

Vacancy Engineering Activates π -*d* Conjugated Coordination Polymers for CO₂ Reduction: An Ab Initio Study

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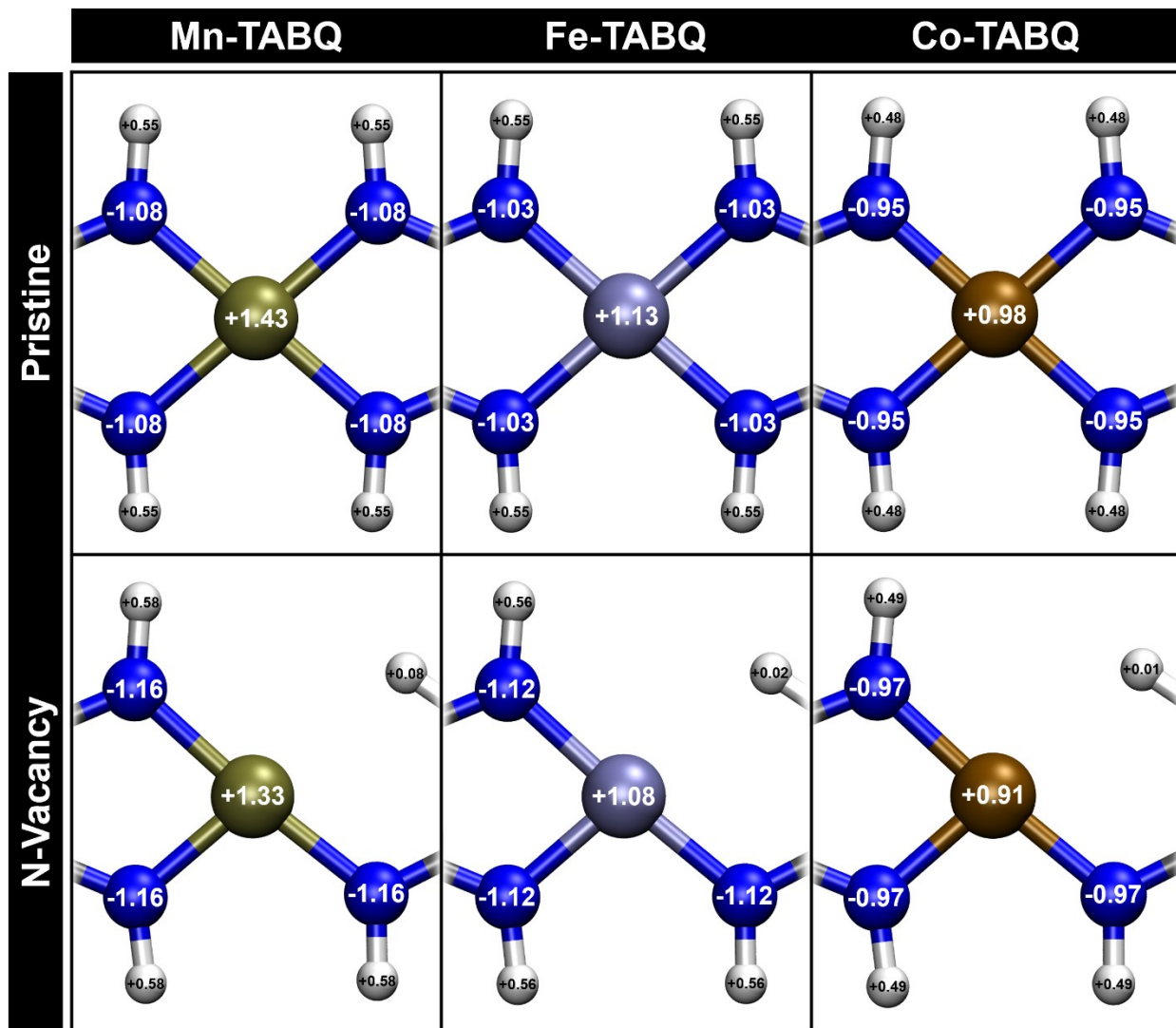


Figure S1. Calculated Bader charge distributions for the pristine and nitrogen-vacancy-modified systems.

Atomic coordinates of Mn-TABQ:

H	8.416000	0.959000	10.001000
H	3.335000	0.949000	9.999000
C	4.636000	2.524000	9.999000
C	7.107000	3.953000	10.000000
C	4.634000	3.948000	9.999000
C	7.109000	2.526000	10.000000
C	5.876000	1.744000	9.999000
C	5.869000	4.732000	10.000000
N	3.406000	1.979000	9.999000
N	8.337000	4.496000	10.001000
N	3.402000	4.491000	9.999000
N	8.344000	1.988000	10.001000
O	5.875000	0.481000	9.999000
O	5.865000	5.995000	10.001000
H	8.408000	5.526000	10.001000
H	3.332000	5.520000	9.999000
Mn	1.957000	3.234000	9.999000
H	16.230000	0.948000	9.999000
H	11.160000	0.959000	10.001000
C	12.461000	2.527000	10.001000
C	14.934000	3.951000	10.000000
C	12.464000	3.955000	10.001000
C	14.931000	2.520000	10.000000
C	13.694000	1.741000	10.001000
C	13.703000	4.735000	10.000000
N	11.229000	1.988000	10.002000
N	16.166000	4.489000	9.999000
N	11.236000	4.499000	10.001000
N	16.160000	1.978000	9.999000
O	13.689000	0.478000	10.000000
O	13.704000	5.998000	10.000000
H	16.236000	5.518000	9.999000
H	11.167000	5.529000	10.001000
Mn	9.784000	3.244000	10.001000
H	24.056000	0.957000	10.000000
H	18.988001	0.949000	9.999000
C	20.289000	2.520000	9.999000
C	22.757000	3.955000	10.001000

C	20.287001	3.952000	10.000000
C	22.757999	2.527000	10.001000
C	21.524000	1.741000	10.000000
C	21.518000	4.735000	10.000000
N	19.059000	1.978000	9.999000
N	23.986000	4.498000	10.001000
N	19.056000	4.490000	9.999000
N	23.989000	1.986000	10.001000
O	21.531000	0.478000	9.999000
O	21.518999	5.999000	10.000000
H	24.056000	5.527000	10.001000
H	18.986000	5.519000	9.999000
Mn	17.611000	3.232000	9.998000
H	31.885000	0.949000	10.000000
H	26.804001	0.959000	10.002000
C	28.110001	2.527000	10.001000
C	30.589001	3.950000	9.999000
C	28.113001	3.952000	10.001000
C	30.586000	2.526000	10.000000
C	29.344000	1.746000	10.001000
C	29.354000	4.732000	10.000000
N	26.875999	1.988000	10.002000
N	31.823000	4.492000	9.998000
N	26.884001	4.497000	10.002000
N	31.815001	1.979000	9.999000
O	29.344000	0.485000	10.001000
O	29.355000	5.994000	9.999000
H	31.893999	5.520000	9.998000
H	26.813999	5.527000	10.002000
Mn	25.436001	3.243000	10.001000
H	12.319000	7.564000	9.999000
H	7.252000	7.562000	10.001000
C	8.554000	9.128000	10.000000
C	11.014000	10.557000	10.000000
C	8.554000	10.556000	10.000000
C	11.014000	9.129000	9.999000
C	9.784000	8.344000	10.000000
C	9.784000	11.340000	10.000000
N	7.318000	8.590000	10.001000
N	12.251000	11.094000	10.000000

N	7.317000	11.093000	10.001000
N	12.250000	8.592000	9.999000
O	9.784000	7.077000	10.001000
O	9.784000	12.608000	10.000000
H	12.318000	12.122000	10.000000
H	7.250000	12.120000	10.000000
Mn	5.876000	9.840000	10.001000
H	20.139000	7.555000	10.000000
H	15.085000	7.557000	10.001000
C	16.375999	9.126000	10.001000
C	18.844999	10.557000	10.000000
C	16.377001	10.561000	10.000000
C	18.844999	9.123000	10.000000
C	17.611000	8.343000	10.000000
C	17.611000	11.340000	10.001000
N	15.149000	8.586000	10.001000
N	20.073000	11.097000	10.000000
N	15.149000	11.101000	10.000000
N	20.073000	8.584000	10.000000
O	17.608999	7.078000	10.000000
O	17.614000	12.606000	10.001000
H	20.136999	12.126000	10.000000
H	15.085000	12.130000	10.000000
Mn	13.692000	9.844000	10.000000
H	27.974001	7.564000	10.000000
H	22.902000	7.564000	10.000000
C	24.205999	9.129000	10.001000
C	26.667999	10.555000	10.000000
C	24.205000	10.557000	10.001000
C	26.667999	9.128000	10.000000
C	25.437000	8.345000	10.000000
C	25.436001	11.340000	10.000000
N	22.971001	8.592000	10.000000
N	27.903000	11.092000	10.000000
N	22.968000	11.092000	10.001000
N	27.905001	8.592000	10.000000
O	25.436001	7.077000	10.000000
O	25.438000	12.607000	9.999000
H	27.972000	12.120000	9.999000
H	22.896999	12.120000	10.001000

Mn	21.528999	9.841000	10.000000
H	35.785000	7.554000	10.000000
H	30.733999	7.556000	10.000000
C	32.028999	9.124000	9.999000
C	34.500000	10.560000	10.000000
C	32.030998	10.557000	9.999000
C	34.498001	9.125000	10.000000
C	33.262001	8.344000	10.000000
C	33.265999	11.340000	10.000000
N	30.799000	8.585000	10.000000
N	35.729000	11.098000	10.001000
N	30.804001	11.099000	9.999000
N	35.723999	8.583000	10.001000
O	33.264000	7.078000	10.000000
O	33.262001	12.605000	10.000000
H	35.794998	12.127000	10.001000
H	30.740999	12.128000	9.999000
Mn	29.346001	9.842000	10.000000
H	16.242001	14.166000	10.001000
H	11.161000	14.156000	9.999000
C	12.462000	15.731000	9.999000
C	14.933000	17.160000	10.000000
C	12.460000	17.155001	9.999000
C	14.935000	15.733000	10.000000
C	13.702000	14.951000	9.999000
C	13.695000	17.938999	10.000000
N	11.232000	15.186000	9.999000
N	16.163000	17.702999	10.001000
N	11.228000	17.698000	9.999000
N	16.170000	15.195000	10.001000
O	13.701000	13.688000	9.999000
O	13.691000	19.202000	10.001000
H	16.233999	18.733000	10.001000
H	11.158000	18.726999	9.999000
Mn	9.783000	16.441000	9.999000
H	24.056000	14.155000	9.999000
H	18.986000	14.166000	10.001000
C	20.287001	15.734000	10.001000
C	22.760000	17.158001	10.000000
C	20.290001	17.162001	10.001000

C	22.757000	15.727000	10.000000
C	21.520000	14.948000	10.001000
C	21.528999	17.941999	10.000000
N	19.055000	15.195000	10.002000
N	23.992001	17.695999	9.999000
N	19.062000	17.705999	10.001000
N	23.986000	15.185000	9.999000
O	21.514999	13.685000	10.000000
O	21.530001	19.205000	10.000000
H	24.062000	18.725000	9.999000
H	18.993000	18.736000	10.001000
Mn	17.610001	16.451000	10.001000
H	31.882000	14.164000	10.000000
H	26.813999	14.156000	9.999000
C	28.115000	15.727000	9.999000
C	30.583000	17.162001	10.001000
C	28.113001	17.159000	10.000000
C	30.584000	15.734000	10.001000
C	29.350000	14.948000	10.000000
C	29.344000	17.941999	10.000000
N	26.885000	15.185000	9.999000
N	31.812000	17.705000	10.001000
N	26.882000	17.697001	9.999000
N	31.815001	15.193000	10.001000
O	29.357000	13.685000	9.999000
O	29.344999	19.205999	10.000000
H	31.882000	18.733999	10.001000
H	26.812000	18.726000	9.999000
Mn	25.437000	16.438999	9.998000
H	39.710999	14.156000	10.000000
H	34.630001	14.166000	10.002000
C	35.936001	15.734000	10.001000
C	38.415001	17.157000	9.999000
C	35.938999	17.159000	10.001000
C	38.411999	15.733000	10.000000
C	37.169998	14.953000	10.001000
C	37.180000	17.938999	10.000000
N	34.702000	15.195000	10.002000
N	39.648998	17.698999	9.998000
N	34.709999	17.704000	10.002000

N	39.640999	15.186000	9.999000
O	37.169998	13.692000	10.001000
O	37.181000	19.201000	9.999000
H	39.720001	18.726999	9.998000
H	34.639999	18.733999	10.002000
Mn	33.262001	16.450001	10.001000
H	20.145000	20.771000	9.999000
H	15.078000	20.768999	10.001000
C	16.379999	22.334999	10.000000
C	18.840000	23.764000	10.000000
C	16.379999	23.763000	10.000000
C	18.840000	22.336000	9.999000
C	17.610001	21.551001	10.000000
C	17.610001	24.547001	10.000000
N	15.144000	21.797001	10.001000
N	20.077000	24.301001	10.000000
N	15.143000	24.299999	10.001000
N	20.076000	21.799000	9.999000
O	17.610001	20.284000	10.001000
O	17.610001	25.815001	10.000000
H	20.143999	25.329000	10.000000
H	15.076000	25.327000	10.000000
Mn	13.702000	23.047001	10.001000
H	27.965000	20.761999	10.000000
H	22.910999	20.764000	10.001000
C	24.202000	22.333000	10.001000
C	26.671000	23.764000	10.000000
C	24.202999	23.768000	10.000000
C	26.671000	22.330000	10.000000
C	25.437000	21.549999	10.000000
C	25.437000	24.547001	10.001000
N	22.975000	21.792999	10.001000
N	27.899000	24.304001	10.000000
N	22.975000	24.308001	10.000000
N	27.899000	21.791000	10.000000
O	25.434999	20.285000	10.000000
O	25.440001	25.813000	10.001000
H	27.962999	25.333000	10.000000
H	22.910999	25.337000	10.000000
Mn	21.518000	23.051001	10.000000

H	35.799999	20.771000	10.000000
H	30.728001	20.771000	10.000000
C	32.032001	22.336000	10.001000
C	34.493999	23.761999	10.000000
C	32.030998	23.764000	10.001000
C	34.493999	22.334999	10.000000
C	33.263000	21.552000	10.000000
C	33.262001	24.547001	10.000000
N	30.797001	21.799000	10.000000
N	35.729000	24.299000	10.000000
N	30.794001	24.299000	10.001000
N	35.730999	21.799000	10.000000
O	33.262001	20.284000	10.000000
O	33.264000	25.813999	9.999000
H	35.798000	25.327000	9.999000
H	30.723000	25.327000	10.001000
Mn	29.355000	23.048000	10.000000
H	43.611000	20.761000	10.000000
H	38.560001	20.763000	10.000000
C	39.855000	22.330999	9.999000
C	42.326000	23.767000	10.000000
C	39.856998	23.764000	9.999000
C	42.324001	22.332001	10.000000
C	41.088001	21.551001	10.000000
C	41.091999	24.547001	10.000000
N	38.625000	21.792000	10.000000
N	43.555000	24.305000	10.001000
N	38.630001	24.306000	9.999000
N	43.549999	21.790001	10.001000
O	41.090000	20.285000	10.000000
O	41.088001	25.812000	10.000000
H	43.620998	25.334000	10.001000
H	38.567001	25.334999	9.999000
Mn	37.172001	23.049000	10.000000

Atomic coordinates of Fe-TABQ:

H	8.340000	0.975000	10.000000
H	3.284000	0.980000	10.000000
C	4.579000	2.527000	10.001000

C	7.041000	3.969000	10.001000
C	4.578000	3.978000	10.000000
C	7.040000	2.528000	10.001000
C	5.804000	1.742000	10.001000
C	5.807000	4.759000	10.000000
N	3.349000	2.010000	10.000000
N	8.267000	4.491000	10.001000
N	3.350000	4.496000	9.999000
N	8.267000	2.006000	10.000000
O	5.813000	0.478000	10.001000
O	5.821000	6.022000	10.000000
H	8.338000	5.522000	10.001000
H	3.281000	5.527000	9.999000
Fe	1.935000	3.253000	10.000000
H	16.094999	0.984000	10.002000
H	11.034000	0.981000	9.999000
C	12.343000	2.531000	10.000000
C	14.797000	3.979000	10.000000
C	12.343000	3.969000	10.000000
C	14.797000	2.529000	10.000000
C	13.575000	1.742000	10.000000
C	13.573000	4.762000	10.000000
N	11.111000	2.012000	9.999000
N	16.031000	4.493000	10.000000
N	11.111000	4.487000	10.000000
N	16.030001	2.015000	10.001000
O	13.566000	0.477000	9.999000
O	13.558000	6.029000	10.000000
H	16.101999	5.523000	10.001000
H	11.037000	5.517000	10.000000
Fe	9.695000	3.249000	9.999000
H	23.841000	0.975000	10.000000
H	18.785999	0.980000	10.002000
C	20.080000	2.527000	10.000000
C	22.542999	3.969000	10.001000
C	20.080000	3.978000	10.000000
C	22.542000	2.528000	10.000000
C	21.305000	1.742000	9.999000
C	21.309000	4.759000	10.000000
N	18.851000	2.010000	10.001000

N	23.768999	4.491000	10.001000
N	18.851999	4.496000	10.001000
N	23.768000	2.006000	10.000000
O	21.313999	0.478000	9.999000
O	21.323000	6.022000	9.999000
H	23.839001	5.522000	10.002000
H	18.784000	5.527000	10.003000
Fe	17.437000	3.253000	10.001000
H	31.597000	0.984000	10.002000
H	26.535999	0.981000	9.998000
C	27.844000	2.531000	10.000000
C	30.298000	3.979000	10.000000
C	27.844000	3.970000	10.000000
C	30.298000	2.529000	10.001000
C	29.076000	1.742000	10.000000
C	29.073999	4.762000	10.000000
N	26.612000	2.012000	9.999000
N	31.532000	4.493000	9.999000
N	26.612000	4.487000	10.001000
N	31.531000	2.015000	10.001000
O	29.066999	0.477000	10.000000
O	29.059999	6.029000	10.000000
H	31.603001	5.523000	9.998000
H	26.538000	5.517000	10.001000
Fe	25.195999	3.249000	10.000000
H	12.217000	7.605000	9.998000
H	7.158000	7.608000	9.999000
C	8.454000	9.155000	9.999000
C	10.916000	10.598000	10.000000
C	8.454000	10.606000	9.999000
C	10.916000	9.158000	10.000000
C	9.680000	8.371000	10.000000
C	9.681000	11.388000	10.000000
N	7.225000	8.638000	9.999000
N	12.142000	11.121000	9.999000
N	7.226000	11.124000	10.000000
N	12.142000	8.636000	9.999000
O	9.691000	7.107000	10.001000
O	9.696000	12.651000	10.001000
H	12.211000	12.152000	9.998000

H	7.158000	12.155000	10.000000
Fe	5.811000	9.881000	10.000000
H	19.969000	7.613000	10.000000
H	14.908000	7.613000	10.001000
C	16.216999	9.162000	10.001000
C	18.672001	10.609000	10.001000
C	16.216999	10.600000	10.000000
C	18.671000	9.159000	10.001000
C	17.448000	8.373000	10.001000
C	17.447001	11.392000	10.001000
N	14.985000	8.643000	10.001000
N	19.906000	11.122000	10.001000
N	14.985000	11.118000	9.999000
N	19.903999	8.643000	10.001000
O	17.438000	7.108000	10.002000
O	17.431999	12.659000	10.001000
H	19.976000	12.152000	10.001000
H	14.911000	12.148000	9.997000
Fe	13.569000	9.880000	9.999000
H	27.719000	7.605000	9.996000
H	22.660000	7.608000	9.999000
C	23.955999	9.154000	10.001000
C	26.417999	10.598000	10.000000
C	23.955999	10.606000	10.000000
C	26.417999	9.157000	10.000000
C	25.181999	8.370000	10.001000
C	25.183001	11.388000	10.001000
N	22.726999	8.638000	10.000000
N	27.643999	11.121000	9.999000
N	22.728001	11.124000	10.000000
N	27.643999	8.636000	9.997000
O	25.193001	7.106000	10.003000
O	25.198000	12.651000	10.002000
H	27.714001	12.151000	9.998000
H	22.660000	12.155000	9.999000
Fe	21.312000	9.881000	10.001000
H	35.471001	7.613000	10.000000
H	30.410000	7.612000	9.999000
C	31.719000	9.162000	10.001000
C	34.174000	10.608000	10.001000

C	31.719000	10.600000	10.001000
C	34.173000	9.159000	10.001000
C	32.950001	8.373000	10.001000
C	32.949001	11.392000	10.001000
N	30.487000	8.643000	10.000000
N	35.407001	11.122000	10.001000
N	30.487000	11.118000	9.999000
N	35.405998	8.643000	10.000000
O	32.939999	7.107000	10.001000
O	32.933998	12.659000	10.002000
H	35.478001	12.152000	10.001000
H	30.413000	12.148000	9.997000
Fe	29.070999	9.879000	9.998000
H	16.091000	14.238000	10.000000
H	11.035000	14.243000	10.000000
C	12.330000	15.790000	10.001000
C	14.792000	17.232000	10.001000
C	12.329000	17.240999	10.000000
C	14.791000	15.791000	10.001000
C	13.555000	15.005000	10.001000
C	13.558000	18.021999	10.000000
N	11.100000	15.273000	10.000000
N	16.018000	17.754000	10.001000
N	11.101000	17.759001	9.999000
N	16.018000	15.269000	10.000000
O	13.564000	13.741000	10.001000
O	13.572000	19.285000	10.000000
H	16.089001	18.785000	10.001000
H	11.032000	18.790001	9.999000
Fe	9.686000	16.516001	10.000000
H	23.846001	14.247000	10.002000
H	18.785000	14.244000	9.999000
C	20.094000	15.794000	10.000000
C	22.548000	17.242001	10.000000
C	20.094000	17.232000	10.000000
C	22.548000	15.792000	10.000000
C	21.326000	15.005000	10.000000
C	21.323999	18.025000	10.000000
N	18.862000	15.275000	9.999000
N	23.782000	17.756001	10.000000

N	18.862000	17.750000	10.000000
N	23.781000	15.278000	10.001000
O	21.316999	13.740000	9.999000
O	21.309000	19.292000	10.000000
H	23.853001	18.785999	10.001000
H	18.788000	18.780001	10.000000
Fe	17.445999	16.511999	9.999000
H	31.591999	14.238000	10.000000
H	26.537001	14.243000	10.002000
C	27.830999	15.790000	10.000000
C	30.294001	17.232000	10.001000
C	27.830999	17.240999	10.000000
C	30.292999	15.791000	10.000000
C	29.056000	15.005000	9.999000
C	29.059999	18.021999	10.000000
N	26.601999	15.273000	10.001000
N	31.520000	17.754000	10.001000
N	26.603001	17.759001	10.001000
N	31.518999	15.269000	10.000000
O	29.065001	13.741000	9.999000
O	29.073999	19.285000	9.999000
H	31.590000	18.785000	10.002000
H	26.535000	18.790001	10.003000
Fe	25.188000	16.516001	10.001000
H	39.348000	14.247000	10.002000
H	34.286999	14.244000	9.998000
C	35.595001	15.794000	10.000000
C	38.049000	17.242001	10.000000
C	35.595001	17.233000	10.000000
C	38.049000	15.792000	10.001000
C	36.827000	15.005000	10.000000
C	36.825001	18.025000	10.000000
N	34.362999	15.275000	9.999000
N	39.283001	17.756001	9.999000
N	34.362999	17.750000	10.001000
N	39.282001	15.278000	10.001000
O	36.818001	13.740000	10.000000
O	36.811001	19.292000	10.000000
H	39.354000	18.785999	9.998000
H	34.289001	18.780001	10.001000

Fe	32.946999	16.511999	10.000000
H	19.968000	20.868000	9.998000
H	14.909000	20.871000	9.999000
C	16.205000	22.417999	9.999000
C	18.667000	23.861000	10.000000
C	16.205000	23.868999	9.999000
C	18.667000	22.421000	10.000000
C	17.431000	21.634001	10.000000
C	17.431999	24.650999	10.000000
N	14.976000	21.900999	9.999000
N	19.893000	24.384001	9.999000
N	14.977000	24.386999	10.000000
N	19.893000	21.899000	9.999000
O	17.441999	20.370001	10.001000
O	17.447001	25.914000	10.001000
H	19.962000	25.415001	9.998000
H	14.909000	25.417999	10.000000
Fe	13.562000	23.143999	10.000000
H	27.719999	20.875999	10.000000
H	22.659000	20.875999	10.001000
C	23.968000	22.424999	10.001000
C	26.423000	23.872000	10.001000
C	23.968000	23.863001	10.000000
C	26.422001	22.422001	10.001000
C	25.198999	21.636000	10.001000
C	25.198000	24.655001	10.001000
N	22.736000	21.906000	10.001000
N	27.657000	24.385000	10.001000
N	22.736000	24.381001	9.999000
N	27.655001	21.906000	10.001000
O	25.188999	20.371000	10.002000
O	25.183001	25.922001	10.001000
H	27.726999	25.415001	10.001000
H	22.662001	25.410999	9.997000
Fe	21.320000	23.143000	9.999000
H	35.470001	20.868000	9.996000
H	30.410999	20.871000	9.999000
C	31.707001	22.417000	10.001000
C	34.168999	23.861000	10.000000
C	31.707001	23.868999	10.000000

C	34.168999	22.420000	10.000000
C	32.932999	21.632999	10.001000
C	32.933998	24.650999	10.001000
N	30.478001	21.900999	10.000000
N	35.395000	24.384001	9.999000
N	30.479000	24.386999	10.000000
N	35.395000	21.899000	9.997000
O	32.944000	20.368999	10.003000
O	32.949001	25.914000	10.002000
H	35.465000	25.414000	9.998000
H	30.410999	25.417999	9.999000
Fe	29.063000	23.143999	10.001000
H	43.222000	20.875999	10.000000
H	38.160999	20.875000	9.999000
C	39.470001	22.424999	10.001000
C	41.924999	23.871000	10.001000
C	39.470001	23.863001	10.001000
C	41.924000	22.422001	10.001000
C	40.701000	21.636000	10.001000
C	40.700001	24.655001	10.001000
N	38.237999	21.906000	10.000000
N	43.158001	24.385000	10.001000
N	38.237999	24.381001	9.999000
N	43.157001	21.906000	10.000000
O	40.691002	20.370001	10.001000
O	40.685001	25.922001	10.002000
H	43.229000	25.415001	10.001000
H	38.164001	25.410999	9.997000
Fe	36.821999	23.142000	9.998000

Atomic coordinates of Co-TABQ:

H	8.295000	0.988000	10.000000
H	3.211000	0.985000	10.001000
C	4.526000	2.525000	10.001000
C	6.988000	3.971000	9.999000
C	4.527000	3.967000	10.001000
C	6.987000	2.529000	10.000000
C	5.757000	1.739000	10.000000
C	5.757000	4.757000	10.000000

N	3.296000	2.015000	10.001000
N	8.219000	4.480000	9.999000
N	3.297000	4.479000	10.002000
N	8.217000	2.017000	9.999000
O	5.760000	0.477000	10.000000
O	5.754000	6.019000	9.999000
H	8.304000	5.510000	9.999000
H	3.217000	5.508000	10.002000
Co	1.917000	3.246000	10.002000
H	15.974000	0.990000	10.001000
H	10.887000	0.993000	9.998000
C	12.203000	2.529000	10.000000
C	14.651000	3.968000	10.000000
C	12.203000	3.972000	10.001000
C	14.651000	2.525000	10.001000
C	13.426000	1.735000	10.000000
C	13.428000	4.762000	10.000000
N	10.969000	2.022000	9.999000
N	15.886000	4.474000	10.000000
N	10.967000	4.477000	10.001000
N	15.887000	2.019000	10.000000
O	13.423000	0.470000	10.000000
O	13.431000	6.027000	10.001000
H	15.968000	5.503000	9.999000
H	10.879000	5.507000	10.001000
Co	9.598000	3.248000	10.000000
H	23.636999	0.988000	9.999000
H	18.551001	0.986000	9.999000
C	19.867001	2.526000	9.999000
C	22.329000	3.971000	10.001000
C	19.868000	3.968000	9.999000
C	22.327999	2.529000	10.000000
C	21.098000	1.739000	10.000000
C	21.098000	4.758000	10.000000
N	18.636000	2.016000	9.999000
N	23.561001	4.480000	10.001000
N	18.638000	4.479000	9.999000
N	23.558001	2.017000	10.000000
O	21.101000	0.478000	10.000000
O	21.094999	6.019000	10.000000

H	23.646000	5.510000	10.002000
H	18.556999	5.508000	9.999000
Co	17.257000	3.247000	10.000000
H	31.316000	0.989000	10.001000
H	26.229000	0.993000	10.001000
C	27.545000	2.528000	10.000000
C	29.993000	3.968000	10.001000
C	27.545000	3.972000	10.000000
C	29.993000	2.524000	10.001000
C	28.768000	1.734000	10.000000
C	28.770000	4.762000	10.000000
N	26.311001	2.022000	10.000000
N	31.228001	4.474000	10.002000
N	26.309000	4.477000	10.001000
N	31.229000	2.019000	10.001000
O	28.764999	0.469000	10.000000
O	28.774000	6.027000	10.000000
H	31.309999	5.503000	10.002000
H	26.222000	5.507000	10.000000
Co	24.938999	3.248000	10.001000
H	12.145000	7.619000	10.002000
H	7.058000	7.623000	9.997000
C	8.374000	9.158000	9.998000
C	10.822000	10.598000	10.001000
C	8.374000	10.602000	9.999000
C	10.822000	9.155000	10.001000
C	9.597000	8.365000	10.000000
C	9.599000	11.392000	10.000000
N	7.139000	8.652000	9.997000
N	12.057000	11.104000	10.001000
N	7.138000	11.107000	9.998000
N	12.058000	8.649000	10.001000
O	9.594000	7.099000	10.000000
O	9.603000	12.657000	10.000000
H	12.139000	12.133000	10.001000
H	7.050000	12.136000	9.999000
Co	5.768000	9.878000	9.998000
H	19.808001	7.617000	9.998000
H	14.722000	7.616000	10.002000
C	16.038000	9.155000	10.001000

C	18.500000	10.600000	10.000000
C	16.039000	10.597000	10.000000
C	18.499001	9.158000	9.999000
C	17.268999	8.369000	10.000000
C	17.268999	11.387000	10.000000
N	14.807000	8.645000	10.001000
N	19.731001	11.110000	10.000000
N	14.809000	11.109000	10.001000
N	19.729000	8.647000	9.999000
O	17.271000	7.107000	9.999000
O	17.266001	12.648000	10.000000
H	19.816000	12.139000	10.000000
H	14.730000	12.138000	10.001000
Co	13.428000	9.877000	10.001000
H	27.485001	7.620000	10.001000
H	22.400000	7.623000	9.999000
C	23.715000	9.158000	9.999000
C	26.162001	10.598000	10.001000
C	23.714001	10.602000	10.000000
C	26.163000	9.155000	10.001000
C	24.938000	8.365000	10.000000
C	24.938999	11.392000	10.000000
N	22.481001	8.652000	9.999000
N	27.396999	11.104000	10.001000
N	22.479000	11.107000	10.000000
N	27.398001	8.649000	10.001000
O	24.936001	7.100000	10.000000
O	24.943001	12.657000	10.000000
H	27.479000	12.133000	10.001000
H	22.391001	12.136000	10.000000
Co	21.110001	9.878000	9.999000
H	35.147999	7.618000	9.998000
H	30.061001	7.616000	10.000000
C	31.378000	9.156000	10.001000
C	33.840000	10.600000	9.999000
C	31.379000	10.597000	10.001000
C	33.839001	9.159000	9.999000
C	32.609001	8.369000	10.000000
C	32.609001	11.387000	10.000000
N	30.146999	8.646000	10.001000

N	35.070999	11.110000	9.998000
N	30.149000	11.109000	10.002000
N	35.068001	8.647000	9.998000
O	32.611000	7.107000	10.000000
O	32.605999	12.649000	10.001000
H	35.155998	12.139000	9.999000
H	30.069000	12.138000	10.002000
Co	28.768000	9.877000	10.001000
H	16.011000	14.309000	10.000000
H	10.927000	14.306000	10.001000
C	12.242000	15.846000	10.001000
C	14.704000	17.292000	9.999000
C	12.243000	17.288000	10.001000
C	14.703000	15.850000	10.000000
C	13.473000	15.060000	10.000000
C	13.473000	18.077999	10.000000
N	11.012000	15.336000	10.001000
N	15.935000	17.801001	9.999000
N	11.013000	17.799999	10.002000
N	15.933000	15.338000	9.999000
O	13.476000	13.798000	10.000000
O	13.470000	19.340000	9.999000
H	16.020000	18.830999	9.999000
H	10.933000	18.829000	10.002000
Co	9.633000	16.566999	10.002000
H	23.690001	14.311000	10.001000
H	18.603001	14.314000	9.998000
C	19.919001	15.850000	10.000000
C	22.367001	17.289000	10.000000
C	19.919001	17.292999	10.001000
C	22.367001	15.846000	10.001000
C	21.142000	15.056000	10.000000
C	21.143999	18.083000	10.000000
N	18.684999	15.343000	9.999000
N	23.601999	17.795000	10.000000
N	18.683001	17.798000	10.001000
N	23.603001	15.340000	10.000000
O	21.139000	13.791000	10.000000
O	21.146999	19.348000	10.001000
H	23.684000	18.823999	9.999000

H	18.594999	18.827999	10.001000
Co	17.313999	16.569000	10.000000
H	31.353001	14.309000	9.999000
H	26.267000	14.307000	9.999000
C	27.583000	15.847000	9.999000
C	30.045000	17.292000	10.001000
C	27.584000	17.289000	9.999000
C	30.044001	15.850000	10.000000
C	28.813999	15.060000	10.000000
C	28.813999	18.079000	10.000000
N	26.351999	15.337000	9.999000
N	31.277000	17.801001	10.001000
N	26.354000	17.799999	9.999000
N	31.274000	15.338000	10.000000
O	28.816999	13.799000	10.000000
O	28.811001	19.340000	10.000000
H	31.362000	18.830999	10.002000
H	26.273001	18.829000	9.999000
Co	24.973000	16.568001	10.000000
H	39.032001	14.310000	10.001000
H	33.945000	14.314000	10.001000
C	35.261002	15.849000	10.000000
C	37.709000	17.289000	10.001000
C	35.261002	17.292999	10.000000
C	37.709000	15.845000	10.001000
C	36.484001	15.055000	10.000000
C	36.486000	18.083000	10.000000
N	34.027000	15.343000	10.000000
N	38.944000	17.795000	10.002000
N	34.025002	17.798000	10.001000
N	38.945000	15.340000	10.001000
O	36.480999	13.790000	10.000000
O	36.490002	19.348000	10.000000
H	39.026001	18.823999	10.002000
H	33.938000	18.827999	10.000000
Co	32.654999	16.569000	10.001000
H	19.861000	20.940001	10.002000
H	14.774000	20.944000	9.997000
C	16.090000	22.479000	9.998000
C	18.538000	23.919001	10.001000

C	16.090000	23.923000	9.999000
C	18.538000	22.476000	10.001000
C	17.313000	21.686001	10.000000
C	17.315001	24.712999	10.000000
N	14.855000	21.973000	9.997000
N	19.773001	24.424999	10.001000
N	14.854000	24.427999	9.998000
N	19.774000	21.969999	10.001000
O	17.309999	20.420000	10.000000
O	17.319000	25.978001	10.000000
H	19.855000	25.454000	10.001000
H	14.766000	25.457001	9.999000
Co	13.484000	23.198999	9.998000
H	27.524000	20.938000	9.998000
H	22.438000	20.937000	10.002000
C	23.754000	22.476000	10.001000
C	26.216000	23.921000	10.000000
C	23.754999	23.917999	10.000000
C	26.215000	22.479000	9.999000
C	24.985001	21.690001	10.000000
C	24.985001	24.708000	10.000000
N	22.523001	21.966000	10.001000
N	27.447001	24.431000	10.000000
N	22.525000	24.430000	10.001000
N	27.445000	21.968000	9.999000
O	24.987000	20.427999	9.999000
O	24.982000	25.969000	10.000000
H	27.532000	25.459999	10.000000
H	22.445999	25.459000	10.001000
Co	21.143999	23.198000	10.001000
H	35.201000	20.941000	10.001000
H	30.115999	20.944000	9.999000
C	31.431000	22.479000	9.999000
C	33.877998	23.919001	10.001000
C	31.430000	23.923000	10.000000
C	33.879002	22.476000	10.001000
C	32.653999	21.686001	10.000000
C	32.654999	24.712999	10.000000
N	30.197001	21.973000	9.999000
N	35.112999	24.424999	10.001000

N	30.195000	24.427999	10.000000
N	35.113998	21.969999	10.001000
O	32.652000	20.421000	10.000000
O	32.659000	25.978001	10.000000
H	35.195000	25.454000	10.001000
H	30.107000	25.457001	10.000000
Co	28.826000	23.198999	9.999000
H	42.863998	20.938999	9.998000
H	37.777000	20.937000	10.000000
C	39.094002	22.476999	10.001000
C	41.556000	23.921000	9.999000
C	39.095001	23.917999	10.001000
C	41.555000	22.480000	9.999000
C	40.325001	21.690001	10.000000
C	40.325001	24.708000	10.000000
N	37.862999	21.966999	10.001000
N	42.786999	24.431000	9.998000
N	37.865002	24.430000	10.002000
N	42.784000	21.968000	9.998000
O	40.327000	20.427999	10.000000
O	40.321999	25.969999	10.001000
H	42.872002	25.459999	9.999000
H	37.785000	25.459000	10.002000
Co	36.484001	23.198000	10.001000