

In [1]:

```
import netCDF4 as nc
import numpy as np
from matplotlib import pyplot as plt
import xarray
import glob
from geopy.distance import geodesic
import datetime as dt
import matplotlib as mpl
from matplotlib.ticker import (MultipleLocator, AutoMinorLocator)
```

## Funktionen zum einlesen von Daten

In [2]:

```
time_threshold = 3600 # in seconds
distance_threshold = 50 # in km
```

In [3]:

```
def cut_useless_variables(DS):
    """
    Preprocessing the IASI dataset before concatenation.
    Removing undesired dimensions and variables.

    Parameters:
    -----
    ds : xarray dataset
        Dataset of IASI data.
    """

    # Remove some nasty variables:
    """
    Remaining variables are:
    pressure_levels_temp
    pressure_levels_humidity
    record_start_time
    record_stop_time
    lat
    lon
    atmospheric_temperature
    atmospheric_water_vapor
    surface_temperature
    surface_pressure
    instrument_mode
    flag_cldnes
    flag_iasibad
    flag_itconv
    flag_landsea
    error_data_index
        # temperature_error
        # water_vapour_error
    surface_z          (useful in combination with surface_pressure)
    co_qflag
    co_bdiv

    Remaining dimensions:
    nlt
    nlq
    along_track
    across_track
        # nerr
        # nerrt
        # nerrw
    """
    useless_vars = ['cloud_formation', 'pressure_levels_ozone', 'surface_emissivity_wave
```

```

lengths',
zenith',
'atmospheric_ozone', 'integrated_water_vapor', 'integrated_ozone', '
integrated_n2o',
'integrated_co', 'integrated_ch4', 'integrated_co2', 'surface_emissi
vity',
'number_cloud_ formations', 'fractional_cloud_cover', 'cloud_top_temp
erature',
'cloud_top_pressure', 'cloud_phase', 'spacecraft_altitude', 'flag_am
subad',
'flag_avhrrbad', 'flag_cdlfrm', 'flag_cdlrst', 'flag_daynit', 'flag_
dustcld',
'flag_fgcheck', 'flag_initia', 'flag_mhsbad', 'flag_numit', 'flag_nw
pbad',
'flag_physcheck', 'flag_recheck', 'flag_satman', 'flag_sunglnt', 'f
lag_thicir',
'lues',
'co_cp_air', 'co_cp_co_a', 'co_x_co', 'co_h_eigenvalues', 'co_h_eige
nvectors',
'temperature_error', 'water_vapour_error']
DS = DS.drop_vars(useless_vars)

# useless_dims = ['npct', 'npcw', 'npco', 'nl_co', 'nl_hno3', 'nl_o3', 'nl_so2', 'new
', 'nlo',
# 'cloud_ formations', 'nerro', 'co_nbr', 'neva_co', 'neve_co']
# DS = DS.squeeze(useless_dims, drop=True)

return DS

```

In [4]:

```

def import_single_NYA_RS_radiosonde(
    filename,
    keys='all',
    verbose=0):

    """
    Imports single NYA-RS radiosonde data for Ny Alesund. Converts to SI units
    and interpolates to a height grid with 5 m resolution from 0 to 15000 m.

    Parameters:
    -----
    filename : str
        Name (including path) of radiosonde data file.
    keys : list of str or str, optional
        This describes which variable(s) will be loaded. Specifying 'all' will import all varia
        bles.
        Specifying 'basic' will load the variables the author consideres most useful for his cu
        rrent
        analysis.
        Default: 'all'
    verbose : int
        If 0, output is suppressed. If 1, basic output is printed. If 2, more output (more warn
        ings,...)
        is printed.
    """

    """
    Loaded values are imported in the following units:
    T: in K
    P: in hPa, will be converted to Pa
    RH: in [0-1]
    Altitude: in m
    time: will be converted to sec since 1970-01-01 00:00:00 UTC
    """

```

```

file_nc = nc.Dataset(filename)

if (not isinstance(keys, str)) and (not isinstance(keys, list)):
    raise TypeError("Argument 'key' must be a list of strings or 'all'.")

if keys == 'all':
    keys = file_nc.variables.keys()
elif keys == 'basic':
    keys = ['time', 'temp', 'press', 'rh', 'alt']

sonde_dict = dict()
for key in keys:
    if not key in file_nc.variables.keys():
        raise KeyError("I have no memory of this key: '%s'. Key not found in radiosonde file."
% key)

    sonde_dict[key] = np.asarray(file_nc.variables[key])
    if key != "IWV" and len(sonde_dict[key]) == 0: # 'and': second condition only evaluate
d if first condition True
        return None

    if key in ['lat', 'lon']: # only interested in the first lat, lon position
        sonde_dict[key] = sonde_dict[key][0]

# convert units:
if 'P' in keys: # from hPa to Pa
    sonde_dict['P'] = sonde_dict['P']*100
if 'time' in keys: # from int64 to float64
    time_unit = file_nc.variables['time'].units
    time_offset = (dt.datetime.strptime(time_unit[-19:], "%Y-%m-%dT%H:%M:%S") - dt.datetim
e(1970,1,1)).total_seconds()
    sonde_dict['time'] = np.float64(sonde_dict['time']) + time_offset
    sonde_dict['launch_time'] = sonde_dict['time'][0]

keys = [*keys] # converts dict_keys to a list
for key in keys:
    if sonde_dict[key].shape == sonde_dict['time'].shape:
        if key not in ['time', 'lat', 'lon', 'alt']:
            sonde_dict[key + "_ip"] = np.interp(np.arange(0,15001,5), sonde_dict['alt'], sonde_d
ict[key])
        elif key == 'alt':
            sonde_dict[key + "_ip"] = np.arange(0, 15001,5)

# Renaming variables to a standard convention
renaming = {'press': 'pres', 'alt': 'height', 'press_ip': 'pres_ip', 'alt_ip': 'height_
ip'}
for ren_key in renaming.keys():
    if ren_key in sonde_dict.keys():
        sonde_dict[renaming[ren_key]] = sonde_dict[ren_key]

return sonde_dict

def import_single_PS122_mosaic_radiosonde_level2(
    filename,
    keys='all',
    verbose=0):

    """
    Imports single level 2 radiosonde data created with PANGAEA_tab_to_nc.py
    ('PS122_mosaic_radiosonde_level2_yyyymmdd_hhmmssZ.nc'). Converts to SI units
    and interpolates to a height grid with 5 m resolution from 0 to 15000 m.

    Parameters:
    -----
    filename : str
        Name (including path) of radiosonde data file.
    keys : list of str or str, optional
        This describes which variable(s) will be loaded. Specifying 'all' will import all varia
bles.
        Specifying 'basic' will load the variables the author consideres most useful for his cu

```

```

rrent
    analysis.
    Default: 'all'
verbose : int
    If 0, output is suppressed. If 1, basic output is printed. If 2, more output (more warn
ings,...)
    is printed.
"""

"""
    Loaded values are imported in the following units:
    T: in deg C, will be converted to K
    P: in hPa, will be converted to Pa
    RH: in %, will be converted to [0-1]
    Altitude: in m
    q: in kg kg-1 (water vapor specific humidity)
    time: in sec since 1970-01-01 00:00:00 UTC
"""

file_nc = nc.Dataset(filename)

if (not isinstance(keys, str)) and (not isinstance(keys, list)):
    raise TypeError("Argument 'key' must be a list of strings or 'all'.")

if keys == 'all':
    keys = file_nc.variables.keys()
elif keys == 'basic':
    keys = ['time', 'T', 'P', 'RH', 'q', 'Altitude']

sonde_dict = dict()
for key in keys:
    if not key in file_nc.variables.keys():
        raise KeyError("I have no memory of this key: '%s'. Key not found in radiosonde file."
% key)

    sonde_dict[key] = np.asarray(file_nc.variables[key])
    if key != "IWV" and len(sonde_dict[key]) == 0: # 'and': second condition only evaluate
d if first condition True
        return None

    if key in ['Latitude', 'Longitude']: # only interested in the first lat, lon position
        sonde_dict[key] = sonde_dict[key][0]
    if key == 'IWV':
        sonde_dict[key] = np.float64(sonde_dict[key])

# convert units:
if 'RH' in keys: # from percent to [0, 1]
    sonde_dict['RH'] = sonde_dict['RH']*0.01
if 'T' in keys: # from deg C to K
    sonde_dict['T'] = sonde_dict['T'] + 273.15
if 'P' in keys: # from hPa to Pa
    sonde_dict['P'] = sonde_dict['P']*100
if 'time' in keys: # from int64 to float64
    sonde_dict['time'] = np.float64(sonde_dict['time'])
    sonde_dict['launch_time'] = sonde_dict['time'][0]

keys = [*keys] # converts dict_keys to a list
for key in keys:
    if sonde_dict[key].shape == sonde_dict['time'].shape:
        if key not in ['time', 'Latitude', 'Longitude', 'ETIM', 'Altitude']:
            sonde_dict[key + "_ip"] = np.interp(np.arange(0,15001,5), sonde_dict['Altitude'], so
nde_dict[key])
        elif key == 'Altitude':
            sonde_dict[key + "_ip"] = np.arange(0, 15001,5)

# Renaming variables: ['Lat', 'Lon', 'p', 'T', 'RH', 'GeopHgt', 'qv', 'time', ...]
renaming = {'T': 'temp', 'P': 'pres', 'RH': 'rh',
            'Altitude': 'height', 'h_geom': 'height_geom',
            'Latitude': 'lat', 'Longitude': 'lon',
            'T_ip': 'temp_ip', 'P_ip': 'pres_ip', 'RH_ip': 'rh_ip',
            'Altitude_ip': 'height_ip', 'h_geom_ip': 'height_geom_ip',

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'IWV': 'iwv'}
for ren_key in renaming.keys():
    if ren_key in sonde_dict.keys():
        sonde_dict[renaming[ren_key]] = sonde_dict[ren_key]

return sonde_dict

####

def import_radiosonde_daterange(
    path_data,
    date_start,
    date_end,
    s_version='level_2',
    with_wind=False,
    verbose=0):

    """
    Imports radiosonde data 'mossonde-curM1' and concatenates the files into time series x h
    eight.
    E.g. temperature profile will have the dimension: n_sondes x n_height

    Parameters:
    -----
    path_data : str
        Path of radiosonde data.
    date_start : str
        Marks the first day of the desired period. To be specified in yyyy-mm-dd (e.g. 2021-01-
    14)!
    date_end : str
        Marks the last day of the desired period. To be specified in yyyy-mm-dd (e.g. 2021-01-1
    4)!
    s_version : str, optional
        Specifies the radiosonde version that is to be imported. Possible options: 'mossonde',
        'psYMMDDwHH', 'level_2'. Default: 'level_2' (published by Marion Maturilli)
    with_wind : bool, optional
        This describes if wind measurements are included (True) or not (False). Does not work w
    ith
    s_version='psYMMDDwHH'. Default: False
    verbose : int, optional
        If 0, output is suppressed. If 1, basic output is printed. If 2, more output (more warn
    ings,...)
        is printed.
    """

    if not isinstance(s_version, str): raise TypeError("s_version in import_radiosonde_dater
    ange must be a string.")

    # extract day, month and year from start date:
    date_start = dt.datetime.strptime(date_start, "%Y-%m-%d")
    date_end = dt.datetime.strptime(date_end, "%Y-%m-%d")

    if s_version == 'level_2':
        all_radiosondes_nc = sorted(glob.glob(path_data + "PS122_mosaic_radiosonde_level2*.nc")
    )

    # inquire the number of radiosonde files (date and time of launch is in filename):
    # And fill a list which will include the relevant radiosonde files.
    radiosondes_nc = []
    for rs_nc in all_radiosondes_nc:
        rs_date = rs_nc[-19:-3] # date of radiosonde from filename
        yyyy = int(rs_date[:4])
        mm = int(rs_date[4:6])
        dd = int(rs_date[6:8])
        rs_date_dt = dt.datetime(yyyy,mm,dd)
        if rs_date_dt >= date_start and rs_date_dt <= date_end:
            radiosondes_nc.append(rs_nc)

    elif s_version == 'nya-rs':
        all_radiosondes_nc = sorted(glob.glob(path_data + "NYA-RS_*.nc"))

    # inquire the number of radiosonde files (date and time of launch is in filename):

```

```

# And fill a list which will include the relevant radiosonde files.
radiosondes_nc = []
for rs_nc in all_radiosondes_nc:
    rs_date = rs_nc[-15:-3] # date of radiosonde from filename
    yyyy = int(rs_date[:4])
    mm = int(rs_date[4:6])
    dd = int(rs_date[6:8])
    rs_date_dt = dt.datetime(yyyy,mm,dd)
    if rs_date_dt >= date_start and rs_date_dt <= date_end:
        radiosondes_nc.append(rs_nc)

# number of sondes:
n_sondes = len(radiosondes_nc)

# count the number of days between start and end date as max. array size:
n_days = (date_end - date_start).days

# basic variables that should always be imported:
if s_version == 'level_2':
    geoinfo_keys = ['lat', 'lon', 'launch_time', 'iwv']
    time_height_keys = ['pres', 'temp', 'rh', 'height', 'rho_v', 'q']
    if with_wind: time_height_keys = time_height_keys + ['wspeed', 'wdir']

elif s_version == 'nya-rs':
    geoinfo_keys = ['lat', 'lon', 'launch_time']
    time_height_keys = ['pres', 'temp', 'rh', 'height']
    if with_wind: time_height_keys = time_height_keys + ['wspeed', 'wdir']
else:
    raise ValueError("s_version in import_radiosonde_daterange must be 'nya-rs' or 'level_2'")
all_keys = geoinfo_keys + time_height_keys

# sonde_master_dict (output) will contain all desired variables on specific axes:
# Time axis (one sonde = 1 timestamp) = axis 0; height axis = axis 1
n_height = len(np.arange(0,15001,5)) # length of the interpolated height grid
sonde_master_dict = dict()
for gk in geoinfo_keys: sonde_master_dict[gk] = np.full((n_sondes,), np.nan)
for thk in time_height_keys: sonde_master_dict[thk] = np.full((n_sondes, n_height), np.nan)

if s_version == 'level_2':
    all_keys_import = ['Latitude', 'Longitude', 'P', 'T', 'RH', 'Altitude', 'rho_v', 'q', 'time', 'IWV']
    if with_wind: all_keys_import = all_keys_import + ['wdir', 'wspeed']

# cycle through all relevant sonde files:
for rs_idx, rs_nc in enumerate(radiosondes_nc):

    if verbose >= 1:
        # rs_date = rs_nc[-19:-3]
        print("Working on Radiosonde, " + rs_nc)

    sonde_dict = import_single_PS122_mosaic_radiosonde_level2(rs_nc, keys=all_keys_import)

    # save to sonde_master_dict:
    for key in all_keys:
        if key in geoinfo_keys:
            sonde_master_dict[key][rs_idx] = sonde_dict[key]

        elif key in time_height_keys:
            sonde_master_dict[key][rs_idx, :] = sonde_dict[key + "_ip"] # must use the interpolated versions!

        else:
            raise KeyError("Key '" + key + "' not found in radiosonde dictionary after importing it with " +
                            "import_single_PS122_mosaic_radiosonde_level2")

if s_version == 'nya-rs':
    all_keys_import = ['lat', 'lon', 'press', 'temp', 'rh', 'alt', 'time']

```

```

if with_wind: all_keys_import = all_keys_import + ['wdir', 'wspeed']

# cycle through all relevant sonde files:
for rs_idx, rs_nc in enumerate(radiosondes_nc):

    if verbose >= 1:
        # rs_date = rs_nc[-19:-3]
        print("Working on Radiosonde, " + rs_nc)

    sonde_dict = import_single_NYA_RS_radiosonde(rs_nc, keys=all_keys_import)

    # save to sonde_master_dict:
    for key in all_keys:
        if key in geoinfo_keys:
            sonde_master_dict[key][rs_idx] = sonde_dict[key]

        elif key in time_height_keys:
            sonde_master_dict[key][rs_idx, :] = sonde_dict[key + "_ip"] # must use the interpolated versions!

        else:
            raise KeyError("Key '" + key + "' not found in radiosonde dictionary after importing it with " +
                            "import_single_NYA_RS_radiosonde")

    return sonde_master_dict

```

In [5]:

```

def numpydatetime64_to_epochtime(npdt_array):

    """
    Converts numpy datetime64 array to array in seconds since 1970-01-01 00:00:00 UTC (type: float).

    Parameters:
    -----
    npdt_array : numpy array of type np.datetime64 or np.datetime64 type
                  Array (1D) or directly a np.datetime64 type variable.
    """

    sec_epochtime = npdt_array.astype(np.timedelta64) / np.timedelta64(1, 's')

    return sec_epochtime

```

In [6]:

```

def create_launch_time(DS):

    time_dif = np.diff(DS.time.values)
    where_jump = np.argwhere(np.abs(time_dif) > time_threshold).flatten()
    launch_time = np.concatenate((np.array([DS.time.values[0]]), DS.time.values[where_jump+1]))

    return xarray.DataArray(launch_time)

```

## Daten einlesen

In [7]:

```

#NyAlesund
path_data = "/Users/charlottebaur/Desktop/Project work/NyAlesund/"
NyAl_sonde_dict = import_radiosonde_daterange(path_data, date_start="2020-08-01", date_end="2020-09-30", s_version='nya-rs', with_wind=False)

#IASI
IASI_DS = xarray.open_mfdataset('/Users/charlottebaur/Desktop/Project work/METRS_IASI/*.nc', concat_dim='along_track', combine='nested', decode_times=False, preprocess=cut_useles

```

```

s_variables)

#Polarstern
path_data = "/Users/charlottebaur/Desktop/Project work/Polarstern/"
date_start = "2020-08-01" # in yyyy-mm-dd
date_end = "2020-09-30" # in yyyy-mm-dd
s_version = 'level_2'

PS_sonde_dict = import_radiosonde_daterange(path_data, date_start, date_end, s_version, w
ith_wind=False)

<ipython-input-4-3e5033df8d41>:59: DeprecationWarning: tostring() is deprecated. Use toby
tes() instead.
    time_unit = file_nc.variables['time'].units
/Users/charlottebaur/opt/anaconda3/lib/python3.8/site-packages/xarray/conventions.py:512:
SerializationWarning: variable 'temperature_error' has multiple fill values {-2147483646,
4294967295}, decoding all values to NaN.
    new_vars[k] = decode_cf_variable(
/Users/charlottebaur/opt/anaconda3/lib/python3.8/site-packages/xarray/conventions.py:512:
SerializationWarning: variable 'water_vapour_error' has multiple fill values {-2147483646
, 4294967295}, decoding all values to NaN.
    new_vars[k] = decode_cf_variable(
/Users/charlottebaur/opt/anaconda3/lib/python3.8/site-packages/xarray/conventions.py:512:
SerializationWarning: variable 'ozone_error' has multiple fill values {-2147483646, 42949
67295}, decoding all values to NaN.
    new_vars[k] = decode_cf_variable(
/Users/charlottebaur/opt/anaconda3/lib/python3.8/site-packages/xarray/conventions.py:512:
SerializationWarning: variable 'surface_z' has multiple fill values {-32767, 32767}, deco
ding all values to NaN.
    new_vars[k] = decode_cf_variable(
/Users/charlottebaur/opt/anaconda3/lib/python3.8/site-packages/xarray/conventions.py:512:
SerializationWarning: variable 'co_cp_air' has multiple fill values {-2, 65535}, decoding
all values to NaN.
    new_vars[k] = decode_cf_variable(
/Users/charlottebaur/opt/anaconda3/lib/python3.8/site-packages/xarray/conventions.py:512:
SerializationWarning: variable 'co_cp_co_a' has multiple fill values {-2, 65535}, decodin
g all values to NaN.
    new_vars[k] = decode_cf_variable(

```

In [15]:

```
print(PS_sonde_dict)
```

```

{'lat': array([78.829, 78.806, 78.835, 78.968, 79.017, 79.037, 79.114, 78.71 ,
       78.656, 78.649, 78.65 , 79.022, 79.047, 79.024, 79.018, 78.812,
       78.714, 78.591, 78.525, 78.42 , 78.386, 78.352, 78.356, 78.796,
       79.41 , 79.753, 79.777, 79.905, 79.881, 79.9 , 79.892, 79.916,
       79.883, 79.882, 79.879, 79.879, 79.908, 79.902, 79.917, 79.921,
       79.946, 79.955, 79.988, 80.001, 80.03 , 80.069, 80.116, 80.182,
       80.233, 80.562, 81.054, 81.277, 81.61 , 82.403, 82.928, 83.397,
       83.992, 84.56 , 85.13 , 85.491, 85.899, 86.36 , 86.662, 86.945,
       87.433, 87.778, 88.118, 88.296, 88.502, 88.916, 88.935, 89.114,
       89.342, 89.644, 89.996, 89.992, 89.821, 89.394, 88.991, 88.581,
       88.154, 87.737, 87.718, 87.717, 87.722, 87.729, 87.749, 87.756,
       87.744, 87.745, 87.757, 87.772, 87.791, 87.798, 87.774, 87.763,
       87.767, 87.776, 87.78 , 87.784, 87.801, 87.827, 87.843, 87.88 ,
       87.906, 87.938, 87.95 , 87.98 , 87.996, 88.025, 88.038, 88.058,
       88.068, 88.093, 88.112, 88.145, 88.168, 88.204, 88.228, 88.253,
       88.266, 88.284, 88.294, 88.311, 88.326, 88.34 , 88.354, 88.375,
       88.392, 88.416, 88.442, 88.474, 88.509, 88.553, 88.591, 88.634,
       88.67 , 88.698, 88.721, 88.743, 88.749, 88.75 , 88.746, 88.742,
       88.733, 88.737, 88.74 , 88.743, 88.752, 88.761, 88.758, 88.746,
       88.734, 88.726, 88.711, 88.696, 88.688, 88.685, 88.675, 88.676,
       88.676, 88.696, 88.71 , 88.729, 88.725, 88.724, 88.71 , 88.713,
       88.708, 88.713, 88.717, 88.735, 88.743, 88.76 , 88.76 , 88.77 ,
       88.772, 88.787, 88.793, 88.811, 88.831, 88.85 , 88.873, 88.908,
       88.935, 88.945, 88.959, 88.987, 89.005, 89.003, 89.009, 89.037,
       89.055, 89.053, 89.047, 89.06 , 89.072, 89.063, 89.079, 89.07 ,
       89.09 , 89.076, 89.07 , 89.034, 89.028, 89.016, 89.031, 89.039,
       89.054, 89.065, 89.075, 89.102, 89.117, 89.153, 89.139, 89.151,
       89.135, 89.146, 89.132, 89.01 , 88.779, 88.595, 88.509, 88.313,
       87.928, 87.502, 87.007, 86.782, 86.555, 86.334, 86.192, 86.005,

```



```
86.036, 85.974, 85.959, 85.959, 85.98 , 85.984, 85.964, 85.984,
85.996, 86.01 , 86.012, 86.032, 86.046, 85.979, 85.949, 85.994,
86.001, 85.958, 85.961, 85.983, 85.979, 85.965, 86.031, 86.032,
85.964, 85.388, 84.742, 84.59 , 84.417, 84.205, 83.942, 83.73 ,
83.523, 83.228, 83.253, 83.255, 83.301, 83.157, 82.996, 82.542,
82.246, 81.667, 81.597, 81.582, 81.589, 81.604, 81.617, 81.625,
81.775, 81.71 , 81.679, 81.535, 81.318, 81.125, 80.965]], 'lon': array([ -2.234,
-2.41 , -2.398, -2.535, -2.591, -2.726, -2.604,
-4.622, -5.038, -4.296, -4.244, -2.965, -3.3 , -3.211,
-3.445, -1.676, -1.16 , -1.578, -2.944, -6.046, -7.04 ,
-7.249, -7.338, -6.598, -5.743, -5.141, -4.65 , -3.555,
-3.531, -3.771, -3.869, -4.062, -4.169, -4.637, -4.857,
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```

## Zeit filtern

In [8]:

```
#IASI in Sekunden seit 01.01.2000 > umwandeln in Zeit wie bei NyAlesund
```

```
record_start_time = np.zeros(IASI_DS['record_start_time'].shape)
time_diff = (dt.datetime(2000,1,1) - dt.datetime(1970,1,1)).total_seconds()
n_time = IASI_DS['record_start_time'].shape[0]
iasi_record_start_time = IASI_DS.record_start_time.values
n_time_print = int(0.15*n_time)
for i in range(n_time):
    if i%n_time_print == 0: print(i)
    record_start_time[i] = iasi_record_start_time[i] + time_diff
```

```
IASI_DS['record_start_time'] = xarray.DataArray(record_start_time, dims=['along_track'])
```

```
0
14857
29714
44571
59428
74285
89142
```

In [12]:

```
n_time_NyAl = len(NyAl_sonde_dict['launch_time'])
time_idx = np.full(n_time_NyAl, np.nan)
for idx in range(n_time_NyAl):
    if np.any(np.abs(record_start_time - NyAl_sonde_dict['launch_time'][idx]) <= time_th
reshold):
        time_idx[idx] = np.argmin(np.abs(record_start_time - NyAl_sonde_dict['launch_tim
e'][idx]))
time_idx = time_idx.astype(np.int32)
```

## Koordinaten filtern

In [13]:

```
coords_nyal = (78.924444, 11.928611)
```

In [14]:

```
#Für jeden IASI Pixel (along und across track )
#<-> 2 for loops: berechne Distanz mit geopy Functions
n_along = len(IASI_DS.along_track)
n_across = len(IASI_DS.across_track)
distance_iasi_nyal = np.full((n_along, n_across), np.nan)
IASI_lon = IASI_DS.lon.values
IASI_lat = IASI_DS.lat.values
for j in range(n_across):
    if j%20 == 0: print(j)
    for i in range(n_along):
        if np.abs(IASI_lat[i,j] <= 90):
            distance_iasi_nyal[i,j] = geodesic(coords_nyal, (IASI_lat[i,j], IASI_lon[i,j]
)).km
        else:
            distance_iasi_nyal[i,j] = 999999.99

IASI_DS['distance_iasi_nyal'] = xarray.DataArray(distance_iasi_nyal, dims=['along_track',
'across_track'])
```

0  
20  
40  
60  
80  
100

In [16]:

```
#NyAlesund from rh to IWP

# constants:
R_d = 287.04    # gas constant of dry air, in J kg^-1 K^-1
R_v = 461.5     # gas constant of water vapour, in J kg^-1 K^-1
M_dv = R_d / R_v # molar mass ratio , in ()
e_0 = 611       # saturation water vapour pressure at freezing point (273.15 K), in Pa
T0 = 273.15     # freezing temperature, in K
g = 9.80665     # gravitation acceleration, in m s^-2

def e_sat(temp):

    """
    Calculates the saturation pressure over water after Goff and Gratch (1946).
    It is the most accurate that you can get for a temperture range from -90°C to +80°C.
    Source: Smithsonian Tables 1984, after Goff and Gratch 1946
    http://cires.colorado.edu/~voemel/vp.html
    http://hurri.kean.edu/~yoh/calculations/satvap/satvap.html
    e_sat_gg_water in Pa.
    Parameters:
    -----
    temp : array of floats
    Array of temperature (in K).
    """

    e_sat_gg_water = 100 * 1013.246 * 10**(-7.90298*(373.16/temp-1) + 5.02808*np.log10(
        373.16/temp) - 1.3816e-7*(10**(11.344*(1-temp/373.16))-1) + 8.1328e-3 * (10*
        *(-3.49149*(373.16/temp-1))-1))

    return e_sat_gg_water

#e_sat(NyAl_temp)

def convert_rh_to_spechum(
    temp,
```

```

pres,
relhum):

"""
Convert array of relative humidity (between 0 and 1) to specific humidity
in kg kg-1.

Saturation water vapour pressure computation is based on: see e_sat(temp).

Parameters:
-----
temp : array of floats
      Array of temperature (in K).
pres : array of floats
      Array of pressure (in Pa).
relhum : array of floats
      Array of relative humidity (between 0 and 1).
"""

e_sat_water = e_sat(temp)

e = e_sat_water * relhum
q = M_dv * e / (e*(M_dv - 1) + pres)

return q

```

In [17]:

```
n_time_ps = PS_sonde_dict['launch_time'].shape[0]
```

In [18]:

```

#IASI_T zu radiosonden(PS)-pixel-selektieren

n_time_ps = len(PS_sonde_dict['launch_time'])

distance_iasi_ps = np.full((n_along, n_across), 999999.99)
record_start_time = IASI_DS.record_start_time.values
which_PS_sonde = np.full((n_along, n_across), np.nan)
for i in range(n_along):
    if i%1000 == 0: print(i)
    # find Polarstern radiosonde launch that has temporally closest to IASI along track scan
    (pixel):
    launch_time_dif = np.abs(PS_sonde_dict['launch_time'] - record_start_time[i])
    idx_ps_time = np.argmin(launch_time_dif)

    if np.abs(PS_sonde_dict['launch_time'][idx_ps_time] - record_start_time[i]) <= 3600:
        # which_PS_sonde[i] = idx_ps_time
        for j in range(n_across):

            if np.abs(IASI_lat[i,j] <= 90):
                disdis = geodesic((PS_sonde_dict['lat'][idx_ps_time], PS_sonde_dict['lat'][idx_ps_time]),
                (IASI_lat[i,j], IASI_lon[i,j])).km
                if disdis < 50:
                    which_PS_sonde[i,j] = idx_ps_time
                    distance_iasi_ps[i,j] = disdis

IASI_DS['distance_iasi_ps'] = xarray.DataArray(distance_iasi_ps, dims=['along_track', 'across_track'])

# remove nans from which_PS_sonde:
which_PS_sonde = which_PS_sonde.astype(np.int32)
which_PS_sonde_nonnan = np.unique(which_PS_sonde[which_PS_sonde >= 0]) # explained below

# what do we have now:
# - distance_iasi_ps (n_along, n_across): distance of IASI to Polarstern for each IASI pixel
  (value is only non-nan if that pixel is temporally within 3600 sec of a
  # Polarstern radiosonde launch AND if it is within 50 km of Polarstern)
# - which_PS_sonde_nonnan (varying dimension): this now indicates which Polarstern sondes

```

```

have IASI pixels that are within 3600 sec of a sonde launch and where IASI
# pixel is within 50 km of Polarstern

# Later, we want to know if there is a IASI pixel for a given Polarstern launch which is
close enough (i.e. < 50 km) and within
# 3600 sec of that sonde launch. So, we would like to have an array with the shape (n_son
des_ps,2) (or (n_time_ps,2)) that tells
# us the exact along track and across track coordinate of IASI that fulfills these condit
ions.
# So, we can now run through all Polarstern sondes again, and check, if the indicated alo
ng track coordinate has one or more IASI_DS['distance_iasi_ps'] < 50 km
iasi_pixels_for_nya = np.full((n_time_ps,2), 0)

ps_iasi_overlap_pixels = list()
for idx in range(n_time_ps):
    if idx in which_PS_sonde_nonnan: # then it's not a fill value and a IASI pixel with
time offset < 3600 sec exists for the current Polarstern sonde launch:

        # find lines where which_PS_sonde is equal to idx:
        ps_iasi_overlap_pixels.append(np.argwhere(which_PS_sonde == idx))

"""
ps_iasi_overlap_pixels must always be considered together with which_PS_sonde_nonnan:
Example: which_PS_sonde_nonnan[0] is 16: then Polarstern sonde number 16 of your array is
within temporal and spatial range of IASI overpasses
Then, ps_iasi_overlap_pixels[0] tells you which coordinates of IASI_DS overlaps with Pola
rstern: For example,
ps_iasi_overlap_pixels[0] can be

array([[372, 108],
       [372, 109],
       [372, 110],
       [372, 111],
       [373, 108],
       [373, 111]])

--> first column: along_track coordinate that fulfills our requirements ; second column:
across_track coordinate that fulfills requirements
--> 6 pixels of IASI fulfill our requirements in this case. You may now select the Polars
tern temperature profile via:

PS_sonde_dict['temp'][which_PS_sonde_nonnan[0], :];

and the IASI temperature profile(s) (dimensions: along_track, across_track, height):
"""

#n_height_iasi = len(IASI_DS.nlt)
#n_detected_pixels = len(ps_iasi_overlap_pixels[0])
#IASI_T = np.zeros((n_detected_pixels, n_height_iasi)) # here, the T prof
iles for the current Polarstern sonde are saved to
#for idx, ps_ol in enumerate(ps_iasi_overlap_pixels[0]):
#    IASI_T[idx,:] = IASI_DS.atmospheric_temperature[ps_ol[0], ps_ol[1],:]

##IASI_T might include many nans because not all pixels of IASI actually have a temperatu
re profile!
##You might now either average over the number of detected pixels (ignore nans):
#IASI_T_avg = np.nanmean(IASI_T, axis=0) # might produce warnings (Runtim
eWarning)

```

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```

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Out[18]:

"\nps\_iasi\_overlap\_pixels must always be considered together with which\_PS\_sonde\_nonnan:\nExample: which\_PS\_sonde\_nonnan[0] is 16: then Polarstern sonde number 16 of your array is within temporal and spatial range of IASI overpasses\nThen, ps\_iasi\_overlap\_pixels[0] tells you which coordinates of IASI\_DS overlaps with Polarstern: For example,\nps\_iasi\_overlap\_pixels[0] can be\n\narray([[372, 108],\n [372, 109],\n [372, 110],\n [372, 111],\n [373, 108],\n [373, 111]])\n\n--> first column: along\_track coordinate that fulfills our requirements ; second column: across\_track coordinate that fulfills requirements\n--> 6 pixels of IASI fulfill our requirements in this case. You may now select the Polarstern temperature profile via:\n\nPS\_sonde\_dict['temp'][which\_PS\_sonde\_nonnan[0], :]\n\nand the IASI temperature profile(s) (dimensions: along\_track, across\_track, height):\n"

In [19]:

```
#IASI_T zu radiosonden(NyAl)-pixel-selektieren

n_time_NyAl = len(NyAl_sonde_dict['launch_time'])

distance_iasi_NyAl = np.full((n_along, n_across), 999999.99)
record_start_time = IASI_DS.record_start_time.values
which_NyAl_sonde = np.full((n_along, n_across), np.nan)
for i in range(n_along):
    if i%1000 == 0: print(i)
    # find NyAlesund radiosonde launch that has temporally closest to IASI along track scan (pixel):
    launch_time_dif = np.abs(NyAl_sonde_dict['launch_time'] - record_start_time[i])
    idx_NyAl_time = np.argmin(launch_time_dif)

    if np.abs(NyAl_sonde_dict['launch_time'][idx_NyAl_time] - record_start_time[i]) <= 3600:
        # which_NyAl_sonde[i] = idx_NyAl_time
        for j in range(n_across):
            if np.abs(IASI_lat[i,j] <= 90):
                disdis = geodesic((NyAl_sonde_dict['lat'][idx_NyAl_time], NyAl_sonde_dict['lat'][idx_NyAl_time]), (IASI_lat[i,j], IASI_lon[i,j])).km
                if disdis < 50:
                    which_NyAl_sonde[i,j] = idx_NyAl_time
                    distance_iasi_NyAl[i,j] = disdis

IASI_DS['distance_iasi_NyAl'] = xarray.DataArray(distance_iasi_NyAl, dims=['along_track', 'across_track'])

# remove nans from which_NyAl_sonde:
which_NyAl_sonde = which_NyAl_sonde.astype(np.int32)
which_NyAl_sonde_nonnan = np.unique(which_NyAl_sonde[which_NyAl_sonde >= 0]) # explained below

# what do we have now:
# - distance_iasi_NyAl (n_along, n_across): distance of IASI to NyAl for each IASI pixel (value is only non-nan if that pixel is temporally within 3600 sec of a NyAl radiosonde launch AND if it is within 50 km of NyAl)
```

```

# - which_NyAl_sonde_nonnan (varying dimension): this now indicates which NyAl sondes have IASI pixels that are within 3600 sec of a sonde launch and where IASI
# pixel is within 50 km of NyAl

# Later, we want to know if there is a IASI pixel for a given NyAl launch which is close enough (i.e. < 50 km) and within
# 3600 sec of that sonde launch. So, we would like to have an array with the shape (n_sondes_NyAl,2) (or (n_time_ps,2)) that tells
# us the exact along track and across track coordinate of IASI that fulfills these conditions.
# So, we can now run through all NyAl sondes again, and check, if the indicated along track coordinate has one or more IASI_DS['distance_iasi_NyAl'] < 50 km
iasi_pixels_for_NyAl = np.full((n_time_ps,2), 0)

NyAl_iasi_overlap_pixels = list()
for idx in range(n_time_NyAl):
    if idx in which_NyAl_sonde_nonnan: # then it's not a fill value and a IASI pixel with time offset < 3600 sec exists for the current NyAl sonde launch:

        # find lines where which_NyAl_sonde is equal to idx:
        NyAl_iasi_overlap_pixels.append(np.argwhere(which_NyAl_sonde == idx))

"""
NyAl_iasi_overlap_pixels must always be considered together with which_PS_sonde_nonnan:
Example: which_PS_sonde_nonnan[0] is 16: then NyAl sonde number 16 of your array is within temporal and spatial range of IASI overpasses
Then, NyAl_iasi_overlap_pixels[0] tells you which coordinates of IASI_DS overlaps with NyAl: For example,
NyAl_iasi_overlap_pixels[0] can be

array([[372, 108],
       [372, 109],
       [372, 110],
       [372, 111],
       [373, 108],
       [373, 111]])

--> first column: along_track coordinate that fulfills our requirements ; second column: across_track coordinate that fulfills requirements
--> 6 pixels of IASI fulfill our requirements in this case. You may now select the NyAl temperature profile via:

NyAl_sonde_dict['temp'][which_NyAl_sonde_nonnan[0], :];

and the IASI temperature profile(s) (dimensions: along_track, across_track, height):
"""

#n_height_iasi = len(IASI_DS.nlt)
#n_detected_pixels = len(NyAl_iasi_overlap_pixels[0])
#IASI_T = np.zeros((n_detected_pixels, n_height_iasi)) # here, the T profiles for the current NyAl sonde are saved to
#for idx, NyAl_ol in enumerate(NyAl_iasi_overlap_pixels[0]):
#    IASI_T[idx,:] = IASI_DS.atmospheric_temperature[NyAl_ol[0], NyAl_ol[1],:]

##IASI_T might include many nans because not all pixels of IASI actually have a temperature profile!
##You might now either average over the number of detected pixels (ignore nans):
#IASI_T_avg = np.nanmean(IASI_T, axis=0) # might produce warnings (RuntimeWarning)

```

```

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```

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Out[19]:

```
"\nNyAl_iasi_overlap_pixels must always be considered together with which_PS_sonde_nonnan
:\nExample: which_PS_sonde_nonnan[0] is 16: then NyAl sonde number 16 of your array is wi
thin temporal and spatial range of IASI overpasses\nThen, NyAl_iasi_overlap_pixels[0] tel
ls you which coordinates of IASI_DS overlaps with NyAl: For example,\nNyAl_iasi_overlap_p
ixels[0] can be\n\narray([[372, 108],\n      [372, 109],\n      [372, 110],\n      [372,
111],\n      [373, 108],\n      [373, 111]])\n\n--> first column: along_track coordinate
that fulfills our requirements ; second column: across_track coordinate that fulfills req
uirements\n--> 6 pixels of IASI fulfill our requirements in this case. You may now select
the NyAl temperature profile via:\n\nNyAl_sonde_dict['temp'][which_NyAl_sonde_nonnan[0],
:];\n\nand the IASI temperature profile(s) (dimensions: along_track, across_track, height
):\n"
```

In [20]:

```
IASI_ST = IASI_DS.surface_temperature.values
IASI_SP= IASI_DS.surface_pressure.values
```

In [22]:

```
# height grid auf eine Größe gebracht werden / interpolieren darauf
```

```
NyAl_T = NyAl_sonde_dict['temp']
```

```
NyAl_alt = NyAl_sonde_dict['height']
```

```
NyAl_q = convert_rh_to_spechum(NyAl_sonde_dict['temp'], NyAl_sonde_dict['pres'], NyAl_so
nde_dict['rh'])
```

```
IASI_T = IASI_DS.atmospheric_temperature.values
IASI_q = IASI_DS.atmospheric_water_vapor.values
```

In [24]:

```
# for schleife für unterschiedliche shapes IASI_T.shape=(2980, 120, 101) along, across, v
ertical IASI_DS.pressure_levels_temp.shape = (101,)
```

```
IASI_alt = np.zeros(IASI_T.shape)
IASI_DS_pressure_levels_temp = IASI_DS.pressure_levels_temp.values
for i in range(n_along):
    for j in range(n_across):
        IASI_alt[i,j,:] = -(R_d / g) * (IASI_T[i,j,:]*np.log(IASI_DS_pressure_levels_tem
p) - IASI_ST[i,j]*np.log(IASI_SP[i,j]))
```

In [25]:

```
#0 0
#1 1
#2 4
#3 5
#Die 0,1,4,5 hatten die Überschneidenden along und across wie IASI
```

In [26]:

```
n_sondes_PS= len(which_PS_sonde_nonnan)
```

```

n_height_PS = PS_sonde_dict['temp'].shape[1]

PS_T = np.zeros((n_sondes_PS,n_height_PS))
PS_P = np.zeros((n_sondes_PS,n_height_PS))
PS_q = np.zeros((n_sondes_PS,n_height_PS))

for i, which_PS in enumerate(which_PS_sonde_nonnan):
    # print(i,which_PS)
    PS_T[i,:] = PS_sonde_dict['temp'][which_PS,:]
    PS_P[i,:] = PS_sonde_dict['pres'][which_PS,:]
    PS_q[i,:] = PS_sonde_dict['q'][which_PS,:]

n_sondes_NyAl = len(which_NyAl_sonde_nonnan)
n_height_NyAl = NyAl_sonde_dict['temp'].shape[1]

NyAl_T = np.zeros((n_sondes_NyAl,n_height_NyAl))
NyAl_P = np.zeros((n_sondes_NyAl,n_height_NyAl))
NyAl_q = np.zeros((n_sondes_NyAl,n_height_NyAl))

for i, which_NyAl in enumerate(which_NyAl_sonde_nonnan):
    # print(i,which_NyAl)
    NyAl_T[i,:] = NyAl_sonde_dict['temp'][which_NyAl,:]
    NyAl_P[i,:] = NyAl_sonde_dict['pres'][which_NyAl,:]
    NyAl_q[i,:] = NyAl_sonde_dict['rh'][which_NyAl,:]

```



In [27]:

```
len(ps_iasi_overlap_pixels) #IASI überlappt mit PS
```

```

n_height_IASI = len(IASI_DS_pressure_levels_temp)
IASI_T_PS = np.zeros((n_sondes_PS,n_height_IASI))
IASI_q_PS = np.zeros((n_sondes_PS,n_height_IASI))
for idx, ps_iasi_overlap in enumerate(ps_iasi_overlap_pixels):
    along_chosen = ps_iasi_overlap[:,0]
    across_chosen = ps_iasi_overlap[:,1]
    IASI_T_PS[idx,:] = np.nanmean(IASI_T[along_chosen, across_chosen,:], axis=0)
    IASI_q_PS[idx,:] = np.nanmean(IASI_q[along_chosen, across_chosen,:], axis=0)

```

```

<ipython-input-27-636a800aa1f5>:9: RuntimeWarning: Mean of empty slice
    IASI_T_PS[idx,:] = np.nanmean(IASI_T[along_chosen, across_chosen,:], axis=0)
<ipython-input-27-636a800aa1f5>:10: RuntimeWarning: Mean of empty slice
    IASI_q_PS[idx,:] = np.nanmean(IASI_q[along_chosen, across_chosen,:], axis=0)

```

In [28]:

```
len(NyAl_iasi_overlap_pixels) #IASI überlappt mit NyAl
```

```

n_height_IASI = len(IASI_DS_pressure_levels_temp)
IASI_T_NyAl = np.zeros((n_sondes_NyAl,n_height_IASI))
IASI_q_NyAl = np.zeros((n_sondes_NyAl,n_height_IASI))
for idx, NyAl_iasi_overlap in enumerate(NyAl_iasi_overlap_pixels):
    along_chosen = NyAl_iasi_overlap[:,0]
    across_chosen = NyAl_iasi_overlap[:,1]
    IASI_T_NyAl[idx,:] = np.nanmean(IASI_T[along_chosen, across_chosen,:], axis=0)
    IASI_q_NyAl[idx,:] = np.nanmean(IASI_q[along_chosen, across_chosen,:], axis=0)

```

```

<ipython-input-28-55e26a30ab36>:9: RuntimeWarning: Mean of empty slice
    IASI_T_NyAl[idx,:] = np.nanmean(IASI_T[along_chosen, across_chosen,:], axis=0)
<ipython-input-28-55e26a30ab36>:10: RuntimeWarning: Mean of empty slice
    IASI_q_NyAl[idx,:] = np.nanmean(IASI_q[along_chosen, across_chosen,:], axis=0)

```

In [29]:

```

#interpolation über druck koordinaten
IASI_DS_pressure_levels_humidity = IASI_DS.pressure_levels_humidity.values
IASI_T_PS_grid = np.zeros((n_sondes_PS,n_height_PS))
IASI_q_PS_grid = np.zeros((n_sondes_PS,n_height_PS))

for idx in range(n_sondes_PS):
    IASI_T_PS_grid[idx,:] = np.interp(PS_P[idx,:],IASI_DS_pressure_levels_temp,IASI_T_PS[
idx,:])

```



```
IASI_q_PS_grid[idx,:] = np.interp(PS_q[idx,:],IASI_DS_pressure_levels_humidity,IASI_q_PS[idx,:])
```

In [30]:

```
#interpolation über druck koordinaten
IASI_DS_pressure_levels_humidity = IASI_DS.pressure_levels_humidity.values
IASI_T_NyAl_grid = np.zeros((n_sondes_NyAl,n_height_NyAl))
IASI_q_NyAl_grid = np.zeros((n_sondes_NyAl,n_height_NyAl))

for idx in range(n_sondes_NyAl):
    IASI_T_NyAl_grid[idx,:] = np.interp(NyAl_P[idx,:],IASI_DS_pressure_levels_temp,IASI_T_NyAl[idx,:])
    IASI_q_NyAl_grid[idx,:] = np.interp(NyAl_q[idx,:],IASI_DS_pressure_levels_humidity,IASI_q_NyAl[idx,:])
```

## RMSE

$$\bar{s}^2 = \frac{1}{n} * [(T_{Sonde} - T_{IASI})^2 + (x_{Sonde} - T_{IASI})^2 + .. (x_{Sonde_n} - T_{IASI})^2]$$

In [31]:

```
# Polarstern und IASI

def RMSE(X_sonde,X_IASI):

    RMSE_X = np.sqrt( np.nanmean((X_sonde - X_IASI)**2, axis=0) ) # for RMSE PROFILE, we average over time (which is axis 0)

    return RMSE_X

RMSE_T_IASI_PS = RMSE(IASI_T_PS_grid, PS_T)
RMSE_pres = np.nanmean(PS_P, axis=0) # zugehöriger Druck
RMSE_q_IASI_PS = RMSE(IASI_q_PS_grid,PS_q)

RMSE_T_IASI_NyAl = RMSE(IASI_T_NyAl_grid, NyAl_T)
RMSE_pres = np.nanmean(NyAl_P, axis=0) # zugehöriger Druck
RMSE_q_IASI_NyAl = RMSE(IASI_q_NyAl_grid,NyAl_q)
```

## Plot

In [32]:

```
fig, (ax1, ax2) = plt.subplots(1, 2, constrained_layout=True, sharey=True)
ax1.plot(RMSE_T_IASI_PS, RMSE_pres)
ax1.set_title('xxx')
ax1.set_xlabel('RMSE T')
ax1.set_ylabel('pressure level [Pa]')

ax2.plot(RMSE_q_IASI_PS, RMSE_pres)
ax2.set_xlabel('q')
ax2.set_title('xxx')

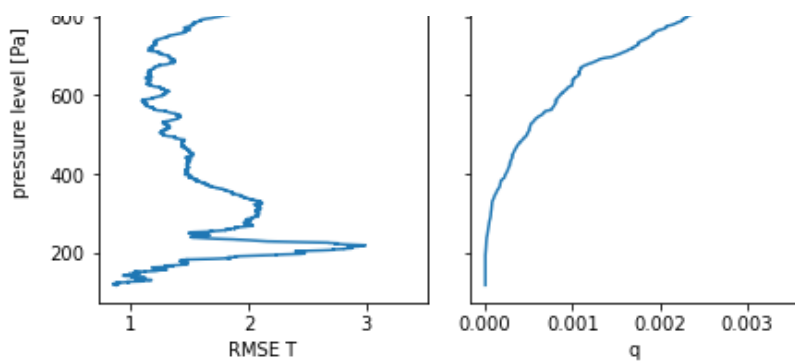
fig.suptitle('RMSE Comparison of IASI and Radiosonde Polarstern', fontsize=16)
```

Out[32]:

Text(0.5, 0.98, 'RMSE Comparison of IASI and Radiosonde Polarstern')

### RMSE Comparison of IASI and Radiosonde Polarstern





In [33]:

```
fig, (ax1, ax2) = plt.subplots(1, 2, constrained_layout=True, sharey=True)
ax1.plot(RMSE_T_IASI_NyAl, RMSE_pres)
ax1.set_title('RMSE Profil')
ax1.set_xlabel('RMSE T')
ax1.set_ylabel('pressure level [Pa]')

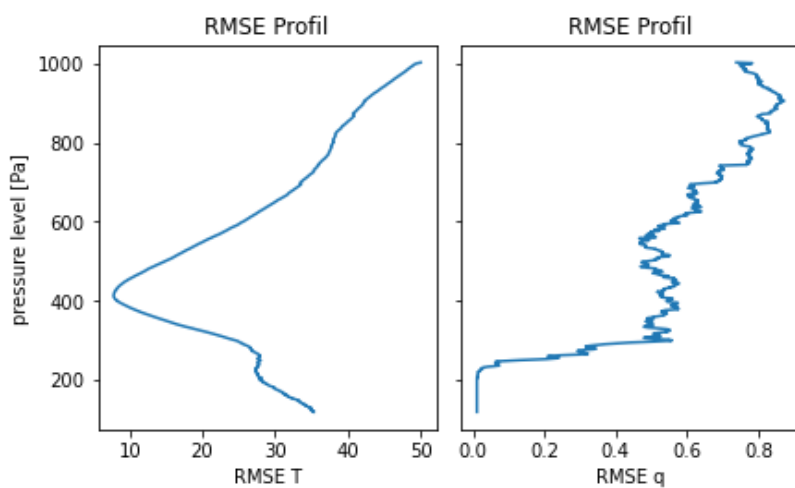
ax2.plot(RMSE_q_IASI_NyAl, RMSE_pres)
ax2.set_xlabel('RMSE q')
ax2.set_title('RMSE Profil')

fig.suptitle('RMSE Comparison of IASI and Radiosonde Polarstern', fontsize=16)
```

Out[33]:

Text(0.5, 0.98, 'RMSE Comparison of IASI and Radiosonde Polarstern')

## RMSE Comparison of IASI and Radiosonde Polarstern



In [ ]: