Supporting Information for

Can aromaticity be a kinetic trap? Example of mechanically interlocked aromatic [2-5]catenanes built of cyclo[18]carbon

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Computational methods

For a choice of a proper theoretical method we would like to refer to recent work by Sundholm and co-workers[1]. As it turned out, many popular DFT-functionals (B3LYP, PBE0) tested for years in organic chemistry fail to reproduce true ground state polyynic structure of C_{9h} symmetry. Instead, B3LYP, for example, equalizes all bonds and leads to D_{18h} structure. While this result may look correct for the $4n+2$ ring, the bond alternation was confirmed experimentally. These non-trivial results were explained in terms of Hartee-Fock exchange (HFE) which percentage should be sufficiently high.

In contrast, family of Minnesota functionals performs well, and by that reason we used M06-2X for all the further DFT-calculations. Even the default value of HFE is enough to fully reproduce bond alternating picture. To treat mechanic bonds all calculations were adjusted with the Grimme's empirical dispersion correction (GD3). All calculations if not stated otherwise were carried out using Gaussian16 software package[2].

Wave function stability tests were performed for all structures discussed in the paper. [2-5]catenanes and Borromean rings are stable in terms of wavefunction. For all species Hessian-based vibration analysis was performed and no imaginary frequencies were found except the TS for which NIMAG=1.

As one may expect, transition state (TS) and following adduct have state lower than closed-shell singlet used as initial guess. Therefore, TS was reoptimized using broken-symmetry approach. Technically, it is done through following commands [UDFT, guess=mix, scf=vshift] which equally mix HOMO and LUMO. To some extent, it gives quasi-two-determinant description, which, of course, is a simple mixing of singlet and triplet states with <S^2> expectation value in range from 0 to 1.0 (as a result of equal mixing 0.0 and 2.0 values of singlet and triple, respectively). Although BS-UDFT is not a true multi-reference method, it was shown many times that it provides reasonable qualitative and quantitative description of open-shell singlets. However, one should be careful, because <S^2> values are not eigenvalues anymore and, being a useful metric of open-shell character in some cases, it does not have strict physical meaning.

To furtherly confirm open-shell singlet character of TS and adduct and CASSCF(8,8)/6-31G* calculations using ORCA package[3] were done. Diffuse functions were deleted on purpose because in CASSCF in Gaussian they immediately cause error ("MCSCF cannot handle deleting basis function") while calculations in ORCA are unstable and CAS energy fluctuates sometimes by a hundred of hartrees. Without diffuse functions single-point calculations converge rapidly. Remarkably, that DFT calculations are also sensitive to the inclusion of diffuse basis function but in the other way. For example, DFT-calculations without them could not locate adduct at all and the discussed reaction pathway do not exist. This is true not only for M06-2X functional used for all calculations but also for ωB97XD functional which was tested as well. It also converged to polyynic ground state structure and located the same TS but only when basis set was augmented with the diffuse functions. So, one should keep that in mind when doing preliminary optimization in smaller basis sets.

To get accurate values of energy of different possible states, CASSCF(8,8)/6-31G* results were dressed with the dynamic correlation treatment according to the NEVPT2. In each case two singlet roots and two triplet roots were considered and transition energies between them were corrected by NEVPT2 approach. For example, in TS transition from ground state to the next lowest energy state, which is triplet, requires 2.425 eV. All other states are higher in energy, so the ground state for each species is not mixed with higher states significantly.

According to the CASSCF(8,8)/6-31G* results, we have the following configurations (few largest CSFs are specified):

- [2]catenane: first CSF = 0.89612: 22220000 | second CSF = 0.02233: 22111100 | third CSF = 0.01522: 22202000, forth CSF = 0.01426: 22020200 → almost pure HF solution, might be considered as closed-shell singlet, wave function is stable
- TS: first CSF = 0.84077: 22220000 | second CSF = 0.08665: 22202000 → high percentage of closed-shell singlet mixed with open-shell singlet, RHF → UHF instability
- Adduct: first CSF = 0.53060: 22220000 | second CSF = 0.33551: 22202000 → typical open-shell singlet, RHF → UHF instability

These results confirm open-shell singlet state of TS and adduct. In case of TS and adduct, ground states have only two CSF with significant contributions, and, therefore, we believe that BS-DFT approach should provide energies comparable with true multireference methods.

Chemical bonding pattern were obtained by the AdNDP2.0[4] method based on M062X/6-31G** calculations of NBO and canonical MO.

Figure S1 Bonding pattern of Borromean rings. AdNDP2.0 analysis.

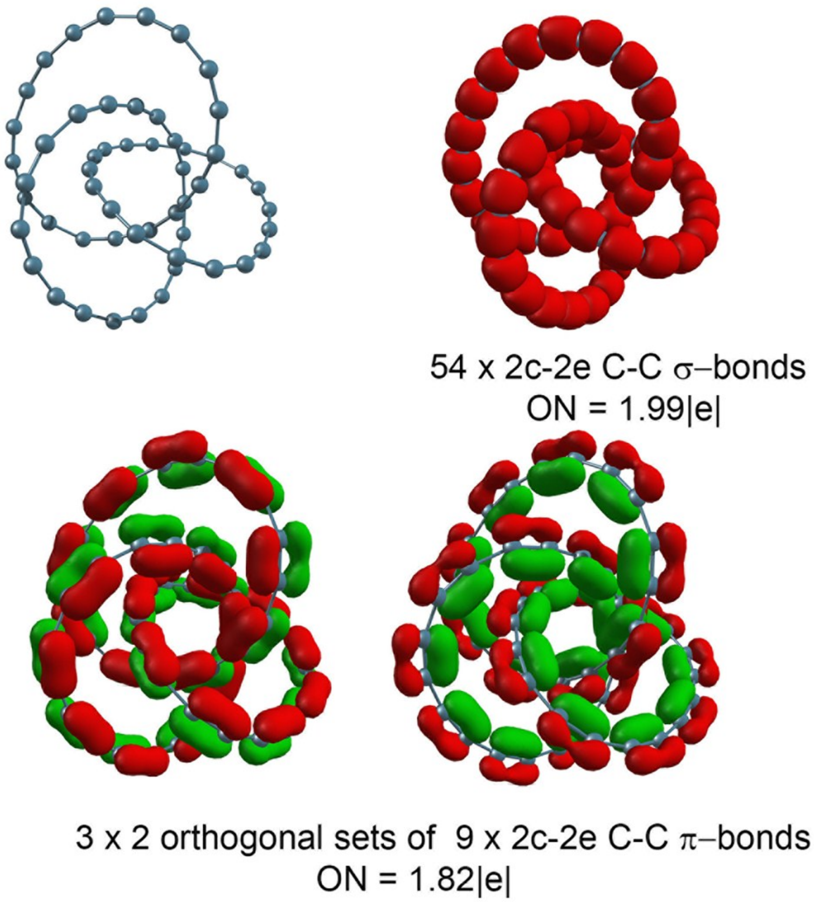

Table S1 C_{18}. M06-2X/6-31+G*.

6	-3.195344000	1.844503000	0.000000000
6	-3.672892000	0.706411000	0.000000000
6	-1.261761000	3.466193000	0.000000000
6	-2.359080000	2.901280000	0.000000000
6	3.633854000	-0.640658000	0.000000000
6	3.692918000	0.592137000	0.000000000

6	3.195427000	1.844533000	0.000000000
6	2.448109000	2.826806000	0.000000000
6	1.261828000	3.466196000	0.000000000
6	0.058058000	3.738562000	0.000000000
6	-3.634158000	-0.640685000	0.000000000
6	-3.267774000	-1.819247000	0.000000000
6	-2.371518000	-2.825674000	0.000000000
6	-1.333379000	-3.493176000	0.000000000
6	0.000000000	-3.688461000	0.000000000
6	1.224409000	-3.532989000	0.000000000
6	3.209620000	-1.919784000	0.000000000
6	2.371684000	-2.825948000	0.000000000

Table S2 [2]catenane. M06-2X/6-31+G*.

6	3.808726000	-2.513923000	1.725260000
6	4.727360000	-1.834688000	1.257197000
6	1.368957000	-3.029781000	2.087325000
6	2.603268000	-3.007494000	2.066092000
6	-1.276651000	1.762039000	-1.225794000
6	-1.859056000	0.873777000	-0.596076000
6	-1.943439000	-0.219084000	0.185889000
6	-1.694196000	-1.211410000	0.877443000
6	-0.901131000	-2.113706000	1.484869000
6	0.062475000	-2.756737000	1.911945000
6	5.261415000	-0.816704000	0.555862000
6	5.434090000	0.189216000	-0.138816000
6	5.061058000	1.252836000	-0.875444000
6	4.419262000	2.119633000	-1.476405000
6	3.304365000	2.740832000	-1.905405000
6	2.133902000	3.064395000	-2.127728000
6	-0.349969000	2.564551000	-1.781837000
6	0.795541000	2.943859000	-2.043026000

6	-2.973928000	2.897608000	2.011523000
6	-1.751398000	3.034606000	2.114807000
6	-4.933088000	1.551505000	1.066703000
6	-4.107143000	2.303037000	1.593071000
6	-1.745404000	-3.088792000	-2.126116000
6	-2.952637000	-2.876634000	-1.978850000
6	-4.144538000	-2.358372000	-1.626680000
6	-4.893107000	-1.547448000	-1.073296000
6	-5.394483000	-0.517068000	-0.366233000
6	-5.342124000	0.497703000	0.334953000
6	-0.416705000	2.886824000	2.016462000
6	0.624542000	2.340166000	1.640429000
6	1.526876000	1.518949000	1.071502000
6	1.898131000	0.557065000	0.391960000
6	1.946202000	-0.536801000	-0.391785000
6	1.477016000	-1.473351000	-1.045487000
6	-0.431528000	-2.841187000	-1.967216000
6	0.657339000	-2.355421000	-1.647098000

Table S3 [3]catenane. M06-2X/6-31+G*.

6	-1.881836000	0.013526000	3.130816000
6	-2.972489000	0.015179000	2.543553000
6	0.695969000	-0.003352000	3.384915000
6	-0.542319000	0.005400000	3.374417000
6	3.029038000	-0.018701000	-2.101610000
6	3.824969000	-0.017545000	-1.151815000
6	4.207028000	-0.015286000	0.157476000
6	3.908557000	-0.014233000	1.360778000
6	3.108575000	-0.013754000	2.463900000
6	2.014203000	-0.010659000	3.044833000
6	-3.870616000	0.015054000	1.517978000
6	-4.174763000	0.014657000	0.316325000

6	-3.923797000	0.016015000	-1.023916000
6	-3.128519000	0.015791000	-1.974734000
6	-1.972077000	0.013085000	-2.694164000
6	-0.757154000	0.004665000	-2.934898000
6	1.815373000	-0.015456000	-2.721404000
6	0.602967000	-0.007679000	-2.973818000
6	-7.533722000	2.508729000	-0.338080000
6	-8.250583000	1.506994000	-0.404488000
6	-5.300960000	3.666971000	-0.135623000
6	-6.490007000	3.356234000	-0.243214000
6	-1.491846000	-1.453857000	0.198279000
6	-1.240017000	-0.249307000	0.223494000
6	-1.398428000	1.087449000	0.212375000
6	-1.837407000	2.238753000	0.173500000
6	-2.845123000	3.129683000	0.085035000
6	-3.958544000	3.651617000	-0.015355000
6	-8.510094000	0.184587000	-0.429865000
6	-8.419748000	-1.045737000	-0.424180000
6	-7.776052000	-2.228586000	-0.368234000
6	-6.919628000	-3.113304000	-0.293039000
6	-5.670536000	-3.606867000	-0.181855000
6	-4.448718000	-3.739922000	-0.072364000
6	-2.158646000	-2.621963000	0.136793000
6	-3.174687000	-3.316807000	0.043427000
6	2.832452000	-3.121840000	0.080718000
6	3.943865000	-3.648431000	-0.017509000
6	1.394990000	-1.072955000	0.204397000
6	1.828605000	-2.226289000	0.167099000
6	5.686556000	3.603859000	-0.187082000
6	4.465081000	3.741976000	-0.080371000
6	3.189137000	3.323927000	0.033688000

6	2.170192000	2.633303000	0.126185000
6	1.498033000	1.468147000	0.188191000
6	1.241796000	0.264580000	0.214296000
6	5.286490000	-3.668714000	-0.135195000
6	6.476912000	-3.362513000	-0.240418000
6	7.524229000	-2.519198000	-0.333360000
6	8.245745000	-1.520763000	-0.398833000
6	8.510920000	-0.199460000	-0.424731000
6	8.425997000	1.031235000	-0.420306000
6	6.933942000	3.105122000	-0.294965000
6	7.786695000	2.216637000	-0.367041000

Table S4 [4]catenane. M06-2X/6-31+G*.

6	9.140926000	-0.799410000	-2.705795000
6	10.015144000	-0.038074000	-2.282770000
6	6.820050000	-1.792781000	-2.680965000
6	7.992762000	-1.476009000	-2.900364000
6	4.286403000	1.503345000	2.242864000
6	3.766144000	0.639449000	1.531740000
6	3.722191000	-0.266098000	0.539951000
6	3.949453000	-1.015570000	-0.411597000
6	4.662217000	-1.585992000	-1.396298000
6	5.576589000	-1.881091000	-2.172199000
6	10.530482000	0.909662000	-1.476083000
6	10.696583000	1.764826000	-0.602120000
6	10.339367000	2.540539000	0.439796000
6	9.722034000	3.089864000	1.356147000
6	8.660471000	3.333524000	2.148811000
6	7.548084000	3.323524000	2.682797000
6	5.178065000	2.364506000	2.770016000
6	6.273578000	2.925724000	2.861659000
6	3.602151000	-3.116451000	2.370201000

6	2.397961000	-3.398140000	2.334389000
6	5.826188000	-1.900018000	1.871450000
6	4.833153000	-2.564968000	2.193402000
6	2.908615000	1.817850000	-1.725673000
6	4.126430000	1.876636000	-1.514715000
6	5.378276000	1.617389000	-1.044550000
6	6.231505000	1.012331000	-0.382001000
6	6.697409000	0.062646000	0.477581000
6	6.493766000	-0.910433000	1.216415000
6	1.055583000	-3.509441000	2.135762000
6	-0.078067000	-3.269855000	1.701013000
6	-1.061475000	-2.640506000	0.996785000
6	-1.368155000	-1.741586000	0.204009000
6	-1.211245000	-0.668517000	-0.622773000
6	-0.581201000	0.224131000	-1.199980000
6	1.593270000	1.471546000	-1.731399000
6	0.451827000	1.009613000	-1.608209000
6	-5.787762000	-1.302886000	-2.253340000
6	-4.786501000	-1.887849000	-2.685291000
6	-2.346897000	-2.689647000	-2.895884000
6	-3.548048000	-2.396338000	-2.928930000
6	-1.016585000	-2.863160000	-2.663030000
6	0.100753000	-2.761905000	-2.141892000
6	1.064746000	-2.344940000	-1.271710000
6	1.370551000	-1.682131000	-0.273690000
6	1.219094000	-0.841484000	0.791063000
6	0.589979000	-0.097838000	1.550576000
6	-0.455307000	0.587446000	2.091602000
6	-1.603631000	1.017409000	2.254138000
6	-4.124107000	1.490558000	2.000410000
6	-2.919306000	1.364898000	2.250441000

6	-5.359701000	1.380655000	1.436729000
6	-6.204857000	0.980194000	0.625953000
6	-6.668671000	0.282730000	-0.450025000
6	-6.465005000	-0.486612000	-1.398798000
6	-10.353110000	-0.166442000	1.652264000
6	-10.765341000	0.951894000	1.024372000
6	-10.639814000	1.948063000	0.307093000
6	-10.163050000	2.914296000	-0.501688000
6	-9.305047000	3.495134000	-1.171760000
6	-8.162025000	3.859067000	-1.784794000
6	-6.972571000	3.758752000	-2.097588000
6	-5.693822000	3.357244000	-2.233433000
6	-4.718986000	2.623535000	-2.047601000
6	-3.908056000	1.631417000	-1.631810000
6	-3.675617000	0.594520000	-1.005560000
6	-3.761526000	-0.502942000	-0.232739000
6	-4.219392000	-1.374030000	0.507459000
6	-5.054130000	-2.103056000	1.270128000
6	-6.144886000	-2.355411000	1.791253000
6	-7.433374000	-2.319980000	2.181112000
6	-8.577951000	-1.861317000	2.236027000
6	-9.686581000	-1.112010000	2.081645000

Tables S5 [5]catenane. M06-2X/6-31+G*.

6	7.091387000	0.095784000	3.272024000
6	8.195062000	0.190033000	2.719457000
6	4.547171000	-0.123315000	3.629607000
6	5.780022000	-0.015788000	3.614175000
6	2.381128000	-0.389225000	-1.851043000
6	1.574111000	-0.452441000	-0.916000000
6	1.236915000	-0.467450000	0.403354000
6	1.366321000	-0.438991000	1.633047000

6	2.162640000	-0.351029000	2.733310000
6	3.216061000	-0.245063000	3.375349000
6	9.054862000	0.258519000	1.666195000
6	9.454639000	0.281479000	0.493986000
6	9.202748000	0.238442000	-0.844909000
6	8.490297000	0.155311000	-1.854330000
6	7.324904000	0.036237000	-2.549221000
6	6.122305000	-0.076671000	-2.818255000
6	3.559336000	-0.293606000	-2.525613000
6	4.768066000	-0.193005000	-2.770718000
6	13.000079000	-1.836103000	-0.499037000
6	13.591760000	-0.758591000	-0.605543000
6	10.927696000	-3.241977000	-0.191160000
6	12.067314000	-2.796950000	-0.351736000
6	6.568862000	1.400388000	0.253716000
6	6.452829000	0.175434000	0.304112000
6	6.759881000	-1.134020000	0.299387000
6	7.336071000	-2.223366000	0.251261000
6	8.437039000	-2.989976000	0.127988000
6	9.599261000	-3.379865000	-0.014058000
6	13.694083000	0.583915000	-0.655212000
6	13.460637000	1.795524000	-0.658026000
6	12.685632000	2.895254000	-0.587092000
6	11.735245000	3.675474000	-0.484738000
6	10.443025000	4.021135000	-0.325986000
6	9.219199000	4.012820000	-0.166210000
6	7.087355000	2.637624000	0.151141000
6	8.010384000	3.445283000	0.007905000
6	1.946955000	2.471409000	0.273290000
6	0.758035000	2.772043000	0.121429000
6	3.763068000	0.735272000	0.512501000

6	3.110288000	1.779964000	0.421720000
6	-0.692423000	-3.730470000	-0.075308000
6	0.533864000	-3.761427000	0.078479000
6	1.844988000	-3.445028000	0.245418000
6	2.938053000	-2.884808000	0.389358000
6	3.756557000	-1.803826000	0.500313000
6	4.027808000	-0.600031000	0.543363000
6	-0.590956000	2.757782000	-0.047348000
6	-1.795937000	2.530047000	-0.200582000
6	-2.954362000	1.832317000	-0.353022000
6	-3.713904000	0.864382000	-0.459505000
6	-4.004956000	-0.465034000	-0.498275000
6	-3.852301000	-1.690756000	-0.479094000
6	-2.009605000	-3.439051000	-0.241851000
6	-3.049587000	-2.783665000	-0.377119000
6	-7.316418000	0.018301000	2.556598000
6	-6.115484000	-0.102203000	2.829727000
6	-3.551790000	-0.334012000	2.556392000
6	-4.761525000	-0.226389000	2.793450000
6	-2.372937000	-0.435788000	1.883479000
6	-1.569563000	-0.500325000	0.945408000
6	-1.235248000	-0.509245000	-0.374901000
6	-1.370296000	-0.471985000	-1.603690000
6	-2.167319000	-0.371060000	-2.702518000
6	-3.219974000	-0.252827000	-3.343619000
6	-4.548884000	-0.120554000	-3.604302000
6	-5.781138000	-0.005900000	-3.597342000
6	-8.198530000	0.208005000	-2.711678000
6	-7.093899000	0.111055000	-3.261912000
6	-9.057175000	0.274741000	-1.657178000
6	-9.452334000	0.292536000	-0.483313000

6	-9.195702000	0.240004000	0.854471000
6	-8.480506000	0.147116000	1.861061000
6	-12.677972000	2.914162000	0.529815000
6	-13.460316000	1.818626000	0.587023000
6	-13.701208000	0.608616000	0.576079000
6	-13.606299000	-0.734448000	0.521622000
6	-13.019610000	-1.814765000	0.417087000
6	-12.090361000	-2.780248000	0.276186000
6	-10.951529000	-3.230754000	0.126634000
6	-9.621695000	-3.374862000	-0.036109000
6	-8.456083000	-2.990563000	-0.163439000
6	-7.349491000	-2.229171000	-0.271158000
6	-6.768847000	-1.141857000	-0.307812000
6	-6.451867000	0.165228000	-0.303471000
6	-6.560818000	1.390606000	-0.249465000
6	-7.072921000	2.630781000	-0.147322000
6	-7.992824000	3.442893000	-0.010397000
6	-9.200885000	4.015729000	0.152944000
6	-10.426282000	4.028851000	0.299018000
6	-11.722180000	3.689362000	0.441741000

Tables S6 Borromean rings. M06-2X/6-31+G*.

6	3.590689000	2.530771000	1.177164000
6	3.721488000	1.324699000	1.429255000
6	1.897772000	4.311238000	0.449667000
6	2.869711000	3.624487000	0.790459000
6	-3.751574000	1.361938000	-1.433735000
6	-3.570596000	2.556644000	-1.161923000
6	-2.875480000	3.669153000	-0.778484000
6	-1.867192000	4.301517000	-0.438591000
6	-0.596662000	4.679540000	-0.118569000
6	0.614300000	4.644160000	0.132018000

6	3.401678000	-0.000691000	1.497809000
6	2.648356000	-0.943161000	1.222232000
6	1.668587000	-1.757756000	0.730948000
6	0.609991000	-2.173441000	0.250310000
6	-0.649738000	-2.184427000	-0.275141000
6	-1.691141000	-1.724170000	-0.753521000
6	-3.414364000	0.038990000	-1.499908000
6	-2.682098000	-0.926070000	-1.250344000
6	1.264683000	-2.911040000	3.290828000
6	0.283001000	-2.161587000	3.214801000
6	3.366821000	-3.606811000	2.033902000
6	2.427495000	-3.458504000	2.826580000
6	3.224668000	1.152376000	-2.948660000
6	3.943118000	0.242565000	-2.514786000
6	4.391751000	-0.835804000	-1.812594000
6	4.602290000	-1.802045000	-1.069847000
6	4.497664000	-2.713380000	-0.061402000
6	4.150615000	-3.342959000	0.945763000
6	-0.606931000	-1.256202000	2.714160000
6	-1.092176000	-0.472432000	1.891948000
6	-1.388135000	0.379182000	0.866006000
6	-1.329758000	1.112029000	-0.123852000
6	-0.898597000	1.732424000	-1.262075000
6	-0.240957000	2.189698000	-2.205555000
6	2.120955000	1.936083000	-3.127139000
6	0.949544000	2.245385000	-2.869161000
6	-3.944892000	0.214160000	2.519606000
6	-3.232830000	1.127256000	2.957059000
6	-4.587740000	-1.830494000	1.067628000
6	-4.385148000	-0.865038000	1.813537000
6	-0.266750000	-2.160062000	-3.218408000

6	-1.243190000	-2.916178000	-3.296055000
6	-2.402912000	-3.469814000	-2.831704000
6	-3.341413000	-3.623854000	-2.039222000
6	-4.126373000	-3.365111000	-0.950826000
6	-4.476783000	-2.738636000	0.057098000
6	-2.133847000	1.917000000	3.137436000
6	-0.964596000	2.234397000	2.879617000
6	0.225178000	2.186790000	2.214133000
6	0.884366000	1.733863000	1.269672000
6	1.317316000	1.116327000	0.130703000
6	1.381416000	0.388101000	-0.862146000
6	0.615443000	-1.248200000	-2.715962000
6	1.092977000	-0.462907000	-1.890731000

Tables S7 TS. M06-2X/6-31+G*.

6	-0.243800000	2.119772000	1.997023000
6	0.884230000	2.476323000	2.346086000
6	-2.077467000	0.820841000	0.790735000
6	-1.337133000	1.545287000	1.454881000
6	2.196437000	-2.634326000	-2.299852000
6	0.953595000	-2.633451000	-2.285464000
6	-0.285436000	-2.278627000	-1.957310000
6	-1.299285000	-1.725038000	-1.474029000
6	-2.110872000	-0.949930000	-0.793447000
6	-2.695622000	-0.087470000	-0.043846000
6	2.230861000	2.488170000	2.371984000
6	3.430361000	2.271162000	2.174462000
6	4.477962000	1.653252000	1.597024000
6	5.196587000	0.919577000	0.908949000
6	5.403440000	-0.058049000	0.008276000
6	5.215583000	-0.959527000	-0.817475000
6	3.488838000	-2.367039000	-2.076559000

6	4.444967000	-1.777733000	-1.553178000
6	-1.069489000	-3.284684000	1.770899000
6	-2.311238000	-3.263359000	1.754996000
6	1.115328000	-2.099282000	1.170188000
6	0.151542000	-2.792081000	1.522809000
6	-0.811526000	3.437172000	-1.827473000
6	0.297703000	2.948984000	-1.587446000
6	1.303316000	2.152240000	-1.182379000
6	1.797291000	1.155910000	-0.643728000
6	2.010521000	0.004070000	0.015847000
6	1.723084000	-1.042219000	0.608181000
6	-3.589689000	-2.915863000	1.584724000
6	-4.429345000	-2.091619000	1.165240000
6	-4.996396000	-1.023458000	0.614306000
6	-4.558080000	0.017101000	-0.019870000
6	-4.752142000	1.221863000	-0.660281000
6	-4.259307000	2.225815000	-1.183622000
6	-2.158308000	3.427564000	-1.812336000
6	-3.336512000	3.098652000	-1.638314000

Tables S8 Adduct. M06-2X/6-31+G*.

6	-0.144721000	2.037826000	1.969681000
6	0.978575000	2.371795000	2.348118000
6	-2.062249000	0.853940000	0.743217000
6	-1.238344000	1.492018000	1.392155000
6	2.163066000	-2.622137000	-2.371699000
6	0.908385000	-2.511812000	-2.251711000
6	-0.317653000	-2.206187000	-1.952686000
6	-1.315248000	-1.603989000	-1.408774000
6	-2.180296000	-0.897973000	-0.795092000
6	-2.842871000	0.007155000	-0.059976000
6	2.327139000	2.399253000	2.414005000

6	3.515901000	2.155294000	2.193298000
6	4.595199000	1.572795000	1.630832000
6	5.217606000	0.808593000	0.884499000
6	5.485845000	-0.137752000	-0.031345000
6	5.172609000	-1.004251000	-0.863347000
6	3.420149000	-2.322521000	-2.104282000
6	4.473687000	-1.829133000	-1.645629000
6	-1.343921000	-3.299168000	1.765540000
6	-2.585394000	-3.254195000	1.698407000
6	0.908676000	-2.202745000	1.261553000
6	-0.090103000	-2.860738000	1.579703000
6	-0.612034000	3.422797000	-1.736927000
6	0.463112000	2.864949000	-1.508282000
6	1.412035000	1.994368000	-1.100073000
6	1.857757000	0.981779000	-0.555198000
6	1.982676000	-0.176509000	0.125729000
6	1.619238000	-1.195220000	0.721038000
6	-3.833711000	-2.852402000	1.457145000
6	-4.600013000	-1.975387000	0.983236000
6	-5.048947000	-0.864110000	0.423738000
6	-4.367844000	0.173501000	-0.095501000
6	-4.657137000	1.432115000	-0.667774000
6	-4.142480000	2.444965000	-1.142976000
6	-1.961325000	3.526541000	-1.731067000
6	-3.157366000	3.276546000	-1.569556000

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