

1,3- γ -Silyl-Elimination in Electron-Deficient Cationic Systems

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Supporting Information: Computational Studies

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General Considerations:

General:

Quantum chemical calculations were performed using Gaussian 09.¹ All optimized geometries were calculated using B3LYP², a hybrid density functional, with the 6-31+g(d) basis set. For γ -stannyl systems, geometry optimizations were carried out using B3LYP and a mixed basis set of LANL2DZ for Sn and 6-31+g(d) for all other atoms. This modified calculation was employed to more accurately describe the electronic nature of the γ -stannyl group. The addition of diffuse functions to the double split-valence basis set ensured an adequate description of the charged systems and the effect of the $-CF_3$ group. Stationary points were characterized by frequency calculations at 298 K, with structures at energy minima showing no negative frequencies and transition-states showing one negative frequency. Intrinsic reaction coordinate (IRC) calculations followed by optimization and frequency calculation were performed on transition state structures to connect the two respective ground states. Thermal energies, enthalpies and Gibbs free energies were corrected using the appropriate thermodynamic correction factor. Solvation energies were evaluated using a self consistent field (SCRF) using the polarization continuum model (PCM)^{3,4} model. All energetic values shown are in kcal mol⁻¹; bond lengths are reported in Ångstrom, bond and pyramidalization angles in degrees. Figures were generated using CYLView.⁵

Complete Citation for Gaussian 09:

Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

¹ Frisch, M. J. et al. Gaussian 09, revision A.1; Gaussian, Inc.:Wallingford, CT, **2009**

² (a) Becke, A. D. J. *Chem. Phys.* **1993**, 98, 5648; (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, 37, 785; (c) Vosko, S. H.; Wilk, L.; Nusair, M. *Can. J. Phys.* **1980**, 58, 1200; (d) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, 98, 11623.

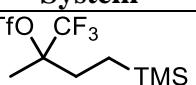
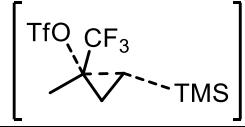
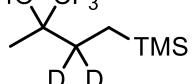
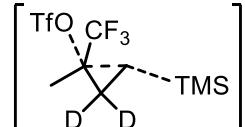
³ Miertuš, S.; Scrocco, E.; Tomasi, J. *Chem. Phys.* **1981**, 55, 117.

⁴ Cammi, R.; Tomasi, J. *J. Chem. Phys.* **1994**, 100, 7495.

⁵ Legault, C. Y. CYLview, 1.0b. Université de Sherbrooke; **2009**. <http://www.cylview.org>.

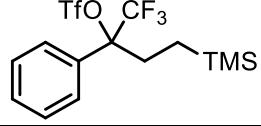
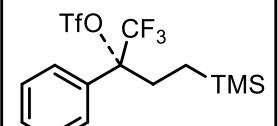
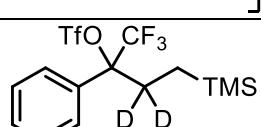
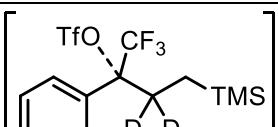
Calculated Kinetic Isotope Effect (KIE)

Table S1: Energies of methyl system stationary points used in the theoretically derived KIE.

| System | E ^a | ΔE |
|---|----------------|----------|
|  | -1170160.858 | - |
|  | -1170141.649 | 19.20869 |
|  | -1170165.159 | - |
|  | -1170145.962 | 19.19677 |

^a Sum of electronic and zero point energies (E, in kcal mol⁻¹, solvent = CF₃CH₂OH) using B3LYP/6-31+g(d).

Table S2: Energies of phenyl system stationary points used in the theoretically derived KIE.

| System | E ^a | ΔE |
|---|----------------|----------|
|  | -1290442.213 | - |
|  | -1290434.513 | 7.700169 |
|  | -1290446.536 | - |
|  | -1290438.86 | 7.675696 |

^a Sum of electronic and zero point energies (E, in kcal mol⁻¹, solvent = CF₃CH₂OH) using B3LYP/6-31+g(d).

Derived from the Arrhenius equation:

$$\frac{k(\text{H})}{k(\text{D})} = e^{\left(\frac{\Delta E(\text{D}) - \Delta E(\text{H})}{RT}\right)}$$

For methyl system (Data provided in Table S1):

$$\frac{k(\text{H})}{k(\text{D})} = e^{\left(\frac{19.19677 - 19.20869}{0.0019872041 * 298.15}\right)}$$

$$\frac{k(\text{H})}{k(\text{D})} = \mathbf{0.980}$$

EXPERIMENTAL VALUE = 1.00

For phenyl system (Data provided in Table S2):

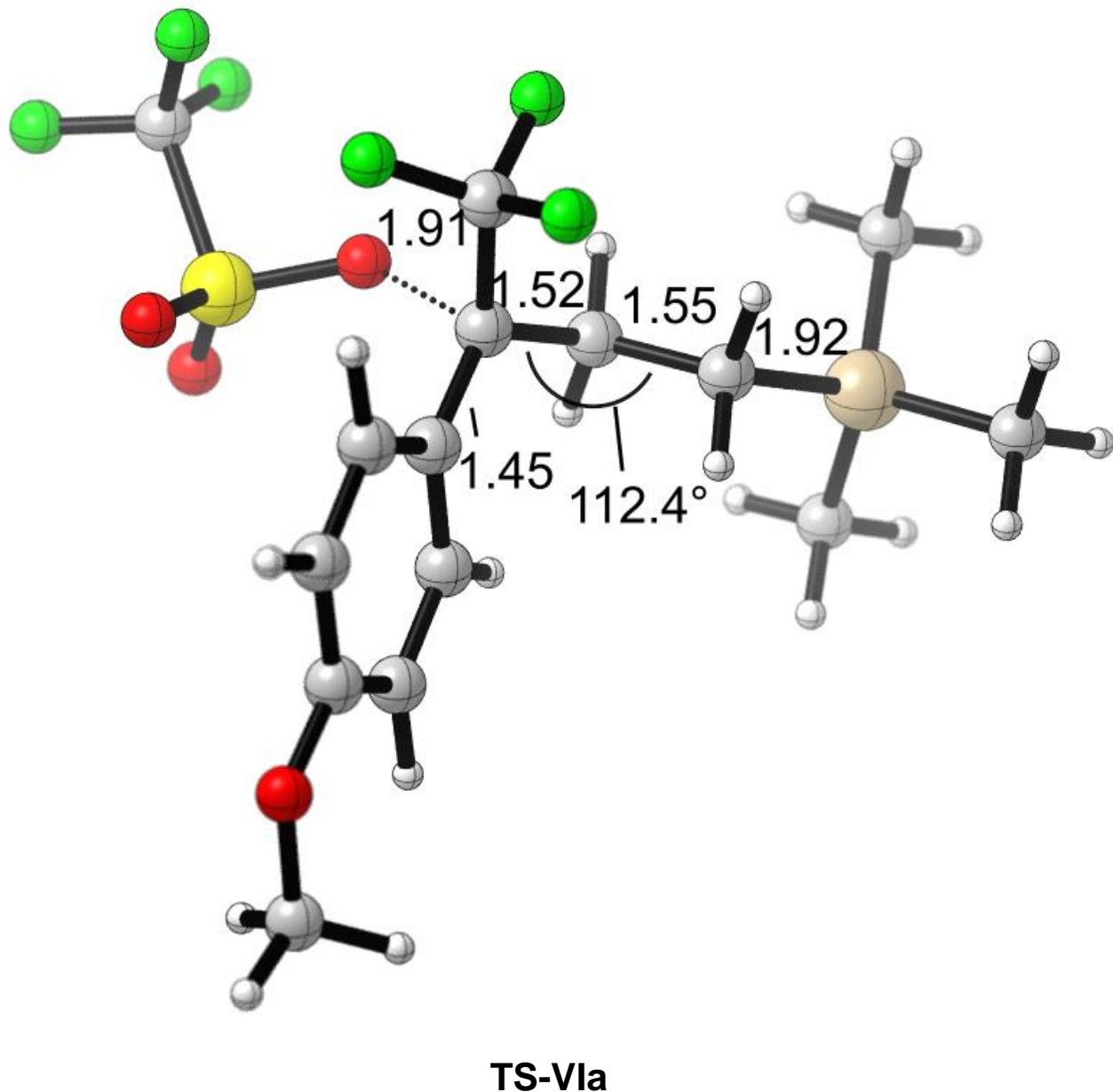
$$\frac{k(\text{H})}{k(\text{D})} = e^{\left(\frac{7.675696 - 7.700169}{0.0019872041 * 298.15}\right)}$$

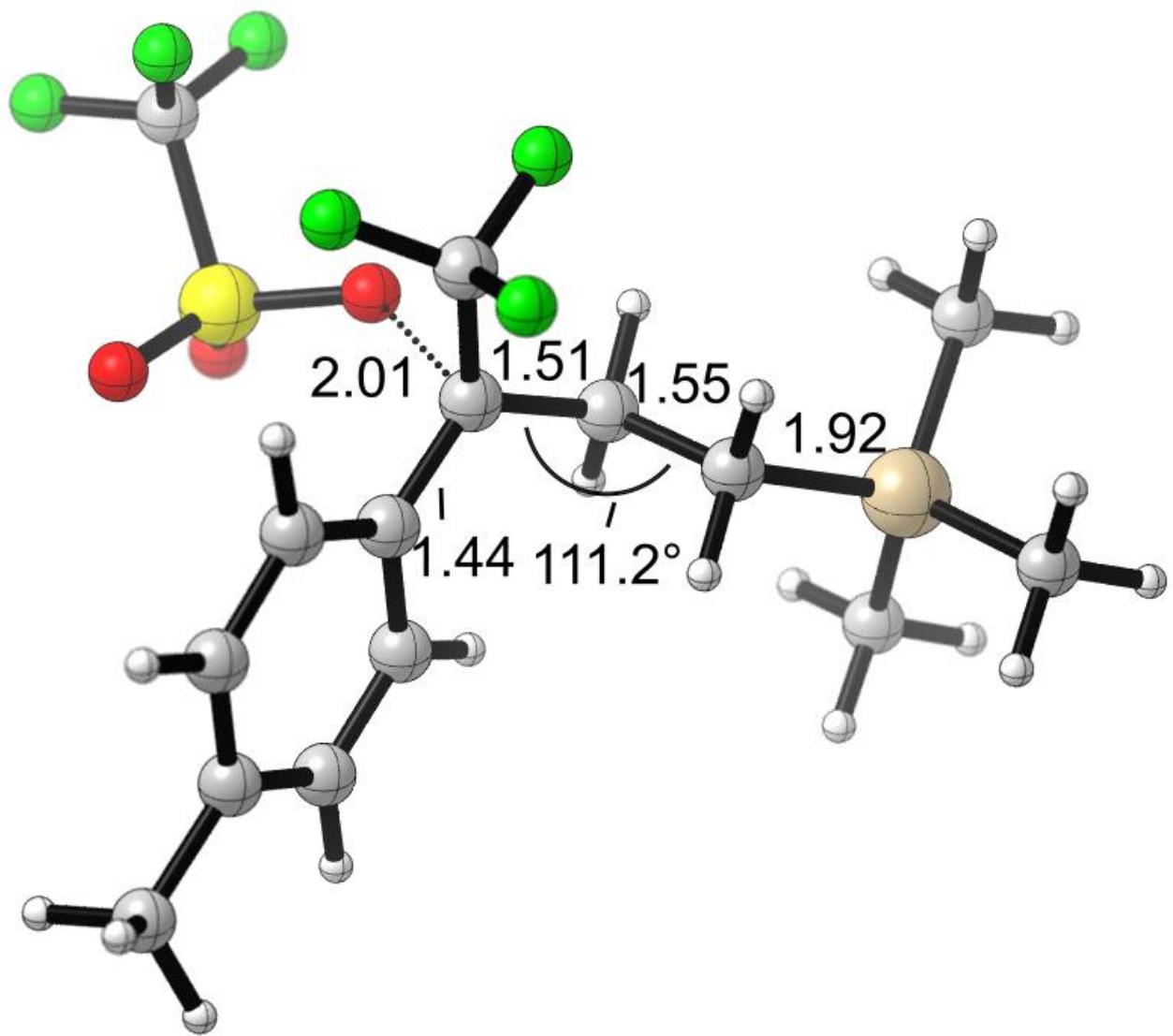
$$\frac{k(\text{H})}{k(\text{D})} = \mathbf{0.960}$$

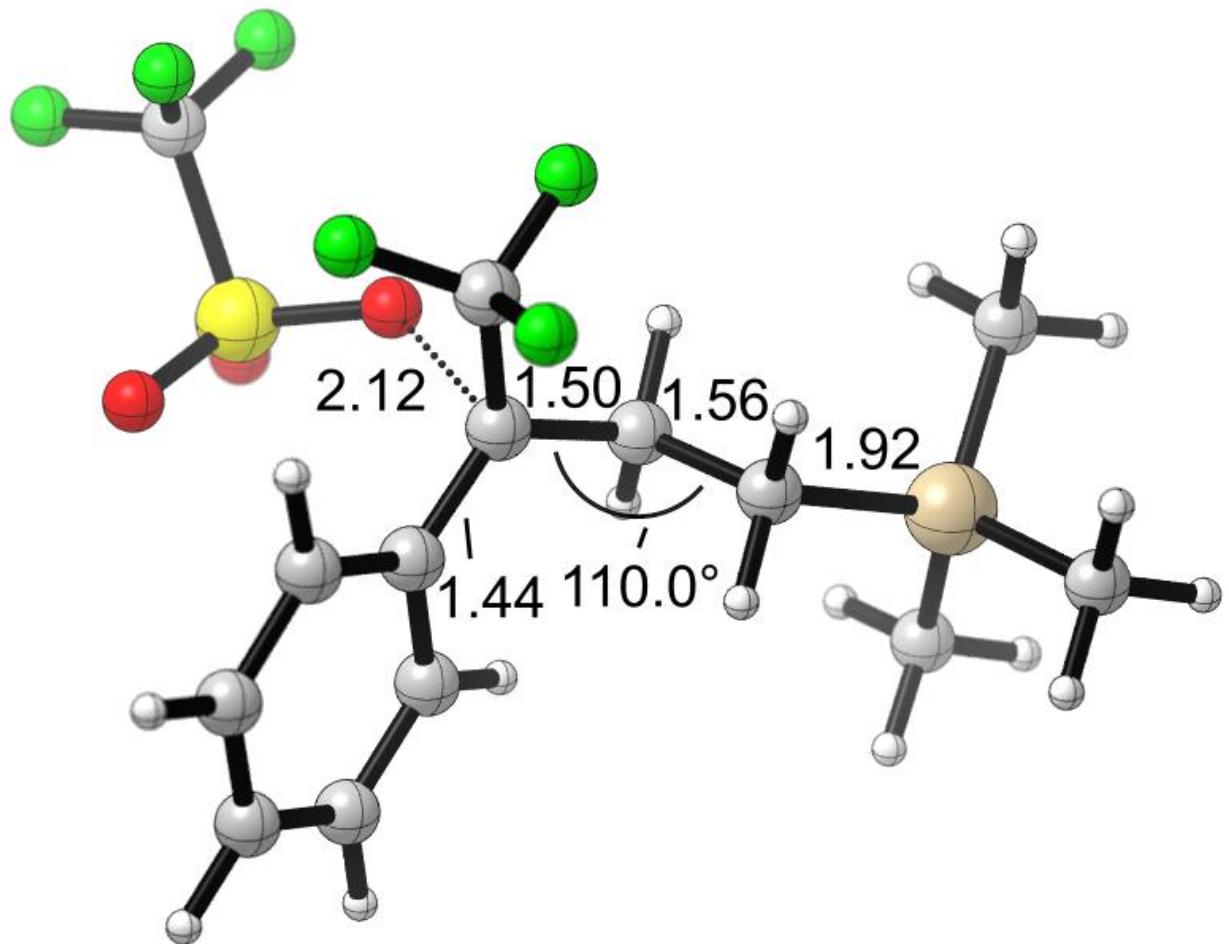
EXPERIMENTAL VALUE = 0.980

Transition State Geometries

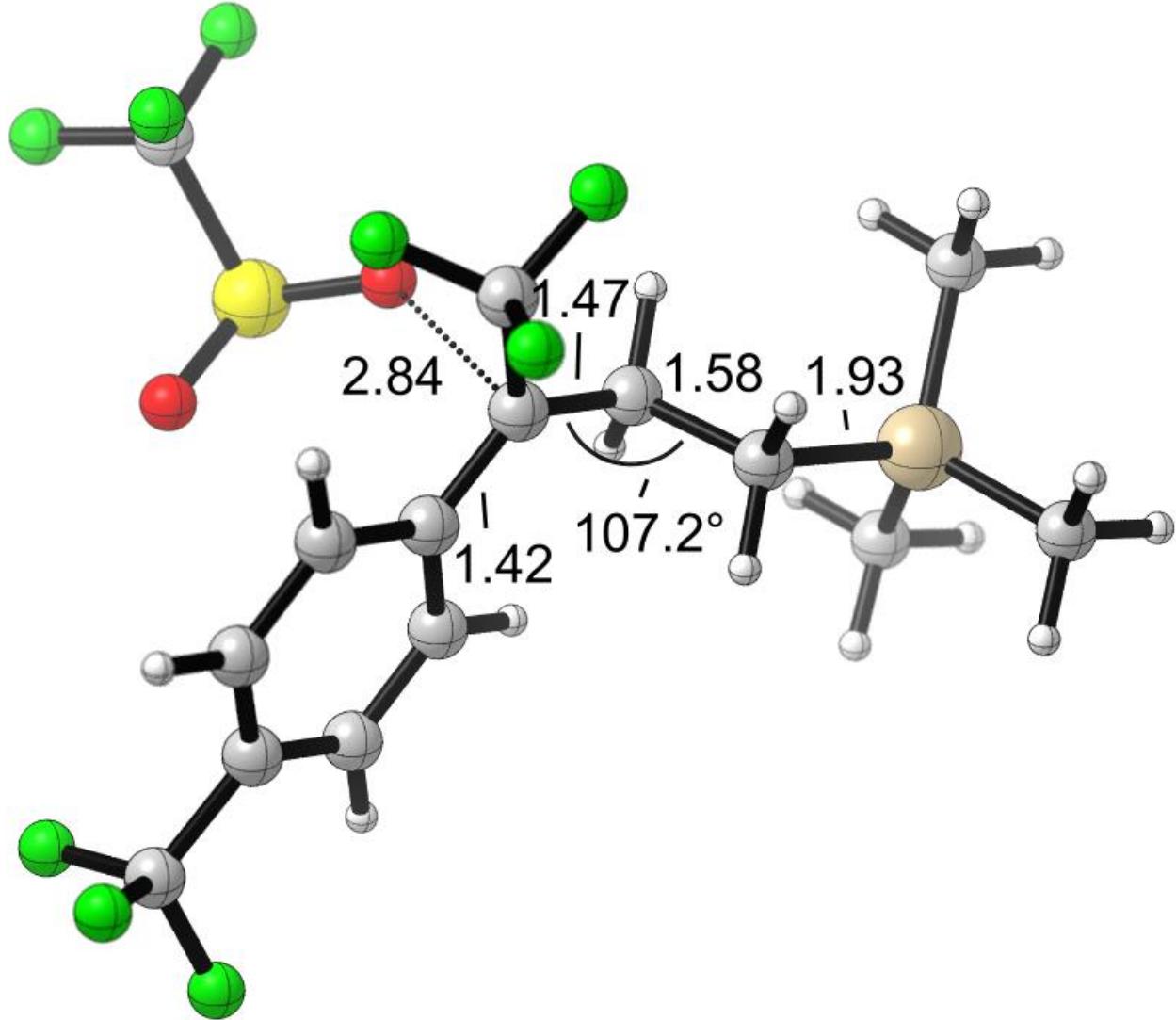
Figure S1. Optimized transition state geometries for the ionization step leading to the discrete carbenium ion intermediate **VIIa-e**. These structures are presented in Figure 4 of the manuscript.

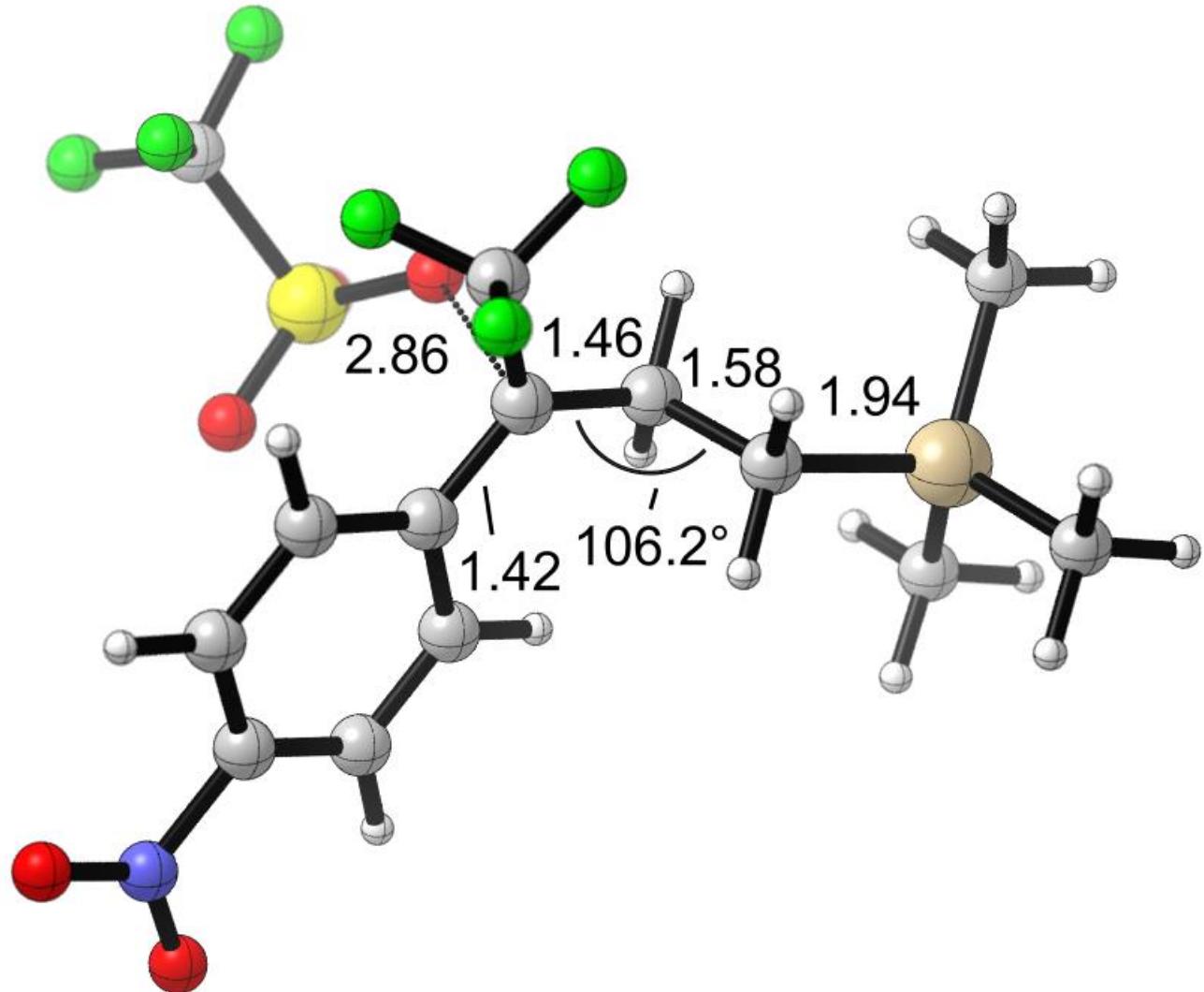






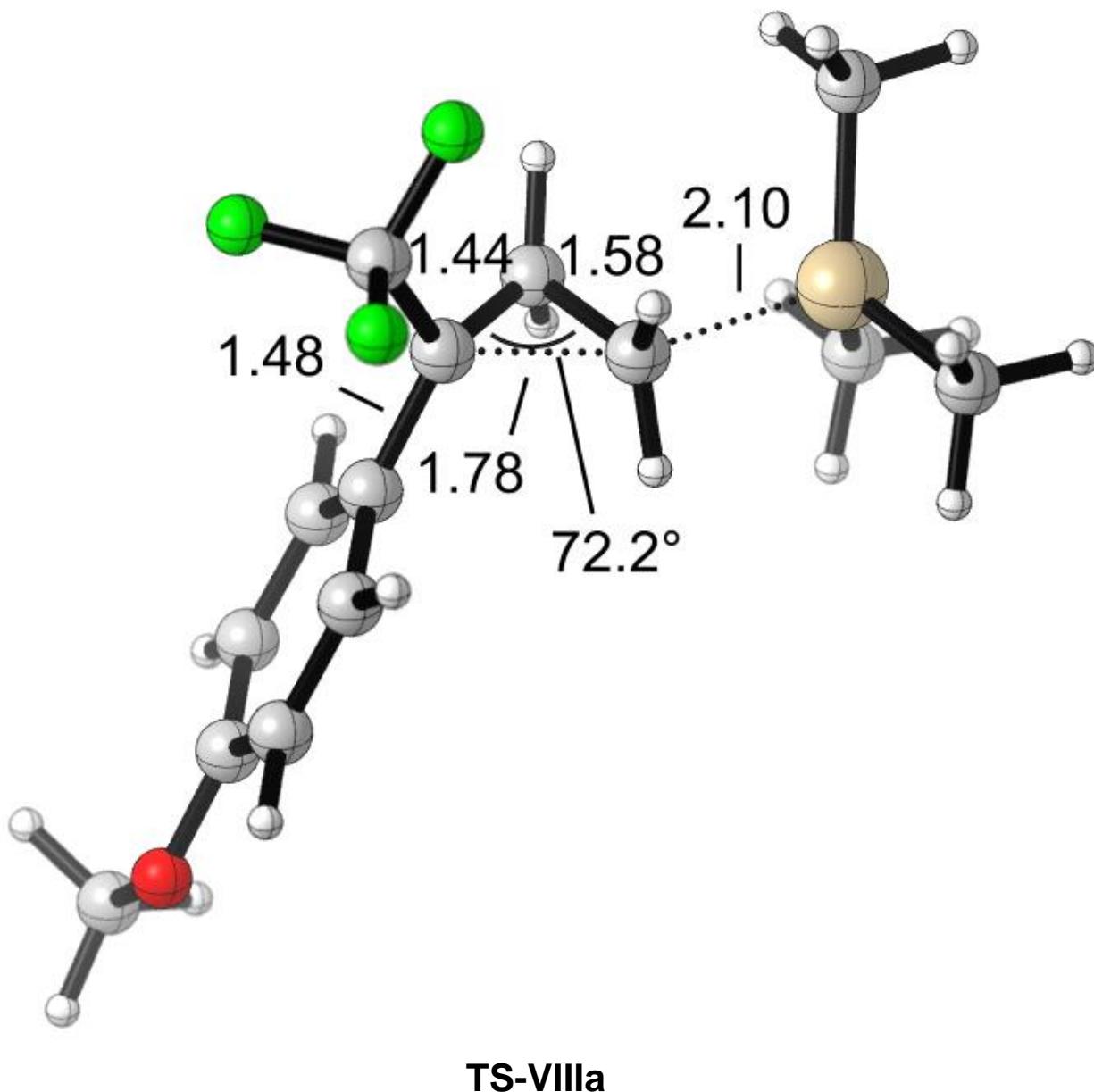
TS-Vlc

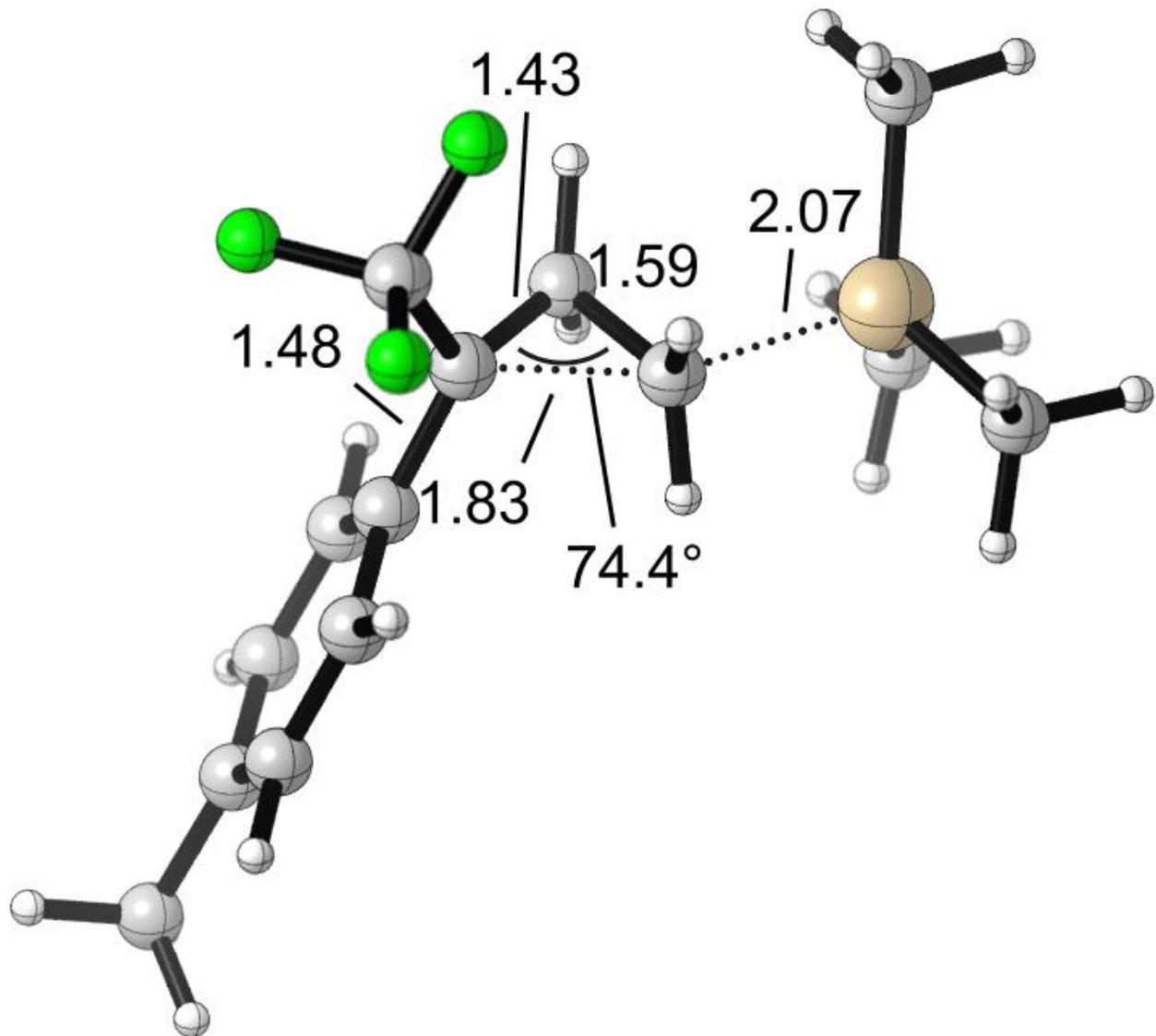




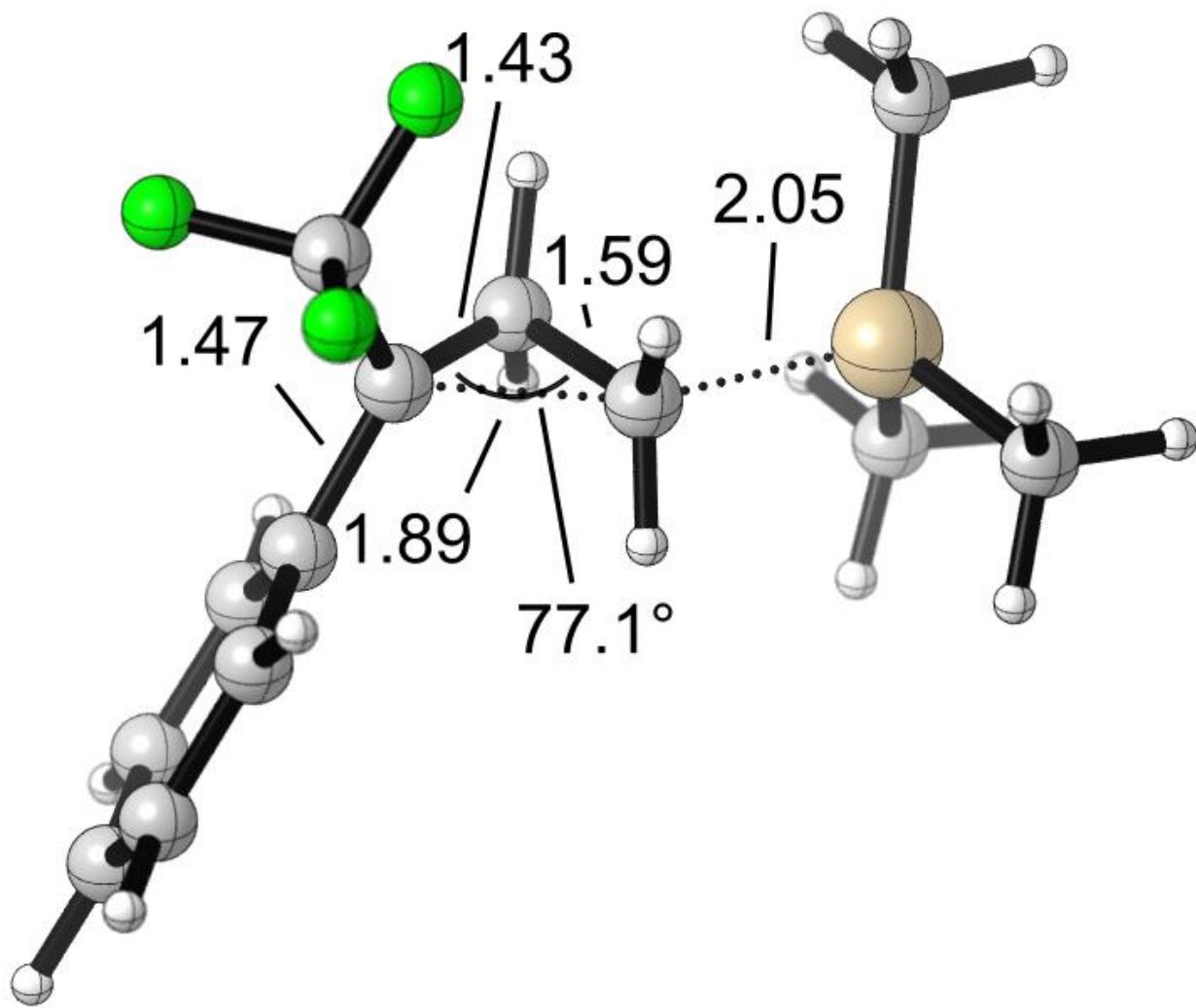
TS-Vle

Figure S2. Optimized transition state geometries for 1,3- γ -silyl-elimination leading to trifluoromethyl cyclopropanes **IXa-e**. These structures are presented in Figure 4 of the manuscript.

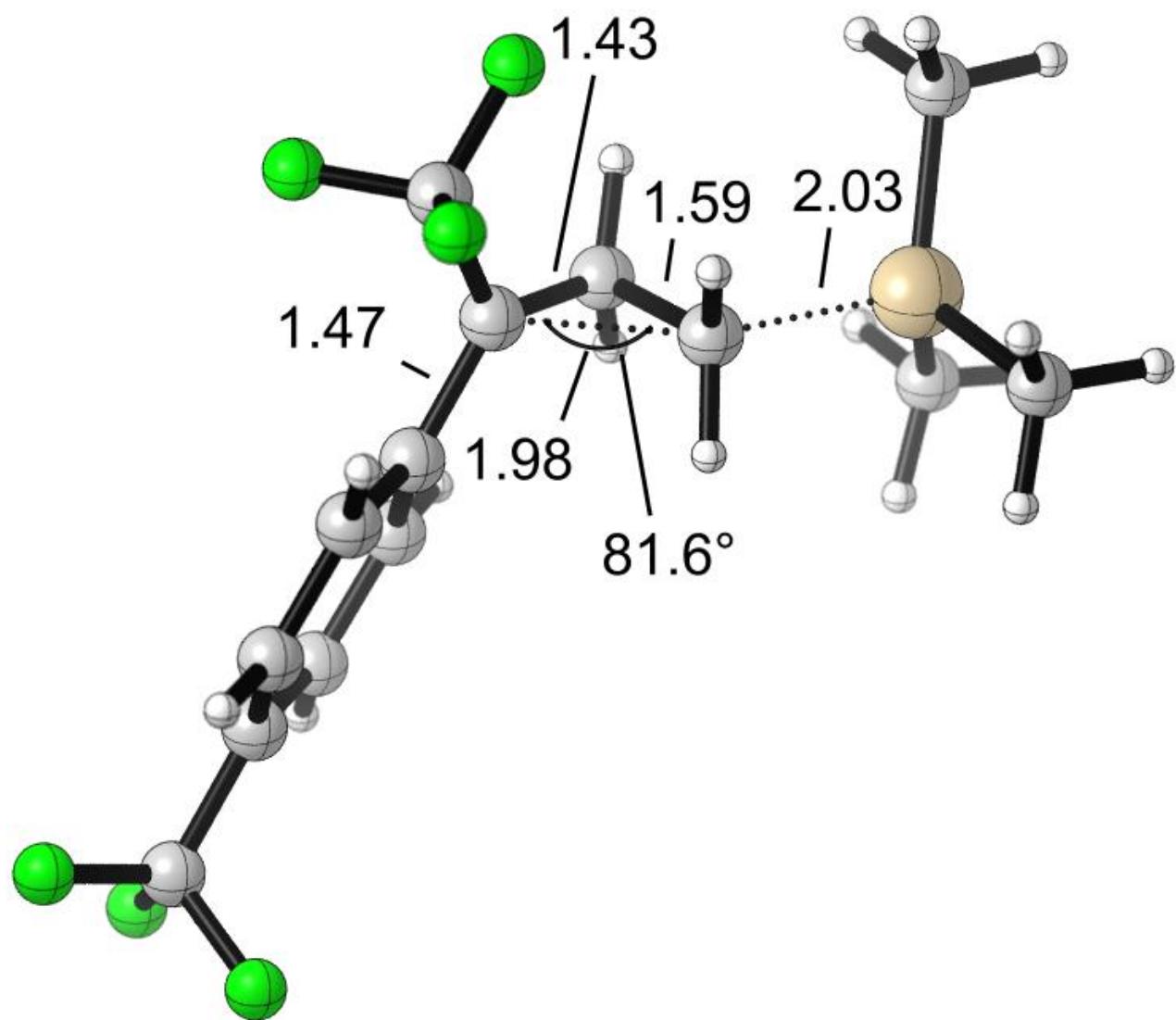




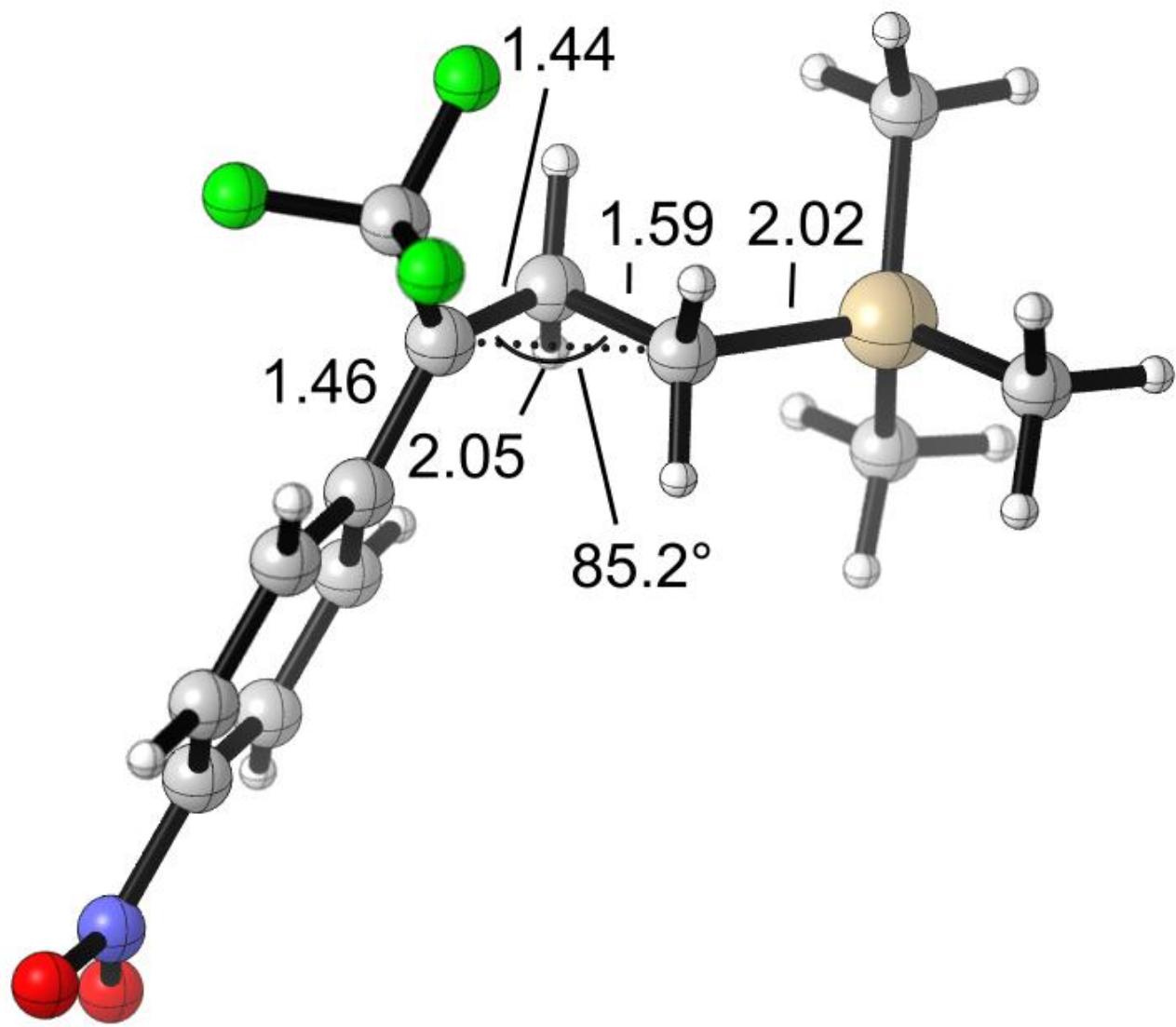
TS-VIIIb



TS-VIIIc

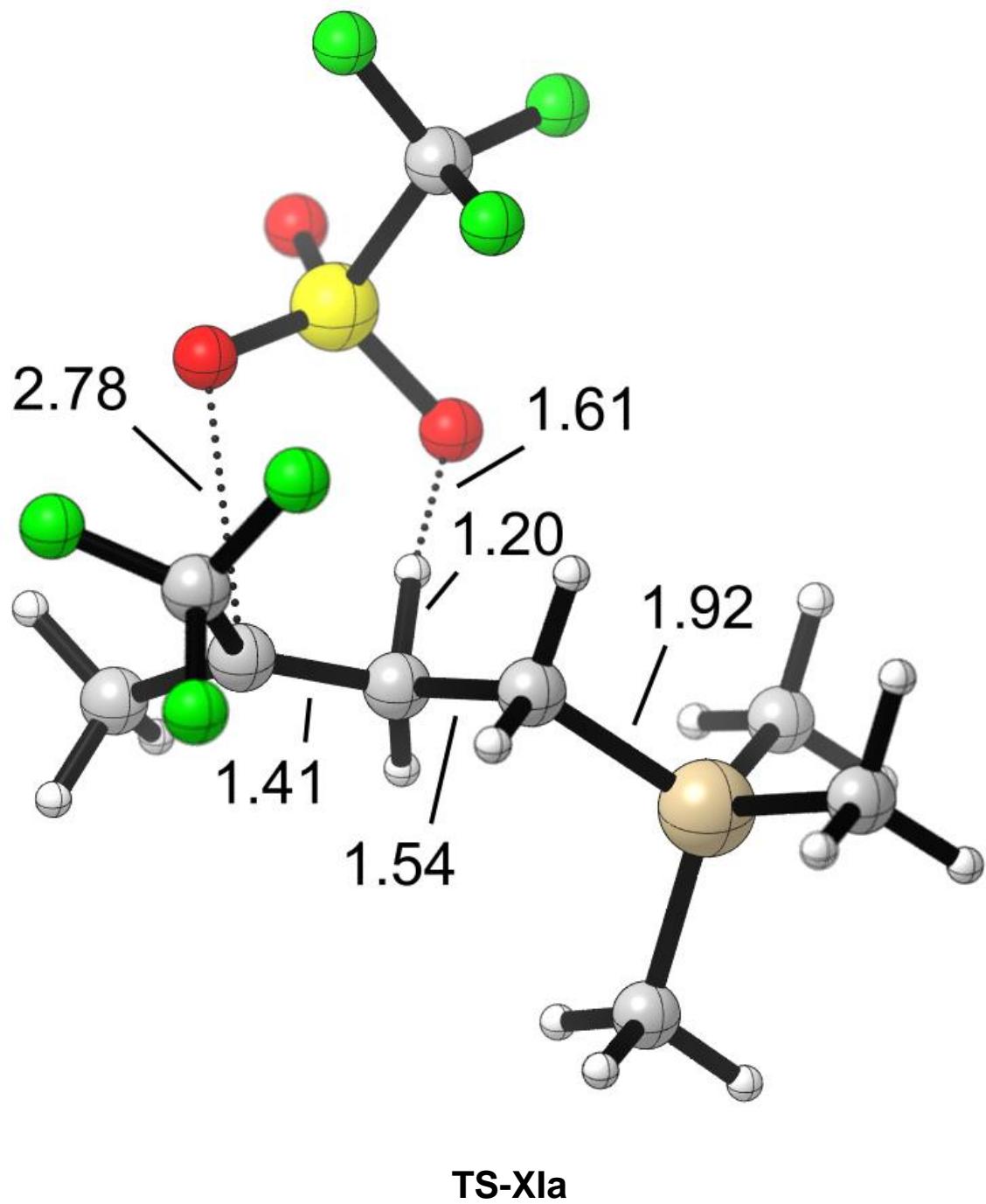


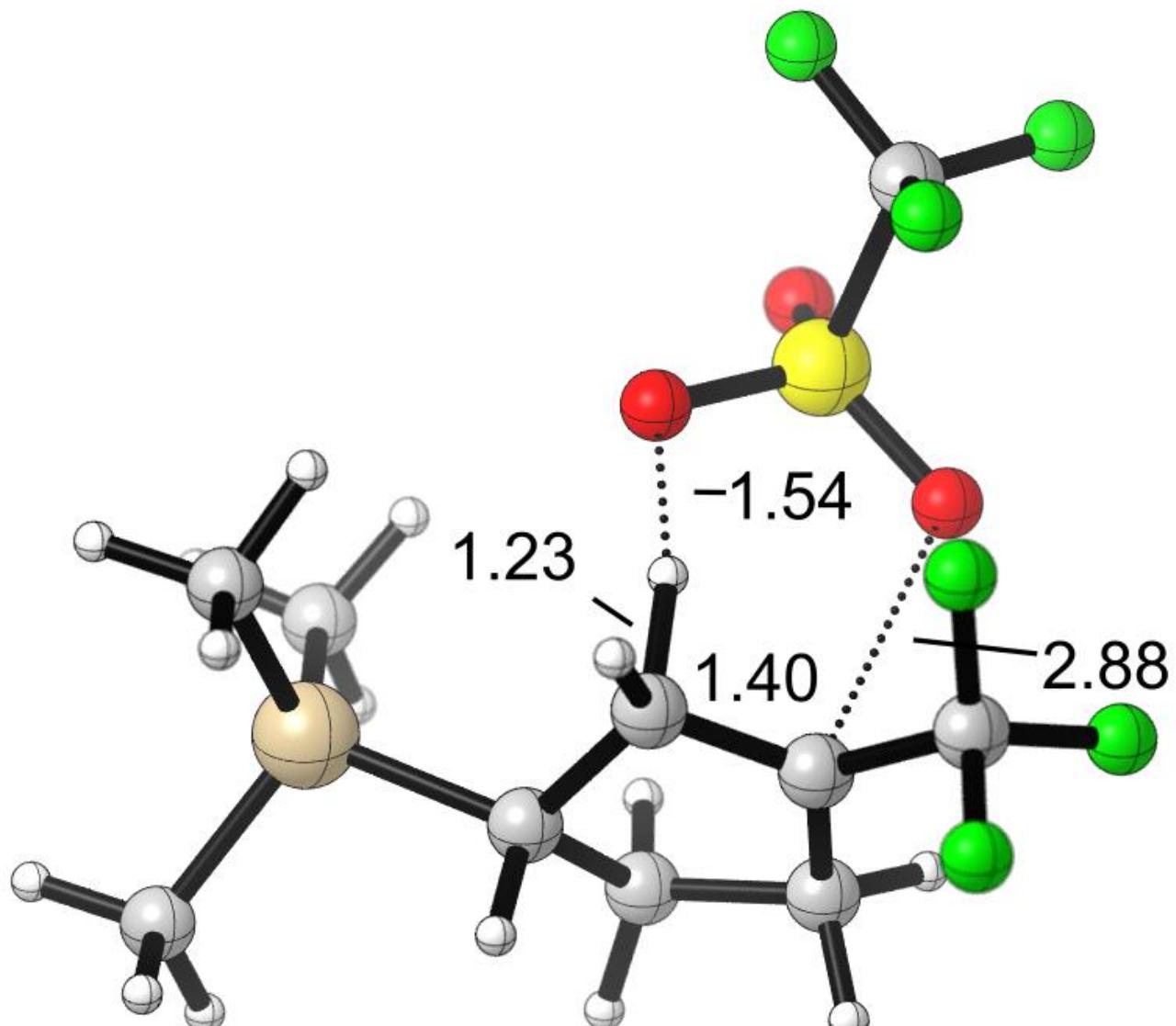
TS-VIIId



TS-VIIIe

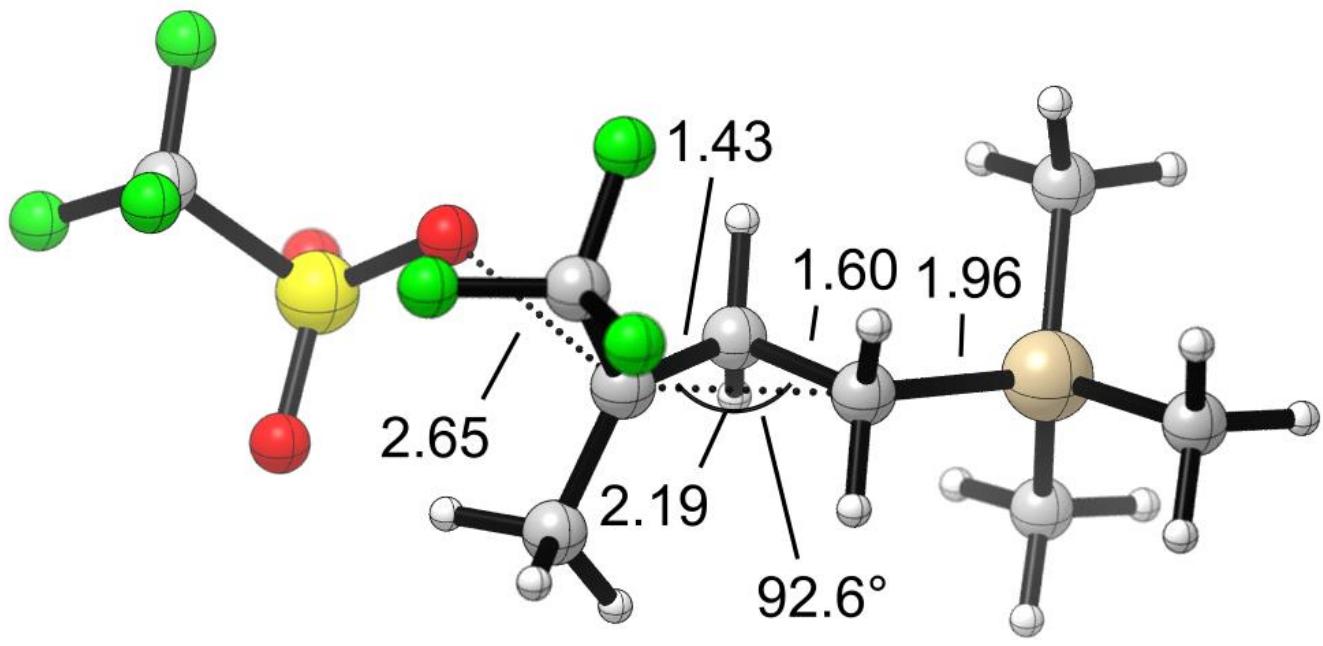
Figure S3. Optimized transition state geometries for the E1-like elimination leading to trifluoromethyl alkenes **XIIa-b**. These structures are presented in Figure 5 of the manuscript.



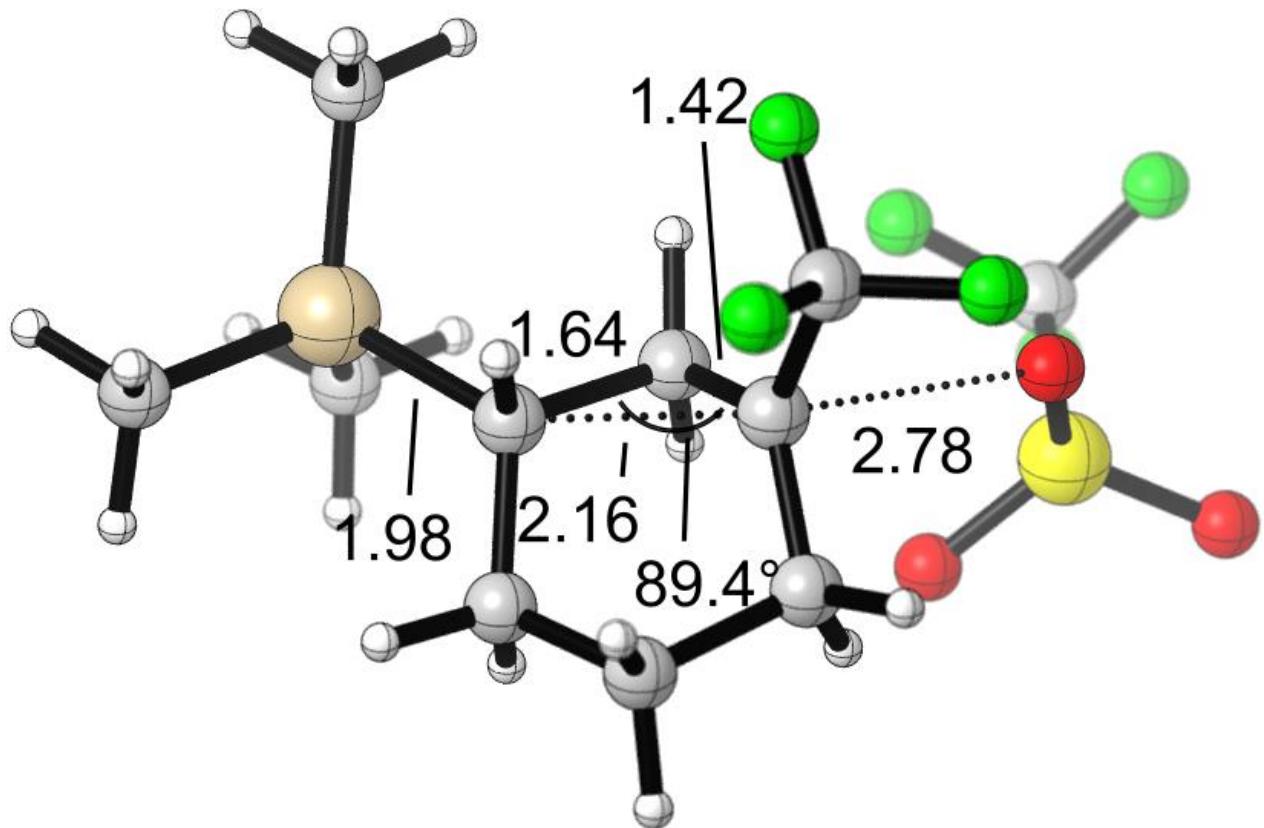


TS-XIb

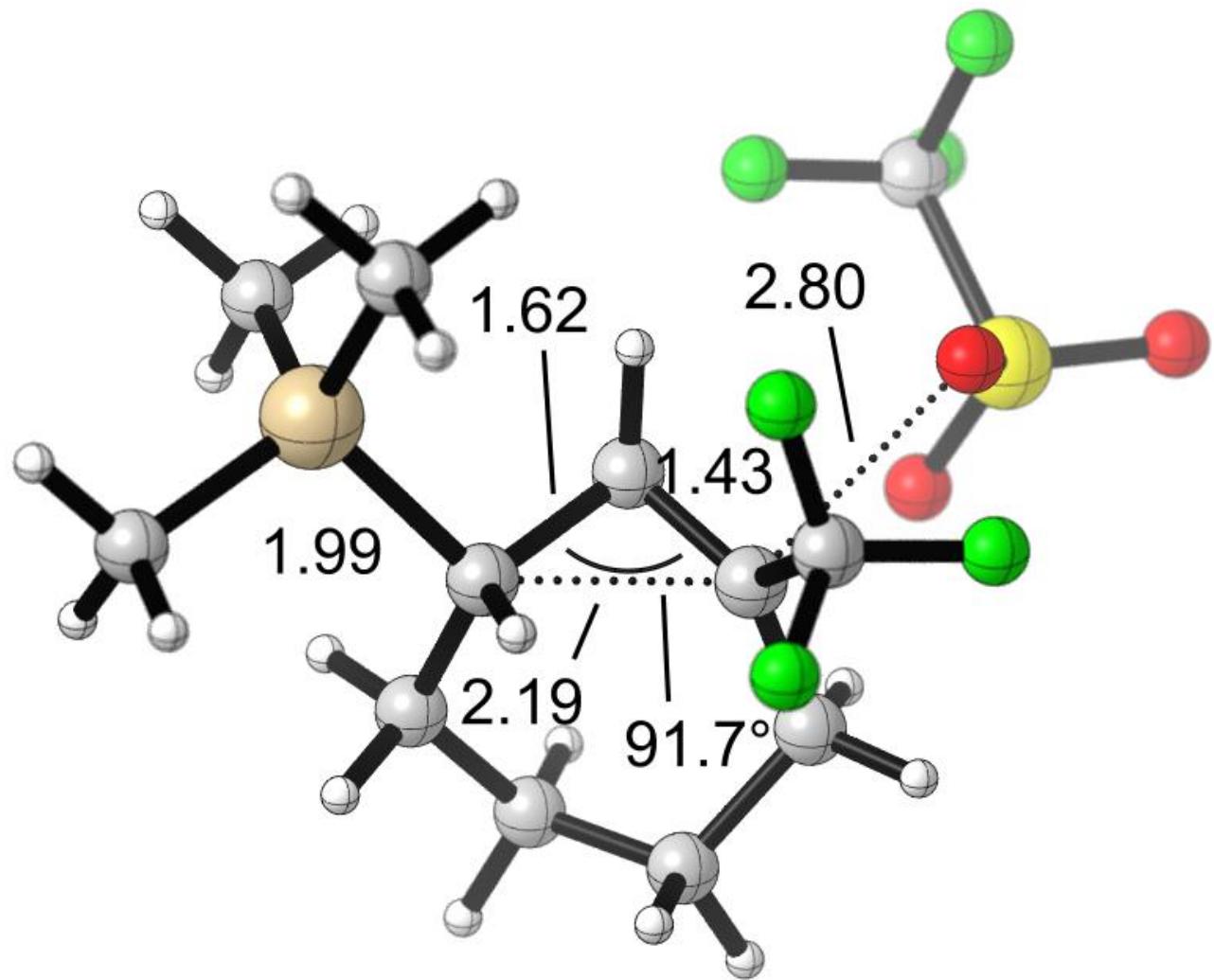
Figure S4. Optimized transition state geometries for the 1,3- γ -silyl-elimination leading to trifluoromethyl cyclopropanes **XIVa, c-e**. These structures are presented in Figure 5 of the manuscript.



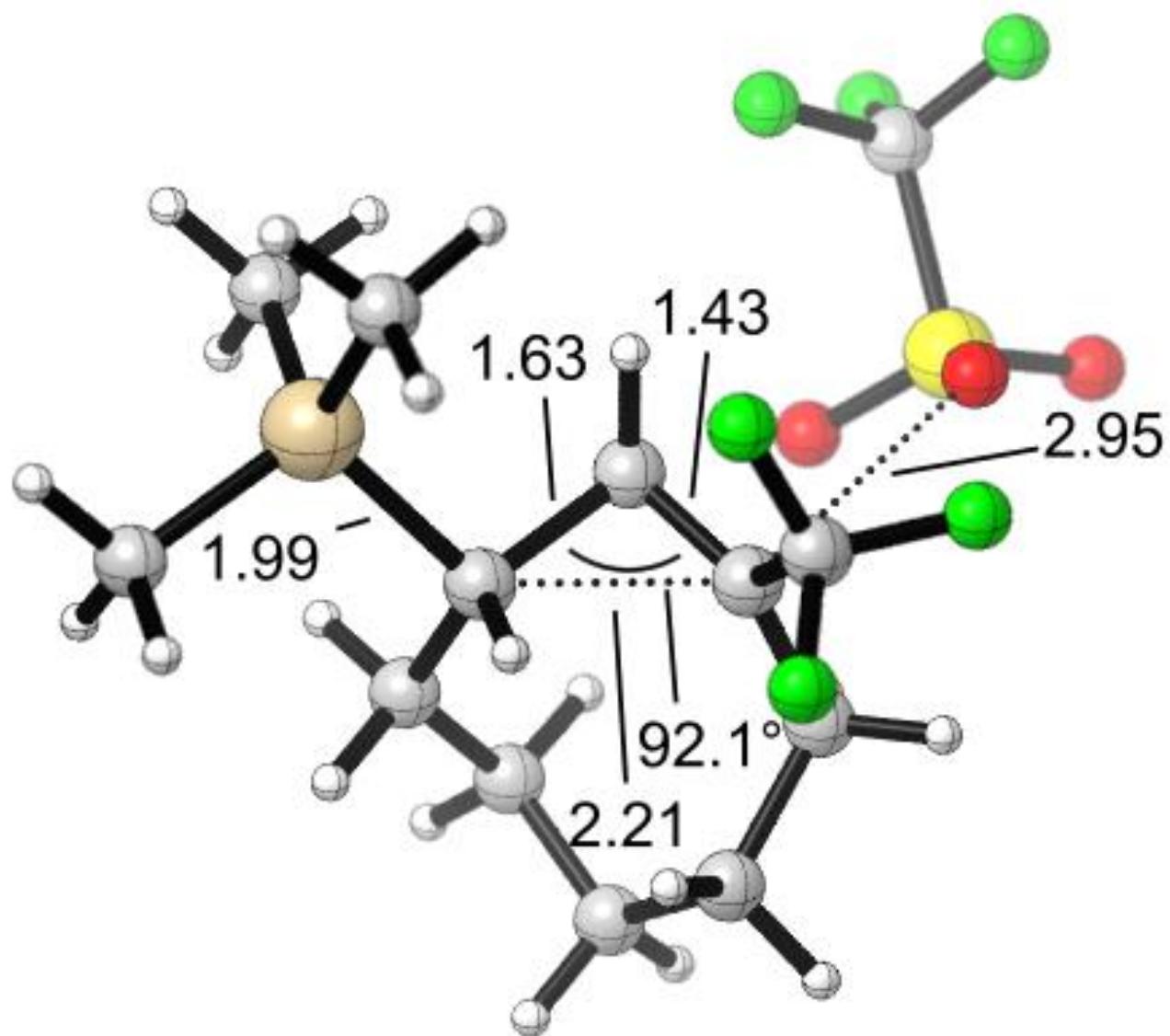
TS-XIIIa



TS-XIIIc

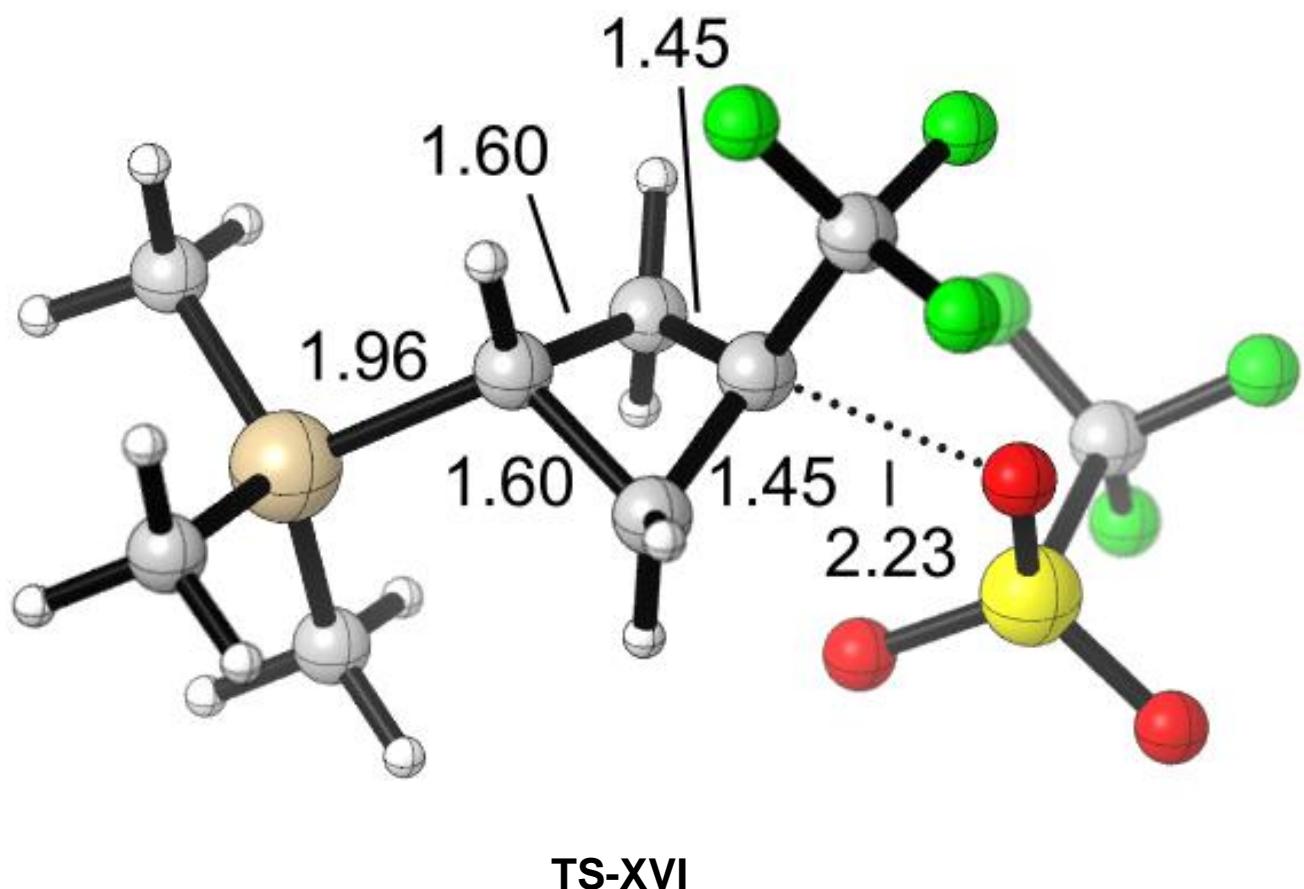


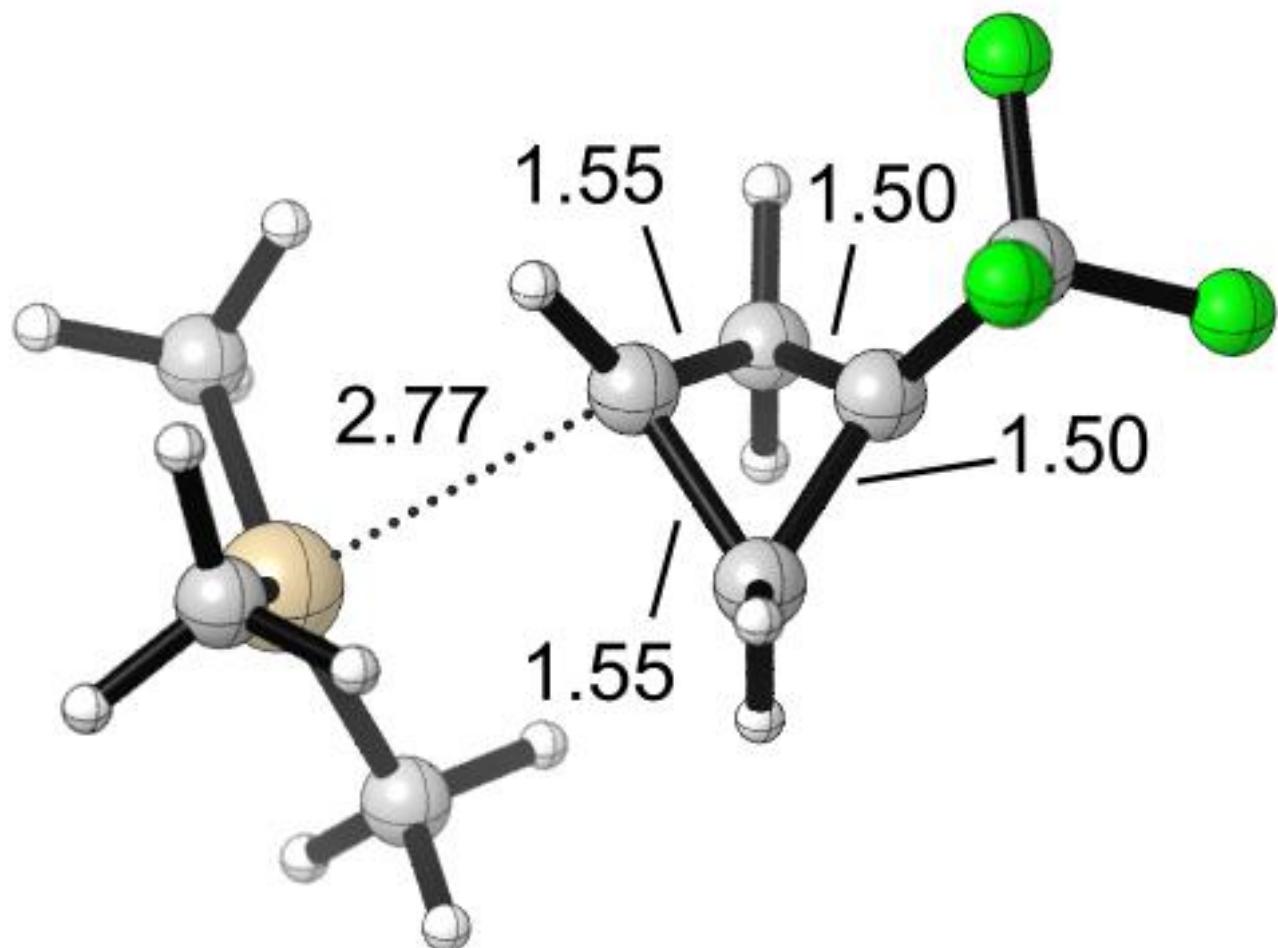
TS-XIIId



TS-XIIIe

Figure S5. Optimized transition state geometries for the stepwise elimination leading to the ionized cyclobutyl intermediate, **XVII**, then to the trifluoromethyl bicyclobutane, **XIX**. These structures are presented in Figure 6 of the manuscript.





TS-XVIII

Stationary Point Energies

Table S3. Summary of stationary point energies: sum of electronic and zero point energies (E, in Hartree, solvent = CF₃CH₂OH), sum of electronic and thermal enthalpies (H, in Hartree, solvent = CF₃CH₂OH), and sum of electronic and thermal free energies (G, in Hartree, solvent = CF₃CH₂OH).

| Structure | E ^a | H ^a | G ^a |
|-------------|----------------|----------------|----------------|
| Ia | -1210.149244 | -1210.125917 | -1210.2022 |
| Ib | -1134.944301 | -1134.921756 | -1134.996507 |
| Ic | -1095.653142 | -1095.632461 | -1095.702679 |
| Id | -1432.710285 | -1432.685876 | -1432.766023 |
| Ie | -1300.166399 | -1300.143089 | -1300.220471 |
| If | -797.882379 | -797.863771 | -797.929035 |
| Ig | -511.719268 | -511.699161 | -511.769909 |
| IIa | -957.903577 | -957.882881 | -957.952736 |
| IIb | -882.687859 | -882.667958 | -882.735984 |
| IIc | -843.389056 | -843.371009 | -843.434457 |
| IID | -1180.433702 | -1180.411874 | -1180.485704 |
| IIe | -1047.883321 | -1047.862506 | -1047.934933 |
| IIIf | -545.654296 | -545.638034 | -545.698027 |
| IIIa | -1209.337124 | -1209.313894 | -1209.389922 |
| IIIb | -1134.121806 | -1134.099424 | -1134.173601 |
| IIIc | -1094.823544 | -1094.803024 | -1094.872517 |
| IIId | -1431.869336 | -1431.845056 | -1431.924899 |
| IIIe | -1299.319812 | -1299.296594 | -1299.374072 |
| IIIf | -797.087729 | -797.069162 | -797.133663 |
| IIIg | -510.926419 | -510.906374 | -510.976535 |
| IVa | -958.71636 | -958.695505 | -958.765799 |
| IVb | -883.511564 | -883.491377 | -883.561371 |
| IVc | -844.220278 | -844.202038 | -844.266453 |
| IVd | -1181.277328 | -1181.25536 | -1181.329807 |
| IVe | -1048.733351 | -1048.712481 | -1048.784162 |
| IVf | -546.44966 | -546.433494 | -546.492849 |
| Va | -2170.947979 | -2170.916289 | -2171.012676 |
| Vb | -2095.74253 | -2095.711533 | -2095.807745 |
| Vc | -2056.450481 | -2056.421462 | -2056.511639 |
| Vd | -2393.505412 | -2393.472661 | -2393.572564 |

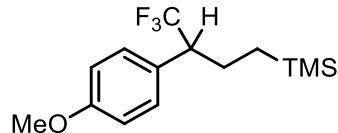
| | | | |
|------------------|--------------|--------------|--------------|
| Ve | -2260.960059 | -2260.928366 | -2261.025848 |
| TS-VIa | -2170.942146 | -2170.910529 | -2171.008537 |
| TS-VIb | -2095.733296 | -2095.702367 | -2095.799427 |
| TS-VIc | -2056.43821 | -2056.409249 | -2056.500721 |
| TS-VId | -2393.48531 | -2393.452915 | -2393.556112 |
| TS-VIe | -2260.935951 | -2260.904517 | -2261.00724 |
| VIIa | -1209.33719 | -1209.313924 | -1209.390225 |
| VIIb | -1134.121906 | -1134.099482 | -1134.173749 |
| VIIc | -1094.82369 | -1094.803124 | -1094.872992 |
| VIId | -1431.86922 | -1431.84498 | -1431.924647 |
| VIIe | -1299.319839 | -1299.29664 | -1299.373937 |
| TS-VIIIa | -1209.315261 | -1209.292726 | -1209.365927 |
| TS-VIIIb | -1134.108726 | -1134.086925 | -1134.15906 |
| TS-VIIIc | -1094.815881 | -1094.795915 | -1094.863778 |
| TS-VIIIId | -1431.867362 | -1431.843768 | -1431.920988 |
| TSVIIIe | -1299.319763 | -1299.297259 | -1299.372278 |
| IXa | -800.352507 | -800.338213 | -800.39292 |
| IXb | -725.148057 | -725.134524 | -725.188005 |
| IXc | -685.861889 | -685.850047 | -685.899504 |
| IXd | -1022.914197 | -1022.898873 | -1022.957385 |
| IXe | -890.370626 | -890.356427 | -890.411631 |
| Xa | -1864.769948 | -1864.74421 | -1864.82668 |
| Xb | -1902.864399 | -1902.839781 | -1902.919705 |
| Xc | -1942.152266 | -1942.125928 | -1942.20959 |
| Xd | -1981.422772 | -1981.395249 | -1981.481082 |
| Xe | -2020.697708 | -2020.669032 | -2020.756922 |
| TS-XIa | -1864.734469 | -1864.708489 | -1864.792357 |
| TS-XIb | -1902.832532 | -1902.806986 | -1902.889592 |
| XIIa | -902.761395 | -902.744264 | -902.805789 |
| XIIb | -940.858156 | -940.841157 | -940.902448 |
| TS-XIIIa | -1864.739337 | -1864.713288 | -1864.797226 |
| TS-XIIIc | -1942.123702 | -1942.096925 | -1942.183393 |
| TS-XIID | -1981.399763 | -1981.371819 | -1981.460291 |
| TS-XIIIe | -2020.673753 | -2020.64453 | -2020.736641 |
| XIVa | -494.172561 | -494.163793 | -494.204833 |
| XIVc | -571.553088 | -571.543394 | -571.58724 |
| XIVd | -610.843457 | -610.832875 | -610.87847 |
| XIVE | -650.120556 | -650.10885 | -650.156761 |
| XV | -1863.554247 | -1863.529792 | -1863.609789 |
| TS-XVI | -1863.529698 | -1863.504987 | -1863.586241 |
| XVII | -901.918478 | -901.902411 | -901.960548 |
| TS-XVIII | -901.887367 | -901.872325 | -901.928072 |

| | | | |
|------------------------|-------------|-------------|-------------|
| XIX | -492.932161 | -492.924202 | -492.964057 |
| XXa | -902.748289 | -902.732076 | -902.791739 |
| XXIa | -650.464621 | -650.451389 | -650.502628 |
| XXIIa | -901.918478 | -901.902411 | -901.960548 |
| XXIIIa | -651.31932 | -651.305566 | -651.358494 |
| XXb | -942.039661 | -942.021157 | -942.086386 |
| XXIb | -689.767559 | -689.751813 | -689.809439 |
| XXIIb | -941.203975 | -941.185666 | -941.249645 |
| XXIIIb | -690.606839 | -690.59089 | -690.649451 |
| XXIV | -942.039661 | -942.021157 | -942.086386 |
| XXV | -689.767559 | -689.751813 | -689.809439 |
| XXVI | -941.203975 | -941.185666 | -941.249645 |
| XXVII | -690.606839 | -690.59089 | -690.649451 |
| OTf | -961.609638 | -961.601423 | -961.642198 |
| HOTf | -962.005744 | -961.996921 | -962.039088 |
| TMS⁺ | -408.960647 | -408.951919 | -408.993126 |

^a Computed at the B3LYP/6-31+g(d) level.

Cartesian Coordinates of Stationary Points

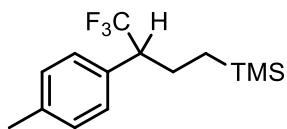
Ia. trimethyl(4,4,4-trifluoro-3-(4-methoxyphenyl)butyl)silane



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.00009100 | 0.00295700 | 0.03232100 |
| C | -0.00391600 | -0.00398900 | 1.55775200 |
| F | 1.26349300 | 0.01202000 | 2.05967400 |
| F | -0.61751600 | -1.07869000 | 2.12441400 |
| F | -0.62481100 | 1.09672700 | 2.06745400 |
| C | 0.86065700 | -1.14681100 | -0.57991100 |
| H | 0.96449000 | -0.89053200 | -1.64136700 |
| H | 1.86618400 | -1.06628900 | -0.14941000 |
| C | 0.34558400 | -2.58963200 | -0.44757600 |
| H | 0.23745900 | -2.86371400 | 0.61042100 |
| H | -0.65762500 | -2.67396500 | -0.88800800 |
| C | -1.39270100 | 0.14598000 | -0.56891800 |
| C | -2.47292900 | -0.70064000 | -0.25563200 |
| C | -1.61390300 | 1.15132100 | -1.51795000 |
| C | -3.71295100 | -0.54371200 | -0.86828800 |
| H | -2.35660300 | -1.48980100 | 0.47917300 |
| C | -2.85114900 | 1.31912400 | -2.15038600 |
| H | -0.80373400 | 1.82821400 | -1.78055200 |
| C | -3.91174400 | 0.46538200 | -1.82360700 |
| H | -4.54105500 | -1.20017500 | -0.61621400 |
| H | -2.96990800 | 2.11286600 | -2.87904200 |
| C | 1.52547700 | -3.62686700 | -3.14402000 |
| H | 0.52392900 | -3.63690800 | -3.59335100 |
| H | 1.99131100 | -2.66323800 | -3.38658700 |
| H | 2.11751300 | -4.41202500 | -3.63227600 |
| C | 3.18887500 | -3.87363300 | -0.54115600 |
| H | 3.16820600 | -4.01124300 | 0.54781400 |
| H | 3.80901400 | -4.67352500 | -0.96647400 |
| H | 3.69143600 | -2.92039400 | -0.74841000 |
| C | 0.65498500 | -5.61010200 | -0.93247200 |
| H | 1.24444100 | -6.41671600 | -1.38735500 |
| H | 0.59132200 | -5.81038100 | 0.14499200 |
| H | -0.36116200 | -5.66690000 | -1.34385000 |
| Si | 1.43904400 | -3.91792100 | -1.27173300 |
| H | 0.54149500 | 0.92851000 | -0.20015300 |
| O | -5.16222600 | 0.53583900 | -2.37103600 |
| C | -5.42276900 | 1.54418000 | -3.35024500 |
| H | -4.77666700 | 1.41895700 | -4.22722400 |
| H | -6.46499900 | 1.40939900 | -3.64198900 |
| H | -5.28592200 | 2.54738800 | -2.92966100 |

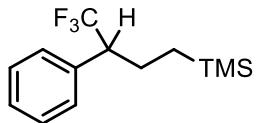
Ib. trimethyl(4,4,4-trifluoro-3-(p-tolyl)butyl)silane



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | 0.00481000 | 0.00269900 | -0.00700200 |
| C | 0.00962100 | 0.00555600 | 1.51814800 |
| F | 1.28048900 | 0.00270300 | 2.01146400 |
| F | -0.61913000 | -1.05341400 | 2.09681900 |
| F | -0.58825500 | 1.12116700 | 2.02326200 |
| C | 0.83744700 | -1.16832300 | -0.61834700 |
| H | 0.93233600 | -0.92471900 | -1.68357900 |
| H | 1.84936200 | -1.10002200 | -0.20106000 |
| C | 0.30036400 | -2.60090000 | -0.46399400 |
| H | 0.20463100 | -2.86285700 | 0.59822600 |
| H | -0.71106800 | -2.67264800 | -0.88746600 |
| C | -1.38796600 | 0.16714800 | -0.60382200 |
| C | -2.48091500 | -0.64957200 | -0.27376600 |
| C | -1.58953700 | 1.16954600 | -1.56565900 |
| C | -3.72323600 | -0.46620900 | -0.88800200 |
| H | -2.37735700 | -1.42993800 | 0.47252800 |
| C | -2.82996200 | 1.34513400 | -2.18236200 |
| H | -0.76533400 | 1.82648300 | -1.83604700 |
| C | -3.92254300 | 0.52778400 | -1.85681600 |
| H | -4.55239100 | -1.11113800 | -0.60433700 |
| H | -2.95007800 | 2.13537700 | -2.92069500 |
| C | 1.42624200 | -3.68254100 | -3.16687400 |
| H | 0.41884100 | -3.68426000 | -3.60304600 |
| H | 1.90118700 | -2.72762200 | -3.42555400 |
| H | 2.00161500 | -4.48030100 | -3.65464000 |
| C | 3.12010600 | -3.93186100 | -0.58313200 |
| H | 3.11066000 | -4.05908800 | 0.50726100 |
| H | 3.72174800 | -4.74581400 | -1.00835200 |
| H | 3.63575100 | -2.98903200 | -0.80535800 |
| C | 0.55388600 | -5.63049600 | -0.92615800 |
| H | 1.12514600 | -6.45031000 | -1.38067500 |
| H | 0.49994900 | -5.82018800 | 0.15373300 |
| H | -0.46786900 | -5.67489700 | -1.32500500 |
| Si | 1.36050400 | -3.95434100 | -1.29091000 |
| H | 0.56328600 | 0.91566400 | -0.24882500 |
| C | -5.25958600 | 0.70013000 | -2.54063900 |
| H | -6.07789900 | 0.31983000 | -1.92000100 |
| H | -5.46105800 | 1.75323200 | -2.76610400 |
| H | -5.28840700 | 0.15286100 | -3.49262500 |

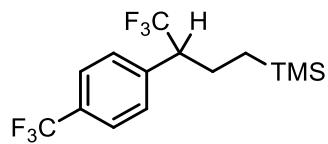
Ic. trimethyl(4,4,4-trifluoro-3-phenylbutyl)silane



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | -0.00126500 | 0.00115300 | -0.00277100 |
| C | 0.00074600 | 0.00312900 | 1.52249700 |
| F | 1.27089600 | 0.01227200 | 2.01640500 |
| F | -0.61834200 | -1.06201800 | 2.09985600 |
| F | -0.60857800 | 1.11281800 | 2.02656300 |
| C | 0.83505900 | -1.16730200 | -0.61434600 |
| H | 0.93470000 | -0.92029000 | -1.67833100 |
| H | 1.84480300 | -1.09853700 | -0.19210100 |
| C | 0.29901900 | -2.60085400 | -0.46649200 |
| H | 0.19960700 | -2.86631100 | 0.59446600 |
| H | -0.71057200 | -2.67296900 | -0.89429300 |
| C | -1.39327800 | 0.16141300 | -0.60400900 |
| C | -2.48425900 | -0.65607100 | -0.26463600 |
| C | -1.58414200 | 1.15468000 | -1.57838700 |
| C | -3.72610100 | -0.48162400 | -0.88391000 |
| H | -2.37597200 | -1.42930800 | 0.48806200 |
| C | -2.82203400 | 1.32594800 | -2.20400700 |
| H | -0.75397400 | 1.80245800 | -1.85170500 |
| C | -3.90036300 | 0.50672800 | -1.85705200 |
| H | -4.55767100 | -1.12299200 | -0.60319400 |
| H | -2.94306700 | 2.10220500 | -2.95520200 |
| C | 1.43643400 | -3.67279800 | -3.16837800 |
| H | 0.43069000 | -3.67515500 | -3.60832800 |
| H | 1.91050700 | -2.71619200 | -3.42240100 |
| H | 2.01522000 | -4.46794100 | -3.65636000 |
| C | 3.12124200 | -3.92689100 | -0.57922000 |
| H | 3.10802600 | -4.05638300 | 0.51086300 |
| H | 3.72549800 | -4.73915400 | -1.00395200 |
| H | 3.63643200 | -2.98294700 | -0.79772200 |
| C | 0.55874500 | -5.62849900 | -0.93604800 |
| H | 1.13161200 | -6.44613500 | -1.39244400 |
| H | 0.50329100 | -5.82194300 | 0.14309300 |
| H | -0.46229500 | -5.67256100 | -1.33673400 |
| Si | 1.36437400 | -3.95041600 | -1.29356000 |
| H | 0.55501000 | 0.91575900 | -0.24288300 |
| H | -4.86645100 | 0.63890400 | -2.33711300 |

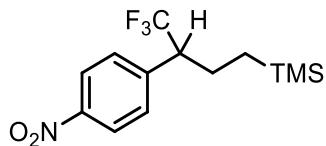
Id. trimethyl(4,4,4-trifluoro-3-(4-(trifluoromethyl)phenyl)butyl)silane



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.00108900 | -0.00310900 | -0.00678900 |
| C | -0.00518000 | -0.00005200 | 1.51900200 |
| F | 1.26261300 | -0.00667100 | 2.01413000 |
| F | -0.64031200 | -1.05697000 | 2.09286700 |
| F | -0.60327900 | 1.11752500 | 2.01736200 |
| C | 0.81222100 | -1.18879400 | -0.61800400 |
| H | 0.92258200 | -0.94208000 | -1.68083800 |
| H | 1.82038100 | -1.13995400 | -0.18995800 |
| C | 0.24513300 | -2.61032500 | -0.47354400 |
| H | 0.13715900 | -2.87537200 | 0.58651100 |
| H | -0.76388700 | -2.66279000 | -0.90576200 |
| C | -1.38691800 | 0.17544900 | -0.61385100 |
| C | -2.49615500 | -0.60746700 | -0.25825900 |
| C | -1.55092300 | 1.14638000 | -1.61542000 |
| C | -3.73186300 | -0.42379000 | -0.88191600 |
| H | -2.41115400 | -1.36569700 | 0.51139600 |
| C | -2.77750600 | 1.33136600 | -2.24999400 |
| H | -0.70744400 | 1.76696300 | -1.90647000 |
| C | -3.87309900 | 0.54216600 | -1.88190000 |
| H | -4.57651500 | -1.03843100 | -0.58895100 |
| H | -2.87726400 | 2.08707000 | -3.02307300 |
| C | 1.36192800 | -3.70306300 | -3.17476900 |
| H | 0.35576000 | -3.69113800 | -3.61356900 |
| H | 1.84985800 | -2.75383300 | -3.43019100 |
| H | 1.92836400 | -4.50699600 | -3.66281100 |
| C | 3.04512500 | -3.98102000 | -0.58637500 |
| H | 3.03061800 | -4.10577300 | 0.50422800 |
| H | 3.63516600 | -4.80520500 | -1.00809300 |
| H | 3.57627000 | -3.04700600 | -0.80934900 |
| C | 0.45557300 | -5.64271100 | -0.93937700 |
| H | 1.01549600 | -6.46966700 | -1.39502800 |
| H | 0.39796600 | -5.83372100 | 0.14003400 |
| H | -0.56622400 | -5.67154000 | -1.33946300 |
| Si | 1.28813500 | -3.97899400 | -1.30001100 |
| H | 0.57077000 | 0.90129800 | -0.24737600 |
| C | -5.20459300 | 0.77868900 | -2.53587000 |
| F | -5.09213200 | 1.00635000 | -3.87245300 |
| F | -6.05953100 | -0.26357900 | -2.38661400 |
| F | -5.84312600 | 1.87296000 | -2.02390000 |

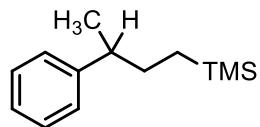
Ie. trimethyl(4,4,4-trifluoro-3-(4-nitrophenyl)butyl)silane



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.00151000 | -0.00275400 | -0.00221900 |
| C | -0.00319700 | -0.00275200 | 1.52417300 |
| F | 1.26518700 | -0.00819400 | 2.01457000 |
| F | -0.63580800 | -1.06158700 | 2.09623300 |
| F | -0.60275400 | 1.11304700 | 2.02371100 |
| C | 0.80094600 | -1.19446300 | -0.61906500 |
| H | 0.91572600 | -0.94379000 | -1.68037100 |
| H | 1.80816600 | -1.15507300 | -0.18823100 |
| C | 0.22020100 | -2.61079000 | -0.48090800 |
| H | 0.10550500 | -2.87818300 | 0.57772500 |
| H | -0.78700200 | -2.65425900 | -0.91835100 |
| C | -1.38590600 | 0.18109300 | -0.60739800 |
| C | -2.49986600 | -0.59376600 | -0.23904900 |
| C | -1.54266100 | 1.14518000 | -1.61828900 |
| C | -3.73414900 | -0.41227700 | -0.85861800 |
| H | -2.41638100 | -1.34362900 | 0.53835700 |
| C | -2.76567600 | 1.33655200 | -2.25448400 |
| H | -0.69545200 | 1.75742600 | -1.91420500 |
| C | -3.85063800 | 0.55072400 | -1.86219400 |
| H | -4.59164600 | -1.00825700 | -0.57114600 |
| H | -2.87997800 | 2.08141700 | -3.03241300 |
| C | 1.33838700 | -3.70553400 | -3.18037800 |
| H | 0.33393600 | -3.68126500 | -3.62255500 |
| H | 1.83778700 | -2.76109500 | -3.43136600 |
| H | 1.89753900 | -4.51426500 | -3.66885500 |
| C | 3.00944000 | -4.00339300 | -0.58617300 |
| H | 2.98994900 | -4.12935800 | 0.50420100 |
| H | 3.59391900 | -4.83211600 | -1.00672800 |
| H | 3.54950600 | -3.07380300 | -0.80620500 |
| C | 0.40750100 | -5.64322300 | -0.95242200 |
| H | 0.96286900 | -6.47397200 | -1.40671600 |
| H | 0.34366600 | -5.83516600 | 0.12644400 |
| H | -0.61268400 | -5.66342200 | -1.35707900 |
| Si | 1.25568500 | -3.98638100 | -1.30690500 |
| H | 0.57506800 | 0.89811500 | -0.24346200 |
| N | -5.14454600 | 0.74292400 | -2.51903800 |
| O | -5.22942100 | 1.59777700 | -3.40729500 |
| O | -6.09556500 | 0.04174600 | -2.15748800 |

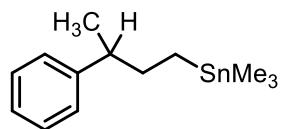
If. trimethyl(3-phenylbutyl)silane



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | -0.01866800 | 0.00520100 | 0.05897300 |
| C | 0.07402500 | -0.11110000 | 1.58947800 |
| C | 1.38819900 | 0.04311200 | -0.61200800 |
| H | 1.24361600 | 0.26441800 | -1.67817900 |
| H | 1.92341300 | 0.90602000 | -0.19053400 |
| C | 2.25230800 | -1.22230800 | -0.46253000 |
| H | 2.42655200 | -1.43916100 | 0.60186100 |
| H | 1.71195600 | -2.09342900 | -0.86181000 |
| C | -0.92998800 | -1.03347500 | -0.58626900 |
| C | -1.07212800 | -2.34005900 | -0.09114000 |
| C | -1.64995200 | -0.69211600 | -1.74491100 |
| C | -1.89824900 | -3.27144400 | -0.73145500 |
| H | -0.53807800 | -2.64159800 | 0.80536500 |
| C | -2.47540300 | -1.61691500 | -2.39044600 |
| H | -1.56476600 | 0.31719100 | -2.14433300 |
| C | -2.60301000 | -2.91549900 | -1.88491400 |
| H | -1.99069400 | -4.27586300 | -0.32475600 |
| H | -3.02293100 | -1.32191800 | -3.28256100 |
| C | 3.74463000 | -0.90848600 | -3.18492500 |
| H | 3.15126600 | -1.71776700 | -3.63029300 |
| H | 3.24063600 | 0.03917900 | -3.41389800 |
| H | 4.72018600 | -0.89478300 | -3.68852900 |
| C | 4.99303600 | 0.26260500 | -0.60587700 |
| H | 5.12798000 | 0.15418500 | 0.47833900 |
| H | 5.99019700 | 0.28343700 | -1.06492000 |
| H | 4.52446600 | 1.23829900 | -0.78766800 |
| C | 4.84572600 | -2.80249500 | -1.00055700 |
| H | 5.83564100 | -2.81388200 | -1.47529300 |
| H | 4.98934500 | -2.97842100 | 0.07357300 |
| H | 4.27359100 | -3.64845400 | -1.40345400 |
| Si | 3.95365200 | -1.15800900 | -1.31528400 |
| H | -0.46880800 | 0.98501200 | -0.15676600 |
| H | -3.24723500 | -3.63753400 | -2.38039600 |
| H | 0.66551100 | 0.72015900 | 1.99236600 |
| H | -0.92100100 | -0.07141900 | 2.04849100 |
| H | 0.55317400 | -1.04091500 | 1.91434400 |

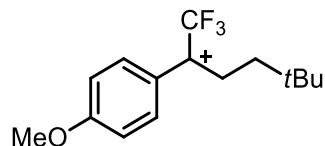
Ig. trimethyl(3-phenylbutyl)stannane



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | -0.13327400 | 0.01918100 | 0.06379600 |
| C | -0.06214400 | -0.05653100 | 1.59824700 |
| C | 1.28546700 | 0.02785100 | -0.58762400 |
| H | 1.15666000 | 0.22965200 | -1.66004300 |
| H | 1.82029900 | 0.89625100 | -0.17592300 |
| C | 2.13228600 | -1.24118300 | -0.40017500 |
| H | 2.29703800 | -1.44665500 | 0.66584900 |
| H | 1.60678500 | -2.11561400 | -0.80598300 |
| C | -1.04283300 | -1.03013600 | -0.56536900 |
| C | -1.18813500 | -2.32698400 | -0.04493000 |
| C | -1.75741800 | -0.71125800 | -1.73395500 |
| C | -2.01268100 | -3.27024700 | -0.67017200 |
| H | -0.65820700 | -2.61098600 | 0.85967800 |
| C | -2.58118100 | -1.64831300 | -2.36480500 |
| H | -1.66934700 | 0.28971900 | -2.15317100 |
| C | -2.71246000 | -2.93664100 | -1.83386600 |
| H | -2.10792500 | -4.26631700 | -0.24405000 |
| H | -3.12443600 | -1.37064000 | -3.26504600 |
| C | 3.87201800 | -0.83201300 | -3.46058600 |
| H | 3.28265100 | -1.63137600 | -3.92470000 |
| H | 3.37033500 | 0.12229800 | -3.65842500 |
| H | 4.85564200 | -0.80693600 | -3.94412200 |
| C | 5.26095600 | 0.42253800 | -0.48610100 |
| H | 5.40444000 | 0.26585800 | 0.58938600 |
| H | 6.24855800 | 0.46581200 | -0.96025700 |
| H | 4.77120700 | 1.39281300 | -0.62842600 |
| C | 5.08589400 | -3.05104600 | -1.01414600 |
| H | 6.08353500 | -3.04358800 | -1.46855200 |
| H | 5.19974600 | -3.24815200 | 0.05820600 |
| H | 4.51497900 | -3.87648300 | -1.45523600 |
| H | -0.57176700 | 0.99645800 | -0.18530800 |
| H | -3.35527100 | -3.66785800 | -2.31752800 |
| H | 0.52497900 | 0.78452500 | 1.98723500 |
| H | -1.06335300 | -0.00390700 | 2.04248500 |
| H | 0.41162200 | -0.97801000 | 1.95338300 |
| Sn | 4.08353300 | -1.17031800 | -1.34068300 |

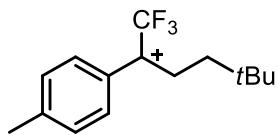
IIa. 1,1,1-trifluoro-2-(4-methoxyphenyl)-5,5-dimethylhexan-2-ylum



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | 0.00538400 | 0.01773400 | -0.01162700 |
| C | 0.01219100 | 0.01860100 | 1.52644900 |
| F | 1.25880500 | 0.01426000 | 2.03240100 |
| F | -0.62098100 | -1.06812200 | 2.02808400 |
| F | -0.60829300 | 1.11894700 | 2.01390200 |
| C | 1.35065600 | -0.00734600 | -0.65326300 |
| H | 1.30593200 | 0.41078700 | -1.65793400 |
| H | 2.03068000 | 0.61849900 | -0.06906400 |
| C | 1.91401600 | -1.46606900 | -0.70873700 |
| H | 1.88459900 | -1.90619500 | 0.29486900 |
| H | 1.24186000 | -2.06272500 | -1.33781000 |
| C | -1.20860200 | -0.00036000 | -0.67914300 |
| C | -2.48948800 | -0.00290900 | 0.00553500 |
| C | -1.24463400 | -0.03141500 | -2.12659100 |
| C | -3.66213900 | -0.03947300 | -0.68592300 |
| H | -2.53159300 | 0.02565600 | 1.08570300 |
| C | -2.41817300 | -0.07591300 | -2.82474900 |
| H | -0.31898700 | -0.02658600 | -2.68698000 |
| C | -3.65359800 | -0.08172200 | -2.11295000 |
| H | -4.61982400 | -0.04086800 | -0.17722500 |
| H | -2.40195800 | -0.10340700 | -3.90693200 |
| C | 3.46775300 | -1.02485800 | -2.68753100 |
| H | 2.73059000 | -1.49338000 | -3.35210000 |
| H | 3.31632200 | 0.06069700 | -2.72122000 |
| H | 4.46425000 | -1.22449500 | -3.09973800 |
| C | 4.36466600 | -0.86002300 | -0.33447700 |
| H | 4.30159300 | -1.23593600 | 0.69446700 |
| H | 5.38997200 | -1.02214100 | -0.68835900 |
| H | 4.19801700 | 0.22355800 | -0.31150300 |
| C | 3.70425700 | -3.09042000 | -1.27894900 |
| H | 4.72402000 | -3.24504900 | -1.65215500 |
| H | 3.64362200 | -3.52841200 | -0.27486600 |
| H | 3.01866900 | -3.64336900 | -1.93306100 |
| C | 3.36361400 | -1.58399500 | -1.25521200 |
| O | -4.83405600 | -0.12326700 | -2.68262000 |
| C | -4.98105900 | -0.17464700 | -4.12693000 |
| H | -4.49887500 | -1.07338000 | -4.51716000 |
| H | -6.05535800 | -0.21641900 | -4.29234500 |
| H | -4.56079700 | 0.72859400 | -4.57389300 |

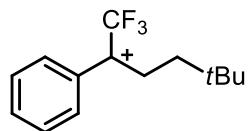
IIb. 1,1,1-trifluoro-5,5-dimethyl-2-(p-tolyl)hexan-2-ylion



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | 0.00139600 | 0.00495800 | -0.02837900 |
| C | 0.01180800 | -0.00595900 | 1.51406000 |
| F | 1.25793900 | 0.03323000 | 2.01536100 |
| F | -0.57854600 | -1.12047100 | 2.00072900 |
| F | -0.64866000 | 1.06720900 | 2.00279300 |
| C | 1.33759400 | 0.02205200 | -0.66910700 |
| H | 1.28457300 | 0.43149700 | -1.67633200 |
| H | 2.00760100 | 0.65542400 | -0.08154700 |
| C | 1.92861500 | -1.43356700 | -0.71837500 |
| H | 1.91413800 | -1.86649900 | 0.28800200 |
| H | 1.26363100 | -2.04334300 | -1.34115200 |
| C | -1.21970500 | -0.04538200 | -0.69879400 |
| C | -2.48777400 | -0.09852600 | -0.00773700 |
| C | -1.25633100 | -0.05481000 | -2.14149200 |
| C | -3.66846400 | -0.15640600 | -0.70573400 |
| H | -2.52520400 | -0.09453800 | 1.07302600 |
| C | -2.44752700 | -0.12000100 | -2.81980700 |
| H | -0.33550000 | -0.01631400 | -2.70849200 |
| C | -3.68148600 | -0.16771700 | -2.12297800 |
| H | -4.60898700 | -0.19751500 | -0.16572700 |
| H | -2.44906200 | -0.13224100 | -3.90504900 |
| C | 3.45775500 | -0.97499500 | -2.71310000 |
| H | 2.72751600 | -1.46889800 | -3.36662500 |
| H | 3.28129900 | 0.10629200 | -2.75896200 |
| H | 4.45587600 | -1.15609100 | -3.12957100 |
| C | 4.36660900 | -0.76107600 | -0.36793500 |
| H | 4.31630800 | -1.12301000 | 0.66656600 |
| H | 5.39309400 | -0.90711700 | -0.72495000 |
| H | 4.17855000 | 0.31929500 | -0.36074700 |
| C | 3.74997800 | -3.01844700 | -1.28121700 |
| H | 4.76998300 | -3.15345300 | -1.66098500 |
| H | 3.70756100 | -3.44491400 | -0.27148400 |
| H | 3.07214400 | -3.59406700 | -1.92344800 |
| C | 3.37769200 | -1.51858300 | -1.27376000 |
| C | -4.97327300 | -0.19839600 | -2.86882600 |
| H | -5.30838800 | 0.83642400 | -3.04025000 |
| H | -4.86477200 | -0.67013800 | -3.84933600 |
| H | -5.75839700 | -0.70128500 | -2.29739300 |

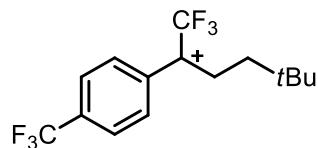
IIe. 1,1,1-trifluoro-5,5-dimethyl-2-phenylhexan-2-ylum



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|--------------|-------------|-------------|
| 1 1 | | | |
| C | 0.00522100 | 0.00606000 | -0.02587600 |
| C | 0.01886200 | -0.01568800 | 1.51915100 |
| F | 1.26504600 | 0.02618000 | 2.01692100 |
| F | -0.565556800 | -1.13622500 | 1.99497000 |
| F | -0.64572000 | 1.05207200 | 2.01030200 |
| C | 1.33507200 | 0.03128900 | -0.66567000 |
| H | 1.28571500 | 0.44115700 | -1.67244900 |
| H | 2.00971400 | 0.65401000 | -0.07227700 |
| C | 1.92058700 | -1.43263500 | -0.71842600 |
| H | 1.90659400 | -1.86671900 | 0.28695500 |
| H | 1.25225700 | -2.03617600 | -1.34286500 |
| C | -1.22296700 | -0.04576500 | -0.69694700 |
| C | -2.48236800 | -0.11295600 | 0.00373500 |
| C | -1.25438500 | -0.03840600 | -2.13745600 |
| C | -3.67029800 | -0.16733400 | -0.69355200 |
| H | -2.51206700 | -0.12058400 | 1.08448200 |
| C | -2.45146500 | -0.10061200 | -2.81703100 |
| H | -0.33318000 | 0.01379200 | -2.70228500 |
| C | -3.66008300 | -0.16195700 | -2.09971600 |
| H | -4.61190700 | -0.21552500 | -0.15771700 |
| H | -2.46257800 | -0.09699600 | -3.90142900 |
| C | 3.44703100 | -0.96978400 | -2.71520200 |
| H | 2.71409000 | -1.46085600 | -3.36768200 |
| H | 3.27455400 | 0.11219500 | -2.75978100 |
| H | 4.44377000 | -1.15358600 | -3.13354800 |
| C | 4.35966200 | -0.75981000 | -0.37065300 |
| H | 4.30987500 | -1.12241800 | 0.66353600 |
| H | 5.38528600 | -0.90750100 | -0.72914300 |
| H | 4.17423100 | 0.32104400 | -0.36294000 |
| C | 3.73718000 | -3.01598500 | -1.28528700 |
| H | 4.75629100 | -3.15131100 | -1.66713500 |
| H | 3.69616400 | -3.44293000 | -0.27585900 |
| H | 3.05743300 | -3.58951900 | -1.92709700 |
| C | 3.36923500 | -1.51437700 | -1.27650400 |
| H | -4.60083300 | -0.20433200 | -2.64074500 |

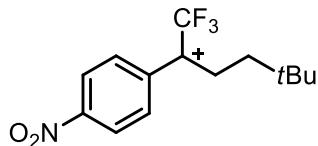
IIId. 1,1,1-trifluoro-5,5-dimethyl-2-(4-(trifluoromethyl)phenyl)hexan-2-ylium



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | -0.00087800 | -0.00151100 | 0.01026700 |
| C | -0.00639600 | -0.01515900 | 1.55729700 |
| F | 1.23290500 | 0.00952700 | 2.06831300 |
| F | -0.61609700 | -1.12471200 | 2.02390300 |
| F | -0.66108800 | 1.06529700 | 2.02844500 |
| C | 1.32500600 | -0.04420600 | -0.61512800 |
| H | 1.30696600 | 0.33769700 | -1.63308400 |
| H | 2.03177500 | 0.54431600 | -0.02484700 |
| C | 1.83321300 | -1.54863100 | -0.63081400 |
| H | 1.80976800 | -1.94944800 | 0.38718200 |
| H | 1.12919300 | -2.13174400 | -1.23380700 |
| C | -1.23172000 | -0.00286500 | -0.67730100 |
| C | -2.49243600 | -0.05254000 | 0.00875900 |
| C | -1.24889100 | 0.04181400 | -2.11131700 |
| C | -3.67947500 | -0.06513800 | -0.69736800 |
| H | -2.53811700 | -0.08728200 | 1.08817600 |
| C | -2.44091000 | 0.02524000 | -2.80671100 |
| H | -0.32543700 | 0.09252600 | -2.67220100 |
| C | -3.65300400 | -0.02893400 | -2.09972600 |
| H | -4.62241800 | -0.10885100 | -0.16527300 |
| H | -2.43593100 | 0.05468600 | -3.89011100 |
| C | 3.35199800 | -1.22438100 | -2.66155800 |
| H | 2.59223100 | -1.71080600 | -3.28594100 |
| H | 3.22445800 | -0.13880800 | -2.74824300 |
| H | 4.33533400 | -1.46635600 | -3.08165200 |
| C | 4.30322300 | -0.96295100 | -0.33668900 |
| H | 4.24975000 | -1.28088700 | 0.71177600 |
| H | 5.31669400 | -1.17128000 | -0.69925200 |
| H | 4.16710300 | 0.12469900 | -0.37212800 |
| C | 3.56925300 | -3.22490600 | -1.15271100 |
| H | 4.57487800 | -3.41849200 | -1.54484300 |
| H | 3.52758500 | -3.60697800 | -0.12576000 |
| H | 2.85468300 | -3.79327700 | -1.75991000 |
| C | 3.27091700 | -1.70737100 | -1.20190100 |
| C | -4.96154500 | -0.00267900 | -2.87119300 |
| F | -4.85091900 | -0.61954000 | -4.06588900 |
| F | -5.96025300 | -0.60185900 | -2.19184100 |
| F | -5.34041100 | 1.27633100 | -3.10836300 |

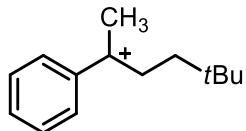
IIe. 1,1,1-trifluoro-5,5-dimethyl-2-(4-nitrophenyl)hexan-2-ylum



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | 0.00762700 | 0.03057700 | -0.05711600 |
| C | 0.05170800 | 0.07373900 | 1.48929600 |
| F | 1.30608500 | 0.06020500 | 1.95954500 |
| F | -0.59331000 | -0.98294800 | 2.02213200 |
| F | -0.53914600 | 1.20419300 | 1.92618400 |
| C | 1.30696200 | -0.01289900 | -0.72720200 |
| H | 1.25946100 | 0.38102300 | -1.74021000 |
| H | 2.04276500 | 0.55496000 | -0.15356400 |
| C | 1.79273800 | -1.52952700 | -0.77876200 |
| H | 1.74504900 | -1.96411200 | 0.22448600 |
| H | 1.08749700 | -2.07791600 | -1.41205200 |
| C | -1.24917200 | -0.00937100 | -0.70563000 |
| C | -2.48492100 | 0.00635900 | 0.02251600 |
| C | -1.30510800 | -0.07038600 | -2.13610300 |
| C | -3.69663600 | -0.03945800 | -0.64239700 |
| H | -2.49707100 | 0.05736100 | 1.10206800 |
| C | -2.51653600 | -0.12826700 | -2.79850700 |
| H | -0.39784100 | -0.07706500 | -2.72449800 |
| C | -3.68733300 | -0.11029900 | -2.03671800 |
| H | -4.63247700 | -0.02488400 | -0.09868400 |
| H | -2.56289400 | -0.18103700 | -3.87862100 |
| C | 3.36108600 | -1.12592300 | -2.75777000 |
| H | 2.60349900 | -1.55675900 | -3.42403900 |
| H | 3.26227800 | -0.03409800 | -2.78508900 |
| H | 4.34714700 | -1.36856400 | -3.17082400 |
| C | 4.26964800 | -1.02329700 | -0.40299200 |
| H | 4.18765700 | -1.40220000 | 0.62302400 |
| H | 5.28454200 | -1.23487000 | -0.75920400 |
| H | 4.16073900 | 0.06752900 | -0.37514700 |
| C | 3.49459500 | -3.21494900 | -1.36142800 |
| H | 4.50437500 | -3.41156200 | -1.74112400 |
| H | 3.41860500 | -3.65376900 | -0.35953600 |
| H | 2.78096900 | -3.72782000 | -2.01689200 |
| C | 3.23790100 | -1.68843900 | -1.33054100 |
| N | -4.99293200 | -0.17132300 | -2.74884900 |
| O | -4.96373700 | -0.26682700 | -3.97271900 |
| O | -6.01176800 | -0.12380800 | -2.06531900 |

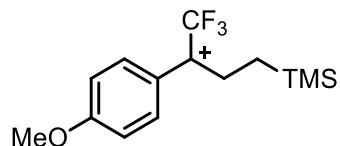
IIf. 5,5-dimethyl-2-phenylhexan-2-ylum



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| 1 1 | | | |
| C | 0.09920500 | -0.07389700 | -0.00406000 |
| C | 0.15634800 | -0.00166600 | 1.48244900 |
| C | 1.41621200 | -0.06593900 | -0.68979700 |
| H | 1.36301400 | 0.35308300 | -1.69413500 |
| H | 2.10678000 | 0.54305400 | -0.09739000 |
| C | 1.96981400 | -1.53237600 | -0.75502200 |
| H | 1.94876800 | -1.96768500 | 0.25125400 |
| H | 1.28934700 | -2.12738500 | -1.37572700 |
| C | 4.42500100 | -0.90856800 | -0.43042600 |
| H | 4.26489600 | 0.17611600 | -0.44280900 |
| H | 4.36885300 | -1.24987400 | 0.61105100 |
| H | 5.44624600 | -1.08859800 | -0.78714700 |
| C | 3.75653400 | -3.16279100 | -1.31173200 |
| H | 3.05888100 | -3.73356100 | -1.93704000 |
| H | 4.76846300 | -3.32403000 | -1.70288200 |
| H | 3.71889100 | -3.57526400 | -0.29585500 |
| C | 3.49426500 | -1.13141100 | -2.76509800 |
| H | 4.48907500 | -1.32734100 | -3.18308200 |
| H | 2.75697800 | -1.62636300 | -3.40995100 |
| H | 3.32670000 | -0.04934700 | -2.82305900 |
| C | -1.13458300 | -0.15167000 | -0.70762200 |
| C | -2.38019500 | -0.12750100 | -0.00779900 |
| C | -1.16686700 | -0.24626400 | -2.13312000 |
| C | -3.57990400 | -0.18678600 | -0.69531500 |
| H | -2.39793500 | -0.05037800 | 1.07216600 |
| C | -2.37178300 | -0.32218200 | -2.81049300 |
| H | -0.24589600 | -0.26650900 | -2.70211300 |
| C | -3.57837000 | -0.28907000 | -2.09512200 |
| H | -4.51906500 | -0.15900400 | -0.15267600 |
| H | -2.38217900 | -0.40120400 | -3.89254000 |
| H | -4.52198400 | -0.34244200 | -2.63050400 |
| H | 1.13358500 | -0.31870400 | 1.85371300 |
| H | 0.04057200 | 1.05781300 | 1.76580300 |
| H | -0.62850800 | -0.56365400 | 1.99020000 |
| C | 3.41301000 | -1.65662400 | -1.31878600 |

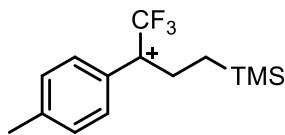
IIIa. 1,1,1-trifluoro-2-(4-methoxyphenyl)-4-(trimethylsilyl)butan-2-ylum



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | -0.00140900 | -0.01689400 | -0.02081500 |
| C | 0.01291700 | -0.01614500 | 1.51709300 |
| F | 1.26131000 | -0.02870900 | 2.01880700 |
| F | -0.62855800 | -1.09488300 | 2.02557500 |
| F | -0.59524500 | 1.09183800 | 2.00355000 |
| C | 1.34056800 | -0.09639200 | -0.66609300 |
| H | 1.30881000 | 0.29091500 | -1.68381400 |
| H | 2.04827000 | 0.52066600 | -0.10588300 |
| C | 1.83254700 | -1.58103600 | -0.67070600 |
| H | 1.87372000 | -1.97347800 | 0.35299400 |
| H | 1.10930400 | -2.20060000 | -1.21610700 |
| C | -1.22067100 | 0.00482500 | -0.68286300 |
| C | -2.49639800 | 0.01517200 | 0.00860600 |
| C | -1.26518200 | 0.01846700 | -2.12884100 |
| C | -3.67404100 | 0.04304300 | -0.67636600 |
| H | -2.53233300 | 0.00232200 | 1.08930600 |
| C | -2.44382100 | 0.04201200 | -2.82108100 |
| H | -0.34308500 | 0.00862800 | -2.69498600 |
| C | -3.67447300 | 0.05999200 | -2.10295900 |
| H | -4.62821100 | 0.05416300 | -0.16117500 |
| H | -2.43365000 | 0.05177100 | -3.90366300 |
| C | 3.52818400 | -1.26175400 | -3.26512600 |
| H | 2.78100900 | -1.82683400 | -3.83664700 |
| H | 3.29396400 | -0.19446200 | -3.36434700 |
| H | 4.50500400 | -1.42906900 | -3.73704300 |
| C | 4.83565100 | -0.79450000 | -0.48564000 |
| H | 4.84963600 | -1.08008100 | 0.57380000 |
| H | 5.84425600 | -0.95572900 | -0.88773700 |
| H | 4.62788700 | 0.28145500 | -0.54259400 |
| C | 3.98003500 | -3.65714200 | -1.33869100 |
| H | 4.96640300 | -3.86007600 | -1.77532000 |
| H | 3.99934300 | -3.99570200 | -0.29525800 |
| H | 3.24351000 | -4.26569900 | -1.87802400 |
| Si | 3.57198100 | -1.81434000 | -1.45589400 |
| O | -4.85949600 | 0.09489700 | -2.66703100 |
| C | -5.01214600 | 0.12412800 | -4.11057600 |
| H | -4.59359100 | -0.78537800 | -4.54657700 |
| H | -6.08707500 | 0.16338500 | -4.27297200 |
| H | -4.53179800 | 1.01692400 | -4.51667500 |

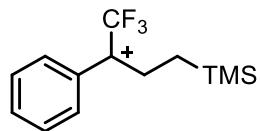
IIIb. 1,1,1-trifluoro-2-(p-tolyl)-4-(trimethylsilyl)butan-2-ylium



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | 0.01384300 | 0.05634400 | -0.03217700 |
| C | 0.04605300 | 0.09636800 | 1.50906800 |
| F | 1.29903900 | 0.08706200 | 1.99499500 |
| F | -0.59800700 | -0.96262600 | 2.04899700 |
| F | -0.54836700 | 1.22318500 | 1.96153400 |
| C | 1.33734100 | -0.05490400 | -0.68849100 |
| H | 1.30936900 | 0.30831000 | -1.71444200 |
| H | 2.07934000 | 0.53206700 | -0.14214100 |
| C | 1.74139700 | -1.57312600 | -0.66270100 |
| H | 1.76411300 | -1.95185800 | 0.36620900 |
| H | 0.98608200 | -2.15827200 | -1.20072700 |
| C | -1.22057300 | 0.06459200 | -0.68760600 |
| C | -2.47703700 | 0.08447700 | 0.02005300 |
| C | -1.27736900 | 0.05109400 | -2.12802300 |
| C | -3.67108600 | 0.08868100 | -0.66183400 |
| H | -2.49927000 | 0.09432700 | 1.10125600 |
| C | -2.47987600 | 0.04920500 | -2.78966800 |
| H | -0.36369600 | 0.03862600 | -2.70778600 |
| C | -3.70537000 | 0.06881900 | -2.07621500 |
| H | -4.60400000 | 0.10287300 | -0.10769200 |
| H | -2.49718600 | 0.03486000 | -3.87502000 |
| C | 3.51445600 | -1.23910200 | -3.20823500 |
| H | 2.71022300 | -1.66492700 | -3.82113700 |
| H | 3.42041200 | -0.14658200 | -3.23490900 |
| H | 4.46889300 | -1.49676700 | -3.68529200 |
| C | 4.79843500 | -1.08355500 | -0.38139000 |
| H | 4.76970600 | -1.45200400 | 0.65163100 |
| H | 5.79621700 | -1.29843200 | -0.78523000 |
| H | 4.68349200 | 0.00711500 | -0.35468900 |
| C | 3.68883600 | -3.79076300 | -1.43765400 |
| H | 4.66688200 | -4.06202400 | -1.85567400 |
| H | 3.63497500 | -4.19663200 | -0.42004600 |
| H | 2.91728900 | -4.28416400 | -2.04144800 |
| Si | 3.47269800 | -1.91286400 | -1.44241300 |
| C | -5.00324400 | 0.08674600 | -2.81468700 |
| H | -5.14725300 | 1.07533000 | -3.27482900 |
| H | -4.99645400 | -0.64012900 | -3.63480500 |
| H | -5.85309300 | -0.11098700 | -2.15769400 |

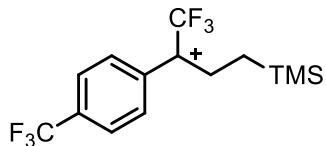
IIIc. 1,1,1-trifluoro-2-phenyl-4-(trimethylsilyl)butan-2-ylum



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | 0.02732200 | 0.05720300 | -0.05137400 |
| C | 0.07505300 | 0.11163100 | 1.49140700 |
| F | 1.33194700 | 0.15133500 | 1.96279900 |
| F | -0.52592400 | -0.96370800 | 2.04514700 |
| F | -0.55377400 | 1.22227000 | 1.93292500 |
| C | 1.33988500 | -0.02895400 | -0.71666500 |
| H | 1.30457400 | 0.31071000 | -1.74967000 |
| H | 2.08597400 | 0.56203000 | -0.18184800 |
| C | 1.73004100 | -1.55540400 | -0.65780300 |
| H | 1.75734000 | -1.91508400 | 0.37729200 |
| H | 0.97371200 | -2.14690900 | -1.18593700 |
| C | -1.22180800 | 0.02924400 | -0.69627800 |
| C | -2.46296500 | 0.00041200 | 0.03225600 |
| C | -1.28565100 | 0.03834500 | -2.13265800 |
| C | -3.66968900 | -0.01456400 | -0.63744700 |
| H | -2.46790800 | -0.01194600 | 1.11343000 |
| C | -2.50029900 | 0.01878000 | -2.78559800 |
| H | -0.37656000 | 0.06310600 | -2.71882700 |
| C | -3.69358200 | -0.00661700 | -2.04226100 |
| H | -4.59876300 | -0.03506200 | -0.07827300 |
| H | -2.53475000 | 0.02685800 | -3.86961400 |
| C | 3.50096700 | -1.26530000 | -3.21135100 |
| H | 2.69423300 | -1.70042200 | -3.81410300 |
| H | 3.41028300 | -0.17326500 | -3.25730600 |
| H | 4.45360700 | -1.53397400 | -3.68600100 |
| C | 4.78731500 | -1.06191600 | -0.38548800 |
| H | 4.75410300 | -1.41061600 | 0.65408300 |
| H | 5.78535500 | -1.28820500 | -0.78242600 |
| H | 4.67651200 | 0.02937700 | -0.38086900 |
| C | 3.66834500 | -3.78681900 | -1.39313100 |
| H | 4.64443200 | -4.06998000 | -1.80794700 |
| H | 3.61504000 | -4.17218200 | -0.36773100 |
| H | 2.89315500 | -4.28712200 | -1.98616100 |
| Si | 3.46594600 | -1.90868900 | -1.43563200 |
| H | -4.64748700 | -0.01936500 | -2.56135900 |

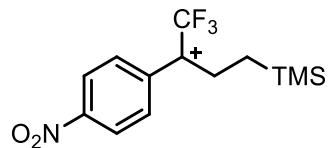
IIIId. 1,1,1-trifluoro-2-(4-(trifluoromethyl)phenyl)-4-(trimethylsilyl)butan-2-ylum



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | -0.00506100 | -0.01792300 | 0.01460900 |
| C | -0.01524300 | -0.03867000 | 1.56004600 |
| F | 1.22237600 | -0.03635400 | 2.07797000 |
| F | -0.65200100 | -1.12686000 | 2.04002000 |
| F | -0.64766600 | 1.06186100 | 2.01769200 |
| C | 1.31447900 | -0.09581700 | -0.60767800 |
| H | 1.33716900 | 0.27882100 | -1.62768600 |
| H | 2.08084500 | 0.40692600 | -0.01740500 |
| C | 1.56510400 | -1.66125400 | -0.58350300 |
| H | 1.58158500 | -2.05174500 | 0.43935900 |
| H | 0.77446600 | -2.18412800 | -1.13069000 |
| C | -1.24289100 | 0.01832000 | -0.68127400 |
| C | -2.50018400 | -0.05463700 | -0.00298600 |
| C | -1.25493100 | 0.15633500 | -2.10489200 |
| C | -3.68902500 | 0.01038800 | -0.70866600 |
| H | -2.54960900 | -0.16553600 | 1.07128500 |
| C | -2.44641400 | 0.21647000 | -2.80160500 |
| H | -0.32965200 | 0.22055300 | -2.66184500 |
| C | -3.66173800 | 0.14329000 | -2.10303500 |
| H | -4.63281500 | -0.04811700 | -0.17943300 |
| H | -2.43638000 | 0.32050700 | -3.88060700 |
| C | 3.30908900 | -1.44429700 | -3.16046300 |
| H | 2.477678900 | -1.84230400 | -3.75354300 |
| H | 3.26181000 | -0.34929800 | -3.19426700 |
| H | 4.24339200 | -1.74607300 | -3.65141200 |
| C | 4.65000600 | -1.33791800 | -0.34889800 |
| H | 4.58766300 | -1.66684800 | 0.69546800 |
| H | 5.62899700 | -1.64564000 | -0.73869700 |
| H | 4.62172100 | -0.24176200 | -0.36402800 |
| C | 3.35114300 | -3.98996400 | -1.35578700 |
| H | 4.30285700 | -4.33261100 | -1.78249700 |
| H | 3.28389400 | -4.37357300 | -0.33091300 |
| H | 2.53865700 | -4.43400500 | -1.94288800 |
| Si | 3.28036900 | -2.10388500 | -1.39407100 |
| C | -4.96246400 | 0.25670100 | -2.87515400 |
| F | -4.88720400 | -0.35932200 | -4.07515500 |
| F | -6.00246900 | -0.28112400 | -2.20542500 |
| F | -5.26262400 | 1.55813100 | -3.11043500 |

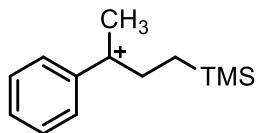
IIIe. 1,1,1-trifluoro-2-(4-nitrophenyl)-4-(trimethylsilyl)butan-2-ylium



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | 0.01544900 | 0.00402000 | -0.01838000 |
| C | 0.02622300 | 0.01652100 | 1.52721300 |
| F | 1.27089000 | 0.03805700 | 2.02695000 |
| F | -0.59971200 | -1.05807700 | 2.04931100 |
| F | -0.60559800 | 1.12781800 | 1.95689000 |
| C | 1.31510600 | -0.07152100 | -0.65955500 |
| H | 1.33774600 | 0.27188900 | -1.68964200 |
| H | 2.11584700 | 0.39210700 | -0.08582200 |
| C | 1.43867500 | -1.65524700 | -0.58814200 |
| H | 1.45094800 | -2.03100800 | 0.43912700 |
| H | 0.62790200 | -2.14648700 | -1.13252600 |
| C | -1.24482400 | 0.04023000 | -0.70144100 |
| C | -2.48311100 | -0.08677000 | -0.00614100 |
| C | -1.27745500 | 0.24673200 | -2.11157700 |
| C | -3.68885200 | -0.00927200 | -0.68548500 |
| H | -2.51176100 | -0.25229500 | 1.06177600 |
| C | -2.48037700 | 0.32738700 | -2.79185000 |
| H | -0.36261700 | 0.35403000 | -2.67905600 |
| C | -3.66444900 | 0.19653600 | -2.06438900 |
| H | -4.63024800 | -0.10672300 | -0.16008700 |
| H | -2.50666100 | 0.49103200 | -3.86154200 |
| C | 3.19846900 | -1.60585700 | -3.17487800 |
| H | 2.32526300 | -1.93813600 | -3.74884100 |
| H | 3.25801200 | -0.51297300 | -3.23691700 |
| H | 4.09364400 | -2.00928900 | -3.66606600 |
| C | 4.54202900 | -1.51147700 | -0.36027000 |
| H | 4.45526900 | -1.80846400 | 0.69150200 |
| H | 5.50159700 | -1.88904000 | -0.73706700 |
| H | 4.58027700 | -0.41667700 | -0.40675900 |
| C | 3.06647000 | -4.10406300 | -1.30511000 |
| H | 3.99166700 | -4.52278500 | -1.72272300 |
| H | 2.97295000 | -4.45579800 | -0.27127200 |
| H | 2.22460800 | -4.50163000 | -1.88360200 |
| Si | 3.14037600 | -2.22169400 | -1.39669600 |
| N | -4.95454900 | 0.28293100 | -2.79121700 |
| O | -4.91332600 | 0.53079800 | -3.99459800 |
| O | -5.98479500 | 0.10087400 | -2.14585300 |

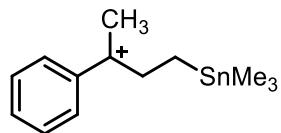
IIIIf. 2-phenyl-4-(trimethylsilyl)butan-2-ylum



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | -0.02579700 | -0.03360500 | 0.07020400 |
| C | -0.01574200 | 0.03585400 | 1.55888200 |
| C | 1.30794500 | -0.02783300 | -0.57826800 |
| H | 1.29061400 | 0.38202400 | -1.58804600 |
| H | 1.99760600 | 0.57112000 | 0.02475200 |
| C | 1.80541900 | -1.51578800 | -0.60393400 |
| H | 1.82883000 | -1.92366500 | 0.41459100 |
| H | 1.09857100 | -2.13144900 | -1.17358800 |
| C | 4.79959200 | -0.71319400 | -0.35661500 |
| H | 4.58572000 | 0.36237400 | -0.39277500 |
| H | 4.79928300 | -1.02305500 | 0.69606100 |
| H | 5.81521400 | -0.85922500 | -0.74659400 |
| C | 3.97385300 | -3.56225600 | -1.28461800 |
| H | 3.25003000 | -4.16156200 | -1.85071700 |
| H | 4.96872500 | -3.75052900 | -1.70832500 |
| H | 3.97644700 | -3.92403400 | -0.24888900 |
| C | 3.53484000 | -1.12911500 | -3.16617000 |
| H | 4.51884800 | -1.28149900 | -3.62804800 |
| H | 2.79880200 | -1.68679000 | -3.75888600 |
| H | 3.29549200 | -0.06148800 | -3.24680200 |
| Si | 3.55913900 | -1.71930300 | -1.36914600 |
| C | -1.24266300 | -0.11775500 | -0.66859100 |
| C | -2.50404700 | -0.09475900 | -0.00097100 |
| C | -1.23886300 | -0.20227700 | -2.09366700 |
| C | -3.68728300 | -0.14061300 | -0.71926300 |
| H | -2.54901100 | -0.02644000 | 1.07899300 |
| C | -2.42701200 | -0.26505800 | -2.80243600 |
| H | -0.30397000 | -0.22897100 | -2.63960600 |
| C | -3.65160500 | -0.23023400 | -2.11882500 |
| H | -4.63934800 | -0.11166000 | -0.19949400 |
| H | -2.40947000 | -0.33633500 | -3.88501900 |
| H | -4.58134700 | -0.27339500 | -2.67882200 |
| H | 0.96671600 | -0.22094700 | 1.95967100 |
| H | -0.21276300 | 1.08309800 | 1.84153000 |
| H | -0.77859500 | -0.57966200 | 2.03876500 |

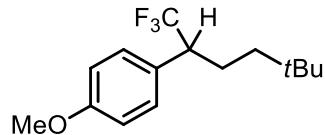
IIIg. 2-phenyl-4-(trimethylstannylyl)butan-2-ylium



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | -0.09002900 | 0.03924600 | 0.08541400 |
| C | -0.10063700 | 0.12714200 | 1.57611100 |
| C | 1.24119700 | 0.06493000 | -0.55562100 |
| H | 1.23059000 | 0.44238500 | -1.57780600 |
| H | 1.93499400 | 0.67030000 | 0.03427000 |
| C | 1.68106500 | -1.44005000 | -0.51564500 |
| H | 1.72004600 | -1.81012600 | 0.51466600 |
| H | 0.96664300 | -2.06461900 | -1.06180400 |
| C | 5.08695700 | -0.64011600 | -0.23634200 |
| H | 4.84500600 | 0.42825100 | -0.24924800 |
| H | 5.09273400 | -0.98314000 | 0.80396800 |
| H | 6.09468300 | -0.76785200 | -0.64759500 |
| C | 4.03140500 | -3.87782600 | -1.27459300 |
| H | 3.27006100 | -4.43157400 | -1.83443300 |
| H | 5.01397600 | -4.11705400 | -1.69668600 |
| H | 4.01133900 | -4.21336000 | -0.23210000 |
| C | 3.61375500 | -1.08206900 | -3.43340000 |
| H | 4.58535800 | -1.25135000 | -3.91121200 |
| H | 2.85101300 | -1.62533100 | -4.00169000 |
| H | 3.38985800 | -0.01091800 | -3.48399800 |
| C | -1.30604200 | -0.09196900 | -0.65948200 |
| C | -2.56439800 | -0.12817800 | 0.00894700 |
| C | -1.30162000 | -0.15215700 | -2.08404500 |
| C | -3.74828100 | -0.20464700 | -0.70869000 |
| H | -2.60988400 | -0.08319000 | 1.09020400 |
| C | -2.48916900 | -0.24187400 | -2.79342000 |
| H | -0.36795000 | -0.13486500 | -2.63259100 |
| C | -3.71370000 | -0.26493000 | -2.10940500 |
| H | -4.69900600 | -0.22157800 | -0.18569300 |
| H | -2.46973900 | -0.29053200 | -3.87735500 |
| H | -4.64224700 | -0.33045300 | -2.66920000 |
| H | 0.90207600 | 0.00815800 | 1.98933400 |
| H | -0.45214500 | 1.13444200 | 1.85004200 |
| H | -0.77532600 | -0.58910000 | 2.05149700 |
| Sn | 3.67159000 | -1.76401900 | -1.39706500 |

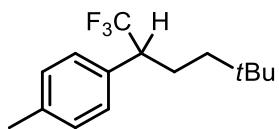
IVa. 1-methoxy-4-(1,1,1-trifluoro-5,5-dimethylhexan-2-yl)benzene



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | 0.00005500 | 0.00098000 | 0.01388800 |
| C | 0.00312600 | -0.00402100 | 1.54009400 |
| F | 1.27243700 | 0.00979000 | 2.03629000 |
| F | -0.61083600 | -1.07682500 | 2.11050800 |
| F | -0.61351800 | 1.09849400 | 2.04946000 |
| C | 0.86419200 | -1.13895700 | -0.60474100 |
| H | 0.94747600 | -0.88901700 | -1.66833200 |
| H | 1.87314900 | -1.04799300 | -0.18747400 |
| C | 0.35472200 | -2.58019000 | -0.45048400 |
| H | 0.28064000 | -2.83139500 | 0.61505100 |
| H | -0.66242200 | -2.64819800 | -0.85762600 |
| C | -1.39713800 | 0.14541000 | -0.57998500 |
| C | -2.47992800 | -0.69366100 | -0.25589700 |
| C | -1.61973200 | 1.14938100 | -1.53001900 |
| C | -3.72353100 | -0.53133100 | -0.85946000 |
| H | -2.36352600 | -1.48162100 | 0.48037100 |
| C | -2.86059000 | 1.32236000 | -2.15390600 |
| H | -0.80778900 | 1.82101800 | -1.80047700 |
| C | -3.92368700 | 0.47603300 | -1.81641200 |
| H | -4.55345100 | -1.18215400 | -0.59900400 |
| H | -2.98007900 | 2.11455700 | -2.88409500 |
| C | 1.26660200 | -3.47422200 | -2.66448500 |
| H | 0.25674800 | -3.42648600 | -3.09275800 |
| H | 1.79283900 | -2.55221500 | -2.93803700 |
| H | 1.79515700 | -4.30709300 | -3.14558100 |
| C | 2.64647600 | -3.70490000 | -0.56815100 |
| H | 2.63649200 | -3.82019500 | 0.52370200 |
| H | 3.21200000 | -4.54659900 | -0.98806600 |
| H | 3.19967300 | -2.78856900 | -0.80528800 |
| C | 0.54233800 | -5.03942200 | -0.84530100 |
| H | 1.10357100 | -5.86079000 | -1.30891700 |
| H | 0.49320100 | -5.23321800 | 0.23409700 |
| H | -0.48204200 | -5.06775900 | -1.23895900 |
| H | 0.53679500 | 0.92865700 | -0.22002900 |
| C | 1.21307100 | -3.68063900 | -1.13706800 |
| O | -5.17771700 | 0.55217700 | -2.35435900 |
| C | -5.44018400 | 1.55968200 | -3.33402500 |
| H | -4.80257100 | 1.42784300 | -4.21620900 |
| H | -6.48577200 | 1.43096400 | -3.61628700 |
| H | -5.29305900 | 2.56300400 | -2.91726800 |

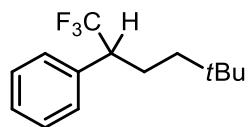
IVb. 1-methyl-4-(1,1,1-trifluoro-5,5-dimethylhexan-2-yl)benzene



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | 0.00016300 | 0.00010900 | -0.00113100 |
| C | 0.00108500 | 0.00025100 | 1.52469800 |
| F | 1.27047300 | 0.00148600 | 2.02082900 |
| F | -0.62504600 | -1.06264700 | 2.09957500 |
| F | -0.60280000 | 1.11224900 | 2.02888800 |
| C | 0.84387900 | -1.15716300 | -0.61609400 |
| H | 0.92739600 | -0.91506800 | -1.68144800 |
| H | 1.85557200 | -1.07941900 | -0.20285900 |
| C | 0.31168200 | -2.58885800 | -0.45020000 |
| H | 0.25066700 | -2.83584600 | 0.61711800 |
| H | -0.71307300 | -2.64009100 | -0.84032800 |
| C | -1.39309200 | 0.16281300 | -0.60128900 |
| C | -2.49142100 | -0.64146000 | -0.26297100 |
| C | -1.58509900 | 1.15173100 | -1.58003200 |
| C | -3.73140500 | -0.45905000 | -0.88404500 |
| H | -2.39479100 | -1.41604900 | 0.49040800 |
| C | -2.82143700 | 1.32562100 | -2.20334300 |
| H | -0.75393000 | 1.79490600 | -1.86198700 |
| C | -3.92240900 | 0.52348000 | -1.86484000 |
| H | -4.56371800 | -1.09840300 | -0.59753400 |
| H | -2.93195200 | 2.10054500 | -2.95931900 |
| C | 1.17010500 | -3.50591100 | -2.67620300 |
| H | 0.15382900 | -3.44135500 | -3.08661000 |
| H | 1.70798000 | -2.59464700 | -2.96279500 |
| H | 1.67486600 | -4.34993700 | -3.16334900 |
| C | 2.58247400 | -3.75052000 | -0.60325700 |
| H | 2.58990800 | -3.86255100 | 0.48898000 |
| H | 3.12778200 | -4.60189800 | -1.03036000 |
| H | 3.14499400 | -2.84328000 | -0.85297700 |
| C | 0.45227200 | -5.05213600 | -0.83835200 |
| H | 0.99216600 | -5.88446000 | -1.30769500 |
| H | 0.41807000 | -5.24069400 | 0.24256200 |
| H | -0.57891400 | -5.06537500 | -1.21472600 |
| H | 0.55273600 | 0.91773500 | -0.23772500 |
| C | 1.13995000 | -3.70567800 | -1.14726200 |
| C | -5.26650100 | 0.72778800 | -2.52579600 |
| H | -5.72578200 | 1.67197500 | -2.20499400 |
| H | -5.17206000 | 0.77073000 | -3.61742300 |
| H | -5.96080300 | -0.08112600 | -2.27631100 |

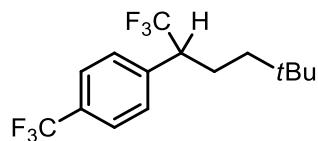
IVc. (1,1,1-trifluoro-5,5-dimethylhexan-2-yl)benzene



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | -0.00150000 | 0.00087000 | -0.00328500 |
| C | 0.00130500 | 0.00251200 | 1.52272200 |
| F | 1.27141700 | 0.01135500 | 2.01578000 |
| F | -0.61795000 | -1.06297700 | 2.09986800 |
| F | -0.60803800 | 1.11188500 | 2.02576200 |
| C | 0.84062700 | -1.15700500 | -0.61944600 |
| H | 0.92543900 | -0.91377400 | -1.68442000 |
| H | 1.85190300 | -1.08024500 | -0.20521300 |
| C | 0.30721100 | -2.58854900 | -0.45563000 |
| H | 0.24126500 | -2.83551700 | 0.61133200 |
| H | -0.71565500 | -2.63999000 | -0.85068600 |
| C | -1.39559600 | 0.16277300 | -0.60324100 |
| C | -2.49160800 | -0.64381000 | -0.25475200 |
| C | -1.58207100 | 1.15077100 | -1.58365700 |
| C | -3.73396800 | -0.46442900 | -0.87132100 |
| H | -2.38764200 | -1.41307300 | 0.50279300 |
| C | -2.82044400 | 1.32664100 | -2.20709800 |
| H | -0.74808600 | 1.79069800 | -1.86375300 |
| C | -3.90376300 | 0.51811100 | -1.85110500 |
| H | -4.56934700 | -1.09753600 | -0.58338900 |
| H | -2.93781000 | 2.09837900 | -2.96348400 |
| C | 1.17656100 | -3.50516200 | -2.67759700 |
| H | 0.16232600 | -3.44073400 | -3.09305300 |
| H | 1.71573500 | -2.59379000 | -2.96140200 |
| H | 1.68388200 | -4.34901600 | -3.16234500 |
| C | 2.57861000 | -3.75047400 | -0.59761600 |
| H | 2.58051200 | -3.86236400 | 0.49464300 |
| H | 3.12570000 | -4.60209300 | -1.02189600 |
| H | 3.14277300 | -2.84352500 | -0.84467000 |
| C | 0.44933300 | -5.05163900 | -0.84353700 |
| H | 0.99121100 | -5.88392100 | -1.31062300 |
| H | 0.41010700 | -5.24049200 | 0.23714900 |
| H | -0.58007600 | -5.06449900 | -1.22471500 |
| H | 0.55071000 | 0.91818000 | -0.24125400 |
| C | 1.13884600 | -3.70529900 | -1.14886400 |
| H | -4.87024300 | 0.65397600 | -2.32930000 |

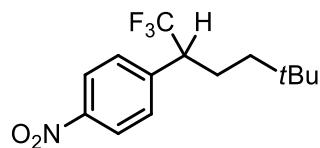
IVd. 1-(1,1,1-trifluoro-5,5-dimethylhexan-2-yl)-4-(trifluoromethyl)benzene



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | 0.00028600 | -0.00020900 | -0.00027800 |
| C | -0.00194100 | 0.00023400 | 1.52614600 |
| F | 1.26633800 | -0.00469900 | 2.01911800 |
| F | -0.63407200 | -1.05958300 | 2.09861200 |
| F | -0.60204900 | 1.11527700 | 2.02597100 |
| C | 0.81624800 | -1.17650800 | -0.61788900 |
| H | 0.91493200 | -0.93060300 | -1.68089600 |
| H | 1.82581200 | -1.12654900 | -0.19600800 |
| C | 0.24333800 | -2.59357600 | -0.46216400 |
| H | 0.18434700 | -2.84946700 | 0.60299900 |
| H | -0.78562000 | -2.61309400 | -0.84441000 |
| C | -1.38731300 | 0.18258500 | -0.60658700 |
| C | -2.50756700 | -0.57420500 | -0.22998800 |
| C | -1.53966500 | 1.13387900 | -1.62837800 |
| C | -3.74237300 | -0.38445800 | -0.85321100 |
| H | -2.43281800 | -1.31761800 | 0.55522200 |
| C | -2.76546900 | 1.32429400 | -2.26315300 |
| H | -0.68753500 | 1.73441700 | -1.93590300 |
| C | -3.87196400 | 0.56109900 | -1.87417000 |
| H | -4.59545800 | -0.97914100 | -0.54382400 |
| H | -2.85580800 | 2.06406300 | -3.05253100 |
| C | 1.04869100 | -3.51475700 | -2.70611900 |
| H | 0.02872000 | -3.42570400 | -3.10243900 |
| H | 1.60229400 | -2.61342600 | -2.99422500 |
| H | 1.52853800 | -4.36588100 | -3.20576800 |
| C | 2.48253900 | -3.80856200 | -0.65408100 |
| H | 2.50222100 | -3.92708200 | 0.43728600 |
| H | 3.00065900 | -4.67050600 | -1.09344400 |
| H | 3.06352300 | -2.91396100 | -0.90696200 |
| C | 0.31742000 | -5.05624200 | -0.86944000 |
| H | 0.82861000 | -5.89778800 | -1.35402400 |
| H | 0.29533200 | -5.25301600 | 0.21028800 |
| H | -0.71940400 | -5.04035800 | -1.22980800 |
| H | 0.56960400 | 0.90632100 | -0.23781400 |
| C | 1.03453400 | -3.72525500 | -1.17836000 |
| C | -5.20335600 | 0.80357900 | -2.52641200 |
| F | -5.09202400 | 1.03448900 | -3.86211100 |
| F | -6.06082600 | -0.23705100 | -2.37848800 |
| F | -5.83863200 | 1.89766900 | -2.00998500 |

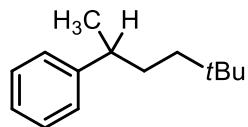
IVe. 1-nitro-4-(1,1,1-trifluoro-5,5-dimethylhexan-2-yl)benzene



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | 0.00043400 | -0.00000500 | -0.00430900 |
| C | 0.00001500 | 0.00144800 | 1.52270800 |
| F | 1.26873600 | -0.00142200 | 2.01126900 |
| F | -0.63002000 | -1.05866500 | 2.09595100 |
| F | -0.60135000 | 1.11618200 | 2.02063600 |
| C | 0.80359200 | -1.18522300 | -0.62389100 |
| H | 0.90894400 | -0.93808800 | -1.68587800 |
| H | 1.81190500 | -1.14700800 | -0.19816700 |
| C | 0.21252500 | -2.59526100 | -0.47192800 |
| H | 0.15065700 | -2.85335900 | 0.59239900 |
| H | -0.81662400 | -2.60163700 | -0.85425400 |
| C | -1.38525000 | 0.18890200 | -0.61011500 |
| C | -2.51324100 | -0.55117400 | -0.21470100 |
| C | -1.52656600 | 1.12562800 | -1.64846300 |
| C | -3.74618300 | -0.36285500 | -0.83481100 |
| H | -2.44299200 | -1.28015100 | 0.58381800 |
| C | -2.74808900 | 1.32298000 | -2.28579900 |
| H | -0.66829000 | 1.71123900 | -1.96575500 |
| C | -3.84718900 | 0.57185700 | -1.86627900 |
| H | -4.61429000 | -0.93240500 | -0.52640400 |
| H | -2.85031100 | 2.04636600 | -3.08537000 |
| C | 1.00244400 | -3.52101800 | -2.71936200 |
| H | -0.01751000 | -3.42196900 | -3.11333000 |
| H | 1.56382400 | -2.62445100 | -3.00735300 |
| H | 1.47326800 | -4.37567300 | -3.22147700 |
| C | 2.43777300 | -3.83447200 | -0.67104900 |
| H | 2.45874800 | -3.95378400 | 0.42018300 |
| H | 2.94461800 | -4.70215400 | -1.11214700 |
| H | 3.02851600 | -2.94663500 | -0.92512900 |
| C | 0.25814400 | -5.05750300 | -0.88351300 |
| H | 0.75777400 | -5.90362100 | -1.37205500 |
| H | 0.23787400 | -5.25664000 | 0.19580000 |
| H | -0.77972900 | -5.02885800 | -1.23999400 |
| H | 0.57599000 | 0.90156300 | -0.24448900 |
| C | 0.98968600 | -3.73426400 | -1.19197300 |
| N | -5.13977000 | 0.77081900 | -2.52411500 |
| O | -5.21216200 | 1.60473400 | -3.43301400 |
| O | -6.10171100 | 0.09580200 | -2.14249600 |

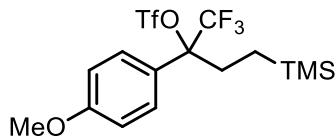
IVf. (5,5-dimethylhexan-2-yl)benzene



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | -0.01433200 | -0.00159600 | 0.06935800 |
| C | 0.08850100 | -0.13093300 | 1.59897200 |
| C | 1.38367300 | 0.04613400 | -0.61588700 |
| H | 1.22763200 | 0.27404400 | -1.67794200 |
| H | 1.92209900 | 0.90346300 | -0.19017400 |
| C | 2.23530700 | -1.22515700 | -0.47824100 |
| H | 2.40592100 | -1.43242800 | 0.58771400 |
| H | 1.66560300 | -2.08022600 | -0.86856700 |
| C | -0.93858800 | -1.02972800 | -0.57798200 |
| C | -1.10648500 | -2.33152900 | -0.07885900 |
| C | -1.64856700 | -0.67902200 | -1.73987600 |
| C | -1.94731700 | -3.24987100 | -0.71875400 |
| H | -0.58081100 | -2.64032700 | 0.82016000 |
| C | -2.48850900 | -1.59084200 | -2.38517100 |
| H | -1.54407000 | 0.32733600 | -2.14215500 |
| C | -2.64153800 | -2.88512700 | -1.87580000 |
| H | -2.05943000 | -4.25095200 | -0.30884400 |
| H | -3.02757300 | -1.28885500 | -3.28008200 |
| C | 3.46915300 | -1.05031900 | -2.70802400 |
| H | 2.81577400 | -1.82685800 | -3.12726200 |
| H | 3.04599900 | -0.07463300 | -2.97398200 |
| H | 4.44513000 | -1.13088000 | -3.20412700 |
| C | 4.52052600 | -0.09359800 | -0.62835500 |
| H | 4.63062200 | -0.17641800 | 0.46110700 |
| H | 5.52375100 | -0.14839600 | -1.07075400 |
| H | 4.11716700 | 0.90108100 | -0.85130000 |
| C | 4.29766500 | -2.57570400 | -0.90041200 |
| H | 5.28491100 | -2.63050600 | -1.37709500 |
| H | 4.43588500 | -2.73222900 | 0.17741100 |
| H | 3.69199800 | -3.40651500 | -1.28551800 |
| C | 3.62171200 | -1.21758400 | -1.18248300 |
| H | -3.29712100 | -3.59697100 | -2.37107500 |
| H | 0.69513900 | 0.68870600 | 2.00291000 |
| H | -0.90295300 | -0.07815000 | 2.06428700 |
| H | 0.55467600 | -1.06957500 | 1.91671800 |
| H | -0.46521200 | 0.98079400 | -0.13107800 |

Va. 1,1,1-trifluoro-2-(4-methoxyphenyl)-4-(trimethylsilyl)butan-2-yl trifluoromethanesulfonate

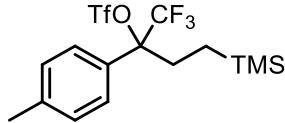


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | 0.00742500 | 0.00772200 | -0.00447100 |
| C | 0.01553200 | 0.01129800 | 1.55003000 |
| F | 1.27980300 | 0.01341600 | 2.02898400 |
| F | -0.59838800 | -1.08210300 | 2.05751900 |
| F | -0.59618600 | 1.09589100 | 2.07429800 |
| O | 0.76074200 | 1.28398900 | -0.32367000 |
| S | 0.13944000 | 2.70436300 | -0.77539700 |
| O | -1.04714300 | 3.08773300 | -0.02195900 |
| O | 0.17336700 | 2.83057500 | -2.22798000 |
| C | 0.98086800 | -1.06861800 | -0.55506000 |
| H | 1.10274500 | -0.83989000 | -1.61726400 |
| H | 1.95739100 | -0.89802900 | -0.09279900 |
| C | 0.54062300 | -2.53038500 | -0.37159900 |
| H | 0.48628400 | -2.78616600 | 0.69353600 |
| H | -0.47225000 | -2.67066400 | -0.77283100 |
| C | -1.37376900 | -0.03151700 | -0.63611700 |
| C | -2.57351600 | -0.00359000 | 0.10057100 |
| C | -1.47088300 | -0.11043500 | -2.03443400 |
| C | -3.80737300 | -0.06139900 | -0.53478500 |
| H | -2.56777600 | 0.06273600 | 1.18098200 |
| C | -2.70276700 | -0.15569800 | -2.68687800 |
| H | -0.57637900 | -0.12281900 | -2.64834200 |
| C | -3.88578700 | -0.13658100 | -1.93438100 |
| H | -4.72541000 | -0.04390800 | 0.04472200 |
| H | -2.72296000 | -0.20724100 | -3.76903700 |
| C | 1.74248300 | -3.52641600 | -3.07527900 |
| H | 0.73943500 | -3.57270400 | -3.51851300 |
| H | 2.17542300 | -2.54944400 | -3.32501100 |
| H | 2.35785600 | -4.29318300 | -3.56374500 |
| C | 3.42561300 | -3.70683400 | -0.47516400 |
| H | 3.40999400 | -3.84835200 | 0.61323500 |
| H | 4.07470000 | -4.48195500 | -0.90285800 |
| H | 3.89248600 | -2.73517100 | -0.68023100 |
| C | 0.94698100 | -5.52996600 | -0.85086200 |
| H | 1.56055800 | -6.32078200 | -1.30129700 |
| H | 0.89041700 | -5.72499400 | 0.22782900 |
| H | -0.06698000 | -5.61967500 | -1.26134700 |
| Si | 1.68018500 | -3.81978000 | -1.20408600 |
| C | 1.58682100 | 3.71900800 | -0.10561200 |
| F | 1.69218000 | 3.55615900 | 1.21349400 |
| F | 1.33424400 | 5.00366000 | -0.37662800 |
| F | 2.72508800 | 3.35537600 | -0.69732500 |
| O | -5.13698800 | -0.18571400 | -2.46197200 |
| C | -5.28396800 | -0.26472500 | -3.88468700 |
| H | -6.35857800 | -0.29402100 | -4.06609400 |

| | | | |
|---|-------------|-------------|-------------|
| H | -4.85141200 | 0.61584700 | -4.37248000 |
| H | -4.81869300 | -1.17614700 | -4.27654300 |

Vb. 1,1,1-trifluoro-2-(p-tolyl)-4-(trimethylsilyl)butan-2-yl trifluoromethanesulfonate



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | 0.00213800 | 0.00190900 | -0.00087100 |
| C | 0.00418200 | 0.00379300 | 1.55301600 |
| F | 1.26776500 | 0.00764300 | 2.03391600 |
| F | -0.60817600 | -1.09110100 | 2.05872600 |
| F | -0.61168900 | 1.08622700 | 2.07643600 |
| O | 0.78780400 | 1.24690700 | -0.33243900 |
| S | 0.21913800 | 2.71347400 | -0.71086300 |
| O | -1.00853400 | 3.06335100 | -0.01017200 |
| O | 0.35250400 | 2.93235100 | -2.14601100 |
| C | 0.94010400 | -1.10719500 | -0.55128500 |
| H | 1.07138500 | -0.87598700 | -1.61200200 |
| H | 1.92023300 | -0.97384600 | -0.08396900 |
| C | 0.44791600 | -2.55363700 | -0.38015400 |
| H | 0.38793700 | -2.81776900 | 0.68242800 |
| H | -0.57022400 | -2.65454100 | -0.78011700 |
| C | -1.37615900 | 0.00074300 | -0.64659400 |
| C | -2.57680200 | -0.04050200 | 0.07518800 |
| C | -1.45089200 | 0.02434400 | -2.05165300 |
| C | -3.80656800 | -0.06166100 | -0.58828100 |
| H | -2.58231600 | -0.05472300 | 1.15779000 |
| C | -2.68034500 | 0.01480300 | -2.70441100 |
| H | -0.54657100 | 0.06577000 | -2.65058700 |
| C | -3.88594200 | -0.03287800 | -1.98560800 |
| H | -4.71929800 | -0.09493600 | 0.00151500 |
| H | -2.70189800 | 0.04304700 | -3.79135000 |
| C | 1.58292600 | -3.58021800 | -3.10146700 |
| H | 0.57296000 | -3.60335100 | -3.53056000 |
| H | 2.03460200 | -2.61344500 | -3.35751600 |
| H | 2.17360000 | -4.36085800 | -3.59841700 |
| C | 3.29871600 | -3.80452200 | -0.52619800 |
| H | 3.29506300 | -3.94205200 | 0.56283000 |
| H | 3.92110200 | -4.59775300 | -0.96034400 |
| H | 3.78788000 | -2.84615300 | -0.74148200 |
| C | 0.76846000 | -5.56332500 | -0.86587000 |
| H | 1.35224600 | -6.36892400 | -1.32947800 |
| H | 0.72708400 | -5.75950400 | 0.21327500 |
| H | -0.25505900 | -5.62498700 | -1.25737900 |
| Si | 1.54041000 | -3.87270800 | -1.22962700 |
| C | 1.63543800 | 3.65784000 | 0.11155000 |
| F | 1.65315700 | 3.41260700 | 1.42194500 |
| F | 1.42195900 | 4.96110500 | -0.09477400 |

| | | | |
|---|-------------|-------------|-------------|
| F | 2.80276100 | 3.30711900 | -0.42893200 |
| C | -5.21420700 | -0.06332700 | -2.70273600 |
| H | -6.04871600 | 0.05112500 | -2.00411200 |
| H | -5.27981800 | 0.73693000 | -3.44924500 |
| H | -5.34987100 | -1.01307700 | -3.23602900 |

Vc. 1,1,1-trifluoro-2-phenyl-4-(trimethylsilyl)butan-2-yl trifluoromethanesulfonate

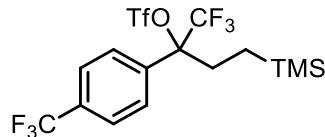


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.00060000 | -0.00032900 | -0.00003000 |
| C | -0.00072500 | -0.00072600 | 1.55387200 |
| F | 1.26248100 | -0.00141600 | 2.03492900 |
| F | -0.61650900 | -1.09443400 | 2.05762500 |
| F | -0.61418100 | 1.08272600 | 2.07776400 |
| O | 0.80230300 | 1.22698200 | -0.33655100 |
| S | 0.26196600 | 2.71493000 | -0.68029300 |
| O | -0.98326600 | 3.05440000 | -0.00668400 |
| O | 0.44264000 | 2.97147800 | -2.10352600 |
| C | 0.91715200 | -1.12736900 | -0.55046800 |
| H | 1.05890500 | -0.89298300 | -1.60922700 |
| H | 1.89687100 | -1.01635100 | -0.07648200 |
| C | 0.39507900 | -2.56460200 | -0.39166100 |
| H | 0.31937800 | -2.83329800 | 0.66864500 |
| H | -0.62033700 | -2.64448500 | -0.80308100 |
| C | -1.37874100 | 0.01968400 | -0.65202100 |
| C | -2.58023600 | -0.04805700 | 0.06911800 |
| C | -1.43877300 | 0.08308500 | -2.05575100 |
| C | -3.80819600 | -0.05399500 | -0.59871600 |
| H | -2.58421200 | -0.09518300 | 1.15063300 |
| C | -2.66556000 | 0.08759900 | -2.71910600 |
| H | -0.52774500 | 0.14248800 | -2.64280000 |
| C | -3.85744500 | 0.01590100 | -1.99207600 |
| H | -4.72627200 | -0.10846300 | -0.02051700 |
| H | -2.68654200 | 0.14430300 | -3.80376500 |
| H | -4.81392000 | 0.01549500 | -2.50741000 |
| C | 1.52930300 | -3.60236100 | -3.10861100 |
| H | 0.52125400 | -3.60954600 | -3.54274000 |
| H | 1.99657500 | -2.64181700 | -3.36010000 |
| H | 2.11082600 | -4.39052100 | -3.60449800 |
| C | 3.22807100 | -3.85536300 | -0.52490400 |
| H | 3.21725700 | -3.99476600 | 0.56385200 |
| H | 3.84199900 | -4.65601700 | -0.95746100 |
| H | 3.73100400 | -2.90324700 | -0.73618400 |
| C | 0.67527000 | -5.57846800 | -0.88120300 |
| H | 1.25100700 | -6.39122800 | -1.34235800 |
| H | 0.62473500 | -5.77538000 | 0.19738400 |
| H | -0.34654000 | -5.62575900 | -1.27912800 |

| | | | |
|----|------------|-------------|-------------|
| Si | 1.47279900 | -3.89844200 | -1.23773700 |
| C | 1.66164800 | 3.62117800 | 0.21067700 |
| F | 1.62555700 | 3.35224500 | 1.51591200 |
| F | 1.47729900 | 4.93096000 | 0.02002400 |
| F | 2.84218800 | 3.25946900 | -0.29223500 |

Vd. 1,1,1-trifluoro-2-(4-(trifluoromethyl)phenyl)-4-(trimethylsilyl)butan-2-yl trifluoromethanesulfonate

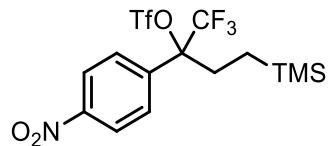


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.00380400 | -0.00337000 | 0.00203600 |
| C | -0.00510500 | -0.00622100 | 1.55616200 |
| F | 1.25726600 | -0.01008100 | 2.03536900 |
| F | -0.62443300 | -1.09933900 | 2.05592500 |
| F | -0.61871900 | 1.07705400 | 2.07967500 |
| O | 0.80991600 | 1.20327600 | -0.34705000 |
| S | 0.29282600 | 2.71281900 | -0.65381300 |
| O | -0.96624900 | 3.03659900 | 0.00049900 |
| O | 0.50816000 | 2.99947000 | -2.06560500 |
| C | 0.88809100 | -1.15115800 | -0.55171600 |
| H | 1.03985200 | -0.91221000 | -1.60828300 |
| H | 1.86754000 | -1.06347000 | -0.07234200 |
| C | 0.33477700 | -2.57781200 | -0.40542100 |
| H | 0.24364700 | -2.85099700 | 0.65228700 |
| H | -0.67749700 | -2.63735600 | -0.82790300 |
| C | -1.38391000 | 0.03448800 | -0.65013300 |
| C | -2.58425500 | -0.05622800 | 0.06679000 |
| C | -1.44093200 | 0.13349100 | -2.05099500 |
| C | -3.81155100 | -0.04833300 | -0.59829800 |
| H | -2.59301000 | -0.13383200 | 1.14597700 |
| C | -2.66216700 | 0.15043800 | -2.71814400 |
| H | -0.53110000 | 0.20817100 | -2.63695800 |
| C | -3.85227600 | 0.05473800 | -1.98954000 |
| H | -4.72855600 | -0.12261600 | -0.02384300 |
| H | -2.68140900 | 0.22993900 | -3.80005500 |
| C | 1.46016400 | -3.62713200 | -3.12041900 |
| H | 0.45302400 | -3.62145800 | -3.55664300 |
| H | 1.93963500 | -2.67187600 | -3.36910100 |
| H | 2.03315000 | -4.42123400 | -3.61672300 |
| C | 3.15024700 | -3.90664500 | -0.53363900 |
| H | 3.13554400 | -4.04168200 | 0.55560300 |
| H | 3.75256700 | -4.71826400 | -0.96204400 |
| H | 3.66823200 | -2.96332400 | -0.74795500 |
| C | 0.57496500 | -5.59524200 | -0.89716300 |
| H | 1.14078700 | -6.41491300 | -1.35832800 |
| H | 0.52017800 | -5.79261900 | 0.18108000 |
| H | -0.44665600 | -5.62866800 | -1.29693100 |

| | | | |
|----|-------------|-------------|-------------|
| Si | 1.39645800 | -3.92657300 | -1.25049500 |
| C | 1.68036900 | 3.58348100 | 0.29179300 |
| F | 1.60345600 | 3.29036500 | 1.58941600 |
| F | 1.51879300 | 4.89803600 | 0.11962000 |
| F | 2.86751200 | 3.21212500 | -0.18640600 |
| C | -5.17293300 | 0.10975900 | -2.70922200 |
| F | -6.17326700 | -0.47959500 | -2.00937600 |
| F | -5.12575500 | -0.49925400 | -3.92171000 |
| F | -5.57175900 | 1.39304200 | -2.94379800 |

Ve. 1,1,1-trifluoro-2-(4-nitrophenyl)-4-(trimethylsilyl)butan-2-yl trifluoromethanesulfonate

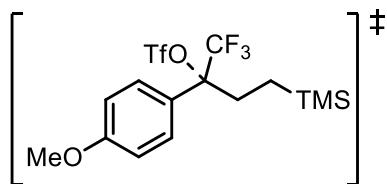


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.00464400 | -0.00407300 | 0.00038400 |
| C | -0.00596100 | -0.00720900 | 1.55471500 |
| F | 1.25612500 | -0.01402300 | 2.03216600 |
| F | -0.62828300 | -1.09896000 | 2.05303800 |
| F | -0.61814900 | 1.07698600 | 2.07771500 |
| O | 0.82040100 | 1.18670700 | -0.35820300 |
| S | 0.32534800 | 2.71184100 | -0.63869800 |
| O | -0.94686000 | 3.02702200 | -0.00643300 |
| O | 0.57518000 | 3.02110600 | -2.03943300 |
| C | 0.86794100 | -1.16769400 | -0.55441700 |
| H | 1.02950400 | -0.92559900 | -1.60890500 |
| H | 1.84589900 | -1.09837800 | -0.06903900 |
| C | 0.28979000 | -2.58538200 | -0.41873500 |
| H | 0.18141200 | -2.86019500 | 0.63674800 |
| H | -0.71759300 | -2.62918500 | -0.85455900 |
| C | -1.38514600 | 0.04787400 | -0.65247400 |
| C | -2.58612500 | -0.05311500 | 0.06502400 |
| C | -1.43664000 | 0.16895700 | -2.05274000 |
| C | -3.81294500 | -0.03184100 | -0.59639600 |
| H | -2.59454200 | -0.14657300 | 1.14268600 |
| C | -2.65303800 | 0.19975200 | -2.72577700 |
| H | -0.52476900 | 0.25145800 | -2.63399400 |
| C | -3.82890700 | 0.09698300 | -1.98298700 |
| H | -4.73950900 | -0.10820800 | -0.04115300 |
| H | -2.68885100 | 0.29853900 | -3.80351800 |
| C | 1.42418900 | -3.64735300 | -3.12433900 |
| H | 0.42054200 | -3.62909300 | -3.56817900 |
| H | 1.91732400 | -2.69798800 | -3.36885200 |
| H | 1.99106400 | -4.44819000 | -3.61679600 |
| C | 3.09094900 | -3.94587300 | -0.52471500 |
| H | 3.06673800 | -4.07639800 | 0.56490200 |
| H | 3.68586100 | -4.76686300 | -0.94555100 |
| H | 3.62272700 | -3.01026500 | -0.73911100 |

| | | | |
|----|-------------|-------------|-------------|
| C | 0.49982500 | -5.60590300 | -0.90767600 |
| H | 1.06066500 | -6.43181600 | -1.36375800 |
| H | 0.43450300 | -5.80179900 | 0.17021600 |
| H | -0.51886100 | -5.62895500 | -1.31555600 |
| Si | 1.34286100 | -3.94707400 | -1.25527700 |
| C | 1.69868000 | 3.55421700 | 0.35373200 |
| F | 1.58755200 | 3.24165100 | 1.64384700 |
| F | 1.55404700 | 4.87231000 | 0.19747200 |
| F | 2.89191600 | 3.17652900 | -0.10286400 |
| N | -5.11986500 | 0.12495500 | -2.68310700 |
| O | -6.14927600 | 0.02708200 | -2.01017600 |
| O | -5.11236500 | 0.24470700 | -3.91107700 |

TS-VIa

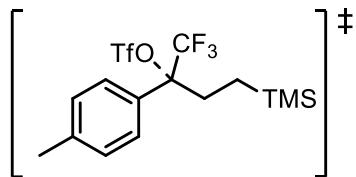


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | 0.01273600 | 0.00983600 | -0.02241900 |
| C | 0.01779200 | 0.01804600 | 1.52483300 |
| F | 1.26691200 | 0.01815700 | 2.02747400 |
| F | -0.59117600 | -1.10916400 | 1.97971900 |
| F | -0.62731100 | 1.06591700 | 2.07011400 |
| O | 0.84907200 | 1.71804300 | -0.16508600 |
| S | 0.23661300 | 3.08471500 | -0.52625400 |
| O | -1.17031700 | 3.23800500 | -0.13892700 |
| O | 0.63861400 | 3.52675500 | -1.86869200 |
| C | 1.18717000 | -0.73886800 | -0.62223600 |
| H | 1.28925900 | -0.43923300 | -1.66653700 |
| H | 2.09810200 | -0.41732400 | -0.11578600 |
| C | 1.02503200 | -2.27618800 | -0.51431500 |
| H | 0.94362300 | -2.57969800 | 0.53705500 |
| H | 0.09105400 | -2.58926100 | -0.99881300 |
| C | 2.61074800 | -2.86861200 | -3.13243700 |
| H | 1.68094000 | -3.10486000 | -3.66560800 |
| H | 2.83789000 | -1.80912500 | -3.30549300 |
| H | 3.41632000 | -3.45641600 | -3.59137800 |
| C | 4.08603700 | -2.84037700 | -0.40226600 |
| H | 4.01323700 | -3.03491300 | 0.67544900 |
| H | 4.91194800 | -3.44726100 | -0.79551100 |
| H | 4.35975100 | -1.78608800 | -0.53546600 |
| C | 2.06900300 | -5.10611400 | -1.05346900 |
| H | 2.86233500 | -5.73395500 | -1.47921100 |
| H | 1.97457600 | -5.36250800 | 0.00945400 |
| H | 1.12757100 | -5.37572100 | -1.54891100 |
| Si | 2.46837500 | -3.27073900 | -1.28732200 |
| C | 1.21171400 | 4.18785500 | 0.65193800 |

| | | | |
|---|-------------|-------------|-------------|
| C | -1.27255200 | 0.01376500 | -0.69033100 |
| C | -2.50498500 | 0.20707700 | -0.00486500 |
| C | -1.33630000 | -0.18587400 | -2.09286000 |
| C | -3.70968300 | 0.17385100 | -0.67447500 |
| H | -2.52492700 | 0.37462600 | 1.06344500 |
| C | -2.53892100 | -0.20416300 | -2.77874000 |
| H | -0.42862200 | -0.31604500 | -2.66965700 |
| C | -3.74452900 | -0.02824100 | -2.07041900 |
| H | -4.64551000 | 0.30829100 | -0.14175900 |
| H | -2.53542800 | -0.35348100 | -3.85147900 |
| F | 2.52821600 | 4.07256400 | 0.42606900 |
| F | 0.85121500 | 5.46641300 | 0.45693100 |
| F | 0.96125500 | 3.86092700 | 1.92712300 |
| O | -4.96363600 | -0.03594800 | -2.63206500 |
| C | -5.09291700 | -0.23193400 | -4.05164700 |
| H | -6.16365800 | -0.19756300 | -4.24924400 |
| H | -4.58692200 | 0.56966100 | -4.59836000 |
| H | -4.69081600 | -1.20685600 | -4.34383600 |

TS-VIb

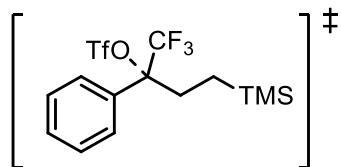


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.00160500 | -0.00052000 | -0.00103200 |
| C | -0.00497500 | -0.00397800 | 1.54521100 |
| F | 1.23932600 | -0.00606600 | 2.05542500 |
| F | -0.61413800 | -1.13986700 | 1.98026300 |
| F | -0.65993800 | 1.03413500 | 2.09382600 |
| O | 0.88694900 | 1.80374200 | -0.08359900 |
| S | 0.31863700 | 3.17899100 | -0.43529500 |
| O | -1.14346400 | 3.27816500 | -0.32668900 |
| O | 0.95734300 | 3.74544000 | -1.63369300 |
| C | 1.18565000 | -0.69763200 | -0.61141600 |
| H | 1.28887300 | -0.37896200 | -1.64932100 |
| H | 2.08945500 | -0.38225700 | -0.08956100 |
| C | 1.03167500 | -2.24273000 | -0.53459800 |
| H | 0.96870400 | -2.56965500 | 0.51068100 |
| H | 0.09314300 | -2.54969400 | -1.01370400 |
| C | 2.55796200 | -2.75685700 | -3.19829600 |
| H | 1.61487700 | -2.98982800 | -3.70903100 |
| H | 2.77094000 | -1.69177500 | -3.35417700 |
| H | 3.35459900 | -3.32697400 | -3.69361700 |
| C | 4.10322900 | -2.76736100 | -0.50442500 |
| H | 4.06031200 | -2.98923600 | 0.56955800 |
| H | 4.92763700 | -3.35201200 | -0.93291200 |
| H | 4.35825800 | -1.70624100 | -0.61854600 |

| | | | |
|----|-------------|-------------|-------------|
| C | 2.09802100 | -5.04599500 | -1.15331000 |
| H | 2.88618000 | -5.65555200 | -1.61380000 |
| H | 2.03624700 | -5.32458400 | -0.09367300 |
| H | 1.14621600 | -5.31581700 | -1.62818100 |
| Si | 2.47228400 | -3.20269200 | -1.36041400 |
| C | 0.99312000 | 4.22398300 | 0.98122300 |
| C | -1.26951900 | 0.06628600 | -0.68660700 |
| C | -2.50654200 | 0.22295800 | -0.00556900 |
| C | -1.31029500 | -0.04279700 | -2.10305700 |
| C | -3.70385800 | 0.24478900 | -0.70252400 |
| H | -2.54043000 | 0.31033200 | 1.07193300 |
| C | -2.51168600 | -0.00144200 | -2.78862000 |
| H | -0.39481100 | -0.14394900 | -2.67316200 |
| C | -3.73505300 | 0.14350700 | -2.10519900 |
| H | -4.63498200 | 0.34777300 | -0.15244100 |
| H | -2.50966600 | -0.08110900 | -3.87209400 |
| F | 2.33150600 | 4.13852200 | 1.03730000 |
| F | 0.65390000 | 5.50973000 | 0.78672500 |
| F | 0.48819800 | 3.82350100 | 2.15728600 |
| C | -5.03514600 | 0.21603500 | -2.85622200 |
| H | -5.26895600 | 1.26176600 | -3.10001800 |
| H | -4.98529600 | -0.33587100 | -3.79981000 |
| H | -5.86536500 | -0.17281000 | -2.25869000 |

TS-VIc

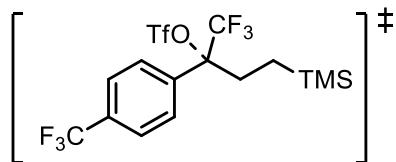


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.00286000 | -0.00083000 | 0.00587800 |
| C | -0.01034100 | -0.00303400 | 1.55246500 |
| F | 1.23146300 | -0.00244000 | 2.06535500 |
| F | -0.61807400 | -1.14282900 | 1.98072500 |
| F | -0.67155400 | 1.03081800 | 2.09811300 |
| O | 0.90834800 | 1.91672600 | -0.03612500 |
| S | 0.33290900 | 3.28196800 | -0.37263000 |
| O | -1.13748900 | 3.34545700 | -0.35135800 |
| O | 1.02088400 | 3.91336500 | -1.51239500 |
| C | 1.20658700 | -0.63593600 | -0.60553800 |
| H | 1.30818400 | -0.31074700 | -1.64082300 |
| H | 2.09715500 | -0.30524700 | -0.07141200 |
| C | 1.08565500 | -2.18948000 | -0.53837700 |
| H | 1.02560200 | -2.52474900 | 0.50414000 |
| H | 0.15783800 | -2.51415300 | -1.02598000 |
| C | 2.63947900 | -2.64157600 | -3.19751000 |
| H | 1.70486000 | -2.89485900 | -3.71397300 |
| H | 2.82668000 | -1.57060000 | -3.34547000 |

| | | | |
|----|-------------|-------------|-------------|
| H | 3.45237500 | -3.18827800 | -3.69278000 |
| C | 4.16975100 | -2.63267800 | -0.49281500 |
| H | 4.12331700 | -2.86019600 | 0.57976000 |
| H | 5.01089500 | -3.19620200 | -0.91703300 |
| H | 4.40091600 | -1.56555800 | -0.60095300 |
| C | 2.22528800 | -4.95685400 | -1.17053700 |
| H | 3.03177200 | -5.54381300 | -1.62865200 |
| H | 2.16239900 | -5.24306000 | -0.11311000 |
| H | 1.28409000 | -5.24620500 | -1.65471200 |
| Si | 2.55837500 | -3.10474700 | -1.36450300 |
| C | 0.88318400 | 4.30889400 | 1.10804300 |
| C | -1.25680700 | 0.09775700 | -0.69035100 |
| C | -2.49892600 | 0.24089000 | -0.01043400 |
| C | -1.27522600 | 0.03255300 | -2.11230800 |
| C | -3.69080500 | 0.29295500 | -0.71888400 |
| H | -2.53773400 | 0.29501400 | 1.06878400 |
| C | -2.46935400 | 0.10158700 | -2.81130200 |
| H | -0.35084100 | -0.05186700 | -2.66987200 |
| C | -3.68130100 | 0.22868100 | -2.11738800 |
| H | -4.62976900 | 0.38957600 | -0.18331100 |
| H | -2.46285800 | 0.06012300 | -3.89576300 |
| H | -4.61630700 | 0.28036900 | -2.66779400 |
| F | 2.21920200 | 4.26788800 | 1.24375900 |
| F | 0.51229500 | 5.58961800 | 0.93238000 |
| F | 0.32608800 | 3.85875900 | 2.24320200 |

TS-VId

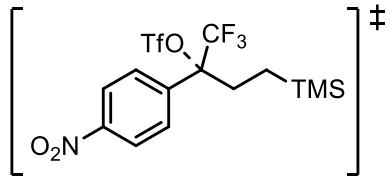


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | 0.00000000 | 0.00000000 | 0.00000000 |
| C | 0.00000000 | 0.00000000 | 1.54558400 |
| F | 1.24196300 | 0.00000000 | 2.05384800 |
| F | -0.62720100 | -1.10287200 | 2.01702100 |
| F | -0.63495400 | 1.08433100 | 2.02711800 |
| O | 0.69097800 | 2.70209000 | -0.51225200 |
| S | -0.16082900 | 3.85081900 | -0.92677900 |
| O | -1.59129300 | 3.52056900 | -1.12422000 |
| O | 0.44266800 | 4.71929600 | -1.96435200 |
| C | 1.31417400 | -0.15704700 | -0.63255800 |
| H | 1.32653700 | 0.26485200 | -1.63499200 |
| H | 2.08309200 | 0.34395100 | -0.04515200 |
| C | 1.61976800 | -1.70287900 | -0.69178000 |
| H | 1.62899300 | -2.13770500 | 0.31522300 |
| H | 0.83178000 | -2.21547700 | -1.25503600 |
| C | 3.34339400 | -1.41502800 | -3.27414500 |

| | | | |
|----|-------------|-------------|-------------|
| H | 2.52809300 | -1.84319800 | -3.87034400 |
| H | 3.25223500 | -0.32246900 | -3.30569800 |
| H | 4.28928300 | -1.67796400 | -3.76530300 |
| C | 4.69166200 | -1.27113500 | -0.47416400 |
| H | 4.65220100 | -1.60549500 | 0.56995100 |
| H | 5.67770300 | -1.54067600 | -0.87414100 |
| H | 4.62255600 | -0.17631000 | -0.48306800 |
| C | 3.49389400 | -3.96168900 | -1.48915600 |
| H | 4.44781500 | -4.26244700 | -1.94145000 |
| H | 3.46768900 | -4.35594000 | -0.46601500 |
| H | 2.68682600 | -4.43820000 | -2.05892500 |
| Si | 3.33153900 | -2.07842600 | -1.50608600 |
| C | -0.17452300 | 4.95065200 | 0.59964300 |
| C | -1.24001500 | 0.02323000 | -0.68509200 |
| C | -2.49356600 | 0.04949900 | 0.00315300 |
| C | -1.25963200 | 0.02577000 | -2.11457900 |
| C | -3.68539700 | 0.07465000 | -0.69903800 |
| H | -2.53756200 | 0.04746100 | 1.08335700 |
| C | -2.45391700 | 0.04433200 | -2.80846600 |
| H | -0.33611300 | 0.01359500 | -2.67804600 |
| C | -3.66500500 | 0.07198500 | -2.10001900 |
| H | -4.62663900 | 0.09235600 | -0.16213800 |
| H | -2.44945700 | 0.04159700 | -3.89251500 |
| F | 1.07444300 | 5.33648800 | 0.92861400 |
| F | -0.90798200 | 6.06060400 | 0.38273900 |
| F | -0.70221900 | 4.30571700 | 1.65870600 |
| C | -4.97119600 | 0.14333600 | -2.86756400 |
| F | -4.90367900 | -0.52704300 | -4.03879700 |
| F | -6.00241200 | -0.37093100 | -2.16411600 |
| F | -5.28430600 | 1.42993100 | -3.15939600 |

TS-VIe

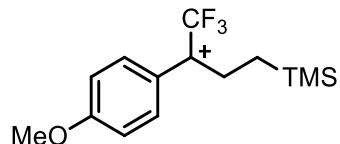


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | 0.00000000 | 0.00000000 | 0.00000000 |
| C | 0.00000000 | 0.00000000 | 1.54576200 |
| F | 1.24137600 | 0.00000000 | 2.05389400 |
| F | -0.63155200 | -1.09733700 | 2.02158900 |
| F | -0.63444100 | 1.08849500 | 2.01733500 |
| O | 0.75517500 | 2.70803000 | -0.49971900 |
| S | -0.12728400 | 3.79455300 | -1.00905100 |
| O | -1.47162000 | 3.34662600 | -1.44074400 |
| O | 0.54632100 | 4.75727500 | -1.91092700 |
| C | 1.31048100 | -0.12968500 | -0.63529900 |
| H | 1.32196500 | 0.30326000 | -1.63276800 |

| | | | |
|----|-------------|-------------|-------------|
| H | 2.07949900 | 0.36313400 | -0.04067200 |
| C | 1.61410900 | -1.67834600 | -0.70873400 |
| H | 1.63494400 | -2.12127300 | 0.29413300 |
| H | 0.82426400 | -2.18911000 | -1.27098900 |
| C | 3.28460000 | -1.40893200 | -3.32596000 |
| H | 2.46232300 | -1.85819800 | -3.89635100 |
| H | 3.17910800 | -0.31833200 | -3.37603900 |
| H | 4.22316200 | -1.66964300 | -3.83220800 |
| C | 4.68801700 | -1.19869000 | -0.55600700 |
| H | 4.65711600 | -1.49347000 | 0.50011400 |
| H | 5.66972900 | -1.48613500 | -0.95426200 |
| H | 4.62151500 | -0.10508100 | -0.60679200 |
| C | 3.50543600 | -3.92221200 | -1.49945700 |
| H | 4.44347600 | -4.21828600 | -1.98690600 |
| H | 3.52930700 | -4.29581100 | -0.46864200 |
| H | 2.68176800 | -4.42059200 | -2.02475300 |
| Si | 3.32114900 | -2.04174700 | -1.54755100 |
| C | -0.48313900 | 4.82059100 | 0.52718900 |
| C | -1.24546700 | -0.00299000 | -0.68721700 |
| C | -2.49574700 | 0.01525800 | 0.00437700 |
| C | -1.26170300 | -0.01750700 | -2.11469200 |
| C | -3.69163200 | 0.01376600 | -0.69371400 |
| H | -2.53777200 | 0.03067900 | 1.08440500 |
| C | -2.45487000 | -0.03278900 | -2.81378000 |
| H | -0.33786800 | -0.01854100 | -2.67729300 |
| C | -3.64710200 | -0.01415300 | -2.08785900 |
| H | -4.64086000 | 0.03017300 | -0.17377300 |
| H | -2.46953400 | -0.04783200 | -3.89595600 |
| F | 0.65785400 | 5.29152700 | 1.06848900 |
| F | -1.26615000 | 5.87553700 | 0.22549800 |
| F | -1.11660200 | 4.08870600 | 1.46421000 |
| N | -4.92962400 | -0.02484700 | -2.83609600 |
| O | -5.96950200 | 0.02834300 | -2.18303300 |
| O | -4.87116300 | -0.08738500 | -4.06228600 |

VIIa. 1,1,1-trifluoro-2-(4-methoxyphenyl)-4-(trimethylsilyl)butan-2-ylum

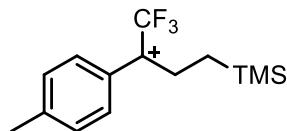


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | 0.00979200 | 0.03983500 | -0.02562200 |
| C | 0.02871200 | 0.05972900 | 1.51203200 |
| F | 1.27863400 | 0.06091800 | 2.01003100 |
| F | -0.60411200 | -1.01645900 | 2.03630100 |
| F | -0.58539000 | 1.16989500 | 1.98598100 |
| C | 1.35072900 | -0.02244900 | -0.67530500 |
| H | 1.31086000 | 0.36812700 | -1.69166000 |
| H | 2.05290100 | 0.60142300 | -0.11591000 |

| | | | |
|----|-------------|-------------|-------------|
| C | 1.86006400 | -1.50128200 | -0.68548100 |
| H | 1.90526200 | -1.89659600 | 0.33705800 |
| H | 1.14305100 | -2.12674400 | -1.23224100 |
| C | 4.86027900 | -0.71397600 | -0.47395700 |
| H | 4.64965600 | 0.36251000 | -0.50426000 |
| H | 4.87203500 | -1.02618500 | 0.57797600 |
| H | 5.87042500 | -0.86238800 | -0.87709300 |
| C | 4.01277000 | -3.55752500 | -1.39569500 |
| H | 3.28159900 | -4.15408100 | -1.95532800 |
| H | 5.00280900 | -3.74810300 | -1.82957000 |
| H | 4.02460300 | -3.92124600 | -0.36064900 |
| C | 3.56238600 | -1.12047900 | -3.26858100 |
| H | 4.54086100 | -1.27712400 | -3.74072900 |
| H | 2.81757400 | -1.67341500 | -3.85487000 |
| H | 3.32782600 | -0.05142800 | -3.34570100 |
| Si | 3.60158200 | -1.71312300 | -1.47177200 |
| C | -1.21141600 | 0.02773800 | -0.68421900 |
| C | -2.48547900 | 0.03279500 | 0.01028600 |
| C | -1.25926600 | 0.00241000 | -2.12993600 |
| C | -3.66494000 | 0.01297500 | -0.67190800 |
| H | -2.51867200 | 0.05428000 | 1.09095700 |
| C | -2.43952700 | -0.02515200 | -2.81912500 |
| H | -0.33837500 | -0.00095200 | -2.69814600 |
| C | -3.66870500 | -0.02160400 | -2.09819200 |
| H | -4.61801700 | 0.01840600 | -0.15462100 |
| H | -2.43193400 | -0.04716200 | -3.90151400 |
| O | -4.85520600 | -0.04877000 | -2.65956900 |
| C | -5.01101600 | -0.09475500 | -4.10240200 |
| H | -6.08662400 | -0.12436300 | -4.26228200 |
| H | -4.58355900 | 0.80468600 | -4.55052000 |
| H | -4.54116100 | -0.99771800 | -4.49823600 |

VIIb. 1,1,1-trifluoro-2-(p-tolyl)-4-(trimethylsilyl)butan-2-ylium

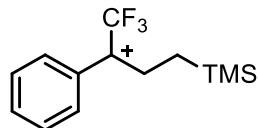


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | 0.00148200 | -0.01474400 | -0.01011400 |
| C | 0.00328500 | -0.04007500 | 1.53177100 |
| F | 1.24642600 | -0.02001800 | 2.04227800 |
| F | -0.60741100 | -1.14690900 | 2.01101900 |
| F | -0.64398500 | 1.04123700 | 2.02117800 |
| C | 1.34052700 | -0.06478100 | -0.64171800 |
| H | 1.32151100 | 0.32518600 | -1.65781900 |
| H | 2.05084200 | 0.53111900 | -0.06382600 |
| C | 1.80027800 | -1.56667900 | -0.64606100 |
| H | 1.83812400 | -1.96228000 | 0.37584600 |
| H | 1.06944600 | -2.17110300 | -1.19660900 |
| C | 4.81155000 | -0.81355600 | -0.45816200 |

| | | | |
|----|-------------|-------------|-------------|
| H | 4.61849100 | 0.26505000 | -0.51485300 |
| H | 4.81829800 | -1.10145600 | 0.60055500 |
| H | 5.81902300 | -0.98761900 | -0.85773200 |
| C | 3.91526100 | -3.66507800 | -1.32018000 |
| H | 3.16820900 | -4.26007800 | -1.85973900 |
| H | 4.89772900 | -3.88210000 | -1.75893500 |
| H | 3.93103700 | -4.00474400 | -0.27726700 |
| C | 3.49474600 | -1.25408700 | -3.24053400 |
| H | 4.46766900 | -1.43167700 | -3.71670500 |
| H | 2.73841600 | -1.80754400 | -3.81111000 |
| H | 3.27426100 | -0.18346400 | -3.33401200 |
| Si | 3.54197800 | -1.81576400 | -1.43590500 |
| C | -1.22067100 | -0.00643100 | -0.68805900 |
| C | -2.49160700 | -0.05452500 | -0.00563300 |
| C | -1.24987100 | 0.05742800 | -2.12702000 |
| C | -3.67075500 | -0.03545600 | -0.70959500 |
| H | -2.53439200 | -0.10900400 | 1.07362400 |
| C | -2.44048900 | 0.07129000 | -2.81278500 |
| H | -0.32565500 | 0.09511400 | -2.68870800 |
| C | -3.67764000 | 0.02976600 | -2.12518900 |
| H | -4.61470600 | -0.07313900 | -0.17481400 |
| H | -2.43644100 | 0.11751900 | -3.89705700 |
| C | -4.97065300 | 0.07716500 | -2.87061700 |
| H | -5.40126100 | 1.08597300 | -2.78344000 |
| H | -4.84028100 | -0.14309700 | -3.93260600 |
| H | -5.70173400 | -0.61376100 | -2.43727800 |

VIIc. 1,1,1-trifluoro-2-phenyl-4-(trimethylsilyl)butan-2-ylium

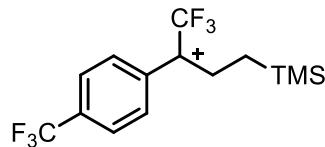


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | 0.00337600 | 0.02616300 | -0.02538500 |
| C | 0.02707500 | 0.08972700 | 1.51766800 |
| F | 1.27666400 | 0.11817400 | 2.00908800 |
| F | -0.59516100 | -0.97567600 | 2.06750100 |
| F | -0.59547100 | 1.20992600 | 1.94333800 |
| C | 1.32357900 | -0.10040300 | -0.66771200 |
| H | 1.31093200 | 0.21811500 | -1.70783400 |
| H | 2.07490000 | 0.48477100 | -0.13357800 |
| C | 1.68351700 | -1.63213200 | -0.56662000 |
| H | 1.71732600 | -1.95645900 | 0.47965900 |
| H | 0.91156000 | -2.22822300 | -1.06639700 |
| C | 4.73177900 | -1.04050500 | -0.45312700 |
| H | 4.61120900 | 0.03879600 | -0.60893300 |
| H | 4.71626600 | -1.23160700 | 0.62699600 |
| H | 5.72643000 | -1.31604200 | -0.82677700 |
| C | 3.64929100 | -3.89554300 | -1.08092400 |
| H | 2.86094800 | -4.47815700 | -1.57300800 |

| | | | |
|----|-------------|-------------|-------------|
| H | 4.61313300 | -4.21422500 | -1.49859000 |
| H | 3.64491500 | -4.14945800 | -0.01395400 |
| C | 3.37580100 | -1.62373100 | -3.19069900 |
| H | 4.32960000 | -1.91085100 | -3.65211400 |
| H | 2.57691800 | -2.16470800 | -3.71269600 |
| H | 3.23543100 | -0.55096400 | -3.37143000 |
| Si | 3.40416700 | -2.04090200 | -1.34926900 |
| C | -1.23517800 | 0.02871800 | -0.69111300 |
| C | -2.48847800 | 0.02479700 | 0.01689200 |
| C | -1.27522900 | 0.04859300 | -2.12832400 |
| C | -3.68412700 | 0.04353900 | -0.67222900 |
| H | -2.51152900 | 0.00359200 | 1.09773800 |
| C | -2.47933000 | 0.06532500 | -2.80073500 |
| H | -0.35666200 | 0.05541400 | -2.69989900 |
| C | -3.68481600 | 0.06388700 | -2.07713000 |
| H | -4.62249400 | 0.04089500 | -0.12840700 |
| H | -2.49588500 | 0.08352000 | -3.88504200 |
| H | -4.63008500 | 0.07958300 | -2.61168600 |

VIIId. 1,1,1-trifluoro-2-(4-(trifluoromethyl)phenyl)-4-(trimethylsilyl)butan-2-ylum

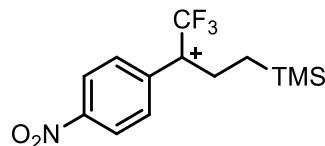


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | -0.00898900 | -0.02069800 | 0.02001000 |
| C | -0.02168400 | -0.04088500 | 1.56557700 |
| F | 1.21507900 | -0.05987500 | 2.08523200 |
| F | -0.67791300 | -1.11790500 | 2.04510500 |
| F | -0.63564900 | 1.07030800 | 2.02213400 |
| C | 1.30828800 | -0.13414500 | -0.60090700 |
| H | 1.34246800 | 0.23557000 | -1.62240000 |
| H | 2.08886100 | 0.34685800 | -0.01127200 |
| C | 1.50854300 | -1.70701900 | -0.56925600 |
| H | 1.50702400 | -2.09373300 | 0.45510200 |
| H | 0.70520600 | -2.20710300 | -1.11917300 |
| C | 4.60034600 | -1.47492200 | -0.31936300 |
| H | 4.60596200 | -0.37879500 | -0.35354300 |
| H | 4.52041900 | -1.78359100 | 0.72992500 |
| H | 5.57202200 | -1.81942600 | -0.69648300 |
| C | 3.22159300 | -4.10105000 | -1.29493400 |
| H | 2.39914400 | -4.52558000 | -1.88270100 |
| H | 4.16424200 | -4.48181300 | -1.70933700 |
| H | 3.13330500 | -4.46798700 | -0.26554500 |
| C | 3.27863900 | -1.58690800 | -3.13904800 |
| H | 4.20469500 | -1.93161100 | -3.61725900 |
| H | 2.43660900 | -1.96474300 | -3.73155800 |
| H | 3.27224900 | -0.49181600 | -3.19279600 |
| Si | 3.21485000 | -2.21431000 | -1.36236400 |

| | | | |
|---|-------------|-------------|-------------|
| C | -1.24579300 | 0.04580200 | -0.67647000 |
| C | -2.50543300 | -0.01266800 | 0.00024500 |
| C | -1.25405200 | 0.19820700 | -2.09761100 |
| C | -3.69044400 | 0.07623700 | -0.70647400 |
| H | -2.55791200 | -0.13352500 | 1.07326100 |
| C | -2.44431700 | 0.28674900 | -2.79649600 |
| H | -0.32731600 | 0.25291700 | -2.65326100 |
| C | -3.65984200 | 0.22442000 | -2.10103600 |
| H | -4.63580900 | 0.02553700 | -0.17804400 |
| H | -2.43057600 | 0.40391600 | -3.87357400 |
| C | -4.97293700 | 0.35511700 | -2.84918200 |
| F | -4.83484300 | 0.13659900 | -4.17246800 |
| F | -5.48744900 | 1.60030100 | -2.69542800 |
| F | -5.89528600 | -0.51773500 | -2.38580500 |

VIIe. 1,1,1-trifluoro-2-(4-nitrophenyl)-4-(trimethylsilyl)butan-2-ylium

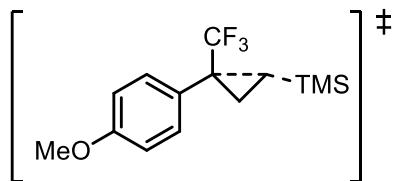


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | 0.00246600 | 0.02629500 | -0.07160400 |
| C | 0.05797600 | 0.10346300 | 1.47142000 |
| F | 1.31636500 | 0.11044700 | 1.93568700 |
| F | -0.58103600 | -0.93172300 | 2.05410000 |
| F | -0.53215200 | 1.24779000 | 1.87227500 |
| C | 1.28091500 | -0.11548200 | -0.74442100 |
| H | 1.28461200 | 0.18315600 | -1.78870700 |
| H | 2.10902900 | 0.35008300 | -0.21246000 |
| C | 1.36543600 | -1.69735000 | -0.61314400 |
| H | 1.37423100 | -2.03545200 | 0.42735300 |
| H | 0.53734000 | -2.18545400 | -1.13381200 |
| C | 4.47137000 | -1.61933100 | -0.40096300 |
| H | 4.53010400 | -0.52721500 | -0.47950300 |
| H | 4.38546600 | -1.88379900 | 0.65959500 |
| H | 5.42144200 | -2.02571500 | -0.77172800 |
| C | 2.93608500 | -4.20976500 | -1.24644200 |
| H | 2.08061400 | -4.61022900 | -1.80247000 |
| H | 3.84822200 | -4.66309100 | -1.65657900 |
| H | 2.84536100 | -4.52165700 | -0.19966100 |
| C | 3.11205300 | -1.78479300 | -3.20664100 |
| H | 3.99253200 | -2.23062900 | -3.68766900 |
| H | 2.22634700 | -2.11514500 | -3.76230200 |
| H | 3.19967700 | -0.69681000 | -3.31178200 |
| Si | 3.04925300 | -2.33384400 | -1.40650600 |
| C | -1.27555900 | 0.06947500 | -0.71909700 |
| C | -2.49587800 | 0.01499500 | 0.01660000 |
| C | -1.34409200 | 0.20911500 | -2.13600300 |
| C | -3.71832800 | 0.10005200 | -0.63113600 |

| | | | |
|---|-------------|-------------|-------------|
| H | -2.49732800 | -0.09900100 | 1.09153200 |
| C | -2.56372800 | 0.29243200 | -2.78554800 |
| H | -0.44344900 | 0.26298600 | -2.73284000 |
| C | -3.72896200 | 0.23657000 | -2.01885600 |
| H | -4.64603300 | 0.05947500 | -0.07484900 |
| H | -2.61673300 | 0.40391500 | -3.86094100 |
| N | -5.03735500 | 0.33021400 | -2.71158000 |
| O | -6.05217300 | 0.28398400 | -2.01955000 |
| O | -5.02546500 | 0.44840500 | -3.93516200 |

TS-VIIIa

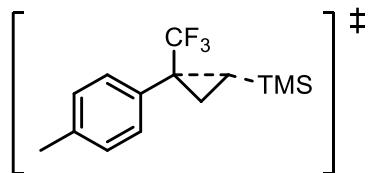


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | 0.00027700 | 0.01464400 | 0.01186600 |
| C | -0.00244500 | 0.00886400 | 1.54433600 |
| F | 1.24337500 | -0.01438400 | 2.06892300 |
| F | -0.67100500 | -1.03923200 | 2.06998700 |
| F | -0.60289100 | 1.13712000 | 1.98068300 |
| C | 1.21822200 | 0.41556500 | -0.63670300 |
| H | 1.14418300 | 0.80007300 | -1.64823600 |
| H | 2.01285400 | 0.85459000 | -0.04229700 |
| C | 1.19104300 | -1.16705500 | -0.59196000 |
| H | 1.39788300 | -1.69701300 | 0.33530000 |
| H | 0.55127800 | -1.69546400 | -1.29274700 |
| C | 4.36308500 | -0.92803800 | -0.35967600 |
| H | 4.41044400 | 0.16530700 | -0.39548500 |
| H | 4.23950200 | -1.24311100 | 0.68205700 |
| H | 5.33109300 | -1.31025200 | -0.71067500 |
| C | 2.94510600 | -3.50525400 | -1.44748800 |
| H | 2.10123600 | -3.88422900 | -2.03397500 |
| H | 3.86848400 | -3.90019100 | -1.89170300 |
| H | 2.86924000 | -3.89595800 | -0.42693900 |
| C | 3.00091600 | -0.89892100 | -3.19540900 |
| H | 3.88543800 | -1.26463600 | -3.73410800 |
| H | 2.11502400 | -1.21292700 | -3.75803500 |
| H | 3.04893900 | 0.19495400 | -3.19011800 |
| Si | 3.03391400 | -1.63327500 | -1.47367700 |
| C | -1.31668800 | 0.03745500 | -0.66176600 |
| C | -2.31158800 | -0.93190800 | -0.40598700 |
| C | -1.60640500 | 1.06907000 | -1.57096300 |
| C | -3.53994100 | -0.86854700 | -1.04171500 |
| H | -2.11594800 | -1.75238100 | 0.27552400 |
| C | -2.84490800 | 1.15008000 | -2.20519400 |
| H | -0.87199800 | 1.84277300 | -1.77318300 |
| C | -3.82058500 | 0.17473800 | -1.94591200 |
| H | -4.30038900 | -1.62050500 | -0.85557400 |

| | | | |
|---|-------------|------------|-------------|
| H | -3.03601000 | 1.97016200 | -2.88672600 |
| O | -5.05001300 | 0.15052000 | -2.51038900 |
| C | -5.40817000 | 1.17561300 | -3.44805600 |
| H | -6.42423700 | 0.93836100 | -3.76293500 |
| H | -5.38901900 | 2.16193500 | -2.97231500 |
| H | -4.73878200 | 1.16153800 | -4.31486800 |

TS-VIIIb

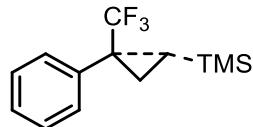


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | 0.00385800 | 0.01169800 | 0.00690000 |
| C | 0.00412900 | 0.01773000 | 1.54117900 |
| F | 1.25092800 | 0.01550600 | 2.06007100 |
| F | -0.64974900 | -1.03211000 | 2.08072700 |
| F | -0.60860200 | 1.14416900 | 1.96318500 |
| C | 1.23889200 | 0.33548200 | -0.64635200 |
| H | 1.18506700 | 0.70482500 | -1.66479300 |
| H | 2.04534000 | 0.76035100 | -0.05758500 |
| C | 1.18795700 | -1.24907400 | -0.58829000 |
| H | 1.34508200 | -1.76118700 | 0.35950800 |
| H | 0.50770300 | -1.75810000 | -1.26587400 |
| C | 4.34498600 | -1.13457300 | -0.31466300 |
| H | 4.42304700 | -0.04234500 | -0.32426800 |
| H | 4.20403700 | -1.46957500 | 0.71877400 |
| H | 5.30482200 | -1.53545000 | -0.66714900 |
| C | 2.85703100 | -3.64765300 | -1.44719500 |
| H | 2.00558200 | -3.99575000 | -2.04191500 |
| H | 3.77104100 | -4.06353300 | -1.89181000 |
| H | 2.76527800 | -4.04797700 | -0.43165400 |
| C | 3.02573000 | -1.02902700 | -3.16635800 |
| H | 3.90444100 | -1.42332100 | -3.69414300 |
| H | 2.13809300 | -1.30319500 | -3.74711100 |
| H | 3.11590400 | 0.06219800 | -3.15045700 |
| Si | 3.00027900 | -1.77755500 | -1.44919600 |
| C | -1.30856400 | 0.05022600 | -0.67162000 |
| C | -2.35229600 | -0.83809000 | -0.34260700 |
| C | -1.53854900 | 1.02302200 | -1.66330400 |
| C | -3.57828100 | -0.75218500 | -0.99292200 |
| H | -2.19996400 | -1.61308200 | 0.39993600 |
| C | -2.77624000 | 1.10748100 | -2.29665900 |
| H | -0.76303100 | 1.73603100 | -1.92461800 |
| C | -3.81827700 | 0.22368600 | -1.97651500 |
| H | -4.36384700 | -1.45782500 | -0.73522500 |
| H | -2.93363700 | 1.87519300 | -3.04971000 |
| C | -5.16454200 | 0.32781400 | -2.64744100 |
| H | -5.86387000 | 0.89496000 | -2.01857200 |

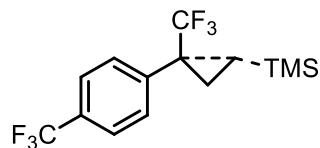
| | | | |
|---|-------------|-------------|-------------|
| H | -5.09451300 | 0.84255400 | -3.61051700 |
| H | -5.60524800 | -0.66117600 | -2.81146300 |

TS-VIIIc

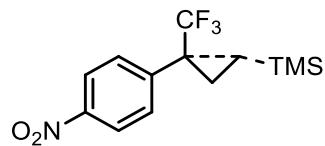


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | -0.00731300 | -0.01513600 | 0.00813100 |
| C | -0.01247900 | -0.04431500 | 1.54384000 |
| F | 1.23152500 | -0.07592800 | 2.06415200 |
| F | -0.68381500 | -1.09432000 | 2.05973600 |
| F | -0.60913400 | 1.08364800 | 1.98308000 |
| C | 1.25039500 | 0.22654900 | -0.63508600 |
| H | 1.22597200 | 0.60655200 | -1.65103500 |
| H | 2.06920100 | 0.61459300 | -0.03779600 |
| C | 1.16444800 | -1.35878800 | -0.60589200 |
| H | 1.25860700 | -1.87213900 | 0.35061500 |
| H | 0.44545700 | -1.82182800 | -1.27783100 |
| C | 4.30814700 | -1.36005200 | -0.30028600 |
| H | 4.41720800 | -0.27021500 | -0.29110400 |
| H | 4.15213100 | -1.70720900 | 0.72708300 |
| H | 5.25773200 | -1.78261100 | -0.65491200 |
| C | 2.74559000 | -3.81289700 | -1.46030300 |
| H | 1.88326300 | -4.12809400 | -2.05775200 |
| H | 3.64560900 | -4.25453200 | -1.90846100 |
| H | 2.64016000 | -4.21862500 | -0.44817200 |
| C | 3.01490900 | -1.19230300 | -3.16014100 |
| H | 3.88273400 | -1.61406900 | -3.68443200 |
| H | 2.12204600 | -1.43191000 | -3.74856600 |
| H | 3.14268400 | -0.10479200 | -3.13869000 |
| Si | 2.94481800 | -1.94630300 | -1.44531400 |
| C | -1.30681500 | 0.07407200 | -0.68115700 |
| C | -2.40372200 | -0.73999700 | -0.32726200 |
| C | -1.46424700 | 1.03320000 | -1.70377800 |
| C | -3.62107800 | -0.59767300 | -0.98785300 |
| H | -2.30077000 | -1.49763400 | 0.44052300 |
| C | -2.69078500 | 1.17902900 | -2.34852100 |
| H | -0.64353000 | 1.68985200 | -1.97237400 |
| C | -3.76933200 | 0.36211100 | -1.99594800 |
| H | -4.45525900 | -1.23751600 | -0.71653700 |
| H | -2.80369100 | 1.93287800 | -3.12174600 |
| H | -4.72334400 | 0.47339300 | -2.50322800 |

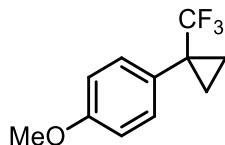
TS-VIII^d**Coordinates (from last standard orientation):**

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | 0.02402200 | 0.04878000 | -0.06587600 |
| C | 0.08318600 | 0.10320400 | 1.47208000 |
| F | 1.34662600 | 0.09821300 | 1.93437800 |
| F | -0.56137000 | -0.92099600 | 2.06967600 |
| F | -0.49776600 | 1.25179300 | 1.87267900 |
| C | 1.27506400 | 0.06127500 | -0.76796900 |
| H | 1.25673900 | 0.36967200 | -1.80809600 |
| H | 2.14699300 | 0.42280700 | -0.23142200 |
| C | 1.09547300 | -1.51326600 | -0.64053200 |
| H | 1.10708300 | -1.94143700 | 0.36286500 |
| H | 0.29795600 | -1.93175200 | -1.25205900 |
| C | 4.18559400 | -1.85082400 | -0.22374500 |
| H | 4.36831500 | -0.77132100 | -0.18329100 |
| H | 3.98477600 | -2.20920400 | 0.79221500 |
| H | 5.11210300 | -2.32718100 | -0.57055900 |
| C | 2.39858700 | -4.14284800 | -1.40048100 |
| H | 1.55428700 | -4.37514800 | -2.05905900 |
| H | 3.27450600 | -4.69517100 | -1.76583200 |
| H | 2.16787500 | -4.50628100 | -0.39312000 |
| C | 3.02485900 | -1.60744700 | -3.13072600 |
| H | 3.85957200 | -2.13353100 | -3.61243700 |
| H | 2.13350300 | -1.76044500 | -3.74991700 |
| H | 3.27034700 | -0.53952200 | -3.12473800 |
| Si | 2.80116300 | -2.30743600 | -1.40462300 |
| C | -1.28457800 | 0.17475400 | -0.71285300 |
| C | -2.46369400 | -0.34533900 | -0.13184500 |
| C | -1.37808100 | 0.87142300 | -1.93693600 |
| C | -3.68948700 | -0.18021100 | -0.76339300 |
| H | -2.42791700 | -0.89748200 | 0.79835000 |
| C | -2.60893800 | 1.04577500 | -2.56129900 |
| H | -0.49957500 | 1.31143000 | -2.39340300 |
| C | -3.76199700 | 0.51585400 | -1.97638000 |
| H | -4.58480900 | -0.59178700 | -0.30959200 |
| H | -2.66514100 | 1.59825300 | -3.49208300 |
| C | -5.10214200 | 0.65797600 | -2.65832100 |
| F | -5.48939900 | -0.51169300 | -3.23504900 |
| F | -6.08010000 | 1.00002300 | -1.78363900 |
| F | -5.09368900 | 1.59299100 | -3.63428100 |

TS-VIIIe**Coordinates (from last standard orientation):**

| ATOM | X | Y | Z |
|-------------|-------------|-------------|-------------|
| 1 1 | | | |
| C | -0.01030400 | -0.01233000 | 0.01214500 |
| C | -0.02193300 | -0.03654900 | 1.55457100 |
| F | 1.21818800 | -0.04020400 | 2.07149100 |
| F | -0.66949300 | -1.10619200 | 2.06232500 |
| F | -0.64575900 | 1.07632800 | 1.98953300 |
| C | 1.27748200 | -0.03007100 | -0.62618700 |
| H | 1.32296700 | 0.32720500 | -1.64974500 |
| H | 2.11883600 | 0.31359500 | -0.03132400 |
| C | 1.13956800 | -1.61276200 | -0.55906600 |
| H | 1.18819400 | -2.04028200 | 0.44341200 |
| H | 0.30277300 | -2.02616600 | -1.12284800 |
| C | 4.27712100 | -1.69019800 | -0.59918900 |
| H | 4.40608000 | -0.61359200 | -0.75611900 |
| H | 4.24192500 | -1.88492000 | 0.47887000 |
| H | 5.16932600 | -2.18932300 | -0.99971600 |
| C | 2.53112400 | -4.21824200 | -1.21323100 |
| H | 1.60124500 | -4.58034500 | -1.66577100 |
| H | 3.36709500 | -4.74956500 | -1.68751100 |
| H | 2.52649200 | -4.47755200 | -0.14876600 |
| C | 2.66871300 | -1.87500100 | -3.28591700 |
| H | 3.48341600 | -2.37097500 | -3.82987100 |
| H | 1.72307200 | -2.18984000 | -3.74166400 |
| H | 2.78492700 | -0.79578100 | -3.43477700 |
| Si | 2.76500200 | -2.37077500 | -1.47797900 |
| C | -1.28224900 | 0.13389900 | -0.68741900 |
| C | -2.51058800 | -0.22995600 | -0.08385000 |
| C | -1.30056600 | 0.69508000 | -1.98746200 |
| C | -3.71221400 | -0.04393200 | -0.75489200 |
| H | -2.53729500 | -0.67385200 | 0.90209400 |
| C | -2.49852500 | 0.88930800 | -2.66119800 |
| H | -0.38536900 | 1.00979100 | -2.47230600 |
| C | -3.68465000 | 0.51272900 | -2.03238500 |
| H | -4.65189400 | -0.32689300 | -0.29774700 |
| H | -2.51464000 | 1.32949000 | -3.65013800 |
| N | -4.96244000 | 0.71402300 | -2.74770700 |
| O | -6.00101200 | 0.40282100 | -2.16525500 |
| O | -4.91485600 | 1.18131800 | -3.88537900 |

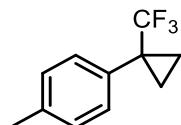
IXa. 1-methoxy-4-(1-(trifluoromethyl)cyclopropyl)benzene



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | -0.00016000 | 0.00003700 | -0.00002100 |
| C | -0.00077800 | -0.00024800 | 1.50797500 |
| F | 1.25347300 | -0.00054900 | 2.03261400 |
| F | -0.62561600 | -1.09107900 | 2.03710300 |
| F | -0.62529800 | 1.09054800 | 2.03751900 |
| C | 1.16523900 | 0.74864700 | -0.64181900 |
| H | 0.93962200 | 1.27945300 | -1.56131300 |
| H | 1.86552500 | 1.25881800 | 0.01233000 |
| C | 1.16460800 | -0.74929000 | -0.64216900 |
| H | 1.86448400 | -1.26039600 | 0.01169100 |
| H | 0.93844200 | -1.27941800 | -1.56192300 |
| C | -1.34948100 | 0.00069500 | -0.68437100 |
| C | -2.57077200 | 0.00083300 | 0.01689000 |
| C | -1.42380200 | 0.00115600 | -2.08596800 |
| C | -3.79387600 | 0.00142100 | -0.64913100 |
| H | -2.59106700 | 0.00051300 | 1.09977100 |
| C | -2.64339700 | 0.00172600 | -2.76972400 |
| H | -0.51887200 | 0.00103000 | -2.68670700 |
| C | -3.84391300 | 0.00187300 | -2.04912800 |
| H | -4.72340500 | 0.00153900 | -0.08691000 |
| H | -2.63620100 | 0.00207000 | -3.85372500 |
| O | -5.09041300 | 0.00243800 | -2.61089900 |
| C | -5.19548500 | 0.00321000 | -4.03626200 |
| H | -6.26435400 | 0.00373100 | -4.25326900 |
| H | -4.73335200 | 0.89996700 | -4.46583000 |
| H | -4.73405600 | -0.89347400 | -4.46674500 |

IXb. 1-methyl-4-(1-(trifluoromethyl)cyclopropyl)benzene

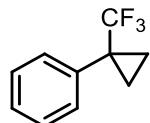


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | -0.00003400 | 0.00069700 | -0.00008200 |
| C | -0.00024700 | 0.01224500 | 1.50807400 |
| F | 1.25451700 | 0.02334300 | 2.03169000 |
| F | -0.61813400 | -1.07782700 | 2.04620900 |
| F | -0.63035300 | 1.10370800 | 2.02903600 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.16188000 | 0.75006900 | -0.64851300 |
| H | 0.93351500 | 1.27289500 | -1.57177700 |
| H | 1.85813900 | 1.26902000 | 0.00289100 |
| C | 1.16884800 | -0.74706100 | -0.63768800 |
| H | 1.86992600 | -1.25005200 | 0.02109300 |
| H | 0.94566900 | -1.28549200 | -1.55325700 |
| C | -1.34772500 | -0.01117500 | -0.68631500 |
| C | -2.56613200 | -0.01289300 | 0.01073400 |
| C | -1.41590800 | -0.01954700 | -2.09304500 |
| C | -3.79001300 | -0.02282700 | -0.66793800 |
| H | -2.58834000 | -0.00482000 | 1.09374300 |
| C | -2.63795300 | -0.02955700 | -2.76317700 |
| H | -0.50829000 | -0.01649400 | -2.68986400 |
| C | -3.85586700 | -0.03276700 | -2.06505200 |
| H | -4.70954700 | -0.02196600 | -0.08655400 |
| H | -2.64148800 | -0.03394400 | -3.85132600 |
| C | -5.17690900 | -0.05706900 | -2.79873400 |
| H | -6.01666900 | 0.09129100 | -2.11206900 |
| H | -5.22268900 | 0.72608300 | -3.56513700 |
| H | -5.32941800 | -1.01660500 | -3.30999500 |

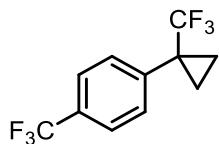
IXc. (1-(trifluoromethyl)cyclopropyl)benzene



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | 0.00019600 | 0.00178500 | -0.00030800 |
| C | -0.00045400 | -0.00600600 | 1.50773500 |
| F | 1.25009100 | -0.01389700 | 2.04271500 |
| F | -0.64061300 | -1.09439500 | 2.02147900 |
| F | -0.63164800 | 1.08214700 | 2.03287300 |
| C | 1.13194600 | 0.75332800 | -0.67668200 |
| H | 0.87743100 | 1.27561200 | -1.59382800 |
| H | 1.85996400 | 1.26028900 | -0.05073200 |
| C | 1.12647000 | -0.75117500 | -0.68431200 |
| H | 1.85075700 | -1.26957600 | -0.06346500 |
| H | 0.86809400 | -1.26235200 | -1.60661800 |
| C | -1.38067200 | 0.00979200 | -0.61021600 |
| C | -2.04102900 | -1.19471400 | -0.89515500 |
| C | -2.03105100 | 1.22166600 | -0.88687900 |
| C | -3.32565800 | -1.18895000 | -1.44610400 |
| H | -1.54539700 | -2.13989400 | -0.68875500 |
| C | -3.31564000 | 1.23025400 | -1.43787700 |
| H | -1.52764200 | 2.16128400 | -0.67397100 |
| C | -3.96646900 | 0.02426100 | -1.71809200 |
| H | -3.82322800 | -2.13026500 | -1.66457000 |
| H | -3.80541500 | 2.17711800 | -1.64989200 |
| H | -4.96440400 | 0.02988200 | -2.14875200 |

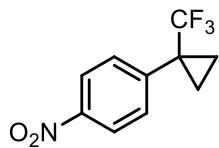
IXd. 1-(trifluoromethyl)-4-(1-(trifluoromethyl)cyclopropyl)benzene



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | 0.00000000 | -0.00032100 | -0.00002000 |
| C | -0.00013800 | -0.00341000 | 1.50925200 |
| F | 1.25412200 | -0.00546600 | 2.02931600 |
| F | -0.62597100 | -1.09484200 | 2.03367200 |
| F | -0.62448700 | 1.08658800 | 2.03821800 |
| C | 1.16755900 | 0.74522400 | -0.64628300 |
| H | 0.94198700 | 1.28083100 | -1.56277600 |
| H | 1.86386400 | 1.25429700 | 0.01254000 |
| C | 1.16384800 | -0.74936300 | -0.64920700 |
| H | 1.85766600 | -1.26461200 | 0.00745800 |
| H | 0.93500400 | -1.27998200 | -1.56778400 |
| C | -1.34383800 | 0.00424000 | -0.68644900 |
| C | -2.56066200 | 0.00120100 | 0.01757700 |
| C | -1.40636800 | 0.00895600 | -2.09321900 |
| C | -3.78495600 | 0.00240700 | -0.65193700 |
| H | -2.57911200 | -0.00460900 | 1.09962800 |
| C | -2.62386500 | 0.01038100 | -2.76817000 |
| H | -0.49905600 | 0.00899100 | -2.68831000 |
| C | -3.82290500 | 0.00423900 | -2.04765500 |
| H | -4.70480100 | -0.00315500 | -0.07618500 |
| H | -2.63316200 | 0.01145700 | -3.85339400 |
| C | -5.13741100 | 0.05375200 | -2.76998500 |
| F | -5.09458500 | -0.56864900 | -3.97699900 |
| F | -6.14455500 | -0.52374300 | -2.06522200 |
| F | -5.54131700 | 1.33547700 | -3.02287900 |

IXe. 1-nitro-4-(1-(trifluoromethyl)cyclopropyl)benzene

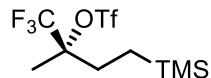


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | -0.00003200 | -0.00011300 | -0.00009000 |
| C | -0.00041200 | 0.00055500 | 1.51007100 |
| F | 1.25356600 | 0.00112900 | 2.02824500 |
| F | -0.62568700 | -1.09005200 | 2.03535100 |
| F | -0.62625600 | 1.09131700 | 2.03436100 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.16759800 | 0.74623900 | -0.65031200 |
| H | 0.94018400 | 1.28067600 | -1.56690600 |
| H | 1.85864400 | 1.25979700 | 0.01045400 |
| C | 1.16809100 | -0.74617500 | -0.64974100 |
| H | 1.85944400 | -1.25877200 | 0.01143600 |
| H | 0.94109200 | -1.28147900 | -1.56593800 |
| C | -1.33923200 | -0.00075900 | -0.68706400 |
| C | -2.55766300 | -0.00074500 | 0.01956100 |
| C | -1.39796900 | -0.00141000 | -2.09652700 |
| C | -3.78092500 | -0.00137300 | -0.64515900 |
| H | -2.57499600 | -0.00028400 | 1.10122100 |
| C | -2.60979800 | -0.00205000 | -2.77562500 |
| H | -0.48957800 | -0.00133800 | -2.68898600 |
| C | -3.79641800 | -0.00203600 | -2.03929900 |
| H | -4.70918400 | -0.00139200 | -0.08702100 |
| H | -2.63612400 | -0.00253600 | -3.85838800 |
| N | -5.07584300 | -0.00277700 | -2.74214300 |
| O | -5.06605100 | -0.00365300 | -3.97868700 |
| O | -6.11458500 | -0.00246500 | -2.07146700 |

Xa. (S)-1,1,1-trifluoro-2-methyl-4-(trimethylsilyl)butan-2-yl trifluoromethanesulfonate



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | 0.00004100 | -0.00061400 | -0.00176800 |
| C | -0.01291700 | -0.00113300 | 1.54931300 |
| F | 1.23442100 | -0.00065600 | 2.06925800 |
| F | -0.64916900 | -1.09496200 | 2.02647900 |
| F | -0.65353700 | 1.07944200 | 2.04905000 |
| O | 0.68550400 | 1.31169500 | -0.23739200 |
| S | 0.48973300 | 2.22925700 | -1.54372700 |
| O | -0.61541000 | 3.16461200 | -1.37366600 |
| O | 0.62319300 | 1.45851100 | -2.77593400 |
| C | 0.91795700 | -1.08755200 | -0.59993900 |
| H | 0.99779500 | -0.84284400 | -1.66400500 |
| H | 1.91539800 | -0.94776700 | -0.16994300 |
| C | 0.45992100 | -2.54824500 | -0.43817700 |
| H | 0.38047700 | -2.81609700 | 0.62250200 |
| H | -0.54248400 | -2.68339100 | -0.86682400 |
| C | -1.42892800 | -0.00381300 | -0.53700700 |
| H | -1.99293700 | 0.86299400 | -0.18508600 |
| H | -1.42388100 | -0.01520600 | -1.62990300 |
| H | -1.94080200 | -0.90747600 | -0.19778000 |
| C | 2.09310100 | 3.19586900 | -1.28376900 |
| F | 2.16694100 | 4.10894100 | -2.25607600 |
| F | 2.07835100 | 3.80496100 | -0.09910700 |
| F | 3.14080500 | 2.37637300 | -1.36029700 |
| C | 3.33863100 | -3.74451700 | -0.50339700 |
| H | 3.81526300 | -2.77381900 | -0.68955400 |
| H | 3.30424300 | -3.89902600 | 0.58280400 |

| | | | |
|----|-------------|-------------|-------------|
| H | 3.98962000 | -4.51875300 | -0.92982400 |
| C | 0.85524900 | -5.54608500 | -0.95069400 |
| H | -0.15038200 | -5.62438100 | -1.38344900 |
| H | 1.47343100 | -6.33473300 | -1.39859700 |
| H | 0.77525300 | -5.75467000 | 0.12393500 |
| C | 1.70623000 | -3.51306600 | -3.12996800 |
| H | 2.31590900 | -4.28204800 | -3.62203200 |
| H | 0.71032800 | -3.53223800 | -3.59111600 |
| H | 2.16096300 | -2.53966300 | -3.35356700 |
| Si | 1.60604700 | -3.83611300 | -1.26537000 |

Xb. (1R,3S)-1-(trifluoromethyl)-3-(trimethylsilyl)cyclopentyl trifluoromethanesulfonate

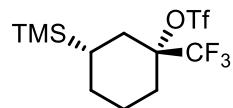


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | 0.00000000 | 0.00000000 | 0.00000000 |
| C | 0.00000000 | 0.00000000 | 1.54441100 |
| C | 1.51055200 | 0.00000000 | 1.87593500 |
| C | 2.18549100 | -0.82230000 | 0.73850700 |
| C | 1.10623300 | -1.00850500 | -0.35665600 |
| H | -0.96373500 | -0.28883200 | -0.43040300 |
| H | 0.25380100 | 0.99332600 | -0.39301200 |
| H | -0.42162200 | -0.96120900 | 1.87822100 |
| H | 1.89688900 | 1.02266300 | 1.84524400 |
| H | 1.74587500 | -0.39793700 | 2.86603700 |
| H | 1.54174400 | -0.88216000 | -1.35110800 |
| H | 0.70718400 | -2.02649200 | -0.29715900 |
| Si | -1.03804100 | 1.36195500 | 2.40339200 |
| C | -2.83470700 | 1.18326700 | 1.83189000 |
| H | -3.47793300 | 1.91460800 | 2.33820300 |
| H | -2.93156800 | 1.34754400 | 0.75134500 |
| H | -3.22770200 | 0.18307800 | 2.05554700 |
| C | -0.93375100 | 1.11717900 | 4.27904700 |
| H | 0.09548900 | 1.22002200 | 4.64572200 |
| H | -1.54790600 | 1.86121000 | 4.80267400 |
| H | -1.29515300 | 0.12250400 | 4.57041600 |
| C | -0.38741400 | 3.08127200 | 1.94258700 |
| H | -0.40722400 | 3.24920500 | 0.85843000 |
| H | -1.01228400 | 3.85485800 | 2.40782000 |
| H | 0.64172700 | 3.24027700 | 2.28832000 |
| C | 2.74949900 | -2.17105400 | 1.21803500 |
| F | 1.77693800 | -2.89727400 | 1.82062400 |
| F | 3.75579200 | -2.03336400 | 2.10765600 |
| F | 3.22778500 | -2.91110100 | 0.19059400 |
| O | 3.33283900 | -0.15776900 | 0.07004800 |
| S | 4.28275100 | 0.99409600 | 0.69199800 |
| O | 3.83860300 | 2.30387500 | 0.23046700 |
| O | 4.60587700 | 0.76910600 | 2.09515000 |
| C | 5.79721700 | 0.52468600 | -0.33670700 |
| F | 6.74436300 | 1.43329600 | -0.08748800 |

| | | | |
|---|------------|-------------|-------------|
| F | 6.23216100 | -0.68335400 | 0.01950300 |
| F | 5.49979500 | 0.53473200 | -1.63549000 |

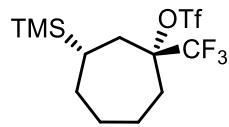
Xc. (1R,3S)-1-(trifluoromethyl)-3-(trimethylsilyl)cyclohexyl trifluoromethanesulfonate



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.00021000 | -0.00476600 | 0.00236700 |
| C | 0.00094000 | -0.01252400 | 1.55131500 |
| C | 1.41260700 | -0.00759500 | 2.16846100 |
| C | 2.29745300 | 1.09661900 | 1.57044500 |
| C | 2.29904000 | 1.11245200 | 0.03181200 |
| C | 0.87037000 | 1.15344500 | -0.53171300 |
| H | -0.48895500 | 0.90295400 | 1.90438700 |
| H | -0.56975100 | -0.86011200 | 1.93931300 |
| H | 0.43693000 | -0.94961000 | -0.35116100 |
| H | 1.87998900 | 2.04165600 | 1.93684400 |
| H | 3.31281900 | 1.01735300 | 1.97103700 |
| H | 2.83090100 | 0.23843500 | -0.36093100 |
| H | 0.41097200 | 2.11653000 | -0.26408900 |
| H | 0.91290200 | 1.11960600 | -1.62675200 |
| C | 2.09211800 | -1.40092400 | 2.15228100 |
| O | 1.40880900 | 0.29520800 | 3.63907700 |
| S | 0.13637700 | 0.34858900 | 4.62441100 |
| O | -0.53842900 | 1.63970500 | 4.54090600 |
| O | -0.63615500 | -0.88820400 | 4.62071800 |
| C | 1.18865000 | 0.36386700 | 6.19444800 |
| F | 0.34992800 | 0.45813600 | 7.23074500 |
| F | 1.88887600 | -0.76585700 | 6.28910200 |
| F | 2.01397000 | 1.41029600 | 6.19282900 |
| F | 3.28879700 | -1.37988100 | 2.78344700 |
| F | 1.33643100 | -2.33737600 | 2.76874100 |
| F | 2.31964800 | -1.83944400 | 0.89280200 |
| H | 2.86272400 | 1.99510100 | -0.29376300 |
| Si | -1.78933600 | 0.00177300 | -0.70643400 |
| C | -1.68755400 | -0.15649700 | -2.59161600 |
| H | -2.69480400 | -0.22071500 | -3.02321800 |
| H | -1.18505200 | 0.70370300 | -3.05062800 |
| H | -1.14108100 | -1.06169500 | -2.88632800 |
| C | -2.67929000 | 1.61057900 | -0.24454300 |
| H | -3.70037500 | 1.60675200 | -0.64777100 |
| H | -2.75547800 | 1.74172600 | 0.84239600 |
| H | -2.16579300 | 2.48992100 | -0.65331100 |
| C | -2.74140200 | -1.48113300 | -0.00852900 |
| H | -2.22306400 | -2.42476200 | -0.22287300 |
| H | -2.87824400 | -1.41289400 | 1.07791800 |
| H | -3.73919000 | -1.53999800 | -0.46252800 |

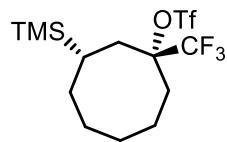
Xd. (1R,3S)-1-(trifluoromethyl)-3-(trimethylsilyl)cycloheptyl trifluoromethanesulfonate



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.00450900 | 0.00579600 | 0.00223300 |
| C | 0.00346800 | -0.02169200 | 1.53981200 |
| C | 1.35990200 | -0.01791900 | 2.26303500 |
| C | 0.70058600 | 1.22931700 | -0.62364600 |
| C | 2.30051400 | 1.15195500 | 1.93300100 |
| C | 2.24761400 | 1.24239300 | -0.71948800 |
| C | 3.05294400 | 1.00829200 | 0.59909200 |
| H | -0.55611700 | 0.87204200 | 1.83933000 |
| H | 1.88868100 | -0.96463300 | 2.09964400 |
| H | 1.75179900 | 2.10351600 | 1.97535400 |
| H | 0.34254500 | 2.09569900 | -0.05789700 |
| H | -0.58418800 | -0.88462600 | 1.87075500 |
| H | 1.11735900 | 0.01230000 | 3.33266600 |
| H | 0.32537300 | 1.33997700 | -1.64476200 |
| H | 3.05422500 | 1.20520800 | 2.72934400 |
| H | 2.53325900 | 0.45154200 | -1.42640200 |
| H | 3.90945900 | 1.69413400 | 0.63009600 |
| H | 3.49578500 | 0.00411600 | 0.57568900 |
| Si | 2.82464100 | 2.85768700 | -1.60428900 |
| C | 0.41372800 | -1.34252100 | -0.63550400 |
| C | 1.85184600 | 3.10776600 | -3.21207100 |
| H | 0.79444600 | 3.33564800 | -3.03024000 |
| H | 2.27514300 | 3.94704400 | -3.77924800 |
| H | 1.89995300 | 2.21782200 | -3.85293200 |
| C | 2.58370600 | 4.36152200 | -0.47542500 |
| H | 3.12989800 | 4.25450300 | 0.46998500 |
| H | 2.95632500 | 5.26737400 | -0.97137700 |
| H | 1.52626800 | 4.52954400 | -0.23562500 |
| C | 4.66176400 | 2.66877700 | -2.03118300 |
| H | 4.83131000 | 1.79838600 | -2.67814000 |
| H | 5.01695100 | 3.55740500 | -2.56906300 |
| H | 5.28835500 | 2.55065900 | -1.13880700 |
| O | -1.48339800 | 0.01654100 | -0.29599100 |
| S | -2.29342300 | 0.97649100 | -1.29910800 |
| O | -2.35215900 | 2.34797600 | -0.80398900 |
| O | -1.98545900 | 0.71325800 | -2.70090100 |
| C | -3.95896100 | 0.16491100 | -0.92378200 |
| F | 0.33921700 | -1.30449300 | -1.98568100 |
| F | 1.68290200 | -1.67745900 | -0.31278100 |
| F | -0.37595800 | -2.36004000 | -0.22258900 |
| F | -3.92928900 | -1.12714400 | -1.24844500 |
| F | -4.26231300 | 0.30170800 | 0.36663400 |
| F | -4.87690300 | 0.79104700 | -1.66677200 |

Xe. (1R,3S)-1-(trifluoromethyl)-3-(trimethylsilyl)cyclooctyl trifluoromethanesulfonate

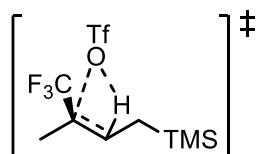


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | 0.00689200 | 0.01598200 | -0.00665400 |
| C | -0.00364400 | 0.00900900 | 1.54005700 |
| C | 3.04983300 | -0.00477200 | -0.26928000 |
| C | 1.09129700 | 0.75778900 | 2.33178100 |
| C | 3.50778000 | 0.46351600 | 1.14419900 |
| C | 2.53763000 | 0.20335700 | 2.32581400 |
| H | 0.35672200 | 0.97835800 | -0.38862700 |
| H | 0.01666700 | -1.02521600 | 1.89826800 |
| H | -1.04204700 | -0.05149800 | -0.31956300 |
| H | -0.95300100 | 0.43334500 | 1.88055700 |
| H | 3.01134100 | 0.61450700 | 3.22172600 |
| H | 2.43730600 | -0.87396600 | 2.49321400 |
| C | 0.75937500 | -1.13768500 | -0.69452600 |
| C | 2.24116500 | -1.32413600 | -0.31509800 |
| H | 2.30730900 | -1.84661800 | 0.64586800 |
| H | 2.68910600 | -2.01204400 | -1.04276400 |
| O | 0.59923500 | 0.74771800 | 3.76703900 |
| S | 0.79292600 | -0.43950300 | 4.82956900 |
| O | 0.59549600 | -1.75804800 | 4.23540900 |
| O | 1.93632100 | -0.18359000 | 5.69722000 |
| C | -0.75813000 | -0.02108600 | 5.82345300 |
| F | -1.84218000 | -0.14200300 | 5.05787600 |
| F | -0.67930800 | 1.21955300 | 6.30408100 |
| F | -0.82775000 | -0.88973400 | 6.83683100 |
| H | 0.68876700 | -0.96466400 | -1.77762000 |
| H | 2.46298400 | 0.79217100 | -0.74154100 |
| H | 3.93807800 | -0.10244200 | -0.90447000 |
| H | 3.68176600 | 1.54753600 | 1.08760500 |
| C | 1.05368200 | 2.29551700 | 2.11275100 |
| F | -0.18280400 | 2.80548800 | 2.31202700 |
| F | 1.42029200 | 2.62951700 | 0.85601700 |
| F | 1.89192400 | 2.94158600 | 2.95438800 |
| Si | 5.25422500 | -0.23323000 | 1.59389300 |
| C | 5.26417100 | -2.12883900 | 1.59167000 |
| H | 5.00565100 | -2.53408800 | 0.60587000 |
| H | 6.26501900 | -2.49829700 | 1.85105700 |
| H | 4.55947300 | -2.54647000 | 2.32183700 |
| C | 5.77765000 | 0.39952700 | 3.30368600 |
| H | 6.82783400 | 0.14033000 | 3.49157200 |
| H | 5.68887600 | 1.49159300 | 3.37243000 |
| H | 5.18286200 | -0.03844200 | 4.11448000 |
| C | 6.49535800 | 0.40666300 | 0.31153700 |
| H | 6.49698700 | 1.50357400 | 0.27062800 |
| H | 7.50957200 | 0.08227100 | 0.57860900 |
| H | 6.28580800 | 0.03311200 | -0.69809300 |

H 0.22506600 -2.07834400 -0.50061300

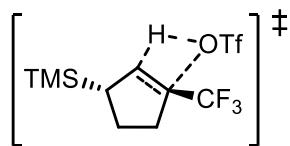
TS-XIa.



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | -0.01363000 | 0.01004200 | -0.01959000 |
| C | -0.03259600 | -0.00008300 | 1.51729200 |
| F | 1.18734600 | -0.00696600 | 2.06757500 |
| F | -0.67074400 | -1.14264200 | 1.88563200 |
| F | -0.71949600 | 1.02998100 | 2.03423400 |
| O | 2.72150100 | 1.34521100 | -1.39524400 |
| S | 2.50634800 | 2.56585100 | -0.53551800 |
| O | 1.28362400 | 2.45039100 | 0.29544200 |
| O | 2.71933800 | 3.84233000 | -1.23222000 |
| C | 0.95028100 | -0.73049500 | -0.73558600 |
| H | 0.59959200 | -0.89684900 | -1.76236400 |
| H | 1.67016900 | 0.20489000 | -0.96689100 |
| C | 1.81802500 | -1.84563700 | -0.13086800 |
| H | 2.67365500 | -1.41762700 | 0.40388700 |
| H | 1.24154200 | -2.40798200 | 0.61367300 |
| C | -1.10751500 | 0.74141100 | -0.68289700 |
| H | -1.23173300 | 1.74510100 | -0.26784300 |
| H | -0.96834600 | 0.77570400 | -1.76445400 |
| H | -2.04468000 | 0.19608500 | -0.47282200 |
| C | 3.92502600 | 2.46792400 | 0.69420200 |
| F | 3.82989900 | 3.46409200 | 1.59055400 |
| F | 3.90353400 | 1.29795100 | 1.35301400 |
| F | 5.10342200 | 2.57654800 | 0.05864100 |
| C | 3.56790000 | -2.22029000 | -2.68765700 |
| H | 2.99999900 | -1.47101900 | -3.25307400 |
| H | 4.41429300 | -1.71020000 | -2.21097700 |
| H | 3.97412600 | -2.94040500 | -3.40968400 |
| C | 3.52827600 | -4.35961600 | -0.43577800 |
| H | 2.92484900 | -4.87209600 | 0.32399200 |
| H | 3.94083000 | -5.12361100 | -1.10689700 |
| H | 4.36895500 | -3.87166900 | 0.07327000 |
| C | 1.04017400 | -3.97366500 | -2.25486700 |
| H | 1.40364400 | -4.72686800 | -2.96561800 |
| H | 0.40312000 | -4.48506700 | -1.52205800 |
| H | 0.41042100 | -3.27078400 | -2.81506300 |
| Si | 2.49564200 | -3.10903500 | -1.40746700 |

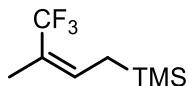
TS-XIb.



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | -0.00424200 | 0.00863300 | -0.03480900 |
| C | -0.01739900 | -0.01145500 | 1.51835200 |
| C | 1.49590000 | -0.02987600 | 1.84405300 |
| C | 2.15672500 | -0.61346400 | 0.75848100 |
| C | 1.28511800 | -0.75526900 | -0.42656200 |
| H | -0.89513200 | -0.44974500 | -0.47017900 |
| H | 0.06285700 | 1.03409400 | -0.41382100 |
| H | -0.39055200 | -0.99508400 | 1.84833100 |
| H | 1.93141200 | 1.10866200 | 1.65269600 |
| H | 1.86624800 | -0.20776400 | 2.85691400 |
| H | 1.76908700 | -0.45148900 | -1.36073600 |
| H | 1.09384900 | -1.84188500 | -0.52098400 |
| Si | -1.14441300 | 1.26962700 | 2.41702700 |
| C | -2.87155100 | 0.49961500 | 2.50123000 |
| H | -3.57520500 | 1.18314300 | 2.99332300 |
| H | -3.26528700 | 0.28245000 | 1.50005000 |
| H | -2.86381200 | -0.43859300 | 3.07053100 |
| C | -0.47466100 | 1.54532300 | 4.16572100 |
| H | 0.51256400 | 2.02344800 | 4.15199100 |
| H | -1.15070800 | 2.19877500 | 4.73206400 |
| H | -0.38618700 | 0.60103600 | 4.71807000 |
| C | -1.22448300 | 2.90603600 | 1.47422000 |
| H | -1.67360700 | 2.77806200 | 0.48139100 |
| H | -1.84638000 | 3.62210300 | 2.02731000 |
| H | -0.23131300 | 3.35035900 | 1.34594400 |
| C | 3.55785100 | -1.19711100 | 0.82448100 |
| F | 3.42176700 | -2.49405000 | 1.20665600 |
| F | 4.33360700 | -0.57974100 | 1.72888500 |
| F | 4.18741400 | -1.18555900 | -0.35966100 |
| O | 2.89867800 | 4.14130000 | -0.24550500 |
| S | 3.22426700 | 2.89719400 | 0.46438500 |
| O | 2.30823100 | 2.59776700 | 1.63338000 |
| O | 3.47696900 | 1.69139000 | -0.35576400 |
| C | 4.86379900 | 3.26831900 | 1.30862400 |
| F | 5.25524100 | 2.23737400 | 2.07273300 |
| F | 5.81038700 | 3.49853200 | 0.38365900 |
| F | 4.75138900 | 4.35773100 | 2.08565600 |

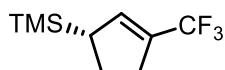
XIIa. (Z)-trimethyl(4,4,4-trifluoro-3-methylbut-2-en-1-yl)silane



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | 0.00051400 | 0.00245100 | -0.00390700 |
| C | -0.00970200 | 0.01211300 | 1.50165500 |
| F | 1.24862300 | 0.01080300 | 2.04591000 |
| F | -0.64589500 | -1.06106000 | 2.05705600 |
| F | -0.62763100 | 1.11361600 | 2.00796800 |
| C | 0.46502300 | -1.06470700 | -0.68266600 |
| H | 0.45915800 | -0.96239500 | -1.76839800 |
| C | 0.97796000 | -2.37604300 | -0.18485500 |
| H | 1.94555100 | -2.58070300 | -0.66767600 |
| H | 1.15160400 | -2.38181100 | 0.89591100 |
| C | -0.49164300 | 1.26010300 | -0.68390300 |
| H | 0.08476900 | 2.14195000 | -0.37717100 |
| H | -0.39849700 | 1.15464400 | -1.76848900 |
| H | -1.54343700 | 1.46678800 | -0.45071900 |
| C | -0.32099700 | -3.98642600 | -2.51115600 |
| H | -0.82967800 | -3.10374900 | -2.91878200 |
| H | 0.65533100 | -4.06996200 | -3.00576700 |
| H | -0.91247000 | -4.86768600 | -2.79139100 |
| C | 0.74875500 | -5.43077900 | 0.01650500 |
| H | 0.88278300 | -5.38779900 | 1.10492400 |
| H | 0.17045400 | -6.33500600 | -0.21322600 |
| H | 1.74047700 | -5.54269200 | -0.44002000 |
| C | -1.83382700 | -3.71843100 | 0.18244100 |
| H | -2.46768800 | -4.57628800 | -0.07729900 |
| H | -1.75272100 | -3.67947600 | 1.27560400 |
| H | -2.35058200 | -2.80874800 | -0.14735000 |
| Si | -0.13359200 | -3.88519900 | -0.62905800 |

XIIb. (S)-trimethyl(3-(trifluoromethyl)cyclopent-2-en-1-yl)silane

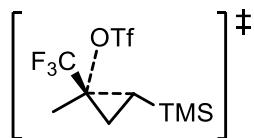


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | 0.00190700 | 0.00429400 | -0.00172100 |
| C | -0.00039900 | 0.00073600 | 1.56168100 |
| C | 1.46826600 | 0.00117500 | 1.89876600 |
| C | 2.23829800 | -0.20511000 | 0.82070300 |
| C | 1.42581100 | -0.43844700 | -0.43791500 |
| H | -0.77808600 | -0.64186500 | -0.41479500 |
| H | -0.18442300 | 1.01602000 | -0.38201000 |
| H | -0.43724900 | -0.93998100 | 1.94065500 |

| | | | |
|----|-------------|-------------|-------------|
| H | 1.79363400 | 0.13169700 | -1.29872600 |
| H | 1.46053800 | -1.50054000 | -0.72059700 |
| Si | -1.03055800 | 1.39765700 | 2.38605300 |
| C | -2.80644500 | 1.28106200 | 1.73890400 |
| H | -3.43856000 | 2.05193000 | 2.19832800 |
| H | -2.84871400 | 1.42067900 | 0.65149000 |
| H | -3.25036700 | 0.30405600 | 1.96930600 |
| C | -1.01346400 | 1.14645800 | 4.26363100 |
| H | 0.00205800 | 1.21117600 | 4.67449800 |
| H | -1.62077300 | 1.91382700 | 4.76101700 |
| H | -1.42454200 | 0.16660100 | 4.53849600 |
| C | -0.29166600 | 3.08922000 | 1.96023100 |
| H | -0.27153700 | 3.26848900 | 0.87797500 |
| H | -0.88611200 | 3.89107100 | 2.41709600 |
| H | 0.73572900 | 3.18261000 | 2.33412100 |
| C | 3.72014600 | -0.28445100 | 0.83121300 |
| F | 4.17705200 | -1.49309200 | 0.37807100 |
| F | 4.26700600 | -0.10378200 | 2.06106900 |
| F | 4.29963500 | 0.64898300 | 0.01326000 |
| H | 1.85005400 | 0.12675000 | 2.90799800 |

TS-XIIIa.

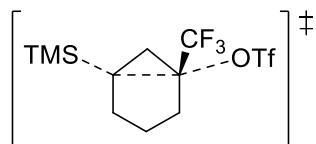


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.00725500 | 0.00527200 | -0.01718300 |
| C | -0.06197400 | -0.00294300 | 1.52368500 |
| F | 1.15547800 | -0.01383300 | 2.08814500 |
| F | -0.72674100 | -1.10419800 | 1.95043800 |
| F | -0.73221900 | 1.06891500 | 1.97034100 |
| O | 1.00581600 | 2.45554300 | 0.06003700 |
| S | 0.34706900 | 3.69090000 | -0.45260200 |
| O | -1.04156700 | 3.47499400 | -0.93317500 |
| O | 1.19973500 | 4.53429400 | -1.31655600 |
| C | 1.21186200 | -0.33321000 | -0.68830700 |
| H | 1.23409600 | -0.01539400 | -1.72964100 |
| H | 2.12551400 | -0.07815300 | -0.15663700 |
| C | 0.92950000 | -1.89997000 | -0.56244200 |
| H | 1.01906000 | -2.25057700 | 0.46805400 |
| H | -0.04347100 | -2.20118000 | -0.96103000 |
| C | -1.28224400 | 0.25250400 | -0.70271500 |
| H | -1.40597600 | 1.35524700 | -0.70265200 |
| H | -1.25372700 | -0.06919400 | -1.74552300 |
| H | -2.14404200 | -0.16916000 | -0.17732300 |
| C | 0.11998600 | 4.74055500 | 1.09151600 |
| F | -0.45033300 | 5.92073100 | 0.78107200 |
| F | -0.66700100 | 4.12036000 | 1.98961700 |
| F | 1.30678400 | 4.99081600 | 1.67696700 |

| | | | |
|----|------------|-------------|-------------|
| C | 3.98198200 | -2.30511100 | -1.06193500 |
| H | 4.18271200 | -1.25834500 | -1.31875000 |
| H | 4.11041900 | -2.42560400 | 0.02031900 |
| H | 4.74590800 | -2.91720600 | -1.55873900 |
| C | 1.95389700 | -4.67790100 | -1.22481500 |
| H | 0.93488700 | -4.97621100 | -1.49757300 |
| H | 2.65256400 | -5.30558000 | -1.79335500 |
| H | 2.10235900 | -4.88835100 | -0.15927000 |
| C | 1.96752100 | -2.48102700 | -3.44266800 |
| H | 2.67257500 | -3.05301800 | -4.05966800 |
| H | 0.95232000 | -2.76372600 | -3.74559300 |
| H | 2.11388100 | -1.42004100 | -3.67669800 |
| Si | 2.27387100 | -2.86271600 | -1.62380400 |

TS-XIIIc.

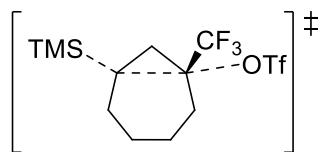


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | -0.01105700 | -0.02822700 | 0.00703200 |
| C | -0.01317500 | -0.08204300 | 1.64698000 |
| C | 1.40817200 | -0.06259100 | 1.63347900 |
| C | 2.15204100 | 1.18641400 | 1.36268900 |
| C | 1.93662400 | 1.55819500 | -0.15005700 |
| C | 0.460444800 | 1.33556500 | -0.49434000 |
| H | -0.47673000 | 0.83043400 | 2.01716300 |
| H | -0.48100300 | -0.98787000 | 2.02321900 |
| H | 0.59196800 | -0.83006100 | -0.43938700 |
| H | 1.72690700 | 1.97951900 | 1.98520400 |
| H | 3.21764600 | 1.08030200 | 1.57727700 |
| H | 2.57166100 | 0.91392500 | -0.76691900 |
| H | -0.16021500 | 2.13205200 | -0.06685500 |
| H | 0.33795500 | 1.37705600 | -1.58294100 |
| C | 2.20284400 | -1.37499700 | 1.67457900 |
| O | 1.43351400 | 0.25179000 | 4.39324300 |
| S | 0.71959200 | 1.40444400 | 5.00698900 |
| O | 1.44587200 | 2.07651000 | 6.10765000 |
| O | 0.06661700 | 2.30771500 | 4.02649200 |
| C | -0.73466600 | 0.59074700 | 5.87862200 |
| F | -1.50676400 | 1.51201600 | 6.48722100 |
| F | -1.50568900 | -0.08262100 | 5.00056400 |
| F | -0.31178400 | -0.28185300 | 6.81374300 |
| F | 3.11300000 | -1.32261200 | 2.65967700 |
| F | 1.42285800 | -2.45067400 | 1.87608300 |
| F | 2.87084000 | -1.56352400 | 0.51030500 |
| H | 2.25510400 | 2.59352700 | -0.30444500 |
| Si | -1.85418700 | -0.55654200 | -0.49862000 |
| C | -1.91393200 | -0.34348900 | -2.37201200 |
| H | -2.87182900 | -0.73216400 | -2.74169100 |

| | | | |
|---|-------------|-------------|-------------|
| H | -1.84148900 | 0.70848000 | -2.66919300 |
| H | -1.11177700 | -0.90115300 | -2.86953900 |
| C | -3.06963700 | 0.58152400 | 0.37878300 |
| H | -4.08555300 | 0.34394400 | 0.03700200 |
| H | -3.05292100 | 0.45658600 | 1.46752700 |
| H | -2.88283100 | 1.63721900 | 0.14993700 |
| C | -2.09487900 | -2.36163100 | -0.02026100 |
| H | -1.33213500 | -3.00470400 | -0.47523100 |
| H | -2.08053400 | -2.52530400 | 1.06320100 |
| H | -3.07369100 | -2.69597600 | -0.38784300 |

TS-XIIIId.

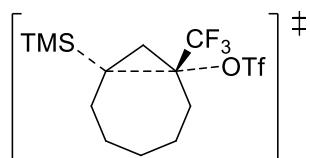


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|--------------|
| 0 1 | | | |
| C | 0.02376100 | 0.00177100 | -0.04262400 |
| C | 0.00461800 | 0.01328000 | 1.43917500 |
| C | 1.40480800 | 0.08479700 | 2.12349500 |
| C | 0.44905100 | 1.08562900 | -0.87348000 |
| C | 2.22417200 | 1.29334500 | 1.68594300 |
| C | 1.98289700 | 0.56666700 | -0.84773300 |
| C | 2.84529700 | 1.16650100 | 0.27493700 |
| H | -0.55645300 | 0.91326800 | 1.72753400 |
| H | 1.95194200 | -0.84930000 | 1.94943000 |
| H | 1.60261700 | 2.19560900 | 1.75212100 |
| H | 0.39725500 | 2.06622300 | -0.40495500 |
| H | -0.52717700 | -0.86476200 | 1.81084200 |
| H | 1.19235100 | 0.14244500 | 3.19539000 |
| H | 0.02336500 | 1.09344900 | -1.87355500 |
| H | 3.05189500 | 1.44111200 | 2.38843100 |
| H | 2.06313200 | -0.52930400 | -0.850555600 |
| H | 3.18143000 | 2.16645600 | -0.02453100 |
| H | 3.74054000 | 0.53914500 | 0.34788300 |
| Si | 2.71940900 | 1.00161100 | -2.63983000 |
| C | -0.41565700 | -1.32075300 | -0.70154900 |
| C | 1.83548300 | -0.01885600 | -3.95123400 |
| H | 0.77517900 | 0.23485200 | -4.05661700 |
| H | 2.31550500 | 0.17861700 | -4.91884300 |
| H | 1.91502700 | -1.09398200 | -3.75400900 |
| C | 2.48596600 | 2.84793700 | -2.92730400 |
| H | 2.97324800 | 3.45483800 | -2.15581800 |
| H | 2.93838300 | 3.11298600 | -3.89187400 |
| H | 1.42839200 | 3.13308600 | -2.97248300 |
| C | 4.54121900 | 0.52347800 | -2.54240300 |
| H | 4.66717700 | -0.52536600 | -2.24875700 |
| H | 4.99351200 | 0.65079700 | -3.53466900 |
| H | 5.09758300 | 1.14967500 | -1.83663700 |

| | | | |
|---|-------------|-------------|-------------|
| O | -2.55051800 | 1.02951500 | -0.45192400 |
| S | -3.06288200 | 2.18397400 | 0.33423600 |
| O | -4.45682300 | 2.04639700 | 0.81292200 |
| O | -2.09757600 | 2.72278300 | 1.32455700 |
| C | -3.17963000 | 3.55477600 | -0.94850500 |
| F | -0.49471700 | -1.24447000 | -2.03941000 |
| F | 0.46340200 | -2.30646400 | -0.39378700 |
| F | -1.61675600 | -1.68987600 | -0.23129200 |
| F | -1.97498600 | 3.80219900 | -1.50245900 |
| F | -4.02944200 | 3.21791300 | -1.93816200 |
| F | -3.62221900 | 4.69849300 | -0.39075700 |

TS-XIIIe.



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.02873400 | 0.00226900 | -0.00304700 |
| C | 0.00208200 | -0.02139600 | 1.56877800 |
| C | 3.15718700 | 0.02855300 | 0.11990800 |
| C | 0.93949900 | 0.94081800 | 2.19846500 |
| C | 2.83179400 | 1.19263600 | 1.08884900 |
| C | 2.30312200 | 0.71931800 | 2.55874800 |
| H | 0.22398600 | 1.00251200 | -0.36379800 |
| H | 0.24377800 | -1.02665800 | 1.92121700 |
| H | -1.06252000 | -0.18148700 | -0.31000000 |
| H | -0.99927000 | 0.23324500 | 1.92982500 |
| H | 2.67733200 | 1.35807300 | 3.35546400 |
| H | 2.56712500 | -0.32490300 | 2.71629000 |
| C | 0.89005800 | -1.06067000 | -0.62347300 |
| C | 2.26201200 | -1.22201600 | 0.03965300 |
| H | 2.14793600 | -1.65893400 | 1.03983900 |
| H | 2.82309500 | -1.97174400 | -0.53177200 |
| O | 0.35907200 | -0.29773300 | 4.81041800 |
| S | 0.87600100 | -1.66407500 | 5.08282100 |
| O | -0.09643600 | -2.59573300 | 5.69865200 |
| O | 1.69596100 | -2.23593300 | 3.98409000 |
| C | 2.13134800 | -1.38043200 | 6.45451300 |
| F | 1.54290200 | -0.85553100 | 7.54725100 |
| F | 3.09811000 | -0.52892000 | 6.05539000 |
| F | 2.72138200 | -2.53708600 | 6.81520800 |
| H | 1.01593500 | -0.81936900 | -1.68751500 |
| H | 3.23635100 | 0.46866400 | -0.88146600 |
| H | 4.15880300 | -0.33590300 | 0.37978400 |
| H | 2.17241300 | 1.93161900 | 0.61011400 |
| C | 0.31905000 | 2.32262600 | 2.49243300 |
| F | -0.65939100 | 2.16814500 | 3.40313200 |
| F | -0.23149900 | 2.85691800 | 1.37941700 |

| | | | |
|----|------------|-------------|-------------|
| F | 1.19988000 | 3.20897700 | 2.97931700 |
| Si | 4.47842600 | 2.25796300 | 1.42536700 |
| C | 5.66180200 | 1.17252500 | 2.41315200 |
| H | 5.91161900 | 0.23986700 | 1.89549100 |
| H | 6.59736500 | 1.72677600 | 2.56501200 |
| H | 5.26891500 | 0.91864700 | 3.40453700 |
| C | 4.10419500 | 3.85298100 | 2.35105700 |
| H | 5.03695500 | 4.43019200 | 2.40414000 |
| H | 3.36177700 | 4.46832000 | 1.83127000 |
| H | 3.76219000 | 3.69082200 | 3.37842200 |
| C | 5.15210000 | 2.65549900 | -0.29172600 |
| H | 4.41342200 | 3.18924300 | -0.90159100 |
| H | 6.02837000 | 3.30773700 | -0.18186500 |
| H | 5.46804500 | 1.75964200 | -0.83629200 |
| H | 0.38548900 | -2.03465200 | -0.58567200 |

XIVa. 1-methyl-1-(trifluoromethyl)cyclopropane



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.00042000 | -0.00002900 | 0.00010200 |
| C | 0.00020600 | 0.00000600 | 1.50171600 |
| F | 1.24676200 | 0.00069800 | 2.04549500 |
| F | -0.63980900 | -1.08911000 | 2.02069900 |
| F | -0.64084600 | 1.08854900 | 2.02062400 |
| C | 1.11674900 | 0.75534700 | -0.68985700 |
| H | 0.84881600 | 1.27796800 | -1.60385200 |
| H | 1.85754900 | 1.26216000 | -0.07852800 |
| C | 1.11832700 | -0.75294000 | -0.69000200 |
| H | 1.86017000 | -1.25836900 | -0.07881700 |
| H | 0.85139100 | -1.27589000 | -1.60410300 |
| C | -1.39279900 | -0.00139600 | -0.61304300 |
| H | -1.96122600 | 0.88744700 | -0.31735400 |
| H | -1.31206100 | -0.00132900 | -1.70415300 |
| H | -1.95957300 | -0.89126200 | -0.31730000 |

XIVc. (1R)-1-(trifluoromethyl)bicyclo[3.1.0]hexane



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|------------|
| O 1 | | | |
| C | 0.00126900 | -0.00058900 | 0.00133400 |
| C | -0.00029300 | 0.00099100 | 1.50818700 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.31882500 | 0.00107500 | 0.76617300 |
| C | 2.00256100 | 1.36093000 | 0.54312300 |
| C | 1.30753900 | 1.94481000 | -0.71121600 |
| C | -0.12033100 | 1.34335700 | -0.72652200 |
| H | -0.26361800 | 0.91841500 | 2.03066600 |
| H | -0.30389700 | -0.91201200 | 2.01351500 |
| H | -0.33460700 | -0.90557100 | -0.49760500 |
| H | 1.85862200 | 2.00489300 | 1.41871200 |
| H | 3.08191700 | 1.25424400 | 0.39655300 |
| H | 1.84731700 | 1.60887600 | -1.60533900 |
| H | -0.83214900 | 1.99907900 | -0.20874300 |
| H | -0.49114100 | 1.20760200 | -1.74776000 |
| C | 2.18540900 | -1.21077700 | 0.82232000 |
| F | 3.01525000 | -1.21155600 | 1.90986700 |
| F | 1.48020600 | -2.37320700 | 0.88317600 |
| F | 3.00606500 | -1.31964700 | -0.26495100 |
| H | 1.30883400 | 3.04048000 | -0.71932800 |

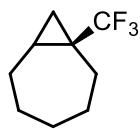
XIVd. (1R)-1-(trifluoromethyl)bicyclo[4.1.0]heptanes



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | -0.00057700 | 0.00042900 | 0.00040700 |
| C | 0.00013400 | 0.00053900 | 1.54071800 |
| C | 1.41276800 | -0.00154000 | 2.14915600 |
| C | 0.08808200 | 1.32433800 | -0.73944400 |
| C | 2.32675600 | 1.02900200 | 1.47573200 |
| C | 1.26314800 | 0.38540700 | -0.76404400 |
| C | 2.55020300 | 0.66661100 | -0.00127000 |
| H | -0.54990200 | 0.88192100 | 1.89402800 |
| H | 1.85934300 | -1.00031300 | 2.03825900 |
| H | 1.88446600 | 2.03177800 | 1.56469900 |
| H | 0.13514500 | 2.21140700 | -0.11229800 |
| H | -0.55126700 | -0.87136500 | 1.90870000 |
| H | 1.33560400 | 0.19403600 | 3.22573600 |
| H | -0.48301000 | 1.45038900 | -1.65498800 |
| H | 3.29637700 | 1.07086600 | 1.98645900 |
| H | 1.41302900 | -0.12940100 | -1.71082600 |
| H | 3.10559800 | 1.46339700 | -0.51416000 |
| H | 3.17820500 | -0.23418100 | -0.04779700 |
| C | -0.87523100 | -1.05577300 | -0.60259200 |
| F | -0.90314500 | -1.03608800 | -1.96280800 |
| F | -0.48686300 | -2.31888300 | -0.25117300 |
| F | -2.17688700 | -0.94547400 | -0.19732100 |

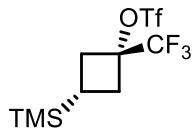
XIVe. (1R)-1-(trifluoromethyl)bicyclo[5.1.0]octane



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.00064800 | 0.00019800 | 0.00050800 |
| C | 0.00045300 | -0.00094400 | 1.54140400 |
| C | 3.01663500 | 0.00004000 | 0.40002900 |
| C | 1.14357700 | 0.81584700 | 2.17331400 |
| C | 2.57214200 | 0.77484900 | 1.63915400 |
| C | 2.24805500 | 0.13526900 | 2.96398800 |
| H | 0.30691400 | 0.99237200 | -0.35299200 |
| H | 0.04040700 | -1.03104600 | 1.91454200 |
| H | 2.97640700 | 0.67628500 | -0.46594100 |
| H | 3.10504800 | 1.71928700 | 1.73328900 |
| H | -1.02659900 | -0.14538000 | -0.36161100 |
| H | -0.95064000 | 0.40215900 | 1.90580900 |
| H | 2.61907000 | 0.61020900 | 3.86813500 |
| H | 2.18095900 | -0.94791000 | 3.02432100 |
| C | 0.89815100 | -1.08538600 | -0.62537600 |
| C | 2.25757800 | -1.29335200 | 0.06827400 |
| H | 2.12403400 | -1.88695100 | 0.98231400 |
| H | 2.88764500 | -1.90898500 | -0.58655300 |
| H | 4.07971000 | -0.23695800 | 0.54691900 |
| C | 0.67565700 | 2.14300300 | 2.70240600 |
| F | 1.66445900 | 2.90196900 | 3.24784500 |
| F | 0.09620800 | 2.91518800 | 1.73476000 |
| F | -0.27114800 | 2.00904900 | 3.68075600 |
| H | 0.36172200 | -2.04454800 | -0.62146400 |
| H | 1.06519700 | -0.83272600 | -1.68177000 |

XV. (1s,3s)-1-(trifluoromethyl)-3-(trimethylsilyl)cyclobutyl trifluoromethanesulfonate

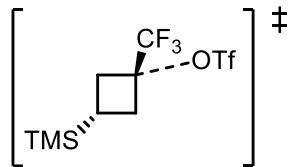


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.00206500 | -0.00332300 | 0.00083800 |
| C | -0.00106800 | -0.00214500 | 1.56564200 |
| C | 1.54607100 | -0.00286900 | 1.53068200 |
| C | 1.51001800 | 0.39930700 | 0.04138300 |
| H | -0.09623100 | -1.03300400 | -0.36245400 |
| H | -0.47480500 | -0.83807600 | 2.08563200 |
| H | -0.37926500 | 0.93095000 | 1.99090800 |

| | | | |
|----|-------------|-------------|-------------|
| H | 2.20260600 | -0.12293100 | -0.62334500 |
| H | 1.67495600 | 1.47661400 | -0.04576800 |
| C | 2.21260800 | -1.36077900 | 1.79008300 |
| F | 1.67763500 | -2.32348600 | 1.00417300 |
| F | 2.07471600 | -1.76815200 | 3.07152000 |
| F | 3.53927400 | -1.31741700 | 1.52569500 |
| Si | -1.24253900 | 1.08176600 | -0.96195600 |
| C | -0.82235500 | 0.95910700 | -2.80406000 |
| H | -1.51650000 | 1.56183200 | -3.40376800 |
| H | 0.19345300 | 1.32049200 | -3.00916600 |
| H | -0.88732700 | -0.07726400 | -3.15949200 |
| C | -2.98823600 | 0.42206700 | -0.64127700 |
| H | -3.73377500 | 1.00760300 | -1.19464700 |
| H | -3.08146900 | -0.62394800 | -0.95994300 |
| H | -3.24968700 | 0.47268900 | 0.42343500 |
| C | -1.11755900 | 2.88393400 | -0.39279100 |
| H | -1.35220600 | 2.99796400 | 0.67293900 |
| H | -0.11727100 | 3.30148100 | -0.56379700 |
| H | -1.83094900 | 3.50190800 | -0.95347700 |
| O | 2.29993900 | 0.97408800 | 2.33200200 |
| S | 1.86087400 | 1.50593800 | 3.79916000 |
| O | 0.93110800 | 0.59930500 | 4.45881700 |
| O | 1.59659300 | 2.93530900 | 3.71383000 |
| C | 3.55243300 | 1.32571200 | 4.62454200 |
| F | 3.91086000 | 0.04321700 | 4.66201700 |
| F | 3.44867700 | 1.79851700 | 5.86928100 |
| F | 4.46284000 | 2.03025000 | 3.95267300 |

TS-XVI.

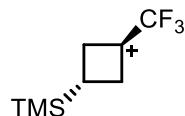


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | 0.18562500 | -0.02906700 | 0.01273000 |
| C | 0.23398900 | 0.06279300 | 1.61252900 |
| C | 1.60839300 | -0.07762200 | 1.15701500 |
| C | 1.62696200 | 0.66130700 | -0.09547800 |
| H | 0.17425200 | -1.05300300 | -0.35768900 |
| H | -0.19065100 | -0.73863900 | 2.21308500 |
| H | -0.05216300 | 1.05894600 | 1.94474400 |
| H | 2.32244400 | 0.34234800 | -0.86860600 |
| H | 1.53874100 | 1.74272600 | -0.00768300 |
| C | 2.35751500 | -1.41694000 | 1.30815800 |
| F | 1.78913100 | -2.39567600 | 0.56017700 |
| F | 2.33567300 | -1.83289500 | 2.58375700 |
| F | 3.63285900 | -1.30195900 | 0.90856200 |
| Si | -1.28242300 | 0.96203300 | -0.83609900 |
| C | -0.92300500 | 0.88081500 | -2.68129100 |

| | | | |
|---|-------------|-------------|-------------|
| H | -1.72325700 | 1.38720300 | -3.23596000 |
| H | 0.02263500 | 1.37629800 | -2.93025400 |
| H | -0.87306700 | -0.15551600 | -3.03542300 |
| C | -2.84651300 | 0.02841300 | -0.36278600 |
| H | -3.71480100 | 0.49596100 | -0.84463300 |
| H | -2.80450200 | -1.01734100 | -0.68924200 |
| H | -3.01570600 | 0.04475100 | 0.72025200 |
| C | -1.28941500 | 2.72842700 | -0.19088700 |
| H | -1.45920100 | 2.78267700 | 0.89031200 |
| H | -0.36602500 | 3.27015400 | -0.42476000 |
| H | -2.11414400 | 3.26614000 | -0.67715500 |
| O | 3.09206100 | 0.84135300 | 2.55209600 |
| S | 2.80569000 | 2.16430200 | 3.20987600 |
| O | 1.63300600 | 2.87020000 | 2.65264900 |
| O | 4.01604800 | 2.97178200 | 3.44937800 |
| C | 2.25095800 | 1.65378400 | 4.93266900 |
| F | 1.15461700 | 0.87447000 | 4.86570700 |
| F | 1.95222200 | 2.73830500 | 5.66985000 |
| F | 3.21805400 | 0.96660000 | 5.56464300 |

XVII. 1-(trifluoromethyl)-3-(trimethylsilyl)cyclobutan-1-ylium

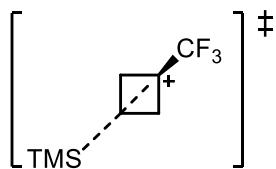


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | -0.00850400 | -0.00340800 | 0.01646700 |
| C | 0.05271300 | 0.11027900 | 1.61944800 |
| C | 1.33093000 | 0.01447100 | 0.95680800 |
| C | 1.30820700 | 0.89649800 | -0.18517400 |
| H | -0.01867200 | -0.99810500 | -0.42824400 |
| H | -0.28750400 | -0.73889100 | 2.20361400 |
| H | -0.28200900 | 1.08407100 | 1.96510800 |
| H | 1.95681900 | 0.66603400 | -1.02435000 |
| H | 1.10526000 | 1.95145100 | -0.02607900 |
| C | 2.21959600 | -1.21958800 | 1.03976500 |
| F | 1.55824900 | -2.29544000 | 1.50462600 |
| F | 3.22449000 | -0.94233100 | 1.89428000 |
| F | 2.75807100 | -1.54230700 | -0.15029500 |
| Si | -1.65370600 | 0.91965700 | -0.72786500 |
| C | -1.28596400 | 1.04931600 | -2.55978200 |
| H | -2.16623800 | 1.46587000 | -3.06632200 |
| H | -0.43799100 | 1.71267600 | -2.76153700 |
| H | -1.07709000 | 0.06900800 | -3.00190600 |
| C | -3.02657100 | -0.28604500 | -0.31489100 |
| H | -3.97102600 | 0.10833700 | -0.71169500 |
| H | -2.85599200 | -1.26779800 | -0.77039900 |
| H | -3.14464100 | -0.41614000 | 0.76635100 |
| C | -1.83811200 | 2.58118000 | 0.11753200 |
| H | -2.06411100 | 2.49290500 | 1.18535400 |
| H | -0.96744000 | 3.23386000 | -0.00842900 |

| | | | |
|---|-------------|------------|-------------|
| H | -2.69089500 | 3.08822500 | -0.35377400 |
|---|-------------|------------|-------------|

TS-XVIII.



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | 0.00000000 | 0.00000000 | 0.00000000 |
| C | 0.00000000 | 0.00000000 | 1.54988400 |
| C | 1.33678500 | 0.00000000 | 0.86087600 |
| C | 1.09239900 | 1.09227100 | -0.14233200 |
| H | -0.32146100 | -0.76134700 | -0.69814200 |
| H | -0.31205800 | -0.92827400 | 2.02402900 |
| H | -0.30833000 | 0.90755800 | 2.07252200 |
| H | 1.67776000 | 1.06173900 | -1.05907800 |
| H | 0.87992200 | 2.09537900 | 0.23223300 |
| C | 2.40966500 | -1.01372900 | 0.89957700 |
| F | 1.95809800 | -2.23540100 | 1.29727600 |
| F | 3.41231300 | -0.68379100 | 1.76728500 |
| F | 3.00644900 | -1.18853500 | -0.31205600 |
| Si | -2.18712700 | 1.49440900 | -0.81280100 |
| C | -1.48450400 | 1.15229900 | -2.48201600 |
| H | -2.00777200 | 1.79104500 | -3.20965500 |
| H | -0.42366600 | 1.42474500 | -2.51902600 |
| H | -1.61769500 | 0.10838900 | -2.77818600 |
| C | -3.35830900 | 0.29366600 | -0.04875100 |
| H | -4.16686300 | 0.07030600 | -0.75683700 |
| H | -2.83316900 | -0.65225800 | 0.14261200 |
| H | -3.78112600 | 0.66672200 | 0.88754600 |
| C | -1.75570100 | 3.04997300 | 0.07588000 |
| H | -1.33558800 | 2.80307300 | 1.05999900 |
| H | -1.04384300 | 3.66282600 | -0.48210700 |
| H | -2.67255800 | 3.62709200 | 0.25773000 |

XIX. 1-(trifluoromethyl)bicyclo[1.1.0]butane

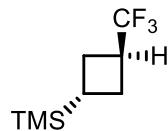


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|------------|------------|------------|
| 0 1 | | | |
| C | 0.00000000 | 0.00000000 | 0.00000000 |
| C | 0.00000000 | 0.00000000 | 1.49955500 |
| C | 1.29790900 | 0.00000000 | 0.73749000 |

| | | | |
|---|-------------|-------------|-------------|
| C | 0.99286900 | 1.09601600 | -0.24817100 |
| H | -0.37217900 | -0.75191500 | -0.68265200 |
| H | -0.28622300 | -0.92874800 | 1.98903400 |
| H | -0.27872700 | 0.90758400 | 2.03877900 |
| H | 1.52392200 | 1.06920900 | -1.19754500 |
| H | 0.79903300 | 2.09747600 | 0.14132400 |
| C | 2.37831400 | -1.00423300 | 0.72283300 |
| F | 1.95715800 | -2.23213100 | 1.13717900 |
| F | 3.41926000 | -0.67031600 | 1.54447800 |
| F | 2.92069000 | -1.17153700 | -0.51572900 |

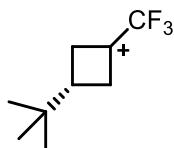
XXa. trimethyl((1r,3r)-3-(trifluoromethyl)cyclobutyl)silane



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | 0.00555800 | 0.01061300 | 0.00824000 |
| C | 0.00791100 | 0.01971100 | 1.57414500 |
| C | 1.56503300 | -0.00185300 | 1.57166800 |
| C | 1.55635700 | 0.22891000 | 0.03136700 |
| H | -0.21936700 | -1.00076100 | -0.35505000 |
| H | -0.48538400 | -0.82612900 | 2.06289800 |
| H | -0.37450900 | 0.94159100 | 2.02280200 |
| H | 2.15145900 | -0.47039300 | -0.56394100 |
| H | 1.87545000 | 1.24533000 | -0.21882200 |
| C | 2.18209200 | -1.30019200 | 2.01447500 |
| F | 1.67951800 | -2.38972200 | 1.36778700 |
| F | 1.99529000 | -1.53008000 | 3.34607200 |
| F | 3.53044100 | -1.32594700 | 1.80791300 |
| Si | -1.10187700 | 1.23464200 | -0.93787600 |
| C | -0.71773200 | 1.10509300 | -2.78975400 |
| H | -1.34238200 | 1.79677700 | -3.36988000 |
| H | 0.33156300 | 1.35021500 | -2.99921100 |
| H | -0.90510600 | 0.09090900 | -3.16558500 |
| C | -2.91748800 | 0.78941200 | -0.62251100 |
| H | -3.58939600 | 1.47577900 | -1.15405800 |
| H | -3.14239100 | -0.22923700 | -0.96431600 |
| H | -3.16312600 | 0.84475400 | 0.44584500 |
| C | -0.77261000 | 3.00774900 | -0.34906000 |
| H | -0.99476300 | 3.13225200 | 0.71849600 |
| H | 0.27216500 | 3.30259300 | -0.50982800 |
| H | -1.40360200 | 3.71610200 | -0.90165400 |
| H | 2.04694300 | 0.78294200 | 2.16233000 |

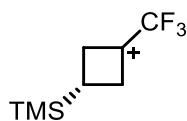
XXIa. 3-(tert-butyl)-1-(trifluoromethyl)cyclobutan-1-ylium



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | -0.00209700 | -0.00394900 | 0.00360200 |
| C | 0.00181800 | 0.00418200 | 1.63494500 |
| C | 1.33638200 | -0.00327100 | 1.11242500 |
| C | 1.38836700 | 0.85419300 | -0.03347500 |
| H | 0.07679800 | -0.99533100 | -0.43658000 |
| H | -0.34121100 | -0.86990900 | 2.17899600 |
| H | -0.41649300 | 0.95070900 | 1.96688800 |
| H | 2.12816600 | 0.64477500 | -0.79943200 |
| H | 1.13755400 | 1.90380600 | 0.09450400 |
| C | 2.25335400 | -1.22634900 | 1.24868700 |
| F | 1.59845300 | -2.31159800 | 1.68531400 |
| F | 3.18649400 | -0.88905700 | 2.15896200 |
| F | 2.86764200 | -1.53676300 | 0.09747700 |
| C | -0.93677100 | 0.84680600 | -2.16253000 |
| H | -1.81176700 | 1.24589000 | -2.68707300 |
| H | -0.09322300 | 1.51650300 | -2.35959200 |
| H | -0.71026300 | -0.13668900 | -2.58788600 |
| C | -2.46522000 | -0.16470800 | -0.41363900 |
| H | -3.33970000 | 0.25628000 | -0.92171400 |
| H | -2.29628000 | -1.16968000 | -0.81488100 |
| H | -2.70298100 | -0.24824000 | 0.65184600 |
| C | -1.52761000 | 2.15149400 | -0.08695200 |
| H | -1.81363300 | 2.13304200 | 0.96942400 |
| H | -0.68897700 | 2.84269400 | -0.21787800 |
| H | -2.37414900 | 2.57938500 | -0.63485300 |
| C | -1.25803500 | 0.75914100 | -0.65944900 |

XXIIa. 1-(trifluoromethyl)-3-(trimethylsilyl)cyclobutan-1-ylium

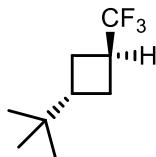


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | -0.00850400 | -0.00340800 | 0.01646700 |
| C | 0.05271300 | 0.11027900 | 1.61944800 |
| C | 1.33093000 | 0.01447100 | 0.95680800 |
| C | 1.30820700 | 0.89649800 | -0.18517400 |

| | | | |
|----|-------------|-------------|-------------|
| H | -0.01867200 | -0.99810500 | -0.42824400 |
| H | -0.28750400 | -0.73889100 | 2.20361400 |
| H | -0.28200900 | 1.08407100 | 1.96510800 |
| H | 1.95681900 | 0.66603400 | -1.02435000 |
| H | 1.10526000 | 1.95145100 | -0.02607900 |
| C | 2.21959600 | -1.21958800 | 1.03976500 |
| F | 1.55824900 | -2.29544000 | 1.50462600 |
| F | 3.22449000 | -0.94233100 | 1.89428000 |
| F | 2.75807100 | -1.54230700 | -0.15029500 |
| Si | -1.65370600 | 0.91965700 | -0.72786500 |
| C | -1.28596400 | 1.04931600 | -2.55978200 |
| H | -2.16623800 | 1.46587000 | -3.06632200 |
| H | -0.43799100 | 1.71267600 | -2.76153700 |
| H | -1.07709000 | 0.06900800 | -3.00190600 |
| C | -3.02657100 | -0.28604500 | -0.31489100 |
| H | -3.97102600 | 0.10833700 | -0.71169500 |
| H | -2.85599200 | -1.26779800 | -0.77039900 |
| H | -3.14464100 | -0.41614000 | 0.76635100 |
| C | -1.83811200 | 2.58118000 | 0.11753200 |
| H | -2.06411100 | 2.49290500 | 1.18535400 |
| H | -0.96744000 | 3.23386000 | -0.00842900 |
| H | -2.69089500 | 3.08822500 | -0.35377400 |

XXIIIa. (1r,3r)-1-(tert-butyl)-3-(trifluoromethyl)cyclobutane

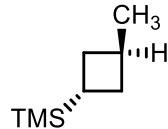


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.00064800 | -0.00003100 | 0.00010300 |
| C | 0.00005200 | 0.00018400 | 1.55990800 |
| C | 1.55754800 | 0.00036900 | 1.54777600 |
| C | 1.52907300 | 0.30373500 | 0.02038700 |
| H | -0.15569700 | -1.02630200 | -0.35640500 |
| H | -0.48698000 | -0.84704100 | 2.05220000 |
| H | -0.38454900 | 0.92255800 | 2.00279500 |
| H | 2.16296000 | -0.32151500 | -0.61558300 |
| H | 1.77460000 | 1.35121800 | -0.17288600 |
| C | 2.19701700 | -1.30805900 | 1.92406300 |
| F | 1.70602300 | -2.37466800 | 1.23211600 |
| F | 2.02563100 | -1.60154700 | 3.24517200 |
| F | 3.54383100 | -1.30310800 | 1.70621300 |
| C | -0.64045800 | 0.78624600 | -2.28993200 |
| H | -1.33546300 | 1.38455200 | -2.89279700 |
| H | 0.37594900 | 1.14033100 | -2.50375200 |
| H | -0.71292200 | -0.25554900 | -2.62808300 |
| C | -2.41163300 | 0.40896400 | -0.54142900 |
| H | -3.13523500 | 1.00984200 | -1.10696700 |
| H | -2.52648900 | -0.63719000 | -0.85374300 |

| | | | |
|---|-------------|------------|-------------|
| H | -2.68126100 | 0.47496400 | 0.52032600 |
| C | -0.87886300 | 2.39046400 | -0.37314400 |
| H | -1.14072300 | 2.54000700 | 0.68084100 |
| H | 0.12504700 | 2.80030500 | -0.53443400 |
| H | -1.57653900 | 2.99049300 | -0.97059200 |
| H | 2.03372300 | 0.76257500 | 2.17117900 |
| C | -0.97262500 | 0.90823000 | -0.78814000 |

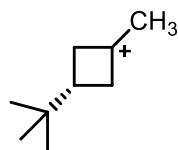
XXb. trimethyl((1r,3r)-3-methylcyclobutyl)silane



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | 0.01037400 | 0.00226900 | -0.01039400 |
| C | 0.01393500 | 0.00470300 | 1.55595900 |
| C | 1.57212200 | 0.01718800 | 1.54408200 |
| C | 1.52511300 | 0.39776900 | 0.03392800 |
| H | -0.08784100 | -1.03043400 | -0.37422600 |
| H | -0.46197800 | -0.85252300 | 2.04858500 |
| H | -0.40601800 | 0.92163100 | 1.98713800 |
| H | 2.19724500 | -0.16029900 | -0.63000700 |
| H | 1.69578300 | 1.46872400 | -0.12955000 |
| C | 2.21376800 | -1.33927400 | 1.83255700 |
| Si | -1.23097600 | 1.07582200 | -0.96374800 |
| C | -0.84210100 | 0.98993100 | -2.81949600 |
| H | -1.54435900 | 1.60239800 | -3.40020300 |
| H | 0.17116700 | 1.35495200 | -3.03200000 |
| H | -0.91036300 | -0.04010100 | -3.19337000 |
| C | -2.98794400 | 0.42546700 | -0.65653000 |
| H | -3.73230200 | 1.02368400 | -1.19842800 |
| H | -3.08922200 | -0.61529600 | -0.99094500 |
| H | -3.24702600 | 0.45936200 | 0.40977000 |
| C | -1.12917500 | 2.88314200 | -0.39244500 |
| H | -1.35639900 | 2.98537900 | 0.67631400 |
| H | -0.13249300 | 3.30921000 | -0.56466900 |
| H | -1.85151400 | 3.49913200 | -0.94410800 |
| H | 2.06290300 | -1.63249000 | 2.87986900 |
| H | 1.78156300 | -2.12662000 | 1.20029800 |
| H | 3.29474700 | -1.31394900 | 1.64156000 |
| H | 2.02669500 | 0.77834400 | 2.19184500 |

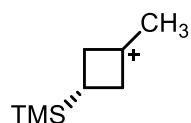
XXIb. 3-(tert-butyl)-1-methylcyclobutan-1-ylum



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | -0.22040600 | 0.09871700 | -0.13832500 |
| C | -0.10553900 | -0.12027100 | 1.45313300 |
| C | 1.26239600 | -0.05178300 | 0.97183800 |
| C | 1.15965900 | 0.92723700 | -0.09599400 |
| H | -0.11110400 | -0.83891100 | -0.68318600 |
| H | -0.43456600 | -1.04638800 | 1.91876900 |
| H | -0.50318400 | 0.77333200 | 1.93366600 |
| H | 1.87684000 | 0.86613300 | -0.91123900 |
| H | 0.92096600 | 1.95004100 | 0.19595300 |
| C | 2.24940800 | -1.14119600 | 1.04072300 |
| C | -1.27526500 | 1.08705200 | -2.17493200 |
| H | -2.17270100 | 1.53515500 | -2.61617500 |
| H | -0.43595700 | 1.76768900 | -2.35709900 |
| H | -1.07686300 | 0.14550600 | -2.69990000 |
| C | -2.69361200 | -0.09328100 | -0.44504600 |
| H | -3.59981700 | 0.35100100 | -0.87223700 |
| H | -2.53282300 | -1.06233400 | -0.93127000 |
| H | -2.87679800 | -0.26808300 | 0.62110400 |
| C | -1.76369300 | 2.19530500 | 0.03241000 |
| H | -1.94504500 | 2.08234400 | 1.10681300 |
| H | -0.95305700 | 2.91732500 | -0.11346900 |
| H | -2.66773100 | 2.64153400 | -0.39673200 |
| H | 1.81746900 | -2.09089900 | 1.36493500 |
| H | 2.83230100 | -1.24908100 | 0.12295300 |
| H | 2.94934800 | -0.81692500 | 1.83232500 |
| C | -1.50011700 | 0.85684600 | -0.66739600 |

XXIIb. 1-methyl-3-(trimethylsilyl)cyclobutan-1-ylum

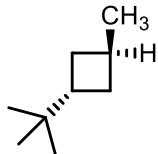


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | -0.01897100 | 0.01571400 | -0.04127700 |
| C | -0.03145000 | -0.14889400 | 1.56075600 |
| C | 1.31566300 | -0.05938700 | 1.03922400 |
| C | 1.26193900 | 0.98868000 | 0.04263700 |
| H | 0.12927100 | -0.90592600 | -0.60425200 |

| | | | |
|----|-------------|--------------|-------------|
| H | -0.34729400 | -1.09588800 | 1.99025100 |
| H | -0.47806700 | 0.72969100 | 2.02091500 |
| H | 1.99591600 | 0.96503200 | -0.75851900 |
| H | 0.95033000 | 1.98593500 | 0.34486000 |
| C | 2.29232600 | -1.18488900 | 1.02595100 |
| Si | -1.63190300 | 0.90376200 | -0.75061000 |
| C | -1.28197400 | 1.13764500 | -2.58233900 |
| H | -2.15623500 | 1.59127400 | -3.06645400 |
| H | -0.42507600 | 1.80081600 | -2.74780200 |
| H | -1.08095800 | 0.18189300 | -3.08021300 |
| C | -3.03042100 | -0.30881000 | -0.42455000 |
| H | -3.96032200 | 0.07907900 | -0.85950600 |
| H | -2.82921100 | -1.28559800 | -0.87958200 |
| H | -3.19811700 | -0.455556100 | 0.64863400 |
| C | -1.87559400 | 2.53971800 | 0.14151300 |
| H | -2.00042100 | 2.42430400 | 1.22391600 |
| H | -1.05991700 | 3.24784500 | -0.04259800 |
| H | -2.79608900 | 2.99861700 | -0.24293800 |
| H | 1.82686500 | -2.14087300 | 1.27900100 |
| H | 2.82765100 | -1.25661100 | 0.07549200 |
| H | 3.03072800 | -0.95549700 | 1.80747600 |

XXIIIa. (1r,3r)-1-(tert-butyl)-3-methylcyclobutane

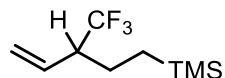


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.08792000 | 0.14936800 | -0.06505300 |
| C | -0.07722000 | 0.12597800 | 1.49326000 |
| C | 1.48030000 | 0.06411200 | 1.45958600 |
| C | 1.42647800 | 0.51464900 | -0.03178800 |
| H | -0.19371200 | -0.88127900 | -0.43108200 |
| H | -0.59267200 | -0.71040600 | 1.98157700 |
| H | -0.44079800 | 1.06000200 | 1.93551200 |
| H | 2.08228200 | -0.01784500 | -0.73187100 |
| H | 1.60453400 | 1.58993800 | -0.14176700 |
| C | 2.06353300 | -1.33150700 | 1.68112800 |
| C | -0.77190400 | 0.90983200 | -2.35436500 |
| H | -1.49387700 | 1.47794400 | -2.95547300 |
| H | 0.22788900 | 1.30912500 | -2.56721500 |
| H | -0.79727300 | -0.13317600 | -2.69634300 |
| C | -2.51937800 | 0.44676600 | -0.60349100 |
| H | -3.27217900 | 1.01298800 | -1.16746800 |
| H | -2.58669200 | -0.60396100 | -0.91514700 |
| H | -2.78808500 | 0.49997400 | 0.45918400 |
| C | -1.08065100 | 2.49481100 | -0.43389000 |
| H | -1.34169700 | 2.62766100 | 0.62265400 |
| H | -0.09778000 | 2.95179700 | -0.59893400 |

| | | | |
|---|-------------|-------------|-------------|
| H | -1.80986700 | 3.06329700 | -1.02526100 |
| H | 1.91316800 | -1.66108700 | 2.71761900 |
| H | 1.59002200 | -2.07326800 | 1.02418300 |
| H | 3.14216000 | -1.34608900 | 1.47638500 |
| H | 1.97819000 | 0.77473000 | 2.13127700 |
| C | -1.10465700 | 1.01043800 | -0.85120000 |

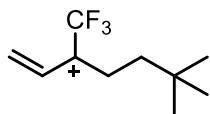
XXIV. trimethyl(3-(trifluoromethyl)pent-4-en-1-yl)silane



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| O 1 | | | |
| C | -0.00042700 | -0.00247500 | 0.00792000 |
| C | -0.02424800 | -0.01934100 | 1.53371000 |
| F | 1.22677200 | -0.03005600 | 2.07028900 |
| F | -0.67706700 | -1.09142400 | 2.06074100 |
| F | -0.64278500 | 1.08435300 | 2.04041500 |
| C | 0.93992500 | -1.08976600 | -0.59541900 |
| H | 1.01508400 | -0.84432100 | -1.66149800 |
| H | 1.94065100 | -0.93454800 | -0.17489800 |
| C | 0.51899800 | -2.56144900 | -0.43255200 |
| H | 0.43659800 | -2.82199100 | 0.63121300 |
| H | -0.48123000 | -2.71914900 | -0.86090000 |
| C | 3.41118300 | -3.73108900 | -0.45848600 |
| H | 3.87587600 | -2.75171600 | -0.62927400 |
| H | 3.36649300 | -3.89599500 | 0.62593100 |
| H | 4.07800700 | -4.49223800 | -0.88421700 |
| C | 0.95957400 | -5.56063200 | -0.94305400 |
| H | -0.03689200 | -5.65491000 | -1.39378500 |
| H | 1.59808100 | -6.33935000 | -1.38001500 |
| H | 0.86283200 | -5.77198500 | 0.12981400 |
| C | 1.81679400 | -3.51645100 | -3.10580900 |
| H | 2.43933200 | -4.28155300 | -3.58788700 |
| H | 0.82882700 | -3.54112300 | -3.58380000 |
| H | 2.26854200 | -2.53973600 | -3.32122600 |
| Si | 1.68667600 | -3.83543100 | -1.24074300 |
| H | 0.43624500 | 0.97222900 | -0.24327900 |
| C | -1.40694400 | -0.05248800 | -0.54516300 |
| H | -1.99841700 | -0.93284500 | -0.29881900 |
| C | -1.93102700 | 0.89462000 | -1.32878000 |
| H | -1.37506800 | 1.79072900 | -1.59926200 |
| H | -2.93678600 | 0.80253100 | -1.73084200 |

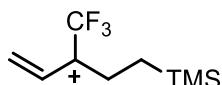
XXV. 6,6-dimethyl-3-(trifluoromethyl)hept-1-en-3-ylidium



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | -0.00602000 | -0.01146500 | -0.02429400 |
| C | 0.08697700 | 0.10163100 | 1.50996700 |
| F | 1.34186700 | -0.00514800 | 1.96627500 |
| F | -0.65947600 | -0.84778700 | 2.10428900 |
| F | -0.39159200 | 1.30925900 | 1.87352500 |
| C | 1.23759900 | -0.08754800 | -0.78082700 |
| H | 1.10177100 | 0.21796500 | -1.81757600 |
| H | 2.00088000 | 0.53648700 | -0.30658200 |
| C | 1.75444500 | -1.59476400 | -0.75029600 |
| H | 1.78717600 | -1.95229300 | 0.28303600 |
| H | 1.02114200 | -2.20176400 | -1.29077400 |
| C | 4.24022200 | -1.02567300 | -0.57842900 |
| H | 4.10443700 | 0.06237300 | -0.60339200 |
| H | 4.24286600 | -1.34629500 | 0.47039600 |
| H | 5.23215000 | -1.23374000 | -0.99634500 |
| C | 3.44765000 | -3.28721200 | -1.33976500 |
| H | 2.70743600 | -3.85229400 | -1.91826700 |
| H | 4.43723100 | -3.49078700 | -1.76602900 |
| H | 3.43932100 | -3.66273700 | -0.30970500 |
| C | 3.17784100 | -1.29495900 | -2.85370100 |
| H | 4.13654900 | -1.55219700 | -3.31904100 |
| H | 2.38272700 | -1.77525000 | -3.43759600 |
| H | 3.06041800 | -0.20816000 | -2.94114800 |
| C | -1.32124000 | -0.05471000 | -0.52489300 |
| H | -2.14335100 | -0.07536700 | 0.18367100 |
| C | -1.60676800 | -0.05222700 | -1.86604300 |
| H | -0.84222200 | -0.00838900 | -2.63509300 |
| H | -2.63890500 | -0.08618500 | -2.20200400 |
| C | 3.16196200 | -1.76656000 | -1.38855000 |

XXVI. 3-(trifluoromethyl)-5-(trimethylsilyl)pent-1-en-3-ylidium

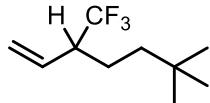


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| C | -0.00093200 | 0.00375800 | -0.01462200 |
| C | 0.03759200 | 0.06358900 | 1.52205700 |
| F | 1.28255600 | 0.07426700 | 2.02030100 |
| F | -0.62577600 | -0.97115300 | 2.07241600 |

| | | | |
|----|-------------|-------------|-------------|
| F | -0.57340200 | 1.20573500 | 1.90450800 |
| C | 1.25961200 | 0.03694200 | -0.73149300 |
| H | 1.16789700 | 0.34449300 | -1.77133100 |
| H | 2.02816300 | 0.62186500 | -0.22552200 |
| C | 1.60531000 | -1.50999000 | -0.63415800 |
| H | 1.72867000 | -1.84214600 | 0.40117000 |
| H | 0.82447100 | -2.11598300 | -1.10148500 |
| C | 4.67120800 | -0.97073400 | -0.62399400 |
| H | 4.54282500 | 0.11806200 | -0.64527500 |
| H | 4.72331600 | -1.28933600 | 0.42398500 |
| H | 5.63908500 | -1.19536400 | -1.09077600 |
| C | 3.49356400 | -3.74603100 | -1.44174800 |
| H | 2.67548900 | -4.26530700 | -1.95442000 |
| H | 4.43576300 | -4.04364300 | -1.92045800 |
| H | 3.52141300 | -4.08855300 | -0.40085400 |
| C | 3.15014800 | -1.28620400 | -3.33399700 |
| H | 4.05379700 | -1.56717000 | -3.89027500 |
| H | 2.29198500 | -1.74940900 | -3.83577300 |
| H | 3.04568400 | -0.19721300 | -3.40880400 |
| Si | 3.29992100 | -1.87245800 | -1.54906500 |
| C | -1.30359500 | -0.11770000 | -0.56677200 |
| H | -2.12997700 | -0.29316500 | 0.11525800 |
| C | -1.56487400 | 0.03188100 | -1.89629400 |
| H | -0.79271600 | 0.22063900 | -2.63523400 |
| H | -2.58604000 | -0.02633300 | -2.26012800 |

XXVII. 6,6-dimethyl-3-(trifluoromethyl)hept-1-ene

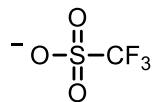


Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| C | 0.00103900 | 0.00211900 | -0.00494300 |
| C | 0.02313200 | 0.01400400 | 1.52158500 |
| F | 1.28917600 | 0.02556100 | 2.02065500 |
| F | -0.60305800 | -1.05453600 | 2.08753000 |
| F | -0.59190000 | 1.12072100 | 2.02428800 |
| C | 0.93605700 | -1.07992100 | -0.61959800 |
| H | 0.98136800 | -0.84688800 | -1.68892600 |
| H | 1.94387100 | -0.91578200 | -0.22300300 |
| C | 0.51605700 | -2.54632500 | -0.42474600 |
| H | 0.46223900 | -2.77398700 | 0.64731100 |
| H | -0.49887400 | -2.68652700 | -0.82113200 |
| C | 2.85897000 | -3.56064100 | -0.50306400 |
| H | 3.36800200 | -2.61808300 | -0.73630300 |
| H | 2.84110400 | -3.67376400 | 0.58885000 |
| H | 3.47162700 | -4.37356800 | -0.91333300 |
| C | 0.82560200 | -4.99791000 | -0.79029500 |
| H | -0.18887700 | -5.08286500 | -1.20118300 |
| H | 1.43511800 | -5.79612900 | -1.23283100 |

| | | | |
|---|-------------|-------------|-------------|
| H | 0.76672700 | -5.18017200 | 0.29060400 |
| C | 1.49607200 | -3.41853500 | -2.61823500 |
| H | 2.06560100 | -4.23299900 | -3.08380500 |
| H | 0.49062900 | -3.41847000 | -3.05948300 |
| H | 1.98590000 | -2.47763700 | -2.89505200 |
| H | 0.41900900 | 0.97692800 | -0.28496200 |
| C | -1.42288100 | -0.06720300 | -0.51268100 |
| H | -2.00874500 | -0.93514700 | -0.21460300 |
| C | -1.96942700 | 0.85172100 | -1.31405700 |
| H | -1.42031100 | 1.73513500 | -1.63542600 |
| H | -2.98748900 | 0.74785300 | -1.68061400 |
| C | 1.43330900 | -3.61139000 | -1.08944300 |

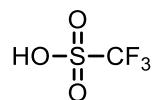
OTf. trifluoromethanesulfonate



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| -1 1 | | | |
| O | -0.00076600 | 0.00000000 | -0.00001700 |
| S | -0.00003600 | 0.00029800 | 1.48384000 |
| O | 1.34442600 | 0.00029100 | 2.11162400 |
| O | -0.98738600 | -0.91137500 | 2.11301600 |
| C | -0.66829200 | 1.70691000 | 1.90905100 |
| F | 0.12295600 | 2.67834200 | 1.40911500 |
| F | -0.74077100 | 1.88091700 | 3.24503900 |
| F | -1.90638500 | 1.88251200 | 1.40300400 |

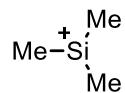
HOTf. triflic acid



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 0 1 | | | |
| O | 0.01534700 | 0.00697900 | -0.00440100 |
| S | 0.00155600 | 0.00387800 | 1.45201100 |
| O | 1.50804900 | -0.00201100 | 2.03604900 |
| O | -0.75074200 | -0.96205600 | 2.23307600 |
| C | -0.56414700 | 1.71599500 | 2.01239600 |
| F | 0.19256200 | 2.65222000 | 1.43687200 |
| F | -0.46660900 | 1.81243800 | 3.33812400 |
| F | -1.83605300 | 1.87797900 | 1.64208000 |
| H | 2.15161000 | 0.28984300 | 1.35576700 |

TMS⁺. trimethylsilyl cation:



Coordinates (from last standard orientation):

| ATOM | X | Y | Z |
|------|-------------|-------------|-------------|
| 1 1 | | | |
| Si | -0.00107400 | 0.00651800 | -0.00356700 |
| C | 0.00432700 | 0.03257600 | 1.83923400 |
| H | 1.01701800 | 0.06858100 | 2.24851100 |
| H | -0.57645900 | 0.88943400 | 2.20289100 |
| H | -0.49937600 | -0.87294000 | 2.20706900 |
| C | -1.59226400 | 0.13462200 | -0.92414500 |
| H | -1.53528400 | 0.96400300 | -1.64151700 |
| H | -1.74317600 | -0.78224300 | -1.51062800 |
| H | -2.44574600 | 0.28289100 | -0.25807800 |
| C | 1.58633000 | -0.15357900 | -0.92592800 |
| H | 2.17361100 | -0.98543700 | -0.51701900 |
| H | 1.43018900 | -0.29920200 | -1.99787300 |
| H | 2.17720200 | 0.76074900 | -0.77105000 |