

Electronic Supplementary Information

Complex phase transition and asymmetric ferroelectricity of homochiral secondary ammonium salts

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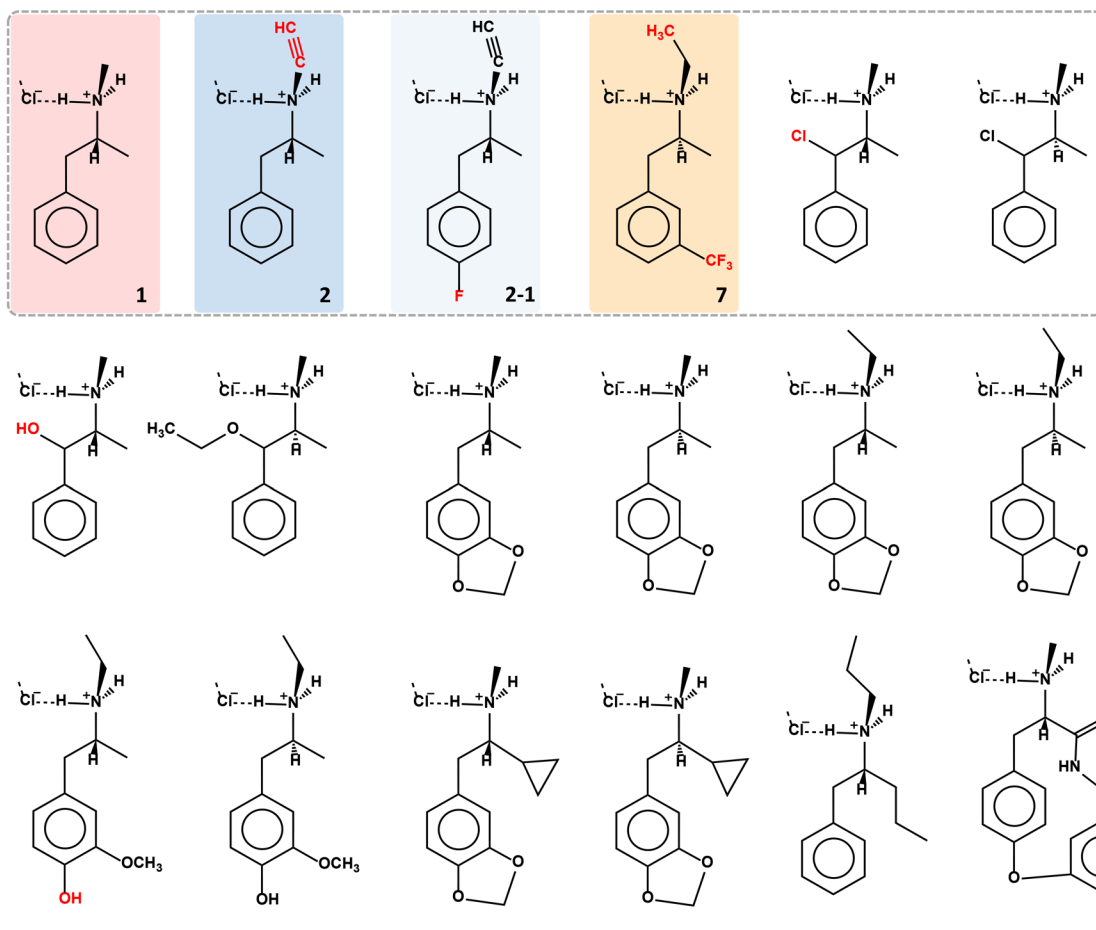
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Computational details

All the first-principles calculations within the framework of the density functional theory (DFT) were performed by using a projector-augmented wave (PAW) method,¹ as implemented in the Vienna ab-initio simulation package (VASP, Version 5.4.4). The electron exchange and correlation effects were described based on the Perdew-Burke-Ernzerh (PBE) functional² of the general gradient approximation (GGA). The Grimme's correlation (DFT-D3)³ was also applied to account for weak van de Waals interactions. An energy cutoff of 520 eV was used for each calculation with the energy precision of 10^{-6} eV for geometry optimization and with a lower energy precision of 10^{-7} eV for further single point calculations of ferroelectric properties. The atomic positions were fully relaxed until the maximum force on each atom was less than 0.02 eV/Å for geometry optimization. The Brillouin zone was sampled with Γ -centered Monkhorst-Pack k -points mesh with a grid spacing of $0.02 \times 2\pi \text{ \AA}^{-1}$ for initial structure relaxation and further single point calculations.

Generally, the experiments can supply exact structure information of low-temperature and high-

temperature phases, corresponding to the ferroelectric and paraelectric phases respectively, of model systems like DIPAC and DIPAB. Their structure difference can be distinguished to generate the ferroelectric-paraelectric phase transition pathway according to their subgroup-group relationship. Further confirmed by the climbing-image nudged elastic band (CI-NEB) calculations,^{4, 5} we believe this phase transition pathway for a specific ferroelectric is the most energetically favorable. The experimental information first helps us eliminate redundant reaction degrees of freedom for studied phase transition. Then, the computation further ensures the rationality of this phase transition pathway. Referring to the phase transition pathway of model system DIPAC, the reaction pathway of each new secondary ammonium salt (SAS, **1-8**) has been constructed. Then, the CI-NEB calculations were employed to locate each possible phase transition pathway connecting the left ferroelectric phase (local minimum), the paraelectric phase (a stationary point), to the right ferroelectric phase (the other local minimum) (see **Fig. 1c** in the main text). The quick convergence of these CI-NEB calculations also proves the rationality of ferroelectric-paraelectric phase transition pathway construction for studied SASs. For time-consuming CI-NEB calculations, we adopted the same computational setting for geometry optimization but a lower k -mesh resolution of $0.04 \times 2\pi \text{ \AA}^{-1}$ to sample the Brillouin zone. Subsequently, the spontaneous polarizations of SAS molecular crystals were calculated using the Berry phase method⁶⁻⁹ for each crystal structure along a certain phase transition pathway.



Scheme S1. Formulae of located 18 SASs with the space group of $P2_1$ and freely rotated -NH_2^+ sites.

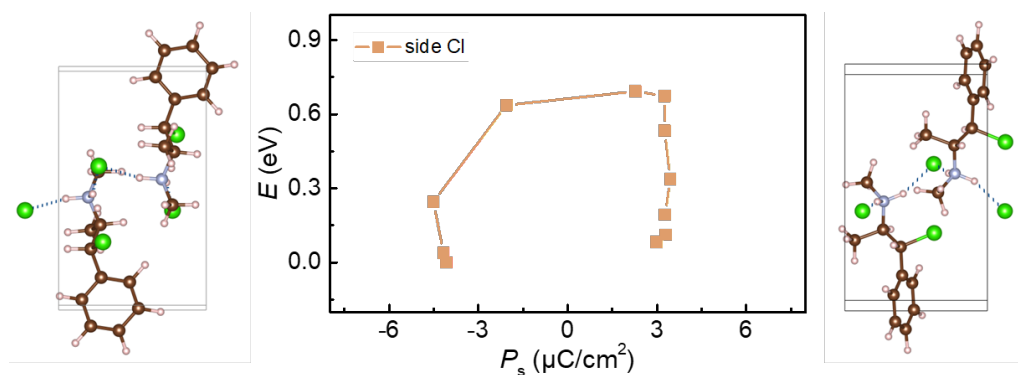


Fig. S1 Crystal structures of the left and right ferroelectric phases viewed along the a axis of a mined SAS with a chlorine substitution on the methylene connecting chiral C* and benzene ring and its variation of energy (E) with polarization (P_s).

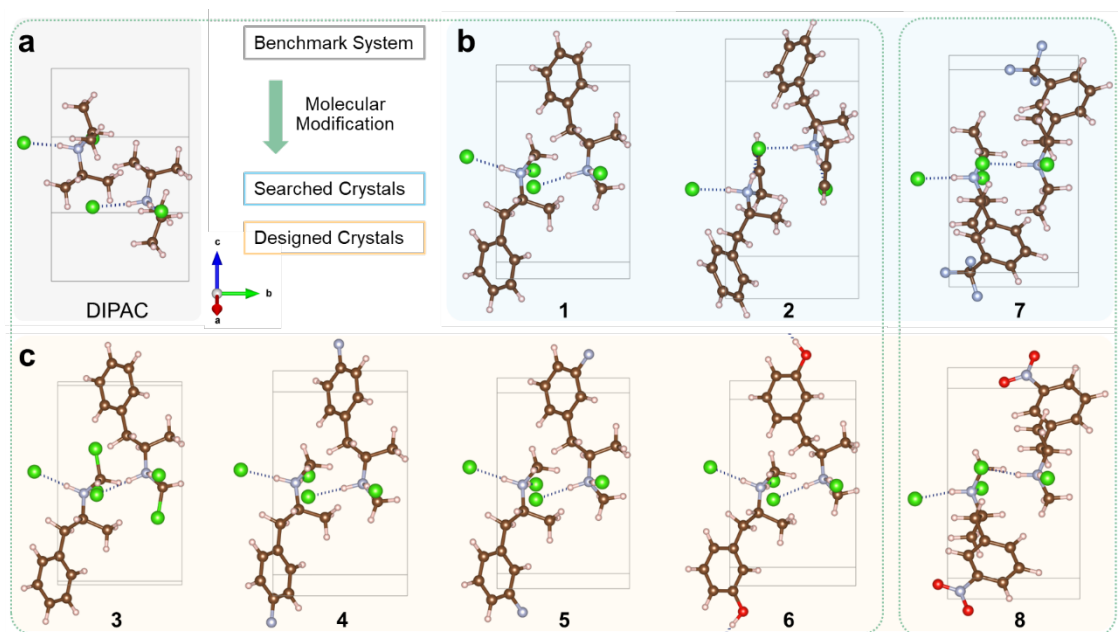


Fig. S2 Crystal structures of secondary ammonium salts (SASs) viewed along the a direction. (a) Benchmark, (b) data-mined, and (c) designed SAS molecular crystals are marked by square shadows in light grey, light blue, and light orange respectively.

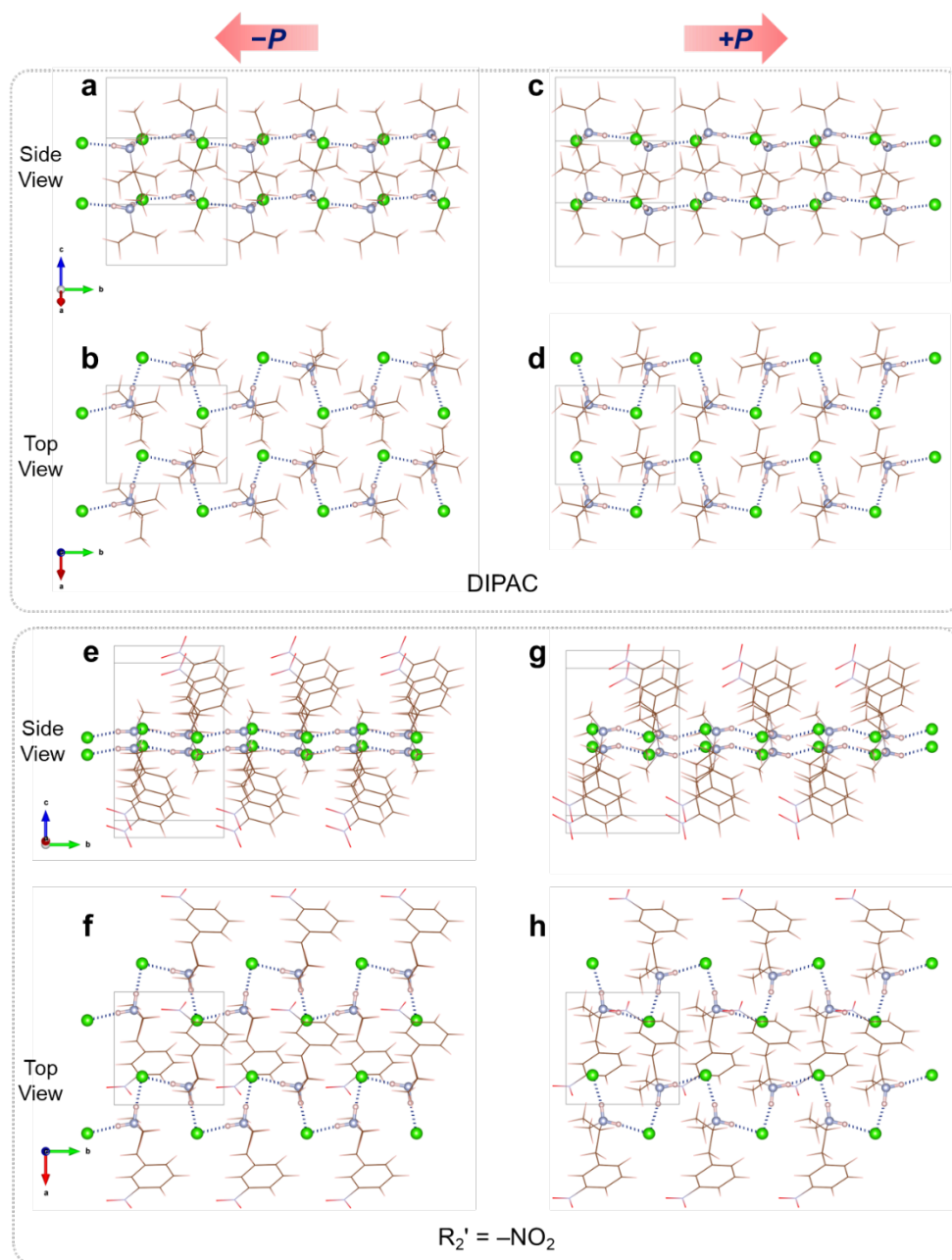


Fig. S3 Hydrogen-bonded networks in (a–d) DIPAC with two symmetric ferroelectric phases and (e–h) NO_2 -substituted SAS with two unsymmetric ferroelectric phases. Hydrogen bonds are marked by dark-blue dotted lines.

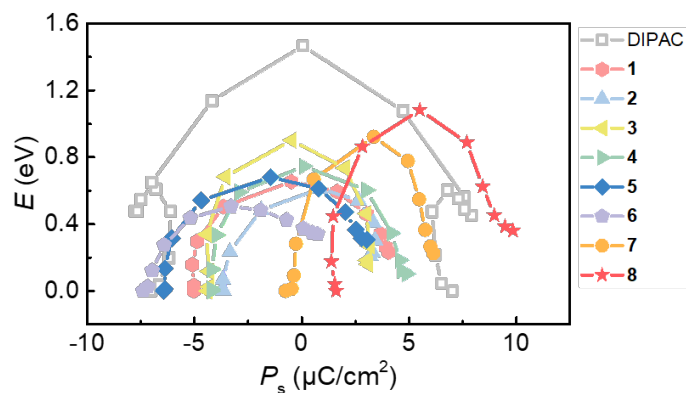


Fig. S4 Spontaneous polarization (P_s) dependent energy (E) curves of all studied SAs.

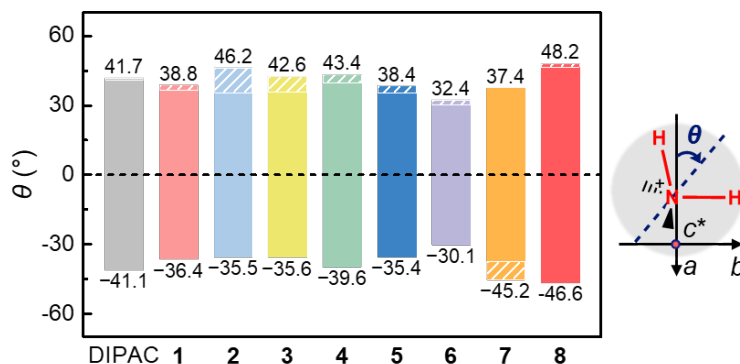


Fig. S5 Ranges of the projected rotation angle (ϑ) of $-\text{NH}_2^+$ sites in all studied SAs. The projected rotation angle (ϑ) is defined as the changed angle of the projection of angle bisector of $\angle\text{H}\text{N}\text{H}$ on the ab plane (marked by a grey disc) with reference to the paraelectric phase. The projected angle bisector is marked by a dark-blue dashed line. The 0° rotation angle indicates the projected angle bisector perpendicular to the b axis.

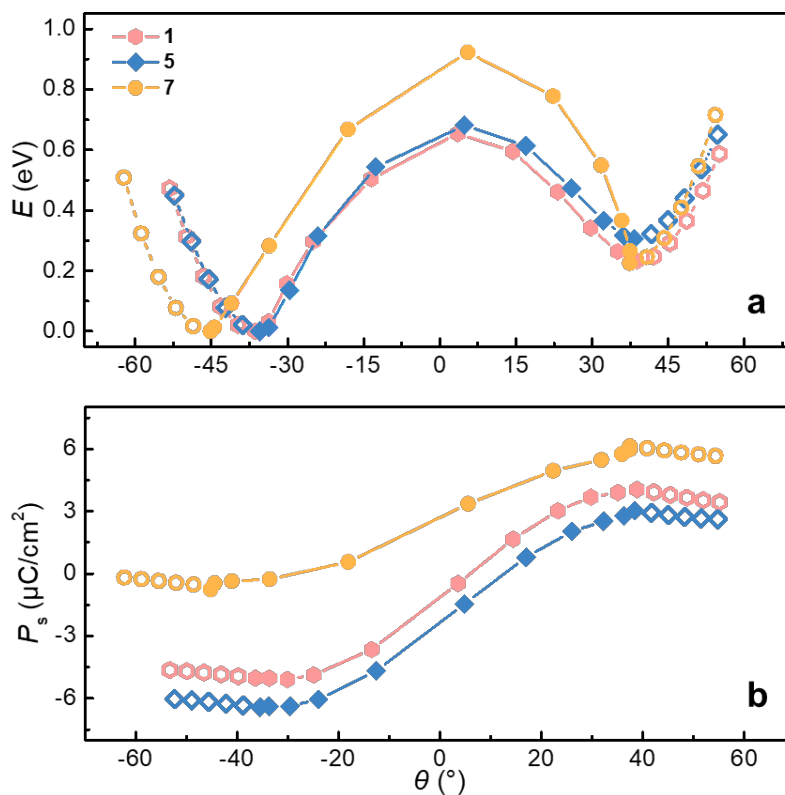


Fig. S6 Variations of (a) energy and (b) polarization of studied SASs (1, 5, and 7) with the projected rotation angle (ϑ) of the $-\text{NH}_2^+$ group. The solid lines/symbols taken from **Fig. 3** in the main text are obtained by CI-NEB calculations, and the dashed lines/hollow symbols are estimated only by single-point calculations.

Crystal structures of all studied SASs (POSCAR files)

DIPAC_FE1_POSCAR

1.0

7.4129500389	0.0000000000	0.0000000000
0.0000000000	7.7936072350	0.0000000000
-4.28810909729	0.0000000000	6.9622700246

Cl	H	C	N
2	32	12	2

Direct

0.283377528	0.800045133	0.619566441
0.716622472	0.300045162	0.380433559
0.588471532	0.335204393	0.663159311
0.411528438	0.835204422	0.336840689
0.612628341	0.153569430	0.805028737
0.387371659	0.653569460	0.194971249
0.652388692	0.363015056	0.903560221
0.347611278	0.863015056	0.096439794
0.271633416	0.433264673	0.673495650
0.728366554	0.933264732	0.326504320
0.381774366	0.310325027	0.998277307
0.618225634	0.810325027	0.001722666
0.339450389	0.100699767	0.901927948
0.660549581	0.600699723	0.098072022
0.119885445	0.243223920	0.819851339
0.880114496	0.743223906	0.180148646
0.217439860	0.063059896	0.567455411
0.782560170	0.563059866	0.432544589
0.027965093	0.218830585	0.487819135
0.972034872	0.718830585	0.512180865
0.269096285	0.501785815	0.406110942
0.730903745	0.001785821	0.593889117
0.998853803	0.443426669	0.249443755
0.001146211	0.943426669	0.750556290
0.182027102	0.425715953	0.171703190
0.817972898	0.925715923	0.828296840
0.372889668	0.192753911	0.405282050
0.627110362	0.692753911	0.594717920
0.092544861	0.968034804	0.250645518
0.907455146	0.468034804	0.749354541

0.892349660	0.130193383	0.157408997
0.107650332	0.630193412	0.842590988
0.073870137	0.116831459	0.077381141
0.926129878	0.616831481	0.922618866
0.557724357	0.287094980	0.772386789
0.442275643	0.787094951	0.227613240
0.325690776	0.299507767	0.710621059
0.674309254	0.799507737	0.289378941
0.288043678	0.235059440	0.866320968
0.711956322	0.735059440	0.133679003
0.162734270	0.410375059	0.294964194
0.837265670	0.910375059	0.705035746
0.208623648	0.224480644	0.360133052
0.791376352	0.724480629	0.639866889
0.057240367	0.101731546	0.202141732
0.942759633	0.601731539	0.797858238
0.187610656	0.194630727	0.531814635
0.812389314	0.694630742	0.468185365

DIPAC_FE2_POSCAR

1.0

7.4128999710	0.0000000000	0.0000000000
0.0000000000	7.7936000824	0.0000000000
-4.2881898263	0.0000000000	6.9622640105

Cl	H	C	N
2	32	12	2

Direct

0.282042831	0.672010481	0.626352847
0.717957139	0.172010481	0.373647183
0.099498950	0.218337163	0.808417141
0.900501013	0.718337178	0.191582829
0.313293546	0.368173897	0.903464735
0.686706424	0.868173897	0.096535295
0.359776825	0.157704353	0.997724414
0.640223145	0.657704353	0.002275601
0.282277614	0.039501350	0.681661129
0.717722416	0.539501309	0.318338841
0.653121233	0.127966404	0.929622829
0.346878767	0.627966404	0.070377164
0.603018224	0.336022258	0.826722860

0.396981746	0.836022258	0.173277140
0.605808616	0.155711740	0.694212556
0.394191384	0.655711710	0.305787444
0.031092666	0.251390249	0.487883806
0.968907297	0.751390278	0.512116194
0.218339801	0.409038633	0.571627676
0.781660199	0.909038603	0.428372324
0.115281858	0.502759576	0.261168748
0.884718120	0.002759592	0.738831282
0.912481070	0.343222916	0.160195976
0.087518908	0.843222857	0.839803994
0.103497446	0.353853285	0.090877332
0.896502554	0.853853285	0.909122705
0.389895469	0.275702924	0.423365593
0.610104561	0.775702953	0.576634347
0.282205164	0.968225658	0.418484151
0.717794895	0.468225628	0.581515849
0.012964825	0.027449686	0.258857548
0.987035155	0.527449727	0.741142452
0.199242562	0.043704640	0.184720725
0.800757468	0.543704689	0.815279305
0.269603014	0.232825786	0.865149856
0.730396986	0.732825756	0.134850159
0.326051027	0.175074354	0.719276786
0.673949003	0.675074339	0.280723214
0.560490489	0.199914411	0.795121610
0.439509511	0.699914396	0.204878390
0.079579107	0.369428694	0.211451441
0.920420885	0.869428694	0.788548529
0.223581940	0.245662421	0.371844321
0.776418090	0.745662391	0.628155649
0.177631646	0.059783943	0.306567192
0.822368324	0.559783936	0.693432808
0.191931963	0.277025253	0.537375987
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SAS_1_FE1-POSCAR

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-1.3611819954	0.0000000000	10.5858317926

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0.201136425	0.182666242	0.468371928
0.685026824	0.790691853	0.430331141
0.314973146	0.290691882	0.569668889
0.749122858	0.895284832	0.707995057
0.250877142	0.395284832	0.292004943
0.738672018	0.696294963	0.661824524
0.261328012	0.196294993	0.338175476
0.868444741	0.562665224	0.746399105
0.131555244	0.062665217	0.253600895
0.807476640	0.535793483	0.875534117
0.192523345	0.035793480	0.124465905
0.892677367	0.638168573	0.979337931
0.107322618	0.138168558	0.020662082
0.839355767	0.609843075	0.099438287
0.160644248	0.109843060	0.900561690
0.700557530	0.478279024	0.118159287
0.299442440	0.978278995	0.881840706
0.613297880	0.376706839	0.015092169
0.386702091	0.876706839	0.984907806
0.666321754	0.405788124	0.894898057
0.333678246	0.905788124	0.105101921
0.715076387	0.938629270	0.442745239
0.284923583	0.438629270	0.557254791
0.792442918	0.541701913	0.504618585
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0.532595038	0.764409006	0.433619142
0.467404991	0.264409006	0.566380858
0.944537938	0.720669746	0.537266970
0.055462036	0.220669731	0.462733001
0.725640833	0.745499074	0.339471549

0.274359167	0.245499104	0.660528421
0.646804869	0.983702362	0.649776876
0.353195131	0.483702362	0.350223124
0.893517435	0.951485991	0.706861138
0.106482588	0.451485991	0.293138832
0.715622425	0.901214242	0.805516124
0.284377575	0.401214242	0.194483891
0.589581430	0.647857189	0.652670145
0.410418570	0.147857189	0.347329885
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0.133540794	0.928298295	0.302418292
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0.983818769	0.115086369	0.244883716
0.003707048	0.738793075	0.966340065
0.996292949	0.238793090	0.033659946
0.909584522	0.690034628	0.178731874
0.090415470	0.190034643	0.821268141
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0.335991055	0.951143265	0.787249207
0.505952358	0.272444516	0.028312054
0.494047672	0.772444487	0.971687973
0.600140750	0.323067933	0.815463722
0.399859279	0.823067963	0.184536308

SAS_1_FE2-POSCAR

1.0

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0.687626719	0.712543964	0.429446042
0.312373251	0.212543964	0.570553958
0.715670943	0.921722829	0.753781021
0.284329057	0.421722829	0.246218964

0.726750970	0.745128155	0.673951924
0.273249030	0.245128125	0.326048076
0.855797887	0.593680143	0.740787506
0.144202098	0.093680173	0.259212464
0.803743541	0.536638021	0.871226609
0.196256444	0.036638018	0.128773361
0.879728496	0.630545676	0.984280527
0.120271519	0.130545661	0.015719490
0.833292544	0.578107893	0.105472125
0.166707426	0.078107893	0.894527853
0.712976277	0.428402483	0.116645530
0.287023693	0.928402543	0.883354485
0.634685755	0.335104048	0.004587178
0.365314245	0.835103989	0.995412827
0.678647816	0.390291899	0.883022666
0.321352184	0.890291870	0.116977334
0.540536284	0.746817589	0.429230303
0.459463716	0.246817559	0.570769727
0.935654342	0.764555931	0.547768831
0.064345658	0.264555961	0.452231139
0.707430780	0.560609519	0.432562411
0.292569220	0.060609501	0.567437530
0.787724376	0.944613457	0.532922328
0.212275609	0.444613457	0.467077672
0.738479376	0.771586716	0.343312860
0.261520624	0.271586716	0.656687140
0.620320022	0.022179509	0.701080084
0.379680008	0.522179484	0.298919886
0.851796508	0.988542140	0.775134444
0.148203507	0.488542169	0.224865571
0.665543020	0.890285730	0.846386492
0.334457010	0.390285760	0.153613538
0.586254537	0.687708259	0.648718417
0.413745433	0.187708274	0.351281583
0.852181375	0.471470952	0.676000834
0.147818640	0.971470952	0.323999137
0.998845637	0.647566199	0.753022075
0.001154390	0.147566184	0.246977940
0.977605402	0.744552076	0.977404475
0.022394571	0.244552046	0.022595551
0.894377589	0.653590620	0.191723734

0.105622418	0.153590649	0.808276236
0.683236778	0.382871985	0.212107360
0.316763222	0.882872045	0.787892640
0.540478885	0.217864513	0.011560311
0.459521115	0.717864513	0.988439679
0.617907405	0.316323280	0.796007276
0.382092625	0.816323280	0.203992754

SAS_2_FE1_POSCAR

1.0

7.4405922890	0.0000000000	0.0000000000
0.0000000000	7.2310051918	0.0000000000
-3.6367861873	0.0000000000	11.2051261705

Cl	N	H	C
2	2	32	24

Direct

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0.419131845	0.165794358	0.376440614
0.613568068	0.523690462	0.619708300
0.386431962	0.023690449	0.380291700
0.507199645	0.705748916	0.534851611
0.492800355	0.205748886	0.465148389
0.039835338	0.736695647	0.451739252
0.960164666	0.236695677	0.548260748
0.732110679	0.916252136	0.679388821
0.267889321	0.416252136	0.320611149
0.845148206	0.711722851	0.754737735
0.154851779	0.211722821	0.245262280
0.322703034	0.600762606	0.642203808
0.677296937	0.100762621	0.357796192
0.593758941	0.460107327	0.805854142
0.406241030	0.960107386	0.194145858
0.638053596	0.680091202	0.876375437
0.361946434	0.180091187	0.123624563
0.503056467	0.726250172	0.029472223
0.496943533	0.226250187	0.970527768
0.257885337	0.660476208	0.126506567
0.742114663	0.160476223	0.873493433
0.986598969	0.452260315	0.026761986
0.013400983	0.952260315	0.973237991
0.968552351	0.309088051	0.829958022
0.031447634	0.809088051	0.170041978
0.215422660	0.370743692	0.736391187
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0.321854740	0.941960871	0.611655951
0.678145230	0.441960841	0.388344049
0.497269332	0.970245063	0.753081143

0.502730608	0.470245093	0.246918857
0.270674139	0.883385956	0.744396269
0.729325891	0.383385956	0.255603701
0.955067933	0.744492292	0.511143863
0.044932041	0.244492278	0.488856107
0.868703604	0.754703164	0.582813799
0.131296396	0.254703134	0.417186230
0.763609827	0.769876242	0.667743206
0.236390173	0.269876212	0.332256824
0.444501847	0.682971656	0.694974780
0.555498123	0.182971641	0.305025220
0.527265191	0.591864169	0.817813456
0.472734839	0.091864154	0.182186544
0.376302361	0.554858208	0.875977695
0.623697639	0.054858238	0.124022335
0.385222793	0.635076702	0.985741019
0.614777207	0.135076717	0.014259004
0.246522561	0.598281920	0.040096819
0.753477454	0.098281942	0.959903181
0.095640384	0.481009960	0.984895825
0.904359639	0.981009901	0.015104203
0.085557982	0.399901897	0.875301957
0.914442003	0.899901867	0.124698021
0.224686027	0.436399162	0.821530879
0.775313973	0.936399221	0.178469107
0.381511778	0.881864786	0.700896025
0.618488193	0.381864786	0.299103975

SAS_2_FE2_POSCAR

1.0

7.5117330551	0.0000000000	0.0000000000
0.0000000000	7.2758727074	0.0000000000
-3.0999379795	0.0000000000	10.7130465982

Cl	N	H	C
2	2	32	24

Direct

0.655912876	0.225712568	0.636816144
0.344087124	0.725712538	0.363183856
0.588220954	0.801272988	0.630635440
0.411779076	0.301272988	0.369364560

0.518790543	0.786804616	0.534350336
0.481209427	0.286804587	0.465649664
0.618185639	0.942662179	0.644349813
0.381814331	0.442662179	0.355650216
0.055426471	0.772841096	0.439459920
0.944573522	0.272841066	0.560540080
0.846895278	0.723793328	0.754040599
0.153104722	0.223793343	0.245959401
0.731328368	0.546739101	0.651698112
0.268671602	0.046739120	0.348301888
0.354047984	0.647731483	0.632484555
0.645951986	0.147731453	0.367515445
0.612275958	0.518139243	0.801295519
0.387724072	0.018139239	0.198704481
0.628671348	0.726287305	0.888248861
0.371328652	0.226287290	0.111751124
0.452533185	0.746277690	0.034099262
0.547466815	0.246277690	0.965900719
0.201680377	0.634200275	0.119264401
0.798319638	0.134200260	0.880735576
0.978880882	0.395989031	0.003338065
0.021119129	0.895989060	0.996661901
0.021545433	0.262723148	0.806971192
0.978454590	0.762723148	0.193028793
0.280189544	0.368246287	0.726478219
0.719810426	0.868246317	0.273521811
0.281435609	0.986418009	0.630327404
0.718564332	0.486417979	0.369672626
0.429859072	0.005988538	0.785045803
0.570140898	0.505988538	0.214954227
0.224613845	0.870464087	0.754119039
0.775386155	0.370464057	0.245880976
0.965641022	0.758420110	0.499215335
0.034358960	0.258420110	0.500784695
0.871626079	0.736986041	0.570430398
0.128373951	0.236986041	0.429569572
0.765823781	0.694491386	0.657599866
0.234176204	0.194491372	0.342400134
0.446960062	0.741954148	0.698412955
0.553039908	0.241954148	0.301587045
0.533409536	0.636855900	0.820228219

0.466590464	0.136855930	0.179771766
0.382256210	0.567195535	0.873804390
0.617743790	0.067195550	0.126195624
0.357748181	0.640254378	0.984257400
0.642251849	0.140254393	0.015742572
0.214554653	0.578002155	0.031377509
0.785445333	0.078002140	0.968622506
0.092023388	0.443360269	0.967484474
0.907976627	0.943360269	0.032515522
0.116364986	0.368049532	0.857680619
0.883634984	0.868049562	0.142319396
0.260941714	0.428855479	0.811643481
0.739058316	0.928855479	0.188356534
0.340010345	0.911879301	0.717873156
0.659989655	0.411879271	0.282126844

SAS_3_FE1_POSCAR

1.0

7.1833963394	0.0000000000	0.0000000000
0.0000000000	7.0826487541	0.0000000000
-0.3177360619	0.0000000000	11.3137126135

Cl	N	C	H
4	2	20	30

Direct

0.208039865	0.813547373	0.553024948
0.791960120	0.313547403	0.446975082
0.707971454	0.804131746	0.330598921
0.292028576	0.304131776	0.669401050
0.789682448	0.711333036	0.555781484
0.210317567	0.211333036	0.444218487
0.675198734	0.844028473	0.483301699
0.324801266	0.344028473	0.516698301
0.745789707	0.899566770	0.738475919
0.254210263	0.399566770	0.261524081
0.734168291	0.703250706	0.683962345
0.265831709	0.203250721	0.316037685
0.862230539	0.556507885	0.745580733
0.137769476	0.056507863	0.254419267
0.808434010	0.514306605	0.870830178
0.191566005	0.014306595	0.129169807
0.894189060	0.610060513	0.966166675
0.105810918	0.110060498	0.033833336
0.844357550	0.571661890	0.082041517
0.155642435	0.071661867	0.917958498
0.708763123	0.436116904	0.105083041
0.291236907	0.936116874	0.894916952
0.622425079	0.339379430	0.010726755
0.377574950	0.839379370	0.989273250
0.672007918	0.378674239	0.894731104
0.327992111	0.878674269	0.105268896
0.717819273	0.990004659	0.501722515
0.282180727	0.490004689	0.498277545
0.781690478	0.573426306	0.518700182
0.218309551	0.073426321	0.481299877
0.527417302	0.821311593	0.501336515
0.472582698	0.321311593	0.498663455
0.932179928	0.750316858	0.552441776

0.067820102	0.250316858	0.447558254
0.640703738	0.995587528	0.699910522
0.359296262	0.495587528	0.300089508
0.884712636	0.960612059	0.726894617
0.115287386	0.460612029	0.273105383
0.721683264	0.890747964	0.833524108
0.278316766	0.390747964	0.166475907
0.589250505	0.652066410	0.682542861
0.410749495	0.152066395	0.317457139
0.857415199	0.425846189	0.692825973
0.142584771	0.925846159	0.307174027
0.006401422	0.608980596	0.744459629
0.993598580	0.108980574	0.255540341
0.002227595	0.714247704	0.949806988
0.997772396	0.214247718	0.050193019
0.914350569	0.647086382	0.154509678
0.085649416	0.147086367	0.845490336
0.673996091	0.404503644	0.196232140
0.326003939	0.904503703	0.803767860
0.604642510	0.301709056	0.821795702
0.395357519	0.801709056	0.178204283
0.517762780	0.231457472	0.026943544
0.482237220	0.731457412	0.973056495

SAS_3_FE2_POSCAR

1.0

7.0798301697	0.0000000000	0.0000000000
0.0000000000	7.2118983269	0.0000000000
0.3241540098	0.0000000000	11.5337004718

Cl	N	C	H
4	2	20	30

Direct

0.234205991	0.675506711	0.535105348
0.765793979	0.175506726	0.464894652
0.798529565	0.706369817	0.311616778
0.201470450	0.206369802	0.688383222
0.800880253	0.763625979	0.540883362
0.199119732	0.263625979	0.459116638
0.705479264	0.652067721	0.451882303
0.294520706	0.152067721	0.548117697

0.777072430	0.892164290	0.737967968
0.222927585	0.392164320	0.262032032
0.728979945	0.724535882	0.664322853
0.271020055	0.224535882	0.335677147
0.818776429	0.541650593	0.704770029
0.181223586	0.041650612	0.295230001
0.775019884	0.492917657	0.829790294
0.224980146	0.992917657	0.170209676
0.897381544	0.549581170	0.916578352
0.102618426	0.049581192	0.083421662
0.859521389	0.505608976	0.032637764
0.140478581	0.005608974	0.967362225
0.699922502	0.400919378	0.063923314
0.300077528	0.900919318	0.936076701
0.578001440	0.341671824	0.978217602
0.421998560	0.841671765	0.021782419
0.614871979	0.388548762	0.862218857
0.385128021	0.888548732	0.137781113
0.554077804	0.684614599	0.455570579
0.445922166	0.184614614	0.544429362
0.948293984	0.737602115	0.536130369
0.051706027	0.237602100	0.463869631
0.729373634	0.503777981	0.466855764
0.270626366	0.003777956	0.533144236
0.783366084	0.905951083	0.520934165
0.216633931	0.405951083	0.479065835
0.711109340	0.018809536	0.705283582
0.288890630	0.518809557	0.294716388
0.930543661	0.914344966	0.738283455
0.069456361	0.414344966	0.261716515
0.726926684	0.870434761	0.827620029
0.273073316	0.370434731	0.172379985
0.574571550	0.709405482	0.659217834
0.425428450	0.209405467	0.340782195
0.773567140	0.427459270	0.648652911
0.226432845	0.927459240	0.351347089
0.972862005	0.554543972	0.692028582
0.027137978	0.054544002	0.307971418
0.024053518	0.628924727	0.893310964
0.975946486	0.128924742	0.106689028
0.956351399	0.552951694	0.098206460

0.043648575	0.052951690	0.901793540
0.671104133	0.365936875	0.154757738
0.328895837	0.865936875	0.845242202
0.518386185	0.342144251	0.796013892
0.481613815	0.842144251	0.203986093
0.454135627	0.258029938	0.001159996
0.545864344	0.758029938	0.998840034

SAS_4_FE1_POSCAR

1.0

6.9674272537	0.0000000000	0.0000000000
0.0000000000	7.3553781509	0.0000000000
-1.8407995040	0.0000000000	10.9865502711

Cl	N	C	H	F
2	2	20	30	2

Direct

0.237046584	0.762455761	0.538889408
0.762953401	0.262455732	0.461110562
0.806116879	0.668162882	0.529350102
0.193883121	0.168162867	0.470649898
0.691647768	0.777220070	0.430332065
0.308352232	0.277220100	0.569667876
0.785507798	0.887926698	0.697368979
0.214492202	0.387926728	0.302631021
0.755605340	0.691935778	0.654809296
0.244394630	0.191935778	0.345190674
0.882034719	0.555622339	0.738771200
0.117965288	0.055622354	0.261228830
0.818964124	0.536914647	0.861301482
0.181035876	0.036914635	0.138698503
0.913533628	0.632443964	0.963114917
0.086466357	0.132443964	0.036885090
0.853200972	0.617611825	0.076268166
0.146799013	0.117611848	0.923731863
0.696154952	0.505113840	0.085831493
0.303845018	0.005113813	0.914168477
0.598370790	0.407347828	0.987615466
0.401629239	0.907347798	0.012384566
0.661413252	0.424224198	0.875469625
0.338586748	0.924224198	0.124530390
0.727788627	0.921737373	0.442672431
0.272211373	0.421737403	0.557327569
0.789842904	0.528991938	0.505680323
0.210157096	0.028991938	0.494319677
0.536138892	0.756628036	0.431708336
0.463861138	0.256628007	0.568291664
0.955775976	0.698580325	0.532974899
0.044224050	0.198580310	0.467025101
0.728548586	0.728882253	0.344033271

0.271451384	0.228882268	0.655966699
0.690226853	0.982055664	0.638931155
0.309773177	0.482055664	0.361068875
0.937318861	0.929480493	0.698360085
0.062681124	0.429480523	0.301639915
0.752139330	0.900391698	0.789841652
0.247860685	0.400391728	0.210158348
0.600799441	0.655508101	0.647208512
0.399200588	0.155508071	0.352791488
0.871805727	0.422383040	0.692809224
0.128194243	0.922383070	0.307190776
0.035066538	0.599666715	0.749445617
0.964933455	0.099666685	0.250554383
0.037145551	0.719770432	0.954626441
0.962854505	0.219770461	0.045373566
0.927015543	0.691440761	0.155391648
0.072984435	0.191440746	0.844608366
0.476602733	0.320122868	0.999627233
0.523397267	0.820122838	0.000372785
0.587417841	0.346740544	0.797799885
0.412582129	0.846740544	0.202200115
0.634594500	0.489929885	0.195851713
0.365405500	0.989929855	0.804148316

SAS_4_FE2_POSCAR

1.0

6.9383888245	0.0000000000	0.0000000000
0.0000000000	7.2822880745	0.0000000000
-0.3565993667	0.0000000000	11.1512058200

Cl	N	C	H	F
2	2	20	30	2

Direct

0.252587885	0.710058153	0.545404792
0.747412145	0.210058123	0.454595178
0.817540228	0.808542311	0.528648198
0.182459801	0.308542311	0.471351802
0.727265775	0.699182987	0.429594785
0.272734255	0.199182972	0.570405185
0.817880332	0.938602507	0.729346037
0.182119653	0.438602477	0.270653963

0.746981025	0.776471317	0.653623104
0.253019005	0.276471287	0.346376866
0.820908844	0.588256299	0.699593544
0.179091170	0.088256299	0.300406426
0.776077688	0.553058445	0.828969240
0.223922327	0.053058468	0.171030760
0.900477827	0.618689775	0.921163261
0.099522173	0.118689783	0.078836739
0.857917786	0.596708417	0.041691858
0.142082214	0.096708432	0.958308101
0.690547526	0.502617717	0.069052123
0.309452474	0.002617722	0.930947900
0.565091074	0.431921452	0.981154323
0.434908956	0.931921482	0.018845672
0.608653545	0.459298044	0.860960364
0.391346425	0.959298015	0.139039606
0.571374714	0.723501623	0.427070558
0.428625286	0.223501608	0.572929382
0.968056083	0.785437703	0.530807197
0.031943910	0.285437703	0.469192833
0.755088806	0.552362204	0.442462891
0.244911194	0.052362222	0.557537079
0.795991421	0.948873341	0.507445216
0.204008594	0.448873311	0.492554754
0.789982200	0.744505823	0.345665038
0.210017815	0.244505823	0.654334962
0.765264869	0.068509877	0.690479696
0.234735116	0.568509877	0.309520334
0.976393163	0.941897511	0.734098196
0.023606809	0.441897482	0.265901834
0.765572846	0.928143680	0.820602775
0.234427169	0.428143680	0.179397225
0.588490248	0.775807321	0.646287978
0.411509782	0.275807321	0.353711993
0.758835196	0.478692383	0.642467916
0.241164789	0.978692412	0.357532114
0.978368044	0.585283935	0.689609051
0.021631941	0.085283950	0.310390949
0.032653514	0.690330684	0.898765564
0.967346489	0.190330699	0.101234436
0.952659786	0.651397467	0.112699576

0.047340207	0.151397467	0.887300432
0.436322957	0.357468516	0.006346799
0.563677073	0.857468486	0.993653178
0.510244489	0.406661451	0.790762544
0.489755511	0.906661451	0.209237471
0.648238063	0.478639126	0.187221840
0.351761937	0.978639126	0.812778115

SAS_5_FE1_POSCAR

1.0

7.0576171875	0.0000000000	0.0000000000
0.0000000000	7.2808256149	0.0000000000
-1.2585730241	0.0000000000	10.6693519952

Cl	N	C	H	F
2	2	20	30	2

Direct

0.225768030	0.793529570	0.561617613
0.774231970	0.293529540	0.438382417
0.794320822	0.693025827	0.530738711
0.205679163	0.193025827	0.469261318
0.680394232	0.804588497	0.433235288
0.319605798	0.304588467	0.566764712
0.741139352	0.896428347	0.709410548
0.258860648	0.396428347	0.290589452
0.732971311	0.700231731	0.660424352
0.267028719	0.200231716	0.339575648
0.863166451	0.565284193	0.741291940
0.136833549	0.065284170	0.258708060
0.802885771	0.531981170	0.869376242
0.197114199	0.031981185	0.130623773
0.886906326	0.631533861	0.973229051
0.113093644	0.131533876	0.026770972
0.831690013	0.593733609	0.090464167
0.168309987	0.093733624	0.909535885
0.698352456	0.460367501	0.111290611
0.301647514	0.960367501	0.888709366
0.613898337	0.362980008	0.007043058
0.386101693	0.862979949	0.992956936
0.664797544	0.398783594	0.887627721
0.335202456	0.898783624	0.112372287
0.708698153	0.951144040	0.449609131
0.291301817	0.451144040	0.550390899
0.789549470	0.554274678	0.500879467
0.210450530	0.054274708	0.499120533
0.528468907	0.775855720	0.436399460
0.471531093	0.275855690	0.563600540
0.939377785	0.732161045	0.536916435
0.060622238	0.232161045	0.463083565
0.723711431	0.766198099	0.342229664

0.276288569	0.266198099	0.657770336
0.635034084	0.983807623	0.655180156
0.364965886	0.483807594	0.344819874
0.883085728	0.956408143	0.705747187
0.116914250	0.456408143	0.294252813
0.710777164	0.898150921	0.807253003
0.289222866	0.398150921	0.192747027
0.584554911	0.650756180	0.650740862
0.415445089	0.150756180	0.349259168
0.862839818	0.433521986	0.691020191
0.137160152	0.933521986	0.308979809
0.010279871	0.618259251	0.749990523
0.989720166	0.118259229	0.250009507
0.995907843	0.735111475	0.963906467
0.004092168	0.235111460	0.036093555
0.666940093	0.431010753	0.206296578
0.333059877	0.931010783	0.793703437
0.600406647	0.318683356	0.807816505
0.399593353	0.818683326	0.192183495
0.509771049	0.256055474	0.019867452
0.490228951	0.756055474	0.980132520
0.915106058	0.692743421	0.191187724
0.084893957	0.192743421	0.808812261

SAS_5_FE2_POSCAR

1.0

7.1744275093	0.0000000000	0.0000000000
0.0000000000	7.1323685646	0.0000000000
-1.1536477494	0.0000000000	10.7697385031

Cl	N	C	H	F
2	2	20	30	2

Direct

0.221769065	0.659156799	0.553826630
0.778230906	0.159156784	0.446173370
0.794428766	0.753822863	0.548609912
0.205571264	0.253822833	0.451390058
0.689617634	0.649834931	0.444667459
0.310382396	0.149834946	0.555332541
0.744064152	0.906144202	0.745311558
0.255935878	0.406144172	0.254688472
0.726941943	0.721589863	0.674750328

0.273058057	0.221589863	0.325249642
0.840087354	0.558196902	0.738950968
0.159912661	0.058196887	0.261049032
0.788757265	0.514178813	0.867272556
0.211242750	0.014178840	0.132727414
0.866897285	0.619453073	0.969519496
0.133102715	0.119453073	0.030480519
0.818609059	0.576660573	0.086907588
0.181390956	0.076660581	0.913092434
0.703024983	0.427307278	0.110474952
0.296974987	0.927307308	0.889525056
0.625640213	0.322885484	0.008302583
0.374359787	0.822885454	0.991697371
0.665178955	0.367882937	0.888215542
0.334821075	0.867882907	0.111784473
0.541033983	0.687367618	0.441728860
0.458966047	0.187367633	0.558271170
0.938608110	0.720575571	0.552237988
0.061391864	0.220575586	0.447762012
0.707800150	0.498396873	0.458877951
0.292199820	0.998396873	0.541122019
0.786023378	0.897735834	0.525294244
0.213976592	0.397735834	0.474705786
0.745527625	0.691464126	0.358659536
0.254472345	0.191464096	0.641340494
0.661830008	0.015337567	0.693170667
0.338170022	0.515337586	0.306829363
0.889882147	0.954315424	0.758680880
0.110117853	0.454315454	0.241319090
0.692854762	0.892492890	0.836574376
0.307145238	0.392492861	0.163425609
0.578237653	0.681762218	0.656878114
0.421762317	0.181762189	0.343121886
0.820303917	0.432460219	0.680021524
0.179696068	0.932460189	0.319978476
0.990167558	0.593737483	0.744657397
0.009832409	0.093737490	0.255342633
0.965229750	0.733351052	0.958915234
0.034770276	0.233351037	0.041084740
0.676997602	0.392500162	0.205113217
0.323002398	0.892500162	0.794886768

0.602324247	0.285729408	0.809688747
0.397675753	0.785729408	0.190311268
0.534590423	0.204410657	0.023063591
0.465409607	0.704410672	0.976936400
0.891119301	0.687365174	0.184172451
0.108880728	0.187365144	0.815827549

SAS_6_FE1_POSCAR

1.0

7.3198151588	0.0000000000	0.0000000000
0.0000000000	7.1875877380	0.0000000000
-1.5364599759	0.0000000000	10.5249625354

Cl	N	C	H	O
2	2	20	32	2

Direct

0.209897593	0.846418977	0.557814956
0.790102422	0.346418947	0.442185044
0.791084111	0.743968427	0.551552653
0.208915889	0.243968457	0.448447317
0.670954704	0.856841922	0.455818564
0.329045266	0.356841922	0.544181466
0.704564393	0.918079615	0.737981558
0.295435578	0.418079615	0.262018442
0.731910765	0.727875113	0.681386471
0.268089205	0.227875084	0.318613499
0.877249658	0.607715547	0.763473272
0.122750312	0.107715569	0.236526728
0.808240294	0.529501498	0.879568934
0.191759691	0.029501479	0.120431058
0.863775790	0.605711877	0.000080636
0.136224225	0.105711870	0.999919355
0.803047001	0.526366651	0.107164815
0.196952999	0.026366627	0.892835200
0.688599229	0.368845761	0.094075784
0.311400771	0.868845761	0.905924261
0.631212652	0.294941276	0.973513544
0.368787348	0.794941306	0.026486440
0.689334095	0.375101775	0.866674781
0.310665905	0.875101745	0.133325189
0.687967539	0.004816893	0.478914827
0.312032461	0.504816890	0.521085143
0.796788514	0.607316256	0.516036570
0.203211501	0.107316278	0.483963460
0.526855469	0.815072060	0.455661178
0.473144531	0.315072030	0.544338822
0.927599788	0.793182790	0.560031652
0.072400190	0.293182820	0.439968348
0.713248074	0.831289351	0.362529099

0.286751896	0.331289381	0.637470961
0.583564281	0.989253163	0.686607778
0.416435719	0.489253134	0.313392222
0.827282608	0.006200868	0.738384664
0.172717407	0.506200850	0.261615366
0.680681825	0.900955617	0.836789429
0.319318175	0.400955588	0.163210586
0.599438310	0.652660012	0.665497661
0.400561661	0.152660012	0.334502310
0.915282726	0.490568757	0.705620587
0.084717296	0.990568697	0.294379413
0.002649157	0.690892398	0.791296721
0.997350812	0.190892398	0.208703294
0.956847906	0.725016832	0.012652636
0.043152064	0.225016817	0.987347364
0.645885110	0.305536151	0.178303659
0.354114890	0.805536151	0.821696341
0.647630453	0.314476460	0.772958994
0.352369577	0.814476430	0.227041006
0.541740000	0.172939673	0.963958740
0.458260030	0.672939658	0.036041304
0.174137235	0.022293821	0.709276199
0.825862765	0.522293806	0.290723860
0.859419048	0.606410444	0.223150462
0.140580982	0.106410451	0.776849568

SAS_6_FE2_POSCAR

1.0

7.6668248177	0.0000000000	0.0000000000
0.0000000000	7.0709519386	0.0000000000
-1.1388495180	0.0000000000	9.9183297756

Cl	N	C	H	O
2	2	20	32	2

Direct

0.204991013	0.774710417	0.525838554
0.795009017	0.274710447	0.474161446
0.795917034	0.838175833	0.555796564
0.204082951	0.338175863	0.444203436
0.670327842	0.790577352	0.435965687
0.329672188	0.290577352	0.564034283
0.699806511	0.938007772	0.773345053

0.300193489	0.438007772	0.226654962
0.736818254	0.768225968	0.688152730
0.263181746	0.268225968	0.311847270
0.872771680	0.630778193	0.758615792
0.127228305	0.130778208	0.241384193
0.805907726	0.536617756	0.878665388
0.194092259	0.036617801	0.121334627
0.871666610	0.585982502	0.010583406
0.128333390	0.085982554	0.989416599
0.811624467	0.491927713	0.120335534
0.188375548	0.991927743	0.879664481
0.686118841	0.347638339	0.098477125
0.313881159	0.847638309	0.901522875
0.617169142	0.302714318	0.967021883
0.382830858	0.802714288	0.032978129
0.676207900	0.396281540	0.857748449
0.323792100	0.896281540	0.142251566
0.542203784	0.851358473	0.450116277
0.457796186	0.351358503	0.549883723
0.921715021	0.787565291	0.543329060
0.078284986	0.287565261	0.456670970
0.659685314	0.636439443	0.428601861
0.340314686	0.136439443	0.571398079
0.809271514	0.985632300	0.556961477
0.190728486	0.485632300	0.443038493
0.719450533	0.848168671	0.345694512
0.280549467	0.348168671	0.654305518
0.588905513	0.020468684	0.724680424
0.411094517	0.520468652	0.275319546
0.815152705	0.030166859	0.789695323
0.184847280	0.530166805	0.210304677
0.665885985	0.891385794	0.871659219
0.334114045	0.391385823	0.128340796
0.614398837	0.689908803	0.658758044
0.385601163	0.189908817	0.341241986
0.901034176	0.521030545	0.685701966
0.098965801	0.021030575	0.314298004
0.995478332	0.706222117	0.790465236
0.004521653	0.206222162	0.209534779
0.971458256	0.695920885	0.029552616
0.028541727	0.195920929	0.970447361

0.644075215	0.272052348	0.184454605
0.355924785	0.772052348	0.815545380
0.626902878	0.356607467	0.754929841
0.373097152	0.856607437	0.245070159
0.518126130	0.191763595	0.950639188
0.481873870	0.691763580	0.049360842
0.161124349	0.955728114	0.685100138
0.838875651	0.455728114	0.314899892
0.881008267	0.543752134	0.247294888
0.118991710	0.043752182	0.752705097

SAS_7_FE1_POSCAR

1.0

8.1680736542	0.0000000000	0.0000000000
0.0000000000	6.9374852180	0.0000000000
1.1033595893	0.0000000000	11.6023844676

Cl	F	N	C	H
2	6	2	24	34

Direct

0.773853004	0.257876009	0.517377019
0.226146996	0.757875979	0.482623011
0.765847027	0.971242011	0.015150000
0.234153003	0.471242011	0.984849989
0.831179023	0.218189999	0.901467979
0.168821007	0.718190014	0.098531999
0.964459002	0.166504994	0.053438999
0.035541002	0.666504979	0.946560979
0.157066002	0.190750003	0.494080007
0.842934012	0.690750003	0.505919993
0.500496984	0.323821992	0.258197993
0.499502987	0.823822021	0.741801977
0.607873976	0.209492996	0.186649993
0.392125994	0.709492981	0.813350022
0.690141976	0.285652012	0.086003996
0.309857994	0.785651982	0.913995981
0.665534973	0.477205008	0.054651000
0.334464997	0.977205992	0.945348978
0.558140993	0.591522992	0.125688002
0.441859007	0.091522999	0.874311984
0.477063000	0.516556025	0.226569995
0.522937000	0.016556000	0.773429990
0.415993005	0.241644993	0.367969990
0.584007025	0.741644979	0.632030010
0.229418993	0.273443997	0.380912989
0.770581007	0.773443997	0.619086981
0.143260002	0.181534007	0.284204006
0.856739998	0.681533992	0.715795994
0.220405996	0.268757999	0.601255000
0.779594004	0.768757999	0.398745000
0.117187001	0.192316994	0.706695020
0.882812977	0.692317009	0.293305010
0.810800016	0.161818996	0.014265000

0.189199999	0.661818981	0.985734999
0.028724000	0.212825000	0.500182986
0.971275985	0.712825000	0.499817014
0.175644994	0.039319001	0.491964012
0.824355006	0.539318979	0.508036017
0.627656996	0.059413999	0.209698007
0.372343004	0.559414029	0.790301979
0.537582994	0.740697026	0.101492003
0.462417006	0.240696996	0.898508012
0.394405991	0.608722985	0.281636000
0.605593979	0.108723000	0.718364000
0.441172987	0.086006001	0.372449994
0.558826983	0.586005986	0.627550006
0.472103000	0.308095008	0.440481007
0.527897000	0.808094978	0.559518993
0.202876002	0.428772002	0.386029005
0.797124028	0.928771973	0.613970995
0.182859004	0.253333986	0.202429995
0.817140996	0.753333986	0.797569990
0.009103000	0.197146997	0.299474001
0.990897000	0.697147012	0.700525999
0.173121005	0.027370000	0.275638014
0.826879025	0.527369976	0.724362016
0.216486007	0.426822007	0.595445991
0.783514023	0.926822007	0.404554009
0.349321008	0.224102005	0.601382971
0.650678992	0.724102020	0.398616999
0.986827016	0.227107003	0.702934980
0.013173000	0.727106988	0.297064990
0.129761994	0.035241999	0.714224994
0.870238006	0.535242021	0.285775006
0.157212004	0.257259995	0.785090029
0.842787981	0.757260025	0.214910001
0.729658008	0.536171019	0.976297021
0.270341992	0.036171000	0.023703000

SAS_7_FE2_POSCAR

1.0

8.3783588409	0.0000000000	0.0000000000
0.0000000000	7.3202595711	0.0000000000

1.0739391465					0.0000000000	11.1361248465
Cl	F	N	C	H		
2	6	2	24	34		
Direct						
	0.807264030			0.200143099		0.469035536
	0.192735955			0.700143099		0.530964494
	0.779907703			0.943034172		0.061683103
	0.220092297			0.443034172		0.938316882
	0.864762068			0.130634844		0.915918767
	0.135237962			0.630634844		0.084081233
	0.976809800			0.132889509		0.085822009
	0.023190193			0.632889509		0.914178014
	0.165206477			0.291618049		0.486584991
	0.834793568			0.791618049		0.513415039
	0.521438301			0.361824155		0.249602646
	0.478561729			0.861824155		0.750397384
	0.628544033			0.229660928		0.199534029
	0.371455967			0.729660928		0.800465941
	0.714093447			0.259202302		0.087716021
	0.285906583			0.759202302		0.912284017
	0.695358694			0.421434641		0.024747049
	0.304641336			0.921434641		0.975252926
	0.587993801			0.553312182		0.073818572
	0.412006229			0.053312182		0.926181436
	0.501436710			0.523341000		0.185007960
	0.498563290			0.023341000		0.814992011
	0.431413531			0.331947505		0.371194661
	0.568586469			0.831947505		0.628805339
	0.255570978			0.277210534		0.363826573
	0.744429052			0.777210534		0.636173427
	0.233917683			0.089909792		0.308846802
	0.766082287			0.589909792		0.691153169
	0.226576671			0.184331059		0.586373329
	0.773423314			0.684331000		0.413626701
	0.111578681			0.200757980		0.699355066
	0.888421297			0.700757980		0.300644964
	0.831979871			0.117855191		0.037782341
	0.168020144			0.617855191		0.962217689
	0.164778635			0.432155430		0.510022938
	0.835221350			0.932155430		0.489977062
	0.044014517			0.255730867		0.479700178

0.955985487	0.755730867	0.520299792
0.647424996	0.104951978	0.249451503
0.352575004	0.604951918	0.750548482
0.573060751	0.680573642	0.025690122
0.426939279	0.180573583	0.974309862
0.418016076	0.627488256	0.223133221
0.581983924	0.127488256	0.776866794
0.494106650	0.227325380	0.419335634
0.505893350	0.727325380	0.580664337
0.432834715	0.459273815	0.423606426
0.567165256	0.959273815	0.576393604
0.198462620	0.380881131	0.310524553
0.801537395	0.880881131	0.689475417
0.299067110	0.086880088	0.219018623
0.700932860	0.586880088	0.780981362
0.106804304	0.062989712	0.299748003
0.893195689	0.562989712	0.700251997
0.280237973	0.979443610	0.362321705
0.719762027	0.479443669	0.637678266
0.345518798	0.238049984	0.600989401
0.654481173	0.738050044	0.399010569
0.239315331	0.041037381	0.558079481
0.760684669	0.541037381	0.441920549
0.101145819	0.342443824	0.731314898
0.898854196	0.842443824	0.268685132
0.991455615	0.152287483	0.683376551
0.008544364	0.652287483	0.316623479
0.155191764	0.117791772	0.771007240
0.844808221	0.617791772	0.228992775
0.765298307	0.444429457	0.939083159
0.234701693	0.944429457	0.060916822

SAS_8_FE1_POSCAR

1.0

7.3961668015	0.0000000000	0.0000000000
0.0000000000	7.1087198257	0.0000000000
1.6942712583	0.0000000000	11.1687475580

Cl	O	N	C	H
2	4	4	20	30

Direct

0.748672009	0.255237013	0.549929976
0.251327991	0.755236983	0.450069994
0.845326006	0.928879023	0.985782981
0.154673994	0.428878993	0.014217000
0.911279023	0.156066999	0.854983985
0.088721000	0.656067014	0.145016000
0.161226004	0.181572005	0.494044006
0.838774025	0.681572020	0.505955994
0.837219000	0.096083000	0.953719020
0.162781000	0.596082985	0.046280999
0.531421006	0.281614989	0.223239005
0.468578994	0.781615019	0.776760995
0.636084020	0.158985004	0.143966004
0.363916010	0.658985019	0.856033981
0.732255995	0.228191003	0.037094001
0.267744005	0.728191018	0.962906003
0.729076028	0.417802006	0.006277000
0.270924002	0.917801976	0.993723989
0.625555992	0.540157974	0.085741997
0.374444008	0.040158000	0.914258003
0.526974022	0.473233014	0.192605004
0.473026007	0.973232985	0.807394981
0.435176015	0.207537994	0.340772986
0.564823985	0.707538009	0.659227014
0.232353002	0.259680003	0.371365994
0.767647028	0.759679973	0.628633976
0.114446998	0.181927994	0.283124000
0.885553002	0.681927979	0.716875970
0.235738993	0.266512990	0.597016990
0.764261007	0.766512990	0.402983010
0.156712994	0.212294996	0.679827988
0.843286991	0.712294996	0.320172012
0.017533001	0.200009003	0.509586990

0.982466996	0.700008988	0.490413010
0.185886994	0.035386000	0.490745991
0.814113021	0.535386026	0.509253979
0.643203974	0.009632000	0.164148003
0.356795996	0.509631991	0.835852027
0.623273015	0.689191997	0.063538000
0.376727015	0.189191997	0.936461985
0.445675999	0.571255982	0.253428996
0.554323971	0.071255997	0.746571004
0.446348011	0.053204998	0.341574013
0.553651989	0.553205013	0.658425987
0.510196984	0.259315997	0.411518008
0.489802986	0.759316027	0.588482022
0.216529995	0.413300008	0.379188001
0.783469975	0.913299978	0.620811999
0.156777993	0.244480997	0.194564998
0.843222022	0.744481981	0.805435002
0.969739020	0.217901006	0.310526013
0.030261001	0.717900991	0.689473987
0.127480999	0.027968001	0.276583999
0.872519016	0.527967989	0.723415971
0.221570998	0.419817001	0.592810988
0.778428972	0.919816971	0.407189012
0.380387008	0.230042994	0.593006015
0.619612992	0.730042994	0.406993985
0.806474984	0.466522008	0.922581971
0.193525001	0.966521978	0.077418000

SAS_8_FE2_POSCAR

1.0

7.4087104797	0.0000000000	0.0000000000
0.0000000000	7.4064083099	0.0000000000
1.6829557098	0.0000000000	10.6605358165

Cl	O	N	C	H
2	4	4	20	30

Direct

0.738552272	0.263668776	0.551422477
0.261447757	0.763668776	0.448577553
0.836452484	0.910789430	0.024164876
0.163547516	0.410789400	0.975835085

0.922038615	0.086724162	0.862206221
0.077961400	0.586724222	0.137793720
0.148203388	0.357287347	0.493615985
0.851796627	0.857287407	0.506383955
0.839299440	0.059523225	0.969892502
0.160700604	0.559523225	0.030107459
0.540508986	0.320419788	0.219421014
0.459491014	0.820419788	0.780579031
0.637925029	0.178378969	0.155357510
0.362074941	0.678378999	0.844642460
0.738558054	0.209618121	0.036725659
0.261441916	0.709618151	0.963274360
0.744396687	0.378070086	0.978730023
0.255603284	0.878070116	0.021270016
0.649232507	0.519956470	0.043853682
0.350767463	0.019956499	0.956146300
0.548933625	0.491847426	0.162824348
0.451066345	0.991847456	0.837175667
0.434256524	0.293114245	0.348464042
0.565743506	0.793114305	0.651535988
0.228855819	0.327372372	0.357048631
0.771144211	0.827372372	0.642951369
0.127231315	0.182063401	0.296127260
0.872768700	0.682063460	0.703872740
0.210876644	0.237623006	0.589650869
0.789123297	0.737623036	0.410349131
0.122037612	0.260587752	0.679362416
0.877962351	0.760587811	0.320637614
0.177314103	0.493089348	0.510118842
0.822685897	0.993089318	0.489881098
0.004365973	0.342916936	0.504046321
0.995634019	0.842916965	0.495953679
0.635313392	0.043614388	0.195993304
0.364686638	0.543614388	0.804006696
0.655283749	0.654364169	0.002708907
0.344716251	0.154364139	0.997291088
0.475847632	0.604456127	0.213575453
0.524152339	0.104456097	0.786424577
0.457637280	0.155996531	0.381462872
0.542362630	0.655996561	0.618537188
0.490144432	0.386051953	0.412382126

0.509855568	0.886052012	0.587617874
0.207085267	0.458223403	0.313632160
0.792914689	0.958223403	0.686367810
0.173368186	0.187188983	0.194562986
0.826631784	0.687189102	0.805437028
0.979481578	0.208171278	0.311440170
0.020518405	0.708171308	0.688559890
0.155014858	0.046365172	0.329942286
0.844985127	0.546365142	0.670057714
0.353334278	0.267838657	0.597916484
0.646665692	0.767838657	0.402083486
0.200353459	0.095936775	0.562001288
0.799646497	0.595936775	0.437998682
0.823210359	0.395351708	0.885796905
0.176789641	0.895351768	0.114203095

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