**References:**

Should be given for known products, for the repetition of known procedures ("According to [Ref], …") and for the application of specific reaction conditions for the preparation of new compounds.
Use The formatting for Chemistry a European Journal.
It is strongly recommended to use http://www.refworks.com/ to insert the references in the reports. At the end of the document.
All references in pdf should be included in a folder named References. The name the pdf files will be the year_journal_abbreviation-article_title of the article.
Abbreviations of Journal Titles (CAS)
http://www.cas.org/expertise/cascontent/caplus/corejournals.html

**NMR Spectra:**

NMR spectra should be included: $^{1}H$, $^{13}C$, DEPT, amd any other like $^{19}F$, $^{31}P$ when corresponding nucleolus is present in the compound. Therefore, pictures of $^{1}H$ and $^{13}C$ NMR shall be included as an appendix in the half-year reports (each spectrum provided with formula drawing and the product number on a A4 page in the landscape format). Make sure that the solvent and any other measurement conditions (like temperature) are properly indicated.

Data files of all spectra should be enclosed into the compound's folder. A text file indicating all measurement conditions should be also included in the folder.

**ECD, UV/Vis, IR, and any other needed Spectra:**

Figures of all spectra (Origin) should be included. Make sure that the concentration, solvent and any other measurement conditions (like cell dimension, $t^a$) are properly indicated.

Data files (Origin) of all spectra should be enclosed into the compound's folder. A text file indicating all measurement conditions should be also included in the folder.

**Guide Lines for Writing the Experimental Part**

**Compound Names**

- According to *ACD Name*. Assign compound names as early as possible.
- Brackets: Use {…{…[…(…)]}}, not (…(…(…(…)))).
- Use di, tri, tetra, … for unsubstituted and bis, tris, tetrakis, … for substituted radicals. No hyphen between the prefix and a substituent in parenthesis.
- Notation:
  1,2,4,5-Tetrakis(bromomethyl)benzene.
  Ethyl (*S*)-(–)-3,3,3-Trifluoro-2-hydroxypropanoate.

**Numbering of Compounds**

- For simple structures, use the systematic numbering; use primes for the assignment of different units.

For complex structures, an arbitrary numbering may be advantageous; simple substituents (like OMe, Ac, CN, CHO) do not need an arbitrary number.

**Text Items**

- Use American English.
- Use – for minus sign, ratios, and bonds (e.g. –78 °C, $cm^{-1}$, 7.41–7.50 ppm, but –10 to –20 °C, H–C(3), $CH_2$–C(5)). Use C(1)–C(2)–C(3)–C(4) for torsion angles, but C(1)-C(2)-C(3) for bond angles.
- EtOAc, $(CD_3)_2CO$, $(CD_3)_2SO$.
- 'quench' for destroying an excess of a reagent is slang (better: 'treated with …'). 'reflux' is only a noun ('kept at reflux', 'heated to reflux', not '~~refluxed~~'). Use 'brine' for saturated NaCl solution. ~~reaction~~ mixture, ~~unreacted~~ starting material.
- Use a space beween the numerary and the extension (3.5 g, 4.25 mL, 50 °C, 12 h, …) and in front and behind a mathematical operator ($c$ = 1.2, $R_f$ = 0.53, but +25 and –50 for positive and negative numbers).
- Italicize symbols for physical quantities ($T$, $c$, $\lambda_{max}$), stereochemical information (*cis*, *trans*, *E*, *Z*, *syn*, *anti*,$\alpha$, $\beta$), configurational prefixes (*erythro*, *ribo*, *myo*), locants (*N*-methyl, *tert*-butyl), symmetry ($C_{2v}$), and conformational symbols ($^4C_1$, $^{1,4}B$, $B_{1,4}$). See the difference between 2-deoxy-$\alpha$-D-*erythro*-pentofuranose (= '$\alpha$-D-2-deoxyribo-furanose') and $\alpha$-D-ribofuranose.
- Use *n*Bu, *i*Pr, *t*Bu, Me, Et, Ac, Ph, Bn (benzyl), Bz (benzoyl).
- Use small caps for the stereodescriptors D and L (D-glucose, L-alanine), and the concentration descriptors N and M (2 N HCl, 3 M $H_2SO_4$).
- Dimensions with negative exponents: $JK^{-1}mol^{-1}$, $molL^{-1}$.

**Procedure**

- Describe a single experiment, if possible of a larger batch size (past tense). General procedures only for experiments run under the same conditions (e.g. exact same batch size).
- Give exact description of reagents and substrates (for enzymes and biological substrates with supplier), e.g. $TsOH \cdot H_2O$, $CaSO_4 \cdot 0.5\ H_2O$ vs. $CaSO_4 \cdot 2\ H_2O$, 60% NaH in mineral oil, saturated (at 0 °C) ammonia in MeOH, …
- Use exact quantitative terms: 8 mg instead of ~~a spatula~~, 27 µL instead of ~~2 drops~~, batchwise or dropwise addition within 12 min instead of slow addition, exact temperature instead ~~room temperature~~ (in Canada: room temperature is 25–28 °C in winter times, but ca. –18 °C in summer times!)
- Quantities of reactands and solvents should be given in parenthesis: a solution of $I_2$ (220 mg, 2 equiv, 0.9 mmol) in toluene (300 mL) was cooled ….
- The ratio of products mixtures must be reflected by spectroscopic data.
- Yields (without decimal place) within the procedure: FC (…) and crystallization from $Et_2O$/hexane gave **25** (843 mg, 77%) as colorless fine needles.
- Best quality of products (sublimed, distilled or crystallized material) is required for m.p., $[\alpha]_D$, UV/Vis, and elemental analysis. Drying of solid material after chromatography is insufficient.
- Drying a sample at a Turbovac pump for several days is rather a placebo (slow laminar flow through narrow tubular connections); releasing pressure and re-evacuation every 2–

3 h is far more effective. Drying over powdered (!) $P_2O_5$ in an evacuated dessicator is presumably more effective than the Turbovac-pump drying also for the removal of other polar solvents.
Small amounts (2–20 mg) are best sublimed with the good old sublimation block.

**Sequence of Analytical and Spectroscopic Data**

- $R_f$; m.p. or b.p.; $[\alpha]_D$; $^1H$; $^{13}C$; other NMR; IR; UV/Vis; MS; elemental analysis.

***R*$_f$ and *t*$_R$ of HPLC**

- Two decimal places for $R_f$ values.
- Give $t_R$ values for HPLC separations.
- Notation:
  $R_f$ = 0.38 ($SiO_2$; heptane/$CH_2Cl_2$ 1:1);
  prep. HPLC: $t_R$ = 15.2 min ($SiO_2$; column size, flow = xx $mLmin^{-1}$, heptane/$CH_2Cl_2$ 1:1);

**M.p. or b.p.**

- Best quality of material required.
- For known products, with m.p. of the literature in parenthesis.
- Simultaneous measuring of mixtures ('mixed m.p.') allows to determine identity of two samples.
- Decomposition (decomp) should be corroborated by TLC; important information for purification by sublimation.
- Notation:
  m.p. 185.5–186.5 °C ($Et_2O$/hexane, [ref]: 185–187 °C);

**Optical Rotation**

- Best quality of material required.
- For known products, with $[\alpha]_D$ of the literature in parenthesis.
- For $[\alpha]_D$ values up to 300: one decimal place, for large values: without decimal place.
- If $[\alpha]_D < 1$, measurement of $[\alpha]_{546}$, $[\alpha]_{436}$, or $[\alpha]_{365}$ (Hg lamp) recommended.
- Notation:
  $[\alpha]_D^{20} = -13.5$ ($c$ = 0.2 in acetone, [ref]: –13.2 ($c$ = 0.5 in acetone));

**NMR**

- If aggregations is expected, exact weighting of the samples recommended (association influences the $\delta$ values).
- If acid sensitive samples are studied, filter $CDCl_3$ through basic $Al_2O_3$ immediately before use (removes DCl, but not water).
- Put down the interpretations and assignments on a hardcopy of the spectrum even for an on-line analysis (when possible).
- Assign signals of solvents and impurities according to *JOC* **1997**, *62*, 7212.
- Important NMR experiments (DQF-COSY, HSQC, HMBC, NOE, selective homodecouplings) should be mentionend with each compound.
- Broad signals hint at equilibria in the NMR scale (some signals may even be hidden by coalescence) → measuring NMR spectra at higher and/or lower temperature.
- HSQC and HMBC spectra require the assignment of $^{13}C$ NMR signals.

**$^{1}$H NMR**

- Two decimal places and in ambiguous cases three decimal places for $\delta$ values, one decimal place for $J$ values.
- Give an exact description of the signals (d, br. d, t ($J$ = 9.5 Hz), t ($J \approx$ 9.5 Hz), dt *vs*. td, ddt, …). Avoid m (range must be given) if possible.
- Check for correct binomial ratios; e.g. 1:1:1:1 for a dd ($J$ = 9.0, 4.5 Hz) and 1:3:3:1 for a q ($J$ = 4.5 Hz). The asymmetry of splitted signals (roof effect) helps in finding coupling partners.
- Exchangeable H-atoms are easily detected by H/D exchange.
- For new members: list 1H NMR data with increasing $\delta$ and decreasing $J$ values.
- Notation (new beginnings of lines only for enhanced reading): $^{1}$H NMR (400 MHz, $(CD_3)_2SO$, 0 °C; assignments based on a DQF-COSY spectrum): $\delta$ = –0.15, 0.02 (2 s, 6 H; $SiMe_2$), 2.06 (s, 3 H; OAc)), 7.55–7.20 (m, 5 arom. H), 3.72 (q, $J \approx$ 4.2 Hz, 1 H, irradiation at 1.33 → n.O.e. of 5.5%; H–C(2)), 4.55 (dd, $J$ = 8.5, 3.8 Hz, 1 H, addition of $D_2O$ → d, $J$ = 8.7 Hz; H–C(1)), 8.34 (dd, $^{3}J$(H,F) = 15.2, $J$ = 4.5 Hz; H–C(3'), 9.52 ppm (d, $J$ = 8.3 Hz, 1 H, exchange with $D_2O$; NHC=O);

**$^{13}$C NMR**

- One decimal place for $\delta$ values; with multiplicity and intensity (reflecting the local symmetry). s for quart. C and d for CH are usually easily assigned from a H-decoupled spectrum by the intensity; in ambiguous cases, a DEPT spectrum is required.
- With assignments for simple structures.
- Give $^{x}J$(F,C) and $^{x}J$(P,C) couplings.
- For new members: list $^{13}$C NMR data with increasing $\delta$ values.
- CP-MAS solid-state $^{13}$C NMR spectra may be measured of solids.
- Notation (new beginnings of lines only for enhanced reading): $^{13}$C NMR (150 MHz, $CDCl_3$; assignments based on a DEPT and a HSQC spectrum): $\delta$ = 59.82 (t; O*C*$H_2$Me), 128.45 (d, 2 C, C(2'',6'')), 136.55 (s; C(1'') or C(1) of Ph), 159.22 (q, $^{2}J$(C,F) = 37.3 Hz; $CF_3$*C*=O), 169.21, 169.43, 170.52 ppm (3 s; 3 NHC=O), signal of *C*(=NH)$CCl_3$ hidden by the noise;

**$^{19}$F NMR**

- H-coupled spectra (full range) give more information. $J$(F,H) couplings are similar in $^{1}$H and $^{19}$F NMR spectra, but $J$(F,H) < 2 Hz are usually not visible in $^{19}$F NMR spectra.
- Notation (new beginnings of lines only for enhanced reading): $^{19}$F NMR (141.1 MHz, $CDCl_3$): $\delta$ = –199.63 (ddd, $^{1}J$(H,F) = 48.9, $^{3}J$(H,F) = 29.7, $^{2}J$(H,F) = 14.2 Hz; F–C(2)), –74.80 ppm (s, $CF_3$);

**IR**

- ATR spectra (solid state) ok. For investigation of associations, solution spectra (2–3 mg/100 µL of solvent) must be measured; artifacts if cell is leaking during the measurement.
- List bands from 4000 to 600 $cm^{-1}$ with intensities (s, m, w, very w; br. for broad and sh for shoulder). Identify diagnostic signals.
- Check for expected bands (e.g. very weak bands for S–H, C–D, and isolated C≡C bonds). Do not list bands stemming from impurities (acetone, EtOAc, $H_2O$).

- Give range for the OH absorption of acids ('Säuresack').
- Notation: IR (ATR): $\tilde{\nu}$ = 3300–2400 (m), 2990 (m), 2100 (very w), 1740 (m, sh), 1725 (s), 1150 (br. s), 890 $cm^{-1}$ (w);

**UV/Vis and ECD**

- Best quality of material required. Exactly weighted samples (special accuracy weighing machine).
  The concentration has to be adjusted to the highest sensitivity (0.5–1.5 A range) of the apparatus.
  The validity of the Lambert-Beer law is evidenced by measuring UV/Vis spectra at different concentrations.
- For measuring at $T < 20°$ (e.g. UV melting curves), the cell compartment must be floated with $N_2$; otherwise artifacts due to condensation of $H_2O$ from air.
- $\lambda_{max}$ in nm, without decimal place.
- The molar absorption coefficient $\varepsilon$ and $\Delta\varepsilon$ has the dimension $M^{-1}cm^{-1}$ (i.e. $c$ in M), but is usually given without dimension. Round the last two digits (for $\varepsilon < 1000$, the last digit).
- Notation:
  UV/Vis (MeOH): $\lambda_{max}$ ($\varepsilon$) = 465 (325), 320 (17200), 270 nm (12400); ECD (MeOH): $\lambda_{max}$ ($\Delta\varepsilon$) = 450 (45), 340 (–45);

**MS**

- Give specification for different types (HR-MALDI-MS, HR-ESI-MS, HR-EI-MS, …) in the *General Remarks* (be careful in copying data from earlier theses!).
- List peaks from large to small with intensities (usually peaks > 20%; for EI-MS, also important peaks of lower intensity). Assign important peaks ($[M + Na]^+$, $[M + H]^+$, $[M – OMe]^+$, …). Do not list matrix peaks or peaks of solvents and impurities (e.g. *m/z* 149 of dioctyl phthalate, an abundant softener).
- For HR-MS: four decimal places for compounds of low molecular mass.
- Calculate the important peaks for the most abundant isotopomer.
- Notation: HR-EI-MS: *m/z* (%): 229.9758 (3), 227.9781 (3, $[M]^+$, calcd for $C_9H_9{}^{79}BrO_2{}^+$: 227.9786), 149.0606 (2, $[M – Br]^+$, calcd for $C_9H_9O_2{}^+$: 149.0603), … (…), 91.xxxx (100, $[C_7H_7]^+$); 57.xxxx (55), 43.xxxx (63); HR-MALDI-MS: *m/z* (%): 399.0202 (39), 397.0215 (58), 395.0246 (100, $[M + Na]^+$, calcd for $C_{20}H_{12}N_4Na^{68}Zn^+$: 395.0251), 377.0389 (25), 375.0396 (37), 373.0426 (100, $[M + H]^+$, calcd for $C_{20}H_{13}N_4{}^{68}Zn^+$: 373.0432);

**Elemental Analysis**

- Best quality of material required.
- As a rule, elemental analysis is measured for crystalline, important, and final products.
- Notation: elemental analysis (%) calcd for $C_{20}H_{32}N_2O_5$ (733.4): C 63.14, H 8.48, N 7.36; found: C 62.88, H 8.41, N 7.44.

**Calculations**

- Figures of all predicted spectra (Origin) should be included. Oscillator strength and Rotational strength should be depicted with bars (for an example see Figure 2 in http://onlinelibrary.wiley.com/doi/10.1002/anie.200906191/pdf).
- Data files (Origin) of all spectra should be enclosed into the compound's folder.

- Calculation files (optimization, frequency and any onther like ECD or ORD should be included (input and output) with a clear nomenclature. A text file indicating calculation parameters should be also included in the folder.
- Z matrix of the optimized geometries should be included in the text.