Effects of Electrostatic Interactions on Gas Adsorption and Permeability of MOF
Membranes

Ilknur Erucar, Thomas A. Manz, Seda Keskin*

Figure S1. Structure of CECYOY in (1,0,0) direction. Carbon atoms (gray) and hydrogen atoms (white) were not labeled.

Figure S2. Structure of FEVVIM in (0,1,0) direction (top) and in (0,0,1) direction (bottom). Carbon atoms (gray) and hydrogen atoms (white) were not labeled.

Figure S3. Structure of IDUDOA in (0,1,0) direction. Carbon atoms (gray) and hydrogen atoms (white) were not labeled.

Figure S4. Structure of IJOMOJ02 in (0,1,0) direction. Carbon atoms (gray) and hydrogen atoms (white) were not labeled.

Figure S5. Structure of KEXFAU in (0,1,0) direction. Carbon atoms (gray) and hydrogen atoms (white) were not labeled.

Figure S6. Structure of ZUQPOQ in (0,0,1) direction. Carbon atoms (gray) and hydrogen atoms (white) were not labeled.

Figure S7. Structure of OHETIE in (1,0,0) direction (top left) and in (0,1,0) direction (top right) and in (0,0,1) direction (bottom). Carbon atoms (gray) and hydrogen atoms (white) were not labeled.

Figure S8. Structure of YARYEV in (1,0,0) direction (top left) and in (0,1,0) direction (top right) and in (0,0,1) direction (bottom). Carbon atoms (gray) and hydrogen atoms (white) were not labeled.

Figure S9. Comparison of experiments and molecular simulation results for CO₂ and H₂ adsorption in IJOMOJ02. Experimental data is taken from the literature.[1]

Figure S10. Effects of electrostatic interactions on CO₂ uptake in ZIF-8.*

*Experimental data is taken from [2]. As discussed before in the literature [2], molecular simulations based on UFF overestimated the CO₂ adsorption in ZIF-8. Molecular simulations employing the same force field were used to predict CO₂ permeability of ZIF-8/Matrimid and ZIF-8/Ultem MMMs and results agreed well with the experimental measurements as shown in Figure 1a of this paper.

Figure S11. Adsorption isotherms of CO₂ in MOFs computed from molecular simulations.

Table S1. Structural properties of MOFs calculated using MOFomics.[3]

MOFs	Total Pore Volume		LCD (Å)	PLD (Å)
	% of			
	cm ³ /g	Total Volume		
CECYOY	0.099	16	3.9	-
FEVVIM	0.456	35	5.6	2.3
IDUDOA	-	-	-	-
IJOMOJ02	-	-	5.5*	4.5*
KEXFAU	0.476	43	4.8	-
OHETIE	0.115	17	4.5	-
YARYEV	0.445	50	4.7	2.7
ZUQPOQ	-	-	-	3.389*

*Data for IJOMOJ02 and ZUQPOQ were taken from the study of Dybtsev et al.[1] and Haldoupis et al.[4], respectively.

Table S2. Permeability and selectivity of pure polymers for CO₂/N₂ separation.

Polymer	P(CO ₂)	S (CO ₂ /N ₂)
Poly(bis(2-(2-methoxyethoxy)ethoxy)phosphazene)	250	62.5
PIM-7	1100	26.2
Modified poly (dimethylsiloxane)	2000	34.2
PIM-1	2300	25
Poly(trimethylgermylpropyne)	11000	14
Poly(trimethylsilylpropyne)	11000	10.7
Matrimid	9	36
PSF	6.49	20
PDMS	2519.8	8.37
Silicon rubber	4550	12.96
PTMSP	37000	5.37
PPO	65.5	18.71

Permeability unit is Barrer.

Data for all polymers were taken from Robeson et al.[5-6] except Matrimid,[7] PSF,[8] and PDMS.[8]

Table S3. Permeability and selectivity of pure polymers for CO₂/CH₄ separation.

Polymer	P(CO ₂)	S (CO ₂ /CH ₄)
PVSH doped polyaniline	0.029	2200
Polypyrrole 6FDA/PMDA (25/75)-TAB	3.13	140
Polyimide TADATO/DSDA (1/1)-DDBT	45	60
Poly(diphenyl acetylene) 3a	110	47.8
Polyimide 6FDA-PMDA/DAT (3:1)	187.6	33.9
Poly(diphenyl acetylene) 3e	290	31.5
Polyimide 6FDA-TADATO	555.7	22.7
6FDA-based polyimide	958	24
PIM-7	1100	17.7
PIM-1	2300	18.4
PDMS	2519.89	3.18
Silicon rubber	4550	3.18
PTMSP	37000	2.01
6FDA-DAM poly(imide)	407.2	17.61

Permeability unit is Barrer.

Data for all polymers were taken from Robeson et al.[5-6] except 6FDA-DAM poly(imide)[9] and PDMS.[8]

Table S4. Permeability and selectivity of pure polymers for H₂/CO₂ separation.

Polymer	P (H ₂)	S (H ₂ /CO ₂)
Liquid crystalline polyester (HBA/HNA 30/70)	0.05	100.9
Polyaniline (redoped)	1.75	23.1
Polyimide(1,1-6FDA-DIA)	31.4	8.05
Poly(trimethylsilylpropyne)	13900	0.495
PTMSP	16200	0.489
PDMS	577.55	0.23

Permeability unit is Barrer.

Data for all polymers were taken from Robeson et al.[5-6] except PSF[8] and PDMS.[8]

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Table S5. Net atomic charges (NAC) and atomic spin moments (ASM) for IJOMOJ02
Lattice vectors: [{ 11.720300, 0.000000, 0.000000 }, { 0.000000, 10.207000, 0.000000 },
{ -0.375500, 0.000000, 14.950800 }]

atom	X (Å)	Y (Å)	Z (Å)	NAC	ASM
C	0.162644	10.06047	3.132566	0.6719	0.0028
C	0.489655	3.763464	4.719564	0.6612	-0.0057
C	0.621649	7.934462	6.650564	0.6688	0.0023
C	0.890653	2.92747	0.731558	0.6644	-0.0044
C	0.91651	6.873465	2.555555	0.6686	0.0043
C	2.475148	9.185463	14.46636	0.6742	0.0016
C	2.47155	4.081463	7.959357	0.6659	-0.0102
C	3.72155	1.769465	4.920562	0.6688	-0.0035
C	4.781647	8.03047	6.74456	0.6453	-0.0063
C	5.05065	2.831463	0.825553	0.6511	-0.0036
C	5.182647	8.866464	2.755567	0.6549	-0.0002
C	5.509655	9.956468	4.343566	0.6557	-0.0078
C	5.835447	10.0471	10.60735	0.6459	-0.0119
C	6.162455	11.346165	12.19535	0.6546	-0.0015
C	6.294451	7.375466	14.12537	0.6479	-0.0020
C	6.563455	2.176466	8.20636	0.6445	-0.0097
C	7.613445	8.437463	10.03036	0.6578	-0.0099
C	8.522952	6.125466	6.990561	0.6673	-0.0129
C	8.869954	1.021466	14.484555	0.6725	0.0022
C	9.403451	3.333463	11.39136	0.6584	-0.0069
C	10.45345	7.279469	11.11936	0.6633	-0.0026
C	10.72345	2.272466	8.30115	0.6603	-0.0085
C	10.85545	6.443465	10.23037	0.6550	-0.0056
C	11.18245	0.14647	11.81835	0.6718	-0.0031
H	-0.10135	8.108471	7.224555	0.0158	-0.0050
H	-0.04686	0.344466	11.04136	0.0101	-0.0016
H	0.208649	3.139469	4.075558	0.0034	-0.0005
H	0.720652	3.842466	0.597554	0.0028	0.0027
H	1.592654	7.565469	2.024563	0.0027	0.0037
H	1.999155	8.645472	13.86237	0.0123	0.0057
H	3.297148	3.541472	8.563355	0.0111	-0.0050
H	4.079646	2.461469	5.451555	0.0057	-0.0040
H	4.95165	8.946466	6.877562	0.0129	-0.0031
H	5.464649	8.243469	3.399558	0.0057	0.0004
H	5.343144	5.448466	11.38536	0.0133	-0.0031
H	5.774649	3.004471	0.251562	0.0195	0.0008
H	5.570452	7.202467	14.69936	0.0207	0.0029
H	6.001946	4.758463	3.565556	0.0123	-0.0016
H	5.880453	1.96347	11.55136	0.0063	-0.0026
H	6.393452	1.260462	8.073357	0.0144	-0.0064

H	7.264448	7.74547	9.499365	0.0062	-0.0053
H	8.046948	6.665467	6.386563	0.0106	-0.0045
H	9.34495	1.561467	1.088553	0.0128	0.0067
H	9.752448	2.64147	12.92636	0.0041	0.0010
H	10.62346	6.364463	14.35236	0.0122	0.0024
H	11.13645	7.06747	10.87536	0.0047	-0.0022
H	11.39095	9.862463	3.909559	0.0085	0.0012
H	11.44646	2.098467	7.726364	0.0139	-0.0052
Mn	2.592644	9.113463	4.680557	0.9382	-1.9783
Mn	5.11651	5.913466	5.515559	0.8327	0.2185
Mn	2.80649	0.809466	1.960558	0.8556	1.3719
Mn	2.50656	4.009463	2.79556	0.8835	1.4682
Mn	5.67554	5.103469	7.475564	0.8824	0.9510
Mn	5.485153	0.00047	14.95037	0.8970	-1.0212
Mn	8.36544	6.197466	12.15536	0.8170	1.2409
Mn	8.383444	9.397462	12.99036	0.8518	-0.9931
Mn	8.633451	2.293462	9.43536	0.8304	0.0784
Mn	8.652446	5.3466	10.27036	0.8506	1.0170
Mn	11.34445	0.00047	14.95037	1.1393	-5.5590
Mn	11.53245	5.103469	7.475355	0.9502	0.9771
O	-0.08885	6.220467	9.314363	-0.5442	-0.0181
O	0.246648	2.140469	0.044553	-0.5825	-0.0219
O	0.096149	10.19047	12.84337	-0.5897	-0.0194
O	0.997646	6.723463	5.53564	-0.5659	-0.0038
O	1.106652	8.902464	2.5556	-0.5511	-0.0011
O	1.415655	10.13147	3.25567	-0.5733	0.0016
O	1.629648	4.278468	4.54555	-0.5737	-0.0131
O	1.599149	4.028468	8.00135	-0.5521	-0.0069
O	1.766654	2.630466	1.604565	-0.5708	-0.0061
O	2.110653	5.777468	2.00556	-0.5485	0.0069
O	2.170646	9.910466	0.307553	-0.5161	-0.0233
O	2.193653	7.150463	3.763565	-0.5808	-0.0004
O	3.478648	2.046463	3.711566	-0.5236	0.0011
O	3.501644	4.807466	7.167563	-0.5380	-0.0060
O	3.561647	0.673468	5.470558	-0.5326	-0.0073
O	3.905647	7.733466	5.870566	-0.5711	-0.0026
O	3.697153	9.132468	14.42437	-0.5474	0.0103
O	4.042652	9.382468	2.928563	-0.5747	0.0012
O	4.256645	5.027468	4.220566	-0.5680	-0.0051
O	4.565649	3.799464	1.40856	-0.5415	-0.0048
O	4.674655	1.619463	0.921567	-0.5508	0.0055
O	5.201148	5.087465	9.583358	-0.5363	-0.0065
O	5.42665	7.243469	7.430563	-0.5273	-0.0079
O	5.385154	1.116462	13.11136	-0.5397	0.0059
O	5.958952	9.090466	1.839561	-0.5354	0.0091

O	5.918452	2.96347	7.520357	-0.5296	-0.0051
O	6.143954	5.119464	5.367561	-0.5345	-0.0052
O	6.670446	8.587466	14.02937	-0.5507	0.0034
O	6.778444	6.407465	13.54236	-0.5247	-0.0063
O	7.088445	5.179471	10.73035	-0.5533	-0.0064
O	7.30245	0.82447	12.02236	-0.5669	-0.0113
O	7.646952	1.07447	0.526567	-0.5487	0.0095
O	7.439454	2.473462	9.080353	-0.5649	-0.0105
O	7.783455	9.533471	9.480362	-0.5391	-0.0177
O	7.83446	5.399462	7.783357	-0.5583	-0.0115
O	7.855445	8.160466	11.23935	-0.5522	-0.0032
O	9.07449	3.056466	11.18736	-0.5636	-0.0064
O	9.17712	0.296462	14.64337	-0.6118	-0.0199
O	9.234449	4.429471	12.94536	-0.5393	-0.0091
O	9.57745	7.576462	13.34636	-0.5601	-0.0090
O	9.745952	6.178471	6.949565	-0.5543	-0.0089
O	9.715453	9.928471	10.40337	-0.5570	-0.0112
O	9.929447	7.55471	11.69535	-0.5658	-0.0070
O	10.23845	1.301465	8.884363	-0.5424	-0.0078
O	10.34645	3.433465	8.396354	-0.5671	-0.0029
O	11.24895	0.01646	2.107554	-0.5873	-0.0156
O	11.09845	8.06647	14.90637	-0.5813	-0.0187
O	11.43295	3.986466	5.635555	-0.5466	-0.0170

Table S6. Net atomic charges (NAC) for FEVVIM
Lattice vectors: [{ 24.403900, 0.000000, 0.000000 }, { 0.000000, 11.262000, 0.000000 },
{ -4.520000, 0.000000, 20.671400 }]

atom	X (Å)	Y (Å)	Z (Å)	NAC
Br	-0.578	7.865966	7.152201	-0.4598
Br	21.3029	10.67497	5.725192	-0.4653
Br	22.7219	7.865966	3.183189	-0.4598
Br	0.840995	10.67497	4.610198	-0.4653
Br	11.6239	2.234966	7.152201	-0.4597
Br	13.0429	5.043968	4.610198	-0.4654
Br	9.100998	5.043968	5.725192	-0.4654
Br	10.52	2.234966	3.183189	-0.4598
Br	-2.83801	3.395966	17.48759	-0.4596
Br	19.04289	0.586964	16.0606	-0.4652
Br	20.46189	3.395966	13.51959	-0.4598
Br	-1.41899	0.586964	14.94561	-0.4653
Br	9.363892	9.026966	17.48759	-0.4596
Br	10.78289	6.217964	14.94561	-0.4653
Br	6.840988	6.217964	16.0606	-0.4652

Br	8.25999	9.026966	13.51959	-0.4597
C	17.7939	6.362962	11.95859	0.6294
C	18.90689	7.54197	13.7876	0.0671
C	20.3429	7.314962	14.1966	-0.1815
C	20.2669	8.217971	15.3936	-0.1313
C	16.44489	10.30897	13.4756	-0.4970
C	17.29991	10.61697	12.2766	0.6168
C	19.24691	0.555971	11.3836	0.0868
C	20.52089	11.05596	11.3836	-0.1762
C	-2.643	8.217971	15.61259	-0.1320
C	-2.71899	7.314962	16.80959	-0.1816
C	-1.28301	7.54197	17.21961	0.0671
C	-0.17	6.362962	19.04859	0.6293
C	-1.55599	10.95996	10.36859	-0.0963
C	-4.49	0.301968	10.30321	-0.0968
C	21.6849	5.65697	9.75719	-0.0979
C	21.012	7.045969	9.536192	-0.1811
C	20.2209	7.088967	8.258204	0.0775
C	18.53391	8.845963	8.374191	0.6348
C	18.1229	10.15796	7.931203	-0.5153
C	-0.637	6.362962	9.288197	-0.1767
C	0.637003	11.05596	9.288197	0.0874
C	2.584003	0.615963	8.395193	0.6167
C	3.438996	0.952962	7.19619	-0.4967
C	1.761006	1.103596	12.7396	-0.5158
C	1.350003	2.415969	12.2976	0.6347
C	-0.337	4.172965	12.4126	0.0776
C	-1.17801	4.215963	11.1356	-0.1811
C	-1.80101	5.604962	10.9146	-0.0975
C	17.68689	5.165969	11.1086	-0.5038
C	-0.06301	5.165969	19.8986	-0.5040
C	11.5649	5.836971	9.288197	-0.1767
C	14.7859	6.275963	8.395193	0.6168
C	15.6409	6.583968	7.19619	-0.4966
C	13.96291	6.734969	12.7396	-0.5154
C	13.5519	8.046969	12.2976	-0.5343
C	11.8649	9.803965	12.4126	0.0777
C	11.02389	9.846963	11.1356	-0.1812
C	10.40089	11.23596	10.9146	-0.0976
C	9.558904	2.586971	15.61259	-0.1319
C	9.482907	1.683962	16.80959	-0.1816
C	10.91889	1.91097	17.21961	0.0674
C	12.03191	0.731962	19.04859	0.6293
C	12.13889	10.79697	19.8986	-0.5038
C	10.60589	5.328964	10.36859	-0.0964

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C	12.8389	5.074961	9.288197	0.0875
C	7.045008	6.186971	11.3836	0.0868
C	9.277997	5.932968	10.30321	-0.0967
C	5.484987	10.79697	11.1086	-0.5034
C	5.592	0.731962	11.95859	0.6294
C	6.70499	1.91097	13.7876	0.0673
C	8.140997	1.683962	14.1966	-0.1816
C	8.064999	2.586971	15.3936	-0.1311
C	4.24299	4.677965	13.4756	-0.4967
C	5.098007	4.985969	12.2766	0.6168
C	8.318989	5.424962	11.3836	-0.1759
C	9.482997	0.02597	9.75719	-0.0979
C	3.859994	1.414969	9.536192	-0.1811
C	8.01006	1.457967	8.258204	0.0776
C	3.45007	3.214963	8.374191	0.6348
C	5.921001	4.526964	7.931203	-0.5153
C	4.02002	10.15796	2.404208	-0.5157
C	3.61001	8.845963	1.962191	0.6347
C	1.923007	7.088967	2.077207	0.0774
C	1.082002	7.045969	0.80019	-0.1814
C	0.458999	0.53597	0.579192	-0.0974
C	19.9469	6.055963	0.773193	-0.5037
C	2.196997	6.055963	9.562197	-0.5039
C	20.05391	4.85397	1.623201	0.6291
C	21.1669	3.7195	3.452206	0.0671
C	22.60291	3.946971	3.86119	-0.1822
C	22.52691	3.043961	5.058188	-0.1319
C	18.7049	0.952968	1.140192	-0.4970
C	19.55989	0.644963	1.140189	0.6161
C	21.50689	10.70596	1.048205	0.0869
C	22.7809	0.205971	1.048205	-0.1761
C	19.21989	10.95996	20.638	-0.0972
C	19.42489	5.604962	20.0926	-0.0978
C	18.80191	4.215963	19.8716	-0.1812
C	17.9609	4.172965	18.59359	-0.0777
C	16.2739	2.415969	18.7096	-0.5349
C	15.8629	1.103969	18.26761	-0.5156
C	-0.38299	3.043961	5.277202	-0.1315
C	-0.45899	3.946971	6.4742	-0.1823
C	0.976993	3.719962	6.883204	0.0669
C	2.09001	4.89897	8.713202	0.6294
C	0.663995	0.301968	0.033198	-0.0961
C	-2.89701	11.05596	19.62361	-0.1767
C	-1.62301	0.555971	19.62361	0.0873
C	0.323993	10.61697	18.7306	0.6166

C	1.179011	10.30897	17.5316	-0.4966
C	16.22289	4.526964	2.404208	-0.5158
C	15.81189	3.214963	1.962191	0.6349
C	14.12491	1.457967	2.077207	0.0774
C	13.2839	1.414969	0.80019	-0.1814
C	12.6609	0.02597	0.579192	-0.0973
C	11.81891	8.674961	5.277202	-0.1316
C	11.74289	9.577971	6.4742	-0.1821
C	13.17889	9.350962	6.883204	0.0668
C	14.29189	10.52997	8.713202	0.6295
C	14.3989	0.464963	9.562197	-0.5044
C	12.8659	5.932968	0.033198	-0.0964
C	10.57889	6.186971	19.62361	0.0873
C	9.30489	5.424962	19.62361	-0.1763
C	13.50089	4.985969	18.7306	0.6167
C	13.50089	4.677965	17.5316	-0.4966
C	7.74432	0.464963	0.773193	-0.5038
C	7.85200	10.52997	1.623201	0.6292
C	8.964996	9.350962	3.452206	0.0672
C	10.40101	9.577971	3.86119	-0.1822
C	10.32501	6.251961	5.058188	-0.1317
C	6.503	6.251968	3.140192	-0.4972
C	7.357993	6.251963	1.941189	0.6162
C	10.57899	5.85397	1.048205	-0.1760
C	7.222987	11.235	20.0926	-0.0977
C	6.600008	9.846963	19.8716	-0.1813
C	5.759001	9.803965	18.59359	0.0777
C	4.071997	8.046969	18.7096	0.6346
C	3.660994	6.734969	11.25761	-0.5156
C	9.304989	5.074961	1.048205	0.0870
C	7.017992	5.328964	20.63192	-0.0972
H	-2.28999	5.861961	11.711	0.0558
H	-1.09101	6.251964	10.7826	0.0588
H	19.29589	5.71997	12.9916	0.2715
H	18.7909	8.380966	13.31459	0.0715
H	18.3029	7.503961	14.5446	0.5712
H	20.9769	7.623969	13.5316	0.0948
H	20.52589	6.391962	14.43261	0.0904
H	-2.29099	9.096971	15.8216	0.0639
H	-2.15201	7.825964	14.8726	0.0784
H	16.82591	10.72297	14.2526	0.1336
H	15.55889	10.64796	13.33059	0.1630
H	16.4069	9.35897	13.6036	0.1597
H	18.51189	0.419971	13.2396	0.2761
H	18.8069	0.436966	10.52759	0.0567

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H	19.4439	1.499963	11.48861	0.0499
H	20.9439	11.13896	12.25359	0.0753
H	20.3329	10.11697	11.23061	0.0788
H	-1.211	11.14396	11.24059	0.0572
H	-1.67199	5.71997	18.0156	0.2714
H	-1.167	8.380966	17.69259	0.0714
H	-0.679	7.503961	16.4626	0.0711
H	-3.353	7.623969	17.4756	0.0949
H	-2.90201	6.391962	16.5746	0.0904
F	19.91489	9.096971	15.1856	0.0636
H	19.77591	7.825964	16.13359	0.0783
H	21.5689	1.26497	10.38959	0.0607
H	1.68501	9.996962	10.2822	0.0606
H	18.5591	10.54196	7.386201	0.1398
H	18.5591	10.08496	7.419193	0.1698
H	17.9689	10.71997	8.694205	0.1626
H	3.0532	0.538966	6.418201	0.1333
H	4.32499	0.61397	7.340207	0.1629
H	3.477011	1.902963	7.0672	0.1595
H	1.371993	10.84196	7.431203	0.2761
H	1.077007	10.84497	10.14321	0.0564
H	0.440009	9.182195	9.182195	0.0497
H	-1.05999	0.182195	8.417208	0.0755
H	-0.44899	1.14396	9.441207	0.0788
H	21.09491	0.1179	9.430189	0.0573
H	20.1979	8.917961	7.483191	0.2666
H	19.4759	6.475965	8.351204	0.0551
H	20.7649	6.785963	10.514199	0.0632
H	21.76789	7.707961	9.72188	0.0695
H	20.49991	7.26997	10.2962	0.0753
H	1.068006	0.719968	13.2872	0.1398
H	2.569007	1.176969	13.252	0.1700
H	1.915008	0.541961	11.9766	0.1627
H	-0.31401	2.343971	13.1886	0.2664
H	0.408011	4.785967	12.3196	0.0552
H	-0.88099	4.475969	13.15759	0.0630
H	-1.88401	3.553961	11.1936	0.0697
H	-0.616	3.991962	10.3746	0.0752
H	18.35491	4.527966	11.3696	0.1414
H	16.81489	4.776969	11.21461	0.1656
H	-0.73101	4.527966	19.6376	0.1415
H	0.809009	4.776969	19.7926	0.1656
H	4.327008	5.412968	0.145196	0.1636
H	17.81691	5.412968	10.19121	0.1635
H	22.17391	5.399971	8.959191	0.0562

H	20.9749	5.009968	9.889198	0.0588
H	15.2599	6.169966	6.418201	0.1334
H	16.5269	6.24497	7.340207	0.1628
H	15.67889	7.533963	7.0672	0.1595
H	11.14191	5.75397	8.417208	0.0754
H	11.75291	6.775962	9.441207	0.0789
H	13.26991	6.350968	13.28559	0.1398
H	14.77091	6.807969	13.2526	0.1698
H	14.11691	6.172961	11.9766	0.1627
F	11.88789	7.974971	13.1886	0.2664
H	12.60991	10.41697	12.3196	0.0552
H	11.32091	10.10697	13.15759	0.0630
H	10.3179	9.184961	11.1936	0.0696
H	11.52591	9.622962	10.3746	0.0752
H	11.11089	0.230961	11.7126	0.0558
H	11.11089	0.620964	10.7826	0.0589
H	9.91089	3.465971	15.8216	0.0638
H	10.0499	2.194964	14.8726	0.0783
H	10.99091	5.512963	11.24059	0.0571
H	11.4709	10.15897	19.6376	0.1415
H	13.01091	10.15897	19.7926	0.1654
H	16.52891	10.15897	0.145196	0.1636
H	10.52991	0.0537	18.0156	0.2718
H	11.03491	2.74396	17.69259	0.0713
H	11.5229	1.8729	16.4626	0.0712
H	8.848906	1.992969	17.4756	0.0948
H	9.299891	0.760962	16.5746	0.0904
H	10.51689	4.365962	10.2822	0.0606
H	13.57389	5.210961	17.2203	0.2762
H	13.27891	5.193967	10.14321	0.0563
H	12.64191	4.130969	9.18225	0.0498
H	6.309991	6.050971	13.23	0.2761
H	6.605001	6.067966	10.52759	0.0566
H	7.241998	7.130963	11.48861	0.0499
H	9.366998	6.89597	10.38959	0.0606
H	8.893007	5.748969	9.430189	0.0573
H	6.153006	10.15897	11.3696	0.1414
H	4.612992	10.40797	11.21461	0.1653
H	7.093991	0.08897	12.9916	0.2716
H	6.589001	2.749966	13.31459	0.0715
H	6.100998	1.872961	14.5446	0.0712
H	8.774995	1.992969	13.5316	0.0947
H	8.323986	0.760962	14.43261	0.0904
H	4.62401	5.091967	14.2526	0.1334
H	3.356989	5.016962	13.33059	0.1629

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H	4.204996	3.72797	13.6036	0.1596
H	8.742001	5.507963	12.25359	0.0752
H	8.131	4.48597	11.23061	0.0786
H	7.712989	3.465971	15.1856	0.0636
H	7.574008	2.194964	16.13359	0.0782
H	5.615008	11.04397	10.19121	0.1634
H	6.614004	4.910964	7.386201	0.1398
H	5.113003	4.453963	7.419193	0.1698
H	5.767	5.088971	8.694205	0.1624
F	7.995996	3.286961	7.483191	0.2666
H	7.273997	0.844965	8.351204	0.0552
H	8.563001	1.154963	7.514199	0.0631
H	2.565992	2.076961	9.478188	0.0695
H	8.269004	1.63897	10.2962	0.0753
H	4.204996	11.03097	8.959191	0.0561
H	8.712995	10.64097	9.889198	0.0588
H	2.066992	5.848965	10.48061	0.1634
H	3.327987	10.54196	2.950202	0.1398
H	4.828995	10.08496	2.917189	0.1699
H	4.174989	10.71997	1.641206	0.1627
H	1.945997	6.733966	2.852198	0.2665
H	2.667992	6.484964	1.984206	0.0552
H	1.378992	6.733966	2.821191	0.0632
H	0.376005	7.707966	0.858194	0.0697
H	1.643989	7.269963	0.039193	0.0754
H	20.61489	6.733966	1.033198	0.1416
H	19.0749	6.484964	0.878204	0.1653
H	15.5569	5.848965	0.05266	0.1634
H	1.529005	6.733966	0.00192	0.1416
H	3.06899	6.484964	9.457207	0.1654
H	19.9139	5.861961	19.29919	0.0559
H	18.71489	6.251964	20.22419	0.0588
H	-0.03001	5.399971	1.377191	0.0558
H	1.168998	5.009968	0.446192	0.0588
H	21.5559	5.541963	2.656192	0.2717
H	21.05091	2.880966	2.979204	0.0715
H	20.56291	3.75796	4.209193	0.0711
H	23.23691	3.637964	3.196191	0.0951
H	22.7859	4.86997	4.097196	0.0905
H	-0.031	2.164962	5.48619	0.0639
H	0.108	3.435969	4.537207	0.0784
H	19.0859	0.538966	3.917189	0.1336
H	17.8189	0.61397	2.995203	0.1630
H	18.66691	1.902963	3.26819	0.1598
H	20.7719	10.84196	2.904208	0.2758

H	21.06691	10.82497	0.192203	0.0565
H	21.70391	9.761969	1.153195	0.0499
H	23.20391	0.12297	1.918203	0.0754
H	22.59291	1.144962	0.895196	0.0786
H	-3.94499	1.26497	20.61759	0.0605
H	1.049011	0.117969	0.905201	0.0573
H	16.5559	0.719968	17.72159	0.1397
H	15.0549	1.176969	17.7546	0.1699
H	15.7089	0.541961	19.0296	0.1628
F	0.587992	5.541963	7.679198	0.2715
H	1.093009	2.880966	7.357199	0.0716
H	1.581012	3.75796	6.127189	0.0713
H	1.09301	3.637964	7.140191	0.0951
H	-0.042	4.86997	6.238194	0.0906
H	0.009	2.164962	4.8492	0.0640
H	22.05589	3.435969	5.798204	0.0785
H	0.79552	10.72297	16.7546	0.1333
H	2.06498	10.64796	17.6756	0.1629
H	1.217004	9.35897	17.4036	0.1596
H	-0.88799	0.419971	17.76659	0.2756
H	-1.183	0.00966	20.47959	0.0565
H	-1.82	0.00963	19.51761	0.0496
H	-3.32	11.00006	18.7526	0.0754
H	-2.709	10.1168	19.7766	0.0788
H	23.8289	9.9965	0.0542	0.0607
H	18.8349	11.14396	19.7656	0.0575
H	17.93789	2.343971	17.8186	0.2664
H	17.21589	4.785967	15.58659	0.0551
H	18.5049	4.475969	15.00959	0.0632
H	19.50791	3.553961	19.8136	0.0696
H	18.2399	3.991962	20.6300	0.0752
H	14.2689	0.217965	10.4800	0.1635
H	15.52989	4.910964	2.950202	0.1399
H	17.03089	4.453963	2.917189	0.1698
H	16.37689	5.088971	1.641206	0.1627
H	14.1479	3.286961	2.852198	0.2665
H	14.86989	0.844965	1.984206	0.0551
H	13.58089	1.154963	2.821191	0.0633
H	12.57791	2.076961	0.858194	0.0697
H	13.84589	1.63897	0.039193	0.0753
H	12.17189	11.03097	1.377191	0.0558
H	13.3709	10.64097	0.446192	0.0588
H	12.1709	7.795962	5.48619	0.0639
H	12.3099	9.066969	4.537207	0.0784
H	8.256909	6.89597	20.61759	0.0606

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H	13.25089	5.748969	0.905201	0.0574
H	13.73091	1.102966	9.302192	0.1418
H	15.27089	0.853964	9.457207	0.1658
H	12.78989	11.17296	7.679198	0.2717
H	13.29491	8.511966	7.357199	0.0716
H	13.78291	9.38896	6.127189	0.0712
H	11.10889	9.268964	7.140191	0.0950
H	11.5599	10.50097	6.238194	0.0906
H	11.31391	6.050971	17.76659	0.2757
F	11.01891	6.067966	20.47959	0.0565
H	10.3819	7.130963	19.51761	0.0496
H	12.99989	5.091967	16.7546	0.1334
H	14.26689	5.016962	17.6756	0.1627
H	13.78891	3.72797	17.4036	0.1596
H	14.8102	5.507963	18.7526	0.0753
H	9.492991	4.48597	19.7766	0.0787
H	8.41192	1.102966	1.033198	0.1416
H	6.87299	0.853964	0.878204	0.1655
H	3.355005	0.217965	20.5266	0.1635
H	9.354001	11.17296	2.656192	0.2718
H	8.849007	6.24497	2.979204	0.0715
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H	11.03501	9.268964	3.196191	0.0950
H	10.584	10.50097	4.097196	0.0905
H	6.883996	6.1695	3.917189	0.1337
H	5.616994	6.24497	2.995203	0.1631
H	6.465006	7.533963	3.26819	0.1598
H	11.00201	5.75397	2.918203	0.0754
H	10.39101	6.775962	6.127189	0.0786
H	4.353999	6.350968	17.72159	0.1398
H	2.852994	6.807969	17.75	0.1698
H	3.506995	6.172961	19.02	0.1628
H	9.972996	7.795962	4.8492	0.0639
H	9.833989	9.066969	5.798204	0.0785
H	5.736011	7.974971	17.8186	0.2665
H	5.013992	10.41697	18.68659	0.552
H	6.302996	10.10697	17.84959	0.0631
H	7.306006	9.184961	19.8136	0.0696
H	6.037997	9.622962	20.6326	0.0753
H	7.711995	0.230961	19.2946	0.0559
H	6.513014	0.620964	20.22459	0.0588
H	8.569996	5.210961	2.904208	0.2760
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H	9.502008	4.130969	1.153195	0.0498
H	11.627	4.365962	0.0542	0.0607

H	6.632997	5.512963	19.7656	0.0575
Mn	-1.13	9.250967	5.168201	0.5105
Mn	11.072	3.619967	5.168201	0.5113
Mn	-3.39001	2.010965	15.50359	0.5109
Mn	8.81199	7.641965	15.50359	0.5115
Mn	6.101003	8.446962	0.000207	0.8166
Mn	16.04289	8.446962	10.3362	0.8150
Mn	3.840989	2.815962	10.3362	0.8173
Mn	18.3029	2.815962	0.000207	0.8149
N	18.76291	6.388966	12.90759	-0.4604
N	18.3489	0.136968	12.4446	-0.4169
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N	19.70989	8.394965	7.960205	-0.4070
N	1.57008	11.12496	8.227197	-0.4170
N	12.7106	2.866967	12.7106	-0.4066
N	12.57589	8.497967	12.7106	-0.4067
N	11.072	0.757966	18.09959	-0.4611
N	13.7369	5.493964	8.227197	-0.4172
N	6.147003	5.767968	12.4446	-0.4172
N	6.561003	0.757966	12.90759	-0.4607
N	7.50799	8.394965	7.960205	-0.4071
N	2.433998	8.394965	2.375206	-0.4067
N	21.02291	4.872966	2.571191	-0.4603
N	20.60891	11.12496	2.108193	-0.4163
N	17.44991	2.866966	18.29661	-0.4069
N	1.121007	4.872966	7.764199	-0.4604
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N	14.6359	2.763965	2.375206	-0.4068
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N	8.821011	10.50397	2.571191	-0.4608
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N	8.40701	5.493964	2.108193	-0.4166
O	17.07791	7.359965	11.8756	-0.5341
O	17.00189	10.18196	11.15259	-0.5433
O	14.26989	8.768965	11.5696	-0.5468
O	0.545995	7.359965	19.13161	-0.5341
O	17.8159	8.123968	9.102196	-0.5471
O	15.00791	9.532968	8.796197	-0.5337
O	2.881996	1.079969	9.5192	-0.5436
O	15.0839	6.710969	9.5192	-0.5432
O	2.067989	3.137965	11.5696	-0.5473
O	12.7479	1.728965	19.13161	-0.5337
O	4.876005	1.728965	11.8756	-0.5344
O	4.79999	4.550963	11.15259	-0.5436

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O	5.613997	2.492968	9.102196	-0.5473
O	2.806005	3.901968	8.796197	-0.5341
O	4.327994	8.123968	1.234207	-0.5473
O	19.33789	3.901968	1.540205	-0.5339
O	19.2619	1.079969	0.81619	-0.5432
O	15.55589	3.137965	19.43761	-0.5470
O	16.5299	2.492968	1.234207	-0.5469
O	0.62199	10.18196	19.85459	-0.5436
O	12.82389	4.550963	19.85459	-0.5432
C	7.135986	9.532968	1.540205	-0.5341
O	7.059998	6.710969	0.81619	-0.5434
O	3.353987	8.768965	19.43761	-0.5471

Table S7. Net atomic charges (NAC) for CECYOY
Lattice vectors: [{ 14.528000, 0.000000, 0.000000 }, { 0.000000, 22.686000, 0.000000 },
{ 0.000000, 0.000000, 13.503000 }]

atom	X (Å)	Y (Å)	Z (Å)	NAC
C	0.159997	18.852	10.87	0.2675
C	7.423997	7.50002	9.385004	0.2676
C	9.239997	5.12003	3.888999	0.2629
C	10.388	0.60098	6.615997	0.2597
C	7.104003	3.82005	10.87	0.2675
C	9.239997	6.222997	2.863001	0.2631
C	10.388	10.742	0.135003	0.2597
C	11.404	11.944	0.135003	0.2597
C	11.404	22.085	6.615997	0.2597
C	14.368	18.852	9.385004	0.2676
C	12.552	17.566	3.888999	0.2629
C	12.552	16.463	2.863001	0.2631
C	0.159997	15.177	9.385004	0.2676
C	5.288003	5.120003	2.863001	0.2631
C	4.140001	0.600998	0.135003	0.2597
C	5.288003	6.222997	3.888999	0.2629
C	4.140001	10.742	6.615997	0.2597
C	3.123999	11.944	6.615997	0.2597
C	7.423997	7.508998	10.87	0.2675
C	7.104003	7.508998	9.385004	0.2676
C	14.368	15.177	10.87	0.2675
C	3.123999	22.085	0.135003	0.2597
C	1.975997	17.566	2.863001	0.2631
C	1.975997	16.463	3.888999	0.2629
C	0.159997	7.508998	2.633004	0.2675
C	12.552	5.120003	10.64	0.2631

C	11.404	0.600998	13.368	0.2597
C	12.552	6.222997	9.614001	0.2629
C	14.368	7.508998	4.117996	0.2676
C	11.404	10.742	6.887003	0.2597
C	10.388	11.944	6.887003	0.2597
C	7.423997	15.177	4.117996	0.2676
C	7.104003	15.177	2.633004	0.2675
C	10.388	22.085	13.368	0.2597
C	9.239997	17.566	10.64	0.2631
C	9.239997	16.463	9.614001	0.2629
C	0.159997	3.834002	4.117996	0.2676
C	1.975997	5.120003	9.614001	0.2629
C	3.123999	0.600998	6.887003	0.2597
C	1.975997	6.222997	10.64	0.2631
C	10.742	13.368	0.2597	
C	4.140001	11.944	13.368	0.2597
C	4.140001	22.085	6.887003	0.2597
C	5.288006	17.566	9.614001	0.2629
C	5.288006	16.463	10.64	0.2631
C	14.368	3.834002	2.633004	0.2675
C	7.423997	3.834002	2.633004	0.2675
C	7.104003	3.834002	4.117996	0.2676
Cl	0.045996	13.81999	0.955	-0.5430
Cl	0.045996	20.20901	5.797	-0.5429
Cl	7.218004	2.476994	5.797	-0.5429
Cl	7.218004	8.866006	0.955	-0.5430
Cl	7.309996	2.476994	0.955	-0.5430
Cl	7.309996	8.866006	5.797	-0.5429
Cl	14.482	13.81999	5.797	-0.5429
Cl	14.482	20.20901	0.955	-0.5430
Cl	0.045996	2.476994	12.548	-0.5430
Cl	0.045996	8.866006	7.706	-0.5429
Cl	7.218004	13.81999	7.706	-0.5429
Cl	7.218004	20.20901	12.548	-0.5430
Cl	7.309996	13.81999	12.548	-0.5430
Cl	7.309996	20.20901	7.706	-0.5429
Cl	14.482	2.476994	7.706	-0.5429
Cl	14.482	8.866006	12.548	-0.5430
Cu	9.190006	3.573	6.676005	0.2308
Cu	9.190006	7.77	0.075995	0.2311
Cu	12.60199	14.916	0.075995	0.2311
Cu	12.60199	19.113	6.676005	0.2308
Cu	1.926006	14.916	6.676005	0.2308
Cu	1.926006	19.113	0.075995	0.2311
Cu	5.337994	3.573	0.075995	0.2311

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Cu	5.337994	7.77	6.676005	0.2309
Cu	12.60199	3.573	13.42701	0.2311
Cu	12.60199	7.77	6.826995	0.2308
Cu	9.190006	14.916	6.826995	0.2308
Cu	9.190006	19.113	13.42701	0.2310
Cu	1.926006	3.573	6.826995	0.2308
Cu	1.926006	7.77	13.42701	0.2311
Cu	5.337994	14.916	13.42701	0.2311
Cu	5.337994	19.113	6.826995	0.2308
F	1.758004	18.89701	8.952003	0.2990
H	0.755006	18.852	7.642995	0.3126
H	5.505996	3.788993	8.952003	0.2990
H	5.508994	3.834002	7.642995	0.3126
H	8.977999	3.175995	4.024002	0.3124
H	6.508002	3.788993	2.498001	0.2960
H	8.441001	0.907009	6.980997	0.3087
H	9.021002	3.788993	11.302	0.2989
H	8.019001	3.834002	12.61201	0.3131
H	8.977999	8.167005	2.727998	0.3126
H	8.848002	7.554007	4.252999	0.2958
H	12.82801	6.980997	7.156995	0.2911
H	6.087	0.907009	13.273	0.3085
H	1.699994	0.755006	13.09801	0.2913
H	8.963994	21.96	7.156995	0.2911
H	13.351	21.778	6.980997	0.3087
H	5.564006	21.96	13.09801	0.2913
H	12.814	19.51001	4.024002	0.3124
H	12.944	18.89701	2.498001	0.2960
H	1.177	21.77899	13.273	0.3085
H	12.77	18.89701	11.302	0.2989
H	13.77299	18.852	12.61201	0.3131
H	12.814	14.519	2.727998	0.3126
H	12.944	15.13199	4.252999	0.2958
H	1.758004	15.13199	11.302	0.2989
H	0.755006	15.177	12.61201	0.3131
H	5.550001	3.175995	2.727998	0.3126
H	5.679998	3.788993	4.252999	0.2958
H	5.550001	8.167005	4.024002	0.3124
H	5.679998	7.554007	2.498001	0.2960
H	5.564006	12.069	7.156995	0.2911
H	6.087	10.43599	6.980997	0.3087
H	1.699994	10.617	7.156995	0.2911
H	1.177	12.25001	6.980997	0.3087
H	5.505996	7.554007	11.302	0.2989
H	6.508994	7.508998	12.61201	0.3131

H	8.963994	12.069	13.09801	0.2913
H	8.441	10.43599	13.273	0.3085
H	9.022004	7.554007	8.952003	0.2990
H	8.019006	7.508998	7.642995	0.3126
H	12.82801	10.617	13.09801	0.2913
H	13.351	12.25001	13.273	0.3085
H	12.77	15.13199	8.952003	0.2990
H	13.77299	15.177	7.642995	0.3126
H	1.713999	19.51001	2.727998	0.3126
F	1.584002	18.89701	4.252999	0.2958
H	1.713999	14.519	4.024002	0.3124
H	1.584002	15.13199	2.498001	0.2960
H	1.699994	12.069	0.404995	0.2913
H	1.177	10.43599	0.229997	0.3085
H	0.755006	10.617	0.404995	0.2913
H	6.087	12.25001	0.229997	0.3085
H	1.750002	7.554007	4.550997	0.2990
H	0.755006	7.508998	5.860005	0.3126
H	12.814	3.175995	10.775	0.3126
H	12.944	3.788993	9.250001	0.2958
H	12.814	6.346005	9.478998	0.3124
H	12.944	7.554007	11.005	0.2960
H	12.82801	12.069	6.346005	0.2911
H	13.351	10.43599	6.522003	0.3087
H	12.77	7.554007	2.201003	0.2989
H	13.77299	7.508998	0.890995	0.3131
H	8.963994	10.617	6.346005	0.2911
H	8.441	12.25001	6.522003	0.3087
H	5.505996	15.13199	4.550997	0.2990
H	6.508994	15.177	5.860005	0.3126
H	9.022004	15.13199	2.201003	0.2989
H	8.019006	15.177	0.890995	0.3131
H	8.977999	19.51001	10.775	0.3126
H	8.848002	18.89701	9.250001	0.2958
H	8.977999	14.519	9.478998	0.3124
H	8.848002	15.13199	11.005	0.2960
H	1.758004	3.788993	2.201003	0.2989
H	0.755006	3.834002	0.890995	0.3131
H	1.713999	3.175995	9.478998	0.3124
H	1.584002	3.788993	11.005	0.2960
H	1.177	0.907009	6.522003	0.3087
H	1.713999	8.167005	10.775	0.3126
H	1.584002	7.554007	9.250001	0.2958
H	5.564006	0.725997	6.346005	0.2911
H	1.699994	21.96	6.346005	0.2911

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H	6.087	21.77899	6.522003	0.3087
H	5.550001	19.51001	9.478998	0.3124
H	5.679998	18.89701	11.005	0.2960
H	5.550001	14.519	10.775	0.3126
H	5.679998	15.13199	9.250001	0.2958
H	13.351	0.907009	0.229997	0.3085
H	12.77	3.788993	4.550997	0.2990
H	13.77299	3.834002	5.860005	0.3126
H	8.963994	0.725997	0.404995	0.2913
F	12.82801	21.96	0.404995	0.2913
H	8.441	21.77899	0.229997	0.3085
H	5.505996	18.89701	2.201003	0.2989
H	5.508994	18.852	0.890995	0.3131
H	9.069004	18.89701	4.550997	0.2990
H	5.509006	18.852	5.860005	0.3126
N	0.843002	18.852	8.588003	-0.4911
N	6.420998	3.834002	8.588003	-0.4911
N	9.006997	3.954011	3.442995	-0.4688
N	9.166994	0.230989	6.926998	-0.4844
N	8.107002	3.834002	11.667	-0.4914
N	9.006997	7.508989	3.308005	-0.4685
N	5.361006	11.11201	13.327	-0.4844
N	12.62501	22.455001	6.926998	-0.4845
N	12.785	18.73199	3.442995	-0.4688
N	1.902994	22.455001	13.327	-0.4844
N	13.685	18.852	11.667	-0.4914
N	12.785	15.29701	3.308005	-0.4685
N	0.843002	15.177	11.667	-0.4914
N	5.521003	3.954011	3.442995	-0.4685
N	5.521003	7.388989	3.442995	-0.4688
N	5.361006	11.11201	6.926998	-0.4844
N	1.902994	11.57399	6.926998	-0.4844
N	6.420998	7.508998	11.667	-0.4914
N	9.166994	11.11201	13.327	-0.4844
N	8.107002	7.508998	8.588003	-0.4911
N	12.62501	11.57399	13.327	-0.4844
N	13.685	15.177	8.588003	-0.4911
N	1.742997	18.73199	3.308005	-0.4685
N	1.742997	15.29701	3.442995	-0.4688
N	1.902994	11.11201	0.175998	-0.4844
N	5.361006	11.57399	0.175998	-0.4844
N	0.843002	7.508998	4.914997	-0.4911
N	12.785	3.954011	10.195	-0.4685
N	12.785	7.388989	10.06001	-0.4688
N	12.62501	11.11201	6.576002	-0.4844

N	13.685	7.508998	1.836003	-0.4914
N	9.166994	11.57399	6.576002	-0.4845
N	6.420998	15.177	4.914997	-0.4911
N	8.107002	15.177	1.836003	-0.4914
N	9.006997	18.73199	10.195	-0.4685
N	9.006997	15.29701	10.06001	-0.4688
N	0.843002	3.834002	1.836003	-0.4914
N	1.742997	3.954011	10.06001	-0.4688
N	1.902994	0.230989	6.576002	-0.4845
N	1.742997	7.388989	10.195	-0.4685
N	5.361006	22.45501	6.576002	-0.4845
N	5.521003	18.73199	10.06001	-0.4688
N	5.521003	15.29701	10.195	-0.4685
N	12.26001	0.230989	0.175998	-0.4844
N	6.420998	3.834002	4.914997	-0.4911
N	9.166994	22.45501	0.175998	-0.4844
N	6.420998	18.852	1.836003	-0.4914
N	8.107002	18.852	4.914997	-0.4911
S	1.745002	18.811	11.351	-0.3037
S	9.009002	3.874996	8.904	-0.3036
S	9.531995	5.475992	5.494006	-0.2806
S	10.91601	0.230989	6.348003	-0.2694
S	5.518998	3.874996	11.351	-0.3036
S	9.531995	5.867008	1.256994	-0.2811
S	10.91601	9.226011	0.403996	-0.2694
S	10.876	13.45999	0.403996	-0.2694
S	12.26001	16.81899	1.256994	-0.2811
S	10.876	20.56901	6.348003	-0.2694
S	12.783	18.811	8.904	-0.3036
S	12.26001	17.21001	5.494006	-0.2806
S	1.745002	15.218	8.904	-0.3036
S	4.996005	5.475992	1.256994	-0.2811
S	3.611995	2.116989	0.403996	-0.2694
S	4.996005	5.867008	5.494006	-0.2806
S	5.518998	7.468004	8.904	-0.3036
S	3.611995	9.226011	6.348003	-0.2694
S	3.652005	13.45999	6.348003	-0.2694
S	2.267995	16.81899	5.494006	-0.2806
S	9.009002	7.468004	11.351	-0.3037
S	12.783	15.218	11.351	-0.3037
S	3.652005	20.56901	0.403996	-0.2694
S	2.267995	17.21001	1.256994	-0.2811
S	1.745002	7.468004	2.152	-0.3037
S	5.518998	15.218	2.152	-0.3037
S	12.26001	5.475992	12.24601	-0.2811

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S	10.876	2.116989	13.099	-0.2694
S	12.26001	5.867008	8.008994	-0.2806
S	12.783	7.468004	4.599	-0.3036
S	10.876	9.226011	7.154997	-0.2694
S	10.91601	13.45999	7.154997	-0.2694
S	9.009002	15.218	4.599	-0.3036
S	9.531995	16.81899	8.008994	-0.2806
S	10.91601	20.56901	13.099	-0.2694
S	9.531995	17.21001	12.24601	-0.2811
S	1.745002	3.874996	4.599	-0.3036
S	2.267995	5.475992	8.008994	-0.2806
S	3.652005	2.116989	7.154997	-0.2694
S	2.267995	5.867008	12.24601	-0.2811
S	3.652005	9.226011	13.099	-0.2694
S	4.996005	13.45999	13.099	-0.2694
S	4.996005	16.81899	12.24601	-0.2811
S	3.611002	20.56901	7.154997	-0.2694
S	5.51899	18.811	4.599	-0.3036
S	4.996005	17.21001	8.008994	-0.2806
S	12.783	3.874996	2.152	-0.3037
S	9.009002	15.218	2.152	-0.3036

Table S8. Net atomic charges (NAC) for IDUDOA
Lattice vectors: [{ 15.290500, 0.000000, 0.000000 }, { 0.000000, 15.238600, 0.000000 },
{ -1.909200, 0.000000, 25.576100 }]

atom	X (Å)	Y (Å)	Z (Å)	NAC
Ag	9.88063	9.96036	23.90611	0.6832
Ag	3.500334	5.277752	1.669991	0.6832
Ag	10.19164	2.340756	14.45809	0.6830
Ag	3.190335	12.89736	11.11801	0.6835
Ag	2.546128	9.96036	14.45809	0.6833
Ag	11.14583	12.89736	1.669991	0.6831
Ag	10.83583	5.277752	11.11801	0.6831
Ag	2.235135	2.340756	23.90611	0.6830
C	7.670831	10.06535	2.220005	-0.0219
C	7.800828	9.618361	0.91299	-0.0621
C	9.024837	9.823365	0.179007	0.3939
C	9.23763	6.514761	22.54809	0.2291
C	7.951626	6.108759	23.28709	0.0371
C	6.905626	5.41176	22.66511	-0.1055
C	6.64663	6.279751	25.3051	-0.0678
C	7.801633	6.524757	24.5961	-0.0840
C	10.48563	6.198758	23.38211	0.0403

C	10.53464	5.127758	24.23811	-0.1041
C	11.66464	4.860763	24.97509	-0.0160
C	12.76963	5.702757	24.84511	-0.0689
C	12.74363	6.748764	23.93409	-0.0174
C	11.60963	6.998754	23.21811	-0.0990
C	0.560336	5.478764	0.07701	0.3956
C	9.390629	5.837755	21.18509	0.0286
C	9.622628	4.466754	21.0901	-0.1087
C	9.79063	3.847762	19.86511	-0.0427
C	9.716635	4.601752	18.70109	-0.0749
C	9.46964	5.97376	18.76511	-0.0254
C	9.31763	6.561756	19.99811	-0.1064
C	2.891634	3.96775	17.42211	0.4063
C	4.11327	8.724358	3.028006	0.2294
C	4.11327	9.129354	2.28901	0.0371
C	6.475337	9.827358	2.910995	-0.1064
C	6.73132	8.958361	0.271004	-0.0678
C	5.57937	8.713355	0.979999	-0.0844
C	2.895332	9.039355	2.193995	0.0404
C	2.846342	10.11136	1.337988	-0.1042
C	1.716326	10.11136	0.601013	-0.0162
C	0.612328	9.039362	0.730991	-0.0687
C	0.637335	8.47533	1.642011	-0.0171
C	1.772327	8.25235	2.357989	-0.0998
C	12.82164	9.7603	25.49909	0.3954
C	3.990335	9.400357	4.391007	0.0284
C	3.758336	10.77236	4.485997	-0.1084
C	3.590333	11.39136	4.71099	-0.0437
C	3.664328	10.63636	4.47909	-0.0739
C	3.912333	9.265358	6.810992	-0.0256
C	4.063334	8.677362	5.57799	-0.1061
C	3.489329	11.27036	8.15399	0.4057
C	5.711127	5.173764	23.3561	-0.0226
C	5.58113	5.619752	24.66311	-0.0622
C	4.356127	5.415753	25.39709	-0.3938
C	7.250631	2.140764	12.86511	-0.3954
C	10.83464	14.13437	15.81611	0.2292
C	12.12063	13.72836	15.07711	0.0369
C	13.16563	13.03036	15.6991	-0.1064
C	-0.92887	12.79335	15.00811	-0.0215
C	-0.79987	13.23936	13.70109	-0.0623
C	13.42564	13.89936	13.05911	-0.0678
C	12.27063	14.14436	13.7681	-0.0843
C	0.425136	13.03536	12.96711	0.3938
C	9.586636	13.81836	14.9821	0.0399

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C	9.53763	12.74736	14.12609	-0.1039
C	8.407632	12.48035	13.38909	-0.0161
C	7.302638	13.32136	13.51909	-0.0692
C	7.327629	14.36835	14.43011	-0.0169
C	8.462637	14.61836	15.14609	-0.0993
C	10.68063	13.45736	17.17911	0.0286
C	10.44863	12.08535	17.2741	-0.1085
C	10.28063	11.46735	18.49909	-0.0434
C	10.35464	12.22136	19.66311	-0.0744
C	10.60263	13.59337	19.59909	-0.0258
C	10.75464	14.18136	18.3661	-0.1060
C	10.17964	11.58736	20.94209	0.4060
C	2.546327	1.104753	9.759993	0.2289
C	1.268338	1.509764	10.49899	0.0370
C	2.54632	2.207753	9.877004	-0.1058
C	14.51083	2.445765	10.56799	-0.0220
C	14.1062	1.999761	11.87501	-0.0619
C	-0.04467	1.339762	12.51699	-0.0682
C	1.111339	1.093751	11.808	-0.0840
C	12.95583	2.203761	12.60899	0.3937
C	3.795337	2.207756	10.594	0.0404
C	3.844328	2.207755	11.45001	-0.1039
C	4.974326	2.707756	12.18701	-0.0165
C	6.078326	1.910755	12.05701	-0.0687
C	6.053334	0.869755	11.14599	-0.0164
C	4.918326	0.62076	10.43001	-0.0997
C	2.700335	1.781758	3.396992	0.0290
C	2.932333	3.15276	3.392002	-0.1089
C	3.100336	3.771752	7.777009	-0.0427
C	3.026341	3.017761	5.91299	-0.0749
C	2.778336	1.645754	5.977001	-0.0251
C	2.627335	1.057757	7.21000	-0.1069
C	3.20134	3.650757	4.634006	0.4057
C	6.130333	13.09736	12.71099	-0.3958
C	-0.39486	9.760354	12.86511	-0.3952
C	10.19184	8.724358	9.759993	-0.2294
C	8.905833	9.129354	10.49899	0.0373
C	7.860827	9.827358	9.877004	-0.1061
C	7.600837	8.958361	12.51699	-0.0672
C	8.75584	8.713355	11.808	-0.0844
C	11.43984	9.039355	10.594	0.0399
C	11.48883	10.11136	11.45001	-0.1040
C	12.61883	10.37737	12.18701	-0.0164
C	13.72384	9.536362	12.05701	-0.0688
C	13.69883	8.489363	11.14599	-0.0170

C	12.56384	8.239359	10.43001	-0.0992
C	10.34583	9.400357	8.396992	0.0281
C	10.57783	10.77236	8.302002	-0.1086
C	10.74583	11.39136	7.077009	-0.0435
C	10.67184	10.63636	5.91299	-0.0741
C	10.42383	9.265358	5.977007	-0.0258
C	10.27184	8.677362	7.210005	-0.1058
C	10.84684	11.27036	4.634006	0.4058
C	3.189127	6.514761	15.81611	0.2290
C	4.475131	6.108759	15.07711	0.0373
C	5.521131	5.41176	15.6991	-0.1056
C	5.780127	6.279751	13.05911	-0.0681
C	4.625139	6.524757	13.7681	-0.0841
C	1.94126	6.198758	14.9821	0.0400
C	4.625135	5.127758	14.12609	-0.1037
C	0.762137	4.860763	13.38909	-0.0161
C	-0.34122	5.702757	13.51909	-0.0689
C	-0.31687	6.748764	14.43011	-0.0175
C	0.817127	6.998754	15.14609	-0.0990
C	3.035134	5.837755	17.17911	0.0288
C	2.80413	5.837754	17.2741	-0.1092
C	2.636127	5.837762	18.49909	-0.0422
C	2.709128	4.625132	19.66311	-0.0754
C	2.957133	5.913757	19.59909	-0.0250
C	3.109128	6.561757	18.3661	-0.1067
C	2.534129	3.96775	20.94209	0.4062
C	13.77583	5.478764	12.71099	0.3956
C	8.204837	13.09736	2.07701	0.3956
C	11.78883	1.104753	2.910006	0.2287
C	13.07483	1.509764	2.28901	0.0371
C	14.12083	2.207753	2.910005	-0.1061
C	0.025336	2.445765	2.220005	-0.0220
C	0.155333	1.999761	0.91299	-0.0621
C	14.38084	1.339762	0.271004	-0.0678
C	13.22484	1.093751	0.979999	-0.0839
C	1.379327	2.203761	0.179007	-0.05934
C	10.54083	1.420756	2.193995	0.0410
C	10.49184	2.491755	1.337988	-0.1048
C	9.361836	2.75776	0.601013	-0.0158
C	8.256829	1.916757	0.730991	-0.0695
C	8.282829	0.869758	1.642011	-0.0160
C	9.416828	0.62076	2.357989	-0.0998
C	11.63583	1.781758	4.391007	0.0289
C	11.40383	3.15276	4.485997	-0.1090
C	11.23583	3.771752	5.71099	-0.0425

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C	11.30984	3.017761	6.875009	-0.0751
C	11.55683	1.645754	6.810992	-0.0251
C	11.70883	1.057757	5.577994	-0.1064
C	11.13484	3.650757	8.153993	0.4064
C	1.592136	14.13437	22.54809	0.2294
C	0.306132	13.72836	23.28709	0.0369
C	-0.73887	13.03036	22.66511	-0.1064
C	13.35563	12.79335	23.3561	-0.0216
C	13.22664	13.23936	24.66311	-0.0622
C	-0.99886	13.89936	25.3051	-0.0678
C	0.156139	14.14436	24.5961	-0.0841
C	12.00164	13.03536	25.39709	0.3936
C	2.840137	13.81836	23.38211	0.0398
C	2.89127	12.74736	24.23811	-0.1040
C	5.124135	12.48035	24.97509	-0.0158
C	5.09127	13.32136	24.84511	-0.0691
C	3.96413	14.36835	23.93409	-0.0169
C	1.746128	14.61836	23.21811	-0.0994
C	1.978127	13.45736	21.18509	0.0283
C	2.145136	12.98535	21.0901	-0.1083
C	2.072134	12.73735	19.86511	-0.0429
C	1.82413	12.22136	18.70109	-0.0748
C	1.672135	13.73527	18.76511	-0.0257
C	2.247134	14.11127	19.99811	-0.1063
C	5.176127	11.58735	17.42211	0.4060
C	6.715631	2.140764	25.49909	0.3956
C	6.845628	5.173764	15.00811	-0.0229
C	8.070631	5.619752	18.70109	-0.0617
C	6.665333	5.415753	15.00711	0.3936
C	6.535336	10.06535	10.56799	-0.0224
C	5.311327	9.618361	11.87111	-0.0621
F	-0.09987	9.823365	12.60811	0.3936
F	2.327135	9.027362	22.78611	-0.5028
F	2.007132	9.60236	23.6581	-0.4972
F	0.672128	8.631356	21.2331	-0.4970
F	1.015126	6.584751	22.2131	-0.5034
F	3.090127	7.536753	24.66311	-0.5045
F	1.626334	7.143764	23.0801	-0.5036
F	1.970327	8.654351	9.424997	-0.5038
F	4.045327	7.70136	11.87501	-0.5047
F	0.854326	8.094363	10.292	-0.5037
F	3.282335	6.211756	9.998004	-0.5030
F	2.961338	5.636758	10.87	-0.4971
F	8.317638	6.607762	8.444998	-0.4968
F		14.20436	22.2131	-0.5040

F	7.54563	1.407757	22.78611	-0.5029
F	8.660636	15.15636	24.66311	-0.5049
F	9.972629	1.982755	23.6581	-0.4972
F	10.73564	14.76335	23.0801	-0.5040
F	9.651632	1.011752	21.2331	-0.4971
F	9.271829	1.034762	9.424997	-0.5034
F	8.499836	13.83036	9.998004	-0.5027
F	9.614827	0.082761	11.87501	-0.5046
F	10.92684	13.25636	10.87	-0.4970
F	11.69084	0.475764	10.292	-0.5038
F	10.60683	14.22636	8.444998	-0.4969
F	12.70884	8.654351	3.363001	-0.5038
F	12.36584	7.70136	0.91299	-0.5049
F	10.73564	8.094363	2.495997	-0.5038
F	10.60683	6.211756	2.789994	-0.5030
F	11.69084	5.636758	1.918003	-0.4971
F	11.36584	6.607762	4.343001	-0.4969
F	12.52684	9.027362	15.5781	-0.5027
F	10.09964	9.60236	14.7061	-0.4970
F	10.41963	8.631356	17.1311	-0.4968
F	11.75463	7.70136	16.1511	-0.5032
F	11.41163	7.724355	13.70109	-0.5044
F	9.335637	7.124354	15.2841	-0.5036
F	5.064335	1.034762	3.363001	-0.5036
F	5.836328	13.83036	2.789994	-0.5031
F	4.720327	0.082761	0.91299	-0.5046
F	3.408334	13.25636	1.918003	-0.4969
F	2.645327	0.475764	2.495997	-0.5035
F	3.729331	14.22636	4.343001	-0.4967
F	4.109134	14.20436	16.1511	-0.5040
F	4.881127	1.407757	15.5781	-0.5030
F	3.766136	15.15636	13.70109	-0.5050
F	2.454128	1.982755	14.7061	-0.4972
F	1.691136	14.76335	15.2841	-0.5040
F	2.77514	1.011752	17.1311	-0.4970
H	8.385827	10.52736	2.642011	0.129
H	11.58764	7.724355	22.60411	0.1201
H	7.008638	5.097754	21.77511	0.1188
H	8.476836	6.553756	0.634006	0.1250
H	8.514626	6.989763	25.01811	0.1057
H	9.775634	4.560761	24.3231	0.1118
H	11.69263	4.115763	25.5661	0.0944
H	-1.77586	7.289765	23.8091	0.1058
H	9.666629	3.945761	21.88309	0.1091
H	9.956634	2.913757	19.8191	0.1242

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H	9.405641	6.491766	17.9721	0.1066
H	9.155629	7.497757	20.0411	0.1237
H	6.372341	10.14136	3.800992	0.1192
H	4.904128	8.684356	24.94209	0.1249
H	4.866338	8.248365	0.557994	0.1062
H	3.60533	10.67735	1.252999	0.1119
H	1.689328	11.12237	0.01	0.0947
H	15.15684	7.948362	1.767002	0.1057
H	3.715329	11.29336	3.69301	0.1090
F	3.425339	12.32536	5.757001	0.1246
H	3.975338	8.747353	7.604005	0.1067
H	4.226329	7.741361	5.535001	0.1233
H	1.793328	7.513757	2.971994	0.1203
H	4.905131	4.71176	22.93409	0.1132
H	1.793328	12.71635	16.58909	0.1191
H	-0.21487	12.33137	15.43011	0.1128
H	11.51111	14.60935	13.3461	0.1059
H	10.2956	12.18037	14.0411	0.1118
H	8.379638	11.73535	12.7981	0.0948
H	8.483638	0.194765	15.7601	0.1202
H	10.40564	12.71635	16.48111	0.1092
H	10.11563	11.29336	18.5451	0.1245
H	10.66563	14.60935	20.39211	0.1069
H	10.91664	15.11635	18.3231	0.1236
H	-0.12287	1.06475	13.42211	0.1248
H	13.50383	14.17336	12.15399	0.1250
H	0.318328	2.52176	3.987007	0.1190
H	13.59583	2.907753	5.14599	0.1129
H	1.824332	0.62975	1.22001	0.1060
H	3.085339	3.058753	11.535	0.1117
H	5.002335	3.503766	12.71635	0.0946
H	4.897326	15.13336	9.8160	0.1201
H	2.97534	3.673752	9.094989	0.1091
H	3.26533	4.705756	7.030998	0.1243
H	2.715331	1.127763	5.183994	0.1066
H	2.46434	0.121756	7.252998	0.1239
H	7.52263	8.684356	13.42211	0.1247
H	7.963838	10.14136	8.987007	0.1191
H	9.468832	8.248365	12.23001	0.1058
H	10.73083	10.67735	11.535	0.1119
H	12.64684	11.12237	12.778	0.0948
H	-0.82066	7.948362	11.021	0.1056
H	10.62084	11.29336	9.094989	0.1091
H	10.91084	12.32536	7.030998	0.1245
H	10.36084	8.747353	5.183994	0.1067

H	10.10984	7.741361	7.252998	0.1233
H	12.54284	7.513757	9.816005	0.1201
H	0.839137	7.724355	15.7601	0.1201
H	5.418135	5.097754	16.58909	0.1189
H	3.912131	6.989763	13.3461	0.1057
H	2.65013	4.560761	14.0411	0.1117
H	0.734128	4.115763	12.7981	0.0945
H	14.20263	7.289765	14.5551	0.1058
H	2.760129	3.945761	16.48111	0.1092
F	2.470139	2.913757	18.5451	0.1242
H	3.020138	6.491766	20.39211	0.1066
H	3.271129	7.497757	18.3231	0.1238
H	5.858334	6.553756	12.15399	0.1250
H	5.866635	14.90936	23.8091	0.1056
H	2.51134	2.52176	3.800992	0.1190
H	0.740332	2.907753	2.642011	0.1129
H	12.5665	1.064751	24.94209	0.1249
H	12.5118	0.62975	0.557994	0.1059
H	11.25084	3.058753	1.252999	0.1121
H	9.333829	3.503766	0.01	0.0945
H	9.438838	2.911336	2.971994	0.1201
H	11.36084	2.911336	3.69301	0.1091
H	11.06984	4.711176	5.757001	0.1242
H	11.62083	1.12176	7.604005	0.1066
H	11.87083	0.12176	5.535001	0.1235
H	-0.63586	12.71635	21.77511	0.1191
H	12.64164	12.33137	22.93409	0.1130
H	0.832335	14.17336	22.634006	0.1250
H	0.869131	14.60935	22.60811	0.1057
H	2.131133	12.18037	24.3231	0.1118
H	4.047135	11.73535	25.5661	0.0947
H	3.942126	0.104765	22.604	0.1202
H	2.021134	11.56436	21.88309	0.1090
H	2.311139	10.53336	19.8191	0.1242
H	1.76114	14.11136	17.9721	0.1069
H	1.510134	15.11636	20.0411	0.1236
H	7.511329	0.328758	1.767002	0.1053
H	7.430626	4.711176	15.43011	0.1133
H	5.950337	10.52736	10.14599	0.1130
H	6.823826	0.328758	11.021	0.1053
H	6.557138	14.90936	14.5551	0.1056
N	8.060636	9.954356	25.13609	-0.4310
N	11.89264	9.911353	24.8501	-0.4416
N	10.06363	11.06937	21.9491	-0.4339
N	1.488326	5.327765	0.726003	-0.4415

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N	10.00864	3.44976	16.4151	-0.4343
N	3.372339	11.78835	9.161001	-0.4339
N	5.320328	5.284762	0.440011	-0.4309
N	3.31833	4.169753	3.626998	-0.4338
N	8.17963	2.291764	13.5141	-0.4416
N	12.01064	2.334752	13.22811	-0.4309
N	1.370342	12.90435	12.34799	-0.4310
N	5.202327	12.94636	12.062	-0.4417
N	0.534135	9.911353	13.5141	-0.4413
N	10.96283	11.78835	3.626998	-0.4338
N	9.015836	5.284762	12.34799	-0.4309
N	12.84784	5.327765	12.062	-0.4414
N	11.01783	4.169753	9.161001	-0.4346
N	4.361137	9.954356	13.22811	-0.4309
N	16.613	11.06937	16.4151	-0.4338
N	2.418132	3.44976	21.9491	-0.4340
N	9.13152	12.94636	0.726003	-0.4416
N	0.41613	2.334752	25.13609	-0.4307
N	12.96584	12.90435	0.440011	-0.4307
N	4.247127	2.291764	24.8501	-0.4414
O	9.200638	7.939356	22.40211	-0.4059
O	4.180341	5.284762	3.173994	-0.4057
O	10.87064	0.319752	15.9621	-0.4057
O	2.510328	14.91836	9.614005	-0.4057
O	10.15584	7.299752	9.614005	-0.4056
O	3.226135	7.939356	15.9621	-0.4057
O	11.82584	14.91836	3.173994	-0.4056
O	1.555128	0.319752	22.40211	-0.4051
Sb	1.499128	8.087354	21.9491	2.1539
Sb	2.454328	7.150759	10.161	2.1547
Sb	9.144638	0.468755	22.941	2.1556
Sb	10.09883	14.77036	10.161	2.1540
Sb	11.88184	7.150759	2.626998	2.1552
Sb	10.92763	8.087354	15.4151	2.1534
Sb	4.236326	14.77036	2.626998	2.1538
Sb	3.282135	0.468755	15.4151	2.1557

Table S9. Net atomic charges (NAC) for KEXFAU
Lattice vectors: [{ 28.590200, 0.000000, 0.000000 }, { 0.000000, 9.087000, 0.000000 },
{ -4.774700, 0.000000, 16.564500 }]

atom	X (Å)	Y (Å)	Z (Å)	NAC
C	14.3269	6.880486	8.825218	0.0915
C	15.14791	6.068489	9.796212	-0.1724

C	15.9849	6.91349	10.74022	-0.0904
C	16.90191	6.097486	11.62821	-0.1195
C	17.76991	6.925484	12.55221	-0.0949
C	18.66691	6.083483	13.43722	-0.1259
C	19.5819	6.897487	14.34022	-0.0721
C	20.38591	6.064491	15.31921	-0.2147
C	21.30691	6.880486	16.21121	0.0984
C	11.1719	6.352485	11.17322	0.1101
C	11.16291	8.981491	11.20421	0.0826
C	10.26571	8.981491	13.64222	0.0825
C	10.25671	6.352485	13.67423	0.1101
C	9.488388	2.206487	7.738719	0.0914
C	8.66741	3.018483	6.768719	-0.1733
C	7.867392	2.173483	5.823714	-0.0892
C	6.97713	2.989487	4.936718	-0.1191
C	6.043411	2.161488	4.011723	-0.0952
C	5.14612	3.00349	3.127725	-0.1248
C	4.23341	2.189485	2.224712	-0.0728
C	3.429411	3.022491	1.245717	-0.2146
C	2.508413	2.206487	0.352724	0.0981
C	12.6434	6.749487	5.391712	0.1104
C	0.031688	2.173485	8.825218	0.0915
C	0.852694	1.553489	9.796212	-0.1718
C	1.689712	2.309485	10.74022	-0.0909
C	2.606692	1.553489	11.62821	-0.1191
C	3.474694	2.381485	12.55221	-0.0949
C	4.371691	1.540483	13.43722	-0.1252
C	5.286689	2.353488	14.34022	-0.0719
C	6.090693	1.521491	15.31921	-0.2148
C	7.011692	2.337485	16.21121	0.0982
C	-3.12329	1.809485	11.17322	0.1099
C	-3.13231	4.438491	11.20421	0.0826
C	24.56089	4.438491	13.64222	0.0826
C	24.5519	1.809485	13.67423	0.1104
C	23.7836	6.749487	7.738719	0.0916
C	22.9626	7.562483	6.768719	-0.1735
C	22.12561	6.717483	5.823714	-0.0896
C	21.2096	7.533486	4.936718	-0.1194
C	20.3406	6.705488	4.011723	-0.0943
C	19.44359	7.54649	3.127725	-0.1245
C	18.5286	6.733485	2.224712	-0.0723
C	17.7246	7.565491	1.245717	-0.2147
C	16.8036	6.749487	0.352724	0.0977
C	26.93861	7.277488	5.391712	0.1105
C	16.71461	2.206487	0.543713	0.0908

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C	17.53562	3.018483	1.513714	-0.1731
C	18.37261	2.173483	2.457725	-0.0897
C	19.28861	2.989487	3.345714	-0.1198
C	20.15761	2.161488	4.270726	-0.0944
C	21.05461	3.00349	5.154723	-0.1250
C	21.96961	2.189485	6.05772	-0.0727
C	22.77362	3.022491	7.036716	-0.2145
C	23.69461	2.206487	7.929724	0.0981
C	13.5596	2.734487	2.890721	0.1102
C	7.100709	6.880486	16.02122	0.0914
C	6.279703	6.068489	15.05022	-0.1730
C	5.442714	6.91349	14.10621	-0.0898
C	4.526706	6.097486	13.21822	-0.1194
C	3.657703	6.925484	12.29422	-0.0951
C	2.747706	6.083483	11.40921	-0.1250
C	1.843703	6.897487	10.50723	-0.0726
C	1.047703	6.064491	9.528215	-0.2144
C	0.12170	6.880486	8.635223	0.0979
C	21.3959	2.337485	16.02122	0.0914
C	20.57489	1.52449	15.05022	-0.1735
C	19.7379	6.91349	14.10621	-0.0898
C	18.82189	6.880486	13.21822	-0.1192
C	17.95289	2.337485	12.29422	-0.0944
C	17.05589	1.52449	11.40921	-0.1247
C	16.14089	2.353487	10.50723	-0.0726
C	15.33689	1.521491	9.528215	-0.2145
C	14.41689	2.337485	8.635223	0.0975
C	2.419395	6.749487	7.543713	0.0915
C	3.240402	7.562483	1.513714	-0.1732
C	4.077391	6.717483	2.457725	-0.0902
C	4.993399	7.533486	3.345714	-0.1193
C	5.862396	6.705488	4.270726	-0.0944
C	6.759398	7.54649	5.154723	-0.1241
C	7.674396	6.733485	6.05772	-0.0725
C	8.478401	7.565491	7.036716	-0.2146
C	9.399394	6.749487	7.929724	0.0983
C	-0.73561	7.277488	2.890721	0.1106
C	13.55061	0.105491	2.921713	0.0828
C	12.65241	0.105491	5.360719	0.0829
C	26.9476	4.648491	5.360719	0.0830
C	-0.7446	4.648491	2.921713	0.0830
Cd	11.9079	4.543491	8.282217	0.7975
Cd	-4.7743	0.000491	16.56422	0.7980
Cd	9.52091	4.543491	16.56422	0.7977
Cd	-2.38731	9.086491	8.282217	0.7975

H	13.62791	7.342487	9.259224	0.0669
H	14.9099	7.460491	8.381223	0.0430
H	14.5469	5.479488	10.33622	0.0682
H	15.68091	5.515491	9.276219	0.0645
H	15.4129	7.360488	11.29722	0.0645
H	16.45291	7.551488	10.27022	0.0528
H	17.41491	5.615484	11.09822	0.0621
H	16.32291	5.506486	12.20822	0.0562
H	17.2369	7.487488	13.10222	0.0529
F	18.2769	7.451485	12.07522	0.0549
H	18.1559	5.543488	13.98022	0.0585
H	19.19591	5.515491	12.85422	0.0629
H	20.19091	7.487488	13.76522	0.0390
H	19.7369	7.533486	14.74222	0.0477
H	19.75092	5.479488	14.79221	0.0947
H	19.71089	5.561489	15.91822	0.0794
H	26.4155	6.324488	0.331721	0.0705
H	25.5646	7.560484	0.181713	0.0360
H	22.17691	7.914486	14.80822	0.2936
H	22.93991	6.851489	15.23922	0.2984
H	13.54589	6.714486	10.03822	0.2939
H	12.78391	2.750489	9.607211	0.2981
H	10.2694	5.715507	6.526711	0.2936
H	11.03141	6.715487	6.956726	0.2980
H	10.18841	1.7444	7.304713	0.0671
H	8.905394	1.626491	8.182714	0.0429
H	9.269415	3.607484	5.228716	0.0683
H	8.134414	3.571491	7.288711	0.0646
H	8.402411	1.726485	5.566726	0.0643
H	7.363406	1.535485	6.294725	0.0526
H	6.400405	3.471488	5.466709	0.0618
H	7.492412	3.580487	4.356715	0.0562
H	6.578396	1.599485	3.461715	0.0528
H	5.539391	1.635487	4.488714	0.0547
H	5.659395	3.543485	2.583714	0.0581
H	4.619412	3.571491	3.710713	0.0528
H	3.624409	1.599485	2.799715	0.0390
H	4.678395	1.553486	1.821714	0.0481
H	2.862403	3.607484	1.772716	0.0947
H	4.102403	3.525483	0.645717	0.0795
H	-2.6783	2.762484	16.23323	0.0705
H	-1.74929	1.526489	16.38222	0.0362
H	1.638409	1.172487	1.755721	0.2938
H	0.876408	2.235484	1.324713	0.2982
H	-0.66731	2.798487	9.259224	0.0669

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H	0.614711	2.916491	8.381223	0.0432
H	0.25169	0.935488	10.33622	0.0680
H	1.38569	0.972491	9.276219	0.0643
H	1.117688	2.816488	11.29722	0.0646
H	2.157694	3.007488	10.27022	0.0528
H	3.1197	1.072484	11.09822	0.0621
H	2.027693	0.963486	12.20822	0.0562
H	2.941709	2.944488	13.10222	0.0527
H	3.981686	2.907486	12.07522	0.0547
F	3.86071	0.999488	13.98022	0.0581
H	4.900693	0.972491	12.85422	0.0627
H	5.895696	2.944488	13.76522	0.0388
H	4.84171	2.989487	14.74222	0.0478
H	6.65702	0.935488	14.79221	0.0946
H	12.1984	1.01749	15.91822	0.0794
H	11.2552	1.781488	0.331721	0.0707
H	7.88169	3.016484	0.181713	0.0363
H	8.644698	3.371486	14.80822	0.2935
H	23.79589	2.308489	15.23922	0.2980
H	24.69191	7.996487	9.094225	0.3043
H	-0.7493	7.205723	9.359224	0.3018
H	-1.5113	10.03822	10.03822	0.2940
H	0.019399	6.85509	9.607211	0.2983
H	-0.8766	1.095487	7.470722	0.3043
H	24.4836	2.0084	7.205723	0.3026
H	23.20061	6.288486	7.304713	0.0669
H	23.5646	6.170491	3.182714	0.0431
H	22.4296	8.151484	3.228716	0.0684
H	22.6976	8.114491	7.205711	0.0649
H	21.65859	6.270484	5.267726	0.0643
H	20.69559	6.079485	6.294705	0.0528
H	21.7876	8.014489	5.466711	0.0620
H	20.87361	8.123487	4.356712	0.0563
H	19.83461	6.142485	3.461715	0.0526
H	19.95461	6.179487	4.488714	0.0542
H	18.9146	8.087485	2.583714	0.0577
H	17.9196	8.114491	3.710713	0.0628
H	18.97361	6.142485	2.799715	0.0389
H	17.15759	6.097486	1.821714	0.0478
H	18.39759	8.151484	1.772716	0.0946
H	11.61689	8.069483	0.645717	0.0793
H	12.54589	7.305485	16.23323	0.0708
H	15.9336	6.070489	16.38222	0.0363
H	15.17159	5.715487	1.755721	0.2934
H		6.778484	1.324713	0.2984

H	24.56462	1.172487	6.526711	0.2936
H	25.32659	2.235484	6.956726	0.2981
H	24.1059	2.762484	8.613225	0.0707
H	23.17691	1.526489	8.464211	0.0361
H	11.92691	3.453487	15.75322	0.3041
H	11.03191	2.535491	15.48822	0.3018
H	16.01459	1.744486	0.97772	0.0671
H	17.2966	1.626491	0.099718	0.0432
H	16.93361	3.607484	2.053716	0.0682
F	18.06861	3.571491	0.993721	0.0647
H	17.80061	1.726485	3.014722	0.0644
H	18.83959	1.535485	1.987723	0.0528
H	19.80159	3.471488	2.815717	0.0622
H	18.79961	3.580487	3.92572	0.0561
H	19.666	1.599485	4.820717	0.0527
H	20.60461	1.635487	3.793718	0.0546
H	20.533	3.543485	5.697724	0.0582
H	21.5826	3.571491	4.571719	0.0628
H	22.57859	1.599485	5.482717	0.0390
H	21.5246	1.553486	6.459724	0.0479
H	23.33959	2.235484	6.509716	0.0947
H	22.1006	2.235483	7.636715	0.0793
H	11.88841	5.615486	0.811727	0.3044
H	12.7834	6.554487	1.076726	0.3025
H	7.800703	7.342487	15.58721	0.0669
H	6.518716	7.460491	16.46521	0.0430
H	6.881708	5.479488	14.51022	0.0682
H	5.746707	5.515491	13.557022	0.0645
H	6.014704	7.360488	11.557023	0.0643
H	4.975699	7.551488	14.57722	0.0528
H	4.013698	5.615484	13.747024	0.0623
H	5.105706	5.506486	12.638022	0.0560
H	4.190717	7.487488	11.74421	0.0528
H	3.151712	7.451485	12.77121	0.0547
H	3.271716	5.543488	10.86621	0.0584
H	2.232705	5.515491	11.99222	0.0628
H	1.237703	7.487488	11.08122	0.0391
H	2.290716	7.533486	10.10421	0.0480
H	0.475696	5.479488	10.05422	0.0946
H	1.714695	5.561489	8.928216	0.0794
H	-0.29059	6.324488	7.950712	0.0707
H	0.638386	7.560484	8.099726	0.0362
H	9.81069	7.305485	8.613225	0.0707
H	8.88169	6.070489	8.464211	0.0363
H	26.18359	1.090485	0.811727	0.3041

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H	27.07859	2.008491	1.076726	0.3026
H	22.09592	2.798487	15.58721	0.0670
H	20.8139	2.916491	16.46521	0.0432
H	21.17689	0.935488	14.51022	0.0684
H	20.04189	0.972491	15.57022	0.0648
H	20.30989	2.816488	13.55023	0.0642
H	19.27091	3.007488	14.57722	0.0528
H	18.30891	1.072484	13.74822	0.0623
H	19.40089	0.963486	12.63822	0.0559
F	18.4859	2.944488	11.74421	0.0526
H	17.4469	2.907486	12.77121	0.0545
H	17.5669	0.999488	10.86621	0.0579
H	16.52789	0.972491	11.99222	0.0627
H	15.52789	2.944488	11.08122	0.0391
H	15.52789	2.989487	10.10421	0.0480
H	14.77091	0.935488	10.05422	0.0945
H	16.0022	1.01749	8.928216	0.0794
H	-2.3683	7.996487	15.75322	0.3039
H	-3.2633	7.078491	15.48822	0.3025
H	1.719402	6.288486	0.97772	0.0669
H	3.001389	8.123487	0.099718	0.0432
H	2.638396	8.123484	2.053716	0.0685
H	3.773398	8.123484	0.993721	0.0649
H	3.505396	6.272487	3.014722	0.0643
H	4.544401	6.079487	1.987723	0.0529
H	5.506407	8.014489	2.815717	0.0622
H	4.414399	8.123487	3.92572	0.0559
H	5.329388	6.142485	5.820717	0.0526
H	6.368393	6.179487	5.820718	0.0542
H	6.248389	8.087485	5.697724	0.0577
H	7.287399	8.114491	4.571722	0.0626
H	8.283403	6.142485	5.482722	0.0390
H	7.229389	6.097486	6.459724	0.0478
H	9.044409	8.151484	6.509716	0.0946
H	7.805409	8.069483	7.636715	0.0791
H	14.0046	1.781488	7.950712	0.0710
H	14.9336	3.016484	8.099726	0.0365
H	14.31461	5.633486	7.470722	0.3044
H	13.41859	6.551491	7.205723	0.3022
H	9.500701	3.453487	9.094225	0.3042
H	10.3967	2.535491	9.359224	0.3012
N	22.42391	7.50449	15.51121	-0.6289
N	11.45689	5.565488	10.40121	-0.4429
N	11.4139	0.740491	10.47022	-0.4575
N	13.29992	2.96149	9.336216	-0.6286

N	10.01371	0.740491	14.37621	-0.4576
N	10.5154	6.125483	7.228715	-0.6282
N	1.391409	1.582483	1.053718	-0.6286
N	12.3584	3.521485	6.163717	-0.4430
N	-2.88131	5.28449	10.47022	-0.4575
N	24.3089	5.28449	14.37621	-0.4577
N	8.128696	2.96149	15.51121	-0.6283
N	-2.83829	1.022487	10.40121	-0.4426
N	24.42891	7.607491	8.752218	-0.6332
N	-0.9953	7.50449	9.336216	-0.6289
N	-0.61359	1.479491	7.811719	-0.6341
N	15.68659	6.125483	1.053718	-0.6281
N	26.65361	8.064485	6.163717	-0.4430
N	24.50959	1.582483	7.228715	-0.6283
N	16.0939	3.064491	16.09422	-0.6326
N	13.6446	3.521485	2.118716	-0.4429
N	12.51121	6.022491	0.470713	-0.6340
N	9.97068	5.565488	14.44622	-0.4428
N	26.81661	1.479491	0.470713	-0.6338
N	24.2659	1.022487	14.44622	-0.4431
N	-3.0013	7.607491	16.09422	-0.6335
N	-0.45058	8.064485	2.118716	-0.4432
N	13.80161	8.34501	2.187723	-0.4577
N	12.40139	8.34501	6.093715	-0.4578
N	26.6966	3.802491	6.093715	-0.4577
N	-0.49361	3.802491	2.187723	-0.4578
N	13.6816	6.022491	7.811719	-0.6334
N	10.13369	3.064491	8.752218	-0.6324
Ni	10.71389	7.656488	11.40323	-0.0043
Ni	13.1016	1.430485	4.140711	-0.0050
Ni	25.0089	3.112488	12.4205	-0.0045
Ni	27.39662	5.974484	4.140711	-0.0053

Table S10. Net atomic charges (NAC) for OHETIE

Lattice vectors: [{ 13.193100, 0.000000, 0.000000 }, { -6.596550, 11.425560, 0.000000 },
{ 0.000000, 0.000000, 11.349800 }]

atom	X (Å)	Y (Å)	Z (Å)	NAC
C	-2.80255	10.31256	5.772996	0.6905
C	-3.69355	9.731561	4.689998	-0.3042
C	-3.10055	9.835556	3.292997	-0.1252
C	-1.84755	8.981564	3.084002	0.0385
C	-0.20355	9.633564	1.409997	0.5269
C	0.05045	9.807564	11.2658	-0.1573

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C	-2.15755	7.497555	3.305005	0.6042
C	3.793999	1.112998	9.359998	0.6896
C	2.902997	1.693999	10.443	-0.3030
C	3.496	1.590004	0.490198	-0.1255
C	4.749001	2.443996	0.699204	0.0379
C	6.393	1.791996	2.373198	0.5273
C	6.647	1.617996	3.867195	-0.1571
C	4.438997	3.928005	0.478201	0.6067
Cd	5.594996	0	7.567002	1.0298
C	-2.79754	4.845557	3.784001	0.4210
Cd	3.798993	6.580003	0.000204	0.4216
H	-4.54554	10.19456	4.703005	0.1302
H	3.86255	8.798561	4.891003	0.1184
H	-2.87755	10.76256	3.116996	0.0756
H	0.22345	9.565559	2.647999	0.0836
H	-1.14955	9.266563	3.709001	0.1102
H	-1.91555	9.000565	1.081	0.3229
H	0.22345	8.943563	10.8618	0.1389
H	-0.73854	10.18556	10.8438	0.1492
H	1.335458	10.79156	10.1698	0.3310
H	1.925454	10.78856	0.067997	0.3186
H	7.634009	0.05995	0.058996	0.3410
H	2.050993	1.273001	10.429	0.1304
H	2.734	2.62399	10.242	0.1181
H	3.719003	0.663001	0.666199	0.0752
H	2.825006	1.860001	1.135196	0.0830
H	5.446996	2.158997	0.074205	0.1103
H	4.662	2.424995	2.702194	0.3245
H	6.820002	2.481997	4.272002	0.1384
H	5.857994	1.240005	4.289203	0.1493
H	7.931995	0.634004	4.963002	0.3307
H	8.521991	1.087005	3.715001	0.3191
H	1.037446	11.36157	3.724199	0.3419
N	-1.39055	9.186562	1.720005	0.4027
N	1.200447	10.69456	11.0438	0.3477
N	5.205997	2.238998	2.063201	0.4042
N	7.796997	0.730996	4.089197	-0.3480
O	-2.72455	9.759565	6.886003	-0.5416
O	-2.17455	11.36856	5.529997	-0.6115
O	0.669444	9.90756	2.226002	-0.5778
O	-2.79855	6.884563	2.427995	-0.5541
O	-1.77755	6.955561	4.371001	-0.4844
O	3.871997	1.665995	8.247003	-0.5412
O	4.422004	0.057002	9.602998	-0.6114
O	7.265994	1.518	1.557204	-0.5776

O	3.798003	4.540997	1.3552	-0.5547
O	4.819004	4.469999	10.76201	-0.4856
O	0.76545	10.40656	6.210996	-0.4259
O	7.362	1.019	8.921998	-0.4259
O	0.316443	9.486562	8.154003	-0.3841
O	6.913006	1.938998	6.979003	-0.3838

Table S11. Net atomic charges (NAC) for YARYEV

Lattice vectors: [{ 12.063000, 0.000000, 0.000000 }, { 0.000000, 12.174000, 0.000000 },
 { -0.249000, 0.000000, 14.618800 }]

atom	X (Å)	Y (Å)	Z (Å)	NAC
C	7.117008	10.82801	9.701372	-0.0517
C	5.845011	1.16	12.30038	-0.0531
C	7.117007	11.014	4.990581	-0.0536
C	4.571009	10.82801	12.22737	-0.0517
C	4.617007	1.16	9.62838	-0.0534
C	1.041012	7.247	12.30038	-0.0533
C	10.64801	7.247	9.62838	-0.0535
C	1.083013	4.990006	9.701372	-0.0518
C	10.60601	4.990006	12.22737	-0.0519
C	1.166014	4.990581	4.990581	-0.0538
C	4.741003	11.014	2.318571	-0.0534
C	10.77301	4.921003	2.318571	-0.0535
C	7.239008	1.345994	2.391577	-0.0517
C	4.699002	1.345994	4.917574	-0.0517
C	10.73101	7.432994	4.917574	-0.0517
C	1.208002	7.432994	2.391577	-0.0519
Cd	5.845011	12.095	10.96438	0.4523
Cd	8.923004	9.130001	7.309371	0.9908
Cd	8.798004	3.043001	14.618838	0.9903
Cd	5.969011	0.078997	3.654568	0.4526
Cd	2.767011	9.130999	14.61838	0.9905
Cd	-0.06199	6.165997	3.654568	0.4525
Cd	11.876	6.008003	10.96438	0.4524
Cd	2.891009	3.043001	7.309371	0.9908
H	10.19901	11.64401	8.031379	0.3382
H	11.43801	10.368	8.093377	0.3395
H	6.892007	7.197999	8.09038	0.3331
H	10.95401	11.063	6.528581	0.3327
H	7.64601	6.616995	6.586573	0.3383
H	6.40801	7.893001	6.525569	0.3399
H	4.168005	5.557005	8.031379	0.3384
H	5.406012	4.280999	8.093377	0.3399

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H	0.860013	1.110999	8.09038	0.3329
H	4.922002	4.976001	6.528581	0.3330
H	1.615004	0.529995	6.586573	0.3383
H	0.376003	1.806001	6.525569	0.3396
H	1.490003	11.64401	13.89637	0.3384
H	0.252003	10.368	13.83538	0.3401
H	0.985009	11.063	0.78158	0.3327
H	4.292012	6.616995	0.722578	0.3383
H	5.531013	7.893001	0.783568	0.3396
F	4.798007	7.197999	13.83738	0.3328
H	7.52201	5.557005	13.89637	0.3383
H	6.283008	4.280999	13.83538	0.3397
H	7.016003	4.976001	0.78158	0.3324
H	10.6401	0.529995	0.722578	0.3385
H	10.6401	1.806001	0.783568	0.3399
H	10.82901	1.110999	13.83738	0.3330
N	7.71002	10.177	9.00638	-0.3772
N	10.6040	10.77201	7.518376	-0.8755
N	10.04101	7.856004	8.895379	-0.3742
N	7.68001	1.769004	13.03237	-0.3743
N	7.805007	4.317996	5.723567	-0.3744
N	10.12801	8.083999	5.612581	-0.3770
N	7.241009	7.470004	7.10057	-0.8763
N	3.97201	10.27701	12.92137	-0.3768
N	1.649005	7.856004	13.03237	-0.3744
N	1.68601	4.090001	9.00638	-0.3770
N	4.573012	4.685006	7.518376	-0.8764
N	4.009003	1.769004	8.895379	-0.3745
N	10.003	4.090001	12.92137	-0.3767
N	1.773012	4.317996	5.723567	-0.3740
N	4.096005	1.996999	5.612581	-0.3771
N	1.210004	1.401994	7.10057	-0.8760
N	4.13301	10.405	1.586578	-0.3744
N	1.085008	10.77201	14.40937	-0.8761
N	1.811007	8.083999	1.697579	-0.3769
N	4.697012	7.488994	0.208581	-0.8758
N	10.16501	4.317996	1.586578	-0.3743
N	7.117002	4.685006	14.40937	-0.8754
N	7.842012	1.996999	1.697579	-0.3770
N	10.72901	1.401994	0.208581	-0.8763

Table S12. Net atomic charges (NAC) for ZUQPOQ

Lattice vectors: [{ 11.071000, 0.000000, 0.000000 }, { 0.000000, 21.824000, 0.000000 },
 { 0.000000, 0.000000, 7.953000 }]

atom	X (Å)	Y (Å)	Z (Å)	NAC
Ag	1.444002	0.059994	0.212003	0.3210
Ag	4.091997	21.76401	4.188002	0.3212
Ag	9.626998	10.97199	3.764998	0.3212
Ag	6.979003	10.85201	7.740997	0.3208
C	0.168999	3.411004	0.429001	-0.1681
C	0.034995	5.913998	0.215001	-0.1173
C	1.932	2.84801	6.132002	-0.1826
C	1.517004	4.074999	5.336002	0.0863
C	2.059996	5.301006	5.639003	-0.1466
C	1.429998	6.433999	4.993999	-0.0781
C	0.558001	6.368003	4.072	0.0578
C	0.034995	5.116004	3.753999	-0.1339
C	0.570999	3.984997	4.334003	-0.1274
C	10.607	4.664007	7.825999	0.0643
C	10.603	7.059999	7.563001	-0.1555
C	9.610004	1.429002	6.569003	0.0877
C	9.077999	7.743999	6.306999	-0.1028
C	9.543003	4.575999	6.918999	-0.1332
C	9.239004	8.182999	5.758004	-0.2024
C	10.938	7.614001	3.538998	-0.1711
C	5.366003	18.413	4.406002	-0.1675
C	5.998998	17.15999	3.848998	0.0645
C	5.499995	15.91	3.4191	-0.1174
C	6.004003	14.764	3.389002	-0.1559
C	6.997005	14.847	2.592996	0.0883
C	7.528003	16.08001	2.329008	-0.1036
C	7.062999	17.22601	2.94	-0.1330
C	7.368005	13.64201	1.781003	-0.2037
C	3.603998	18.97599	2.155001	-0.1830
C	4.019005	17.749	1.360003	-0.0867
C	3.475995	16.52299	1.662002	-0.1469
C	3.952004	15.39	1.018	-0.0787
C	4.977998	15.456	0.094999	0.0584
C	4.964004	17.839	0.357996	-0.1270
C	5.440002	16.708	7.729998	-0.1345
C	5.667998	14.21	7.515999	-0.1713
C	5.072002	6.247993	0.127001	0.0640
C	5.066997	3.852001	0.389999	-0.1558
C	4.073995	3.934998	1.383997	0.0887
C	3.542997	5.16801	1.646001	-0.1037

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C	4.008001	6.314011	1.034001	-0.1324
C	3.702995	2.730008	2.194996	-0.2035
C	7.467002	8.06399	1.820998	-0.1824
C	7.051995	6.837001	2.616998	0.0867
C	7.595005	5.610994	2.313997	-0.1473
C	7.118996	4.478001	2.959001	-0.0778
C	6.093002	4.543997	3.881	0.0579
C	5.630998	5.795996	4.199001	-0.1342
C	6.106996	6.927003	3.618997	-0.1273
C	5.403002	3.297999	4.414002	-0.1707
C	5.704997	7.500996	7.523999	-0.1676
C	5.571005	4.998002	7.737999	-0.1170
C	10.902	14.323	3.546998	-0.1673
C	11.05601	16.826	3.762	-0.1172
C	13.76001	13.76001	5.797999	-0.1828
C	9.553996	14.987	6.592997	0.0863
C	9.011002	16.21301	6.290998	-0.1466
C	9.488002	17.346	6.935	-0.0781
C	10.513	17.28	7.858001	0.0582
C	10.5	14.897	7.595004	-0.1269
C	0.463997	11.05601	4.104002	0.0646
C	0.468004	11.0572	4.365998	-0.1559
C	1.460996	17.346	5.360004	0.0878
C	1.993001	16.63599	5.623002	-0.1030
C	1.527997	15.509	5.01	-0.1335
C	1.831996	19.09399	6.171997	-0.2029
C	0.132996	18.526	0.437001	-0.1719
C	10.976	16.028	1.223002	-0.1346
H	0.932001	3.568006	0.047001	0.1050
H	0.647997	6.004001	0.836998	0.0937
H	2.542998	1.904995	5.774999	0.1152
H	2.593005	2.920008	6.792999	0.0976
H	2.714997	5.381995	6.350001	0.0973
H	1.987001	7.13599	5.207998	0.0933
H	0.263003	3.111993	4.146002	0.1169
H	0.361003	7.955001	2.822997	0.1323
H	10.979	7.933002	7.904002	0.1180
H	8.310003	5.714003	5.741	0.0871
H	9.135003	3.720992	6.730004	0.1109
H	8.391995	8.173001	5.186	0.1203
H	9.138003	9.093995	6.454997	0.1174
H	10.433	5.034993	3.020001	0.0864
H	10.066	7.302005	3.163004	0.1019
H	6.031005	18.85399	5.014001	0.1375
H	4.603001	18.25599	4.922	0.1045

H	4.888001	15.82	4.813999	0.0938
H	5.627002	13.891	3.927001	0.1180
H	8.296995	16.11	1.765001	0.0874
H	7.471995	18.10301	2.753003	0.1108
H	8.215003	13.651	1.210001	0.1208
H	7.467998	12.73001	2.478004	0.1178
H	2.992004	19.91901	1.797998	0.1153
H	2.943004	18.90399	2.815998	0.0978
H	2.821002	16.44201	2.374002	0.0974
F	3.548001	14.68801	1.231999	0.0936
H	5.271999	18.71201	0.169001	0.1167
H	6.173001	16.78901	6.996	0.0865
H	5.174995	13.869	6.799004	0.1323
H	6.511001	14.522	7.139002	0.1019
H	2.6098	2.978998	0.048998	0.1178
H	2.714005	5.197997	2.212	0.0873
H	3.591002	7.191008	1.222996	0.1107
H	2.855997	2.738999	2.767	0.1207
H	3.603002	1.818005	1.498003	0.1176
H	8.078996	9.007005	2.178001	0.1151
H	8.127996	5.12992	1.160001	0.0976
H	8.249998	5.129005	1.602999	0.0976
H	7.522999	3.716001	2.745002	0.0931
H	4.897999	5.871002	4.932999	0.0867
H	5.799001	7.800600	3.806998	0.1167
H	5.896005	2.956999	5.130003	0.1322
H	4.529999	3.609995	4.789996	0.1018
H	5.039995	7.941994	6.6916	0.1373
H	6.467999	7.343994	7.140999	0.1047
H	6.182999	4.907999	7.116002	0.0936
H	10.139	14.48001	3.027001	0.1046
H	10.423	16.916	3.139001	0.0937
H	8.528002	12.817	6.155002	0.1153
H	8.477995	13.83201	5.137002	0.0977
H	8.356003	16.294	5.578998	0.0973
H	9.083999	18.04799	6.721001	0.0933
H	10.808	14.02399	7.783999	0.1167
H	0.496003	13.88201	2.938999	0.1373
H	0.092	18.845	4.025999	0.1181
H	2.760997	16.626	6.187999	0.0872
H	1.935997	14.63299	5.199997	0.1110
H	2.679005	19.085	6.742999	0.1204
H	1.932997	20.006	5.474996	0.1177
H	10.575	2.970006	1.037	0.1373
H	0.638	15.94699	0.957	0.0865

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H	1.005003	18.21401	0.813998	0.1021
H	10.71	18.867	1.153996	0.1326
N	1.042003	0.081011	3.198999	0.9042
N	4.493996	21.74299	7.176	0.9040
N	6.577004	10.83099	4.754001	0.9040
N	10.029	10.99301	0.777	0.9038
O	1.150997	0.088998	4.410996	-0.5183
O	0.011005	0.242006	2.612998	-0.5287
O	3.514002	0.05899	6.488002	-0.4955
C	2.021996	21.76501	2.512003	-0.4946
O	5.523997	21.58199	6.588997	-0.5285
O	9.049004	10.85301	1.464998	-0.4948
O	7.556998	10.97099	5.440997	-0.4948
O	6.68995	10.823	3.542004	-0.5186
O	10.03	10.66999	5.340002	-0.5280
O	11.06	11.15401	1.364003	-0.5291
O	9.92002	11.001	7.518997	-0.5173
O	4.38400	21.735	0.434003	-0.5173
S	0.564001	2.160009	7.109004	-0.0096
S	10.609	8.874009	4.792001	0.0183
S	5.074005	6.25991	3.160999	0.0183
S	4.971997	7.05399	3.132997	-0.0101
S	5.996995	12.6599	0.816002	0.0189
S	6.099003	8.75298	0.843996	-0.0099
S	10.507	13.072	4.820003	-0.0101
S	0.462004	19.78601	7.136998	0.0187

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