357497	-3.073287	-4.796291
C	1.831389	-3.799159	-2.493607
C	0.925189	-4.364399	-4.694487
C	0.482412	-2.163022	-3.724151
C	1.237008	-2.523157	-2.584945
C	1.642258	-4.735899	-3.532388
C	0.121541	-4.916469	-6.977340
C	1.145971	-7.508530	-6.729896
C	-0.011488	-5.845634	-8.012485
C	0.774166	-5.307591	-5.782004
C	1.284369	-6.623482	-5.657945
C	0.500710	-7.125505	-7.892689
H	-0.524571	-5.582546	-8.928827
H	0.395633	-7.830289	-8.711675
H	1.548433	-8.512090	-6.672932
C	1.466894	-1.548698	-1.548266
C	2.227204	0.527435	0.217420
C	2.379975	-1.804965	-0.502329
C	0.833859	-0.294371	-1.604345
C	1.255672	0.729565	-0.752394
C	2.739326	-0.763408	0.351006
H	0.829968	1.713793	-0.883875
H	3.483654	-0.942527	1.117718
C	2.633824	-4.137911	-1.336337
C	4.172196	-4.800853	0.905441
C	3.144934	-5.449002	-1.189762
C	2.917068	-3.158489	-0.350824
C	3.672004	-3.517166	0.766951
C	3.919772	-5.753305	-0.066620
H	3.864402	-2.796892	1.552963
H	4.341952	-6.742090	0.062106
H	4.763349	-5.061369	1.778018
C	2.167308	-6.077250	-3.395262
C	3.034598	-8.716895	-3.059997
C	1.953434	-7.030611	-4.419759
C	2.864534	-6.452610	-2.219856
C	3.277636	-7.778928	-2.071678
C	2.387006	-8.344600	-4.225121
H	3.785153	-8.101362	-1.171148
H	2.209789	-9.102037	-4.978245
H	3.353050	-9.745476	-2.921632
C	2.768324	1.662292	1.094940
C	2.042999	2.989842	0.836327
H	2.179008	3.335396	-0.194586
H	2.445191	3.762942	1.499750
H	0.970345	2.912106	1.037216
C	2.598828	1.305334	2.581845
H	3.134200	0.388570	2.850442
H	1.544810	1.161041	2.827202
H	2.987083	2.113423	3.212017
C	4.264082	1.856813	0.780330
H	4.412678	2.098478	-0.277799
H	4.844945	0.955470	1.003713
H	4.673478	2.677197	1.381142
C	-1.749293	-2.892353	0.599724
C	-2.931023	-3.448224	1.417537
H	-2.699333	-3.486899	2.487333
H	-3.173315	-4.465757	1.089561
H	-3.822315	-2.824358	1.289257
C	-2.120842	-2.948757	-0.888546
H	-1.318046	-2.560600	-1.522775
H	-3.035567	-2.385061	-1.103245
H	-2.297373	-3.988762	-1.182659
C	-0.511161	-3.779115	0.817481
H	-0.209062	-3.817501	1.869266
H	0.336966	-3.407520	0.238988
H	-0.719467	-4.805223	0.494051
O	-2.287237	2.651328	-3.650574

[A]⁺• C₉₂H₄₈O

	X	Y	Z
C	-1.676713	3.542740	1.773133
C	-1.021803	3.971887	4.493225
C	-1.242614	2.466433	2.579252
C	-1.839507	4.824701	2.339216
C	-1.503138	5.044830	3.696813
C	-0.925379	2.676825	3.945126
C	-1.899442	3.337754	0.363556
C	-2.216878	3.005709	-2.367830
C	-2.398390	4.401932	-0.447528
C	-1.622483	2.074001	-0.200774
C	-1.576388	1.983017	-1.622801
C	-2.628801	4.186102	-1.828917
H	-3.063050	4.935797	-2.474671
C	-1.190408	1.145853	2.028872
C	-1.483708	-1.478107	0.991673
C	-1.460815	0.932717	0.658657
C	-0.917158	0.024091	2.848076
C	-1.076261	-1.248394	2.314728
C	-1.644510	-0.372962	0.178414
H	-0.932468	-2.108659	2.957108
H	-1.963022	-0.505492	-0.845495
C	-0.497057	1.562141	4.760724
C	0.382187	-0.582540	6.327709
C	-0.485771	0.246212	4.229685
C	-0.080649	1.784268	6.094862
C	0.347731	0.693441	6.859345
C	-0.028268	-0.804895	5.022720
H	0.661658	0.827561	7.886325
H	0.029837	-1.811333	4.626070
H	0.730656	-1.411999	6.934593
C	-0.620370	4.205502	5.862340
C	0.278358	4.683695	8.467368
C	-0.115834	3.138794	6.646555
C	-0.702522	5.507088	6.413463
C	-0.239043	5.722957	7.712575
C	0.332742	3.404906	7.943322
H	-0.264018	6.711351	8.152860
H	0.740154	2.615264	8.561438
H	0.639834	4.872875	9.472877
C	-1.649911	6.361558	4.271231
C	-1.963450	8.906090	5.392077
C	-1.266882	6.597729	5.615457
C	-2.184214	7.421576	3.495287
C	-2.324968	8.684660	4.075539
C	-1.442827	7.873708	6.153792
H	-2.717339	9.517900	3.506787
H	-1.181270	8.080111	7.183430
H	-2.087705	9.891516	5.829051
C	-2.357594	5.899763	1.532249
C	-3.480718	7.961582	-0.007024
C	-2.566993	7.177321	2.104510
C	-2.680255	5.682478	0.163255
C	-3.246473	6.730190	-0.582186
C	-3.137006	8.182539	1.319233
H	-3.516455	6.590162	-1.620711
H	-3.329763	9.162325	1.736684
H	-3.927907	8.759157	-0.590534
C	-1.063394	1.082725	-2.596071
C	-0.954097	-0.505911	-4.913043
C	-1.648095	1.493459	-3.821161
C	-0.155227	-0.015706	-2.632295
C	-0.219865	-0.879365	-3.746614
C	-1.611421	0.748744	-4.960211
H	-2.124925	1.107861	-5.840424
C	-0.996518	-1.410797	-6.040519
C	-1.159627	-3.194355	-8.181272
C	-1.644208	-1.049040	-7.233437
C	-0.400385	-2.698836	-5.935846
C	-0.511243	-3.608052	-7.014832
C	-1.714189	-1.927100	-8.294660
H	-2.094495	-0.071664	-7.347245
H	-2.207283	-1.631998	-9.214710
H	-1.235998	-3.858506	-9.032460
C	0.329264	-3.071694	-4.750911
C	1.855329	-3.754204	-2.462983
C	0.913317	-4.356959	-4.642490
C	0.470160	-2.144353	-3.697167
C	1.247912	-2.476989	-2.565280
C	1.658731	-4.704874	-3.484777
C	0.048793	-4.953758	-6.889561
C	1.127889	-7.521516	-6.637706
C	-0.099579	-5.898318	-7.908203
C	0.747832	-5.315435	-5.709816
C	1.288068	-6.620007	-5.584026
C	0.438528	-7.166338	-7.784591
H	-0.641967	-5.660254	-8.814129
H	0.319755	-7.885334	-8.588588
H	1.544311	-8.518724	-6.580642
C	1.480194	-1.492351	-1.552303
C	2.220462	0.610817	0.201127
C	2.383756	-1.738018	-0.490673
C	0.847315	-0.231116	-1.623900
C	1.261173	0.805960	-0.773651
C	2.733359	-0.687154	0.346958
H	0.843671	1.791490	-0.921256
H	3.475445	-0.855244	1.117846
C	2.661982	-4.073795	-1.306078
C	4.175391	-4.713450	0.958854
C	3.187959	-5.378285	-1.151169
C	2.925896	-3.087401	-0.321050
C	3.667646	-3.432701	0.807653
C	3.946570	-5.670737	-0.012360
H	3.845882	-2.708963	1.593880
H	4.369847	-6.656255	0.131664
H	4.754612	-4.966012	1.841218
C	2.211105	-6.034114	-3.346836
C	3.182170	-8.639185	-3.030176
C	2.004871	-6.997039	-4.363840
C	2.936595	-6.385669	-2.181701
C	3.406950	-7.694974	-2.045148
C	2.491878	-8.292545	-4.179413
H	3.952460	-7.997965	-1.160850
H	2.331866	-9.056939	-4.928807
H	3.548583	-9.652673	-2.903558
C	2.762842	1.746509	1.074822
C	2.033262	3.071185	0.815977
H	2.169561	3.420157	-0.213546
H	2.433294	3.844173	1.479464
H	0.960896	2.989640	1.018374
C	2.598320	1.389295	2.562975
H	3.141843	0.478815	2.835233
H	1.546255	1.239059	2.815363
H	2.984813	2.201545	3.187969
C	4.257598	1.942426	0.754190
H	4.402308	2.192472	-0.302205
H	4.842342	1.042195	0.970449
H	4.667484	2.758993	1.358774
C	-1.776225	-2.906730	0.521613
C	-2.961749	-3.456988	1.338554
H	-2.737672	-3.489979	2.409891
H	-3.199682	-4.476648	1.016287
H	-3.853860	-2.837214	1.199945
C	-2.145203	-2.959045	-0.966932
H	-1.340142	-2.570180	-1.598389
H	-3.061082	-2.397554	-1.182364
H	-2.321046	-3.997852	-1.263225
C	-0.540283	-3.797118	0.742525
H	-0.243319	-3.844183	1.795107
H	0.314236	-3.429456	0.169752
H	-0.753029	-4.820440	0.414970
O	-2.301737	2.682114	-3.689129

[os**A**]$^{2+}$ C$_{92}$H$_{48}$O

	X	Y	Z
C	-1.715364	3.565701	1.792511
C	-1.013052	4.076960	4.495188
C	-1.254790	2.507752	2.620592
C	-1.903187	4.875255	2.353226
C	-1.532488	5.124955	3.688321
C	-0.925411	2.743166	3.964417
C	-1.949198	3.339908	0.403418
C	-2.194652	2.968691	-2.306219
C	-2.480753	4.385478	-0.419703
C	-1.614685	2.072010	-0.157366
C	-1.549475	1.972349	-1.562721
C	-2.666109	4.157377	-1.777600
H	-3.108708	4.883290	-2.445968
C	-1.200268	1.174337	2.095645
C	-1.473274	-1.469372	1.103860
C	-1.440844	0.943735	0.728682
C	-0.960811	0.071640	2.943372
C	-1.101289	-1.222009	2.423800
C	-1.614479	-0.366749	0.269424
H	-0.965632	-2.071054	3.082035
H	-1.909652	-0.515472	-0.759225
C	-0.522031	1.654013	4.806496
C	0.159579	-0.475699	6.486584
C	-0.575235	0.317124	4.322973
C	-0.097503	1.907165	6.136843
C	0.219219	0.833787	6.959530
C	-0.221105	-0.730648	5.187019
H	0.502296	0.992555	7.992472
H	-0.239775	-1.757910	4.846239
H	0.414606	-1.296904	7.147984
C	-0.559401	4.341880	5.820101
C	0.579367	4.917227	8.305624
C	-0.022737	3.289720	6.618389
C	-0.591047	5.672583	6.330821
C	0.000592	5.932867	7.574639
C	0.557309	3.603260	7.837733
H	0.035239	6.938540	7.972434
H	1.021779	2.836451	8.444784
H	1.052194	5.138529	9.256606
C	-1.686933	6.443457	4.242969
C	-2.042597	8.999765	5.344894
C	-1.233716	6.719692	5.555086
C	-2.302091	7.465289	3.480860
C	-2.465553	8.739515	4.057102
C	-1.431578	7.999456	6.087709
H	-2.925288	9.544192	3.498823
H	-1.125594	8.228749	7.100325
H	-2.186676	9.983978	5.776378
C	-2.479884	5.913031	1.553209
C	-3.767781	7.897327	0.052906
C	-2.733100	7.189203	2.125324
C	-2.827943	5.667230	0.195936
C	-3.476036	6.661038	-0.524576
C	-3.392647	8.162211	1.348965
H	-3.779647	6.495235	-1.550718
H	-3.625748	9.134415	1.762019
H	-4.285561	8.652983	-0.527883
C	-1.059789	1.026857	-2.555106
C	-0.896919	-0.484575	-4.925869
C	-1.635250	1.453333	-3.762969
C	-0.166450	-0.062758	-2.608474
C	-0.194270	-0.888418	-3.758596
C	-1.571624	0.749403	-4.936792
H	-2.074815	1.137458	-5.811650
C	-0.890222	-1.346160	-6.091976
C	-0.961086	-3.063725	-8.297239
C	-1.447074	-0.928549	-7.312488
C	-0.327232	-2.647358	-5.998776
C	-0.414180	-3.528373	-7.106981
C	-1.464497	-1.768743	-8.403123
H	-1.854179	0.068081	-7.423019
H	-1.875037	-1.426461	-9.346857
H	-0.991547	-3.694243	-9.176667
C	0.359790	-3.054226	-4.806433
C	1.866873	-3.824495	-2.516661
C	0.940130	-4.368753	-4.719491
C	0.486369	-2.160072	-3.729752
C	1.254223	-2.529634	-2.591041
C	1.670892	-4.749462	-3.556192
C	0.075800	-4.901871	-6.975606
C	1.048085	-7.524671	-6.726085
C	-0.136064	-5.841540	-7.974784
C	0.768518	-5.294274	-5.791783
C	1.274477	-6.624507	-5.678771
C	0.346290	-7.141215	-7.850631
H	-0.694402	-5.587892	-8.866602
H	0.168733	-7.857508	-8.645855
H	1.412146	-8.541769	-6.673867
C	1.470611	-1.583288	-1.551459
C	2.229004	0.474344	0.238747
C	2.383769	-1.853136	-0.496094
C	0.834198	-0.318519	-1.593953
C	1.254665	0.690416	-0.725555
C	2.743327	-0.823566	0.360482
H	0.838455	1.679463	-0.847485
H	3.492780	-1.005130	1.120557
C	2.661398	-4.169214	-1.372028
C	4.166089	-4.873169	0.885441
C	3.192232	-5.479625	-1.248478
C	2.923252	-3.206517	-0.359667
C	3.655663	-3.581354	0.758111
C	3.946347	-5.803437	-0.102886
H	3.832983	-2.878627	1.563024
H	4.366918	-6.792064	0.021838
H	4.739867	-5.141940	1.765919
C	2.219774	-6.075519	-3.449705
C	3.240695	-8.679247	-3.210784
C	2.011657	-7.016646	-4.486392
C	2.955142	-6.449565	-2.298070
C	3.452832	-7.763412	-2.202982
C	2.528747	-8.308228	-4.343997
H	4.013603	-8.080821	-1.334091
H	2.385927	-9.051116	-5.117615
H	3.630784	-9.687157	-3.122393
C	2.776637	1.594668	1.126032
C	2.058788	2.929008	0.883232
H	2.197312	3.289167	-0.141778
H	2.468343	3.690028	1.554580
H	0.985403	2.854555	1.085313
C	2.606492	1.216360	2.608951
H	3.143516	0.298704	2.868973
H	1.551828	1.071084	2.855708
H	2.999790	2.016677	3.244535
C	4.274109	1.781572	0.808807
H	4.423432	2.041535	-0.244112
H	4.853028	0.876554	1.018703
H	4.687338	2.589536	1.421688
C	-1.754625	-2.902695	0.637743
C	-2.953088	-3.450162	1.437529
H	-2.745511	-3.481792	2.512139
H	-3.186985	-4.470126	1.114601
H	-3.843133	-2.831334	1.284089
C	-2.099756	-2.964816	-0.856678
H	-1.288636	-2.573875	-1.479993
H	-3.015174	-2.410318	-1.090170
H	-2.267313	-4.006057	-1.148569
C	-0.520606	-3.788067	0.887061
H	-0.241903	-3.825031	1.945041
H	0.342777	-3.423239	0.324955
H	-0.726795	-4.814980	0.567538
O	-2.284531	2.646988	-3.618561

[csA]²⁺ C₉₂H₄₈O

	X	Y	Z
C	-1.658175	3.542986	1.761111
C	-1.023877	3.956928	4.499482
C	-1.241935	2.457556	2.569456
C	-1.817394	4.823152	2.328376
C	-1.493749	5.039413	3.698853
C	-0.929240	2.665452	3.949752
C	-1.869594	3.342396	0.355670
C	-2.227995	3.018711	-2.388274
C	-2.363764	4.412805	-0.454822
C	-1.620406	2.071389	-0.206294
C	-1.583828	1.976909	-1.640969
C	-2.611019	4.196004	-1.850919
H	-3.035922	4.954390	-2.491912
C	-1.195414	1.151221	2.020485
C	-1.489403	-1.472740	0.968678
C	-1.470718	0.937998	0.641555
C	-0.911383	0.020472	2.836808
C	-1.074751	-1.242015	2.300329
C	-1.651305	-0.373037	0.158506
H	-0.933188	-2.105276	2.938789
H	-1.979012	-0.505090	-0.862370
C	-0.505841	1.551597	4.759429
C	0.385863	-0.594871	6.316840
C	-0.480386	0.237099	4.219978
C	-0.100969	1.768450	6.099614
C	0.336084	0.673376	6.858305
C	-0.016635	-0.812367	5.004842
H	0.645418	0.801683	7.886896
H	0.053029	-1.816479	4.604313
H	0.738021	-1.426007	6.918587
C	-0.643355	4.184076	5.873052
C	0.195139	4.643457	8.503372
C	-0.153970	3.113133	6.660212
C	-0.734873	5.482056	6.430186
C	-0.302486	5.688694	7.741041
C	0.262816	3.370034	7.972110
H	-0.338469	6.673000	8.189038
H	0.651536	2.576258	8.596293
H	0.529171	4.826208	9.518908
C	-1.638117	6.348217	4.271876
C	-1.948865	8.890769	5.394166
C	-1.275666	6.577437	5.626863
C	-2.151131	7.418767	3.488340
C	-2.290720	8.678818	4.069238
C	-1.450151	7.853442	6.163548
H	-2.666411	9.519335	3.500576
H	-1.204089	8.058673	7.196723
H	-2.072156	9.875684	5.831784
C	-2.312002	5.896527	1.522843
C	-3.394308	7.972749	-0.038201
C	-2.513447	7.178693	2.092552
C	-2.626184	5.681787	0.145072
C	-3.174988	6.745595	-0.610456
C	-3.059728	8.184917	1.299870
H	-3.436910	6.611933	-1.651145
H	-3.245331	9.167875	1.713126
H	-3.822509	8.780350	-0.621089
C	-1.061277	1.105803	-2.598687
C	-0.979889	-0.519491	-4.900145
C	-1.654061	1.511496	-3.841056
C	-0.152852	-0.008942	-2.630510
C	-0.240057	-0.887465	-3.732259
C	-1.634454	0.755267	-4.958851
H	-2.154620	1.102827	-5.839270
C	-1.037997	-1.421165	-6.005830
C	-1.224746	-3.219523	-8.130686
C	-1.710880	-1.067591	-7.200009
C	-0.432698	-2.711844	-5.903272
C	-0.555903	-3.626575	-6.979033
C	-1.793620	-1.950363	-8.246668
H	-2.168034	-0.094241	-7.314246
H	-2.303270	-1.669701	-9.161547
H	-1.313222	-3.886831	-8.978241
C	0.309489	-3.073230	-4.735293
C	1.866670	-3.750815	-2.456608
C	0.908161	-4.361857	-4.630382
C	0.454033	-2.142937	-3.686417
C	1.248277	-2.464922	-2.559110
C	1.668377	-4.703098	-3.473103
C	0.018541	-4.965755	-6.862329
C	1.134234	-7.521771	-6.619994
C	-0.132023	-5.911351	-7.876253
C	0.740521	-5.318223	-5.688502
C	1.300204	-6.619219	-5.569041
C	0.424385	-7.173482	-7.756423
H	-0.687584	-5.684567	-8.776759
H	0.303011	-7.894307	-8.558017
H	1.560028	-8.514854	-6.570826
C	1.479804	-1.484784	-1.560882
C	2.212936	0.629356	0.191088
C	2.380221	-1.729686	-0.486190
C	0.845092	-0.214172	-1.636039
C	1.258616	0.825834	-0.779949
C	2.726568	-0.679053	0.340661
H	0.849342	1.813724	-0.933735
H	3.469525	-0.841673	1.111490
C	2.673467	-4.063741	-1.304714
C	4.178955	-4.700649	0.966403
C	3.210949	-5.365558	-1.152586
C	2.926122	-3.077700	-0.313204
C	3.660833	-3.420085	0.816325
C	3.965077	-5.655572	-0.006639
H	3.831916	-2.699299	1.606779
H	4.393722	-6.638060	0.138871
H	4.755562	-4.950084	1.850892
C	2.236370	-6.023768	-3.342558
C	3.263214	-8.611736	-3.047407
C	2.037470	-6.986447	-4.360876
C	2.976099	-6.367837	-2.184775
C	3.476816	-7.669689	-2.059965
C	2.552441	-8.272274	-4.188061
H	4.040059	-7.966245	-1.184999
H	2.403068	-9.036498	-4.939386
H	3.653364	-9.617296	-2.932092
C	2.769028	1.759645	1.059227
C	2.050262	3.090004	0.799898
H	2.187412	3.436823	-0.230101
H	2.459967	3.860427	1.459949
H	0.977424	3.017819	1.006460
C	2.608024	1.404638	2.549085
H	3.142245	0.489182	2.822336
H	1.555449	1.269413	2.809290
H	3.010203	2.212784	3.168722
C	4.265013	1.937596	0.729671
H	4.408054	2.186564	-0.326700
H	4.843198	1.033310	0.945182
H	4.685267	2.749804	1.331756
C	-1.791244	-2.900964	0.510755
C	-2.975808	-3.436617	1.340135
H	-2.746931	-3.466386	2.410250
H	-3.220616	-4.456482	1.025977
H	-3.865534	-2.814165	1.201988
C	-2.168293	-2.959915	-0.975282
H	-1.364132	-2.578271	-1.613131
H	-3.083574	-2.397307	-1.189274
H	-2.350877	-3.999331	-1.263891
C	-0.557930	-3.795764	0.733188
H	-0.254979	-3.839319	1.784008
H	0.296233	-3.439152	0.152170
H	-0.780585	-4.819793	0.416041
O	-2.308946	2.696585	-3.707783

[B] C$_{93}$H$_{48}$O

	X	Y	Z
C	-1.667560	3.498793	1.791013
C	-0.914204	3.839528	4.495018
C	-1.203280	2.397934	2.546193
C	-1.813189	4.760656	2.409749
C	-1.426664	4.932782	3.760327
C	-0.840749	2.560999	3.898087
C	-1.937310	3.345814	0.374961
C	-2.196162	3.132157	-2.355120
C	-2.424250	4.444555	-0.369789
C	-1.654016	2.097079	-0.257190
C	-1.599790	2.069294	-1.656458
C	-2.629099	4.281791	-1.747351
H	-3.077584	5.047898	-2.368119
C	-1.175814	1.085244	1.948286
C	-1.567540	-1.498913	0.868275
C	-1.489592	0.919537	0.587105
C	-0.910472	-0.057966	2.730910
C	-1.116320	-1.320069	2.174477
C	-1.727157	-0.361098	0.086816
H	-0.971744	-2.198272	2.792023
H	-2.068979	-0.457574	-0.933986
C	-0.392081	1.418300	4.666392
C	0.490579	-0.785830	6.147607
C	-0.428871	0.118765	4.101305
C	0.087339	1.596700	5.985366
C	0.509979	0.479130	6.710282
C	0.031715	-0.963572	4.853525
H	0.856205	0.582600	7.731059
H	0.051670	-1.958987	4.426462
H	0.836074	-1.639476	6.722480
C	-0.437404	4.028922	5.847902
C	0.674850	4.444052	8.380950
C	0.117585	2.941330	6.566629
C	-0.482718	5.313132	6.441099
C	0.091049	5.499026	7.701637
C	0.677684	3.176273	7.824443
H	0.109032	6.479897	8.160047
H	1.142265	2.371317	8.380057
H	1.129789	4.610220	9.352504
C	-1.565939	6.227413	4.392951
C	-1.912047	8.704766	5.650313
C	-1.124166	6.417426	5.725100
C	-2.159564	7.304673	3.690334
C	-2.318928	8.531946	4.338859
C	-1.319955	7.658639	6.335805
H	-2.767817	9.373437	3.826599
H	-1.025764	7.818756	7.365569
H	-2.057077	9.662137	6.141087
C	-2.365763	5.870624	1.665733
C	-3.545153	7.978080	0.250057
C	-2.580068	7.118862	2.299453
C	-2.710983	5.708753	0.301637
C	-3.304075	6.772571	-0.383977
C	-3.178557	8.151855	1.574239
H	-3.591833	6.666998	-1.422486
H	-3.370279	9.112013	2.036180
H	-4.015934	8.791574	-0.292940
C	-1.108379	1.083767	-2.675838
C	-0.908165	-0.572480	-4.953127
C	-1.703881	1.421531	-3.902423
C	-0.184250	0.030680	-2.667303
C	-0.195261	-0.875888	-3.770397
C	-1.596703	0.646738	-5.027459
H	-2.090118	0.988068	-5.929295
C	-0.906279	-1.515902	-6.066634
C	-0.970333	-3.358916	-8.164683
C	-1.512856	-1.195744	-7.284324
C	-0.300143	-2.786075	-5.907031
C	-0.359212	-3.726999	-6.963706
C	-1.533765	-2.104337	-8.326712
H	-1.970455	-0.226007	-7.434080
H	-1.998344	-1.836661	-9.270484
H	-1.010973	-4.048743	-8.998063
C	0.389241	-3.111358	-4.677822
C	1.832035	-3.709663	-2.319487
C	0.969014	-4.391543	-4.505713
C	0.494818	-2.145865	-3.651167
C	1.232710	-2.444198	-2.482860
C	1.668107	-4.698490	-3.315915
C	0.210380	-5.063020	-6.773828
C	1.287638	-7.616995	-6.398096
C	0.125305	-6.035220	-7.773475
C	0.848774	-5.386350	-5.551048
C	1.380775	-6.685307	-5.360862
C	0.664818	-7.296439	-7.591090
H	-0.366150	-5.819698	-8.713679
H	0.598324	-8.034692	-8.384151
H	1.712641	-8.606893	-6.290167
C	1.441233	-1.416412	-1.491353
C	2.193176	0.747059	0.168212
C	2.330362	-1.622754	-0.415847
C	0.820992	-0.161310	-1.628279
C	1.242043	0.904521	-0.832326
C	2.688499	-0.537439	0.383205
H	0.827322	1.883585	-1.025314
H	3.419513	-0.680527	1.169766
C	2.604392	-3.991999	-1.126948
C	4.057015	-4.549442	1.199490
C	3.111649	-5.293438	-0.902829
C	2.852797	-2.968278	-0.178284
C	3.563707	-3.274104	0.983728
C	3.842798	-5.544867	0.261428
H	3.723038	-2.518286	1.743414
H	4.258407	-6.526398	0.451232
H	4.612605	-4.770285	2.105711
C	2.201877	-6.027254	-3.104965
C	3.086102	-8.640164	-2.631241
C	2.023189	-7.027699	-4.090465
C	2.871213	-6.343300	-1.896398
C	3.295510	-7.656361	-1.680197
C	2.463008	-8.327667	-3.826346
H	3.786338	-7.932462	-0.755499
H	2.308598	-9.119976	-4.547785
H	3.411560	-9.657807	-2.439085
C	2.724996	1.922374	0.996440
C	1.976087	3.227496	0.694889
H	2.101769	3.540684	-0.347367
H	2.367529	4.029808	1.329064
H	0.905924	3.137390	0.902900
C	2.572377	1.618015	2.496978
H	3.153417	0.742307	2.804097
H	1.527188	1.430139	2.749578
H	2.918127	2.470084	3.092963
C	4.215026	2.126734	0.662168
H	4.349909	2.345034	-0.402786
H	4.808020	1.237174	0.900478
H	4.620633	2.966051	1.238987
C	-1.902545	-2.905866	0.360027
C	-3.100517	-3.445023	1.165098
H	-2.872494	-3.507561	2.234528
H	-3.368679	-4.449950	0.818693
H	-3.974719	-2.795964	1.045403
C	-2.275625	-2.909058	-1.128589
H	-1.463819	-2.519221	-1.749817
H	-3.177565	-2.319578	-1.326682
H	-2.475234	-3.935292	-1.454335
C	-0.693303	-3.837913	0.551916
H	-0.410985	-3.941584	1.604519
H	0.176168	-3.462614	0.008679
H	-0.924690	-4.839235	0.171587
C	-2.355572	2.755515	-3.786599
O	-2.897044	3.393326	-4.664407

[B]⁺· C₉₃H₄₈O

	X	Y	Z
C	-1.624791	3.483305	1.756577
C	-0.900239	3.778398	4.476626
C	-1.176661	2.367897	2.499546
C	-1.772085	4.736448	2.390103
C	-1.409372	4.885797	3.752138
C	-0.816135	2.511998	3.860937
C	-1.879506	3.348552	0.343966
C	-2.202616	3.162732	-2.403065
C	-2.346597	4.465976	-0.397809
C	-1.644158	2.095761	-0.291078
C	-1.596445	2.077410	-1.708663
C	-2.587370	4.310014	-1.788754
H	-3.028656	5.091428	-2.394005
C	-1.162125	1.071661	1.889943
C	-1.587607	-1.502010	0.782459
C	-1.501820	0.917211	0.527014
C	-0.871932	-0.083655	2.651535
C	-1.100026	-1.332419	2.085775
C	-1.753509	-0.362917	0.014433
H	-0.952975	-2.216813	2.693553
H	-2.123409	-0.447697	-0.998031
C	-0.348283	1.364243	4.604900
C	0.634279	-0.842614	6.014918
C	-0.359505	0.075776	4.012698
C	0.141708	1.528114	5.922264
C	0.619668	0.406978	6.608712
C	0.151513	-1.007629	4.726226
H	0.988583	0.496523	7.622308
H	0.196141	-1.992064	4.275562
H	1.023635	-1.695773	6.560870
C	-0.446047	3.946492	5.838538
C	0.607078	4.324515	8.400933
C	0.124990	2.855422	6.538458
C	-0.533862	5.214202	6.461247
C	0.012021	5.382978	7.735330
C	0.652229	3.071849	7.814531
H	-0.001268	6.351817	8.218329
H	1.118380	2.264622	8.364853
H	1.036641	4.477091	9.385603
C	-1.574907	6.162222	4.406130
C	-2.040673	8.584799	5.724225
C	-1.185504	6.320808	5.759406
C	-2.155903	7.251443	3.709201
C	-2.384628	8.449136	4.390862
C	-1.440743	7.534948	6.399117
H	-2.847601	9.292278	3.894424
H	-1.192939	7.670493	7.444197
H	-2.240985	9.516984	6.242174
C	-2.286089	5.858309	1.650436
C	-3.316923	8.030755	0.202929
C	-2.494907	7.102089	2.294051
C	-2.590928	5.723238	0.268086
C	-3.108063	6.825896	-0.433716
C	-3.008367	8.166339	1.550303
H	-3.349619	6.751332	-1.485793
H	-3.170872	9.131509	2.012534
H	-3.715844	8.875466	-0.348205
C	-1.082066	1.146591	-2.699467
C	-0.929238	-0.575221	-4.931449
C	-1.661843	1.485247	-3.955000
C	-0.158708	0.068937	-2.671749
C	-0.207565	-0.866838	-3.743779
C	-1.582600	0.681088	-5.044787
H	-2.065572	1.005684	-5.957456
C	-0.974653	-1.539683	-6.003112
C	-1.124166	-3.436085	-8.042828
C	-1.642219	-1.252109	-7.206185
C	-0.359258	-2.810451	-5.833113
C	-0.452821	-3.773995	-6.866016
C	-1.708596	-2.188154	-8.215537
H	-2.116379	-0.292258	-7.362388
H	-2.221991	-1.954706	-9.142047
H	-1.203384	-4.148033	-8.854122
C	0.358573	-3.110876	-4.622576
C	1.830000	-3.675407	-2.267821
C	0.949437	-4.387346	-4.440768
C	0.477165	-2.129691	-3.613617
C	1.226906	-2.406225	-2.447804

	X	Y	Z
C	1.664484	-4.675553	-3.250046
C	0.145761	-5.095439	-6.679860
C	1.282429	-7.622093	-6.304243
C	0.058024	-6.076714	-7.669792
C	0.822357	-5.393156	-5.469572
C	1.386982	-6.679438	-5.279505
C	0.625324	-7.324818	-7.485629
H	-0.453248	-5.881145	-8.603465
H	0.554733	-8.072561	-8.268691
H	1.721956	-8.605195	-6.197983
C	1.440735	-1.369028	-1.482295
C	2.195744	0.821283	0.152924
C	2.306396	-1.570125	-0.382687
C	0.837430	-0.101244	-1.644362
C	1.261140	0.977125	-0.855065
C	2.668324	-0.476071	0.394068
H	0.868922	1.960270	-1.074392
H	3.393347	-0.614809	1.186637
C	2.589210	-3.944488	-1.066772
C	3.954406	-4.494757	1.312845
C	3.097947	-5.242888	-0.827333
C	2.810130	-2.916757	-0.114780
C	3.475770	-3.216583	1.073067
C	3.777954	-5.491155	0.369670
H	3.609250	-2.458879	1.836104
H	4.174852	-6.474440	0.585673
H	4.469954	-4.715180	2.241974
C	2.223536	-5.992217	-3.037119
C	3.227962	-8.565441	-2.590684
C	2.068413	-6.996077	-4.023208
C	2.907836	-6.289320	-1.832389
C	3.400521	-7.581760	-1.633503
C	2.570029	-8.275332	-3.773332
H	3.926923	-7.840032	-0.723799
H	2.447328	-9.069729	-4.497915
H	3.610912	-9.565416	-2.415350
C	2.755237	1.997336	0.958925
C	2.017429	3.307591	0.652788
H	2.131849	3.608982	-0.394203
H	2.429574	4.112078	1.269887
H	0.949517	3.232991	0.881225
C	2.624518	1.713152	2.465892
H	3.202717	0.837853	2.778336
H	1.582161	1.541968	2.742469
H	2.991720	2.569499	3.041372
C	4.242415	2.173133	0.595039
H	4.363189	2.379047	-0.473786
H	4.825933	1.277637	0.833670
H	4.670721	3.011040	1.155966
C	-1.966233	-2.901494	0.288973
C	-3.182469	-3.386089	1.102443
H	-2.956253	-3.441516	2.172486
H	-3.483812	-4.386000	0.771152
H	-4.034827	-2.710864	0.972694
C	-2.338769	-2.905912	-1.199718
H	-1.513348	-2.549140	-1.823846
H	-3.223098	-2.292480	-1.404166
H	-2.572030	-3.927672	-1.515254
C	-0.790689	-3.873644	0.493936
H	-0.524599	-3.991900	1.548893
H	0.098983	-3.532495	-0.039976
H	-1.055544	-4.865163	0.111752
C	-2.332075	2.810209	-3.843321
O	-2.861380	3.450884	-4.721042

[os**B**]²⁺ $C_{93}H_{48}O$

	X	Y	Z
C	-1.619102	3.538054	1.769156
C	-0.909971	3.849124	4.509958
C	-1.138553	2.422618	2.538303
C	-1.807241	4.782529	2.393651
C	-1.462214	4.951195	3.768291
C	-0.785412	2.587916	3.901030
C	-1.865997	3.384501	0.360636
C	-2.130930	3.163425	-2.369217
C	-2.324081	4.495254	-0.393783
C	-1.598508	2.125828	-0.267308
C	-1.546697	2.087557	-1.661054
C	-2.537520	4.322273	-1.778282
H	-2.990844	5.081935	-2.402694
C	-1.092397	1.129311	1.945661
C	-1.538481	-1.460934	0.904154
C	-1.441216	0.953847	0.585098
C	-0.801441	-0.017143	2.731096
C	-1.035979	-1.282044	2.190000
C	-1.707400	-0.321554	0.110820
H	-0.888995	-2.155978	2.812103
H	-2.080259	-0.428678	-0.897996
C	-0.288828	1.463771	4.651997
C	0.748514	-0.709301	6.089164
C	-0.284421	0.168782	4.079079
C	0.206429	1.653443	5.963270
C	0.718890	0.545883	6.663158
C	0.249306	-0.897279	4.806713
H	1.094570	0.656794	7.671874
H	0.298843	-1.887904	4.370871
H	1.156138	-1.548701	6.641673
C	-0.469984	4.039201	5.860238
C	0.595259	4.472739	8.411026
C	0.152790	2.972659	6.563774
C	-0.615708	5.305021	6.484029
C	-0.061237	5.505786	7.741418
C	0.687667	3.223534	7.840571
H	-0.109446	6.476575	8.219005
H	1.193524	2.442178	8.392103
H	1.029172	4.656573	9.387974
C	-1.687088	6.200953	4.415572
C	-2.357366	8.562047	5.754597
C	-1.334505	6.371396	5.787135
C	-2.314123	7.272278	3.710836
C	-2.649295	8.435142	4.409777
C	-1.695917	7.544371	6.435427
H	-3.161566	9.250642	3.916743
H	-1.492624	7.680173	7.489989
H	-2.643939	9.463621	6.285312
C	-2.330913	5.893813	1.646216
C	-3.316115	8.065767	0.168484
C	-2.584070	7.130466	2.287180
C	-2.587038	5.756825	0.260693
C	-3.079109	6.862035	-0.459477
C	-3.069536	8.199049	1.530418
H	-3.275071	6.788058	-1.521073
H	-3.249119	9.163328	1.987842
H	-3.689418	8.911216	-0.398578
C	-1.084562	1.087093	-2.674166
C	-0.937390	-0.587134	-4.947008
C	-1.688646	1.428700	-3.905636
C	-0.181755	0.021328	-2.667779
C	-0.215193	-0.893372	-3.766682
C	-1.608892	0.651806	-5.022888
H	-2.095355	1.002730	-5.924243
C	-0.958956	-1.525043	-6.045557
C	-1.054127	-3.369015	-8.138765
C	-1.598878	-1.207854	-7.258666
C	-0.344882	-2.792610	-5.895849
C	-0.413486	-3.731369	-6.953542
C	-1.636643	-2.115065	-8.293503
H	-2.067205	-0.243022	-7.401461
H	-2.124527	-1.857761	-9.227218
H	-1.112047	-4.058162	-8.971052
C	0.349911	-3.116430	-4.678848
C	1.803824	-3.752532	-2.308449
C	0.935160	-4.412825	-4.514340
C	0.457782	-2.161749	-3.654255
C	1.208073	-2.471538	-2.469877
C	1.639804	-4.732482	-3.302782
C	0.175247	-5.054760	-6.781348
C	1.300758	-7.601056	-6.423608
C	0.112687	-6.015358	-7.790847
C	0.824367	-5.384606	-5.551871
C	1.377532	-6.689514	-5.376235
C	0.674312	-7.267839	-7.616628
H	-0.371953	-5.802074	-8.733941
H	0.624545	-7.996477	-8.418828
H	1.736804	-8.587332	-6.336353
C	1.419430	-1.461404	-1.489268
C	2.238666	0.699988	0.142558
C	2.306504	-1.680511	-0.401438
C	0.827211	-0.183392	-1.637441
C	1.282773	0.872668	-0.861379
C	2.695438	-0.594417	0.381038
H	0.899482	1.862596	-1.063550
H	3.430642	-0.743846	1.161526
C	2.554849	-4.044038	-1.114555
C	3.947191	-4.638147	1.247889
C	3.049187	-5.350997	-0.891100
C	2.797833	-3.029332	-0.155819
C	3.477379	-3.349738	1.019557
C	3.746000	-5.620992	0.302614
H	3.634376	-2.599144	1.784775
H	4.138964	-6.609147	0.500711
H	4.475527	-4.868411	2.166550
C	2.174921	-6.049521	-3.106416
C	3.112009	-8.653954	-2.665326
C	2.018194	-7.039536	-4.109455
C	2.841300	-6.375241	-1.894279
C	3.299211	-7.692262	-1.700269
C	2.477806	-8.328757	-3.863170
H	3.801817	-7.974774	-0.785150
H	2.344403	-9.115060	-4.594585
H	3.460624	-9.667288	-2.498927
C	2.819301	1.876007	0.932235
C	2.093469	3.193789	0.627469
H	2.204222	3.493722	-0.419788
H	2.519796	3.993947	1.239932
H	1.025082	3.132639	0.860809
C	2.708847	1.605744	2.443602
H	3.262221	0.713470	2.752437
H	1.665940	1.475549	2.742626
H	3.120019	2.452876	3.002251
C	4.303520	2.029315	0.542295
H	4.410978	2.216369	-0.531043
H	4.881890	1.133045	0.788802
H	4.747122	2.872883	1.081553
C	-1.935172	-2.859104	0.422632
C	-3.151030	-3.320300	1.252050
H	-2.913026	-3.380940	2.318898
H	-3.474350	-4.313566	0.923106
H	-3.992892	-2.630796	1.132040
C	-2.321807	-2.872789	-1.062963
H	-1.504295	-2.517300	-1.699193
H	-3.209244	-2.263770	-1.264574
H	-2.557043	-3.896959	-1.368004
C	-0.769974	-3.844435	0.625059
H	-0.480851	-3.943476	1.675663
H	0.112017	-3.530452	0.061197
H	-1.061672	-4.839481	0.273651
C	-2.313731	2.777888	-3.797921
O	-2.848806	3.416128	-4.672346

[csB]$^{2+}$ C$_{93}$H$_{48}$O

	X	Y	Z
C	-1.609181	3.481791	1.752386
C	-0.922373	3.768930	4.495070
C	-1.193599	2.358209	2.505458
C	-1.737947	4.740195	2.377745
C	-1.393469	4.889694	3.753965
C	-0.849493	2.501423	3.884547
C	-1.852402	3.343807	0.344141
C	-2.251212	3.149183	-2.411338
C	-2.321762	4.463501	-0.400435
C	-1.647938	2.083685	-0.283269
C	-1.619065	2.053321	-1.720370
C	-2.598393	4.297148	-1.800809
H	-3.036908	5.083194	-2.401345
C	-1.184189	1.074838	1.900334
C	-1.590647	-1.502423	0.775636
C	-1.518098	0.917745	0.525865
C	-0.884392	-0.088111	2.660183
C	-1.105946	-1.327912	2.090873
C	-1.757483	-0.371084	0.009293
H	-0.962154	-2.213834	2.696887
H	-2.131523	-0.457912	-1.001349
C	-0.404481	1.352714	4.631244
C	0.583624	-0.853961	6.038734
C	-0.387088	0.066934	4.027736
C	0.045389	1.507590	5.965621
C	0.533078	0.384464	6.647303
C	0.126859	-1.013310	4.736519
H	0.887913	0.467204	7.665863
H	0.195837	-1.993362	4.279521
H	0.979234	-1.706209	6.580987
C	-0.517249	3.927868	5.871380
C	0.350654	4.256797	8.511895
C	-0.011665	2.821159	6.596841
C	-0.603451	5.196091	6.493483
C	-0.154643	5.337863	7.807975
C	0.415820	3.011576	7.915846
H	-0.184434	6.298973	8.304249
H	0.807047	2.187506	8.497608
H	0.693576	4.388337	9.532427
C	-1.522204	6.171384	4.389954
C	-1.836230	8.649534	5.647783
C	-1.153449	6.329623	5.752976
C	-2.032393	7.283303	3.664604
C	-2.178226	8.508761	4.313343
C	-1.330362	7.574760	6.358088
H	-2.564091	9.376124	3.794030
H	-1.083701	7.724886	7.400637
H	-1.965472	9.608114	6.138866
C	-2.215084	5.860011	1.629638
C	-3.226544	8.033894	0.155553
C	-2.388261	7.119715	2.256576
C	-2.536174	5.714655	0.245119
C	-3.045580	6.826920	-0.468974
C	-2.895589	8.175677	1.504930
H	-3.300017	6.747441	-1.516929
H	-3.048285	9.147043	1.957242
H	-3.620912	8.881141	-0.394013
C	-1.089722	1.165228	-2.690963
C	-0.966287	-0.592636	-4.910308
C	-1.665766	1.503752	-3.968205
C	-0.163524	0.065115	-2.663086
C	-0.236034	-0.881181	-3.722186
C	-1.610656	0.685865	-5.035346
H	-2.100288	1.000117	-5.947713
C	-1.031364	-1.550210	-5.961714
C	-1.213161	-3.457856	-7.986069
C	-1.725477	-1.267567	-7.163622
C	-0.409409	-2.825657	-5.796180
C	-0.523352	-3.794387	-6.824823
C	-1.807274	-2.205898	-8.159548
H	-2.204956	-0.310798	-7.318089
H	-2.335297	-1.983292	-9.079933
H	-1.303625	-4.170202	-8.795930
C	0.331981	-3.115071	-4.609480
C	1.861934	-3.670544	-2.280915
C	0.945863	-4.391788	-4.439303
C	0.459548	-2.132137	-3.604752
C	1.237610	-2.396648	-2.452713
C	1.691291	-4.670876	-3.258649
C	0.081353	-5.112929	-6.648083
C	1.247782	-7.630871	-6.289015
C	-0.039642	-6.102780	-7.622222
C	0.803495	-5.396974	-5.456121
C	1.390183	-6.678854	-5.278178
C	0.540871	-7.347253	-7.444428
H	-0.588882	-5.924453	-8.537398
H	0.440378	-8.104196	-8.214931
H	1.689938	-8.613257	-6.192611
C	1.449982	-1.366334	-1.499970
C	2.183652	0.832694	0.143929
C	2.317781	-1.564551	-0.391954
C	0.832674	-0.093417	-1.656528
C	1.249966	0.987838	-0.855407
C	2.668112	-0.472806	0.380071
H	0.858927	1.971230	-1.075159
H	3.396874	-0.604182	1.170247
C	2.635203	-3.930896	-1.093483
C	4.019583	-4.476198	1.275634
C	3.173773	-5.221834	-0.869246
C	2.840938	-2.906135	-0.131423
C	3.513386	-3.202587	1.049094
C	3.861706	-5.466715	0.326746
H	3.639468	-2.450796	1.819158
H	4.277363	-6.443327	0.535326
H	4.543183	-4.693272	2.200694
C	2.280494	-5.974608	-3.064359
C	3.390103	-8.514635	-2.669912
C	2.126247	-6.977467	-4.051157
C	3.002428	-6.259739	-1.879420
C	3.549881	-7.536199	-1.707136
C	2.684305	-8.238114	-3.829445
H	4.114068	-7.783164	-0.817477
H	2.576522	-9.029558	-4.559210
H	3.819355	-9.499259	-2.519498
C	2.749939	2.001814	0.951576
C	2.027870	3.318794	0.638561
H	2.151347	3.616877	-0.408285
H	2.446887	4.119888	1.254677
H	0.957923	3.256639	0.863090
C	2.605017	1.716247	2.457759
H	3.171870	0.835547	2.775137
H	1.558417	1.557443	2.727833
H	2.979217	2.567777	3.035018
C	4.241819	2.160361	0.596039
H	4.372270	2.366381	-0.471308
H	4.817977	1.261703	0.839735
H	4.673239	2.993979	1.159850
C	-1.962670	-2.905547	0.293621
C	-3.159611	-3.400807	1.130223
H	-2.917373	-3.456246	2.196544
H	-3.453809	-4.403829	0.803979
H	-4.022412	-2.737078	1.013577
C	-2.361265	-2.916721	-1.187881
H	-1.550434	-2.553374	-1.827850
H	-3.256138	-2.314026	-1.377515
H	-2.590131	-3.941206	-1.496222
C	-0.769919	-3.861064	0.482141
H	-0.479196	-3.969603	1.531442
H	0.103891	-3.513984	-0.074494
H	-1.032171	-4.858292	0.114423
C	-2.364210	2.813352	-3.856580
O	-2.897102	3.450639	-4.730817

[2A] $C_{168}H_{64}O_2$

	X	Y	Z
O	0.653032	6.018693	3.783840
C	4.747915	3.349228	2.966787
H	4.536718	4.403688	3.158743
C	1.894745	6.242928	4.471422
C	2.430314	7.422829	5.015087
H	1.870999	8.359324	4.907883
C	3.665714	7.399329	5.679788
C	4.366115	8.627830	6.052188
C	3.906114	9.869330	5.638688
H	2.975368	9.927331	5.060071
C	4.580115	11.049131	5.910888
C	5.740215	10.959531	6.669688
H	6.270234	11.883764	6.927200
C	6.282015	9.738530	7.078788
C	7.589316	9.661730	7.746088
C	8.368016	10.800131	7.968988
H	7.963792	11.780938	7.696118
C	9.649016	10.727631	8.499789
C	10.118817	9.486130	8.878789
H	11.119045	9.423359	9.328468
C	9.390116	8.318130	8.700789
C	8.112316	8.390130	8.079288
C	7.406016	7.176529	7.747488
C	6.150815	7.258529	7.095388
C	5.588715	8.541430	6.767988
C	5.480215	6.067729	6.720788
C	4.241714	6.132229	5.974288
C	3.651514	4.927528	5.490388
C	2.613214	5.032228	4.549887
C	4.125614	3.647528	6.006588
C	5.363415	3.594028	6.686288
C	6.058215	4.811028	7.010788
C	7.319316	4.735128	7.660188
C	7.996816	5.918829	8.011288
C	9.293816	5.840929	8.642589
C	9.963117	7.021729	9.038289
C	11.193617	6.911629	9.699689
H	11.688481	7.828071	10.042647
C	11.814417	5.698929	9.916389
C	11.169117	4.558128	9.471089
H	11.656397	3.587298	9.623607
C	9.924217	4.589728	8.844489
C	9.239616	3.363128	8.419889
C	7.922416	3.450128	7.896688
C	9.832216	2.111927	8.539589
H	10.862376	2.047697	8.910023
C	9.169916	0.926627	8.229789
C	7.868416	1.021727	7.769988
H	7.323557	0.102085	7.528183
C	7.228016	2.249728	7.602488
C	5.867815	2.332228	7.073688
C	5.063015	1.197227	6.922888
H	5.450608	0.225269	7.244659
C	3.775314	1.262327	6.395488
C	3.337714	2.489328	5.931788
H	2.327684	2.554604	5.514635
C	1.924114	4.073328	3.632787
C	0.670168	4.647468	3.350275
C	-0.334587	3.861828	2.769387
H	-1.319035	4.311271	2.584158
C	-0.096387	2.522928	2.452786
C	-1.172288	1.583627	2.128086
C	-2.512988	1.977827	2.270186
H	-2.739560	3.012225	2.546435
C	-3.560188	1.088327	2.089786
C	-3.249188	-0.203773	1.696486
H	-4.073097	-0.906783	1.519994
C	-1.940088	-0.657874	1.518686
C	-1.639188	-2.041574	1.141986
C	-2.638288	-2.993774	0.909586
H	-3.685782	-2.671559	0.967581
C	-2.368788	-4.320275	0.629786
C	-1.034087	-4.692975	0.520686
H	-0.799731	-5.737079	0.284384
C	0.005713	-3.786075	0.695986
C	-0.280587	-2.450474	1.050586
C	0.784113	-1.529074	1.365786
C	0.495713	-0.188673	1.713786
C	-0.876987	0.258627	1.768186
C	1.540414	0.702227	2.070386
C	1.246813	2.046627	2.488886
C	2.293214	2.881528	2.999287
C	3.681114	2.441628	2.830187
C	3.945114	1.120527	2.457886
C	2.881214	0.216927	2.099386
C	3.162914	-1.113074	1.752086
C	2.121914	-1.997474	1.382586
C	2.425814	-3.350275	1.003186
C	1.407213	-4.231875	0.583386
C	1.743514	-5.484675	0.085586
H	0.946048	-6.141872	-0.284917
C	3.054414	-5.950575	0.035086
C	4.037414	-5.101775	0.545986
H	5.073213	-5.462027	0.551085
C	3.769614	-3.831975	1.036486
C	4.804315	-2.964374	1.576086
C	4.521315	-1.613974	1.853386
C	5.566315	-0.751574	2.248286
C	5.293715	0.671127	2.435086
C	6.314115	1.607827	2.600186
H	7.354628	1.268197	2.543399
C	6.069115	2.950928	2.834487
C	6.096015	-3.452575	1.842586
H	6.304183	-4.512103	1.661176
C	7.100115	-2.646874	2.342186
C	6.825115	-1.299174	2.501786
H	7.626019	-0.637946	2.852052
O	-0.652896	-6.018722	-3.783786
C	-4.747989	-3.349274	-2.966615
H	-4.536768	-4.403759	-3.158524
C	-1.894565	-6.243034	-4.471212
C	-2.430388	-7.422776	-5.014916
H	-1.871574	-8.359429	-4.907969
C	-3.665788	-7.399376	-5.679616
C	-4.366289	-8.627876	-6.052017
C	-3.906189	-9.869277	-5.638517
H	-2.975376	-9.927725	-5.059884
C	-4.580189	-11.049077	-5.910717
C	-5.740289	-10.959577	-6.669517
H	-6.269955	-11.884019	-6.927149
C	-6.282089	-9.738577	-7.078617
C	-7.589490	-9.661777	-7.745917
C	-8.368090	-10.800177	-7.968817
H	-7.963811	-11.781036	-7.695928
C	-9.649191	-10.727677	-8.499618
C	-10.118991	-9.486177	-8.878618
H	-11.119149	-9.423409	-9.328315
C	-9.390290	-8.318076	-8.700618
C	-8.112390	-8.390176	-8.079117
C	-7.406190	-7.176576	-7.747317
C	-6.150989	-7.258576	-7.095217
C	-5.588789	-8.541476	-6.767817
C	-5.480289	-6.067775	-6.720617
C	-4.241789	-6.132276	-5.974117
C	-3.651588	-4.927575	-5.490216
C	-2.613288	-5.032475	-4.549716
C	-4.125689	-3.647575	-6.006417
C	-5.363489	-3.593975	-6.686117
C	-6.058289	-4.811075	-7.010617
C	-7.319490	-4.735175	-7.660017
C	-7.996990	-5.918875	-8.011117
C	-9.293890	-5.840975	-8.642418
C	-9.963191	-7.021776	-9.038118
C	-11.193691	-6.911676	-9.699518
H	-11.688423	-7.828130	-10.042532
C	-11.814591	-5.698975	-9.916218
C	-11.169291	-4.558175	-9.470918
H	-11.656637	-3.587361	-9.623579
C	-9.924391	-4.589675	-8.844318
C	-9.239690	-3.363175	-8.419717
C	-7.922590	-3.450175	-7.896517
C	-9.832391	-2.111974	-8.539418
H	-10.862442	-2.047945	-8.909742
C	-9.170090	-0.926674	-8.229617
C	-7.868590	-1.021774	-7.769817
H	-7.323535	-0.102247	-7.527975
C	-7.228090	-2.249774	-7.602317
C	-5.867989	-2.332274	-7.073517

C	-5.063189	-1.197274	-6.922717
H	-5.450536	-0.225232	-7.244389
C	-3.775388	-1.262374	-6.395317
C	-3.337888	-2.489374	-5.931617
H	-2.327872	-2.554480	-5.514537
C	-1.924188	-4.073375	-3.632616
C	-0.670259	-4.647479	-3.350180
C	0.334513	-3.861875	-2.769215
H	1.318955	-4.311267	-2.583941
C	0.096213	-2.522974	-2.452615
C	1.172213	-1.583674	-2.127915
C	2.512914	-1.977774	-2.270015
H	2.739270	-3.012197	-2.546141
C	3.560114	-1.088374	-2.089615
C	3.249114	0.203827	-1.696315
H	4.072967	0.906795	-1.519692
C	1.939914	0.657827	-1.518515
C	1.639114	2.041527	-1.141815
C	2.638214	2.993728	-0.909415
H	3.685545	2.671490	-0.967445
C	2.368614	4.320228	-0.629615
C	1.034013	4.692928	-0.520515
H	0.799829	5.737275	-0.284308
C	-0.005887	3.786028	-0.695815
C	0.280413	2.450428	-1.050415
C	-0.784187	1.529027	-1.365615
C	-0.495787	0.188627	-1.713615
C	0.876813	-0.258673	-1.768015
C	-1.540588	-0.702274	-2.070215
C	-1.246887	-2.046674	-2.488715
C	-2.293288	-2.881574	-2.999116
C	-3.681188	-2.441574	-2.830015
C	-3.945289	-1.120574	-2.457715
C	-2.881388	-0.216973	-2.099215
C	-3.163088	1.113027	-1.751915
C	-2.121988	1.997527	-1.382415
C	-2.425988	3.350228	-1.003015
C	-1.407388	4.231828	-0.583215
C	-1.743688	5.484629	-0.085414
H	-0.945965	6.141513	0.285108
C	-3.054488	5.950529	-0.034914
C	-4.037589	5.101729	-0.545815
H	-5.073308	5.461766	-0.550556
C	-3.769688	3.832028	-1.036315
C	-4.804389	2.964328	-1.575915
C	-4.521489	1.613927	-1.853215
C	-5.566389	0.751527	-2.248115
C	-5.293789	-0.671174	-2.434915
C	-6.314189	-1.607874	-2.600015
H	-7.354889	-1.268313	-2.543072
C	-6.069189	-2.950974	-2.834315
C	-6.096189	3.452528	-1.842415
H	-6.304171	4.511947	-1.661050
C	-7.100190	2.646828	-2.342015
C	-6.825190	1.299127	-2.501615
H	-7.626036	0.637740	-2.851886
H	4.205254	12.009358	5.563675
H	10.252625	11.624381	8.628606
H	12.777562	5.638817	10.420591
H	9.662713	-0.036125	8.343898
H	8.082540	-3.051022	2.579640
H	6.884765	3.665588	2.930292
H	3.169034	5.042674	-0.486203
H	3.147375	0.375508	6.334372
H	-3.169160	-5.042845	0.487409
H	-6.884776	-3.665448	-2.930197
H	-4.205287	-12.009318	-5.563583
H	-10.252527	-11.624442	-8.628654
H	-12.777917	-5.639008	-10.420047
H	-3.147228	-0.375575	-6.334104
H	-8.082702	3.050896	-2.579071
H	-3.297857	6.927641	0.371077
H	4.593917	-1.399305	-2.229934
H	3.297921	-6.927704	-0.371474
H	-4.593674	1.399628	2.228343
H	-9.662684	0.035932	-8.343504

[2B] C$_{170}$H$_{64}$O$_2$

	X	Y	Z
O	-0.253129	6.852945	3.590201
C	0.636471	6.037545	3.767801
C	4.747973	3.349244	2.966701
H	4.536776	4.403704	3.158657
C	1.935172	6.266745	4.466102
C	2.430372	7.422845	5.015002
H	1.871057	8.359340	4.907798
C	3.665772	7.399345	5.679702
C	4.366172	8.627846	6.052102
C	3.906172	9.869346	5.638602
H	2.975426	9.927347	5059986
C	4.580173	11.049146	5.910802
C	5.740273	10.959546	6.669602
H	6.270292	11.883780	6.927114
C	6.282073	9.738546	7.078702
C	7.589373	9.661746	7.746002
C	8.368074	10.800146	7.968903
H	7.963850	11.780954	7.696033
C	9.649074	10.727646	8.499703
C	10.118874	9.486146	8.878703
H	11.119102	9.423374	9.328382
C	9.390174	8.318146	8.700703
C	8.112374	8.390146	8.079203
C	7.406073	7.176545	7.747402
C	6.150873	7.258545	7.095302
C	5.588773	8.541446	6.767902
C	5.480273	6.067745	6.720702
C	4.241772	6.132245	5.974202
C	3.651572	4.927545	5.490302
C	2.613272	5.032445	4.549802
C	4.125672	3.647544	6.006502
C	5.363473	3.594044	6.686202
C	6.058273	4.811045	7.010702
C	7.319373	4.735145	7.660102
C	7.996874	5.918845	8.011203
C	9.293874	5.840945	8.642503
C	9.963174	7.021745	9.038203
C	11.193674	6.911645	9.699603
H	11.688539	7.828087	10.042561
C	11.814475	5.698945	9.916303
C	11.169174	4.558145	9.471003
H	11.656455	3.587315	9.623521
C	9.924274	4.589745	8.844403
C	9.239674	3.363144	8.419803
C	7.922473	3.450144	7.896603
C	9.832274	2.111944	8.539503
H	10.862434	2.047714	8.909937
C	9.169974	0.926644	8.229703
C	7.868473	1.021744	7.769902
H	7.323615	0.102101	7.528097
C	7.228073	2.249744	7.602402
C	5.867873	2.332244	7.073602
C	5.063073	1.197244	6.922802
H	5.450666	0.225285	7.244573
C	3.775372	1.262344	6.395402
C	3.337772	2.489344	5.931702
H	2.327742	2.554621	5.514549
C	1.924172	4.073344	3.632701
C	0.657671	4.609845	3.351901
C	-0.334529	3.861844	2.769301
H	-1.318977	4.311287	2.584073
C	-0.096329	2.522944	2.452701
C	-1.172229	1.583644	2.128001
C	-2.512930	1.977844	2.270101
H	-2.739502	3.012241	2.546349
C	-3.560130	1.088344	2.089701
C	-3.249130	-0.203757	1.696401
H	-4.073038	-0.906766	1.519909
C	-1.940029	-0.657857	1.518601
C	-1.639129	-2.041557	1.141901
C	-2.638230	-2.993758	0.909501
H	-3.685724	-2.671542	0.967496
C	-2.368729	-4.320258	0.629700
C	-1.034029	-4.692958	0.520600
H	-0.799673	-5.737062	0.284299
C	0.005771	-3.786058	0.695900
C	-0.280529	-2.450457	1.050501
C	0.784171	-1.529057	1.365701

	X	Y	Z
C	0.495771	-0.188657	1.713701
C	-0.876929	0.258643	1.768101
C	1.540472	0.702243	2.070301
C	1.246872	2.046644	2.488801
C	2.293272	2.881544	2.999201
C	3.681172	2.441644	2.830101
C	3.945172	1.120544	2.457801
C	2.881272	0.216943	2.099301
C	3.162972	-1.113057	1.752001
C	2.121972	-1.997457	1.382501
C	2.425872	-3.350258	1.003101
C	1.407272	-4.231858	0.583300
C	1.743572	-5.484658	0.085500
H	0.946106	-6.141855	-0.285002
C	3.054472	-5.950558	0.035000
C	4.037472	-5.101758	0.545900
H	5.073271	-5.462010	0.551000
C	3.769672	-3.831958	1.036401
C	4.804373	-2.964358	1.576001
C	4.521373	-1.613957	1.853301
C	5.566373	-0.751557	2.248201
C	5.293773	0.671143	2.435001
C	6.314173	1.607844	2.600101
H	7.354686	1.268214	2.543313
C	6.069173	2.950944	2.834401
C	6.096073	-3.452558	1.842501
H	6.304240	-4.512086	1.661091
C	7.100173	-2.646857	2.342101
C	6.825173	-1.299157	2.501701
H	7.626077	-0.637929	2.851967
O	0.253171	-6.852859	-3.590201
C	-0.636429	-6.037458	-3.767801
C	-4.747930	-3.349258	-2.966701
H	-4.536710	-4.403742	-3.158609
C	-1.935229	-6.266759	-4.466101
C	-2.430330	-7.422759	-5.015001
H	-1.871515	-8.359412	-4.908054
C	-3.665730	-7.399359	-5.679701
C	-4.366230	-8.627859	-6.052102
C	-3.906130	-9.869260	-5.638601
H	-2.975317	-9.927708	-5.059969
C	-4.580130	-11.049060	-5.910801
C	-5.740230	-10.959560	-6.669602
H	-6.269896	-11.884001	-6.927233
C	-6.282031	-9.738560	-7.078702
C	-7.589431	-9.661760	-7.746002
C	-8.368031	-10.800160	-7.968902
H	-7.963752	-11.781019	-7.696013
C	-9.649132	-10.727660	-8.499702
C	-10.118932	-9.486159	-8.878702
H	-11.119090	-9.423392	-9.328400
C	-9.390232	-8.318059	-8.700702
C	-8.112331	-8.390159	-8.079202
C	-7.406131	-7.176559	-7.747402
C	-6.150931	-7.258559	-7.095302
C	-5.588730	-8.541459	-6.767902
C	-5.480230	-6.067758	-6.720702
C	-4.241730	-6.132259	-5.974201
C	-3.651530	-4.927558	-5.490301
C	-2.613230	-5.032458	-4.549801
C	-4.125630	-3.647558	-6.006501
C	-5.363430	-3.593958	-6.686202
C	-6.058231	-4.811058	-7.010702
C	-7.319431	-4.735158	-7.660102
C	-7.996931	-5.918858	-8.011202
C	-9.293831	-5.840958	-8.642502
C	-9.963132	-7.021759	-9.038202
C	-11.193632	-6.911659	-9.699603
H	-11.688364	-7.828113	-10.042617
C	-11.814532	-5.698958	-9.916303
C	-11.169232	-4.558158	-9.471002
H	-11.656578	-3.587345	-9.623664
C	-9.924332	-4.589658	-8.844402
C	-9.239631	-3.363158	-8.419802
C	-7.922531	-3.450158	-7.896602
C	-9.832332	-2.111957	-8.539502
H	-10.862383	-2.047928	-8.909826
C	-9.170031	-0.926657	-8.229702
C	-7.868531	-1.021757	-7.769902
H	-7.323476	-0.102230	-7.528060

C	-7.228031	-2.249757	-7.602402
C	-5.867930	-2.332257	-7.073602
C	-5.063130	-1.197257	-6.922802
H	-5.450478	-0.225215	-7.244474
C	-3.775330	-1.262357	-6.395402
C	-3.337830	-2.489357	-5.931701
H	-2.327813	-2.554464	-5.514622
C	-1.924129	-4.073358	-3.632701
C	-0.657629	-4.609858	-3.351901
C	0.334571	-3.861858	-2.769301
H	1.319014	-4.311250	-2.584027
C	0.096271	-2.522957	-2.452700
C	1.172272	-1.583657	-2.128000
C	2.512972	-1.977757	-2.270100
H	2.739328	-3.012180	-2.546226
C	3.560172	-1.088357	-2.089700
C	3.249172	0.203843	-1.696400
H	4.073025	0.906812	-1.519778
C	1.939972	0.657844	-1.518600
C	1.639172	2.041544	-1.141900
C	2.638272	2.993744	-0.909500
H	3.685603	2.671506	-0.967530
C	2.368672	4.320245	-0.629700
C	1.034072	4.692945	-0.520600
H	0.799887	5.737291	-0.284394
C	-0.005829	3.786044	-0.695900
C	0.280471	2.450444	-1.050500
C	-0.784129	1.529044	-1.365700
C	-0.495729	0.188643	-1.713700
C	0.876871	-0.258657	-1.768100
C	-1.540529	-0.702257	-2.070300
C	-1.246829	-2.046657	-2.488800
C	-2.293229	-2.881558	-2.999201
C	-3.681130	-2.441557	-2.830101
C	-3.945230	-1.120557	-2.457800
C	-2.881330	-0.216957	-2.099300
C	-3.163030	1.113044	-1.752000
C	-2.121929	1.997544	-1.382500
C	-2.425930	3.350244	-1.003100
C	-1.407329	4.231845	-0.583300
C	-1.743629	5.484645	-0.085500
H	-0.945907	6.141529	0.285023
C	-3.054430	5.950545	-0.035000
C	-4.037530	5.101745	-0.545900
H	-5.073249	5.461782	-0.550642
C	-3.769630	3.832044	-1.036400
C	-4.804330	2.964344	-1.576000
C	-4.521430	1.613944	-1.853300
C	-5.566330	0.751544	-2.248200
C	-5.293730	-0.671157	-2.435000
C	-6.314131	-1.607857	-2.600100
H	-7.354830	-1.268296	-2.543157
C	-6.069131	-2.950958	-2.834401
C	-6.096131	3.452544	-1.842500
H	-6.304112	4.511964	-1.661135
C	-7.100131	2.646844	-2.342100
C	-6.825131	1.299144	-2.501700
H	-7.625977	0.637757	-2.851971
H	4.205312	12.009373	5.563589
H	10.252682	11.624397	8.628520
H	12.777619	5.638833	10.420504
H	9.662771	-0.036109	8.343812
H	8.082598	-3.051005	2.579554
H	6.884823	3.665604	2.930207
H	3.169092	5.042690	-0.486288
H	3.147433	0.375524	6.334286
H	-3.169102	-5.042829	0.487323
H	-6.884717	-3.665431	-2.930282
H	-4.205228	-12.009301	-5.563668
H	-10.252468	-11.624425	-8.628739
H	-12.777857	-5.638991	-10.420132
H	-3.147169	-0.375558	-6.334189
H	-8.082643	3.050912	-2.579156
H	-3.297798	6.927657	0.370992
H	4.593975	-1.399289	-2.230019
H	3.297979	-6.927687	-0.371559
H	-4.593615	1.399645	2.228257
H	-9.662625	0.035949	-8.343589

[AB] $C_{169}H_{64}O_2$

	X	Y	Z
O	-0.252060	6.823790	3.574925
C	0.637540	6.008390	3.752525
C	4.749042	3.320089	2.951425
H	4.537845	4.374549	3.143380
C	1.936241	6.237590	4.450825
C	2.431441	7.393690	4.999725
H	1.872126	8.330185	4.892521
C	3.666841	7.370190	5.664425
C	4.367242	8.598691	6.036825
C	3.907241	9.840191	5.623325
H	2.976495	9.898192	5.044709
C	4.581242	11.019991	5.895525
C	5.741342	10.930391	6.654326
H	6.271361	11.854625	6.911837
C	6.283142	9.709391	7.063426
C	7.590442	9.632591	7.730726
C	8.369143	10.770991	7.953626
H	7.964919	11.751799	7.680756
C	9.650143	10.698491	8.484426
C	10.119943	9.456991	8.863426
H	11.120171	9.394219	9.313105
C	9.391243	8.288991	8.685426
C	8.113443	8.360991	8.063926
C	7.407142	7.147390	7.732126
C	6.151942	7.229390	7.080026
C	5.589842	8.512291	6.752626
C	5.481342	6.038590	6.705426
C	4.242841	6.103090	5.958925
C	3.652641	4.898390	5.475025
C	2.614341	5.003290	4.534525
C	4.126741	3.618389	5.991225
C	5.364542	3.564889	6.670926
C	6.059342	4.781890	6.995426
C	7.320442	4.705990	7.644826
C	7.997943	5.889690	7.995926
C	9.294943	5.811790	8.627226
C	9.964243	6.992590	9.022926
C	11.194744	6.882490	9.684326
H	11.689608	7.798932	10.027284
C	11.815544	5.669790	9.901027
C	11.170244	4.528990	9.455726
H	11.657524	3.558160	9.608244
C	9.925343	4.560590	8.829126
C	9.240743	3.333989	8.404526
C	7.923543	3.420989	7.881326
C	9.833343	2.082789	8.524226
H	10.863503	2.018559	8.894661
C	9.171043	0.897489	8.214426
C	7.869543	0.992589	7.754626
H	7.324684	0.072946	7.512821
C	7.229142	2.220589	7.587126
C	5.868942	2.303089	7.058326
C	5.064142	1.168089	6.907526
H	5.451735	0.196130	7.229297
C	3.776441	1.233189	6.380126
C	3.338841	2.460189	5.916425
H	2.328811	2.525466	5.499273
C	1.925241	4.044189	3.617425
C	0.658741	4.580690	3.336625
C	-0.333460	3.832689	2.754025
H	-1.317908	4.282132	2.568796
C	-0.095260	2.493789	2.437424
C	-1.171160	1.554489	2.112724
C	-2.511860	1.948689	2.254824
H	-2.738433	2.983086	2.531073
C	-3.559061	1.059189	2.074424
C	-3.248061	-0.232912	1.681124
H	-4.071969	-0.935921	1.504632
C	-1.938960	-0.687012	1.503324
C	-1.638060	-2.070712	1.126624
C	-2.637160	-3.022913	0.894224
H	-3.684655	-2.700697	0.952219
C	-2.367660	-4.349413	0.614424
C	-1.032960	-4.722113	0.505324
H	-0.798604	-5.766217	0.269022
C	0.006840	-3.815213	0.680624
C	-0.279460	-2.479612	1.035224
C	0.785241	-1.558212	1.350424

	X	Y	Z
C	0.496840	-0.217812	1.698424
C	-0.875860	0.229488	1.752824
C	1.541541	0.673089	2.055024
C	1.247941	2.017489	2.473524
C	2.294341	2.852389	2.983925
C	3.682241	2.412489	2.814825
C	3.946241	1.091389	2.442524
C	2.882341	0.187788	2.084024
C	3.164041	-1.142212	1.736724
C	2.123041	-2.026612	1.367224
C	2.426941	-3.379413	0.987824
C	1.408341	-4.261013	0.568024
C	1.744641	-5.513813	0.070224
H	0.947175	-6.171010	-0.300279
C	3.055541	-5.979713	0.019724
C	4.038541	-5.130913	0.530624
H	5.074340	-5.491165	0.535723
C	3.770741	-3.861113	1.021124
C	4.805442	-2.993513	1.560724
C	4.522442	-1.643112	1.838024
C	5.567442	-0.780712	2.232924
C	5.294842	0.641989	2.419724
C	6.315242	1.578689	2.584824
H	7.355755	1.239059	2.528037
C	6.070242	2.921789	2.819125
C	6.097142	-3.481713	1.827224
H	6.305310	-4.541241	1.645814
C	7.101242	-2.676012	2.326824
C	6.826242	-1.328312	2.486424
H	7.627146	-0.667084	2.836690
O	-0.651816	-6.047662	-3.799087
C	-4.746861	-3.378413	-2.981977
H	-4.535641	-4.432897	-3.173886
C	-1.893562	-6.272047	-4.486614
C	-2.429260	-7.451914	-5.030278
H	-1.870446	-8.388567	-4.923331
C	-3.664661	-7.428514	-5.694978
C	-4.365161	-8.657014	-6.067378
C	-3.905061	-9.898415	-5.653878
H	-2.974248	-9.956863	-5.075245
C	-4.579061	-11.078215	-5.926078
C	-5.739161	-10.988715	-6.684878
H	-6.268827	-11.913156	-6.942510
C	-6.280961	-9.767715	-7.093978
C	-7.588362	-9.690914	-7.761279
C	-8.366962	-10.829315	-7.984179
H	-7.962683	-11.810174	-7.711290
C	-9.648063	-10.756815	-8.514979
C	-10.117863	-9.515314	-8.893979
H	-11.118021	-9.452547	-9.343676
C	-9.389162	-8.347214	-8.715979
C	-8.111262	-8.419314	-8.094479
C	-7.405062	-7.205714	-7.762679
C	-6.149862	-7.287714	-7.110578
C	-5.587661	-8.570614	-6.783178
C	-5.479161	-6.096913	-6.735978
C	-4.240661	-6.161414	-5.989478
C	-3.650461	-4.956713	-5.505578
C	-2.612160	-5.061613	-4.565078
C	-4.124561	-3.676713	-6.021778
C	-5.362361	-3.623113	-6.701478
C	-6.057161	-4.840213	-7.025978
C	-7.318362	-4.764313	-7.675379
C	-7.995862	-5.948013	-8.026479
C	-9.292762	-5.870113	-8.657779
C	-9.962063	-7.050914	-9.053479
C	-11.192563	-6.940814	-9.714879
H	-11.687295	-7.857268	-10.057893
C	-11.813463	-5.728113	-9.931579
C	-11.168163	-4.587313	-9.486279
H	-11.655509	-3.616499	-9.638941
C	-9.923263	-4.618813	-8.859679
C	-9.238562	-3.392313	-8.435079
C	-7.921462	-3.479313	-7.911879
C	-9.831263	-2.141112	-8.554779
H	-10.861314	-2.077083	-8.925103
C	-9.168962	-0.955812	-8.244979
C	-7.867462	-1.050912	-7.785179
H	-7.322407	-0.131385	-7.543337
C	-7.226962	-2.278912	-7.617679

C	-5.866861	-2.361412	-7.088878
C	-5.062061	-1.226412	-6.938078
H	-5.449409	-0.254370	-7.259750
C	-3.774261	-1.291512	-6.410678
C	-3.336761	-2.518512	-5.946978
H	-2.326744	-2.583619	-5.529899
C	-1.923060	-4.102513	-3.647977
C	-0.668964	-4.676427	-3.365685
C	0.335640	-3.891013	-2.784577
H	1.320083	-4.340405	-2.599303
C	0.097340	-2.552112	-2.467977
C	1.173341	-1.612812	-2.143277
C	2.514041	-2.006912	-2.285377
H	2.740398	-3.041335	-2.561502
C	3.561241	-1.117512	-2.104977
C	3.250241	0.174688	-1.711677
H	4.074094	0.877657	-1.535054
C	1.941041	0.628689	-1.533877
C	1.640241	2.012389	-1.157177
C	2.639341	2.964589	-0.924777
H	3.686672	2.642351	-0.982807
C	2.369741	4.291090	-0.644977
C	1.035141	4.663790	-0.535876
H	0.800956	5.708136	-0.299670
C	-0.004760	3.756889	-0.711176
C	0.281540	2.421289	-1.065777
C	-0.783060	1.499889	-1.380977
C	-0.494660	0.159488	-1.728977
C	0.877941	-0.287812	-1.783377
C	-1.539460	-0.731412	-2.085577
C	-1.245760	-2.075812	-2.504077
C	-2.292160	-2.910713	-3.014477
C	-3.680061	-2.470712	-2.845377
C	-3.944161	-1.149712	-2.473077
C	-2.880261	-0.246112	-2.114577
C	-3.161961	1.083889	-1.767277
C	-2.120860	1.968389	-1.397777
C	-2.424860	3.321089	-1.018377
C	-1.406260	4.202690	-0.598576
C	-1.742560	5.455490	-0.100776
H	-0.944838	6.112374	0.269746
C	-3.053361	5.921390	-0.050276
C	-4.036461	5.072590	-0.561176
H	-5.072180	5.432627	-0.565918
C	-3.768561	3.802889	-1.051677
C	-4.803261	2.935189	-1.591277
C	-4.520361	1.584789	-1.868577
C	-5.565261	0.722389	-2.263477
C	-5.292661	-0.700312	-2.450277
C	-6.313062	-1.637012	-2.615377
H	-7.353761	-1.297451	-2.558433
C	-6.068061	-2.980113	-2.849677
C	-6.095061	3.423389	-1.857777
H	-6.303043	4.482809	-1.676412
C	-7.099062	2.617689	-2.357377
C	-6.824062	1.269989	-2.516977
H	-7.624908	0.608602	-2.867248
H	4.206381	11.980218	5.548313
H	10.253751	11.595242	8.613244
H	12.778689	5.609678	10.405228
H	9.663840	-0.065264	8.328535
H	8.083667	-3.080160	2.564278
H	6.885892	3.636449	2.914930
H	3.170161	5.013535	-0.501565
H	3.148502	0.346369	6.319009
H	-3.168033	-5.071984	0.472047
H	-6.883648	-3.694586	-2.945558
H	-4.204159	-12.038456	-5.578945
H	-10.251399	-11.653580	-8.644015
H	-12.776788	-5.668146	-10.435409
H	-3.146100	-0.404713	-6.349465
H	-8.081574	3.021757	-2.594433
H	-3.296729	6.898502	0.355715
H	4.595044	-1.428444	-2.245296
H	3.299048	-6.956842	-0.386835
H	-4.592546	1.370490	2.212981
H	-9.661556	0.006794	-8.358866

Alternative packing Structure 1

	X	Y	Z
O	-9.924981	3.723258	2.510458
C	-8.970772	2.995452	2.418587
C	-4.806279	0.826881	0.539454
H	-5.051283	1.842541	0.855814
C	-7.587209	3.215488	2.957424
C	-7.111193	4.304835	3.641148
H	-7.748662	5.177463	3.810470
C	-5.769921	4.284273	4.105674
C	-5.167213	5.487229	4.679680
C	-5.926672	6.652597	4.892915
H	-6.993243	6.658224	4.658844
C	-5.331629	7.802465	5.403517
C	-3.965649	7.819038	5.692805
H	-3.512281	8.733773	6.079208
C	-3.176416	6.676994	5.492199
C	-1.732872	6.695367	5.757270
C	-1.089820	7.870484	6.178241
H	-1.670287	8.781507	6.335348
C	0.287205	7.889845	6.398424
C	1.044760	6.738318	6.194621
H	2.122841	6.767265	6.365773
C	0.436622	5.542175	5.777393
C	-0.967974	5.513674	5.568864
C	-1.619937	4.279504	5.162390
C	-3.006947	4.271434	4.862247
C	-3.786624	5.487857	5.007613
C	-3.630007	3.078288	4.425019
C	-5.019865	3.093891	3.996286
C	-5.590632	1.906581	3.412048
C	-6.789302	2.047877	2.716697
C	-4.909509	0.626081	3.642056
C	-3.548293	0.625536	4.040485
C	-2.884318	1.873135	4.376021
C	-1.510249	1.873510	4.702933
C	-0.867666	3.087043	5.057241
C	0.569841	3.108529	5.264913
C	1.230958	4.327791	5.556206
C	2.634294	4.358112	5.606987
H	3.146644	5.302001	5.806712
C	3.397385	3.208876	5.381041
C	2.731009	1.991504	5.176839
H	3.324955	1.084812	5.039523
C	1.333357	1.919892	5.123242
C	0.643906	0.640187	4.906156
C	-0.756833	0.631409	4.680908
C	1.346133	-0.572580	4.924310
H	2.423127	-0.569777	5.108356
C	0.700716	-1.797275	4.707910
C	-0.678898	-1.795517	4.478121
H	-1.188839	-2.747003	4.309409
C	-1.418133	-0.601967	4.452130
C	-2.860619	-0.606906	4.175049
C	-3.576276	-1.806234	4.042416
H	-3.056932	-2.760127	4.160077
C	-4.952148	-1.813527	3.778879
C	-5.602316	-0.590260	3.569684
H	-6.673155	-0.597138	3.357991
C	-7.541255	1.183248	1.771867
C	-8.893088	1.659951	1.736086
C	-9.896530	0.978759	1.096507
H	-10.917481	1.372118	1.087837
C	-9.588050	-0.252886	0.461207
C	-10.655944	-1.085334	-0.091700
C	-11.995669	-0.654979	-0.070778
H	-12.247165	0.323594	0.344026
C	-13.008931	-1.464743	-0.574779
C	-12.706436	-2.722481	-1.099380
H	-13.513687	-3.349740	-1.482581
C	-11.382391	-3.184524	-1.137460
C	-11.060012	-4.512182	-1.672250
C	-12.071938	-5.364178	-2.143173
H	-13.113260	-5.036172	-2.120343
C	-11.764595	-6.630005	-2.640699
C	-10.441472	-7.064334	-2.673908
H	-10.213048	-8.058442	-3.063727
C	-9.401466	-6.238737	-2.212837
C	-9.708573	-4.947444	-1.709066
C	-8.644869	-4.074232	-1.238889

C	-8.957291	-2.794712	-0.708477
C	-10.340080	-2.353959	-0.643597
C	-7.922130	-1.945498	-0.247892
C	-8.242109	-0.666643	0.370589
C	-7.182544	0.137386	0.924519
C	-5.804986	-0.156967	0.512227
C	-5.502853	-1.435212	-0.020642
C	-6.570548	-2.357134	-0.368277
C	-6.257876	-3.629639	-0.898578
C	-7.297803	-4.499696	-1.313701
C	-6.972924	-5.826146	-1.814296
C	-8.008025	-6.694987	-2.247880
C	-7.680590	-7.983158	-2.705175
H	-8.471217	-8.659067	-3.036665
C	-6.355216	-8.410969	-2.738550
C	-5.333708	-7.558002	-2.322550
H	-4.298659	-7.904474	-2.356450
C	-5.621525	-6.262989	-1.861950
C	-4.545907	-5.353994	-1.446900
C	-4.870315	-4.044982	-1.014504
C	-3.823090	-3.142810	-0.689751
C	-4.153382	-1.768072	-0.295982
C	-3.169372	-0.772308	-0.213260
H	-2.132841	-1.015039	-0.456720
C	-3.492452	0.543906	0.142885
C	-3.200784	-5.758662	-1.483268
H	-2.951859	-6.773386	-1.803096
C	-2.167271	-4.890203	-1.123486
C	-2.494465	-3.581386	-0.738646
H	-1.687727	-2.894096	-0.473918
O	8.944961	-2.631515	-2.238463
C	4.712996	-0.489782	-0.526831
H	4.952585	-1.503041	-0.857555
C	7.679090	-2.906981	-2.790703
C	7.375410	-4.091731	-3.429069
H	8.114790	-4.884688	-3.528025
C	6.062595	-4.226207	-3.921875
C	5.611377	-5.512416	-4.462897
C	6.498918	-6.595038	-4.591485
H	7.550366	-6.471793	-4.322531
C	6.053284	-7.828965	-5.060471
C	4.710486	-8.008010	-5.392090
H	4.371729	-8.984330	-5.745259
C	3.794757	-6.949590	-5.279067
C	2.375744	-7.139474	-5.599634
C	1.879281	-8.401132	-5.967105
H	2.556705	-9.254452	-6.031389
C	0.526088	-8.578450	-6.251511
C	-0.354008	-7.500808	-6.169968
H	-1.411185	-7.653258	-6.394992
C	0.105774	-6.223500	-5.808370
C	1.485396	-6.036026	-5.526198
C	1.985070	-4.719333	-5.162938
C	3.341483	-4.548831	-4.789370
C	4.252764	-5.679270	-4.837350
C	3.812439	-3.275398	-4.384470
C	5.169707	-3.118691	-3.884753
C	5.570226	-1.860195	-3.335487
C	6.764496	-1.824529	-2.599434
C	4.768268	-0.671338	-3.640560
C	3.450854	-0.831208	-4.138542
C	2.944601	-2.156709	-4.446190
C	1.602956	-2.316874	-4.864343
C	1.111048	-3.606551	-5.181372
C	-0.297578	-3.787726	-5.486206
C	-0.816151	-5.084114	-5.727006
C	-2.202533	-5.258291	-5.872073
H	-2.605384	-6.260174	-6.036229
C	-3.086010	-4.178100	-5.792390
C	-2.555251	-2.889193	-5.635121
H	-3.240746	-2.038572	-5.608819
C	-1.178507	-2.674295	-5.491794
C	-0.629296	-1.320270	-5.336971
C	0.735710	-1.157913	-4.992054
C	-1.431839	-0.186807	-5.544977
H	-2.480135	-0.313260	-5.824348
C	-0.915813	1.105657	-5.415622
C	0.424050	1.256571	-5.028336
H	0.824574	2.265011	-4.902658
C	1.256458	0.150049	-4.809445

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C     2.655768     0.316603    -4.393961
C     3.227153     1.588257    -4.251468
H     2.625130     2.476558    -4.458561
C     4.565297     1.755015    -3.866159
C     5.317691     0.618329    -3.553944
H     6.360531     0.746039    -3.254644
C     7.443395    -0.907757    -1.688729
C     8.789630    -1.383056    -1.608269
C     9.823515    -0.716082    -0.983978
H    10.832037    -1.126464    -0.971719
C     9.511626     0.519286    -0.382848
C    10.580174     1.351321     0.179019
C    11.912838     0.904010     0.186354
H    12.156937    -0.085461    -0.206915
C    12.932088     1.709075     0.690178
C    12.638232     2.979272     1.184237
H    13.447428     3.605380     1.566870
C    11.318564     3.459718     1.194681
C    11.009058     4.801979     1.697927
C    12.029070     5.654382     2.152666
H    13.066912     5.315998     2.139477
C    11.732639     6.933224     2.620591
C    10.413252     7.381457     2.641714
H    10.194333     8.385913     3.009295
C     9.366764     6.556309     2.196705
C     9.662484     5.251446     1.720650
C     8.592065     4.379019     1.262516
C     8.893943     3.091789     0.750731
C    10.272410     2.633404     0.704538
C     7.852629     2.246298     0.292693
C     8.160934     0.961283    -0.317498
C     7.100155     0.174751    -0.866218
C     5.722704     0.484333    -0.475919
C     5.429300     1.758853     0.067006
C     6.505653     2.670664     0.410964
C     6.201536     3.951260     0.931117
C     7.247124     4.818124     1.331953
C     6.934213     6.155025     1.809995
C     7.977157     7.025577     2.221545
C     7.661037     8.326317     2.648420
H     8.457776     9.003982     2.961141
C     6.338746     8.765557     2.676148
C     5.310030     7.909813     2.286049
H     4.277342     8.263855     2.316375
C     5.586281     6.601557     1.855719
C     4.502265     5.689910     1.469591
C     4.816088     4.374161     1.050186
C     3.760546     3.474114     0.744045
C     4.080462     2.098322     0.344546
C     3.090687     1.110482     0.248709
H     2.055773     1.357199     0.496628
C     3.402825    -0.204039    -0.128904
C     3.158957     6.100020     1.520339
H     2.918767     7.119865     1.829888
C     2.117170     5.230771     1.188453
C     2.434404     3.917327     0.809756
H     1.621468     3.230966     0.564007
H    -5.932330     8.696120     5.573897
H     0.771320     8.807948     6.729790
H    12.533964     7.584131     2.969739
H   -12.560722    -7.279875    -3.002809
H     6.754008    -8.657010    -5.164485
H     0.155800    -9.562328    -6.538260
H     6.108673     9.778445     3.004580
H    13.959922     1.347538     0.694762
H    -6.115939    -9.414092    -3.090894
H   -14.042457    -1.118468    -0.557260
H     1.260383    -2.728497     4.723998
H     4.483729     3.252015     5.381995
H     1.081802     5.559258     1.230749
H     5.003919     2.747312    -3.798148
H    -1.540518     1.975787    -5.597586
H    -4.159763    -4.328611    -5.868677
H    -5.502035    -2.749618     3.721389
H    -2.733814     1.321942     0.143843
H     2.636725    -0.974137    -0.143420
H    -1.130350    -5.215524    -1.152054
```

Alternative packing Structure 2

	X	Y	Z
O	-5.177314	0.783477	3.837701
C	-4.273360	0.027037	3.591585
C	-0.547260	-2.197652	1.052069
H	-0.714556	-1.187270	1.430815
C	-2.813202	0.206311	3.887769
C	-2.188068	1.280046	4.468241
H	-2.754636	2.176898	4.735582
C	-0.787354	1.214776	4.693034
C	-0.051762	2.407701	5.114464
C	-0.718039	3.617283	5.371741
H	-1.807215	3.661647	5.294798
C	-0.018570	4.779589	5.710240
C	1.377781	4.716684	5.804513
H	1.928999	5.624865	6.062154
C	2.078146	3.527258	5.562029
C	3.544732	3.483493	5.635783
C	4.286896	4.647865	5.891211
H	3.765286	5.597654	6.036199
C	5.683245	4.627006	5.948647
C	6.340192	3.402165	5.772761
H	7.430949	3.377647	5.831089
C	5.634893	2.218081	5.513261
C	4.218812	2.252598	5.431660
C	3.472221	1.042207	5.132879
C	2.058027	1.093734	5.015945
C	1.360220	2.347895	5.230332
C	1.330582	-0.075787	4.688883
C	-0.108664	-0.004678	4.481912
C	-0.811157	-1.168364	4.004831
C	-2.103437	-0.983772	3.518938
C	-0.145979	-2.472762	4.104709
C	1.261472	-2.523291	4.271086
C	2.015278	-1.307088	4.525379
C	3.420852	-1.364102	4.664554
C	4.153512	-0.182993	4.948214
C	5.604030	-0.235270	5.046408
C	6.341687	0.946597	5.319510
C	7.743440	0.880233	5.399119
H	8.317855	1.784754	5.608716
C	8.411655	-0.327850	5.213299
C	7.691346	-1.491570	4.947330
H	8.226875	-2.432228	4.805193
C	6.289829	-1.465796	4.862722
C	5.528172	-2.692587	4.595971
C	4.114240	-2.633096	4.518918
C	6.180894	-3.924400	4.424015
H	7.271259	-3.967262	4.477463
C	5.468192	-5.101697	4.179329
C	4.069090	-5.040191	4.138622
H	3.505707	-5.960104	3.965051
C	3.381632	-3.830038	4.305985
C	1.915452	-3.780208	4.256492
C	1.148489	-4.953862	4.211617
H	1.647742	-5.925363	4.212092
C	-0.251365	-4.913367	4.187449
C	-0.883517	-3.665347	4.126308
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C	-3.026947	-1.816801	2.708379
C	-4.352300	-1.308013	2.907492
C	-5.465269	-1.966024	2.450263
H	-6.464013	-1.553665	2.620113
C	-5.296458	-3.199476	1.767516
C	-6.458487	-4.017555	1.422922
C	-7.765523	-3.572724	1.695462
H	-7.923636	-2.590143	2.145102
C	-8.864078	-4.373087	1.397052
C	-8.678962	-5.636520	0.833182
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C	-7.188730	-7.446415	-0.029622
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C	-6.265536	-5.289705	0.824193
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C	-1.562013	-3.160361	1.147995
C	-1.386283	-4.420032	0.520971
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C	-2.325568	-6.581221	-0.258661
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C	-4.330150	-9.634726	-1.231544
C	-4.108930	-10.922583	-1.749684
H	-4.951145	-11.602067	-1.893387
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C	-1.739750	-10.483921	-1.915701
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C	0.097171	-6.092580	-0.577264
C	-0.117770	-4.754297	-0.014677
C	0.901587	-3.791169	-0.022359
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H	4.303543	-0.953504	-4.647538
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C	1.932305	-1.782372	-5.750081
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H	3.943561	-2.544096	-5.498861
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C	1.421790	-4.213017	-7.038584
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C	0.389253	-3.273862	-6.920277
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C	-1.232716	-4.778001	-8.079786
H	-0.447729	-5.529343	-8.185336
C	-2.508169	-5.048245	-8.572842
C	-3.521126	-4.100833	-8.442371
H	-4.517200	-4.324060	-8.829797
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C	0.640271	-2.035781	-6.271535
C	-0.148897	0.187112	-5.491665
C	1.149444	0.430341	-4.879524
C	1.351752	1.621032	-4.113683
C	2.505325	1.699782	-3.318364
C	0.394084	2.720872	-4.251462
C	-0.875812	2.466117	-4.827270
C	-1.167883	1.170620	-5.415625
C	-2.449979	0.916070	-5.959202
C	-2.725065	-0.334236	-6.566970
C	-4.057288	-0.614986	-7.079102
C	-4.340522	-1.868078	-7.682536
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H	-5.867524	-3.099035	-8.602409
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C	-6.374745	0.055387	-7.439613
H	-7.172499	0.795786	-7.352090
C	-5.085955	0.357950	-6.970046
C	-4.788431	1.667770	-6.380764
C	-3.481813	1.940480	-5.898156
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H	-6.785536	2.458437	-6.660950
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C	-4.198549	4.194411	-5.299093
H	-3.979767	5.179613	-4.883433
C	-3.186421	3.222625	-5.363703

C	-1.832435	3.511501	-4.879732		C	-0.464666	10.090129	3.161602
C	-1.461926	4.804115	-4.483088		H	-1.537434	10.289141	3.204136
H	-2.191837	5.615452	-4.536971		C	0.005708	8.927532	2.529613
C	-0.164925	5.091422	-4.035474		C	-0.927110	7.949686	1.958913
C	0.746312	4.037520	-3.913393		C	-0.421368	6.795381	1.306100
H	1.756883	4.256396	-3.560723		C	-1.323809	5.820104	0.804879
C	3.014464	2.530597	-2.230342		C	-0.799333	4.621394	0.142329
C	4.413189	2.240595	-2.161350		C	-1.639690	3.556431	-0.210048
C	5.322328	2.924703	-1.382213		H	-2.706486	3.609849	0.021146
H	6.378956	2.661456	-1.387112		C	-1.141672	2.404183	-0.834945
C	4.817466	3.979022	-0.596084		C	-2.316664	8.126390	2.068292
C	5.742141	4.841294	0.146116		H	-2.714572	9.016984	2.557756
C	7.127800	4.603004	0.118619		C	-3.197867	7.172434	1.561706
H	7.522021	3.749911	-0.438607		C	-2.706721	6.025069	0.941304
C	8.009150	5.443830	0.793658		H	-3.406887	5.281228	0.556125
C	7.520827	6.539214	1.505238		H	-8.938108	-10.222372	-0.987129
H	8.222406	7.196603	2.023383		H	-2.713155	-6.001669	-9.058903
C	6.143203	6.803459	1.563405		H	0.043894	11.897968	4.220281
C	5.628074	7.955756	2.311780		H	9.080434	5.247836	0.763518
C	6.496019	8.818138	2.995296		H	-2.665753	-12.347233	-2.479141
H	7.571826	8.629799	2.973646		H	-9.872000	-4.015139	1.607409
C	6.019389	9.922026	3.716708		H	9.498771	-0.364095	5.276894
C	4.645601	10.172080	3.720280		H	-4.273432	7.322232	1.653762
H	4.266485	11.040243	4.264438		H	-6.261234	4.676215	-5.698719
C	3.743840	9.329247	3.048439		H	-7.655642	-1.404231	-8.375395
C	4.229804	8.198334	2.345810		H	6.246155	5.537882	6.131780
C	3.309155	7.293505	1.677002		H	6.706384	10.573518	4.249404
C	3.806385	6.182045	0.950229		H	-0.545453	5.712082	5.895470
C	5.238848	5.943195	0.884594		H	5.985589	-6.045937	4.035733
C	2.909782	5.300998	0.296082		H	-0.834881	-5.830375	4.200454
C	3.415023	4.207062	-0.521001		H	1.471328	-1.742728	0.407186
C	2.494093	3.392134	-1.252578		H	2.578776	-8.064549	-1.887992
C	1.075044	3.436829	-0.889551		H	3.492101	-4.709770	-6.629186
C	0.589150	4.531495	-0.131695		H	0.120961	6.106677	-3.773549
C	1.512023	5.503266	0.427139		H	-1.796454	1.565770	-1.059667
C	1.014032	6.606351	1.160845					
C	1.914029	7.519811	1.762679					
C	1.404340	8.687316	2.463562					
C	2.302102	9.600761	3.075419					
C	1.793903	10.751187	3.702360					
H	2.479036	11.464140	4.165763					
C	0.423073	10.997321	3.738368					

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