

Redox-responsive Organometallic Foldamers from Ferrocene Amino Acid: Solid-Phase Synthesis, Conformation and Mixed-Valence Properties

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Supporting Information

Experimental general considerations

All reactions were performed under argon atmosphere unless otherwise noted. Dichloromethane was dried over CaH_2 and distilled prior to use; THF was distilled from sodium/benzophenone. All reagents were used as received from commercial suppliers (Acros, Sigma-Aldrich, Iris-Biotech, Rapp Polymere). Microwave accelerated reactions were conducted in heavy-walled glass vials sealed with aluminium crimp caps fitted with a silicon septum. The inner diameter of the vial filled to the height of 8 cm was 1 cm. Microwave heating was performed in a Discover Benchmate Plus (CEM Synthesis) single-mode microwave cavity producing continuous irradiation at 2.455 GHz with 100W (max. power). Reaction mixtures were stirred with a magnetic stir bar during irradiation. Temperature and irradiation power were monitored during the course of the reaction. NMR spectra were recorded on a Bruker Avance DRX 400 spectrometer at 400.13 MHz (^1H) and 100.03 MHz ($^{13}\text{C}\{^1\text{H}\}$). All resonances are reported in ppm versus the solvent signal as internal standard. CDCl_3 (^1H : $\delta = 7.26$; ^{13}C : $\delta = 77.0$ ppm), CD_2Cl_2 (^1H : $\delta = 5.32$; ^{13}C : $\delta = 53.8$ ppm), $[\text{D}]_8\text{-THF}$ (^1H : $\delta = 3.58$; ^{13}C : $\delta = 67.4$ ppm), $[\text{D}]_7\text{-DMF}$ (^1H : $\delta = 2.92$; ^{13}C : $\delta = 35.2, 162.7$ ppm). (s) = singlet, (d) = doublet, (t) = triplet, (pt) = pseudo triplet (unresolved doublet of doublets), (br. s) = broad singlet. IR spectra were recorded with a BioRad Excalibur FTS 3100 spectrometer using KBr cells in CH_2Cl_2 and as CsI disks. (s) = strong, (m) = medium, (w) = weak. Electrochemical experiments were carried out on a BioLogic SP-50 voltammetric analyzer using a glassy carbon working electrode, a platinum wire as counter electrode and a 0.01 M Ag/AgNO_3 electrode as reference electrode. The measurements were carried out at a scan rate of 100 mV s^{-1} for cyclic voltammetry experiments and at 10 mV s^{-1} for square wave voltammetry experiments using 0.1 M $(n\text{Bu}_4\text{N})(\text{PF}_6)$ as supporting electrolyte in CH_2Cl_2 . Potentials are given relative to the ferrocene/ferrocenium couple ($E_{1/2} = 225 \pm 5 \text{ mV}$ under the

experimental conditions). UV/Vis/NIR spectra were recorded on a Varian Cary 5000 spectrometer using 1.0 cm cells (Hellma, suprasil). ESI mass spectra were recorded on a Micromass Q-TOF-Ultima spectrometer; FD mass spectra were recorded on a FD Finnigan MAT90 spectrometer; MALDI-TOF spectra were recorded on a Shimadzu Axima CFR MALDI-TOF spectrometer using a HABA matrix (2-(4-hydroxyphenyl-azo)-benzoic acid) and KI as potassium ion source. Melting points were determined using a Gallenkamp capillary melting point apparatus MFB 595 010 and were not corrected. Elemental analyses were performed by the microanalytical laboratory of the chemical institutes of the University of Mainz.

Table S1 Data of the crystallographic structure determinations.

	Fmoc-Fca-OMe	Boc-Fca₂-OMe
Empirical formula	C ₂₇ H ₂₃ FeNO ₄	C ₂₈ H ₃₀ N ₂ O ₅ Fe ₂
Formula weight	481.31	586.24
Temperature /K	296	173
Crystal color, habit	orange plate	orange plate
Crystal dimensions / mm	0.12 × 0.10 × 0.04	0.10 × 0.10 × 0.05
Crystal system	triclinic	monoclinic
Space group	<i>P</i> −1	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> / Å	10.5978(5)	11.656(3)
<i>b</i> / Å	13.1099(6)	19.486(4)
<i>c</i> / Å	17.8502(8)	11.051(3)
<i>α</i> /°	82.684(1)	90
<i>β</i> /°	74.957(1)	105.010(8)
<i>γ</i> /°	66.876(1)	90
<i>V</i> / Å ³	2201.72(18)	2424.3(9)
<i>Z</i>	4	4
<i>F</i> (000)	1000	1216
Density (calcd) / g cm ^{−3}	1.452	1.606
Absorption coefficient <i>μ</i> / mm ^{−1}	0.720	1.241
2 <i>θ</i> range / °	4.72 – 55.96	4.98 – 56.00
Index ranges	−13 ≤ <i>h</i> ≤ 13 −17 ≤ <i>k</i> ≤ 17 −23 ≤ <i>l</i> ≤ 23	−15 ≤ <i>h</i> ≤ 15 −25 ≤ <i>k</i> ≤ 25 −14 ≤ <i>l</i> ≤ 11
Reflections collected	25637	20545
Independent reflections	10561	5818
Parameters	595	334
Max. / min. transmission	1.15637 / 0.88270	1.07964 / 0.95015
Goodness-of-fit on <i>F</i> ²	0.900	0.622
Largest difference peak and hole / e Å ^{−3}	0.368 / −0.328	0.439 / −0.633
<i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>))	0.0316	0.0506
<i>R</i> ₁ (all data)	0.0640	0.2516
<i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.0795	0.0694
<i>wR</i> ₂ (all data)	0.0881	0.1091



Fig. S1 Photograph of the activation of **Fmoc-Fca-Cl** as acyl pyridinium ion with DMAP and reaction with Hypogel Wang resin (left); Photograph of the Hypogel resin after first Fmoc-Fca coupling as ester (right).

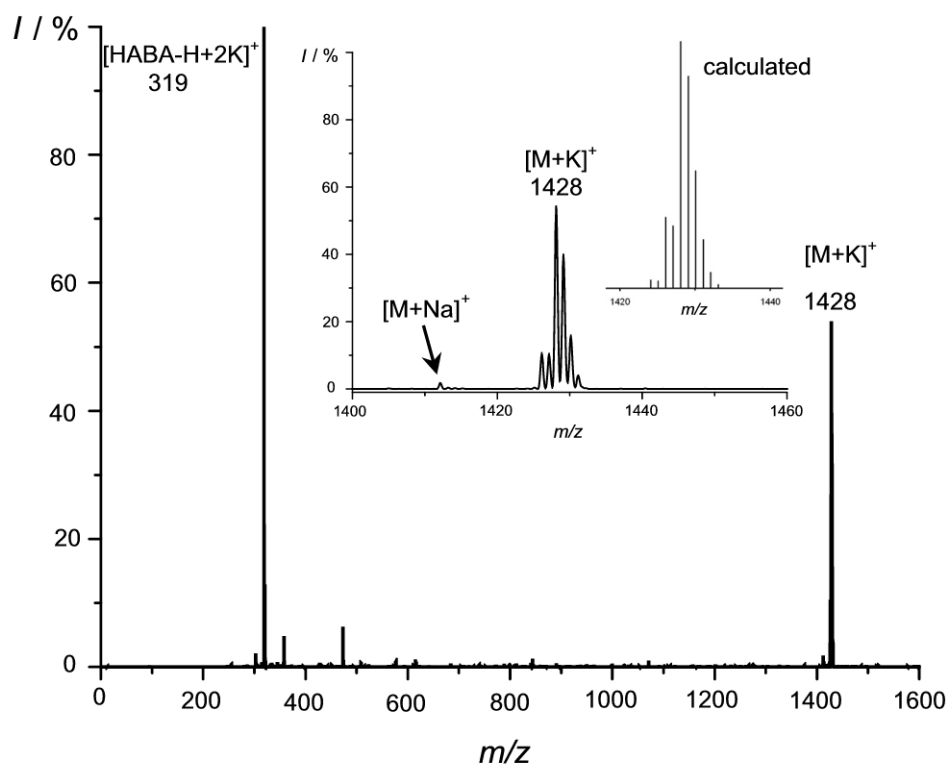


Fig. S2 MALDI-TOF mass spectrum of **Fmoc-Fca₅-OMe** (HABA matrix, KI, HABA = 2-(4-hydroxyphenylazo)benzoic acid) and calculated isotopic pattern of the $[M+K]^+$ peak.

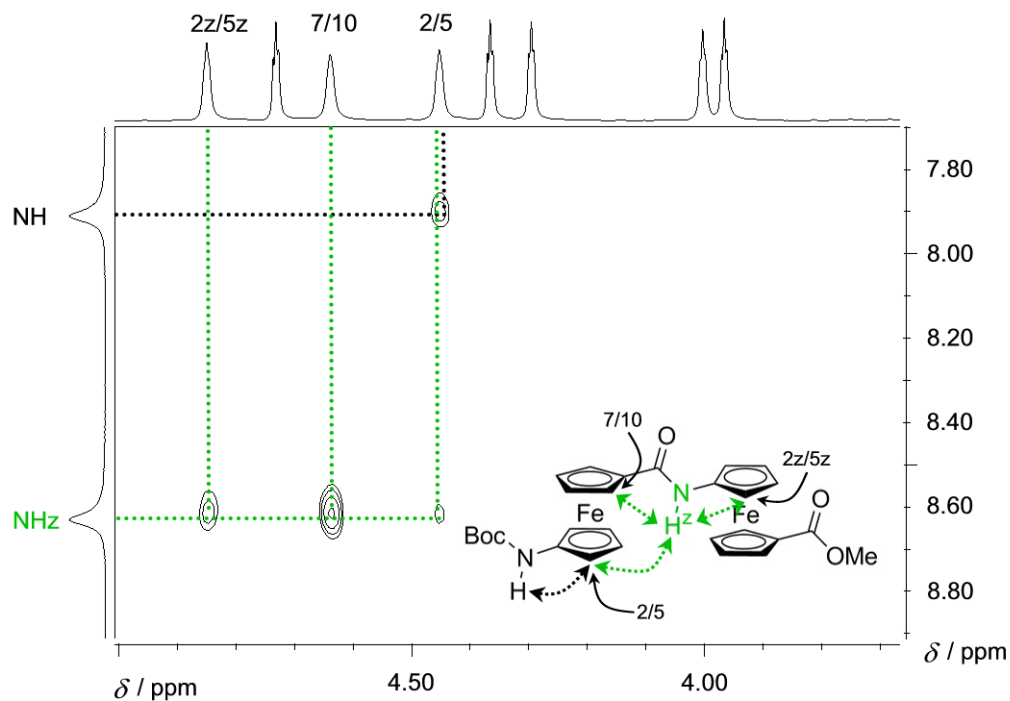


Fig. S3 Partial NOESY spectrum of **Boc-Fca₂-OMe** in [D]₈-THF.

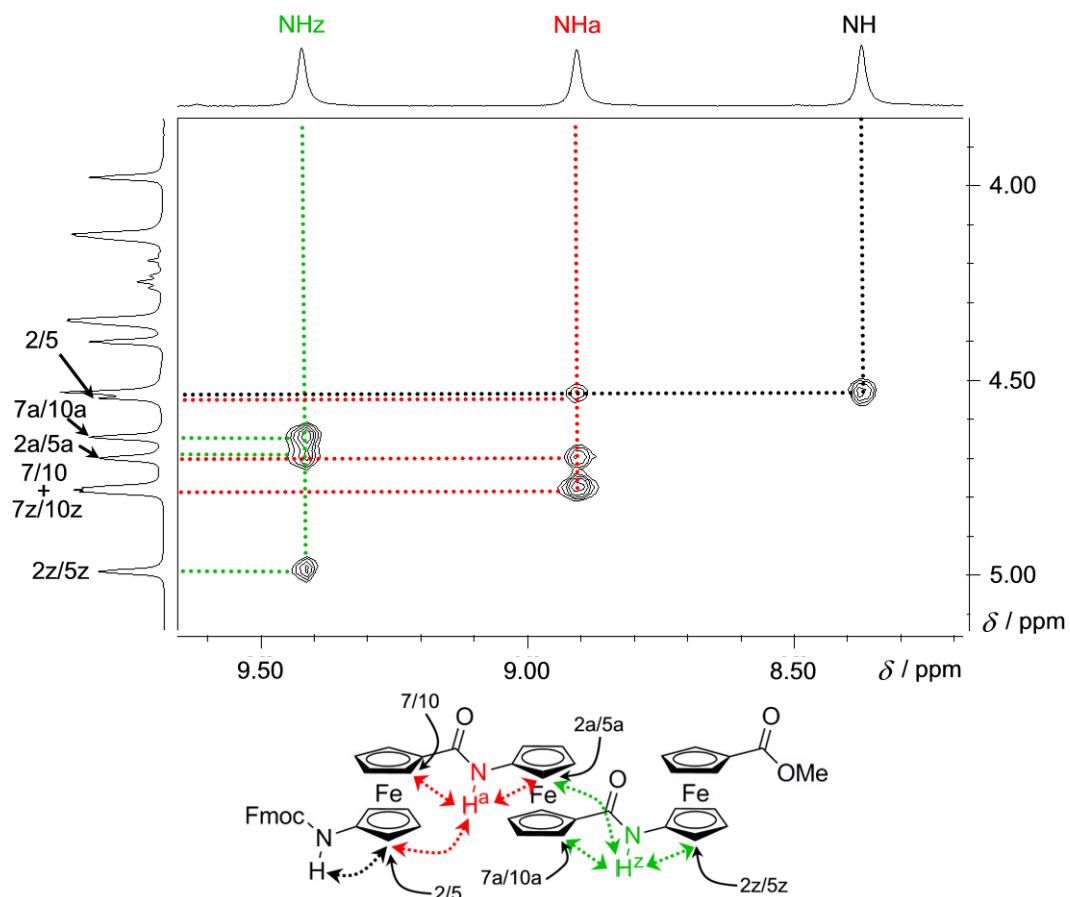


Fig. S4 Partial NOESY spectrum of **Fmoc-Fca₃-OMe** in [D]₈-THF.

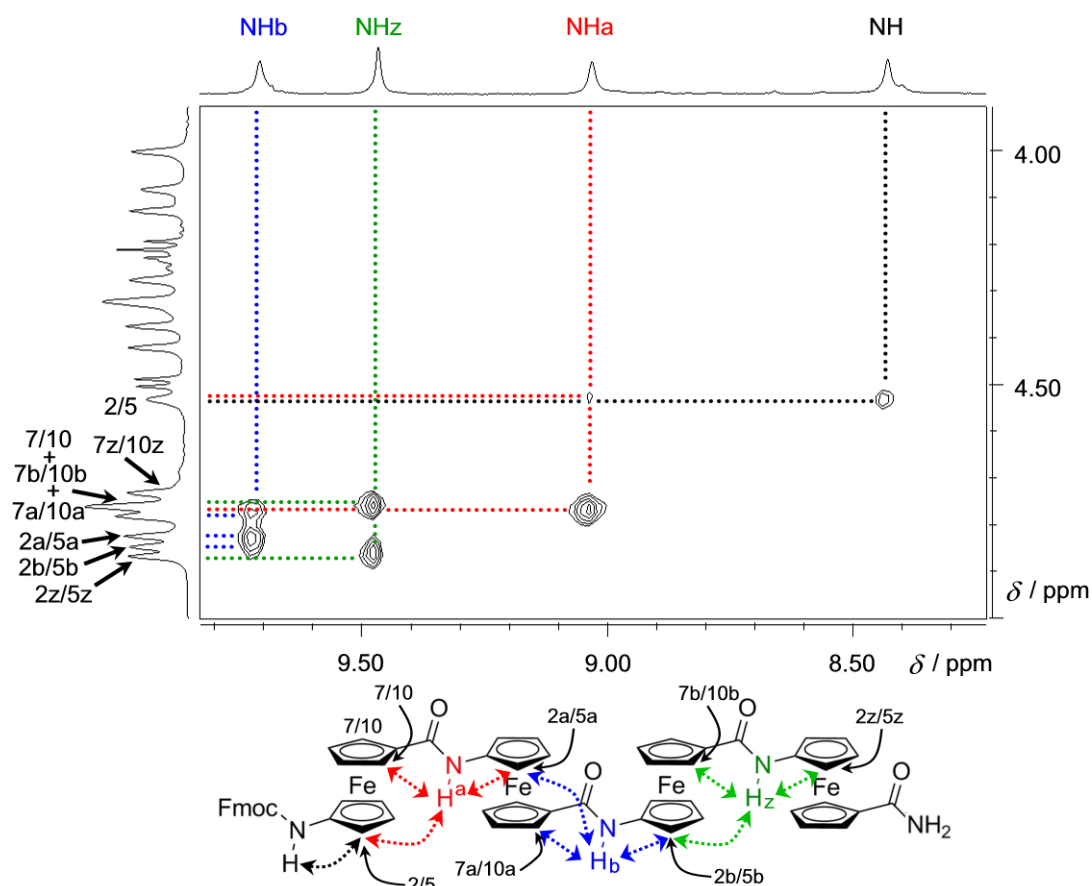


Fig. S5 Partial NOESY spectrum of **Fmoc-Fca₄-NH₂** in [D]₈-THF.

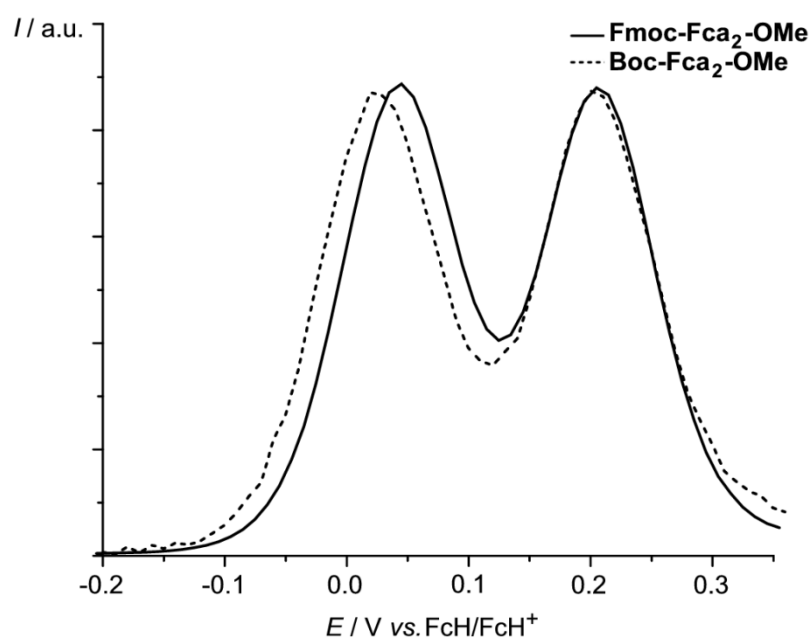


Fig. S6 SWV of **Boc-Fca₂-OMe** and **Fmoc-Fca₂-OMe** in CH₂Cl₂/[*n*Bu₄N][PF₆].

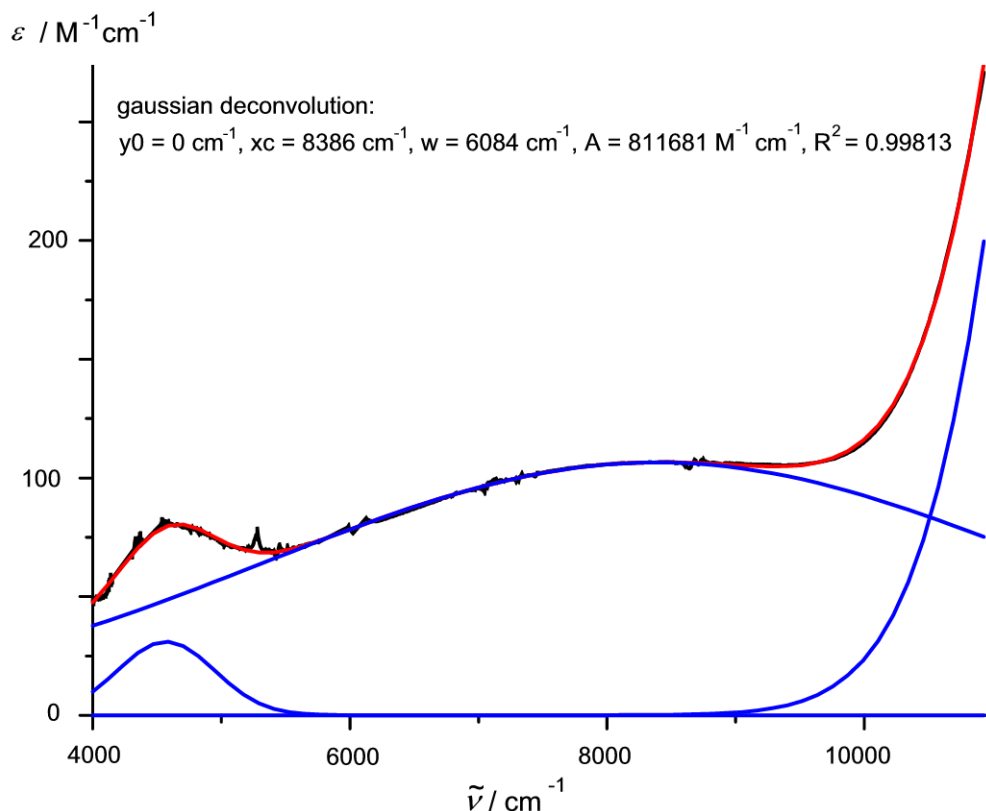


Fig. S7 Gaussian deconvolution of the IVCT band of **[Boc-Fca₂-OMe]⁺** in CH₂Cl₂.

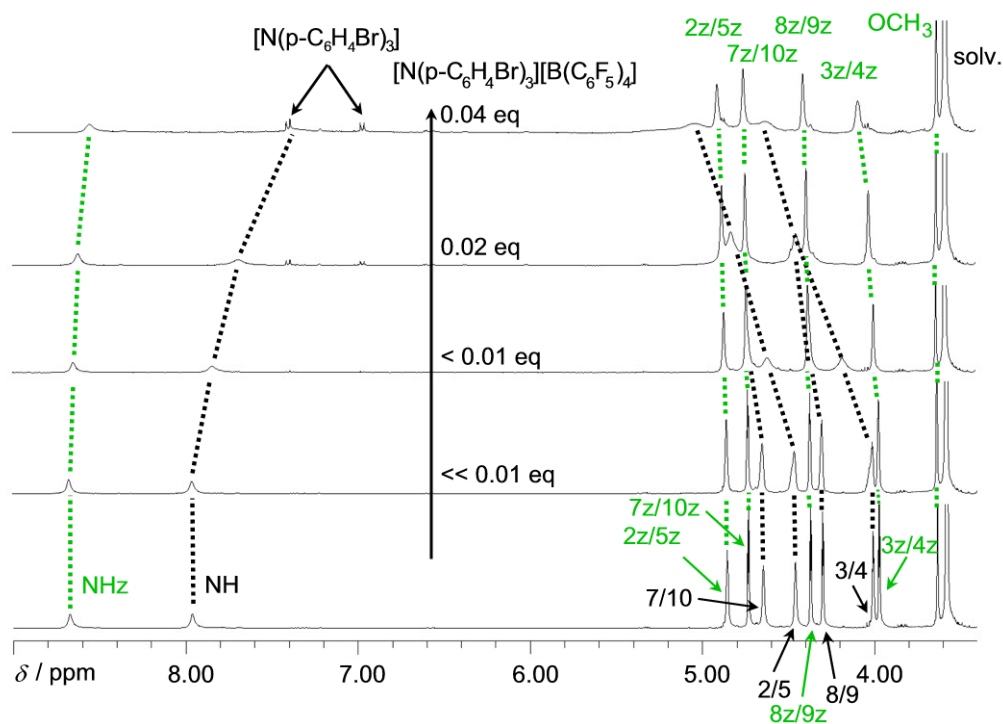


Fig. S8 ¹H NMR spectra during oxidation of **Boc-Fca₂-OMe** with [N(p-C₄H₄Br)₃][B(C₆F₅)₄] in [D]₈-THF.

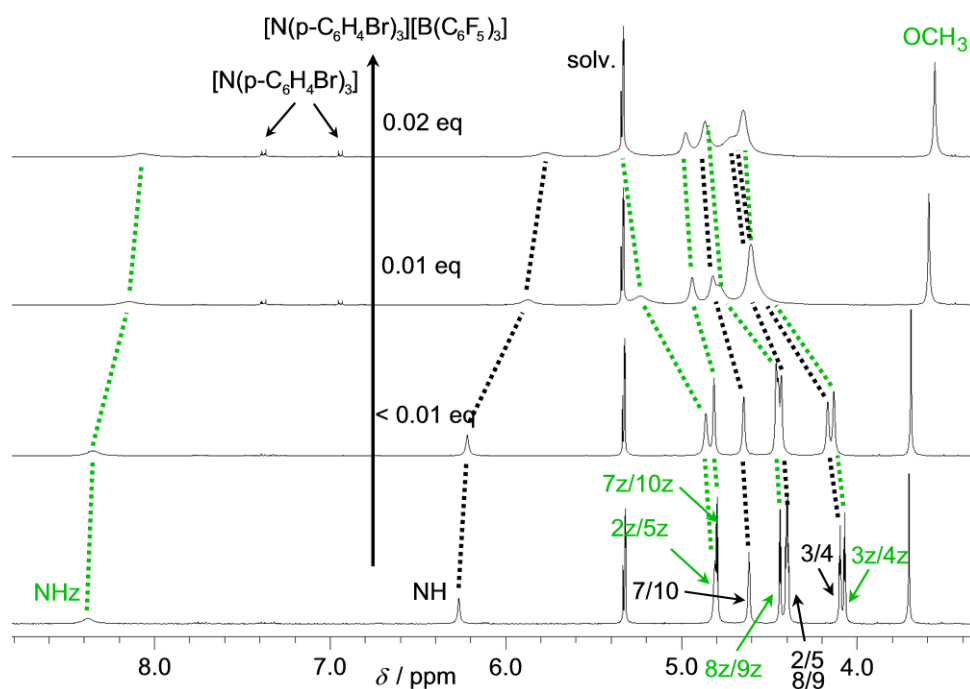


Fig. S9 ^1H NMR spectra during oxidation of **Boc-Fca₂-OMe** with $[\text{N}(\text{p-C}_6\text{H}_4\text{Br})_3][\text{B}(\text{C}_6\text{F}_5)_4]$ in CD_2Cl_2 .

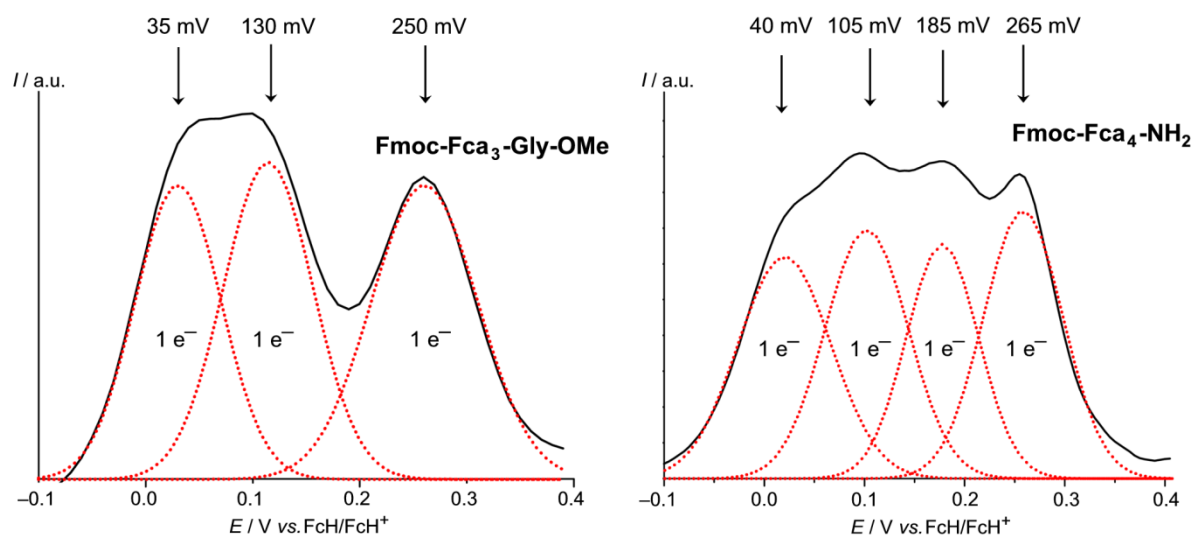


Fig. S10 SWV of **Fmoc-Fca₃-Gly-OMe** and **Fmoc-Fca₄-NH₂** in $\text{CH}_2\text{Cl}_2/[\text{nBu}_4\text{N}][\text{PF}_6]$.

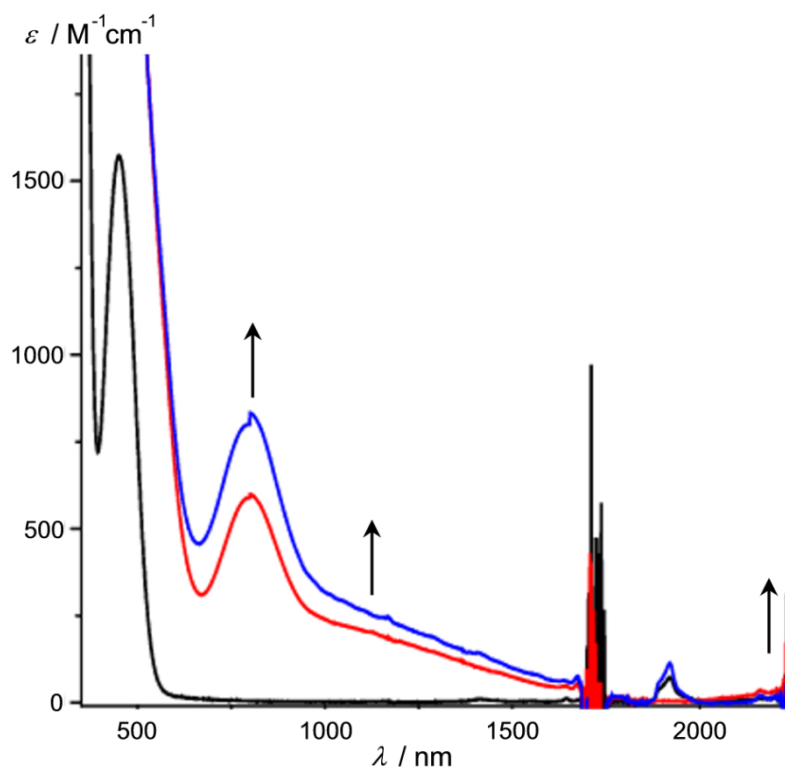


Fig. S11 UV/Vis/NIR spectra of **Fmoc-Fca₄-OMe** upon oxidation with excess $[C_{12}H_8S_2][BF_4]$ in THF.

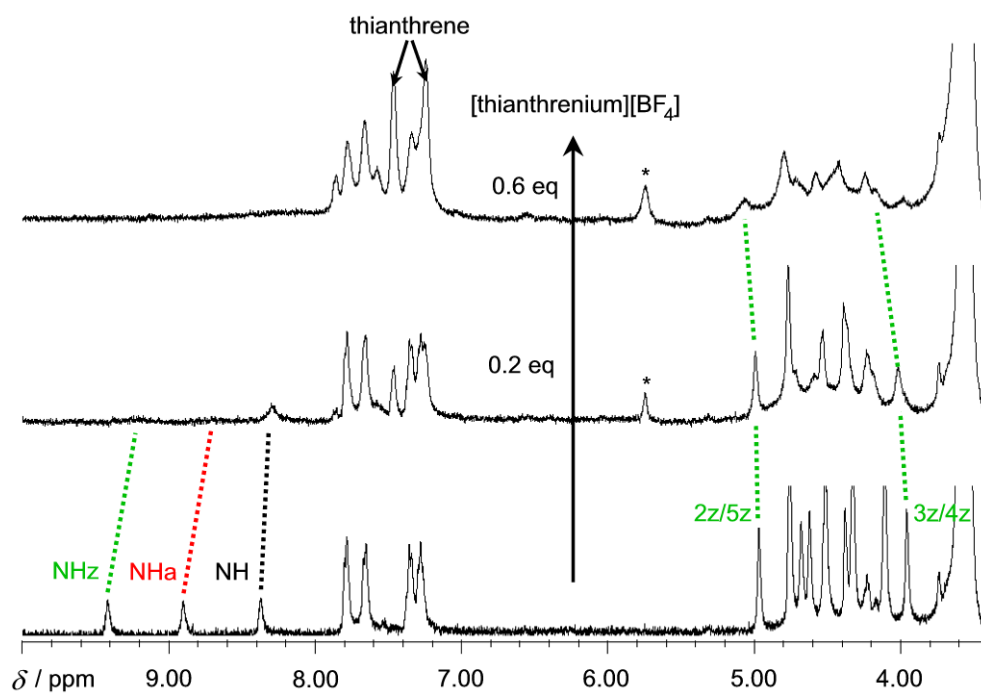


Fig. S12 1H NMR spectra during oxidation of **Fmoc-Fca₃-OMe** with $[C_{12}H_8S_2][BF_4]$ in $[D]_8$ -THF (* denotes residual CH_2Cl_2).

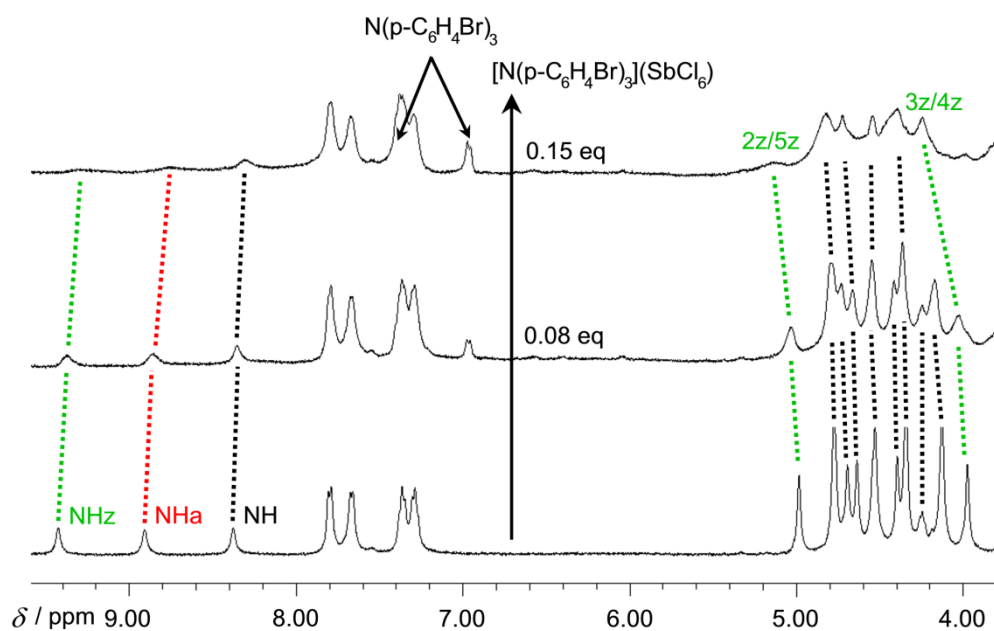


Fig. S13 ^1H NMR spectra during oxidation of **Fmoc-Fca₃-OMe** with $[\text{N}(\text{p-C}_6\text{H}_4\text{Br})_3][\text{SbCl}_6]$ in $[\text{D}]_8\text{-THF}$.

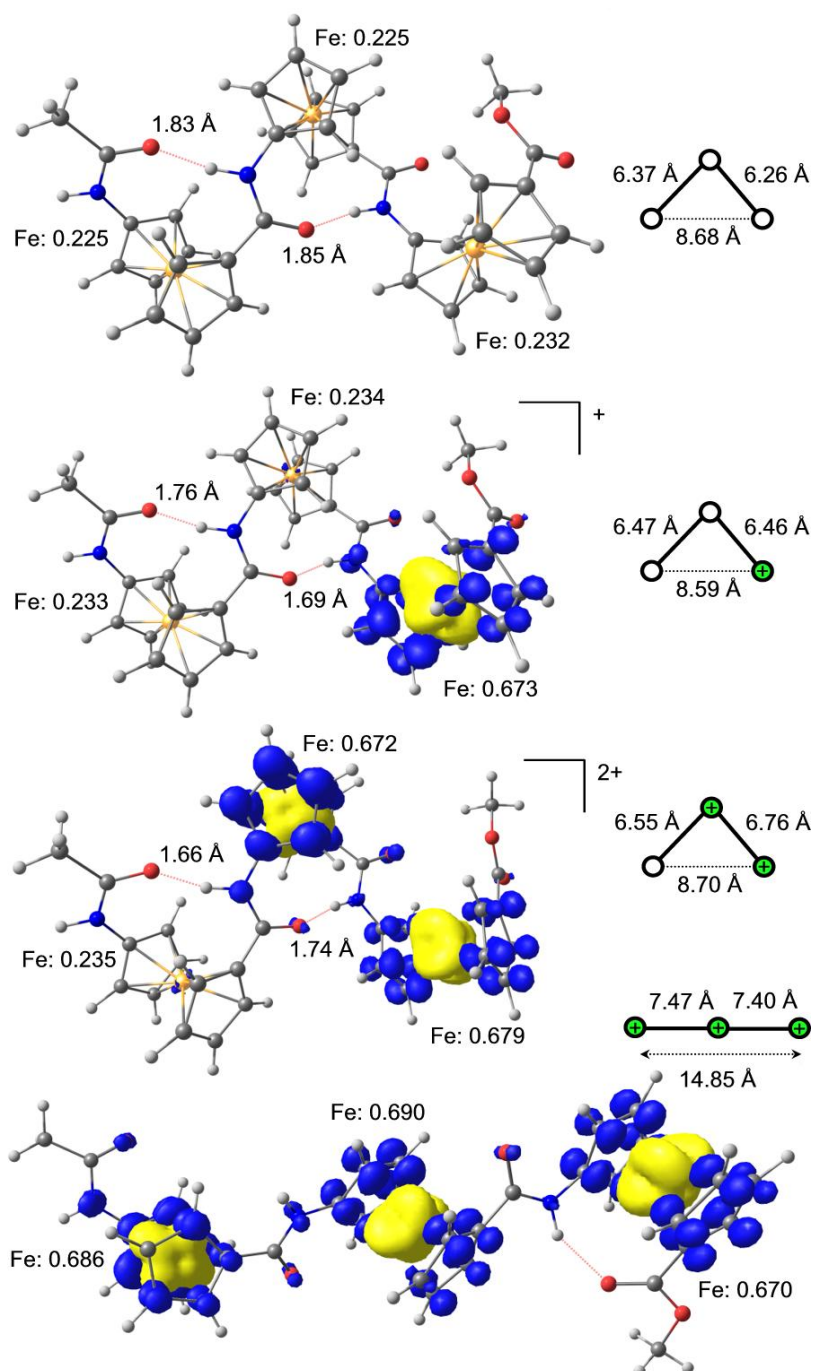


Fig. S14 DFT optimized geometries of computational models of $[\text{Fmoc-Fca}_3\text{-OMe}]^{n+}$ (-O-CH₂-fluorenyl replaced by CH₃; $n = 0 - 3$), relevant interatomic distances, natural charges on Fe centers and spin density surfaces (0.002 a.u.).

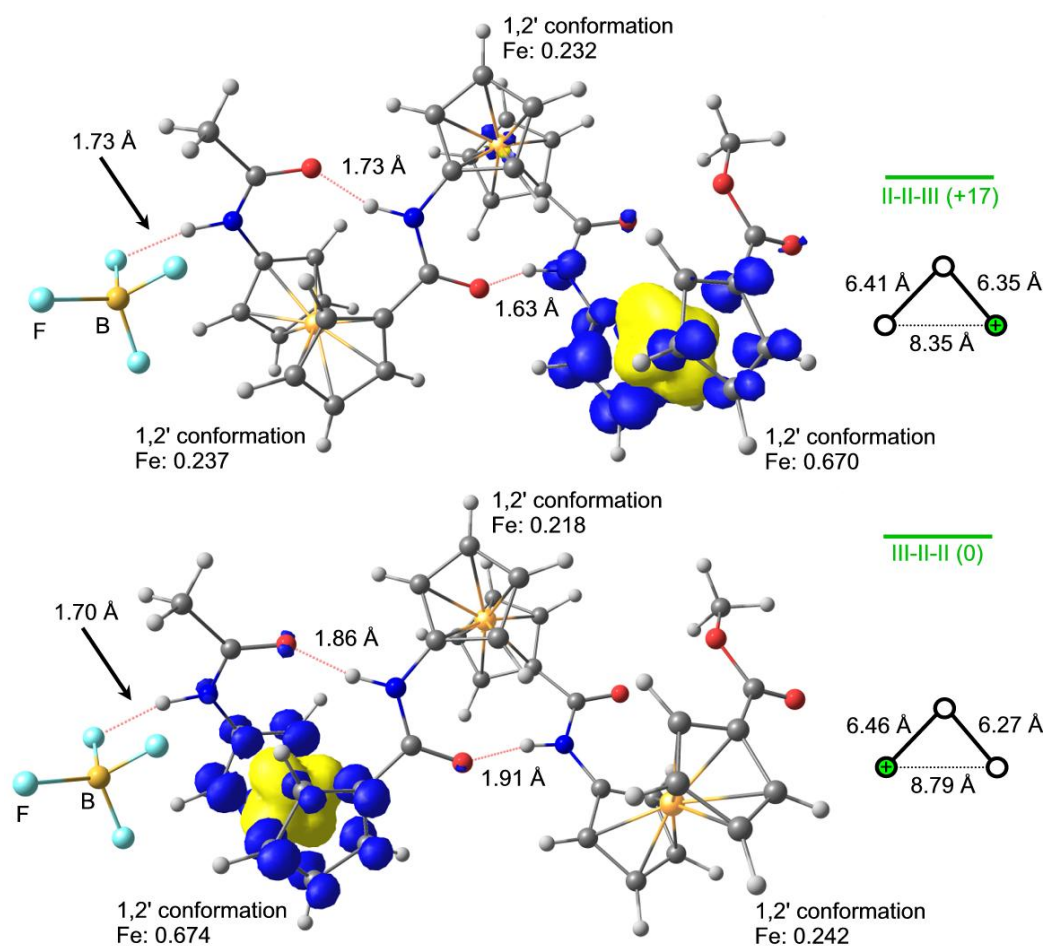


Fig. S15 DFT optimized geometries and relative energies (in parentheses in kJ mol^{-1}) of computational models of **[Fmoc-Fca₃-OMe]⁺** (-O-CH₂-fluorenyl replaced by CH₃) with **[BF₄]⁻** coordinated to NH_{carbamate}, relevant interatomic distances, natural charges on Fe centres and spin density surfaces (0.002 a.u.).

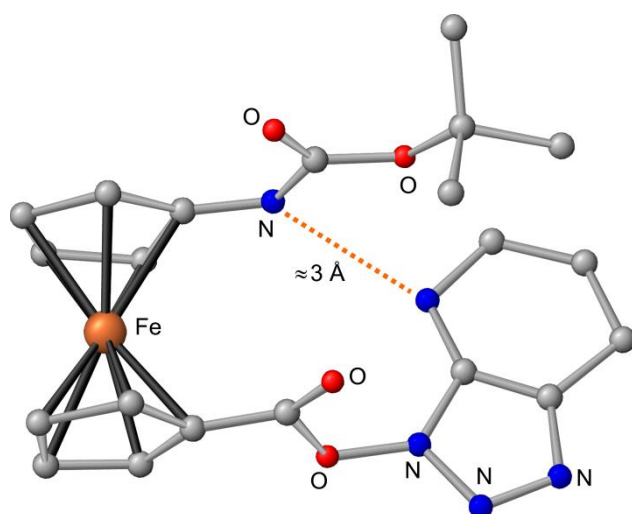


Fig. S16 Molecular structure of **Boc-Fca-OAt** in the crystal.

Cartesian coordinates of a model of Boc-Fca₂-OMe (tBu replaced by Me)

1,2' 8-membered ring $E_{\text{rel}} = 0 \text{ kJ mol}^{-1}$

1	-4.694877000	-2.639014000	1.483748000
6	-3.740929000	-2.172027000	1.282702000
1	-3.672654000	-0.475190000	2.770560000
1	-6.107717000	-0.737476000	-1.103329000
6	-3.199487000	-1.017405000	1.963535000
1	-5.452410000	1.354226000	0.498414000
1	-2.872127000	-3.430582000	-0.381957000
6	-5.196654000	-0.159141000	-1.159425000
6	-2.787556000	-2.590905000	0.292351000
6	-4.851074000	0.950098000	-0.304751000
26	-3.415960000	-0.582869000	-0.092320000
6	-1.917585000	-0.712001000	1.382152000
6	-4.110313000	-0.365651000	-2.083394000
6	-1.663008000	-1.690899000	0.341552000
1	-4.057397000	-1.130452000	-2.844862000
1	-1.241368000	0.074848000	1.688051000
6	-3.554407000	1.434284000	-0.719882000
1	-3.470797000	3.202625000	0.405814000
6	-3.092125000	0.620581000	-1.816925000
7	-2.908414000	2.544297000	-0.120729000
8	-0.029969000	-3.012884000	-0.812433000
6	-0.426086000	-1.862771000	-0.473507000
1	-2.150089000	0.728714000	-2.330609000
6	-1.552046000	2.712067000	-0.051316000
1	-0.199818000	0.201750000	-0.603706000
7	0.243189000	-0.699823000	-0.803247000
8	-0.693560000	1.976123000	-0.591277000
1	2.285672000	-2.711521000	-1.459484000
6	1.450405000	-0.632848000	-1.518936000
6	2.400192000	-1.688286000	-1.776914000
1	4.279896000	-1.850072000	1.375152000
6	3.330875000	0.189398000	1.334215000
6	4.313628000	-0.829765000	1.024406000
6	1.943785000	0.582490000	-2.122640000
1	1.445496000	1.540168000	-2.086408000
26	3.400990000	-0.102504000	-0.751686000
6	3.458371000	-1.131826000	-2.585164000
6	3.732468000	1.415675000	0.673540000
1	3.198858000	2.353027000	0.723801000
1	4.314316000	-1.675665000	-2.959384000
6	3.176588000	0.266201000	-2.802407000
6	5.314530000	-0.231941000	0.188662000
6	4.959211000	1.154212000	-0.024761000
1	3.783710000	0.960196000	-3.366464000
1	6.180677000	-0.733223000	-0.220042000
1	5.516492000	1.868555000	-0.614402000
6	2.129761000	0.034952000	2.156786000
8	1.227967000	0.893351000	2.307001000
8	2.097850000	-1.193278000	2.789432000
6	0.942170000	-1.496527000	3.649635000
1	0.062973000	-1.703116000	3.033240000
1	1.235189000	-2.385340000	4.210425000
1	0.735365000	-0.656026000	4.319754000
8	-1.243050000	3.810468000	0.720870000
6	0.190977000	4.012618000	1.026363000
1	0.735963000	4.242382000	0.105115000
1	0.206206000	4.863390000	1.708897000
1	0.600166000	3.112438000	1.495666000

1,1' 8-membered ring $E_{\text{rel}} = 10 \text{ kJ mol}^{-1}$

1	4.882461000	0.825230000	1.758421000
1	3.044946000	2.701154000	1.319341000
6	4.685932000	0.642262000	0.710767000
7	2.860279000	2.335437000	0.392481000
1	6.233317000	-0.895101000	0.148917000
6	3.682828000	1.299753000	-0.090869000
6	5.409987000	-0.262535000	-0.150644000
6	1.838326000	2.940629000	-0.298021000

1	2.616899000	-1.742851000	2.567668000
6	3.746068000	0.771433000	-1.430888000
6	4.827779000	-0.184368000	-1.466456000
26	3.389486000	-0.833902000	-0.076918000
8	1.383383000	2.598311000	-1.411536000
1	3.108802000	1.069003000	-2.247980000
1	5.132940000	-0.752959000	-2.333431000
6	2.506671000	-1.939876000	1.511302000
1	4.165979000	-3.380474000	1.032731000
6	1.481236000	-1.363527000	0.673264000
6	3.310666000	-2.809897000	0.698788000
6	1.657103000	-1.887602000	-0.669806000
6	2.781788000	-2.781801000	-0.646644000
1	3.163636000	-3.335310000	-1.492824000
1	1.009153000	-1.709561000	-1.516103000
6	-1.972594000	1.901088000	-0.603952000
7	-0.252447000	0.277122000	0.220658000
6	-1.396805000	1.067041000	0.423787000
6	-3.112950000	2.580262000	-0.032660000
6	0.402066000	-0.480268000	1.181493000
6	-2.206993000	1.182973000	1.613025000
6	-3.256892000	2.133294000	1.331487000
26	-3.443882000	0.513849000	0.002592000
8	0.093865000	-0.443853000	2.404788000
6	-4.000637000	-0.624904000	-1.680260000
6	-3.542686000	-1.494936000	-0.616004000
6	-5.149693000	0.087716000	-1.196131000
6	-4.411688000	-1.306554000	0.526476000
6	-5.399124000	-0.329090000	0.166915000
1	-1.575929000	2.030285000	-1.600944000
1	0.134037000	0.284728000	-0.717313000
1	-3.749239000	3.287006000	-0.546370000
1	-2.013491000	0.673358000	2.542319000
1	-4.020595000	2.448547000	2.028280000
1	-3.550753000	-0.554350000	-2.659768000
1	-5.725197000	0.813799000	-1.752916000
1	-4.312498000	-1.819408000	1.471183000
1	-6.188711000	0.038397000	0.807273000
8	1.385729000	4.023452000	0.438285000
6	0.264242000	4.795221000	-0.120685000
1	0.221167000	5.702155000	0.484328000
1	0.455030000	5.031636000	-1.172080000
1	-0.661713000	4.222025000	-0.029849000
6	-2.377781000	-2.380540000	-0.708083000
8	-1.523583000	-2.365490000	-1.621858000
8	-2.323447000	-3.269685000	0.349134000
6	-1.190776000	-4.211257000	0.384618000
1	-1.385949000	-4.849171000	1.247831000
1	-1.157992000	-4.796775000	-0.539902000
1	-0.250838000	-3.666871000	0.506285000

1,1' 6-membered ring $E_{\text{rel}} = 12 \text{ kJ mol}^{-1}$

1	-4.409713000	0.426396000	-2.298918000
1	-2.315084000	1.984749000	-1.593950000
6	-4.508264000	0.401682000	-1.222590000
7	-2.714174000	2.072911000	-0.663980000
1	-6.186456000	-1.060572000	-0.879343000
6	-3.732339000	1.179268000	-0.286566000
6	-5.454242000	-0.382670000	-0.464262000
6	-2.086699000	2.961867000	0.178038000
1	-2.237306000	-2.102844000	-2.204379000
6	-4.167179000	0.850796000	1.050235000
6	-5.242180000	-0.105382000	0.934251000
26	-3.494436000	-0.918234000	0.073597000
8	-2.291778000	3.114670000	1.400409000
1	-3.770989000	1.286418000	1.953242000
1	-5.790080000	-0.536984000	1.759671000
6	-2.294821000	-2.157505000	-1.127210000
1	-3.897611000	-3.680698000	-0.722366000
6	-1.474371000	-1.378534000	-0.222342000
6	-3.165030000	-2.984928000	-0.338545000
6	-1.857047000	-1.730193000	1.134435000
6	-2.897393000	-2.718919000	1.056509000
1	-3.395186000	-3.178123000	1.898957000
1	-1.453089000	-1.317530000	2.048730000

6	2.161546000	1.634433000	1.147191000
7	0.437505000	0.026618000	0.262293000
6	1.448112000	0.990743000	0.069061000
6	3.121186000	2.539005000	0.558570000
6	-0.499134000	-0.363350000	-0.681723000
6	1.984217000	1.467518000	-1.182900000
6	3.010242000	2.433373000	-0.875798000
26	3.542149000	0.569683000	-0.032475000
8	-0.528847000	0.112904000	-1.853645000
6	4.546297000	-0.754104000	1.250602000
6	3.820007000	-1.490092000	0.233747000
6	5.517331000	0.066595000	0.582829000
6	4.347715000	-1.112717000	-1.060342000
6	5.387931000	-0.147744000	-0.841984000
1	1.985331000	1.482119000	2.202926000
1	0.468579000	-0.492450000	1.134979000
1	3.805128000	3.174764000	1.102859000
1	1.631017000	1.172245000	-2.156936000
1	3.593795000	2.981936000	-1.601517000
1	4.378732000	-0.837175000	2.314501000
1	6.219692000	0.733332000	1.062772000
1	4.000456000	-1.495235000	-2.008386000
1	5.970999000	0.338673000	-1.611193000
8	-1.165070000	3.696949000	-0.554449000
6	-0.328206000	4.638307000	0.201939000
1	0.223449000	5.193366000	-0.558252000
1	-0.953369000	5.305249000	0.803475000
1	0.358747000	4.088049000	0.851975000
6	2.696279000	-2.391332000	0.510949000
8	2.046702000	-2.428994000	1.581534000
8	2.405345000	-3.212373000	-0.559487000
6	1.279187000	-4.152040000	-0.396820000
1	1.257087000	-4.722175000	-1.326552000
1	1.457393000	-4.804884000	0.463275000
1	0.344919000	-3.602725000	-0.251477000

1,2' 6-membered ring $E_{\text{rel}} = 12 \text{ kJ mol}^{-1}$

1	-5.714428000	-0.822079000	-0.392325000
1	-2.874051000	1.646332000	0.307959000
6	-4.963846000	-0.994896000	0.362678000
7	-3.838659000	1.306421000	0.365215000
1	-5.289116000	-3.132603000	0.986368000
6	-4.027018000	-0.007278000	0.844830000
6	-4.737438000	-2.210857000	1.104628000
6	-4.825540000	2.052820000	-0.223706000
1	-2.368447000	-0.086382000	-2.238255000
6	-3.216497000	-0.616298000	1.872849000
6	-3.659023000	-1.978969000	2.034105000
26	-2.969673000	-1.660866000	0.061009000
8	-6.021335000	1.730470000	-0.394415000
1	-2.421033000	-0.126009000	2.416044000
1	-3.254297000	-2.695485000	2.734809000
6	-2.101597000	-1.001225000	-1.729107000
1	-3.422735000	-2.558440000	-2.667279000
6	-1.102919000	-1.110127000	-0.686456000
6	-2.654613000	-2.310014000	-1.948896000
6	-1.047175000	-2.499558000	-0.266367000
6	-2.008933000	-3.231559000	-1.044532000
1	-2.214708000	-4.289494000	-0.962722000
1	-0.414822000	-2.908513000	0.509194000
6	2.786982000	0.346534000	1.938064000
7	0.859831000	-0.223103000	0.412748000
6	1.704263000	0.714955000	1.052963000
6	3.460819000	1.555030000	2.339036000
6	-0.394097000	0.050276000	-0.092151000
6	1.714653000	2.151331000	0.901796000
6	2.800551000	2.665962000	1.698724000
26	3.554265000	1.317950000	0.237548000
8	-0.912467000	1.209016000	-0.042990000
6	4.412201000	-0.143989000	-0.964135000
6	3.535680000	0.696192000	-1.758696000
6	5.476726000	0.685582000	-0.434352000
6	4.058971000	2.033010000	-1.711631000
6	5.247670000	2.027130000	-0.889618000
1	3.033813000	-0.659165000	2.248877000

1	1.287025000	-1.116166000	0.161459000
1	4.309267000	1.612557000	3.005831000
1	1.010746000	2.715845000	0.312298000
1	3.063606000	3.708780000	1.803663000
1	6.283523000	0.340282000	0.194701000
1	5.858783000	2.887252000	-0.655128000
1	2.655583000	0.358535000	-2.286475000
1	3.632090000	2.894523000	-2.204757000
8	-4.296285000	3.277255000	-0.629820000
6	-5.239519000	4.200945000	-1.270954000
1	-4.645124000	5.083428000	-1.513965000
1	-5.661595000	3.751645000	-2.175996000
1	-6.053106000	4.454295000	-0.583455000
6	4.146027000	-1.552567000	-0.649523000
8	3.022120000	-2.109088000	-0.698773000
8	5.281941000	-2.230996000	-0.261523000
6	5.125793000	-3.652641000	0.097351000
1	4.703556000	-4.208767000	-0.744898000
1	6.135537000	-3.994212000	0.328098000
1	4.467803000	-3.755556000	0.966491000

extended $E_{\text{rel}} = 14 \text{ kJ mol}^{-1}$

1	-5.491557000	1.394826000	1.719940000
1	-3.092584000	2.694387000	1.714332000
6	-4.819045000	1.513031000	0.885742000
6	-3.547540000	2.197929000	0.868895000
6	-5.056163000	1.014899000	-0.446050000
6	-2.997311000	2.105116000	-0.459367000
1	-3.730099000	-1.454196000	2.675718000
6	-3.922183000	1.354368000	-1.273053000
1	-1.374045000	-0.167204000	2.472329000
26	-3.250611000	0.176652000	0.344869000
1	2.942265000	1.066980000	2.199665000
1	0.628834000	0.038522000	1.515399000
6	-3.125819000	-1.384437000	1.782530000
6	-1.864710000	-0.701923000	1.669606000
1	-3.796336000	1.111467000	-2.319235000
6	2.979259000	1.238009000	1.132106000
7	0.775200000	0.197043000	0.526114000
6	-3.454849000	-1.939153000	0.490242000
1	4.905294000	2.368327000	0.865418000
6	-1.406496000	-0.836567000	0.296472000
1	-4.343696000	-2.507375000	0.255159000
6	1.976785000	0.841092000	0.169534000
6	4.016993000	1.943242000	0.420444000
6	-0.194344000	-0.275073000	-0.347862000
6	-2.400599000	-1.600016000	-0.424391000
1	5.957788000	-0.534743000	-2.224579000
6	2.413962000	1.258106000	-1.140627000
6	3.670927000	1.950964000	-0.978230000
1	-2.328351000	-1.857411000	-1.470840000
26	3.878509000	-0.031808000	-0.298169000
8	-0.053796000	-0.233890000	-1.601245000
1	1.879209000	1.070272000	-2.056772000
1	4.252481000	2.392331000	-1.774868000
6	5.368479000	-0.999935000	-1.449051000
1	3.584793000	-1.838725000	-2.530919000
6	5.713503000	-1.026613000	-0.042214000
6	4.121260000	-1.694335000	-1.603890000
6	4.670596000	-1.740674000	0.665189000
6	3.691519000	-2.152792000	-0.300946000
1	2.784929000	-2.703532000	-0.093269000
1	4.664314000	-1.926841000	1.729237000
6	6.885895000	-0.425460000	0.601957000
8	7.133065000	-0.440347000	1.825059000
1	-2.048215000	2.499566000	-0.792889000
7	-6.193940000	0.336373000	-0.926375000
1	-6.235354000	0.109363000	-1.912872000
6	-7.260683000	-0.076402000	-0.165061000
8	-7.412039000	0.073695000	1.063533000
8	-8.182660000	-0.710658000	-0.993619000
6	-9.405680000	-1.203478000	-0.343075000
1	-9.949851000	-0.374055000	0.119390000
1	-9.988892000	-1.653066000	-1.148000000
1	-9.156249000	-1.945207000	0.422250000

8	7.735429000	0.176554000	-0.318352000
6	8.953860000	0.798338000	0.224103000
1	9.570555000	0.047105000	0.727932000
1	9.470408000	1.210327000	-0.644294000
1	8.694514000	1.586777000	0.938360000

Cartesian coordinates of a model of Fmoc-Fca₃-OMe (O-CH₂-fluorenyl replaced by Me)

1	-5.008819000	-3.825425000	-2.320882000
6	-4.922763000	-2.772999000	-2.089238000
1	-2.871713000	-2.246408000	-2.869098000
1	-3.494861000	-4.569481000	0.684076000
6	-3.783128000	-1.931203000	-2.380663000
1	-1.444618000	-2.807350000	0.313064000
6	1.581787000	-0.722430000	-0.529506000
1	-6.883907000	-2.289736000	-1.068651000
6	-3.492579000	-3.525846000	0.965544000
8	0.453319000	-0.975974000	-0.003099000
6	-5.916125000	-1.972127000	-1.428138000
7	1.892676000	0.485844000	-1.093856000
6	-2.406767000	-2.599170000	0.758788000
26	-4.143011000	-1.961127000	-0.277144000
1	-1.047310000	0.616747000	-1.465483000
6	0.988661000	1.558191000	-1.281452000
6	-4.069620000	-0.606133000	-1.905530000
6	-0.438436000	1.506098000	-1.493113000
6	-4.575441000	-2.808895000	1.596025000
6	-5.389716000	-0.628756000	-1.312203000
1	-5.538031000	-3.215364000	1.872328000
1	-3.436800000	0.265484000	-1.969429000
6	-2.810790000	-1.318898000	1.293437000
6	1.411816000	2.935933000	-1.374069000
1	2.429859000	3.283349000	-1.272460000
1	-1.024563000	-0.351228000	0.920625000
6	-0.892370000	2.853749000	-1.736416000
6	-4.162425000	-1.439419000	1.786151000
7	-1.952551000	-0.204214000	1.331778000
1	-1.916166000	3.145527000	-1.922755000
6	0.247801000	3.734067000	-1.664385000
8	-7.151080000	0.385592000	-0.007934000
6	-6.069907000	0.477013000	-0.623823000
1	0.667947000	0.842198000	2.232331000
26	-0.015232000	2.727745000	0.179997000
1	0.234413000	4.806875000	-1.794291000
1	-4.741792000	-0.634860000	2.208381000
6	-2.300616000	1.063224000	1.746675000
6	0.217557000	1.808428000	2.057146000
6	-1.187944000	2.052731000	1.797391000
1	1.947809000	3.239642000	2.232076000
8	-3.476105000	1.389669000	2.082097000
6	0.892104000	3.080661000	2.060825000
6	-1.369045000	3.475608000	1.650289000
6	-0.088550000	4.109821000	1.801188000
1	-2.315826000	3.956974000	1.454129000
1	0.106904000	5.170851000	1.732672000
1	2.877078000	0.702874000	-1.284660000
6	2.637821000	-1.767148000	-0.568646000
6	3.712443000	-1.921218000	-1.530175000
6	4.429132000	-3.123905000	-1.198517000
6	3.806200000	-3.712731000	-0.035320000
6	2.698105000	-2.882298000	0.345200000
26	4.503875000	-1.752455000	0.416411000
6	4.798322000	0.148186000	1.310540000
6	5.924777000	-0.186493000	0.472326000
6	6.515171000	-1.409632000	0.966575000
6	5.760565000	-1.822750000	2.122107000
6	4.701647000	-0.866814000	2.329983000
7	6.483003000	0.575608000	-0.591036000
1	4.145639000	0.997312000	1.180712000
1	7.373314000	-1.916382000	0.546001000
1	5.949819000	-2.704081000	2.717864000
1	3.955624000	-0.904244000	3.110875000
1	7.490428000	0.528538000	-0.690880000
6	5.791345000	1.366230000	-1.475996000
8	4.532633000	1.458402000	-1.463211000
1	3.914927000	-1.264773000	-2.364134000

1	5.281455000	-3.520959000	-1.732030000
1	4.119145000	-4.620256000	0.461499000
1	2.015314000	-3.042458000	1.166873000
6	6.628928000	2.138358000	-2.481367000
1	6.490126000	3.212717000	-2.313781000
1	7.698432000	1.908790000	-2.423556000
1	6.268689000	1.917972000	-3.491875000
8	-5.362563000	1.662609000	-0.737105000
6	-5.790666000	2.784486000	0.119123000
1	-5.328756000	2.651832000	1.102243000
1	-5.414390000	3.684419000	-0.372696000
1	-6.881094000	2.806090000	0.201330000

Cartesian coordinates of a model of Fmoc-Fca₄-OMe (O-CH₂-fluorenyl replaced by Me)

1	-1.550480000	4.856701000	2.881046000
6	-1.960099000	3.983060000	2.393578000
1	-0.377191000	2.412618000	2.742176000
1	-0.212967000	5.883386000	-0.174368000
6	-1.332273000	2.683332000	2.313706000
1	1.223861000	3.567928000	-0.061406000
6	3.534966000	0.685378000	0.394015000
1	-3.946561000	4.703360000	1.590020000
6	-0.495116000	4.936477000	-0.612562000
8	2.559131000	1.278448000	-0.165451000
6	-3.220824000	3.911520000	1.706711000
7	3.428547000	-0.541682000	0.989017000
6	0.266940000	3.715602000	-0.541311000
26	-1.626101000	3.442114000	0.363567000
1	0.596413000	0.266877000	1.359405000
6	2.226669000	-1.271805000	1.163029000
6	-2.197832000	1.811322000	1.562608000
6	0.889902000	-0.770760000	1.382009000
6	-1.702225000	4.667059000	-1.354927000
6	-3.371205000	2.576667000	1.182767000
1	-2.489470000	5.374590000	-1.573792000
1	-2.041367000	0.761404000	1.359989000
6	-0.466034000	2.695471000	-1.255895000
6	2.186888000	-2.713919000	1.240226000
1	3.039643000	-3.368933000	1.133752000
1	0.991046000	1.237064000	-1.092294000
6	0.024487000	-1.902852000	1.610977000
6	-1.691510000	3.279026000	-1.750128000
7	0.028984000	1.383617000	-1.421654000
1	-1.043590000	-1.857850000	1.777683000
6	0.826854000	-3.097957000	1.523928000
8	-5.737812000	2.515218000	0.796389000
6	-4.591994000	2.078424000	0.489570000
1	2.133506000	-0.441984000	-2.354887000
26	0.907989000	-2.039979000	-0.308005000
1	0.468729000	-4.111195000	1.639726000
1	-2.455082000	2.761821000	-2.307868000
6	-0.732586000	0.282172000	-1.715931000
6	1.397577000	-1.213303000	-2.180968000
1	-3.423648000	0.913124000	-0.783633000
7	-4.382054000	1.106655000	-0.469986000
6	-0.007307000	-0.999218000	-1.883645000
1	2.566726000	-3.120616000	-2.426377000
8	-1.999321000	0.330389000	-1.829688000
6	1.623544000	-2.633614000	-2.220368000
1	-7.323488000	1.080702000	-0.258437000
6	-0.635230000	-2.292678000	-1.749637000
6	0.369718000	-3.298727000	-1.946956000
6	-5.385475000	0.419973000	-1.171110000
6	-6.816903000	0.468616000	-0.985983000
1	-1.678341000	-2.445233000	-1.516042000
1	0.216025000	-4.367570000	-1.897269000
1	-7.445687000	-1.771887000	1.832334000
6	-5.407241000	-2.324363000	1.059060000
6	-6.855750000	-2.317369000	1.111521000
6	-5.094925000	-0.503450000	-2.242013000
1	-4.102396000	-0.736083000	-2.598987000
26	-6.178597000	-1.555782000	-0.750305000
6	-7.411567000	-0.389192000	-1.983971000
6	-5.001557000	-3.166457000	-0.048120000
1	-3.978769000	-3.368676000	-0.330217000

1	-8.471443000	-0.554635000	-2.118825000
6	-6.351402000	-0.985134000	-2.760332000
6	-7.334802000	-3.158167000	0.052442000
6	-6.191448000	-3.683835000	-0.662619000
1	-6.471581000	-1.678327000	-3.581012000
1	-8.372140000	-3.355658000	-0.179178000
1	-6.226721000	-4.343889000	-1.517996000
1	4.287415000	-1.049340000	1.228834000
6	4.872236000	1.333794000	0.432829000
6	5.926283000	1.164373000	1.414287000
6	6.999722000	2.055965000	1.063480000
6	6.617489000	2.772719000	-0.131459000
6	5.304196000	2.334769000	-0.512753000
26	6.642791000	0.675473000	-0.505618000
6	6.312319000	-1.262201000	-1.300455000
6	7.486239000	-1.262025000	-0.460672000
6	8.438106000	-0.320193000	-1.005277000
6	7.855641000	0.251394000	-2.192711000
6	6.545926000	-0.324550000	-2.370476000
7	7.763560000	-2.101670000	0.653563000
1	5.419273000	-1.845071000	-1.136390000
1	9.413463000	-0.093532000	-0.596140000
1	8.318604000	0.992258000	-2.828560000
1	5.850542000	-0.090242000	-3.163813000
1	8.730970000	-2.378907000	0.773250000
6	6.847285000	-2.574607000	1.561841000
8	5.627629000	-2.252727000	1.525800000
1	5.896412000	0.501001000	2.266448000
1	7.928087000	2.173628000	1.604793000
1	7.215004000	3.511171000	-0.647173000
1	4.721228000	2.678188000	-1.354792000
6	-4.489884000	-1.619199000	1.954774000
8	-3.242460000	-1.585617000	1.845688000
8	-5.158896000	-0.986504000	2.984646000
6	7.382231000	-3.523002000	2.621398000
1	6.927461000	-4.510705000	2.481139000
1	8.471997000	-3.631535000	2.596821000
1	7.078854000	-3.163257000	3.610076000
6	-4.356303000	-0.203637000	3.939576000
1	-3.931971000	0.672528000	3.442307000
1	-5.061477000	0.097037000	4.715777000
1	-3.550777000	-0.819214000	4.353291000

Cartesian coordinates of a model of Fmoc-Fca₅-OMe (O-CH₂-fluorenyl replaced by Me)

1	-4.554420000	4.171270000	3.715500000
6	-4.748839000	3.311352000	3.089777000
1	-2.788870000	2.193548000	3.133236000
1	-3.712745000	6.002672000	0.875663000
6	-3.806614000	2.261176000	2.774548000
1	-1.723304000	4.164809000	0.546352000
6	1.297288000	1.981398000	0.364076000
1	-6.900182000	3.590412000	2.453320000
6	-3.768877000	5.103051000	0.279163000
8	0.137757000	2.381206000	0.023757000
6	-5.986279000	3.015242000	2.420657000
7	1.585484000	0.673956000	0.648447000
6	-2.714760000	4.133850000	0.117756000
26	-4.412019000	3.221183000	0.991521000
1	-1.309778000	0.572583000	1.293141000
6	0.643696000	-0.379954000	0.712472000
6	-4.456616000	1.322467000	1.896937000
6	-0.751995000	-0.325308000	1.079756000
6	-4.910994000	4.652318000	-0.478260000
6	-5.811598000	1.793485000	1.674981000
1	-5.866269000	5.152540000	-0.553499000
1	-4.041858000	0.401583000	1.511871000
6	-3.204245000	3.090976000	-0.754202000
6	0.994773000	-1.761589000	0.478396000
1	1.978362000	-2.113297000	0.202506000
1	-1.411990000	2.066243000	-0.887913000
6	-1.260859000	-1.675831000	1.091952000
6	-4.568311000	3.402747000	-1.114053000
7	-2.398717000	2.009722000	-1.171499000
1	-2.282084000	-1.961852000	1.305112000
6	-0.182032000	-2.558406000	0.721503000

8	-8.095468000	1.145524000	1.331042000
6	-6.898208000	1.100841000	0.927819000
1	0.011922000	1.053903000	-2.553390000
26	-0.558561000	-1.185557000	-0.841378000
1	-0.246558000	-3.633400000	0.628022000
1	-5.206371000	2.802750000	-1.742023000
6	-2.869305000	0.823141000	-1.672073000
6	-0.475416000	0.090700000	-2.514856000
1	-5.550944000	0.537217000	-0.559830000
7	-6.501624000	0.400413000	-0.195645000
6	-1.853751000	-0.153255000	-2.129241000
1	1.127710000	-1.333059000	-3.194770000
8	-4.111001000	0.549696000	-1.742333000
6	0.111554000	-1.176136000	-2.860416000
1	-9.293523000	-0.502495000	0.093029000
6	-2.104976000	-1.570237000	-2.249651000
6	-0.892914000	-2.201566000	-2.690104000
6	-7.331769000	-0.407451000	-0.988164000
6	-8.700579000	-0.804590000	-0.754153000
1	-3.045904000	-2.046794000	-2.018320000
1	-0.755004000	-3.259940000	-2.861641000
1	-8.464575000	-3.600819000	1.584608000
6	-6.420373000	-3.395720000	0.668426000
6	-7.805458000	-3.814051000	0.756789000
6	-6.889209000	-1.002961000	-2.226351000
1	-5.904375000	-0.873453000	-2.650613000
26	-7.514809000	-2.569721000	-0.937065000
6	-9.118170000	-1.603551000	-1.882155000
6	-5.886306000	-3.872866000	-0.591593000
1	-4.873421000	-3.718472000	-0.933296000
1	-10.099267000	-2.037996000	-2.014820000
6	-8.003808000	-1.722852000	-2.791143000
6	-8.115118000	-4.552782000	-0.433500000
6	-6.931323000	-4.591078000	-1.265314000
1	-7.997334000	-2.262617000	-3.727664000
1	-9.072283000	-4.994302000	-0.673640000
1	-6.850652000	-5.068864000	-2.231672000
1	2.569983000	0.381785000	0.690344000
6	2.417464000	2.948968000	0.479226000
6	3.596517000	2.856579000	1.319601000
6	4.365087000	4.057589000	1.129587000
6	3.671149000	4.890622000	0.173966000
6	2.467243000	4.212433000	-0.217300000
26	4.161714000	3.008753000	-0.701395000
6	4.235851000	1.255134000	-1.883888000
6	5.470528000	1.405601000	-1.148608000
6	6.077278000	2.658524000	-1.534595000
6	5.223781000	3.278030000	-2.515526000
6	4.087866000	2.415012000	-2.728756000
7	6.087156000	0.497292000	-0.252656000
1	3.549794000	0.427843000	-1.795665000
1	7.014575000	3.041208000	-1.156696000
1	5.400977000	4.228725000	-2.997885000
1	3.262256000	2.603652000	-3.400211000
1	7.114555000	0.480597000	-0.275420000
8	4.158567000	-0.501194000	0.561982000
1	3.838642000	2.041189000	1.985769000
1	5.299544000	4.294170000	1.618934000
1	4.000200000	5.856264000	-0.183449000
1	1.716467000	4.563719000	-0.910021000
6	-5.667073000	-2.628812000	1.661427000
8	-4.487301000	-2.228014000	1.535238000
8	-6.407084000	-2.399571000	2.805849000
6	-5.779694000	-1.604522000	3.875104000
1	-5.669124000	-0.565869000	3.552677000
1	-6.469457000	-1.675557000	4.717410000
1	-4.798377000	-2.017722000	4.130356000
6	5.425050000	-0.386144000	0.554167000
6	6.257856000	-1.216303000	1.463483000
6	7.518821000	-0.866801000	2.090169000
6	5.875978000	-2.524947000	1.936284000
6	6.897612000	-2.992290000	2.830642000
6	7.908110000	-1.965205000	2.933369000
26	7.746772000	-2.597635000	0.913957000
6	8.423344000	-4.402960000	0.032535000
6	7.533274000	-3.716955000	-0.871202000
6	8.096722000	-2.424599000	-1.171460000
6	9.338530000	-2.314171000	-0.444250000

6	9.539226000	-3.534202000	0.305935000
7	10.304423000	-1.270656000	-0.515826000
6	10.049649000	0.075370000	-0.616631000
8	8.882011000	0.553102000	-0.600104000
1	11.274672000	-1.563653000	-0.505179000
6	11.265587000	0.976721000	-0.753019000
1	11.224859000	1.487757000	-1.721867000
1	12.216374000	0.437894000	-0.679227000
1	11.229761000	1.747538000	0.024173000
1	8.055010000	0.061576000	1.959676000
1	8.798003000	-2.009342000	3.545551000
1	6.907226000	-3.945780000	3.339588000
1	4.972500000	-3.043918000	1.651477000
1	8.275532000	-5.390168000	0.446164000
1	6.597873000	-4.098580000	-1.254906000
1	7.667849000	-1.668056000	-1.810786000
1	10.380398000	-3.752500000	0.949864000

Cartesian coordinates of a model of [Boc-Fca₂-OMe]⁺ (tBu replaced by Me)

1,2' 8-membered ring $E_{\text{rel}} = 0 \text{ kJ mol}^{-1}$ II-III

1	4.196469000	-3.453169000	-0.804325000
6	3.348338000	-2.784332000	-0.768589000
1	3.576157000	-1.573871000	-2.656955000
1	5.956705000	-1.274326000	1.247958000
6	3.024897000	-1.773782000	-1.749159000
1	5.696887000	0.461692000	-0.819349000
1	2.299782000	-3.371519000	1.140976000
6	5.176532000	-0.535019000	1.137261000
6	2.352560000	-2.744868000	0.262382000
6	5.039635000	0.381615000	0.035547000
26	3.327945000	-0.849818000	0.145400000
6	1.838862000	-1.089104000	-1.320606000
6	4.085160000	-0.307009000	2.049857000
6	1.419903000	-1.689626000	-0.064766000
1	3.904849000	-0.841260000	2.971722000
1	1.311070000	-0.320348000	-1.864929000
6	3.866280000	1.188688000	0.282366000
1	4.225854000	2.811347000	-0.991406000
6	3.273246000	0.763400000	1.526484000
7	3.486960000	2.283360000	-0.537715000
8	-0.396627000	-2.188239000	1.428611000
6	0.238861000	-1.349591000	0.740723000
1	2.392799000	1.184969000	1.987476000
6	2.220061000	2.721389000	-0.774591000
1	0.442255000	0.687854000	0.205146000
7	-0.158296000	0.007367000	0.701373000
8	1.149815000	2.203815000	-0.352263000
1	-2.182464000	-1.183208000	2.467156000
6	-1.252727000	0.523689000	1.339342000
6	-2.227715000	-0.143082000	2.185800000
1	-5.182078000	-1.646333000	0.202733000
6	-3.682807000	-0.630044000	-1.123874000
6	-4.856214000	-0.740674000	-0.289113000
6	-1.704391000	1.895350000	1.163520000
1	-1.180226000	2.635603000	0.575675000
26	-3.382344000	0.696984000	0.532863000
6	-3.173181000	0.844184000	2.637256000
6	-3.588956000	0.732627000	-1.591897000
1	-2.832775000	1.107794000	-2.266577000
1	-3.971292000	0.667162000	3.344814000
6	-2.848322000	2.106659000	2.012516000
6	-5.487922000	0.543127000	-0.244115000
6	-4.701089000	1.460300000	-1.031637000
1	-3.353480000	3.048809000	2.171466000
1	-6.392457000	0.785737000	0.297344000
1	-4.934536000	2.500446000	-1.212614000
6	-2.676796000	-1.682613000	-1.406770000
8	-1.587733000	-1.456491000	-1.969397000
8	-3.085193000	-2.902954000	-0.952167000
6	-2.136581000	-4.039865000	-1.065293000
1	-1.355647000	-3.919011000	-0.308899000
1	-2.741654000	-4.925424000	-0.872017000
1	-1.701681000	-4.063458000	-2.067932000
8	2.255586000	3.841420000	-1.571527000

6	0.981059000	4.471939000	-1.950570000
1	0.472596000	4.856203000	-1.060613000
1	1.265508000	5.289339000	-2.613063000
1	0.342162000	3.753004000	-2.472724000

1,2' 8-membered ring $E_{\text{rel}} = 42 \text{ kJ mol}^{-1}$ III-II

1	4.066508000	2.811576000	-1.330397000
7	3.414115000	2.365980000	-0.692094000
6	3.875487000	1.379987000	0.178946000
6	2.089014000	2.775780000	-0.778634000
6	5.038986000	0.558243000	-0.063594000
6	3.293953000	0.975425000	1.435404000
8	1.139909000	2.237977000	-0.169488000
8	1.991368000	3.819528000	-1.644184000
1	5.686666000	0.616445000	-0.928367000
6	5.216507000	-0.305699000	1.076231000
6	4.135449000	-0.049345000	1.999149000
1	2.399315000	1.386302000	1.877772000
6	0.650120000	4.400228000	-1.895478000
1	6.032115000	-0.999933000	1.221165000
1	3.990246000	-0.518479000	2.962197000
1	0.251803000	4.816713000	-0.966388000
1	0.826624000	5.182288000	-2.632652000
1	-0.019650000	3.629924000	-2.287550000
1	0.247622000	0.579731000	0.408770000
7	-0.294188000	-0.127021000	0.907748000
6	0.121382000	-1.429024000	0.886476000
6	-1.480486000	0.346005000	1.514078000
6	1.353164000	-1.732484000	0.084317000
8	-0.450994000	-2.383937000	1.482004000
6	-2.504009000	-0.401227000	2.212162000
6	-1.859957000	1.738995000	1.491664000
6	2.349224000	-2.694502000	0.490621000
6	1.695237000	-1.261717000	-1.231994000
1	-2.492805000	-1.464286000	2.387846000
6	-3.501452000	0.545338000	2.640696000
1	-1.289530000	2.537905000	1.040478000
6	-3.108191000	1.860269000	2.200343000
6	3.324573000	-2.799395000	-0.564278000
1	2.324791000	-3.249861000	1.418053000
6	2.917252000	-1.903896000	-1.629274000
1	1.095843000	-0.579290000	-1.817698000
1	-4.396560000	0.302350000	3.195130000
1	-3.651774000	2.778311000	2.370364000
1	4.179713000	-3.460858000	-0.579083000
1	3.416301000	-1.781263000	-2.580906000
26	-3.345670000	0.586931000	0.524374000
6	-3.393424000	-0.509257000	-1.262273000
6	-4.640868000	-0.714340000	-0.555789000
6	-3.267438000	0.904829000	-1.555490000
6	-2.376935000	-1.525693000	-1.550600000
1	-5.005976000	-1.667543000	-0.204535000
6	-5.275057000	0.563227000	-0.413174000
1	-2.448981000	1.359383000	-2.093846000
6	-4.433166000	1.561264000	-1.033149000
8	-1.199934000	-1.290816000	-1.922200000
8	-2.851969000	-2.797290000	-1.343636000
1	-6.218748000	0.749545000	0.079544000
1	-4.647634000	2.618763000	-1.094381000
6	-1.909263000	-3.924284000	-1.467890000
1	-1.227978000	-3.918026000	-0.610758000
1	-2.537394000	-4.815528000	-1.455988000
1	-1.349792000	-3.850696000	-2.405335000
26	3.347290000	-0.801248000	0.169710000

1,2' 6-membered ring $E_{\text{rel}} = 24 \text{ kJ mol}^{-1}$ III-II

1	-5.742892000	-0.844645000	-0.177440000
1	-3.073329000	1.803853000	0.805853000
6	-4.931455000	-1.031789000	0.509288000
7	-3.956650000	1.311176000	0.659250000
1	-5.130870000	-3.209324000	1.015911000
6	-4.026479000	-0.015726000	1.012007000
6	-4.595438000	-2.278734000	1.142785000

6	-4.923106000	1.970595000	-0.113241000
1	-2.463838000	0.038526000	-2.276552000
6	-3.071479000	-0.675678000	1.882764000
6	-3.453710000	-2.061425000	2.000188000
26	-2.879661000	-1.660834000	0.004714000
8	-5.953217000	1.445257000	-0.571215000
1	-2.259331000	-0.184125000	2.399950000
1	-2.985353000	-2.792255000	2.643957000
6	-2.105822000	-0.878129000	-1.829525000
1	-3.327698000	-2.481193000	-2.828842000
6	-1.062172000	-0.968014000	-0.833299000
6	-2.560488000	-2.213708000	-2.115011000
6	-0.879127000	-2.372053000	-0.512907000
6	-1.798824000	-3.131293000	-1.311679000
1	-1.904260000	-4.207849000	-1.306089000
1	-0.155334000	-2.776213000	0.181398000
6	2.618312000	0.810516000	1.871914000
7	0.882386000	0.044853000	0.180014000
6	1.700799000	1.048632000	0.777179000
6	3.340945000	2.032768000	2.103232000
6	-0.417515000	0.222190000	-0.180099000
6	1.852276000	2.416831000	0.343157000
6	2.869842000	3.019854000	1.163572000
26	3.658081000	1.326562000	0.115906000
8	-1.089812000	1.281465000	0.012116000
6	4.421031000	-0.400561000	-0.754328000
6	3.830124000	0.452624000	-1.771692000
6	5.525852000	0.316435000	-0.150338000
6	4.570199000	1.682616000	-1.784975000
6	5.603918000	1.602238000	-0.779491000
1	2.732142000	-0.116739000	2.415731000
1	1.372443000	-0.818941000	-0.104195000
1	4.101821000	2.183434000	2.855475000
1	1.289850000	2.894398000	-0.444820000
1	3.215342000	4.040922000	1.090257000
1	6.161466000	-0.060675000	0.637133000
1	6.316633000	2.378945000	-0.541510000
1	3.005637000	0.184805000	-2.416315000
1	4.387285000	2.522786000	-2.439205000
8	-4.543434000	3.271061000	-0.274280000
6	-5.453444000	4.151626000	-1.042179000
1	-4.952323000	5.118859000	-1.054022000
1	-5.584891000	3.759069000	-2.054440000
1	-6.420908000	4.212427000	-0.536241000
6	3.888875000	-1.706388000	-0.348914000
8	2.680821000	-2.061276000	-0.463628000
8	4.836363000	-2.522237000	0.196037000
6	4.426165000	-3.864788000	0.658732000
1	3.982824000	-4.424874000	-0.169326000
1	5.349722000	-4.332270000	0.999472000
1	3.705379000	-3.776051000	1.477828000

1,1' 6-membered ring $E_{\text{rel}} = 28 \text{ kJ mol}^{-1}$ III-II

8	-1.480263000	2.506171000	1.061500000
1	-3.356704000	-1.710684000	3.016910000
1	-2.086077000	0.558513000	2.210970000
6	-3.692554000	-1.038271000	2.240030000
6	-3.014325000	0.165071000	1.827466000
6	-2.428600000	2.773431000	0.304505000
6	-4.905803000	-1.162705000	1.469064000
6	-3.850479000	0.833972000	0.851335000
1	-5.648565000	-1.942603000	1.559242000
1	-2.651099000	-4.191232000	0.019526000
7	-3.610936000	2.019249000	0.203163000
6	-4.973909000	-0.037579000	0.569872000
1	-0.536597000	-2.533979000	0.326608000
26	-3.225568000	-1.250018000	0.178175000
1	0.784076000	2.321179000	0.478215000
1	0.898521000	-1.082181000	-0.682686000
6	-2.502485000	-3.252713000	-0.497802000
6	-1.387167000	-2.368347000	-0.322768000
1	-5.774983000	0.172096000	-0.126331000
1	-4.268475000	2.348216000	-0.497666000
6	1.553125000	2.058248000	-0.234108000
7	0.586963000	-0.170332000	-1.033980000

6	-3.396638000	-2.669430000	-1.464948000
1	3.051178000	3.731237000	-0.084763000
6	-1.579150000	-1.232173000	-1.201216000
1	-4.317014000	-3.109083000	-1.824252000
6	1.556723000	0.874650000	-1.059410000
6	2.750355000	2.798149000	-0.539773000
6	-0.729998000	-0.003252000	-1.358374000
6	-2.823748000	-1.422440000	-1.908521000
1	1.999056000	-0.402511000	2.422123000
6	2.750414000	0.886303000	-1.878075000
6	3.485702000	2.077540000	-1.550869000
1	-3.215982000	-0.749873000	-2.658069000
26	3.249650000	0.856022000	0.178177000
8	-1.253442000	1.071672000	-1.766505000
1	3.021970000	0.141593000	-2.612957000
1	4.426860000	2.379270000	-1.988000000
6	2.953984000	-0.209736000	1.955820000
1	3.664169000	1.681753000	2.934684000
6	3.594684000	-1.052554000	0.959589000
6	3.843217000	0.882622000	2.229760000
6	4.875402000	-0.463993000	0.626331000
6	5.018388000	0.731326000	1.402680000
1	5.861705000	1.406553000	1.373252000
1	5.582167000	-0.866467000	-0.084060000
6	2.991073000	-2.239900000	0.353802000
8	1.748412000	-2.471304000	0.297973000
8	-2.530963000	3.832063000	-0.539724000
6	-1.327623000	4.670495000	-0.741436000
1	-0.575592000	4.079458000	-1.270078000
1	-1.672542000	5.506849000	-1.348397000
1	-0.946632000	5.013304000	0.224712000
8	3.912155000	-3.093746000	-0.180830000
6	3.429130000	-4.326006000	-0.839154000
1	4.335679000	-4.842864000	-1.153240000
1	2.858725000	-4.929399000	-0.127338000
1	2.802339000	-4.072741000	-1.699931000

1,1' 8-membered ring $E_{\text{rel}} = 29 \text{ kJ mol}^{-1}$ II-III

1	4.771363000	0.407821000	2.017936000
1	3.628461000	2.847164000	1.238199000
6	4.701820000	0.317702000	0.942727000
7	3.192726000	2.290262000	0.509630000
1	6.150245000	-1.333819000	0.456203000
6	3.887052000	1.131820000	0.073492000
6	5.444062000	-0.593437000	0.108951000
6	2.117307000	2.862609000	-0.106681000
1	2.406359000	-2.369218000	2.212277000
6	4.089801000	0.703292000	-1.287705000
6	5.063198000	-0.359188000	-1.261361000
26	3.379067000	-0.943027000	-0.140852000
8	1.379432000	2.324689000	-0.976574000
1	3.616749000	1.125920000	-2.161285000
1	5.431873000	-0.896263000	-2.123747000
6	2.336440000	-2.311197000	1.135513000
1	3.918272000	-3.727872000	0.409657000
6	1.401301000	-1.483676000	0.405687000
6	3.120415000	-3.035780000	0.180201000
6	1.619879000	-1.704758000	-1.014979000
6	2.671215000	-2.670905000	-1.144182000
1	3.061687000	-3.057140000	-2.074910000
1	1.039485000	-1.283814000	-1.822126000
6	-1.848344000	2.148964000	-0.220441000
7	-0.177797000	0.382052000	0.304923000
6	-1.298343000	1.101143000	0.624905000
6	-2.996617000	2.712104000	0.445083000
6	0.296031000	-0.745126000	1.022981000
6	-2.217237000	0.922657000	1.735710000
6	-3.224798000	1.947508000	1.650224000
26	-3.452323000	0.716040000	-0.057566000
8	-0.250762000	-1.090158000	2.101738000
6	-3.709775000	-0.372952000	-1.877339000
6	-3.707691000	-1.293562000	-0.764590000
6	-4.850657000	0.494874000	-1.718007000
6	-4.851161000	-1.000176000	0.066887000
6	-5.559275000	0.093002000	-0.527377000

1	-1.387737000	2.504258000	-1.131584000
1	0.417731000	0.770844000	-0.438902000
1	-3.567314000	3.566279000	0.108990000
1	-2.093909000	0.190918000	2.518194000
1	-4.000240000	2.123665000	2.382697000
1	-2.997067000	-0.374543000	-2.689806000
1	-5.151520000	1.277363000	-2.400906000
1	-5.108454000	-1.528157000	0.974395000
1	-6.463032000	0.546625000	-0.143026000
8	1.931569000	4.139448000	0.377509000
6	0.830335000	4.943222000	-0.176323000
1	1.033771000	5.960637000	0.158202000
1	0.828740000	4.883438000	-1.268534000
1	-0.126099000	4.592634000	0.224969000
6	-2.642901000	-2.293393000	-0.507677000
8	-1.582017000	-2.345206000	-1.158967000
8	-2.960504000	-3.109933000	0.538659000
6	-1.938493000	-4.089167000	0.988901000
1	-2.472596000	-4.754109000	1.667215000
1	-1.538755000	-4.632127000	0.128515000
1	-1.140985000	-3.549248000	1.507878000

extended $E_{\text{rel}} = 57 \text{ kJ mol}^{-1}$ III-II

1	-5.787860000	1.420892000	1.460095000
1	-3.465566000	2.838263000	1.551698000
6	-5.035292000	1.480718000	0.689089000
6	-3.797894000	2.221160000	0.728453000
6	-5.150476000	0.888834000	-0.625976000
6	-3.109496000	2.026537000	-0.526248000
1	-3.669764000	-1.306491000	3.030689000
6	-3.916649000	1.152557000	-1.339345000
1	-1.461338000	0.230696000	2.757755000
26	-3.281692000	0.181952000	0.483277000
1	3.280300000	0.807275000	2.357193000
1	0.903599000	-0.114434000	1.754495000
6	-3.040300000	-1.254149000	2.152429000
6	-1.862123000	-0.437294000	2.006726000
1	-3.676192000	0.826236000	-2.342300000
6	3.219481000	1.124252000	1.324687000
7	0.918143000	0.248840000	0.807100000
6	-3.230462000	-1.991754000	0.934283000
1	5.162181000	2.207873000	1.014529000
6	-1.324268000	-0.666205000	0.682383000
1	-4.022965000	-2.702735000	0.743342000
6	2.116224000	0.899955000	0.417032000
6	4.213555000	1.883753000	0.611937000
6	-0.161121000	-0.007984000	0.003551000
6	-2.191077000	-1.618686000	0.017048000
1	5.901870000	-0.233612000	-2.396997000
6	2.437227000	1.492913000	-0.860993000
6	3.735252000	2.106382000	-0.728652000
1	-2.036414000	-1.993517000	-0.985099000
26	3.888372000	0.026287000	-0.350744000
8	-0.223298000	0.272560000	-1.226664000
1	1.809665000	1.471942000	-1.736497000
1	4.261294000	2.635292000	-1.510296000
6	5.307918000	-0.795939000	-1.692323000
1	3.471689000	-1.375109000	-2.851538000
6	5.680418000	-1.068924000	-0.321836000
6	4.026606000	-1.402193000	-1.924533000
6	4.626985000	-1.850741000	0.287649000
6	3.608482000	-2.055939000	-0.704259000
1	2.691584000	-2.612310000	-0.568095000
1	4.642655000	-2.216760000	1.303965000
6	6.892750000	-0.627733000	0.387835000
8	7.133247000	-0.841698000	1.592006000
1	-2.149049000	2.429281000	-0.815126000
7	-6.196518000	0.146760000	-1.132321000
1	-6.176231000	-0.146039000	-2.104941000
6	-7.347761000	-0.212681000	-0.410449000
8	-7.536104000	0.030131000	0.792115000
8	-8.194494000	-0.872055000	-1.251919000
6	-9.494943000	-1.322798000	-0.697427000
1	-10.059549000	-0.458436000	-0.337980000
1	-9.997562000	-1.803421000	-1.535760000

1	-9.322385000	-2.027266000	0.120778000
8	7.757994000	0.058367000	-0.443154000
6	9.028563000	0.515991000	0.152345000
1	9.595589000	-0.340418000	0.529394000
1	9.558523000	1.009586000	-0.662945000
1	8.832535000	1.211176000	0.974821000

Cartesian coordinates of a model of [Boc-Fca₂-OMe*OMe₂]⁺ (tBu replaced by Me)

1,2' 8-membered ring $E_{\text{rel}} = 0 \text{ kJ mol}^{-1}$ II-III

1	2.802645000	-4.389963000	-1.071025000
6	2.118956000	-3.560445000	-0.958988000
1	2.759988000	-2.149549000	-2.596786000
1	4.827431000	-3.001615000	1.389461000
6	2.104394000	-2.360453000	-1.763889000
1	5.102296000	-0.926892000	-0.349797000
1	0.815312000	-4.187741000	0.772441000
6	4.232456000	-2.099616000	1.376564000
6	1.074342000	-3.458864000	0.018082000
6	4.379467000	-1.007642000	0.449489000
26	2.443631000	-1.840229000	0.273117000
6	1.064944000	-1.499657000	-1.276819000
6	3.143952000	-1.787033000	2.268296000
6	0.423363000	-2.180481000	-0.163634000
1	2.782681000	-2.409501000	3.074498000
1	0.761165000	-0.554836000	-1.701905000
6	3.387375000	-0.010296000	0.781825000
6	2.618529000	-0.493554000	1.903757000
7	3.322885000	1.248585000	0.137108000
8	-1.589428000	-2.474799000	1.117959000
6	-0.720108000	-1.709649000	0.627613000
1	1.810452000	0.030071000	2.391478000
6	2.201921000	1.978499000	-0.053506000
1	-0.008586000	0.284421000	0.493028000
7	-0.798773000	-0.308654000	0.811051000
8	1.016155000	1.668513000	0.270983000
1	-3.240428000	-1.252850000	2.143809000
6	-1.814674000	0.341257000	1.452710000
6	-3.014624000	-0.200975000	2.069463000
1	-5.979753000	-0.558021000	-0.388885000
6	-4.129699000	0.255644000	-1.367987000
6	-5.392428000	0.305496000	-0.668007000
6	-1.919966000	1.791339000	1.514747000
1	-1.172294000	2.467640000	1.125230000
26	-3.738424000	1.169677000	0.532723000
6	-3.759351000	0.894769000	2.632303000
6	-3.664998000	1.609480000	-1.556212000
1	-2.763630000	1.890029000	-2.081821000
1	-4.656861000	0.799966000	3.227697000
6	-3.081282000	2.127095000	2.296432000
6	-5.710212000	1.680420000	-0.429164000
6	-4.639094000	2.488670000	-0.957981000
1	-3.375351000	3.122379000	2.598188000
1	-6.594844000	2.048459000	0.072956000
1	-4.599897000	3.569200000	-0.953502000
6	-3.365279000	-0.951582000	-1.763823000
8	-2.194816000	-0.912870000	-2.190664000
8	-4.090846000	-2.092268000	-1.572272000
6	-3.415263000	-3.392522000	-1.813095000
1	-2.720960000	-3.582881000	-0.989481000
1	-4.221994000	-4.125129000	-1.828268000
1	-2.882129000	-3.364613000	-2.767009000
8	2.499674000	3.167097000	-0.693510000
6	1.393764000	4.094668000	-0.966741000
1	0.936575000	4.428394000	-0.029431000
1	1.858329000	4.934220000	-1.484832000
1	0.640669000	3.617117000	-1.602024000
8	5.771036000	2.010360000	-0.801214000
1	4.222317000	1.624691000	-0.237924000
6	6.941649000	2.068309000	0.072708000
1	7.829715000	1.689007000	-0.451105000
1	7.123764000	3.098917000	0.408513000
1	6.723517000	1.432115000	0.934004000
6	5.901746000	2.808319000	-2.018980000
1	6.092640000	3.862228000	-1.772703000

1	6.717922000	2.420287000	-2.643624000
1	4.951667000	2.723848000	-2.551355000

1,2' 8-membered ring $E_{\text{rel}} = 27 \text{ kJ mol}^{-1}$ III-II

8	-5.557904000	2.008162000	1.066130000
6	-6.664171000	2.607327000	0.311326000
1	-6.579714000	3.702122000	0.309334000
1	-6.592106000	2.228674000	-0.711232000
1	-7.624891000	2.309138000	0.749756000
6	-5.508816000	2.435467000	2.467655000
1	-6.424154000	2.126395000	2.988244000
1	-4.643343000	1.944033000	2.919020000
1	-5.391903000	3.525089000	2.533609000
1	-4.154054000	1.673121000	0.278724000
7	-3.328498000	1.301192000	-0.258632000
6	-3.460961000	0.065976000	-0.876145000
6	-2.156082000	2.030205000	-0.263963000
6	-4.434910000	-0.926802000	-0.478573000
6	-2.685727000	-0.485065000	-1.965102000
8	-1.053108000	1.625159000	-0.703252000
8	-2.355742000	3.251544000	0.313971000
1	-5.155742000	-0.802082000	0.317697000
6	-4.317828000	-2.051060000	-1.371274000
6	-3.237349000	-1.776523000	-2.290510000
1	-1.863096000	0.004882000	-2.462434000
6	-1.195980000	4.166017000	0.405579000
1	-4.947013000	-2.930027000	-1.366402000
1	-2.907522000	-2.411988000	-3.100504000
1	-0.827908000	4.399830000	-0.597170000
1	-1.587502000	5.056715000	0.895884000
1	-0.401536000	3.706057000	1.000119000
1	0.189501000	0.146476000	-0.780171000
7	0.962478000	-0.480869000	-1.012266000
6	0.871527000	-1.810363000	-0.701590000
6	2.096944000	0.143545000	-1.582223000
6	-0.341016000	-2.244478000	0.068092000
8	1.732949000	-2.685254000	-0.996141000
6	3.382776000	-0.449559000	-1.877882000
6	2.149756000	1.546465000	-1.928108000
6	-1.039360000	-3.486921000	-0.161866000
6	-0.907160000	-1.622901000	1.235096000
1	3.637298000	-1.486078000	-1.731333000
6	4.217005000	0.586622000	-2.419313000
1	1.335356000	2.248124000	-1.821122000
6	3.469272000	1.816576000	-2.448428000
6	-2.059763000	-3.617129000	0.846812000
1	-0.797228000	-4.194968000	-0.942138000
6	-1.977666000	-2.453544000	1.707554000
1	-0.544905000	-0.708768000	1.683239000
1	5.241749000	0.460230000	-2.738495000
1	3.826106000	2.773026000	-2.801770000
1	-2.735467000	-4.452463000	0.966934000
1	-2.583604000	-2.269698000	2.584178000
26	3.598872000	1.123988000	-0.449616000
6	3.717382000	0.458886000	1.529067000
6	5.057016000	0.699896000	1.037470000
6	2.979923000	1.706718000	1.474389000
6	3.112058000	-0.826721000	1.893938000
1	5.832453000	-0.046191000	0.953230000
6	5.143397000	2.086694000	0.684632000
1	1.958618000	1.840696000	1.798406000
6	3.867328000	2.709203000	0.953482000
8	1.889334000	-1.000791000	2.122708000
8	4.029138000	-1.847094000	1.928576000
1	6.013608000	2.580648000	0.276036000
1	3.626398000	3.750712000	0.794277000
6	3.525639000	-3.217141000	2.149438000
1	2.963916000	-3.541586000	1.267954000
1	4.421637000	-3.822612000	2.287035000
1	2.889238000	-3.248424000	3.038554000
26	-2.472287000	-1.880353000	-0.317555000

Cartesian coordinates of a model of [Boc-Fca₂-OMe][BF₄] (tBu replaced by Me)

1,2' 8-membered ring $E_{\text{rel}} = 0 \text{ kJ mol}^{-1}$ III-II

1	-3.735334000	-2.548060000	2.656733000
6	-2.865198000	-2.067473000	2.231747000
1	-3.443338000	0.122590000	2.197652000
1	-5.014075000	-3.001082000	-0.648901000
6	-2.699689000	-0.643519000	2.028164000
1	-4.953380000	-0.288657000	-0.810453000
1	-1.415714000	-3.773303000	1.872350000
6	-4.198143000	-2.408763000	-1.037955000
6	-1.649477000	-2.719460000	1.817684000
6	-4.187114000	-0.973531000	-1.147621000
26	-2.588422000	-1.687516000	0.145138000
6	-1.389817000	-0.421535000	1.480512000
6	-2.942881000	-2.908927000	-1.553361000
6	-0.742419000	-1.704639000	1.339478000
1	-2.648610000	-3.945947000	-1.634010000
1	-0.981604000	0.542906000	1.205483000
6	-2.941873000	-0.583570000	-1.777268000
6	-2.154041000	-1.781382000	-1.980794000
7	-2.588347000	0.731032000	-2.018806000
8	1.297997000	-2.923222000	1.507432000
6	0.660720000	-2.013605000	0.905836000
1	-1.160776000	-1.812450000	-2.399753000
6	-1.277188000	1.171119000	-2.064847000
1	0.555487000	-0.602983000	-0.620464000
7	1.162155000	-1.270467000	-0.132097000
8	-0.270086000	0.432361000	-1.917929000
1	3.597315000	-2.646813000	0.814266000
6	2.458148000	-1.408234000	-0.672140000
6	3.594563000	-2.105785000	-0.117400000
1	4.831313000	0.325399000	2.350670000
6	3.579732000	1.494318000	0.892977000
6	4.761423000	0.826460000	1.396997000
6	2.844849000	-0.828876000	-1.936724000
1	2.198738000	-0.246741000	-2.577451000
26	4.103655000	-0.057200000	-0.424868000
6	4.675938000	-1.984260000	-1.064336000
6	3.890683000	2.034084000	-0.416461000
1	3.209011000	2.595759000	-1.037443000
1	5.662875000	-2.409098000	-0.947627000
6	4.214985000	-1.202221000	-2.185272000
6	5.791574000	0.956070000	0.406860000
6	5.258320000	1.707530000	-0.707930000
1	4.794086000	-0.932572000	-3.056979000
1	6.792929000	0.555433000	0.478664000
1	5.794241000	1.972050000	-1.608544000
6	2.275147000	1.599582000	1.552897000
8	1.207436000	1.956624000	1.003347000
8	2.346310000	1.262976000	2.889941000
6	1.109761000	1.340340000	3.688953000
1	0.513252000	0.436528000	3.530001000
1	1.444803000	1.397421000	4.725476000
1	0.527552000	2.223092000	3.409370000
8	-1.231353000	2.510814000	-2.259074000
6	0.065005000	3.189397000	-2.029105000
1	0.771528000	2.902744000	-2.814985000
1	-0.175816000	4.250693000	-2.086604000
1	0.449286000	2.916850000	-1.041748000
9	-4.605152000	2.167264000	-0.981365000
5	-4.384454000	2.290304000	0.474685000
9	-4.833311000	3.533783000	0.938804000
9	-2.963906000	2.102123000	0.693766000
9	-5.085604000	1.186830000	1.098326000
1	-3.312945000	1.448240000	-1.840728000

1,2' 8-membered ring $E_{\text{rel}} = 39 \text{ kJ mol}^{-1}$ II-III

1	-3.349373000	-3.724661000	1.526864000
6	-2.586049000	-2.998277000	1.285362000
1	-3.359265000	-1.083298000	2.231470000
1	-4.891532000	-3.054956000	-1.522274000
6	-2.599994000	-1.604378000	1.664450000
1	-5.153233000	-0.539835000	-0.505655000
1	-1.082097000	-4.194153000	0.097577000
6	-4.215861000	-2.228379000	-1.690011000

6	-1.397024000	-3.252603000	0.524130000
6	-4.365004000	-0.900795000	-1.151199000
26	-2.560216000	-1.759286000	-0.464626000
6	-1.433510000	-0.976702000	1.118150000
6	-3.002091000	-2.264022000	-2.468033000
6	-0.675141000	-2.001543000	0.409302000
1	-2.610180000	-3.117645000	-3.002729000
1	-1.176913000	0.063147000	1.257110000
6	-3.252579000	-0.107577000	-1.619856000
6	-2.401186000	-0.950623000	-2.422632000
7	-3.137914000	1.269557000	-1.347551000
8	1.456607000	-2.751777000	-0.429332000
6	0.592372000	-1.842535000	-0.298520000
1	-1.491177000	-0.644392000	-2.915625000
6	-1.987367000	1.982197000	-1.273683000
1	0.036540000	0.137459000	-0.881203000
7	0.817075000	-0.555393000	-0.858632000
8	-0.805451000	1.527715000	-1.377232000
1	3.339136000	-1.934074000	-1.456903000
6	1.950955000	-0.166605000	-1.499340000
6	3.185402000	-0.903613000	-1.734190000
1	6.034879000	-0.473489000	0.839263000
6	4.043804000	0.349751000	1.483173000
6	5.366655000	0.373921000	0.893598000
6	2.175780000	1.196072000	-1.964614000
1	1.428274000	1.975088000	-1.908800000
26	3.808047000	0.826424000	-0.583650000
6	4.076291000	-0.053569000	-2.480285000
6	3.478780000	1.672431000	1.372869000
1	2.508518000	1.966898000	1.748257000
1	5.036170000	-0.350465000	-2.879464000
6	3.451004000	1.243448000	-2.625526000
6	5.620181000	1.707836000	0.439184000
6	4.447990000	2.502255000	0.705163000
1	3.856266000	2.094180000	-3.154878000
1	6.524705000	2.053030000	-0.043402000
1	4.330068000	3.553502000	0.480702000
6	3.325621000	-0.813296000	2.055790000
8	2.183570000	-0.744624000	2.541468000
8	4.063443000	-1.966679000	1.960012000
6	3.392822000	-3.225081000	2.373316000
1	2.614439000	-3.463625000	1.642367000
1	4.185224000	-3.974234000	2.373212000
1	2.956346000	-3.104818000	3.368626000
8	-2.257520000	3.312026000	-1.089194000
6	-1.261795000	4.134090000	-0.388348000
1	-0.284178000	4.059392000	-0.877720000
1	-1.649138000	5.151715000	-0.451126000
1	-1.213581000	3.802672000	0.652856000
9	-4.759035000	1.961409000	0.704842000
5	-3.948161000	2.014802000	1.931048000
9	-4.247457000	0.856584000	2.717793000
9	-4.207850000	3.218154000	2.625592000
9	-2.543388000	1.967290000	1.528499000
1	-3.932759000	1.705159000	-0.861138000

Cartesian coordinates of a model of [Fmoc-Fca₃-OMe]⁺ (OCH₂-fluorenyl replaced by Me)

1	-5.365482000	-4.072629000	-1.978918000
6	-5.210597000	-3.009805000	-1.853945000
1	-3.309888000	-2.636809000	-3.007756000
1	-3.170356000	-4.523707000	0.888687000
6	-4.119588000	-2.243286000	-2.408032000
1	-1.272507000	-2.659327000	0.276273000
6	1.552409000	-0.638755000	-0.512966000
1	-6.984236000	-2.345190000	-0.612913000
6	-3.225574000	-3.464589000	1.097784000
8	0.388767000	-0.864021000	-0.027572000
6	-6.063594000	-2.110036000	-1.128111000
7	1.927011000	0.576546000	-1.005362000
6	-2.221385000	-2.488652000	0.766593000
26	-4.133400000	-2.056004000	-0.188150000
1	-0.974405000	0.847551000	-1.574425000
6	1.080197000	1.690832000	-1.208728000

6	-4.303366000	-0.868977000	-2.046592000
6	-0.329578000	1.710778000	-1.521646000
6	-4.306194000	-2.779331000	1.773456000
6	-5.494318000	-0.781803000	-1.241095000
1	-5.207747000	-3.229012000	2.165464000
1	-3.672520000	-0.033338000	-2.313723000
6	-2.624174000	-1.212890000	1.330769000
6	1.567480000	3.049716000	-1.239656000
1	2.590429000	3.346502000	-1.060100000
1	-0.906079000	-0.208047000	0.846182000
6	-0.704869000	3.082837000	-1.765773000
6	-3.968709000	-1.379353000	1.857730000
7	-1.845752000	-0.089840000	1.278818000
1	-1.693170000	3.429154000	-2.032521000
6	0.466038000	3.905826000	-1.593426000
8	-7.019814000	0.386259000	0.205624000
6	-6.067239000	0.424137000	-0.592364000
1	0.631349000	1.022255000	2.309564000
26	0.022489000	2.878533000	0.204732000
1	0.511146000	4.980098000	-1.700538000
1	-4.569471000	-0.592042000	2.285869000
6	-2.283713000	1.213394000	1.612686000
6	0.179887000	1.979238000	2.091706000
6	-1.217392000	2.213612000	1.755980000
1	1.872664000	3.429526000	2.372682000
8	-3.505878000	1.466889000	1.764866000
6	0.831850000	3.257702000	2.137853000
6	-1.405364000	3.638791000	1.599730000
6	-0.142210000	4.277329000	1.824074000
1	-2.341524000	4.118834000	1.355220000
1	0.049308000	5.339502000	1.769225000
1	2.930061000	0.757279000	-1.162718000
6	2.550264000	-1.728976000	-0.583712000
6	3.595896000	-1.903870000	-1.576549000
6	4.248207000	-3.156033000	-1.308655000
6	3.621888000	-3.754443000	-0.152722000
6	2.571157000	-2.881346000	0.288504000
26	4.433850000	-1.850026000	0.356677000
6	4.867826000	-0.025214000	1.349187000
6	5.936308000	-0.361477000	0.438815000
6	6.482227000	-1.641104000	0.829304000
6	5.760694000	-2.087754000	1.992508000
6	4.763405000	-1.096042000	2.308545000
7	6.486200000	0.440452000	-0.598662000
1	4.264179000	0.868147000	1.309147000
1	7.292926000	-2.162559000	0.338761000
1	5.932574000	-3.012233000	2.524650000
1	4.058534000	-1.143413000	3.126325000
1	7.488042000	0.365196000	-0.736085000
6	5.797470000	1.311795000	-1.403542000
8	4.541078000	1.443679000	-1.336657000
1	3.815597000	-1.228970000	-2.391168000
1	5.064198000	-3.578697000	-1.877585000
1	3.899238000	-4.694537000	0.302752000
1	1.910645000	-3.038067000	1.128945000
6	6.624553000	2.123685000	-2.382579000
1	6.564449000	3.184491000	-2.112033000
1	7.678903000	1.829377000	-2.407517000
1	6.199538000	2.019787000	-3.386265000
8	-5.414709000	1.562564000	-0.980651000
6	-5.800308000	2.824665000	-0.302906000
1	-5.367082000	2.818276000	0.700955000
1	-5.371706000	3.615733000	-0.918982000
1	-6.889274000	2.905131000	-0.253979000

Cartesian coordinates of a model of [Fmoc-Fca₃-OMe]²⁺ (OCH₂-fluorenyl replaced by Me)

1	-5.365482000	-4.072629000	-1.978918000
6	-5.210597000	-3.009805000	-1.853945000
1	-3.309888000	-2.636809000	-3.007756000
1	-3.170356000	-4.523707000	0.888687000
6	-4.119588000	-2.243286000	-2.408032000
1	-1.272507000	-2.659327000	0.276273000
6	1.552409000	-0.638755000	-0.512966000

1	-6.984236000	-2.345190000	-0.612913000
6	-3.225574000	-3.464589000	1.097784000
8	0.388767000	-0.864021000	-0.027572000
6	-6.063594000	-2.110036000	-1.128111000
7	1.927011000	0.576546000	-1.005362000
6	-2.221385000	-2.488652000	0.766593000
26	-4.133400000	-2.056004000	-0.188150000
1	-0.974405000	0.847551000	-1.574425000
6	1.080197000	1.690832000	-1.208728000
6	-4.303366000	-0.868977000	-2.046592000
6	-0.329578000	1.710778000	-1.521646000
6	-4.306194000	-2.779331000	1.773456000
6	-5.494318000	-0.781803000	-1.241095000
1	-5.207747000	-3.229012000	2.165464000
1	-3.672520000	-0.033338000	-2.313723000
6	-2.624174000	-1.212890000	1.330769000
6	1.567480000	3.049716000	-1.239656000
1	2.590429000	3.346502000	-1.060100000
1	-0.906079000	-0.208047000	0.846182000
6	-0.704869000	3.082837000	-1.765773000
6	-3.968709000	-1.379353000	1.857730000
7	-1.845752000	-0.089840000	1.278818000
1	-1.693170000	3.429154000	-2.032521000
6	0.466038000	3.905826000	-1.593426000
8	-7.019814000	0.386259000	0.205624000
6	-6.067239000	0.424137000	-0.592364000
1	0.631349000	1.022255000	2.309564000
26	0.022489000	2.878533000	0.204732000
1	0.511146000	4.980098000	-1.700538000
1	-4.569471000	-0.592042000	2.285869000
6	-2.283713000	1.213394000	1.612686000
6	0.179887000	1.979238000	2.091706000
6	-1.217392000	2.213612000	1.755980000
1	1.872664000	3.429526000	2.372682000
8	-3.505878000	1.466889000	1.764866000
6	0.831850000	3.257702000	2.137853000
6	-1.405364000	3.638791000	1.599730000
6	-0.142210000	4.277329000	1.824074000
1	-2.341524000	4.118834000	1.355220000
1	0.049308000	5.339502000	1.769225000
1	2.930061000	0.757279000	-1.162718000
6	2.550264000	-1.728976000	-0.583712000
6	3.595896000	-1.903870000	-1.576549000
6	4.248207000	-3.156033000	-1.308655000
6	3.621888000	-3.754443000	-0.152722000
6	2.571157000	-2.881346000	0.288504000
26	4.433850000	-1.850026000	0.356677000
6	4.867826000	-0.025214000	1.349187000
6	5.936308000	-0.361477000	0.438815000
6	6.482227000	-1.641104000	0.829304000
6	5.760694000	-2.087754000	1.992508000
6	4.763405000	-1.096042000	2.308545000
7	6.486200000	0.440452000	-0.598662000
1	4.264179000	0.868147000	1.309147000
1	7.292926000	-2.162559000	0.338761000
1	5.932574000	-3.012233000	2.524650000
1	4.058534000	-1.143413000	3.126325000
1	7.488042000	0.365196000	-0.736085000
6	5.797470000	1.311795000	-1.403542000
8	4.541078000	1.443679000	-1.336657000
1	3.815597000	-1.228970000	-2.391168000
1	5.064198000	-3.578697000	-1.877585000
1	3.899238000	-4.694537000	0.302752000
1	1.910645000	-3.038067000	1.128945000
6	6.624553000	2.123685000	-2.382579000
1	6.564449000	3.184491000	-2.112033000
1	7.678903000	1.829377000	-2.407517000
1	6.199538000	2.019787000	-3.386265000
8	-5.414709000	1.562564000	-0.980651000
6	-5.800308000	2.824665000	-0.302906000
1	-5.367082000	2.818276000	0.700955000
1	-5.371706000	3.615733000	-0.918982000
1	-6.889274000	2.905131000	-0.253979000

Cartesian coordinates of a model of [Fmoc-Fca₃-OMe]³⁺ (OCH₂-fluorenyl replaced by Me)

1	-8.365377000	-1.509273000	3.002641000
6	-8.454958000	-0.830941000	2.164837000
1	-10.423886000	-1.423681000	1.246789000
1	-8.362375000	-2.345441000	-2.355563000
6	-9.558619000	-0.773596000	1.242533000
1	-6.608889000	-0.277587000	-2.431009000
6	3.870961000	0.788945000	0.078736000
1	-6.607751000	0.457704000	2.340295000
6	-7.531866000	-2.194231000	-1.680032000
8	3.591562000	1.591876000	-0.839131000
6	-7.516721000	0.204865000	1.812851000
7	3.004349000	-0.271319000	0.416362000
6	-6.598131000	-1.096264000	-1.724536000
26	-7.611634000	-1.106259000	0.151178000
1	1.022176000	-2.268726000	1.019344000
6	1.871885000	-0.639067000	-0.300246000
6	-9.316237000	0.291999000	0.314090000
6	0.947290000	-1.671595000	0.119584000
6	-7.123735000	-3.079069000	-0.615197000
6	-8.047615000	0.897867000	0.655766000
1	-7.606622000	-4.005945000	-0.336693000
1	-9.965193000	0.603576000	-0.493468000
6	-5.585332000	-1.330307000	-0.715311000
6	1.386780000	-0.095767000	-1.551187000
1	1.842329000	0.717892000	-2.093688000
1	-4.734818000	0.547731000	-0.644333000
6	-0.011301000	-1.870031000	-0.937572000
6	-5.931479000	-2.545868000	-0.011239000
7	-4.534697000	-0.439802000	-0.452833000
1	-0.787098000	-2.623047000	-0.941621000
6	0.258326000	-0.892659000	-1.966740000
8	-6.113906000	2.009716000	-0.283807000
6	-7.353609000	1.995004000	-0.077472000
1	-1.599042000	-0.127333000	2.468681000
26	-0.314216000	0.078923000	-0.173366000
1	-0.263043000	-0.791377000	-2.908681000
1	-5.366894000	-2.979895000	0.800135000
6	-3.394742000	-0.766635000	0.274928000
6	-1.552059000	0.493430000	1.583917000
6	-2.381340000	0.325529000	0.408927000
1	0.002032000	2.034323000	2.083337000
8	-3.213370000	-1.890407000	0.803698000
6	-0.710350000	1.634279000	1.374158000
6	-2.016851000	1.357856000	-0.539025000
6	-0.979784000	2.159669000	0.062901000
1	-2.452958000	1.520091000	-1.515731000
1	-0.507534000	3.022896000	-0.386615000
1	3.219936000	-0.810082000	1.250445000
6	5.096256000	0.910837000	0.910978000
6	5.838874000	-0.119559000	1.619911000
6	6.897944000	0.523098000	2.341460000
6	6.839000000	1.934344000	2.071750000
6	5.734533000	2.181821000	1.188203000
26	7.108833000	0.865190000	0.140242000
6	7.758839000	-0.525353000	-1.401350000
6	8.991914000	-0.098337000	-0.765777000
6	9.012887000	1.353957000	-0.798461000
6	7.896891000	1.804405000	-1.588967000
6	7.123129000	0.642575000	-1.959517000
7	9.956505000	-0.881129000	-0.174323000
1	7.442025000	-1.551495000	-1.500503000
1	9.790739000	1.984286000	-0.386373000
1	7.695883000	2.828125000	-1.872739000
1	6.231514000	0.643169000	-2.571455000
1	10.837468000	-0.438904000	0.076495000
8	8.728630000	-2.841063000	-0.090223000
1	5.650072000	-1.185798000	1.610886000
1	7.622461000	0.025733000	2.972712000
1	7.499496000	2.686582000	2.481954000
1	5.399876000	3.142170000	0.820454000
6	9.827954000	-2.283012000	0.085049000
6	11.089450000	-2.962774000	0.555519000
1	11.788942000	-3.081256000	-0.283289000

1	11.601561000	-2.392340000	1.340519000
1	10.843868000	-3.955604000	0.935911000
8	-8.215946000	2.940252000	-0.496314000
6	-7.706750000	4.140113000	-1.221493000
1	-7.243356000	3.829245000	-2.161879000
1	-8.594693000	4.745082000	-1.396950000
1	-6.985848000	4.664585000	-0.589486000

Cartesian coordinates of a model of [Fmoc-Fca₃-OMe][BF₄] (OCH₂-fluorenyl replaced by Me)

1,2' 8-membered ring $E_{\text{rel}} = 0 \text{ kJ mol}^{-1}$ III-II-II

1	-5.320842000	-4.397769000	-2.074334000
6	-5.310307000	-3.321680000	-1.971819000
1	-3.239535000	-2.764451000	-2.673298000
1	-3.897023000	-4.665639000	1.052659000
6	-4.200037000	-2.450800000	-2.288763000
1	-2.005720000	-2.747878000	0.624119000
6	0.921166000	-0.471828000	-0.151438000
1	-7.367811000	-2.843580000	-1.160781000
6	-4.016465000	-3.604397000	1.219332000
8	-0.230093000	-0.819984000	0.254698000
6	-6.393391000	-2.511258000	-1.487410000
7	1.184433000	0.706317000	-0.783722000
6	-3.012991000	-2.595091000	0.984306000
26	-4.712861000	-2.247932000	-0.228430000
1	-1.693779000	0.460976000	-1.463658000
6	0.203087000	1.646164000	-1.188469000
6	-4.594219000	-1.098665000	-2.004968000
6	-1.178329000	1.405243000	-1.536756000
6	-5.207995000	-2.943957000	1.695624000
6	-5.952308000	-1.133261000	-1.506753000
1	-6.144314000	-3.419502000	1.950934000
1	-4.009042000	-0.201871000	-2.138221000
6	-3.580189000	-1.316217000	1.347352000
6	0.497526000	3.042302000	-1.411762000
1	1.457750000	3.511294000	-1.252573000
1	-1.871960000	-0.206347000	1.006312000
6	-1.731539000	2.656163000	-1.990018000
6	-4.946672000	-1.526980000	1.762583000
7	-2.840431000	-0.117294000	1.322521000
1	-2.751347000	2.807747000	-2.313562000
6	-0.700902000	3.662402000	-1.913652000
8	-7.874609000	-0.079089000	-0.494435000
6	-6.749989000	0.004367000	-1.026459000
1	-0.449528000	1.318842000	2.369623000
26	-1.064048000	2.845005000	0.009384000
1	-0.807949000	4.704636000	-2.178034000
1	-5.633178000	-0.750099000	2.056610000
6	-3.348170000	1.144877000	1.548900000
6	-0.964002000	2.197244000	2.006937000
6	-2.346820000	2.248825000	1.573196000
1	0.585593000	3.826758000	2.166330000
8	-4.575348000	1.378608000	1.739743000
6	-0.420713000	3.527620000	1.907662000
6	-2.646304000	3.613221000	1.217714000
6	-1.459887000	4.399718000	1.411508000
1	-3.605770000	3.958272000	0.861427000
1	-1.361527000	5.458842000	1.219220000
1	2.155098000	1.026657000	-0.875133000
6	2.066780000	-1.413303000	0.048626000
6	3.223701000	-1.625039000	-0.788315000
6	3.990531000	-2.700587000	-0.226988000
6	3.307381000	-3.164425000	0.961550000
6	2.112727000	-2.376347000	1.123734000
26	3.876981000	-1.119137000	1.247462000
6	4.056509000	0.940969000	1.900800000
6	5.265309000	0.642443000	1.163311000
6	5.894585000	-0.502576000	1.786684000
6	5.122546000	-0.856362000	2.948889000
6	3.986797000	0.036445000	3.021526000
7	5.749921000	1.248377000	0.014910000
1	3.355660000	1.723633000	1.657796000
1	6.777414000	-1.005912000	1.414621000

1	5.363515000	-1.645082000	3.647348000
1	3.230492000	0.049660000	3.793830000
1	6.679784000	0.929028000	-0.304528000
6	4.969919000	1.908443000	-0.927282000
8	3.720107000	2.023967000	-0.782552000
1	3.510138000	-1.065109000	-1.667544000
1	4.941858000	-3.049416000	-0.605310000
1	3.621120000	-3.984827000	1.591764000
1	1.351359000	-2.486480000	1.883050000
6	5.712322000	2.404988000	-2.143021000
1	5.082733000	3.103828000	-2.696719000
1	6.658890000	2.885256000	-1.872541000
1	5.948327000	1.545195000	-2.784086000
8	-6.102475000	1.210725000	-1.239492000
6	-6.694718000	2.404981000	-0.608213000
1	-6.372119000	2.431410000	0.436999000
1	-6.294311000	3.254758000	-1.165756000
1	-7.785771000	2.369034000	-0.674785000
9	7.826838000	-0.137248000	-0.961027000
9	5.920804000	-0.908438000	-2.090221000
9	8.052266000	-1.756870000	-2.671041000
9	7.055381000	-2.327038000	-0.601154000
5	7.236913000	-1.321870000	-1.621631000

Cartesian coordinates of a model of [Fmoc-Fca₃-OMe][BF₄] (OCH₂-fluorenyl replaced by Me)

1,2' 8-membered ring $E_{\text{rel}} = 17 \text{ kJ mol}^{-1}$ II-II-III

1	-5.168706000	-4.710860000	-1.805357000
6	-5.133979000	-3.630161000	-1.813495000
1	-3.081048000	-3.197711000	-2.642719000
1	-3.476681000	-4.531676000	1.415662000
6	-4.024483000	-2.824702000	-2.267143000
1	-1.704832000	-2.530248000	0.839289000
6	0.833590000	-0.409465000	-0.033182000
1	-7.164095000	-3.014389000	-1.023889000
6	-3.675115000	-3.470121000	1.463008000
8	-0.362149000	-0.678263000	0.363748000
6	-6.184139000	-2.746149000	-1.392413000
7	1.140682000	0.765339000	-0.657778000
6	-2.733872000	-2.427639000	1.157561000
26	-4.480846000	-2.354811000	-0.136036000
1	-1.710630000	0.630689000	-1.471458000
6	0.217839000	1.729743000	-1.108440000
6	-4.389703000	-1.444948000	-2.149372000
6	-1.157343000	1.555417000	-1.514771000
6	-4.921575000	-2.846314000	1.855031000
6	-5.717522000	-1.388023000	-1.592242000
1	-5.826537000	-3.353422000	2.159193000
1	-3.788775000	-0.587142000	-2.414678000
6	-3.353500000	-1.149426000	1.470057000
6	0.575254000	3.112982000	-1.317983000
1	1.552587000	3.526662000	-1.116427000
1	-1.703556000	-0.026642000	1.032232000
6	-1.638372000	2.827813000	-2.001004000
6	-4.747236000	-1.415974000	1.793872000
7	-2.697110000	0.040492000	1.366461000
1	-2.628737000	3.022192000	-2.387804000
6	-0.566389000	3.785280000	-1.879638000
8	-7.614676000	-0.215833000	-0.686232000
6	-6.502776000	-0.179767000	-1.243215000
1	-0.446038000	1.541895000	2.398522000
26	-1.075260000	3.004427000	0.018481000
1	-0.610200000	4.829765000	-2.153727000
1	-5.484714000	-0.658706000	2.009045000
6	-3.299702000	1.316115000	1.481203000
6	-0.974777000	2.404971000	2.021044000
6	-2.360157000	2.439114000	1.568113000
1	0.546458000	4.047327000	2.180245000
8	-4.553010000	1.443765000	1.495154000
6	-0.455783000	3.738909000	1.919056000
6	-2.672431000	3.801512000	1.192019000
6	-1.496648000	4.595095000	1.397797000
1	-3.628690000	4.139723000	0.820701000

1	-1.401953000	5.652371000	1.194881000
1	2.132348000	1.073093000	-0.694242000
6	1.914943000	-1.384235000	0.161004000
6	3.101718000	-1.574474000	-0.662224000
6	3.830902000	-2.689006000	-0.128287000
6	3.117261000	-3.185908000	1.025328000
6	1.933430000	-2.392447000	1.203318000
26	3.649676000	-1.138093000	1.314878000
6	3.831507000	0.861681000	1.997765000
6	4.987098000	0.506423000	1.207375000
6	5.631723000	-0.627389000	1.829237000
6	4.887652000	-0.958323000	3.016947000
6	3.775503000	-0.044624000	3.120907000
7	5.490895000	1.121889000	0.041408000
1	3.148211000	1.666249000	1.777924000
1	6.498214000	-1.142364000	1.438237000
1	5.118165000	-1.765239000	3.697968000
1	3.034987000	-0.029372000	3.908520000
1	6.417276000	0.792455000	-0.265817000
6	4.776034000	1.850897000	-0.859010000
8	3.527994000	2.091673000	-0.719082000
1	3.398914000	-1.004255000	-1.530347000
1	4.784951000	-3.034747000	-0.501126000
1	3.433040000	-4.004800000	1.656608000
1	1.185024000	-2.506584000	1.974672000
6	5.539382000	2.324290000	-2.078210000
1	4.995991000	3.145050000	-2.551987000
1	6.556576000	2.642128000	-1.826347000
1	5.623147000	1.486225000	-2.782074000
8	-5.846494000	0.967751000	-1.602634000
6	-6.437778000	2.253119000	-1.160944000
1	-6.210553000	2.382965000	-0.099113000
1	-5.944537000	3.012521000	-1.768760000
1	-7.517768000	2.246882000	-1.330217000
9	7.621071000	-0.199867000	-1.015648000
9	5.825407000	-0.907295000	-2.356180000
9	8.017725000	-1.635498000	-2.847353000
9	6.902537000	-2.440284000	-0.927034000
5	7.104144000	-1.329106000	-1.816950000

Cartesian coordinates of a model of [Fmoc-Fca₄-OMe]⁺ (OCH₂-fluorenyl replaced by Me)

1	-1.534159000	4.873125000	2.873903000
6	-1.961965000	4.014829000	2.375780000
1	-0.449521000	2.391546000	2.778586000
1	-0.044050000	5.802942000	-0.168581000
6	-1.380164000	2.693066000	2.319183000
1	1.270696000	3.420765000	0.016365000
6	3.504998000	0.580506000	0.381378000
1	-3.886374000	4.816216000	1.513051000
6	-0.358759000	4.865987000	-0.605478000
8	2.500562000	1.164652000	-0.142588000
6	-3.200008000	3.993711000	1.653443000
7	3.444306000	-0.685168000	0.898274000
6	0.337970000	3.611530000	-0.494696000
26	-1.597544000	3.435885000	0.343580000
1	0.627862000	0.060767000	1.423889000
6	2.265018000	-1.442638000	1.082299000
6	-2.243991000	1.849161000	1.539860000
6	0.932300000	-0.973057000	1.379834000
6	-1.551346000	4.650012000	-1.386085000
6	-3.381339000	2.661188000	1.122587000
1	-2.287048000	5.397119000	-1.647904000
1	-2.108220000	0.794629000	1.345997000
6	-0.420108000	2.619425000	-1.222745000
6	2.247351000	-2.886087000	1.098288000
1	3.104571000	-3.520650000	0.926371000
1	0.990406000	1.117504000	-1.052787000
6	0.095363000	-2.128019000	1.602241000
6	-1.595858000	3.258663000	-1.766765000
7	0.022313000	1.286643000	-1.369493000
1	-0.959208000	-2.104609000	1.840511000
6	0.909580000	-3.305928000	1.428762000
8	-5.705170000	2.696190000	0.504487000

6	-4.553141000	2.221133000	0.352750000
1	2.057154000	-0.532212000	-2.404893000
26	0.879165000	-2.172393000	-0.357788000
1	0.577442000	-4.330052000	1.523663000
1	-2.355487000	2.781765000	-2.365393000
6	-0.762651000	0.205447000	-1.647674000
6	1.319355000	-1.299871000	-2.223141000
1	-3.322133000	0.967047000	-0.862557000
7	-4.305842000	1.188079000	-0.587520000
6	-0.073216000	-1.080073000	-1.870719000
1	2.458472000	-3.206300000	-2.565208000
8	-2.042325000	0.274689000	-1.708112000
6	1.527463000	-2.718212000	-2.313889000
1	-7.237977000	1.273449000	-0.489262000
6	-0.708674000	-2.374302000	-1.751940000
6	0.279038000	-3.381342000	-2.016820000
6	-5.273187000	0.524930000	-1.284794000
6	-6.718637000	0.592030000	-1.144391000
1	-1.744076000	-2.531804000	-1.489245000
1	0.119806000	-4.450221000	-1.996945000
1	-7.550050000	-1.585625000	1.900266000
6	-5.537564000	-2.278580000	1.201830000
6	-6.973123000	-2.186650000	1.211658000
6	-4.980679000	-0.531166000	-2.242122000
1	-3.978079000	-0.814219000	-2.533113000
26	-6.218918000	-1.501451000	-0.758817000
6	-7.299897000	-0.299829000	-2.113330000
6	-5.147367000	-3.170097000	0.141301000
1	-4.128831000	-3.446415000	-0.091953000
1	-8.357455000	-0.409273000	-2.309795000
6	-6.225308000	-0.989316000	-2.798127000
6	-7.477524000	-3.033468000	0.166102000
6	-6.347907000	-3.644120000	-0.499000000
1	-6.333573000	-1.708647000	-3.597655000
1	-8.520603000	-3.204995000	-0.061156000
1	-6.394722000	-4.363090000	-1.304939000
1	4.324215000	-1.187790000	1.080034000
6	4.807112000	1.280329000	0.479899000
6	5.825653000	1.114094000	1.501061000
6	6.859970000	2.080096000	1.248184000
6	6.492566000	2.838139000	0.074528000
6	5.224676000	2.353214000	-0.392112000
26	6.650961000	0.768324000	-0.406800000
6	6.490492000	-1.108144000	-1.384876000
6	7.588451000	-1.128346000	-0.448020000
6	8.530479000	-0.100297000	-0.827265000
6	8.020563000	0.545311000	-2.009043000
6	6.762541000	-0.071099000	-2.348532000
7	7.822316000	-2.054385000	0.605582000
1	5.628070000	-1.755870000	-1.358283000
1	9.455462000	0.133839000	-0.317889000
1	8.495376000	1.359228000	-2.537731000
1	6.128599000	0.197395000	-3.181551000
1	8.791105000	-2.300698000	0.774808000
6	6.867820000	-2.647989000	1.392398000
8	5.637883000	-2.374555000	1.287339000
1	5.789736000	0.414112000	2.323491000
1	7.754951000	2.218624000	1.838232000
1	7.072814000	3.631496000	-0.375048000
1	4.666004000	2.712544000	-1.244055000
6	-4.587556000	-1.568384000	2.090043000
8	-3.347852000	-1.614975000	1.967323000
8	-5.242864000	-0.866922000	3.063626000
6	7.365718000	-3.665112000	2.403312000
1	6.954688000	-4.650485000	2.154594000
1	8.457505000	-3.740676000	2.441073000
1	6.990703000	-3.397786000	3.396868000
6	-4.427896000	-0.117597000	4.050105000
1	-3.897986000	0.695448000	3.547258000
1	-5.151028000	0.268750000	4.767814000
1	-3.713519000	-0.793664000	4.528566000

Cartesian coordinates of a model of [Fmoc-Fca₄-OMe]²⁺ (OCH₂-fluorenyl replaced by Me)

1	-1.393067000	4.761499000	3.001514000
6	-1.850576000	3.930584000	2.483895000
1	-0.360322000	2.271299000	2.787246000
1	-0.023512000	5.818337000	-0.063195000
6	-1.296436000	2.602634000	2.359703000
1	1.299509000	3.444127000	0.018255000
6	3.562694000	0.546486000	0.366011000
1	-3.785648000	4.798186000	1.718405000
6	-0.349040000	4.893660000	-0.517569000
8	2.539231000	1.020893000	-0.213754000
6	-3.111313000	3.958088000	1.803434000
7	3.538349000	-0.742766000	0.913863000
6	0.351135000	3.638949000	-0.461729000
26	-1.557676000	3.416506000	0.421237000
1	0.739115000	0.031903000	1.397648000
6	2.389960000	-1.477778000	1.124927000
6	-2.204397000	1.805064000	1.577687000
6	1.038126000	-1.003873000	1.354589000
6	-1.560579000	4.701005000	-1.273081000
6	-3.337273000	2.652682000	1.230057000
1	-2.300869000	5.457200000	-1.491547000
1	-2.100208000	0.757007000	1.333124000
6	-0.432144000	2.669499000	-1.195248000
6	2.343918000	-2.923422000	1.095394000
1	3.203363000	-3.559790000	0.934042000
1	0.979509000	1.155680000	-1.133695000
6	0.189615000	-2.151113000	1.575429000
6	-1.620196000	3.324507000	-1.694882000
7	-0.000098000	1.331896000	-1.390946000
1	-0.868543000	-2.122773000	1.807046000
6	1.000910000	-3.337111000	1.402917000
8	-5.690240000	2.737323000	0.753961000
6	-4.559781000	2.258931000	0.508722000
1	1.942691000	-0.546275000	-2.648075000
26	0.896567000	-2.209907000	-0.405065000
1	0.665526000	-4.359215000	1.510669000
1	-2.394062000	2.871247000	-2.293733000
6	-0.805009000	0.273833000	-1.670996000
6	1.201727000	-1.294835000	-2.403063000
1	-3.425237000	1.044796000	-0.808992000
7	-4.383091000	1.266782000	-0.489804000
6	-0.135617000	-1.037556000	-1.925092000
1	2.267495000	-3.223031000	-2.830767000
8	-2.078080000	0.332975000	-1.715501000
6	1.377800000	-2.714340000	-2.485539000
1	-7.303488000	1.409672000	-0.232628000
6	-0.795345000	-2.310215000	-1.743847000
6	0.142461000	-3.348617000	-2.075939000
6	-5.403462000	0.661636000	-1.174685000
6	-6.835448000	0.757868000	-0.953587000
1	-1.814230000	-2.429386000	-1.405718000
1	-0.051569000	-4.412132000	-2.070706000
1	-7.335170000	-1.518547000	2.076690000
6	-5.517876000	-2.367856000	1.073860000
6	-6.920581000	-2.118255000	1.278741000
6	-5.189559000	-0.332414000	-2.212330000
1	-4.217569000	-0.620279000	-2.587788000
26	-6.362644000	-1.368060000	-0.722005000
6	-7.490747000	-0.060253000	-1.940499000
6	-5.374676000	-3.217597000	-0.079820000
1	-4.437987000	-3.596124000	-0.463745000
1	-8.559960000	-0.133252000	-2.084066000
6	-6.474081000	-0.728001000	-2.725908000
6	-7.648206000	-2.821877000	0.256569000
6	-6.690826000	-3.510323000	-0.580503000
1	-6.645124000	-1.389450000	-3.563704000
1	-8.724448000	-2.864039000	0.161937000
1	-6.923258000	-4.159444000	-1.413284000
1	4.436349000	-1.265675000	1.000169000
6	4.817316000	1.284413000	0.496787000
6	5.842082000	1.101150000	1.518237000
6	6.854683000	2.090998000	1.293706000
6	6.481622000	2.872430000	0.137071000
6	5.226377000	2.386370000	-0.351003000
26	6.655921000	0.801073000	-0.394868000
6	6.535941000	-1.032994000	-1.454880000
6	7.601978000	-1.089116000	-0.483022000
6	8.552495000	-0.045166000	-0.790601000

6	8.079793000	0.645227000	-1.960973000
6	6.835628000	0.042268000	-2.366828000
7	7.806427000	-2.063893000	0.532727000
1	5.682948000	-1.693082000	-1.489155000
1	9.461578000	0.169883000	-0.245537000
1	8.571004000	1.479305000	-2.440995000
1	6.236540000	0.339061000	-3.215818000
1	8.773041000	-2.308158000	0.722750000
6	6.841289000	-2.721673000	1.241613000
8	5.603142000	-2.459208000	1.107527000
1	5.810090000	0.392630000	2.333598000
1	7.743537000	2.232652000	1.891844000
1	7.054641000	3.684188000	-0.287948000
1	4.672645000	2.763045000	-1.198776000
6	-4.397113000	-1.847407000	1.892754000
8	-3.185986000	-1.975537000	1.601044000
8	-4.858616000	-1.228493000	3.014599000
6	7.312317000	-3.797295000	2.198569000
1	6.969137000	-4.775982000	1.842113000
1	8.400725000	-3.832164000	2.307460000
1	6.860954000	-3.631334000	3.182135000
6	-3.889715000	-0.696655000	4.001931000
1	-3.353035000	0.152214000	3.570368000
1	-4.503476000	-0.380937000	4.844736000
1	-3.191901000	-1.485777000	4.296623000

Cartesian coordinates of a model of [Fmoc-Fca₄-OMe]³⁺ (OCH₂-fluorenyl replaced by Me)

1	2.367517000	5.018689000	-2.380343000
6	2.673735000	4.062969000	-1.977139000
1	1.582995000	2.585007000	-3.284388000
1	-0.070496000	5.259240000	0.273171000
6	2.259644000	2.765069000	-2.459754000
1	-1.279106000	3.026647000	-0.693504000
6	-4.105143000	0.527764000	-0.726206000
1	4.151098000	4.615665000	-0.354689000
6	0.157077000	4.240209000	0.555544000
8	-2.897282000	0.836162000	-0.453323000
6	3.610899000	3.856834000	-0.904508000
7	-4.415281000	-0.766979000	-1.165771000
6	-0.482910000	3.062915000	0.037899000
26	1.708453000	3.031110000	-0.340443000
1	-1.794602000	-0.420423000	-2.472147000
6	-3.509322000	-1.657135000	-1.684493000
6	2.932292000	1.761054000	-1.690139000
6	-2.220667000	-1.397392000	-2.304749000
6	1.135029000	3.826401000	1.535694000
6	3.751502000	2.430252000	-0.709833000
1	1.753032000	4.479873000	2.136223000
1	2.860492000	0.691323000	-1.825017000
6	0.075901000	1.917535000	0.711289000
6	-3.693709000	-3.093486000	-1.661057000
1	-4.558945000	-3.590144000	-1.242655000
1	-1.363948000	0.526785000	0.187445000
6	-1.699501000	-2.653233000	-2.788635000
6	1.109248000	2.384280000	1.611056000
7	-0.379667000	0.607499000	0.517128000
1	-0.809418000	-2.780498000	-3.389222000
6	-2.607190000	-3.701301000	-2.377942000
8	5.796347000	2.425581000	0.509590000
6	4.719995000	1.835520000	0.258040000
1	-2.081454000	-1.410675000	1.972736000
26	-1.751285000	-2.717210000	-0.685230000
1	-2.503278000	-4.756592000	-2.590696000
1	1.702740000	1.769075000	2.270300000
6	0.415009000	-0.516273000	0.598679000
6	-1.477179000	-2.127568000	1.432782000
1	3.441351000	0.225153000	0.651985000
7	4.367283000	0.622207000	0.846539000
6	-0.289736000	-1.829035000	0.661401000
1	-2.503139000	-4.075902000	1.858199000
8	1.679222000	-0.457551000	0.646250000
6	-1.699775000	-3.539789000	1.370636000
1	6.964750000	1.240079000	2.098955000

6	0.226948000	-3.078244000	0.142853000
6	-0.651895000	-4.130556000	0.571158000
6	5.197458000	-0.094697000	1.701952000
6	6.475275000	0.292947000	2.262888000
1	1.131297000	-3.189722000	-0.438701000
1	-0.535065000	-5.184975000	0.360537000
1	9.398999000	-0.684088000	-0.130457000
6	7.390213000	-1.284553000	-0.940945000
6	8.618341000	-1.429808000	-0.195288000
6	4.921232000	-1.450838000	2.129949000
1	4.032544000	-2.015327000	1.882758000
26	6.818631000	-1.546889000	1.106202000
6	6.931212000	-0.782283000	3.103992000
6	6.619344000	-2.498090000	-0.781934000
1	5.677038000	-2.708744000	-1.266608000
1	7.826468000	-0.763789000	3.710589000
6	5.971587000	-1.858330000	3.031084000
6	8.605819000	-2.719086000	0.427972000
6	7.373101000	-3.380634000	0.074616000
1	6.010728000	-2.789129000	3.579332000
1	9.386820000	-3.125709000	1.057125000
1	7.090798000	-4.384142000	0.362483000
1	-5.374483000	-1.150156000	-0.973239000
6	-5.216304000	1.455716000	-0.606018000
6	-6.477362000	1.401875000	-1.344750000
6	-7.244794000	2.549803000	-0.967606000
6	-6.496213000	3.301502000	0.013413000
6	-5.248050000	2.638680000	0.236006000
26	-6.838626000	1.297963000	0.719879000
6	-6.760698000	-0.488110000	1.866509000
6	-8.013508000	-0.409470000	1.153737000
6	-8.702924000	0.786711000	1.579913000
6	-7.881751000	1.437683000	2.564830000
6	-6.682461000	0.657780000	2.736914000
7	-8.584869000	-1.379149000	0.284097000
1	-6.034457000	-1.280764000	1.773845000
1	-9.669413000	1.124185000	1.230692000
1	-8.124398000	2.358030000	3.076365000
1	-5.874814000	0.882770000	3.418627000
1	-9.593609000	-1.483136000	0.339294000
6	-7.916278000	-2.204594000	-0.572335000
8	-6.654544000	-2.123454000	-0.743284000
1	-6.747494000	0.671879000	-2.094127000
1	-8.218869000	2.812962000	-1.354696000
1	-6.828149000	4.208085000	0.499248000
1	-4.464762000	2.951818000	0.911081000
6	6.942914000	-0.085729000	-1.695879000
8	5.749992000	0.125010000	-2.010717000
8	7.984258000	0.737352000	-1.968416000
6	-8.738328000	-3.236503000	-1.312970000
1	-8.449480000	-4.240318000	-0.978683000
1	-9.815505000	-3.120830000	-1.160419000
1	-8.523006000	-3.174859000	-2.384760000
6	7.736184000	2.012930000	-2.688444000
1	7.246940000	2.712342000	-2.004114000
1	8.727283000	2.366540000	-2.969424000
1	7.116743000	1.826419000	-3.569572000

Cartesian coordinates of a model of [Fmoc-Fca₄-OMe]⁴⁺ (OCH₂-fluorenyl replaced by Me)

1	-3.426245000	-2.388102000	2.415784000
6	-4.168540000	-2.300037000	1.633588000
1	-3.721347000	-4.063840000	0.307896000
1	-4.893568000	1.060065000	-1.784144000
6	-4.325024000	-3.190641000	0.516867000
1	-3.134323000	1.633676000	0.167354000
6	7.806804000	0.320731000	0.335420000
1	-5.335984000	-0.464405000	2.233900000
6	-3.990295000	0.502930000	-1.577237000
8	7.424191000	1.504525000	0.454558000
6	-5.173660000	-1.280755000	1.542616000
7	6.947619000	-0.670692000	-0.208964000
6	-3.058543000	0.799443000	-0.518399000
26	-3.973025000	-1.164119000	-0.278620000

1	5.000311000	-2.532777000	-1.210790000
6	5.723355000	-0.428013000	-0.804474000
6	-5.452925000	-2.742258000	-0.262642000
6	4.824504000	-1.466192000	-1.270687000
6	-3.501245000	-0.659080000	-2.282820000
6	-5.992856000	-1.561309000	0.380614000
1	-3.953072000	-1.122004000	-3.149538000
1	-5.829117000	-3.220844000	-1.157844000
6	-1.941978000	-0.114517000	-0.635813000
6	5.085661000	0.848713000	-1.066984000
1	5.492354000	1.811205000	-0.797782000
1	-0.727199000	0.738703000	0.798266000
6	3.736529000	-0.836943000	-1.971710000
6	-2.262990000	-1.074546000	-1.669147000
7	-0.779367000	-0.024000000	0.128488000
1	2.951088000	-1.356714000	-2.502926000
6	3.896618000	0.593590000	-1.843211000
8	-7.108007000	0.537134000	0.017376000
6	-7.160773000	-0.714240000	-0.029714000
1	2.242943000	-2.548824000	1.433981000
26	3.576744000	-0.262129000	0.062994000
1	3.266786000	1.353152000	-2.285511000
1	-1.639508000	-1.904584000	-1.963467000
6	0.327839000	-0.885939000	0.032720000
6	2.377621000	-1.476275000	1.484166000
1	-8.286298000	-2.425092000	-0.346458000
7	-8.295228000	-1.412754000	-0.434767000
6	1.518588000	-0.503479000	0.849503000
1	4.156389000	-1.224935000	2.827015000
8	0.300337000	-1.925524000	-0.662025000
6	3.393068000	-0.771371000	2.209166000
1	-9.069641000	1.377903000	-1.013464000
6	2.041063000	0.811956000	1.153947000
6	3.199846000	0.640672000	1.999160000
6	-9.461923000	-0.839272000	-0.965141000
6	-9.729271000	0.553936000	-1.236238000
1	1.638852000	1.763458000	0.829917000
1	3.787208000	1.438532000	2.432950000
1	-14.293495000	0.270084000	0.375618000
6	-12.474396000	1.357801000	1.127884000
6	-13.360559000	0.236115000	0.921767000
6	-10.615613000	-1.607913000	-1.370388000
1	-10.727027000	-2.682494000	-1.299489000
26	-11.377600000	-0.113457000	0.045958000
6	-11.005270000	0.626320000	-1.907952000
6	-11.355057000	0.908242000	1.929791000
1	-10.553231000	1.544265000	2.278788000
1	-11.455241000	1.530131000	-2.295178000
6	-11.550775000	-0.706864000	-1.994735000
6	-12.784356000	-0.902492000	1.581720000
6	-11.554747000	-0.488371000	2.208631000
1	-12.478978000	-0.992371000	-2.469969000
1	-13.212704000	-1.895866000	1.616054000
1	-10.913908000	-1.114636000	2.814637000
1	7.253747000	-1.638283000	-0.150520000
6	9.131348000	-0.163324000	0.792347000
6	9.909161000	-1.292436000	0.324336000
6	11.100059000	-1.373102000	1.134739000
6	11.060744000	-0.296867000	2.092400000
6	9.869410000	0.463246000	1.866013000
26	11.117289000	0.486598000	0.016976000
6	12.709449000	0.412491000	-1.458430000
6	13.157241000	1.434642000	-0.522850000
6	12.080918000	2.404946000	-0.403801000
6	11.077660000	2.087858000	-1.383153000
6	11.467404000	0.857005000	-2.034916000
7	14.334324000	1.480291000	0.177431000
1	13.272775000	-0.468392000	-1.724819000
1	12.090485000	3.283016000	0.229242000
1	10.204454000	2.686801000	-1.601682000
1	10.947675000	0.366045000	-2.846120000
1	14.558287000	2.337594000	0.677672000
8	15.014067000	-0.691033000	-0.252791000
1	9.657992000	-1.975351000	-0.477630000
1	11.869483000	-2.129138000	1.054737000
1	11.795775000	-0.105312000	2.862478000
1	9.541322000	1.334069000	2.418004000
6	-12.637956000	2.759194000	0.644412000

8	-11.721860000	3.598391000	0.691548000
8	-13.893313000	2.971797000	0.166404000
6	-14.258015000	4.351611000	-0.266278000
1	-13.598927000	4.669627000	-1.078733000
1	-15.292393000	4.270754000	-0.596948000
1	-14.164304000	5.031603000	0.584228000
6	15.304915000	0.416747000	0.228392000
6	16.616522000	0.780138000	0.874912000
1	17.231667000	1.359699000	0.172555000
1	16.485395000	1.382299000	1.782283000
1	17.160812000	-0.132689000	1.123455000

Cartesian coordinates of a model of [Fmoc-Fca₅-OMe]⁺ (OCH₂-fluorenyl replaced by Me)

1	-4.441922000	4.072378000	3.835479000
6	-4.679827000	3.249762000	3.176294000
1	-2.792577000	2.016374000	3.208930000
1	-3.452493000	5.935472000	1.019273000
6	-3.797484000	2.156931000	2.836593000
1	-1.573727000	3.988252000	0.676464000
6	1.322527000	1.856162000	0.341626000
1	-6.795036000	3.693017000	2.528492000
6	-3.554307000	5.053262000	0.403561000
8	0.145089000	2.241756000	0.035554000
6	-5.921317000	3.058939000	2.485308000
7	1.625949000	0.546299000	0.600956000
6	-2.560552000	4.025655000	0.238134000
26	-4.327209000	3.195390000	1.060575000
1	-1.238556000	0.449610000	1.354392000
6	0.688590000	-0.505152000	0.698901000
6	-4.479311000	1.292906000	1.912033000
6	-0.693129000	-0.449828000	1.116037000
6	-4.708913000	4.692425000	-0.380696000
6	-5.806614000	1.856176000	1.691274000
1	-5.624775000	5.259847000	-0.466533000
1	-4.103573000	0.366693000	1.500580000
6	-3.097474000	3.032903000	-0.664544000
6	1.027824000	-1.885888000	0.447673000
1	2.001387000	-2.235172000	0.135825000
1	-1.347337000	1.945919000	-0.832296000
6	-1.201072000	-1.801490000	1.144858000
6	-4.432092000	3.438577000	-1.040128000
7	-2.347545000	1.916153000	-1.093129000
1	-2.208708000	-2.092355000	1.409304000
6	-0.136737000	-2.684244000	0.733467000
8	-8.104180000	1.428753000	1.121118000
6	-6.882800000	1.298233000	0.861124000
1	-0.013918000	0.911412000	-2.551564000
26	-0.583070000	-1.309034000	-0.809657000
1	-0.199612000	-3.759680000	0.645662000
1	-5.089692000	2.909148000	-1.710858000
6	-2.857210000	0.744741000	-1.572178000
6	-0.519164000	-0.041317000	-2.491680000
1	-5.461809000	0.658952000	-0.602572000
7	-6.451303000	0.570030000	-0.277333000
6	-1.890908000	-0.256352000	-2.062115000
1	1.030817000	-1.495527000	-3.219048000
8	-4.116186000	0.496228000	-1.594673000
6	0.029251000	-1.318451000	-2.853540000
1	-9.309563000	-0.084503000	-0.148525000
6	-2.171540000	-1.671766000	-2.169752000
6	-0.986702000	-2.324832000	-2.649014000
6	-7.271304000	-0.152324000	-1.093645000
6	-8.681394000	-0.469191000	-0.936223000
1	-3.109818000	-2.137246000	-1.907251000
1	-0.871287000	-3.385008000	-2.825088000
1	-8.780735000	-3.347128000	1.590110000
6	-6.713070000	-3.398735000	0.728831000
6	-8.129998000	-3.642345000	0.779211000
6	-6.790361000	-0.886640000	-2.254187000
1	-5.766135000	-0.853059000	-2.600404000
26	-7.681428000	-2.411423000	-1.007878000
6	-9.087918000	-1.256120000	-2.071096000
6	-6.204114000	-3.937568000	-0.504556000

1	-5.166756000	-3.916208000	-0.807697000
1	-10.098766000	-1.576244000	-2.282634000
6	-7.920046000	-1.507570000	-2.891054000
6	-8.500306000	-4.347648000	-0.417181000
6	-7.307930000	-4.531484000	-1.214651000
1	-7.899034000	-2.051068000	-3.825225000
1	-9.491724000	-4.703616000	-0.660765000
1	-7.245292000	-5.058273000	-2.156544000
1	2.613923000	0.250900000	0.591827000
6	2.426474000	2.834398000	0.445973000
6	3.619267000	2.744777000	1.270118000
6	4.367056000	3.958762000	1.087860000
6	3.650594000	4.796278000	0.153425000
6	2.450968000	4.109913000	-0.233257000
26	4.149149000	2.927552000	-0.754646000
6	4.231511000	1.200183000	-1.973338000
6	5.462363000	1.336061000	-1.229148000
6	6.069590000	2.597281000	-1.586060000
6	5.221043000	3.236114000	-2.557810000
6	4.086972000	2.377447000	-2.795017000
7	6.071559000	0.418711000	-0.340350000
1	3.551820000	0.365596000	-1.910885000
1	7.006228000	2.969628000	-1.196819000
1	5.401456000	4.195994000	-3.020228000
1	3.269053000	2.578015000	-3.472427000
1	7.100597000	0.450194000	-0.309728000
8	4.147235000	-0.661908000	0.372530000
1	3.879691000	1.925945000	1.925415000
1	5.304486000	4.201349000	1.568074000
1	3.964345000	5.770353000	-0.194345000
1	1.689803000	4.464426000	-0.912907000
6	-5.888206000	-2.690015000	1.736061000
8	-4.677983000	-2.429565000	1.590799000
8	-6.620983000	-2.369176000	2.845639000
6	-5.928699000	-1.675280000	3.958111000
1	-5.593908000	-0.689118000	3.626261000
1	-6.681536000	-1.592008000	4.741460000
1	-5.073503000	-2.271436000	4.289395000
6	5.412365000	-0.505955000	0.417992000
6	6.238808000	-1.321637000	1.343412000
6	7.422506000	-0.904420000	2.072917000
6	5.925807000	-2.672289000	1.743526000
6	6.912845000	-3.095582000	2.697016000
6	7.830734000	-2.001036000	2.908855000
26	7.867826000	-2.567095000	0.863944000
6	8.766254000	-4.285557000	0.007005000
6	7.893155000	-3.656630000	-0.952600000
6	8.363515000	-2.313903000	-1.184207000
6	9.532106000	-2.116829000	-0.360768000
6	9.777722000	-3.332005000	0.382859000
7	10.405357000	-0.993121000	-0.337543000
6	10.044376000	0.326840000	-0.447444000
8	8.840217000	0.701506000	-0.521606000
1	11.393642000	-1.201494000	-0.249780000
6	11.182480000	1.331816000	-0.480137000
1	11.185609000	1.837726000	-1.452682000
1	12.166287000	0.879108000	-0.317856000
1	11.010190000	2.096417000	0.284681000
1	7.894662000	0.065189000	2.012674000
1	8.676285000	-2.003155000	3.582296000
1	6.960306000	-4.064576000	3.173380000
1	5.091135000	-3.249903000	1.374124000
1	8.675175000	-5.291882000	0.389681000
1	7.029710000	-4.109380000	-1.418743000
1	7.926296000	-1.583349000	-1.847607000
1	10.580896000	-3.492678000	1.089151000

Cartesian coordinates of a model of [Fmoc-Fca₅-OMe]²⁺ (OCH₂-fluorenyl replaced by Me)

1	-4.453684000	3.963506000	3.964588000
6	-4.717579000	3.166029000	3.284746000
1	-2.872511000	1.871546000	3.281273000
1	-3.460790000	5.882907000	1.205337000
6	-3.871734000	2.055571000	2.912197000

1	-1.620115000	3.919248000	0.793991000
6	1.400440000	1.798452000	0.184034000
1	-6.822236000	3.687776000	2.663714000
6	-3.580242000	5.022664000	0.562394000
8	0.238030000	2.222293000	-0.098136000
6	-5.968346000	3.028951000	2.598128000
7	1.701797000	0.491691000	0.422325000
6	-2.606719000	3.981684000	0.358120000
26	-4.376332000	3.155179000	1.167772000
1	-1.122472000	0.432672000	1.337149000
6	0.743131000	-0.550151000	0.536955000
6	-4.587225000	1.234805000	1.972641000
6	-0.606105000	-0.470517000	1.051382000
6	-4.745112000	4.707316000	-0.224898000
6	-5.895996000	1.844086000	1.775585000
1	-5.651295000	5.293146000	-0.284444000
1	-4.246614000	0.305819000	1.536979000
6	-3.169365000	3.027695000	-0.570820000
6	1.045100000	-1.934141000	0.257594000
1	1.986147000	-2.307573000	-0.120204000
1	-1.435896000	1.935187000	-0.867129000
6	-1.130141000	-1.812773000	1.102345000
6	-4.497153000	3.471124000	-0.925723000
7	-2.444745000	1.909038000	-1.048730000
1	-2.125727000	-2.090650000	1.422079000
6	-0.112483000	-2.711124000	0.614657000
8	-8.213965000	1.479848000	1.253616000
6	-7.005447000	1.328919000	0.955662000
1	-0.235092000	0.886995000	-2.744780000
26	-0.628500000	-1.306280000	-0.888599000
1	-0.204508000	-3.783625000	0.520419000
1	-5.170724000	2.976179000	-1.606981000
6	-2.986159000	0.746027000	-1.518339000
6	-0.720133000	-0.067245000	-2.596605000
1	-5.634141000	0.684426000	-0.536196000
7	-6.618244000	0.620662000	-0.207893000
6	-2.045723000	-0.269848000	-2.041285000
1	0.752938000	-1.543695000	-3.441776000
8	-4.242020000	0.514612000	-1.509680000
6	-0.204715000	-1.354371000	-2.977728000
1	-9.491009000	0.044449000	-0.036074000
6	-2.334766000	-1.684505000	-2.090673000
6	-1.198433000	-2.352214000	-2.658799000
6	-7.477281000	-0.055602000	-1.029877000
6	-8.891696000	-0.331759000	-0.850116000
1	-3.242579000	-2.139838000	-1.723850000
1	-1.100445000	-3.416611000	-2.818538000
1	-8.931641000	-3.272672000	1.624270000
6	-6.917790000	-3.373275000	0.645125000
6	-8.338386000	-3.564609000	0.769154000
6	-7.045552000	-0.761189000	-2.225593000
1	-6.031349000	-0.749891000	-2.600474000
26	-7.939754000	-2.299427000	-1.006121000
6	-9.347217000	-1.072758000	-1.996947000
6	-6.500556000	-3.895094000	-0.629908000
1	-5.482341000	-3.908522000	-0.991990000
1	-10.371817000	-1.357486000	-2.192429000
6	-8.208297000	-1.330733000	-2.853620000
6	-8.802989000	-4.215837000	-0.425275000
6	-7.664263000	-4.424805000	-1.292295000
1	-8.226746000	-1.843227000	-3.805250000
1	-9.819721000	-4.526756000	-0.621669000
1	-7.675892000	-4.926574000	-2.249754000
1	2.682766000	0.187198000	0.438255000
6	2.510117000	2.797272000	0.306743000
6	3.616931000	2.787346000	1.231368000
6	4.347333000	4.011387000	1.065084000
6	3.688075000	4.793442000	0.040511000
6	2.546774000	4.046156000	-0.416950000
26	4.382127000	2.953578000	-0.832731000
6	4.621831000	1.200265000	-2.061363000
6	5.835926000	1.303865000	-1.277579000
6	6.424796000	2.597787000	-1.549745000
6	5.623835000	3.256658000	-2.546510000
6	4.511823000	2.390007000	-2.867997000
7	6.359396000	0.407866000	-0.360907000
1	3.950683000	0.356541000	-2.058976000
1	7.340303000	2.963185000	-1.104907000

1	5.834802000	4.217781000	-2.994202000
1	3.746248000	2.582348000	-3.606766000
1	7.395498000	0.436518000	-0.233461000
8	4.348852000	-0.614349000	0.157647000
1	3.849952000	1.996454000	1.931839000
1	5.218084000	4.311404000	1.632112000
1	3.973322000	5.784241000	-0.284928000
1	1.813776000	4.357794000	-1.147738000
6	-6.012363000	-2.733425000	1.629632000
8	-4.807095000	-2.484103000	1.418729000
8	-6.664647000	-2.467003000	2.799705000
6	-5.896707000	-1.866408000	3.915671000
1	-5.570408000	-0.860237000	3.639798000
1	-6.599442000	-1.836030000	4.747727000
1	-5.032684000	-2.495241000	4.149291000
6	5.603590000	-0.533170000	0.332899000
6	6.330733000	-1.368674000	1.297892000
6	7.479578000	-0.978722000	2.107124000
6	5.980032000	-2.726978000	1.649689000
6	6.905077000	-3.176282000	2.647799000
6	7.816584000	-2.096206000	2.942431000
26	7.972643000	-2.596348000	0.876475000
6	8.945657000	-4.298450000	0.060156000
6	8.126006000	-3.671875000	-0.946096000
6	8.592739000	-2.321458000	-1.134569000
6	9.702880000	-2.116318000	-0.235012000
6	9.917354000	-3.337316000	0.509037000
7	10.567367000	-0.986668000	-0.154118000
6	10.222461000	0.332573000	-0.251405000
8	9.018178000	0.723484000	-0.360138000
1	11.553272000	-1.198357000	-0.038746000
6	11.361926000	1.332216000	-0.228668000
1	11.419677000	1.836148000	-1.200806000
1	12.333820000	0.875601000	-0.017607000
1	11.157984000	2.098803000	0.526042000
1	7.960861000	-0.011749000	2.109150000
1	8.615584000	-2.123085000	3.669599000
1	6.918577000	-4.156656000	3.102216000
1	5.169197000	-3.295224000	1.217573000
1	8.845511000	-5.310385000	0.425286000
1	7.307415000	-4.136141000	-1.477296000
1	8.200682000	-1.596469000	-1.832027000
1	10.677981000	-3.498611000	1.260781000

Cartesian coordinates of a model of [Fmoc-Fca₅-OMe]³⁺ (OCH₂-fluorenyl replaced by Me)

1	-4.172425000	4.066448000	3.902286000
6	-4.490663000	3.259632000	3.257565000
1	-2.658739000	1.957757000	3.140537000
1	-3.374497000	5.944257000	1.061310000
6	-3.681287000	2.139053000	2.839490000
1	-1.584387000	3.968665000	0.545653000
6	1.331456000	1.568448000	-0.048030000
1	-6.633003000	3.784823000	2.793120000
6	-3.547956000	5.076472000	0.441366000
8	0.178066000	1.851072000	-0.485523000
6	-5.790657000	3.118972000	2.671882000
7	1.682579000	0.232759000	0.202855000
6	-2.600230000	4.026610000	0.181094000
26	-4.307689000	3.208917000	1.120626000
1	-1.101003000	0.180428000	1.129908000
6	0.750722000	-0.793671000	0.291780000
6	-4.473691000	1.308137000	1.970499000
6	-0.614667000	-0.714362000	0.772952000
6	-4.769107000	4.764726000	-0.256198000
6	-5.790317000	1.921558000	1.866317000
1	-5.669489000	5.362480000	-0.258734000
1	-4.174620000	0.372086000	1.518609000
6	-3.241614000	3.065753000	-0.688459000
6	0.985253000	-2.155076000	-0.126819000
1	1.909321000	-2.525063000	-0.549636000
1	-1.542940000	1.951916000	-1.113625000
6	-1.181644000	-2.041299000	0.746060000
6	-4.589054000	3.518790000	-0.955936000

7	-2.563544000	1.935490000	-1.214897000
1	-2.180390000	-2.310040000	1.070574000
6	-0.190863000	-2.929341000	0.178253000
8	-8.142539000	1.523384000	1.614138000
6	-6.978288000	1.384301000	1.178175000
1	-0.483450000	0.880115000	-3.077176000
26	-0.786955000	-1.445054000	-1.235557000
1	-0.302402000	-3.994207000	0.027825000
1	-5.314095000	3.029536000	-1.586721000
6	-3.158222000	0.797049000	-1.657333000
6	-1.009559000	-0.056370000	-2.954138000
1	-5.789084000	0.738167000	-0.451592000
7	-6.722654000	0.666236000	-0.018021000
6	-2.271004000	-0.234142000	-2.277321000
1	0.334022000	-1.532475000	-3.980561000
8	-4.406694000	0.560099000	-1.576370000
6	-0.567382000	-1.339709000	-3.414863000
1	-9.528916000	0.026339000	0.548298000
6	-2.618206000	-1.635405000	-2.346557000
6	-1.562015000	-2.322380000	-3.041648000
6	-7.675073000	-0.022711000	-0.724777000
6	-9.043006000	-0.329200000	-0.346827000
1	-3.520432000	-2.062563000	-1.933236000
1	-1.535991000	-3.375655000	-3.284419000
1	-8.536746000	-3.252572000	2.100874000
6	-6.763049000	-3.388842000	0.734101000
6	-8.135011000	-3.545846000	1.141173000
6	-7.408651000	-0.700617000	-1.981466000
1	-6.467205000	-0.658014000	-2.511164000
26	-8.080998000	-2.275967000	-0.669355000
6	-9.645253000	-1.066050000	-1.426102000
6	-6.626595000	-3.911703000	-0.601154000
1	-5.705965000	-3.951165000	-1.165492000
1	-10.681860000	-1.369987000	-1.475378000
6	-8.639202000	-1.287998000	-2.443334000
6	-8.846785000	-4.176293000	0.062348000
6	-7.910414000	-4.411625000	-1.014499000
1	-8.788887000	-1.783688000	-3.392374000
1	-9.888487000	-4.465881000	0.075932000
1	-8.127385000	-4.909071000	-1.949662000
1	2.679831000	-0.033267000	0.185635000
6	2.341580000	2.590716000	0.227492000
6	3.425680000	2.523053000	1.199298000
6	4.083676000	3.798051000	1.198655000
6	3.433417000	4.647320000	0.227879000
6	2.357170000	3.912758000	-0.364698000
26	4.190263000	2.877392000	-0.722438000
6	4.586829000	1.317626000	-2.096472000
6	5.684537000	1.462767000	-1.165939000
6	6.225157000	2.795964000	-1.303308000
6	5.466252000	3.470827000	-2.320298000
6	4.457663000	2.564513000	-2.807083000
7	6.262419000	0.478956000	-0.317202000
1	3.993730000	0.428386000	-2.241073000
1	7.057892000	3.202103000	-0.746789000
1	5.621424000	4.487430000	-2.651868000
1	3.734207000	2.780265000	-3.580268000
1	7.274703000	0.571844000	-0.163814000
8	4.353927000	-0.792871000	0.076419000
1	3.645706000	1.688517000	1.849606000
1	4.916592000	4.081982000	1.826063000
1	3.713066000	5.663607000	-0.010903000
1	1.671854000	4.267819000	-1.120732000
6	-5.665696000	-2.803035000	1.539327000
8	-4.508014000	-2.579834000	1.113154000
8	-6.076573000	-2.561999000	2.814805000
6	-5.111757000	-2.043488000	3.811399000
1	-4.830520000	-1.019133000	3.553535000
1	-5.653684000	-2.070243000	4.756049000
1	-4.230705000	-2.691090000	3.845779000
6	5.595636000	-0.561442000	0.242743000
6	6.381097000	-1.463596000	1.150640000
6	7.334223000	-1.074918000	2.161349000
6	6.172857000	-2.888029000	1.266158000
6	7.004204000	-3.377501000	2.336957000
6	7.720062000	-2.249916000	2.890167000
26	8.262965000	-2.559328000	0.802466000
6	9.536971000	-4.071396000	-0.032068000

6	8.774159000	-3.420995000	-1.073530000
6	9.152957000	-2.030943000	-1.105847000
6	10.181483000	-1.831718000	-0.111991000
6	10.388643000	-3.083265000	0.576461000
7	10.869693000	-0.642892000	0.167735000
6	10.303501000	0.630820000	0.107036000
8	9.066140000	0.763810000	-0.079711000
1	11.841825000	-0.721751000	0.453327000
6	11.246885000	1.795287000	0.280685000
1	11.436468000	2.251956000	-0.699808000
1	12.211118000	1.510323000	0.712746000
1	10.780518000	2.559114000	0.909313000
1	7.694591000	-0.070361000	2.337203000
1	8.403082000	-2.279280000	3.728680000
1	7.051030000	-4.397325000	2.693688000
1	5.482812000	-3.466516000	0.668347000
1	9.502710000	-5.120419000	0.228118000
1	8.075689000	-3.899425000	-1.745969000
1	8.775683000	-1.277057000	-1.780683000
1	11.087377000	-3.256151000	1.385117000

Cartesian coordinates of a model of [Fmoc-Fca₅-OMe]⁴⁺ (OCH₂-fluorenyl replaced by Me)

1	-5.457385000	4.485042000	2.992990000
6	-5.605106000	3.554807000	2.461109000
1	-4.321782000	2.100078000	3.609336000
1	-3.092085000	5.467245000	0.489022000
6	-5.003066000	2.282919000	2.789065000
1	-1.533182000	3.360413000	1.181426000
6	1.897405000	1.243618000	0.518967000
1	-7.124522000	4.083749000	0.868823000
6	-3.140194000	4.474813000	0.061436000
8	0.649238000	1.341214000	0.299183000
6	-6.480499000	3.351521000	1.337017000
7	2.445898000	-0.003463000	0.860084000
6	-2.312216000	3.359740000	0.430877000
26	-4.470525000	2.906865000	0.737491000
1	-0.101811000	-0.169620000	2.316014000
6	1.688088000	-1.077057000	1.286933000
6	-5.500654000	1.298328000	1.874935000
6	0.423694000	-1.056884000	1.998997000
6	-4.027140000	4.045027000	-0.994786000
6	-6.398350000	1.957034000	0.958940000
1	-4.745247000	4.663410000	-1.515973000
1	-5.263458000	0.244205000	1.879394000
6	-2.663794000	2.244586000	-0.409417000
6	2.032411000	-2.461573000	1.056796000
1	2.913660000	-2.800880000	0.529490000
1	-0.975520000	1.052809000	-0.177531000
6	0.070121000	-2.418254000	2.317703000
6	-3.754909000	2.653356000	-1.267908000
7	-1.985572000	1.014162000	-0.407083000
1	-0.766106000	-2.729056000	2.928747000
6	1.059756000	-3.287267000	1.722535000
8	-8.373152000	1.883474000	-0.362492000
6	-7.262698000	1.364591000	-0.103769000
1	-0.095854000	-0.463417000	-2.217073000
26	0.005819000	-2.190793000	0.221017000
1	1.083493000	-4.366583000	1.787278000
1	-4.230358000	2.045590000	-2.023392000
6	-2.594110000	-0.205779000	-0.612088000
6	-0.531379000	-1.342787000	-1.761371000
1	-5.830085000	-0.081507000	-0.581641000
7	-6.787499000	0.231350000	-0.762481000
6	-1.688721000	-1.361503000	-0.896253000
1	0.758730000	-3.008333000	-2.532584000
8	-3.849424000	-0.357125000	-0.601964000
6	-0.077038000	-2.691131000	-1.923385000
1	-9.381254000	0.735015000	-2.069082000
6	-1.953759000	-2.738277000	-0.540769000
6	-0.952174000	-3.557931000	-1.168214000
6	-7.542343000	-0.501442000	-1.677328000
6	-8.826177000	-0.169973000	-2.259493000
1	-2.782177000	-3.082688000	0.062530000

1	-0.886987000	-4.636309000	-1.115901000
1	-11.758981000	-1.461588000	-0.006477000
6	-9.739683000	-1.969539000	0.841207000
6	-10.929918000	-2.154480000	0.045458000
6	-7.167056000	-1.815043000	-2.157306000
1	-6.253890000	-2.338311000	-1.908719000
26	-9.082798000	-2.081517000	-1.195008000
6	-9.189033000	-1.231864000	-3.160421000
6	-8.882764000	-3.118774000	0.646750000
1	-7.946594000	-3.294940000	1.156613000
1	-10.066738000	-1.241856000	-3.792405000
6	-8.164466000	-2.246676000	-3.106808000
6	-10.808520000	-3.402833000	-0.645881000
6	-9.546356000	-4.000455000	-0.282287000
1	-8.129014000	-3.152151000	-3.696210000
1	-11.539202000	-3.824865000	-1.323637000
1	-9.188019000	-4.966418000	-0.611284000
1	3.453272000	-0.178700000	0.682337000
6	2.811006000	2.374950000	0.439530000
6	4.045874000	2.556165000	1.198883000
6	4.556181000	3.857693000	0.883272000
6	3.673628000	4.476263000	-0.078397000
6	2.596218000	3.574455000	-0.348433000
26	4.441200000	2.624251000	-0.858155000
6	4.783155000	0.891731000	-2.025572000
6	5.990108000	1.270607000	-1.325404000
6	6.364105000	2.599531000	-1.751538000
6	5.395155000	3.037251000	-2.717946000
6	4.420807000	1.989601000	-2.886082000
7	6.790962000	0.486838000	-0.451372000
1	4.271092000	-0.053475000	-1.934786000
1	7.229418000	3.151295000	-1.412705000
1	5.397572000	3.992468000	-3.223189000
1	3.575197000	2.016406000	-3.558482000
1	7.802326000	0.680758000	-0.494081000
8	5.109128000	-0.839430000	0.454921000
1	4.452316000	1.868793000	1.927086000
1	5.445696000	4.307305000	1.300916000
1	3.808637000	5.453035000	-0.520976000
1	1.769583000	3.743512000	-1.023168000
6	-9.407934000	-0.795042000	1.688835000
8	-8.239776000	-0.499079000	2.028466000
8	-10.522432000	-0.100638000	2.018259000
6	-10.402933000	1.118325000	2.859160000
1	-9.928011000	1.909200000	2.271159000
1	-11.430076000	1.378679000	3.110733000
1	-9.820789000	0.891637000	3.756259000
6	6.335771000	-0.496354000	0.363611000
6	7.352225000	-1.175850000	1.235083000
6	8.395433000	-0.542104000	2.006771000
6	7.341313000	-2.579257000	1.580134000
6	8.381192000	-2.809160000	2.551506000
6	9.027830000	-1.544701000	2.814647000
26	9.271363000	-2.120129000	0.714881000
6	10.593869000	-3.609338000	-0.100191000
6	9.591320000	-3.228460000	-1.068983000
6	9.767597000	-1.829443000	-1.370617000
6	10.910914000	-1.358985000	-0.622161000
6	11.392621000	-2.448936000	0.191590000
7	11.479623000	-0.078569000	-0.655881000
6	10.760005000	1.106368000	-0.804389000
8	9.500606000	1.089467000	-0.773129000
1	12.488766000	-0.014497000	-0.548793000
6	11.569494000	2.364335000	-0.995427000
1	11.609274000	2.607605000	-2.065984000
1	12.598949000	2.273291000	-0.634904000
1	11.081731000	3.200450000	-0.487734000
1	8.653305000	0.508208000	1.982422000
1	9.831884000	-1.375963000	3.518797000
1	8.609443000	-3.751052000	3.031770000
1	6.646002000	-3.312558000	1.196666000
1	10.743503000	-4.597343000	0.313637000
1	8.867907000	-3.887061000	-1.529296000
1	9.192596000	-1.245787000	-2.073834000
1	12.230058000	-2.408922000	0.876922000

Cartesian coordinates of a model of [Fmoc-Fca₅-OMe]⁵⁺ (OCH₂-fluorenyl replaced by Me)

1	-7.305915000	-2.347799000	2.263504000
6	-8.019437000	-2.219434000	1.460444000
1	-7.588729000	-3.969704000	0.110853000
1	-8.545815000	1.226880000	-1.897597000
6	-8.168873000	-3.080720000	0.319968000
1	-6.827032000	1.713716000	0.112027000
6	4.184249000	-0.238012000	0.396945000
1	-9.148423000	-0.361144000	2.066039000
6	-7.661699000	0.643445000	-1.680093000
8	3.973999000	0.993541000	0.395969000
6	-8.988957000	-1.166572000	1.361243000
7	3.203987000	-1.156115000	-0.042349000
6	-6.752579000	0.892702000	-0.589722000
26	-7.726394000	-1.050633000	-0.417840000
1	1.099950000	-2.868561000	-0.999176000
6	2.003801000	-0.822415000	-0.659188000
6	-9.256216000	-2.578792000	-0.484382000
6	1.023661000	-1.793461000	-1.102236000
6	-7.182732000	-0.515119000	-2.397842000
6	-9.779019000	-1.395223000	0.168318000
1	-7.622252000	-0.947110000	-3.286628000
1	-9.619787000	-3.025713000	-1.400952000
6	-5.658404000	-0.048692000	-0.696407000
6	1.494282000	0.493966000	-0.985976000
1	1.986950000	1.425852000	-0.754398000
1	-4.466170000	0.740830000	0.794345000
6	0.007644000	-1.096607000	-1.847610000
6	-5.971871000	-0.974932000	-1.760977000
7	-4.510304000	-0.000035000	0.099606000
1	-0.818730000	-1.563992000	-2.365497000
6	0.295696000	0.317429000	-1.770740000
8	-10.802114000	0.747804000	-0.199577000
6	-10.907348000	-0.499580000	-0.256392000
1	-1.656058000	-2.569692000	1.571097000
26	-0.141326000	-0.435370000	0.156906000
1	-0.255277000	1.113064000	-2.253431000
1	-5.360563000	-1.812467000	-2.059756000
6	-3.408091000	-0.861327000	-0.004515000
6	-1.462172000	-1.504994000	1.577384000
1	-12.085892000	-2.164286000	-0.617844000
7	-12.062073000	-1.150281000	-0.680163000
6	-2.233468000	-0.515519000	0.859395000
1	0.266600000	-1.290842000	2.990864000
8	-3.414669000	-1.871781000	-0.742121000
6	-0.440522000	-0.824367000	2.318023000
1	-12.793844000	1.681142000	-1.080113000
6	-1.648116000	0.780949000	1.129373000
6	-0.539658000	0.583883000	2.034876000
6	-13.207880000	-0.526908000	-1.202672000
6	-13.454867000	0.883445000	-1.382068000
1	-1.984358000	1.736044000	0.745940000
1	0.072663000	1.367286000	2.460519000
1	-17.893569000	1.256242000	0.168874000
6	-15.944346000	1.513972000	1.252033000
6	-17.069426000	0.802329000	0.703050000
6	-14.357204000	-1.253880000	-1.694719000
1	-14.476582000	-2.329655000	-1.712024000
26	-15.148779000	0.111805000	-0.192632000
6	-14.711770000	1.017799000	-2.077514000
6	-15.070876000	0.559529000	1.898316000
1	-14.178065000	0.819680000	2.449566000
1	-15.143904000	1.950628000	-2.413182000
6	-15.265479000	-0.298480000	-2.279091000
6	-16.881740000	-0.593731000	0.979041000
6	-15.652589000	-0.746913000	1.725471000
1	-16.180326000	-0.538396000	-2.803004000
1	-17.560206000	-1.389362000	0.700001000
1	-15.276633000	-1.674595000	2.134621000
1	3.395505000	-2.145807000	0.089241000
6	5.448087000	-0.841349000	0.910999000
6	6.127542000	-2.051223000	0.495667000
6	7.273258000	-2.230221000	1.355835000
6	7.304412000	-1.134992000	2.290767000

6	6.201850000	-0.267097000	2.003160000
26	7.507526000	-0.401926000	0.206133000
6	9.153495000	-0.593177000	-1.223046000
6	9.615114000	0.442804000	-0.315784000
6	8.576728000	1.453702000	-0.250747000
6	7.583338000	1.142235000	-1.244363000
6	7.938897000	-0.124435000	-1.843427000
7	10.800005000	0.498499000	0.391487000
1	9.689152000	-1.502506000	-1.448033000
1	8.605823000	2.355639000	0.347408000
1	6.737657000	1.766071000	-1.498990000
1	7.420083000	-0.622945000	-2.650738000
1	10.973112000	1.331634000	0.947977000
8	11.586172000	-1.624020000	-0.131196000
1	5.834899000	-2.723960000	-0.300724000
1	7.959245000	-3.066042000	1.326577000
1	8.022751000	-0.998707000	3.088056000
1	5.940594000	0.643913000	2.525532000
6	-15.678798000	2.981148000	1.204059000
8	-14.593506000	3.481242000	1.548240000
8	-16.765140000	3.661783000	0.751301000
6	-16.710643000	5.151657000	0.737040000
1	-15.905507000	5.483727000	0.075880000
1	-17.687088000	5.458072000	0.364925000
1	-16.540375000	5.515471000	1.753519000
6	11.800074000	-0.513743000	0.399942000
6	13.050860000	-0.175919000	1.119030000
6	13.636469000	1.127671000	1.397728000
6	13.880948000	-1.175637000	1.762941000
6	14.941953000	-0.491153000	2.444544000
6	14.786875000	0.922101000	2.225891000
26	15.034016000	-0.111814000	0.251831000
6	15.957611000	-1.459455000	-1.100713000
6	15.026635000	-0.604980000	-1.801269000
6	15.486541000	0.757120000	-1.691131000
6	16.771126000	0.738989000	-1.013372000
6	16.994858000	-0.623470000	-0.556680000
7	17.615061000	1.794085000	-0.769919000
6	17.289121000	3.173620000	-0.995354000
8	16.117948000	3.482347000	-1.282861000
1	18.551667000	1.585695000	-0.430842000
6	18.443596000	4.132648000	-0.859414000
1	19.108717000	4.048113000	-1.729967000
1	19.043322000	3.938166000	0.038552000
1	18.062590000	5.154497000	-0.822041000
1	13.288769000	2.092026000	1.048001000
1	15.433128000	1.700082000	2.610675000
1	15.713072000	-0.959280000	3.041926000
1	13.692359000	-2.240609000	1.762036000
1	15.907804000	-2.536576000	-1.019774000
1	14.150133000	-0.931673000	-2.343742000
1	15.028721000	1.637154000	-2.114495000
1	17.852809000	-0.967887000	0.007083000