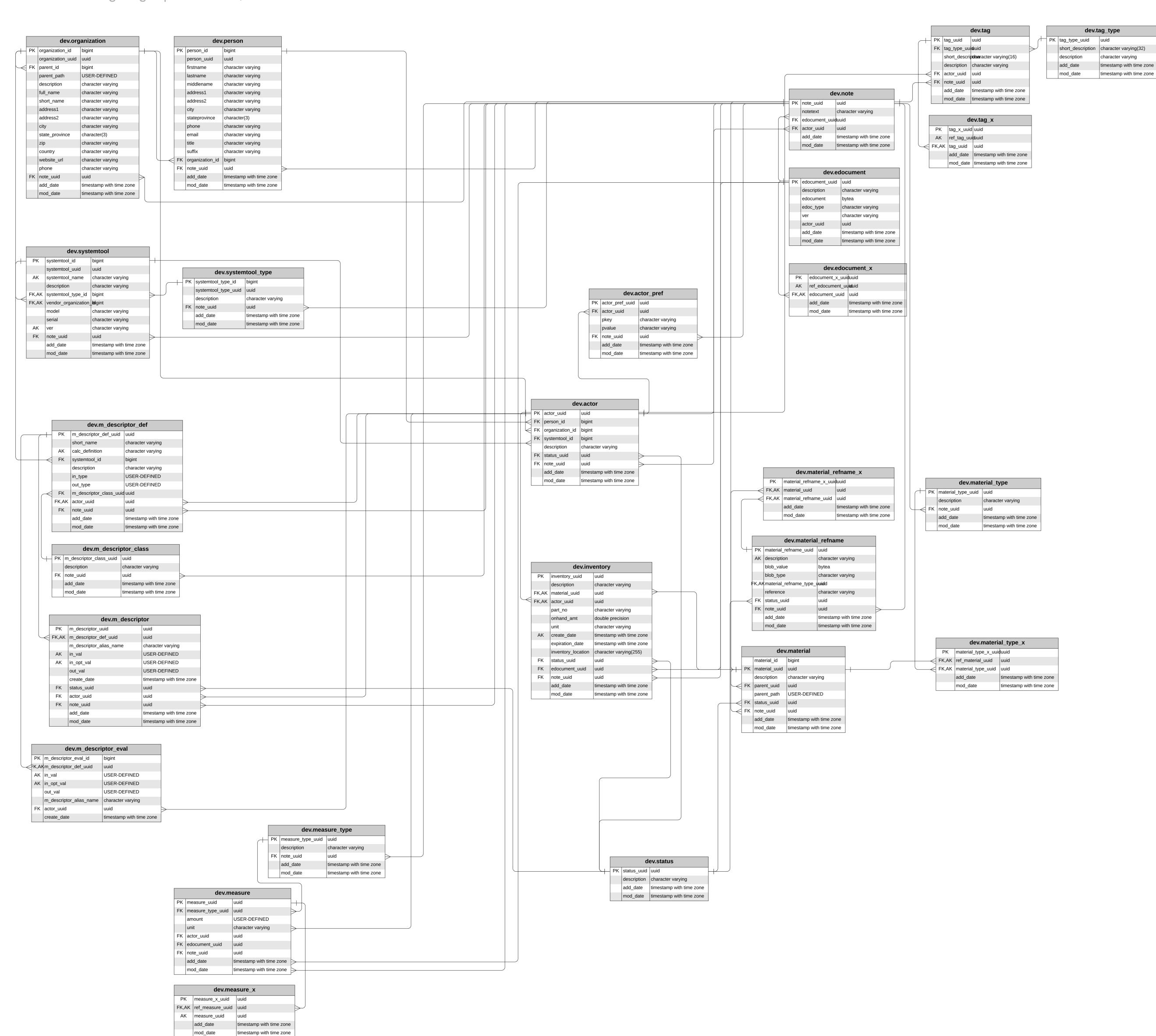
ESCALATE v3 Data Model

Haverford College - gc | March 25, 2020



dev.load_hc_inventory

reagent character varying(255)
part_no character varying(255)
amount double precision
units character varying(255)
update_date timestamp with time zone
create_date updated_by in_stock real

reagent character varying(255)
part_no character varying(255)
amount double precision
units character varying(255)
update_date timestamp with time zone
create_date timestamp with time zone

remaining_stockal

dev.load_perov_mol_image

filename character varying integer
_image bytea

_raw_inchikey character varying(255) _raw_smiles character varying(255) _raw_molweight double precision _raw_smiles_standard character varying(255 _raw_standard_molweight double precision _prototype_ecpf4_256_6 character varying _feat_atomcount_c smallint _feat_atomcount_n smallint _feat_avgpol double precision _feat_molpol double precision _feat_refractivity double precision _feat_aliphaticringcount _feat_aromaticringcount smallint _feat_aliphaticatomcount _feat_aromaticatomcount _feat_bondcount _feat_carboaliphaticringcount _feat_carboaromaticringcount _feat_carboringcount _feat_chainatomcount _feat_chiralcentercount _feat_ringatomcount _feat_smallestringsize _feat_largestringsize _feat_heteroaliphaticringcount _feat_heteroaromaticringcount _feat_rotatablebondcount smallint _feat_balabanindex double precision _feat_cyclomaticnumber smallint _feat_hyperwienerindex smallint _feat_wienerindex smallint _feat_wienerpolarity _feat_minimalprojectionarea double precision _feat_maximalprojectionarea _feat_minimalprojectionradius double precision _feat_maximalprojectionradius double precision _feat_lengthperpendiculartotheminarea | double precision _feat_lengthperpendiculartothemaxarea | double precision _feat_vanderwaalssurfacearea double precision _feat_asa double precision _feat_asa+ double precision _feat_asadouble precision _feat_asa_h _feat_asa_p double precision _feat_polarsurfacearea double precision _feat_acceptorcount smallint _feat_accsitecount smallint _feat_donsitecount _feat_fr_nh2 _feat_fr_nh1 _feat_fr_nh0 _feat_fr_quatn _feat_fr_arn _feat_fr_ar_nh _feat_fr_imine _feat_fr_amidine _feat_fr_dihydropyridine _feat_fr_guanido _feat_fr_piperdine smallint _feat_fr_piperzine _feat_fr_pyridine _feat_maximalprojectionsize _feat_minimalprojectionsize double precision

_feat_molsurfaceareavdwp

_feat_molsurfaceareaasap

_feat_protpolarsurfacearea

_feat_msareavdwp

_feat_msareaasap

_feat_hacceptorcount

_feat_hdonorcount

_calc_chrg_per_vol

_calc_chrg_per_asa

_feat_charge_cnt

_feat_protpsa

double precision

smallint

smallint

smallint

dev.load_perov_desc