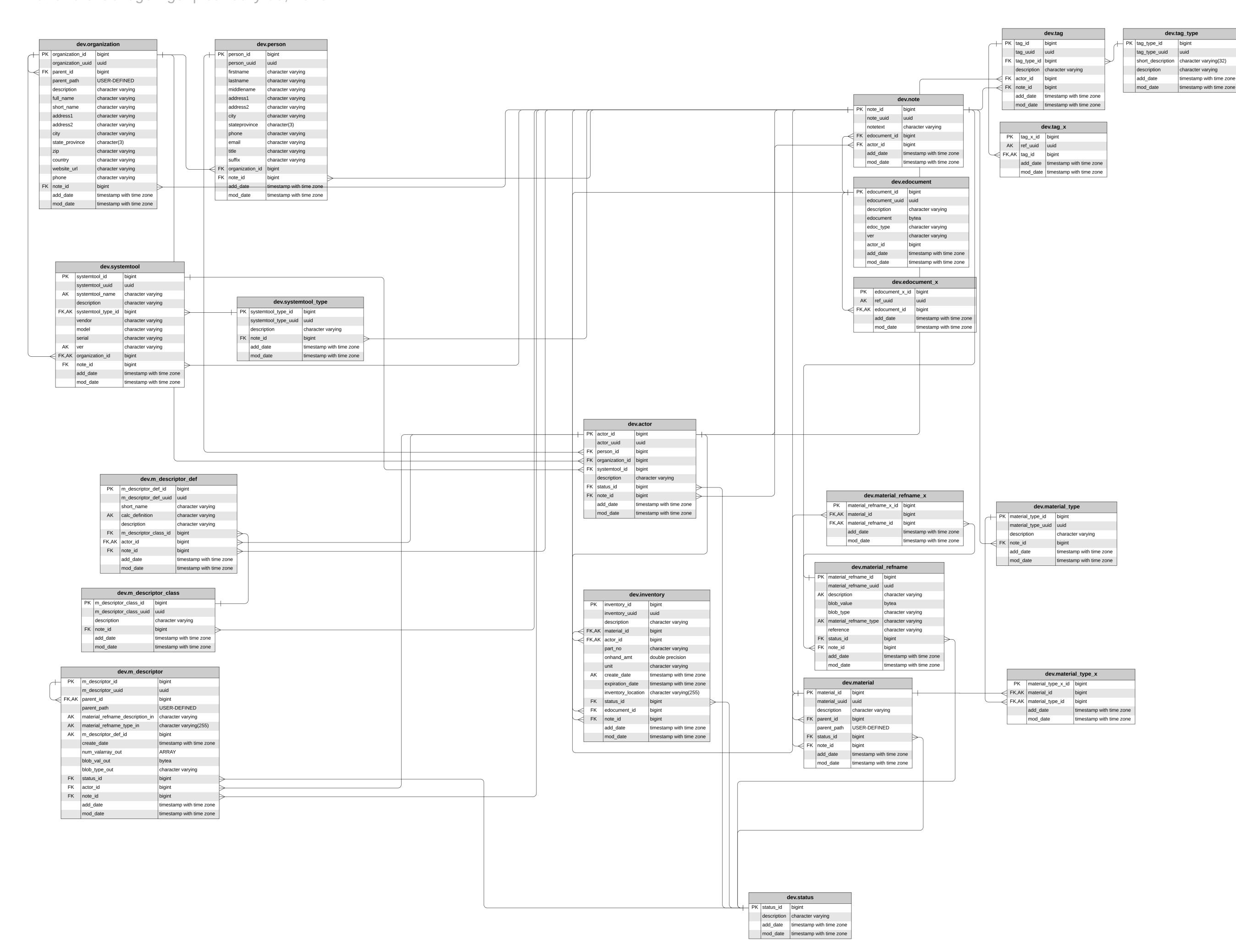
## **ESCALATE v3 Data Model**

Haverford College - gc | January 30, 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	timestamp with time zone

dev.load_lbl_inventory		
reagent	ch	aracter varying(255)
part_no	ch	aracter varying(255)
amount	do	ouble precision
units	ch	aracter varying(255)
update_	_date tin	nestamp with time zone
create_	date tin	nestamp with time zone

dev.load_perov_desc_def		
short_name character varying(25		
calc_definition   character varying(25		
description character varying(25		
systemtool_nameharacter varying(25		
systemtool_ver character varying(25		

dev.load_perov_mol_image		
	filename	character varying
	fileno	integer
	_image	bytea

	de	v.load_chem_i	nventory	
	ChemicalNam	ne	character var	ying(25
	ChemicalAbb	reviation	character var	ying(25
	MolecularWei	ght	character var	ying(25
	Density		character var	ying(25
	InChI		character var	ying(25
	InChlKey		character var	ying(25
	ChemicalCategory		character var	ying(25
	CanonicalSMILES		character var	ying(25
	MolecularFormula		character var	ying(25
	PubChemID		character var	ying(25
	CatalogDescr		character var	ying(25
	Synonyms		character var	ying(25
	CatalogNo		character var	ying(25
	Sigma-Aldrich URL		character var	ying(25
	PrimaryInformationSource		character var	ying(25
	StandardizedSMILES		character var	ying(25
dev.load_hc_inventory				
	reagent	character varying(255)		
	part_no	character var	ying(255)	
	I	l	_	1

_prototype_ecpf4_256_6	character varying(256)
_feat_atomcount_c	double precision
_feat_atomcount_n	double precision
_feat_avgpol	double precision
_feat_molpol	double precision
_feat_refractivity	double precision
feat_aliphaticringcount	double precision
feat aromaticringcount	double precision
feat aliphaticatomcount	
	double precision
feat_aromaticatomcount	double precision
_feat_bondcount	double precision
_feat_carboaliphaticringcount	double precision
_feat_carboaromaticringcount	double precision
_feat_carboringcount	double precision
_feat_chainatomcount	double precision
_feat_chiralcentercount	double precision
feat ringatomcount	double precision
feat smallestringsize	double precision
feat largestringsize	double precision
feat_heteroaliphaticringcount	double precision
	-
_feat_heteroaromaticringcount	double precision
feat_rotatablebondcount	double precision
_feat_balabanindex	double precision
_feat_cyclomaticnumber	double precision
_feat_hyperwienerindex	double precision
_feat_wienerindex	double precision
_feat_wienerpolarity	double precision
_feat_minimalprojectionarea	double precision
	double precision
feat_minimalprojectionradius	double precision
feat maximalprojectionradius	double precision
feat_lengthperpendiculartotheminarea	-
	double precision
feat_lengthperpendiculartothemaxarea	double precision
_feat_vanderwaalsvolume	double precision
_feat_vanderwaalssurfacearea	double precision
_feat_asa	double precision
_feat_asa+	double precision
_feat_asa-	double precision
_feat_asa_h	double precision
_feat_asa_p	double precision
 feat_polarsurfacearea	double precision
feat acceptorcount	double precision
feat accsitecount	double precision
	-
_feat_donorcount	double precision
_feat_donsitecount	double precision
_feat_fr_nh2	double precision
_feat_fr_nh1	double precision
_feat_fr_nh0	double precision
_feat_fr_quatn	double precision
_feat_fr_arn	double precision
_feat_fr_ar_nh	double precision
_feat_fr_imine	double precision
_feat_fr_amidine	double precision
 feat_fr_dihydropyridine	double precision
feat_fr_guanido	double precision
feat fr piperdine	
	double precision
_feat_fr_piperzine	double precision
_feat_fr_pyridine	double precision
_feat_maximalprojectionsize	double precision
_feat_minimalprojectionsize	double precision
_feat_molsurfaceareavdwp	double precision
_feat_msareavdwp	double precision
_feat_molsurfaceareaasap	double precision
 feat_msareaasap	double precision
feat_protpolarsurfacearea	double precision
feat protpsa	double precision
feat hacceptorcount	double precision
feat hdonorcount	double precision
_reat_naonorcount	aouble precision

dev.load\_perov\_desc

character varying(255)

character varying(255)

character varying(256)

double precision

double precision

character varying(255)

\_raw\_inchikey

\_raw\_smiles

\_raw\_molweight

\_raw\_smiles\_standard

\_raw\_standard\_molweight

\_prototype\_ecpf4\_256\_6