

Supporting Information

Insights into the Nucleophilic Substitution of pyridine at an Unsaturated Carbon Center

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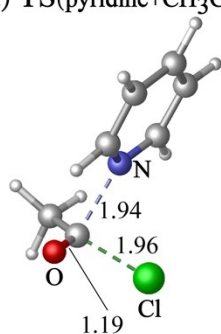
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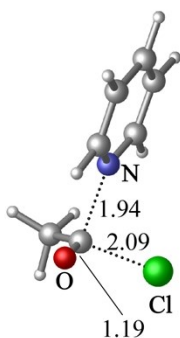
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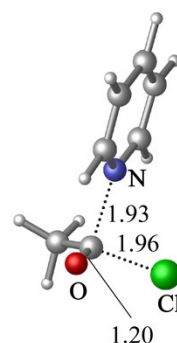
(a) TS(pyridine+CH₃ClCO)



$\Delta G^\ddagger = 13.8$ kcal/mol
M06-2X

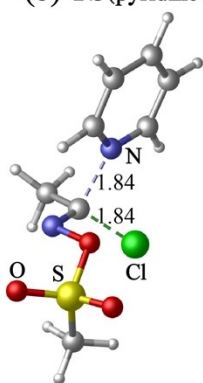


$\Delta G^\ddagger = 15.5$ kcal/mol
B3LYP-*d3*

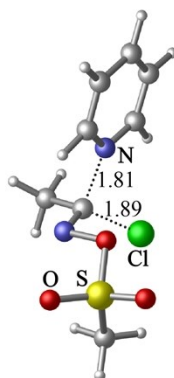


$\Delta G^\ddagger = 13.0$ kcal/mol
wB97XD

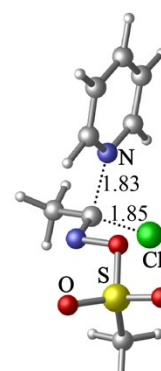
(b) TS(pyridine+s7)



$\Delta G^\ddagger = 22.8$ kcal/mol
M06-2X

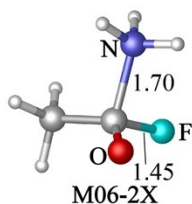


$\Delta G^\ddagger = 24.6$ kcal/mol
B3LYP-*d3*

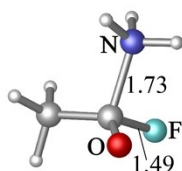


$\Delta G^\ddagger = 23.4$ kcal/mol
wB97XD

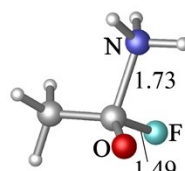
(c) T(NH₃-CH₃FCO)



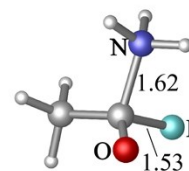
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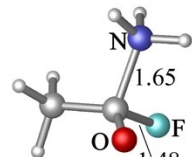
B3LYP



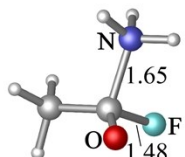
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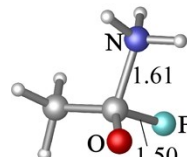
MP2



wB97XD

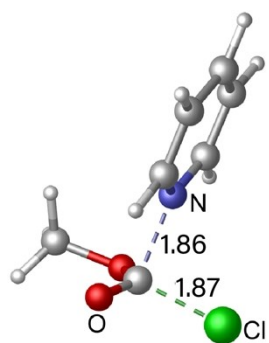


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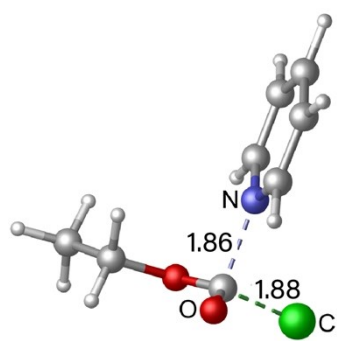


QCISD

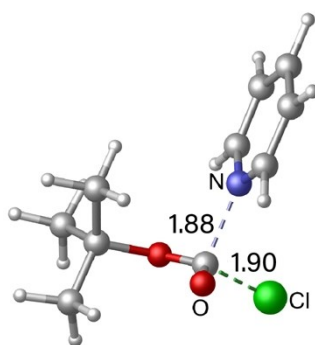
Figure S1. The geometry structures of (a) transition states of pyridine reacting with s1, (b) transition states of pyridine reacting with s7 and (c) tetrahedral intermediates formed from NH₃ and CH₃FCO calculated by other density functionals.



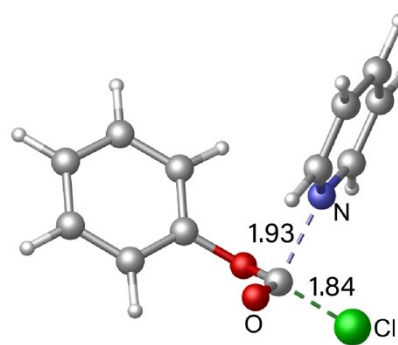
S2



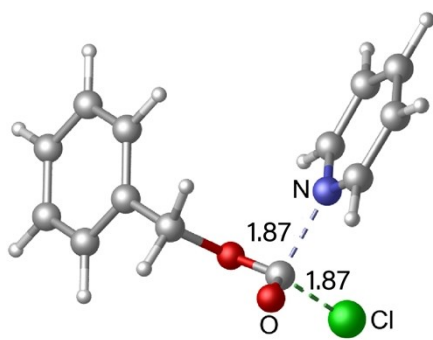
S3



S4

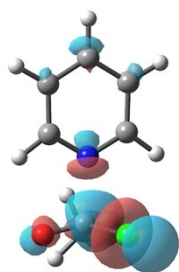


S5

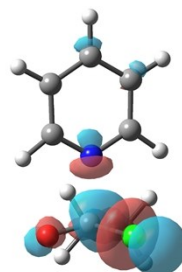


S6

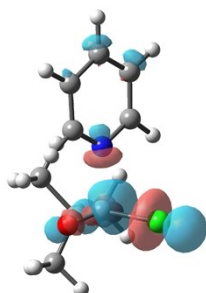
Figure S2. The geometry structures of transition states of the substrates (s2-s7) reacting with pyridine.



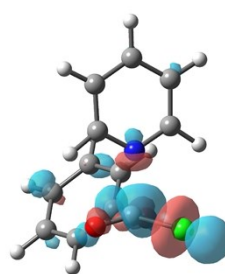
S2



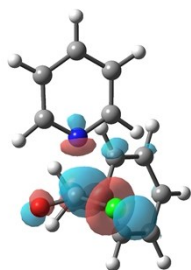
S3



S4

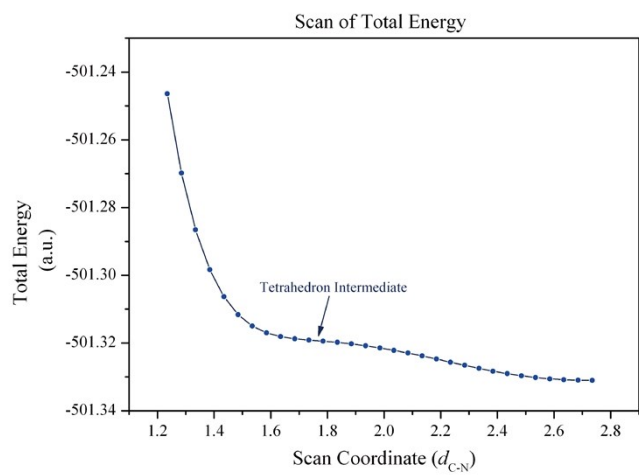


S5

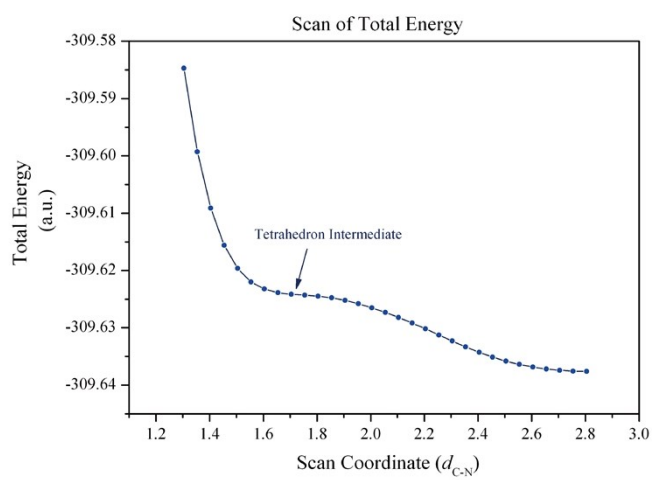


S6

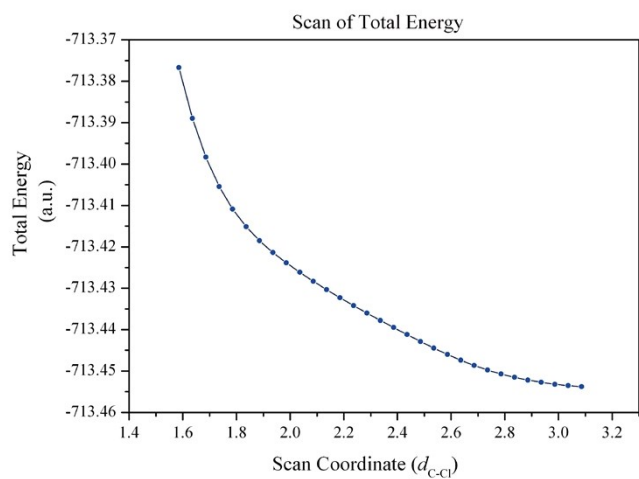
Figure S3. The mixing orbitals of transition states of the substrates (s2-s7) reacting with pyridine.



(a)



(b)



(c)

Figure S4. The potential energy diagrams representing the reaction of acyl fluoride (s1) with different nucleophiles (pyridine, NH_3 , and Cl^-)

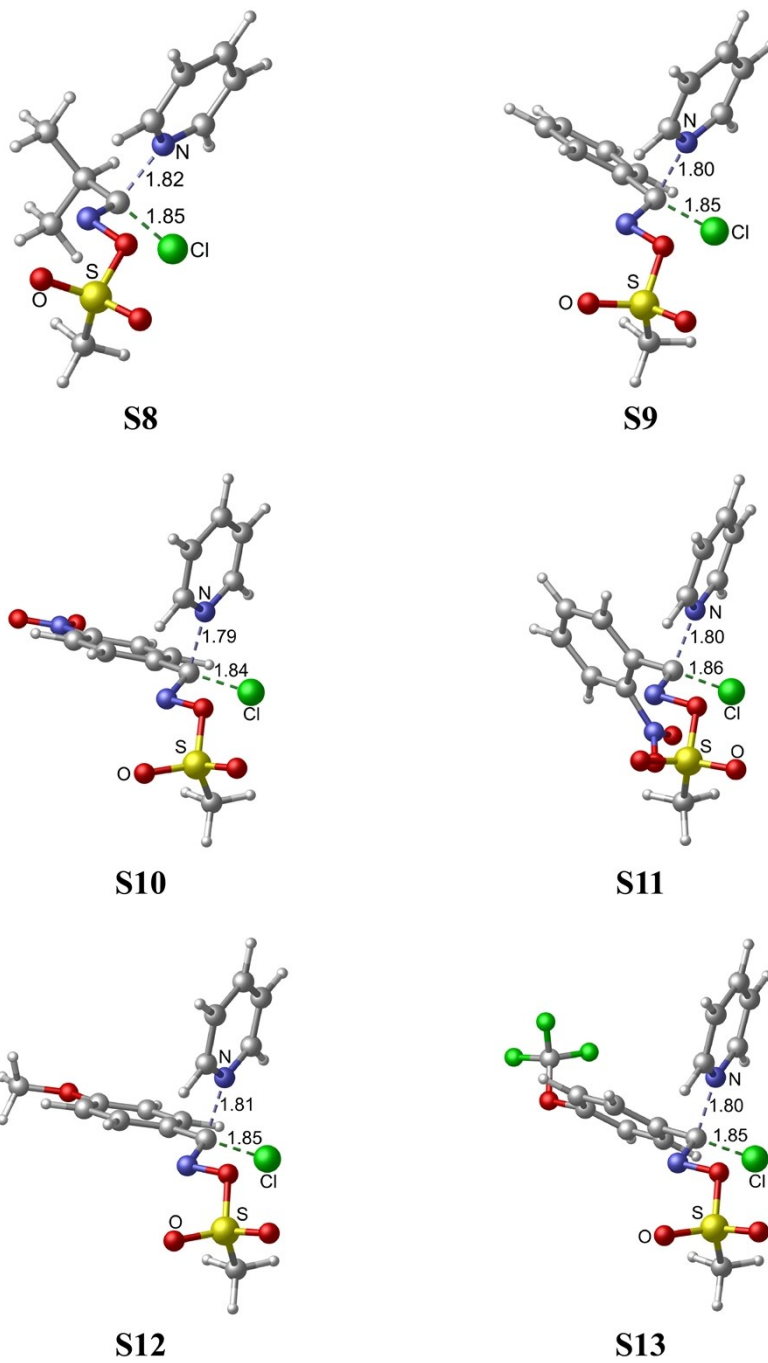


Figure S5. The geometry structures of transition states of the imidoyl substrates (s8-s13) reacting with pyridine.

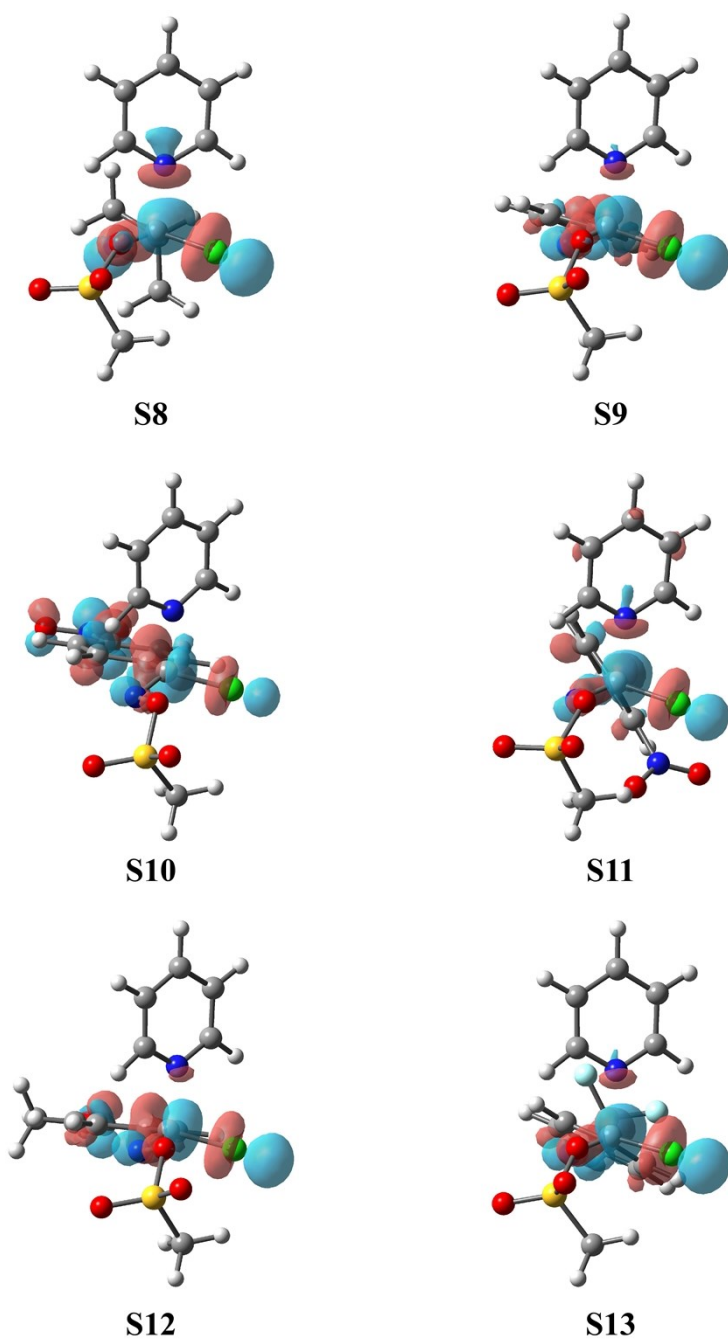
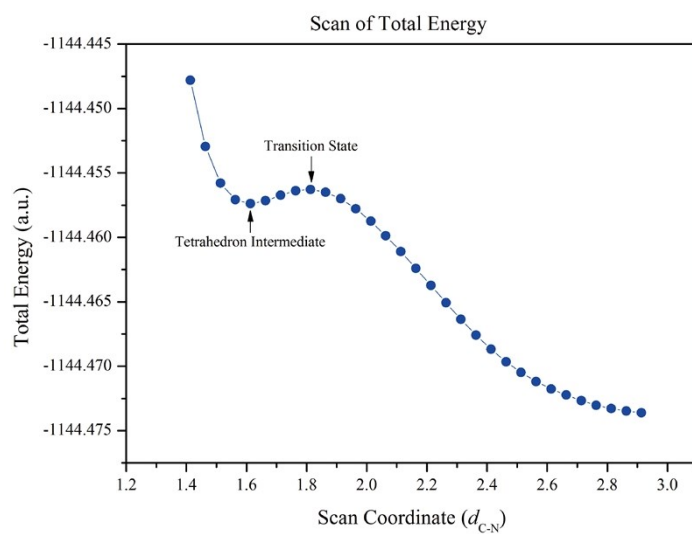
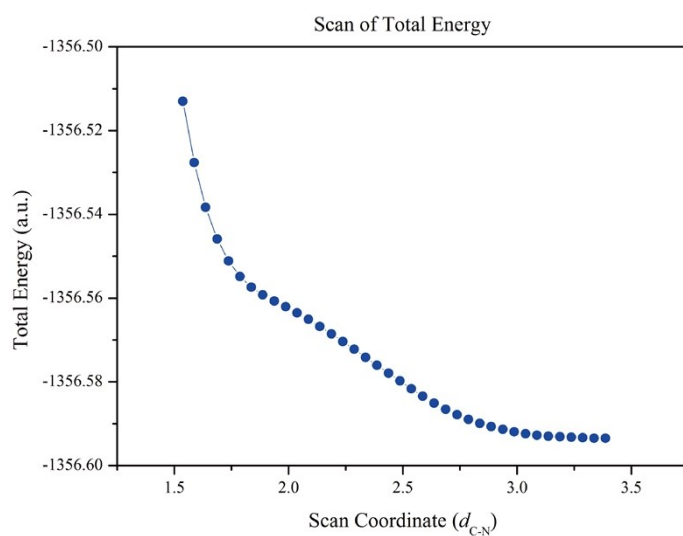


Figure S6. The mixing orbitals of transition states of the imidoyl substrates (s8-s13) reacting with pyridine.



(a)



(b)

Figure S7. The profile scans of nucleophile (pyridine or Cl^-) approach to

$\text{CH}_3\text{FC}=\text{NOTf}$ (s7).

Table S1. Free energies of all species (a.u.).

Species	Free energies	Species	Free energies
Cl	-460.383802	s9	-1448.170274
pyridine	-248.180832	s9-ts	-1696.313281
s1	-613.409228	s9-ts-p	-1696.345615
s1Br-ts	-2975.543871	s9-ts-r	-1696.343195
s1Cl-ts	-1073.767374	s10	-1652.662273
s1Cl-ts-sgm	-1073.76094	s10-ts	-1900.805854
s1-ts	-861.568053	s10-ts-p	-1900.836904
s1-ts-p	-861.582627	s10-ts-r	-1900.836189
s1-ts-r	-861.581646	s11	-1652.654173
s1-ts-sigma	-861.543104	s11-ts	-1900.793016
s2	-688.624292	s11-ts-p	-1900.821010
s2-ts	-936.780512	s11-ts-r	-1900.827239
s2-ts-p	-936.804729	s12	-1562.656498
s2-ts-r	-936.797344	s12-ts	-1810.799682
s3	-727.906730	s12-ts-p	-1810.833169
s3-ts	-976.062437	s12-ts-r	-1810.831501
s3-ts-p	-976.088209	s13	-1860.439383
s3-ts-r	-976.079351	s13-ts	-2108.582137
s4	-806.470158	s13-ts-p	-2108.615738
s4-ts	-1054.624172	s13-ts-r	-2108.611775
s4-ts-p	-1054.650621	s14	-538.150208
s4-ts-r	-1054.641137	s14-ts	-786.263421
s5	-880.284127	s14-ts-sgm	-786.255297
s5-ts	-1128.443643	s14Cl-ts	-998.45768
s5-ts-p	-1128.463958	s14Cl-ts-sgm	-998.466638
s5-ts-r	-1128.455625	s15	-616.717757
s6	-919.565582	s15-ts	-864.825287
s6-ts	-1167.722418	s16	-1916.963926
s6-ts-p	-1167.746239	s16-ts	-2165.083830
s6-ts-r	-1167.736780	d-pyridine	-248.312009
s7	-1256.511927	d-s1	-613.519492
s7Cl-ts	-1716.853471	d-s1-ts	-861.810765
s7Cl-ts-sigma	-1716.832046	d-s7	-1256.768094
s7F	-896.153860	d-s7-ts	-1505.042879
s7-ts	-1504.656378	w-pyridine	-248.198892
s7-ts-p	-1504.686811	w-s1	-613.437474
s7-ts-r	-1504.683555	w-s1-ts	-861.611596
s7-ts-sgm	-1504.61414	w-s7	-1256.570556
s8	-1335.067915	w-s7-ts	-1504.730169
s8-ts	-1583.210553	T(Py+s1F)	-501.21293

s8-ts-p	-1583.243336	T(NH3+s1F)	-309.56656
s8-ts-r	-1583.239846	T(Py+s7F)	-1144.303001

Table S2. Imaginary frequencies of all transition states.

Species	Imaginary frequency
s1-ts	180.80 cm ⁻¹
s2-ts	189.04 cm ⁻¹
s3-ts	190.32 cm ⁻¹
s4-ts	190.61 cm ⁻¹
s5-ts	180.73 cm ⁻¹
s6-ts	190.73 cm ⁻¹
s7-ts	231.67 cm ⁻¹
s8-ts	143.30 cm ⁻¹
s9-ts	213.87 cm ⁻¹
s10-ts	203.58 cm ⁻¹
s11-ts	210.19 cm ⁻¹
s12-ts	217.57 cm ⁻¹
s13-ts	209.04 cm ⁻¹
s1-ts-sgm	181.77 cm ⁻¹
s1Cl-ts	264.63 cm ⁻¹
s1Cl-ts-sgm	75.63 cm ⁻¹
s1Br-ts	162.90 cm ⁻¹
s7-ts-sgm	232.36 cm ⁻¹
s7Cl-ts	237.19 cm ⁻¹
s7Cl-ts-sgm	186.91 cm ⁻¹
s14-ts (S_NV-σ_v)	554.97 cm ⁻¹
s14-ts-sgm (S_NV-σ_b)	689.29 cm ⁻¹
s14Cl-ts (S_NV-σ_v)	629.94 cm ⁻¹
s14Cl-ts-sgm(S_NV-σ_b)	687.66 cm ⁻¹
s15-ts	571.26 cm ⁻¹
s16-ts	385.18 cm ⁻¹

Table S3. Cartesian coordinates of all species (angstroms).

				H	-2.990543	0.822736	-1.670085
s1				H	-2.167624	-1.454910	1.896518
Symbol	X	Y	Z	O	1.469770	1.835483	-0.814975
C	-0.482976	0.237660	-0.000001	Cl	1.413578	-1.916105	-0.789323
O	-0.821045	1.366968	-0.000381	C	2.070547	0.817611	1.273436
C	-1.327001	-0.993650	0.000071	H	3.021904	1.317384	1.112418
H	-2.376031	-0.706607	-0.001001	H	1.624788	1.165163	2.207297
H	-1.087816	-1.589274	-0.881582	H	2.224469	-0.261509	1.311808
H	-1.089245	-1.587987	0.882979	C	1.193546	1.155549	0.116259
Cl	1.290870	-0.143978	0.000317	H	0.132712	-0.529498	1.860908
s1-ts				s1-ts-r			
Symbol	X	Y	Z	Symbol	X	Y	Z
C	1.143514	1.136647	0.304475	C	-1.095632	0.859979	0.414056
C	2.521411	1.011564	0.424060	C	-2.421150	1.272369	0.327254
C	3.108081	-0.202315	0.090680	C	-3.375272	0.351244	-0.088916
C	2.303318	-1.251070	-0.345275	C	-2.965269	-0.939674	-0.400315
C	0.935868	-1.045167	-0.433713	C	-1.614951	-1.252505	-0.280707
N	0.387887	0.129330	-0.117939	N	-0.690825	-0.376603	0.118208
H	4.179964	-0.333886	0.172836	H	-4.418225	0.633942	-0.169022
H	0.610495	2.048846	0.553261	H	-0.321004	1.550258	0.736767
H	3.111523	1.848377	0.772385	H	-2.691871	2.289385	0.580442
H	2.721875	-2.213557	-0.606692	H	-3.671079	-1.691901	-0.728570
O	-1.629625	1.624758	0.318200	O	1.953459	0.519250	1.487612
Cl	-2.078754	-0.972812	0.877292	Cl	2.289836	0.740631	-1.080698
C	-1.788107	0.221951	-1.641866	C	2.175520	-1.607725	0.359997
H	-2.869039	0.277600	-1.781176	H	3.211787	-1.858115	0.121916
H	-1.301820	0.971965	-2.266907	H	1.881187	-2.073850	1.298235
H	-1.446007	-0.774425	-1.906955	H	1.536107	-1.936287	-0.455812
C	-1.503596	0.560263	-0.204114	C	2.076099	-0.126366	0.509225
H	0.255830	-1.829705	-0.745836	H	-1.260672	-2.251848	-0.515821
s1-ts-p				s1-ts-sigm			
Symbol	X	Y	Z	Symbol	X	Y	Z
C	-1.051972	0.999573	-0.819647	C	-1.728636	-1.099664	-0.003683
C	-2.337075	0.511339	-0.867747	C	-3.111123	-1.237254	-0.016227
C	-2.759684	-0.377872	0.116581	C	-3.891063	-0.087442	-0.019027
C	-1.880127	-0.757299	1.123111	C	-3.260020	1.150697	-0.009699
C	-0.599866	-0.247654	1.121828	C	-1.871741	1.185702	0.001823
N	-0.215657	0.626340	0.170627	N	-1.115348	0.085275	0.005166
H	-3.766325	-0.776017	0.094817	H	-4.972117	-0.154537	-0.028157
H	-0.639826	1.682989	-1.547916	H	-1.087758	-1.976416	-0.000191

H	-3.557650	-2.222686	-0.023277
H	-3.825309	2.073226	-0.010968
O	1.362995	-1.295917	0.043795
Cl	4.291799	-0.036997	-0.032982
C	1.507191	1.246483	0.023478
H	2.573273	1.474028	0.042258
H	0.996005	1.598905	-0.874112
H	1.005250	1.616212	0.920367
C	1.382059	-0.182993	0.046556
H	-1.348803	2.137460	0.008931

s1Br-ts

Symbol	X	Y	Z
C	-1.727475	0.988597	-0.596756
C	-3.053061	0.615509	-0.782225
C	-3.511204	-0.534112	-0.151444
C	-2.633391	-1.272547	0.636604
C	-1.325595	-0.829117	0.765045
N	-0.898497	0.280320	0.161678
H	-4.538329	-0.855154	-0.274469
H	-1.301178	1.870397	-1.065934
H	-3.701694	1.214365	-1.407397
H	-2.949367	-2.177239	1.138562
O	0.987453	1.935833	-0.578563
C	1.143087	1.162055	1.715935
H	2.186030	1.406855	1.924991
H	0.497035	1.968745	2.065231
H	0.889385	0.225455	2.202139
C	0.999165	1.073337	0.226149
H	-0.592909	-1.375761	1.349476
Br	1.961586	-0.749957	-0.397317

s1Cl-ts

Symbol	X	Y	Z
O	-0.000229	1.058008	1.360088
Cl	-1.632286	-0.754093	-0.049404
C	-0.000230	1.398552	-1.049686
H	-0.894686	2.023533	-1.065607
H	0.894120	2.023682	-1.065634
H	-0.000181	0.712158	-1.887944
C	-0.000148	0.660398	0.255939
Cl	1.632664	-0.753392	-0.049359

s1Cl-ts-sgm

Symbol	X	Y	Z
O	0.250297	-1.331462	0.926554
Cl	-2.843074	-0.140774	0.916311
C	0.101096	1.203774	0.768080
H	-0.763431	1.489895	1.365969
H	1.057536	1.597465	1.114819
H	-0.050479	1.468932	-0.280464
C	0.190274	-0.227415	0.813061
Cl	2.577752	0.060243	-0.814891

s2

Symbol	X	Y	Z
C	-0.030528	0.306505	-0.001253
O	0.215694	1.467155	0.000229
Cl	-1.690866	-0.303845	0.000276
O	0.802214	-0.703799	-0.000488
C	2.199995	-0.333349	0.000470
H	2.422594	0.247134	0.893738
H	2.738172	-1.274371	0.001025
H	2.423880	0.246821	-0.892680

s2-ts

Symbol	X	Y	Z
C	-1.039635	0.193588	1.107389
C	-2.416653	0.226505	1.254357
C	-3.211364	0.050163	0.124932
C	-2.608879	-0.149974	-1.111128
C	-1.222782	-0.167079	-1.177883
N	-0.481260	0.000426	-0.087984
H	-4.290887	0.069084	0.209754
H	-0.353746	0.320132	1.937317
H	-2.851494	0.385892	2.231677
H	-3.194518	-0.289699	-2.009500
O	1.573248	-0.008400	-1.502812
Cl	1.666113	-1.685961	0.557779
C	1.367982	-0.056694	-0.316634
O	1.735033	0.881407	0.589171
H	-0.669347	-0.312105	-2.099419
C	1.719801	2.210976	0.056424
H	2.010774	2.860520	0.877329
H	2.424706	2.296628	-0.769516
H	0.714078	2.467103	-0.286500

s2-ts-p

Symbol	X	Y	Z
C	0.866337	-0.371524	-1.026513
C	2.181141	-0.765050	-1.146788
C	3.129778	-0.240984	-0.276204
C	2.744084	0.671990	0.702419
C	1.422094	1.040454	0.786413
N	0.522747	0.528244	-0.080174
H	4.165450	-0.547184	-0.353645
H	0.063626	-0.749699	-1.639349
H	2.445293	-1.487107	-1.905857
H	3.454710	1.092921	1.398862
O	-1.236509	1.453205	1.108773
Cl	-1.234778	-2.049367	0.755804
C	-0.888240	0.914406	0.108204
O	-1.566490	0.642300	-0.966584
H	1.028239	1.728958	1.520098
C	-3.000505	0.754419	-0.829121
H	-3.401259	0.480794	-1.799119
H	-3.322548	0.056153	-0.057638
H	-3.262115	1.778192	-0.569332

s2-ts-r

Symbol	X	Y	Z
C	1.538785	0.829245	-0.910644
C	2.913903	0.638760	-0.997927
C	3.536450	-0.140841	-0.029852
C	2.760933	-0.695632	0.981254
C	1.392531	-0.444907	0.980023
N	0.785393	0.302845	0.056637
H	4.605688	-0.313014	-0.063508
H	1.017847	1.431126	-1.649588
H	3.475912	1.090766	-1.805151
H	3.200835	-1.310516	1.755948
O	-1.816699	-0.237672	1.520744
Cl	-1.954030	-1.652803	-0.652540
C	-1.934887	-0.192685	0.340144
O	-2.123697	0.853773	-0.425056
H	0.749617	-0.860069	1.750836
C	-1.998758	2.118720	0.255216
H	-2.176934	2.871486	-0.506045
H	-2.739747	2.187086	1.049981
H	-0.990588	2.196766	0.660132

s3

Symbol	X	Y	Z
C	-0.612968	0.414009	0.000350
O	-0.698902	1.597104	-0.000213
Cl	-2.039358	-0.629772	-0.000454
O	0.466064	-0.328184	0.000252
C	1.727745	0.402441	0.000083
H	1.746736	1.035226	0.887809
H	1.746546	1.035158	-0.887696
C	2.829893	-0.626911	0.000004
H	2.769511	-1.256698	-0.888056
H	3.794559	-0.117910	-0.000082
H	2.769656	-1.256673	0.888091

s3-ts

Symbol	X	Y	Z
C	-1.589197	-0.368900	-1.072414
C	-2.904847	0.063070	-0.980338
C	-3.292065	0.775477	0.148125
C	-2.359238	1.035540	1.148317
C	-1.065390	0.568382	0.985471
N	-0.714495	-0.113327	-0.105446
H	-4.311685	1.126355	0.249210
H	-1.198534	-0.925347	-1.917523
H	-3.602097	-0.156212	-1.777389
H	-2.625606	1.588035	2.039080
O	1.099923	-1.103936	-1.496432
Cl	0.943333	-2.106091	0.964631
C	1.011994	-0.760042	-0.344928
O	1.710606	0.238201	0.242218
C	1.998707	1.336063	-0.646196
H	1.059516	1.681222	-1.090046
H	2.648850	0.977671	-1.445677
H	-0.282069	0.727142	1.718049
C	2.653525	2.418049	0.180183
H	2.895553	3.270281	-0.456671
H	1.983465	2.755477	0.972613
H	3.575479	2.049930	0.632278

s3-ts-p

Symbol	X	Y	Z
C	-1.863313	-0.983794	0.737861
C	-3.153843	-0.648478	0.400776
C	-3.371369	0.175092	-0.700943
C	-2.290301	0.647048	-1.436776

C	-1.013467	0.290698	-1.061641
N	-0.832102	-0.525295	-0.001547
H	-4.380289	0.452829	-0.979234
H	-1.597007	-1.604450	1.581310
H	-3.970818	-1.025599	0.998825
H	-2.424671	1.300249	-2.286880
O	0.701743	-1.340107	1.531699
Cl	0.765059	2.117890	0.957091
C	0.531057	-0.874706	0.451000
O	1.379885	-0.659179	-0.506404
C	2.785419	-0.692376	-0.118755
H	3.018221	-1.708833	0.198776
H	2.890476	-0.004911	0.721525
H	-0.119077	0.635310	-1.556343
C	3.580715	-0.256636	-1.322345
H	4.641276	-0.260010	-1.067052
H	3.424310	-0.935656	-2.161424
H	3.298306	0.754181	-1.618351

s3-ts-r

Symbol	X	Y	Z
C	1.905314	-0.373348	1.255832
C	3.253450	-0.187344	0.966290
C	3.607674	0.194379	-0.322256
C	2.602331	0.372802	-1.265342
C	1.283786	0.161164	-0.875840
N	0.931753	-0.203283	0.359208
H	4.647068	0.348968	-0.586578
H	1.592572	-0.672437	2.251506
H	4.000651	-0.339897	1.734535
H	2.828772	0.667487	-2.282069
O	-2.005142	-0.837336	1.507294
Cl	-1.775586	-1.980824	-0.816755
C	-1.869187	-0.648503	0.343757
O	-1.815368	0.488558	-0.303331
C	-1.737797	1.669128	0.541564
H	-0.914540	1.512887	1.239342
H	-2.674007	1.749602	1.095368
H	0.469377	0.287941	-1.583794
C	-1.501048	2.846627	-0.371237
H	-1.444434	3.758200	0.225405
H	-0.561231	2.727690	-0.912472
H	-2.314947	2.952275	-1.089465

s4

Symbol	X	Y	Z
C	-1.015480	0.339521	0.002289
O	-0.966301	1.526565	0.000761
Cl	-2.576447	-0.507825	-0.004274
O	-0.058477	-0.545998	0.000465
C	1.367942	-0.112763	0.000251
C	2.104038	-1.441996	-0.002594
H	1.847317	-2.019225	-0.892253
H	3.179490	-1.257353	-0.002808
H	1.848217	-2.022544	0.885158
C	1.651700	0.678728	-1.267303
H	1.142889	1.641618	-1.266847
H	2.727176	0.856992	-1.329323
H	1.348666	0.107632	-2.147106
C	1.653564	0.674241	1.270166
H	1.352155	0.099875	2.148408
H	2.729128	0.852394	1.330975
H	1.144583	1.637014	1.274090

s4-ts

Symbol	X	Y	Z
C	-1.888417	0.095379	1.150387
C	-3.135152	-0.512840	1.094963
C	-3.554438	-1.056426	-0.113130
C	-2.722313	-0.975524	-1.226494
C	-1.493349	-0.350308	-1.090628
N	-1.108490	0.161516	0.077912
H	-4.520651	-1.539955	-0.188532
H	-1.478523	0.537194	2.052686
H	-3.754968	-0.557011	1.980162
H	-3.016256	-1.388320	-2.182036
O	0.726841	1.128188	1.479677
Cl	0.160450	2.533486	-0.717397
C	0.570159	0.975844	0.297307
O	1.302421	0.231215	-0.547316
C	2.068283	-0.907611	-0.016853
H	-0.787061	-0.250643	-1.907494
C	2.570560	-1.581949	-1.285500
H	3.170399	-2.455964	-1.025166
H	1.729456	-1.904135	-1.902791
H	3.188247	-0.891739	-1.862872
C	1.171311	-1.854241	0.774205
H	0.765937	-1.372148	1.664185

H	0.349059	-2.220860	0.155628
H	1.768561	-2.712162	1.090218
C	3.233793	-0.394619	0.820543
H	3.804630	0.343269	0.253045
H	2.888065	0.058754	1.748012
H	3.893235	-1.231670	1.061206

s4-ts-p

Symbol	X	Y	Z
C	-2.057161	-0.890553	1.011843
C	-3.389290	-0.852901	0.671931
C	-3.746182	-0.481762	-0.621837
C	-2.758630	-0.151412	-1.541752
C	-1.437052	-0.191992	-1.153937
N	-1.116526	-0.578865	0.097377
H	-4.789891	-0.443168	-0.907222
H	-1.688059	-1.153754	1.992391
H	-4.131203	-1.106085	1.415411
H	-3.000641	0.156830	-2.548618
O	0.530813	-0.749309	1.713382
Cl	-0.565961	2.506005	0.334045
C	0.295481	-0.570548	0.560894
O	1.077474	-0.411705	-0.456328
C	2.554485	-0.276467	-0.275462
H	-0.614412	0.078511	-1.796484
C	3.014303	0.068865	-1.681048
H	4.101285	0.162121	-1.689689
H	2.724879	-0.714784	-2.383345
H	2.577793	1.016955	-2.000054
C	3.102065	-1.617316	0.185823
H	2.732972	-1.878289	1.177391
H	2.836398	-2.404704	-0.522138
H	4.190731	-1.548405	0.232008
C	2.844174	0.856407	0.696431
H	2.268733	1.742366	0.422501
H	2.605931	0.581308	1.722735
H	3.909119	1.089306	0.636190

s4-ts-r

Symbol	X	Y	Z
C	-2.068093	0.087234	1.062490
C	-3.368121	-0.385413	1.216497
C	-4.072538	-0.766509	0.080519
C	-3.450345	-0.658584	-1.157971

C	-2.147236	-0.172708	-1.204300
N	-1.461536	0.193614	-0.120228
H	-5.086677	-1.140271	0.158595
H	-1.481069	0.392101	1.924116
H	-3.810848	-0.450496	2.202292
H	-3.958569	-0.942629	-2.070687
O	1.009758	1.020369	1.473683
Cl	0.795090	2.597126	-0.580711
C	1.168779	1.092948	0.298908
O	1.669175	0.234101	-0.545445
C	2.154389	-1.087352	-0.069315
H	-1.629890	-0.074859	-2.154327
C	2.663805	-1.723240	-1.352816
H	3.042482	-2.723066	-1.134242
H	1.856693	-1.805271	-2.082735
H	3.471818	-1.127706	-1.781119
C	0.997392	-1.882484	0.514903
H	0.592266	-1.407259	1.407693
H	0.200178	-1.991925	-0.221483
H	1.367644	-2.874567	0.783109
C	3.287345	-0.877927	0.925865
H	4.048105	-0.219675	0.501049
H	2.929393	-0.458209	1.864886
H	3.748458	-1.845708	1.132935

s5

Symbol	X	Y	Z
C	1.616384	0.162062	0.305683
O	1.379087	0.796826	1.275317
Cl	3.250350	-0.205493	-0.215208
O	0.762343	-0.383374	-0.551077
C	-0.609457	-0.185341	-0.294078
C	-1.346074	-1.275546	0.131983
C	-1.176113	1.054950	-0.533515
C	-2.714246	-1.111068	0.330429
H	-0.855004	-2.226078	0.298701
C	-2.543453	1.204563	-0.327666
H	-0.560710	1.879439	-0.872211
C	-3.311260	0.125087	0.102777
H	-3.310256	-1.952061	0.662429
H	-3.007823	2.166119	-0.507869
H	-4.375857	0.248071	0.258714

s5-ts

Symbol	X	Y	Z
C	-1.553376	-0.785123	1.305996
C	-2.253041	-1.984692	1.337747
C	-2.778478	-2.477059	0.149906
C	-2.591276	-1.761313	-1.029879
C	-1.881398	-0.572744	-0.976352
N	-1.384461	-0.114491	0.172572
H	-3.329020	-3.409758	0.140473
H	-1.109562	-0.333291	2.187167
H	-2.377256	-2.513480	2.273036
H	-2.986371	-2.113780	-1.973090
O	-0.031119	1.607529	1.447125
Cl	-1.529736	2.651558	-0.459510
C	-0.313869	1.492484	0.288845
O	0.556720	1.202125	-0.731203
H	-1.694828	0.036708	-1.854358
C	1.611694	0.350260	-0.403296
C	1.641939	-0.896532	-1.011320
C	2.623864	0.769371	0.450175
C	2.713188	-1.748154	-0.755318
H	0.840473	-1.182660	-1.681735
C	3.686533	-0.092038	0.701405
H	2.572471	1.750319	0.903694
C	3.733306	-1.349115	0.102604
H	2.747987	-2.721696	-1.229049
H	4.482816	0.223470	1.364681
H	4.565770	-2.013071	0.301167

s5-ts-p

Symbol	X	Y	Z
C	2.558326	0.650086	1.195580
C	3.897729	0.686828	0.888876
C	4.289006	0.587338	-0.443974
C	3.328041	0.447497	-1.438571
C	1.997167	0.405622	-1.087671
N	1.643426	0.529018	0.209936
H	5.339856	0.611096	-0.703629
H	2.163165	0.706230	2.199482
H	4.618951	0.786814	1.687007
H	3.598697	0.351409	-2.480094
O	-0.058573	0.304856	1.762715
Cl	0.868477	-2.471372	-0.246426
C	0.235312	0.427165	0.622085
O	-0.535643	0.580816	-0.429823

H	1.194159	0.267254	-1.794011
C	-1.924056	0.398691	-0.249428
C	-2.737685	1.501134	-0.432501
C	-2.407800	-0.864714	0.041807
C	-4.113912	1.325746	-0.314773
H	-2.301322	2.464784	-0.663463
C	-3.785412	-1.019059	0.159243
H	-1.713545	-1.689637	0.161152
C	-4.635795	0.070160	-0.018303
H	-4.774063	2.172610	-0.455187
H	-4.193235	-1.996385	0.385911
H	-5.707039	-0.060998	0.072417

s5-ts-r

Symbol	X	Y	Z
C	-0.442761	1.285740	1.376958
C	-1.800853	1.572750	1.285491
C	-2.246147	2.331014	0.209460
C	-1.317209	2.769830	-0.726332
C	0.019665	2.429281	-0.543623
N	0.459887	1.701783	0.484788
H	-3.296951	2.572508	0.100153
H	-0.059553	0.684118	2.195453
H	-2.485886	1.203878	2.038344
H	-1.615224	3.361740	-1.582514
O	1.929169	-0.836685	1.405794
Cl	3.542633	0.040620	-0.424587
C	2.069661	-0.646069	0.246802
O	1.248739	-0.923474	-0.756725
H	0.770688	2.751561	-1.258817
C	-0.074078	-1.316407	-0.497109
C	-1.022076	-0.751980	-1.336106
C	-0.407297	-2.241464	0.480748
C	-2.356072	-1.103456	-1.172613
H	-0.707031	-0.041392	-2.089887
C	-1.749674	-2.580723	0.631840
H	0.351358	-2.681461	1.111728
C	-2.723220	-2.012767	-0.184067
H	-3.107388	-0.660365	-1.815006
H	-2.029633	-3.297723	1.393915
H	-3.763902	-2.283189	-0.054210

s6

Symbol	X	Y	Z
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C	-2.367532	0.282860	0.148574
O	-2.830379	1.225310	0.703040
Cl	-3.373361	-0.962570	-0.587574
O	-1.102757	-0.015340	-0.029306
C	-0.158834	0.944766	0.541051
H	-0.360197	1.010503	1.610555
H	-0.345260	1.912438	0.075336
C	1.219002	0.433652	0.254201
C	1.806563	-0.505299	1.102419
C	1.914094	0.875104	-0.870589
C	3.075819	-1.001187	0.826277
H	1.268146	-0.845188	1.980888
C	3.185529	0.381626	-1.147098
H	1.459979	1.608130	-1.528814
C	3.765989	-0.557476	-0.299378
H	3.528135	-1.728672	1.489436
H	3.722228	0.730822	-2.020953
H	4.756777	-0.940653	-0.512866

s6-ts

Symbol	X	Y	Z
C	-2.878147	0.405573	-0.893548
C	-3.562505	1.612411	-0.855517
C	-3.175689	2.565549	0.078796
C	-2.122136	2.288146	0.945704
C	-1.490706	1.058974	0.849050
N	-1.876366	0.158824	-0.056222
H	-3.689337	3.517532	0.132433
H	-3.107098	-0.391182	-1.593194
H	-4.375703	1.793856	-1.545020
H	-1.794433	3.006718	1.684647
O	-1.408021	-1.984709	-1.247889
Cl	-1.693125	-2.243707	1.384140
C	-1.040610	-1.501618	-0.207266
O	0.229221	-1.131692	0.090714
C	0.960651	-0.656916	-1.060930
H	0.356639	0.097734	-1.573223
H	1.129265	-1.495506	-1.738028
H	-0.664143	0.766908	1.487457
C	2.247007	-0.070000	-0.559076
C	2.317151	1.282209	-0.224367
C	3.372220	-0.875892	-0.389218
C	3.497405	1.824001	0.274948
H	1.444562	1.913088	-0.362481

C	4.553646	-0.337329	0.110854
H	3.320629	-1.927564	-0.650699
C	4.616811	1.013311	0.443844
H	3.545269	2.876359	0.528473
H	5.424370	-0.969422	0.238294
H	5.537558	1.433961	0.830383

s6-ts-p

Symbol	X	Y	Z
C	-3.343541	-0.857623	-0.408361
C	-4.401095	-0.051501	-0.758583
C	-4.154603	1.277279	-1.095097
C	-2.854347	1.768759	-1.069029
C	-1.823823	0.928582	-0.708538
N	-2.089059	-0.360143	-0.405670
H	-4.975343	1.927943	-1.369487
H	-3.437720	-1.894810	-0.120263
H	-5.400302	-0.462339	-0.761393
H	-2.632314	2.798701	-1.308398
O	-1.263843	-2.279949	0.595391
Cl	-0.753743	0.707218	2.344547
C	-1.007255	-1.261561	0.039786
O	0.141698	-0.783525	-0.336052
C	1.308419	-1.399500	0.289508
H	1.407422	-2.412309	-0.100154
H	1.103914	-1.421692	1.361239
H	-0.791796	1.233545	-0.631189
C	2.489770	-0.538777	-0.038878
C	3.510128	-1.009323	-0.860828
C	2.563140	0.750739	0.493346
C	4.605513	-0.198035	-1.149317
H	3.451563	-2.011082	-1.272860
C	3.652145	1.561605	0.198269
H	1.760381	1.100050	1.136705
C	4.675289	1.086958	-0.621991
H	5.399968	-0.569305	-1.785529
H	3.709031	2.561174	0.612670
H	5.526630	1.718818	-0.846253

s6-ts-r

Symbol	X	Y	Z
C	-1.049399	2.343956	-1.051283
C	-0.148731	3.385817	-0.850184
C	0.505845	3.468542	0.373791

C	0.235012	2.507850	1.340514
C	-0.676483	1.501198	1.038046
N	-1.313202	1.412314	-0.131864
H	1.213522	4.265610	0.569054
H	-1.579136	2.250312	-1.994450
H	0.029401	4.109426	-1.635394
H	0.721750	2.527199	2.307275
O	-2.673631	-1.310021	-1.379636
Cl	-3.118098	-1.290530	1.181638
C	-2.168088	-1.348772	-0.306871
O	-0.898973	-1.470805	-0.001884
C	0.009981	-1.390941	-1.139582
H	-0.307641	-0.553865	-1.760983
H	-0.081997	-2.322227	-1.700248
H	-0.899564	0.723242	1.762284
C	1.389658	-1.185492	-0.592494
C	1.957631	0.087322	-0.588481
C	2.105217	-2.259897	-0.062353
C	3.228376	0.287347	-0.056923
H	1.403166	0.923795	-1.002769
C	3.373261	-2.061549	0.471976
H	1.666267	-3.252217	-0.069838
C	3.935698	-0.786487	0.475154
H	3.663374	1.279944	-0.058101
H	3.924657	-2.899429	0.881486
H	4.925341	-0.632496	0.888792

s7Cl-ts

Symbol	X	Y	Z
Cl	1.450103	1.506835	-0.758129
C	1.442805	0.005410	0.495510
N	0.262056	-0.365459	0.920241
S	-2.080394	-0.207157	-0.020264
O	-0.561831	-0.668001	-0.238617
O	-2.730271	-0.536429	-1.274519
O	-2.612848	-0.778381	1.201601
C	-1.961506	1.552551	0.162479
H	-2.974360	1.916068	0.327757
H	-1.319733	1.753676	1.017469
H	-1.533643	1.953464	-0.753364
C	2.407964	0.347468	1.602317
H	2.006622	1.184452	2.174750
H	2.526254	-0.520485	2.250546
H	3.374447	0.622918	1.187407

Cl	2.370796	-1.345284	-0.639268
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s7Cl-ts-sigma

Symbol	X	Y	Z
Cl	-0.488023	3.042927	-0.253300
C	2.462987	1.432847	0.650578
H	1.840683	2.303678	0.876349
H	3.065207	1.116220	1.500308
H	3.105235	1.628505	-0.206347
C	1.546977	0.368163	0.302323
N	0.587459	-0.236106	0.118341
S	-1.903386	-0.920608	0.171455
O	-0.188565	-1.213453	-0.220068
O	-2.420116	-2.239340	-0.032863
O	-1.891964	-0.281139	1.453060
C	-2.304908	0.192879	-1.134854
H	-3.368596	0.405055	-1.022106
H	-1.703834	1.098724	-0.988665
H	-2.097190	-0.321089	-2.070959
Cl	3.504777	-1.386365	-0.363433

s7F

Symbol	X	Y	Z
C	-2.116767	0.007471	-0.016618
C	-3.318138	-0.841181	0.149916
H	-3.020996	-1.873083	0.316923
H	-3.897718	-0.477816	1.000069
H	-3.936976	-0.769949	-0.745939
N	-0.936450	-0.443630	0.031527
O	0.001053	0.583225	-0.175954
S	1.528869	0.056982	0.135782
O	2.322521	1.223991	-0.158205
O	1.558949	-0.532682	1.451885
C	1.747399	-1.191444	-1.100293
H	2.750804	-1.590783	-0.961165
H	0.993917	-1.958918	-0.937126
H	1.642533	-0.717842	-2.073866
F	-2.359586	1.295219	-0.226584

s7

Symbol	X	Y	Z
C	1.845851	-0.426234	-0.022152
C	2.845519	-1.527367	-0.109407
H	2.328971	-2.483287	-0.168572

H	3.466170	-1.384622	-0.995056
H	3.491433	-1.505826	0.769375
Cl	2.475391	1.186839	0.075800
N	0.606532	-0.684597	-0.020280
O	-0.188586	0.459997	0.083265
S	-1.783923	0.098077	-0.138477
O	-2.415045	1.381903	0.037078
O	-1.927294	-0.623457	-1.379028
C	-2.112936	-0.968366	1.235938
H	-3.164590	-1.242529	1.167413
H	-1.472453	-1.842513	1.141623
H	-1.909340	-0.408963	2.146296

s7-ts

Symbol	X	Y	Z
C	2.858274	0.578907	-0.498195
C	3.970734	-0.199897	-0.764880
C	3.977798	-1.524051	-0.337872
C	2.879002	-2.023335	0.348362
C	1.804407	-1.180940	0.588685
N	1.811400	0.079854	0.163806
H	4.832389	-2.157826	-0.538767
H	2.786587	1.612053	-0.814853
H	4.808403	0.227080	-1.298766
H	2.846211	-3.046401	0.696450
Cl	0.101955	1.969536	-0.935287
C	0.320443	1.041942	0.636245
N	-0.621945	0.221038	1.023461
S	-2.666216	-0.737802	-0.133616
O	-1.069994	-0.528079	-0.142550
O	-2.916879	-1.495153	-1.339501
O	-3.088812	-1.276485	1.139714
C	-3.275863	0.916808	-0.300523
H	-4.361840	0.860071	-0.259772
H	-2.880271	1.499831	0.528572
H	-2.933363	1.305393	-1.256624
H	0.912063	-1.483966	1.125574
C	0.847217	1.942575	1.717418
H	0.098188	2.701922	1.936204
H	1.039617	1.351480	2.611111
H	1.765475	2.432509	1.401010

s7-ts-p

Symbol	X	Y	Z
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C	2.378741	0.502302	-0.336038
C	3.336936	-0.146495	-1.087390
C	3.482652	-1.522530	-0.964834
C	2.661001	-2.231877	-0.091972
C	1.713395	-1.550739	0.635008
N	1.594629	-0.210300	0.500015
H	4.232438	-2.043599	-1.546625
H	2.162733	1.562837	-0.401569
H	3.953201	0.432044	-1.760614
H	2.747770	-3.302250	0.027579
Cl	0.142275	2.890806	-0.894950
C	0.591840	0.482898	1.300215
N	-0.637364	0.219165	1.172931
S	-2.504263	-0.774509	-0.208048
O	-0.882182	-0.707227	0.164253
O	-2.527464	-1.781458	-1.238192
O	-3.241550	-0.965519	1.015365
C	-2.769877	0.845466	-0.863534
H	-3.821518	0.896616	-1.142071
H	-2.520112	1.565680	-0.086222
H	-2.110441	0.969348	-1.719826
H	1.035181	-2.024593	1.330722
C	1.083551	1.491898	2.272265
H	0.239163	1.875912	2.840002
H	1.819079	1.043517	2.942558
H	1.545700	2.317453	1.726079

s7-ts-r

Symbol	X	Y	Z
C	3.423181	-0.456701	0.525913
C	3.354580	-1.372012	-0.519413
C	2.181804	-2.098242	-0.688144
C	1.132128	-1.881409	0.196162
C	1.303324	-0.947598	1.213547
N	2.423564	-0.238896	1.384508
H	2.087432	-2.817827	-1.492874
H	4.323834	0.129884	0.679693
H	4.200600	-1.504421	-1.181897
H	0.196981	-2.420546	0.110927
Cl	1.145309	1.474300	-1.420429
C	0.274959	1.852239	0.029996
N	-0.822389	1.300864	0.339995
S	-2.420820	-0.611612	-0.005208
O	-1.244978	0.366713	-0.613969

O	-2.709123	-1.476750	-1.121925
O	-1.957421	-1.168744	1.243454
C	-3.744063	0.527573	0.283061
H	-4.572683	-0.056442	0.680473
H	-3.398700	1.263038	1.006282
H	-4.003378	0.983706	-0.669805
H	0.495421	-0.757346	1.912840
C	0.892600	2.865468	0.928828
H	1.051880	3.796881	0.384438
H	0.242541	3.037441	1.784657
H	1.857403	2.482491	1.267064

s7-ts-sgm

Symbol	X	Y	Z
C	3.542104	0.970475	0.502728
C	4.812144	0.441787	0.312120
C	4.931969	-0.772891	-0.352546
C	3.781654	-1.411675	-0.799583
C	2.553493	-0.808615	-0.561196
N	2.435639	0.358152	0.076228
H	5.906868	-1.214463	-0.519448
H	3.408507	1.917740	1.014911
H	5.680021	0.974346	0.677883
H	3.827460	-2.357596	-1.322700
Cl	-2.515965	2.660114	-0.797312
C	0.585585	2.445504	0.665213
H	-0.375036	2.965029	0.706016
H	1.122930	2.508510	1.611051
H	1.192284	2.843208	-0.147065
C	0.268888	1.059068	0.382314
H	1.632290	-1.275860	-0.893908
N	-0.404397	0.133932	0.227561
S	-2.478049	-1.420082	0.295467
O	-0.745090	-1.092669	-0.016326
O	-2.445412	-2.850877	0.293196
O	-2.793951	-0.649737	1.460589
C	-3.166531	-0.735943	-1.176803
H	-4.238058	-0.930738	-1.117675
H	-2.957404	0.341373	-1.163334
H	-2.712649	-1.257844	-2.016429

s8

Symbol	X	Y	Z
Cl	1.613566	1.970056	-0.155271

C	1.363391	0.250331	-0.188553
N	0.214206	-0.271744	-0.102277
S	-2.289661	-0.057454	-0.056053
O	-0.809833	0.667604	0.043644
O	-3.187963	1.047844	0.165135
O	-2.352656	-0.815864	-1.281057
C	-2.260158	-1.145211	1.341102
H	-3.226593	-1.646548	1.360206
H	-1.450705	-1.856734	1.194080
H	-2.113844	-0.538371	2.231967
C	2.594515	-0.607003	-0.313106
H	3.146004	-0.211462	-1.172428
C	2.240524	-2.070013	-0.568902
H	3.161589	-2.636948	-0.711282
H	1.703591	-2.492715	0.282494
H	1.618416	-2.182220	-1.457094
C	3.466796	-0.454956	0.940660
H	4.371278	-1.053123	0.822218
H	3.760993	0.580988	1.110137
H	2.928053	-0.816073	1.820064

s8-ts

Symbol	X	Y	Z
C	2.784017	-0.030540	-0.841535
C	3.872522	-0.879465	-0.765009
C	3.816060	-1.966869	0.101657
C	2.678121	-2.163461	0.872401
C	1.629008	-1.265822	0.758146
N	1.698112	-0.237033	-0.087767
H	4.652341	-2.650872	0.174717
H	2.757686	0.821312	-1.508273
H	4.741448	-0.688494	-1.379371
H	2.594154	-2.994987	1.558274
Cl	0.133416	1.028055	-1.914412
C	0.360442	0.847476	-0.062248
N	-0.642841	0.353612	0.636796
S	-2.751177	-0.967208	0.113285
O	-1.163328	-0.805803	-0.080288
O	-3.073683	-2.135008	-0.682295
O	-3.078634	-0.974941	1.525110
C	-3.428521	0.492979	-0.628571
H	-4.492041	0.488413	-0.395649
H	-2.930163	1.351141	-0.182523
H	-3.254017	0.436970	-1.700183

H	0.717232	-1.330768	1.338682
C	0.929667	2.142116	0.523767
H	1.797823	2.405906	-0.087044
C	1.382968	1.953480	1.973277
H	1.809768	2.889576	2.338619
H	0.534359	1.689236	2.605519
H	2.144868	1.177548	2.070596
C	-0.099975	3.268926	0.422731
H	0.355411	4.207145	0.745286
H	-0.460704	3.395630	-0.598551
H	-0.951655	3.055974	1.071537

s8-ts-p

Symbol	X	Y	Z
C	-2.087921	-0.356525	1.029619
C	-2.908430	-1.389765	1.435186
C	-3.085197	-2.487073	0.601955
C	-2.431330	-2.537809	-0.627184
C	-1.617120	-1.491874	-0.993323
N	-1.467901	-0.432815	-0.166318
H	-3.728009	-3.303276	0.906624
H	-1.855105	0.519794	1.627577
H	-3.394628	-1.324175	2.398103
H	-2.546130	-3.376807	-1.298406
Cl	0.017655	1.847112	2.420487
C	-0.618117	0.672234	-0.597636
N	0.624983	0.506327	-0.746089
S	2.699268	-0.830251	-0.234961
O	1.041421	-0.771236	-0.382099
O	2.914087	-2.203939	0.143536
O	3.280930	-0.308951	-1.446243
C	2.956396	0.276038	1.120078
H	4.032029	0.317687	1.284833
H	2.548056	1.246772	0.842727
H	2.425703	-0.125296	1.980609
H	-1.071518	-1.451498	-1.926312
C	-1.302297	1.973756	-0.884581
H	-1.841258	2.227081	0.036401
C	-2.312129	1.796076	-2.026985
H	-2.830629	2.740567	-2.195087
H	-1.798253	1.517481	-2.950314
H	-3.064847	1.037575	-1.801014
C	-0.287977	3.074717	-1.170414
H	-0.818240	4.016477	-1.317397

H	0.401645	3.181217	-0.332452
H	0.282677	2.852293	-2.074420

s8-ts-r

Symbol	X	Y	Z
C	3.136343	-1.341989	0.526904
C	2.901073	-2.382126	-0.366503
C	1.624289	-2.927398	-0.426624
C	0.641353	-2.414303	0.411233
C	0.981877	-1.380146	1.277681
N	2.203246	-0.841541	1.341146
H	1.399217	-3.734447	-1.113912
H	4.121325	-0.889288	0.590753
H	3.700596	-2.745898	-0.999410
H	-0.370544	-2.799419	0.404220
Cl	1.159673	0.563924	-1.816849
C	0.505698	1.287075	-0.379319
N	-0.659128	1.030592	0.043763
S	-2.664192	-0.482526	0.021408
O	-1.350180	0.122446	-0.766804
O	-3.240375	-1.359701	-0.967071
O	-2.237069	-1.007576	1.296918
C	-3.658693	0.962959	0.255508
H	-4.559748	0.636231	0.772231
H	-3.089150	1.663204	0.862637
H	-3.891335	1.369867	-0.726144
H	0.229413	-0.959459	1.937226
C	1.397211	2.257580	0.345474
H	2.371583	1.763290	0.405904
C	0.892866	2.532846	1.759067
H	1.602348	3.187006	2.268363
H	-0.079998	3.027623	1.738309
H	0.801584	1.605138	2.325817
C	1.538002	3.547808	-0.472820
H	2.229780	4.221955	0.034367
H	1.922458	3.353179	-1.474878
H	0.570362	4.048006	-0.559045

s9

Symbol	X	Y	Z
C	0.566325	0.654094	-0.074295
Cl	0.451351	2.372667	-0.265185
N	-0.458890	-0.088485	0.021542
O	-1.655823	0.614701	-0.066766

S	-2.949345	-0.417358	-0.071958
O	-4.063353	0.493487	-0.142308
O	-2.745786	-1.407315	-1.099917
C	-2.829243	-1.156851	1.531758
H	-3.673939	-1.838442	1.619619
H	-1.884442	-1.693339	1.583561
H	-2.887307	-0.359753	2.269649
C	1.910962	0.040074	-0.033876
C	2.054027	-1.300236	-0.408926
C	3.024915	0.771015	0.380589
C	3.303272	-1.901785	-0.357380
H	1.188638	-1.855455	-0.747897
C	4.272374	0.159494	0.433148
H	2.920490	1.809620	0.667330
C	4.414012	-1.174445	0.065247
H	3.411887	-2.937149	-0.656043
H	5.133389	0.728800	0.760698
H	5.388723	-1.645847	0.101114

s9-ts

Symbol	X	Y	Z
C	1.814284	1.848229	0.934796
C	2.371655	3.094453	0.710613
C	1.938905	3.833001	-0.386947
C	0.974419	3.298263	-1.230805
C	0.468438	2.037736	-0.951321
N	0.883325	1.355267	0.113567
H	2.354823	4.813410	-0.582919
H	2.103140	1.222163	1.770334
H	3.127808	3.472167	1.385020
H	0.614870	3.839473	-2.095084
Cl	-0.182640	-0.234193	2.080714
C	0.218194	-0.314858	0.284507
N	-0.778373	-0.498485	-0.555980
S	-3.301711	-0.327550	-0.308608
O	-1.862725	0.379694	-0.143736
O	-4.231523	0.681747	0.154411
O	-3.445774	-0.847759	-1.651850
C	-3.220573	-1.672532	0.843601
H	-4.156256	-2.220931	0.748661
H	-2.368778	-2.291893	0.569905
H	-3.104853	-1.249958	1.839065
H	-0.271776	1.541684	-1.568571
C	1.418334	-1.163527	-0.041029

C	1.827461	-1.218164	-1.377685
C	2.124415	-1.878074	0.923459
C	2.922092	-1.989763	-1.742024
H	1.280320	-0.658236	-2.125900
C	3.224378	-2.648542	0.552392
H	1.820679	-1.844849	1.960936
C	3.625437	-2.707208	-0.776428
H	3.228127	-2.028770	-2.780459
H	3.764678	-3.203935	1.309417
H	4.481935	-3.306681	-1.060702

s9-ts-p

Symbol	X	Y	Z
C	1.143498	1.877839	0.795979
C	1.158995	3.246624	0.962883
C	0.559549	4.054594	0.004981
C	-0.046109	3.479383	-1.110439
C	-0.046202	2.110952	-1.238455
N	0.543094	1.344980	-0.290825
H	0.565670	5.130916	0.122294
H	1.563716	1.173444	1.500095
H	1.636119	3.661779	1.838997
H	-0.514558	4.080174	-1.876567
Cl	-0.248313	-0.246332	2.752793
C	0.535401	-0.099607	-0.438433
N	-0.543118	-0.748435	-0.590032
S	-3.060870	-0.864941	-0.498850
O	-1.668698	0.050259	-0.480644
O	-4.074066	0.141282	-0.308193
O	-3.051561	-1.670519	-1.694750
C	-2.844918	-1.863752	0.943064
H	-3.788718	-2.386004	1.094319
H	-2.032366	-2.559224	0.742662
H	-2.591668	-1.201229	1.770441
H	-0.492124	1.585741	-2.070930
C	1.833283	-0.788440	-0.402053
C	2.979845	-0.169700	-0.906285
C	1.900847	-2.074939	0.137942
C	4.190501	-0.850869	-0.888584
H	2.929755	0.830526	-1.323043
C	3.114236	-2.747978	0.150314
H	1.008564	-2.518841	0.560947
C	4.257031	-2.138370	-0.363422
H	5.079600	-0.376915	-1.285101

H	3.172470	-3.742571	0.574440
H	5.203589	-2.664974	-0.346510

s9-ts-r

Symbol	X	Y	Z
C	1.534149	1.970962	1.327181
C	2.493513	2.391314	0.410149
C	2.070553	2.789797	-0.851240
C	0.712144	2.742679	-1.143721
C	-0.166067	2.298777	-0.159964
N	0.227414	1.923762	1.060710
H	2.785726	3.121524	-1.595054
H	1.831866	1.649135	2.321258
H	3.541102	2.399893	0.683952
H	0.334708	3.035014	-2.115710
Cl	0.077422	-1.267356	2.423536
C	0.086492	-1.088901	0.700828
N	-0.983895	-0.974842	0.028436
S	-3.451451	-0.545273	-0.080181
O	-2.132173	-0.978472	0.814337
O	-4.519649	-0.636852	0.882432
O	-3.169352	0.704777	-0.743712
C	-3.541871	-1.860624	-1.261919
H	-4.414327	-1.656952	-1.880793
H	-2.628320	-1.843826	-1.851907
H	-3.656359	-2.792999	-0.713488
H	-1.230377	2.225893	-0.362155
C	1.389821	-1.044520	0.000869
C	1.427872	-0.603926	-1.326547
C	2.574020	-1.408095	0.644293
C	2.639866	-0.529120	-1.996978
H	0.510612	-0.303891	-1.816664
C	3.784772	-1.330430	-0.034191
H	2.555392	-1.747596	1.671515
C	3.821333	-0.888828	-1.352782
H	2.663683	-0.176208	-3.021016
H	4.699709	-1.613828	0.471393
H	4.767250	-0.823285	-1.877097

T-NH3+s1F

Symbol	X	Y	Z
O	-0.184278	-0.838029	1.181574
C	-1.191931	0.935854	-0.102464
H	-2.169374	0.455600	-0.160297

H	-1.196840	1.638711	0.731040
H	-0.999885	1.466329	-1.034654
C	-0.166324	-0.147724	0.162554
F	-0.029897	-0.897209	-1.072211
N	1.341032	0.632235	0.029821
H	2.043136	-0.101848	0.111725
H	1.461422	1.280046	0.806509
H	1.484217	1.128706	-0.848299

T-py+s1F

Symbol	X	Y	Z
O	1.009964	1.225618	-0.225719
C	-0.018402	3.205422	-1.123683
H	-0.996959	2.741223	-1.250616
H	0.005346	3.728493	-0.167612
H	0.141765	3.914139	-1.934833
C	1.002414	2.085185	-1.098492
F	1.131069	1.597660	-2.454186
C	2.951761	3.661998	-2.106488
C	4.167159	4.320405	-2.057838
C	4.954108	4.188566	-0.917726
C	4.504846	3.397162	0.132159
C	3.275425	2.768866	0.015220
N	2.530583	2.916877	-1.080006
H	5.910137	4.693079	-0.853303
H	2.306653	3.702709	-2.974817
H	4.485876	4.915864	-2.902194
H	5.091743	3.262982	1.030353
H	2.844286	2.126756	0.774112

T-py+s7F

Symbol	X	Y	Z
C	2.477153	0.436816	-0.947282
C	3.570254	-0.391314	-1.112736
C	3.782084	-1.419277	-0.199990
C	2.895628	-1.586355	0.856553
C	1.821420	-0.724330	0.972819
N	1.633254	0.255204	0.080250
H	4.630031	-2.083112	-0.312437
H	2.246780	1.248368	-1.621845
H	4.237240	-0.227823	-1.947572
H	3.023501	-2.374351	1.585276
C	0.390634	1.240297	0.333175
N	-0.605909	0.662393	1.027665

S	-2.528493	-0.620704	-0.077482
O	-0.962609	-0.530318	0.225163
O	-2.661143	-1.797692	-0.917371
O	-3.283190	-0.574896	1.160300
C	-2.871541	0.841324	-1.020776
H	-3.934113	0.811817	-1.256235
H	-2.623499	1.700909	-0.403340
H	-2.261835	0.810817	-1.920416
H	1.076961	-0.777472	1.757060
C	0.925525	2.471794	1.026753
H	0.108797	3.180646	1.155254
H	1.335261	2.207799	2.000752
H	1.704838	2.929905	0.417174
F	0.107901	1.568844	-1.019537

w-pyridine2

Symbol	X	Y	Z
C	-1.140532	-0.718265	-0.000283
C	-1.194065	0.671326	0.000094
C	0.001448	1.379872	-0.000085
C	1.195291	0.669257	0.000062
C	1.138919	-0.720658	-0.000195
N	-0.001273	-1.414858	0.000156
H	0.002171	2.463319	-0.000060
H	-2.057171	-1.300135	0.000448
H	-2.149568	1.179776	0.000346
H	2.152094	1.175278	0.000277
H	2.055012	-1.303421	0.000339

w-sl

Symbol	X	Y	Z
C	-0.481726	0.234427	0.003530
O	-0.823212	1.366560	-0.001480
C	-1.329064	-0.991908	0.000537
H	-2.379298	-0.705382	-0.002372
H	-1.094568	-1.591411	-0.881066
H	-1.099449	-1.591677	0.883221
Cl	1.292379	-0.141390	-0.002540

w-sl-ts

Symbol	X	Y	Z
C	-1.139353	1.131056	-0.301250
C	-2.514496	1.012369	-0.429320
C	-3.109237	-0.198255	-0.101772

C	-2.311861	-1.249389	0.338236
C	-0.946083	-1.050250	0.436326
N	-0.389450	0.120914	0.124053
H	-4.181452	-0.324887	-0.190940
H	-0.600279	2.041133	-0.544240
H	-3.098672	1.853035	-0.779519
H	-2.736332	-2.210414	0.596951
O	1.622850	1.631814	-0.259430
Cl	2.090527	-0.939842	-0.911282
C	1.791773	0.167803	1.650766
H	2.871792	0.242851	1.792722
H	1.293136	0.886190	2.303729
H	1.474561	-0.843354	1.893337
C	1.494387	0.544472	0.224150
H	-0.274809	-1.838647	0.755953

w-s7

Symbol	X	Y	Z
C	-1.851842	0.427728	-0.025579
C	-2.843996	1.535539	-0.102566
H	-2.322729	2.489498	-0.168074
H	-3.477601	1.401899	-0.981497
H	-3.481760	1.523983	0.783464
Cl	-2.491121	-1.186575	0.076375
N	-0.610597	0.681494	-0.036287
O	0.186166	-0.461458	0.056986
S	1.791475	-0.096211	-0.138552
O	2.411530	-1.387749	0.020535
O	1.958908	0.650687	-1.361140
C	2.111210	0.940388	1.263750
H	3.164792	1.212627	1.213238
H	1.476966	1.821112	1.185434
H	1.897161	0.366045	2.162723

w-s7-ts

Symbol	X	Y	Z
C	2.859438	0.565981	-0.520198
C	3.967461	-0.216394	-0.784271
C	3.978688	-1.533171	-0.338613
C	2.885753	-2.020927	0.363796
C	1.815152	-1.176542	0.598717
N	1.816552	0.077841	0.155417
H	4.831748	-2.170180	-0.537067
H	2.786961	1.594576	-0.849183

H	4.801001	0.202581	-1.331410
H	2.855869	-3.038663	0.728312
Cl	0.120018	2.008457	-0.922879
C	0.335402	1.036524	0.635133
N	-0.620065	0.220255	1.004057
S	-2.675288	-0.741346	-0.141422
O	-1.082572	-0.503934	-0.175203
O	-2.933162	-1.452471	-1.373823
O	-3.070351	-1.337917	1.115167
C	-3.321193	0.908014	-0.230668
H	-4.406242	0.829976	-0.187212
H	-2.933772	1.463500	0.620993
H	-2.993755	1.350944	-1.168745
H	0.925681	-1.469197	1.146061
C	0.858109	1.911189	1.746132
H	0.109900	2.667326	1.985746
H	1.046627	1.297203	2.627254
H	1.780713	2.409577	1.451335

d-pyridine

Symbol	X	Y	Z
C	-1.143243	-0.720428	0.000221
C	-1.196650	0.671622	-0.000038
C	0.000406	1.382335	-0.000006
C	1.196949	0.671162	-0.000064
C	1.142760	-0.721097	0.000096
N	-0.000283	-1.417284	-0.000043
H	0.000495	2.466018	-0.000129
H	-2.060467	-1.302355	-0.000137
H	-2.152812	1.180086	-0.000238
H	2.153517	1.178859	-0.000239
H	2.059913	-1.303181	-0.000202

d-s1

Symbol	X	Y	Z
C	-0.497243	0.241810	-0.000342
O	-0.843538	1.369692	-0.000104
C	-1.328070	-1.002235	-0.000117
H	-2.381267	-0.726671	-0.001125
H	-1.087523	-1.600247	-0.880618
H	-1.089043	-1.598560	0.881990
Cl	1.309295	-0.145265	0.000196

d-s1-ts

Symbol	X	Y	Z
C	-1.165478	1.139473	-0.335752
C	-2.538836	0.988528	-0.484091
C	-3.120094	-0.219670	-0.110915
C	-2.311660	-1.237501	0.392710
C	-0.947542	-1.011032	0.507460
N	-0.407620	0.158951	0.152197
H	-4.187518	-0.369777	-0.214525
H	-0.638827	2.045845	-0.612220
H	-3.130706	1.800790	-0.884138
H	-2.724972	-2.193126	0.686246
O	1.620828	1.659828	-0.285610
Cl	2.081530	-1.010650	-0.931545
C	1.828646	0.211497	1.650415
H	2.913972	0.267373	1.751110
H	1.365235	0.933881	2.325987
H	1.502282	-0.794518	1.894236
C	1.481507	0.604340	0.244627
H	-0.268788	-1.771804	0.869968

d-s7

Symbol	X	Y	Z
C	-1.863491	0.435049	-0.025610
C	-2.858643	1.541801	-0.108025
H	-2.339833	2.497457	-0.169413
H	-3.487571	1.407823	-0.990625
H	-3.503313	1.528613	0.773338
Cl	-2.513498	-1.188885	0.072301
N	-0.619715	0.687458	-0.027585
O	0.181202	-0.473127	0.073261
S	1.807158	-0.098543	-0.138538
O	2.434177	-1.398244	0.030603
O	1.967042	0.644379	-1.377861
C	2.128912	0.959880	1.265890
H	3.178382	1.243879	1.202168
H	1.480032	1.828820	1.184110
H	1.928293	0.385901	2.167708

d-s7-ts

Symbol	X	Y	Z
C	2.831423	0.551022	-0.535999
C	3.930763	-0.244411	-0.813881
C	3.943419	-1.559748	-0.354948
C	2.859324	-2.035054	0.375759

C	1.795682	-1.182083	0.626882
N	1.798790	0.072095	0.168724
H	4.788023	-2.203740	-0.564581
H	2.754286	1.573889	-0.875651
H	4.755523	0.163673	-1.381810
H	2.830837	-3.049284	0.749537
Cl	0.126312	2.034084	-0.935204
C	0.356470	1.039864	0.661356
N	-0.618142	0.253212	1.041308
S	-2.666310	-0.747110	-0.141498
O	-1.053372	-0.528115	-0.140817
O	-2.901405	-1.491731	-1.371796
O	-3.103753	-1.312220	1.128115
C	-3.293628	0.919151	-0.287467
H	-4.379820	0.852450	-0.263575
H	-2.913557	1.488044	0.557420
H	-2.940058	1.332005	-1.228787
H	0.917631	-1.463328	1.193828
C	0.888023	1.940784	1.749447
H	0.143302	2.703462	1.976432
H	1.084488	1.348896	2.643821
H	1.807855	2.430492	1.434680

pyridine

Symbol	X	Y	Z
C	-1.140531	-0.718266	-0.000283
C	-1.194065	0.671325	0.000094
C	0.001447	1.379872	-0.000085
C	1.195291	0.669258	0.000062
C	1.138920	-0.720657	-0.000195
N	-0.001272	-1.414858	0.000156
H	0.002169	2.463319	-0.000060
H	-2.057170	-1.300136	0.000448
H	-2.149569	1.179775	0.000346
H	2.152093	1.175280	0.000277
H	2.055013	-1.303419	0.000339

s10

Symbol	X	Y	Z
C	-0.528677	0.900952	-0.113493
Cl	-0.913048	2.571468	-0.331715
N	-1.414674	0.000978	0.004414
O	-2.706861	0.490378	-0.075100
S	-3.817147	-0.745653	-0.039155

O	-5.062934	-0.030866	-0.137888
O	-3.445499	-1.720665	-1.032795
C	-3.575537	-1.394661	1.589783
H	-4.297504	-2.201224	1.708668
H	-2.555951	-1.768622	1.653331
H	-3.761607	-0.590912	2.298753
C	0.898293	0.503329	-0.073190
C	1.241729	-0.805917	-0.426419
C	1.883737	1.411235	0.314909
C	2.564990	-1.211551	-0.381257
H	0.472245	-1.496725	-0.744180
C	3.212345	1.014053	0.365670
H	1.621365	2.425704	0.583539
C	3.522912	-0.289862	0.016545
H	2.854715	-2.216064	-0.655986
H	3.991602	1.698982	0.668753
N	4.936274	-0.715783	0.063522
O	5.190136	-1.863640	-0.233256
O	5.763227	0.105488	0.397951

s10-ts

Symbol	X	Y	Z
C	0.018210	2.700575	0.836677
C	0.033824	4.033454	0.467199
C	-0.530519	4.396793	-0.752113
C	-1.081430	3.416901	-1.567584
C	-1.051686	2.098629	-1.139637
N	-0.520915	1.774653	0.037896
H	-0.536090	5.433962	-1.063263
H	0.435144	2.351558	1.773524
H	0.479888	4.765892	1.125769
H	-1.528165	3.658958	-2.522006
Cl	-1.052197	0.098049	2.141802
C	-0.466078	0.015261	0.405431
N	-1.189127	-0.665476	-0.459011
S	-3.550118	-1.599431	-0.380914
O	-2.579183	-0.316198	-0.236129
O	-4.867967	-1.054598	-0.131882
O	-3.292649	-2.270980	-1.636650
C	-3.039489	-2.635415	0.963915
H	-3.630044	-3.547409	0.896494
H	-1.978486	-2.841865	0.838390
H	-3.237397	-2.099568	1.889435
H	-1.445186	1.272611	-1.721225

C	1.005921	-0.279389	0.261402
C	1.528638	-0.303661	-1.036821
C	1.839614	-0.514679	1.351506
C	2.870231	-0.573339	-1.247573
H	0.877497	-0.115278	-1.880248
C	3.188719	-0.784993	1.153552
H	1.448173	-0.498582	2.358531
C	3.675299	-0.808306	-0.141486
H	3.289117	-0.599047	-2.243788
H	3.848784	-0.975410	1.988174
N	5.107566	-1.090908	-0.354513
O	5.519245	-1.099881	-1.495496
O	5.795888	-1.298171	0.622662

s10-ts-p

Symbol	X	Y	Z
C	-0.390086	2.263782	0.900933
C	-0.841704	3.551885	1.093895
C	-1.650027	4.140819	0.129165
C	-1.994052	3.430198	-1.018970
C	-1.529049	2.146303	-1.174391
N	-0.742428	1.594693	-0.219966
H	-2.010715	5.152280	0.267156
H	0.215115	1.716137	1.611080
H	-0.559883	4.075860	1.995910
H	-2.616363	3.861352	-1.789816
Cl	-0.837264	-0.367580	2.739322
C	-0.265153	0.236549	-0.394110
N	-1.056690	-0.734376	-0.579748
S	-3.389400	-1.703375	-0.559978
O	-2.382297	-0.368413	-0.492315
O	-4.682793	-1.094670	-0.389885
O	-3.075774	-2.433153	-1.762212
C	-2.882258	-2.594041	0.880015
H	-3.605275	-3.398655	1.009011
H	-1.883426	-2.982340	0.692063
H	-2.873045	-1.896992	1.717468
H	-1.747225	1.527701	-2.033245
C	1.189646	0.010170	-0.335602
C	1.657917	-1.191329	0.200822
C	2.077319	0.978396	-0.808650
C	3.020078	-1.440780	0.240684
H	0.951709	-1.903028	0.607455
C	3.442972	0.738861	-0.769021

H	1.714994	1.912584	-1.221080
C	3.880683	-0.468363	-0.247798
H	3.412533	-2.358649	0.655229
H	4.153638	1.466091	-1.135150
N	5.335586	-0.727031	-0.202101
O	5.704324	-1.800301	0.222776
O	6.076809	0.148559	-0.594450

s10-ts-r

Symbol	X	Y	Z
C	0.241585	2.549789	1.176576
C	0.969174	3.162602	0.160925
C	0.420042	3.198949	-1.115629
C	-0.824128	2.615167	-1.321964
C	-1.467893	2.018962	-0.240891
N	-0.954645	1.985758	0.991691
H	0.954587	3.667260	-1.934013
H	0.641921	2.504326	2.185277
H	1.938258	3.597874	0.371510
H	-1.291299	2.614000	-2.298804
Cl	-0.767344	-1.179541	2.782979
C	-0.500958	-1.046456	1.081933
N	-1.408091	-1.289194	0.229283
S	-3.815876	-1.702856	-0.347231
O	-2.616679	-1.654319	0.798180
O	-4.960377	-2.104399	0.428308
O	-3.812459	-0.448971	-1.060189
C	-3.259376	-3.014418	-1.397866
H	-4.014859	-3.127247	-2.173917
H	-2.301614	-2.720627	-1.821597
H	-3.179424	-3.914081	-0.791613
H	-2.430641	1.534546	-0.375033
C	0.829966	-0.604721	0.598438
C	0.977243	-0.277154	-0.754266
C	1.908844	-0.472617	1.472975
C	2.186837	0.200456	-1.226070
H	0.135233	-0.371873	-1.426423
C	3.129260	-0.002184	1.008612
H	1.802980	-0.723183	2.519351
C	3.238404	0.333611	-0.330168
H	2.313620	0.480690	-2.262566
H	3.974963	0.112204	1.672025
N	4.522248	0.867310	-0.823206
O	4.569593	1.255253	-1.971728

O 5.458608 0.893140 -0.052713

s11

Symbol	X	Y	Z
C	-0.150624	-0.116814	-0.544619
Cl	-0.203031	-1.341796	-1.763546
N	0.914076	0.288662	0.004102
O	2.043389	-0.382055	-0.447472
S	3.422332	0.261070	0.213642
O	4.448011	-0.568513	-0.363542
O	3.415288	1.684686	-0.011437
C	3.196742	-0.097392	1.932135
H	4.081917	0.278580	2.443020
H	2.300468	0.420068	2.267190
H	3.108433	-1.176433	2.037295
C	-1.419166	0.578103	-0.215438
C	-1.506125	1.940522	-0.486277
C	-2.554735	-0.061793	0.285794
C	-2.691882	2.633170	-0.257362
C	-3.746405	0.607385	0.501519
C	-3.810868	1.969256	0.228610
H	-2.738221	3.693761	-0.469432
H	-4.596455	0.066767	0.895168
H	-4.734176	2.506116	0.403127
H	-0.639779	2.448450	-0.890721
N	-2.499978	-1.484179	0.665508
O	-1.422955	-1.934244	0.997999
O	-3.534122	-2.113842	0.644040

s11-ts

Symbol	X	Y	Z
C	-1.415343	2.265408	-1.110477
C	-1.698600	3.614035	-1.225876
C	-1.012501	4.513699	-0.414692
C	-0.077486	4.036516	0.494106
C	0.146354	2.669777	0.566066
N	-0.509258	1.827670	-0.230461
H	-1.210100	5.575731	-0.489411
H	-1.908538	1.513206	-1.714053
H	-2.441017	3.945825	-1.938572
H	0.472842	4.702735	1.143954
Cl	0.136766	-0.295773	-1.794297
C	-0.139745	0.074345	-0.003074
N	0.851886	-0.087162	0.838878

S	3.350263	-0.456932	0.506893
O	2.044735	0.452500	0.212934
O	4.410117	0.253305	-0.177747
O	3.470153	-0.696167	1.929196
C	2.964521	-1.971627	-0.323073
H	3.775041	-2.664520	-0.103296
H	2.014472	-2.327505	0.070505
H	2.898695	-1.758469	-1.387827
H	0.840142	2.216279	1.263934
C	-1.439760	-0.485171	0.532558
C	-2.171427	0.259134	1.458028
C	-1.967405	-1.728018	0.178767
C	-3.372227	-0.206986	1.981337
C	-3.180282	-2.196898	0.657241
C	-3.889051	-1.428339	1.570349
H	-3.905951	0.396082	2.704759
H	-3.542641	-3.162969	0.329812
H	-4.830956	-1.790145	1.961839
H	-1.796948	1.223438	1.774660
O	-1.816613	-3.116329	-1.649590
O	-0.122825	-3.004088	-0.332731
N	-1.236039	-2.679676	-0.681163

s11-ts-p

Symbol	X	Y	Z
C	0.813863	2.133340	0.972937
C	0.693119	3.440006	1.395208
C	-0.120690	4.311966	0.683670
C	-0.794161	3.863068	-0.450506
C	-0.650687	2.552819	-0.838760
N	0.137756	1.716166	-0.121073
H	-0.224955	5.341029	1.003597
H	1.411423	1.389011	1.478437
H	1.234371	3.756715	2.275093
H	-1.422983	4.518436	-1.035609
Cl	-0.189938	-0.372513	2.524488
C	0.283462	0.331906	-0.550765
N	-0.714078	-0.395282	-0.824059
S	-3.174078	-0.903298	-0.603506
O	-1.919173	0.206915	-0.534983
O	-4.304758	-0.077033	-0.266886
O	-3.109937	-1.565214	-1.881940
C	-2.730675	-1.995461	0.710124
H	-3.538220	-2.722330	0.787468

H	-1.784301	-2.464112	0.442566
H	-2.616459	-1.395524	1.611458
H	-1.130915	2.133118	-1.710438
C	1.685280	-0.120092	-0.728411
C	2.542998	0.755183	-1.402658
C	2.248486	-1.290657	-0.205721
C	3.887738	0.462309	-1.580112
C	3.598025	-1.576046	-0.343659
C	4.418750	-0.704706	-1.046328
H	4.517863	1.152284	-2.126164
H	3.990084	-2.483432	0.096010
H	5.468569	-0.938086	-1.167625
H	2.145258	1.681718	-1.800502
O	1.967806	-2.762071	1.530160
O	0.443188	-2.709446	0.018368
N	1.474347	-2.321675	0.518165

s11-ts-r

Symbol	X	Y	Z
C	-1.767622	-2.694470	-1.060704
C	-3.063768	-2.458151	-1.505150
C	-3.950800	-1.814001	-0.650107
C	-3.503006	-1.431531	0.607662
C	-2.184534	-1.709611	0.954367
N	-1.323462	-2.330098	0.145245
H	-4.968347	-1.608763	-0.961041
H	-1.050768	-3.194039	-1.704949
H	-3.363364	-2.771309	-2.497194
H	-4.147597	-0.913281	1.305987
Cl	0.496544	-0.245012	-2.008727
C	0.722446	0.075085	-0.325056
N	-0.127979	0.653275	0.410129
S	-2.294599	1.915353	0.663531
O	-1.281823	1.006489	-0.280987
O	-3.444666	2.070780	-0.190064
O	-2.421895	1.295971	1.959326
C	-1.378499	3.424731	0.792922
H	-1.983619	4.105368	1.389666
H	-0.436669	3.199427	1.289696
H	-1.225938	3.808250	-0.213518
H	-1.800301	-1.395723	1.920587
C	1.954219	-0.456807	0.308216
C	1.812259	-1.499971	1.218745
C	3.245884	-0.020383	0.005132

C	2.933115	-2.071764	1.815006
C	4.370289	-0.589041	0.578577
C	4.207818	-1.621268	1.495435
H	2.804881	-2.878669	2.525517
H	5.349499	-0.211499	0.317662
H	5.079060	-2.066711	1.957923
H	0.815139	-1.872177	1.420458
O	4.530828	1.198242	-1.466294
O	2.543011	1.898815	-1.057801
N	3.455406	1.110864	-0.915530

s12

Symbol	X	Y	Z
C	-0.284354	0.901626	-0.079079
Cl	-0.708607	2.569416	-0.303987
N	-1.162506	-0.010580	0.028689
O	-2.466181	0.467721	-0.093692
S	-3.554326	-0.774594	-0.069464
O	-4.812140	-0.080716	-0.185484
O	-3.165116	-1.752453	-1.055350
C	-3.331696	-1.422049	1.563195
H	-4.044551	-2.238256	1.669706
H	-2.308055	-1.780754	1.644460
H	-3.540670	-0.621461	2.269374
C	1.144271	0.548504	-0.025942
C	1.540371	-0.747360	-0.360242
C	2.115123	1.478598	0.364842
C	2.875192	-1.123168	-0.300071
H	0.797037	-1.466034	-0.681795
C	3.445007	1.112856	0.431554
H	1.829178	2.490046	0.624061
C	3.835777	-0.189818	0.100287
H	3.152559	-2.131177	-0.575011
H	4.204503	1.821565	0.736874
O	5.156081	-0.451125	0.188515
C	5.603543	-1.758167	-0.146240
H	5.369833	-1.994233	-1.187209
H	6.681092	-1.749156	-0.006797
H	5.153915	-2.504095	0.513577

s12-ts

Symbol	X	Y	Z
C	0.267704	2.652391	0.805019
C	0.347571	3.973712	0.402618

C	-0.146007	4.322324	-0.851162
C	-0.691165	3.338647	-1.665726
C	-0.728647	2.032628	-1.201144
N	-0.267027	1.723047	0.008513
H	-0.100678	5.350075	-1.189246
H	0.631169	2.314412	1.767686
H	0.788436	4.708414	1.062266
H	-1.082344	3.568198	-2.647321
Cl	-0.913609	0.122420	2.146674
C	-0.270991	-0.033778	0.421528
N	-1.009712	-0.699941	-0.441789
S	-3.431836	-1.463250	-0.409347
O	-2.383280	-0.246161	-0.281358
O	-4.718586	-0.826586	-0.216806
O	-3.191243	-2.196525	-1.634363
C	-3.031391	-2.486712	0.981742
H	-3.679257	-3.359566	0.922494
H	-1.982876	-2.764927	0.896985
H	-3.220375	-1.909641	1.883951
H	-1.121152	1.204536	-1.780031
C	1.186496	-0.385744	0.346169
C	1.756078	-0.549187	-0.916390
C	1.996292	-0.542252	1.473468
C	3.098482	-0.877310	-1.064662
H	1.140770	-0.423664	-1.798674
C	3.335996	-0.864772	1.337733
H	1.583599	-0.421494	2.465949
C	3.896912	-1.036760	0.070070
H	3.503808	-1.001446	-2.059308
H	3.967771	-0.992907	2.208013
O	5.212769	-1.350896	0.038324
C	5.819844	-1.543940	-1.230882
H	6.859502	-1.789658	-1.031134
H	5.345402	-2.368415	-1.769021
H	5.768080	-0.632162	-1.831417

s12-ts-p

Symbol	X	Y	Z
C	-1.384421	1.963757	0.680888
C	-1.879029	3.252490	0.668295
C	-1.500205	4.120448	-0.347332
C	-0.619902	3.688368	-1.338268
C	-0.138484	2.402159	-1.287241
N	-0.529107	1.575292	-0.289385

H	-1.884582	5.132425	-0.369610
H	-1.602467	1.221209	1.446667
H	-2.553518	3.559363	1.455012
H	-0.305083	4.338077	-2.142245
Cl	-1.129980	-0.376329	3.070566
C	-0.014155	0.213456	-0.292057
N	-0.795622	-0.781695	-0.388859
S	-3.112339	-1.746537	-0.631006
O	-2.126400	-0.410191	-0.496235
O	-4.421343	-1.144011	-0.629705
O	-2.665807	-2.514760	-1.766976
C	-2.779198	-2.598198	0.880653
H	-3.496885	-3.416281	0.929116
H	-1.756482	-2.965925	0.834235
H	-2.894793	-1.888616	1.699554
H	0.551314	1.988334	-2.010242
C	1.438294	0.047954	-0.210141
C	2.036081	-1.100966	-0.728994
C	2.235013	1.016357	0.416454
C	3.405759	-1.292918	-0.630281
H	1.423539	-1.845808	-1.221887
C	3.598523	0.832333	0.520404
H	1.788624	1.906962	0.844512
C	4.194233	-0.322659	-0.002290
H	3.845320	-2.187925	-1.047364
H	4.226767	1.565646	1.009694
O	5.529847	-0.411260	0.140212
C	6.184525	-1.571261	-0.359321
H	7.238123	-1.439762	-0.129189
H	5.809697	-2.470908	0.134159
H	6.052349	-1.656348	-1.440547

s12-ts-r

Symbol	X	Y	Z
C	0.125476	2.415145	1.389016
C	1.189232	2.913257	0.640800
C	1.042387	3.001143	-0.736931
C	-0.154113	2.579768	-1.306916
C	-1.153275	2.089118	-0.472654
N	-1.028670	2.011016	0.855801
H	1.847461	3.380316	-1.356019
H	0.209917	2.330292	2.468842
H	2.104982	3.216921	1.132480
H	-0.313012	2.620003	-2.377382

Cl	-0.680868	-0.913804	2.723857
C	-0.331037	-0.962841	1.025778
N	-1.226650	-1.224869	0.163415
S	-3.647247	-1.463029	-0.446140
O	-2.486573	-1.431139	0.724148
O	-4.845654	-1.718151	0.312894
O	-3.531965	-0.268924	-1.248550
C	-3.179208	-2.884848	-1.392013
H	-3.925607	-2.989653	-2.177908
H	-2.191599	-2.700000	-1.808259
H	-3.185846	-3.743930	-0.724804
H	-2.089968	1.727827	-0.885912
C	1.043536	-0.663579	0.585434
C	1.293376	-0.450197	-0.771383
C	2.103936	-0.554986	1.493784
C	2.565968	-0.131766	-1.223421
H	0.478253	-0.514832	-1.480936
C	3.373669	-0.236628	1.054241
H	1.936511	-0.714157	2.550942
C	3.613655	-0.015690	-0.306484
H	2.722514	0.039565	-2.279485
H	4.198860	-0.147100	1.749641
O	4.882303	0.304272	-0.640208
C	5.168574	0.556256	-2.008970
H	6.227304	0.797014	-2.053473
H	4.967462	-0.328098	-2.618487
H	4.583722	1.402236	-2.379198

s13

Symbol	X	Y	Z
C	-1.237161	0.901375	-0.030226
Cl	-1.625024	2.541796	-0.422705
N	-2.121024	-0.002582	0.077888
O	-3.407663	0.456228	-0.168926
S	-4.496839	-0.793217	-0.150926
O	-5.740630	-0.112444	-0.402956
O	-4.027999	-1.822752	-1.043956
C	-4.393322	-1.337542	1.530322
H	-5.112344	-2.148635	1.634978
H	-3.378715	-1.687481	1.707218
H	-4.652504	-0.495802	2.168717
C	0.183902	0.545036	0.176907
C	0.583626	-0.780262	-0.022861
C	1.113058	1.503070	0.582158

C	1.903031	-1.147286	0.190224
H	-0.139330	-1.515760	-0.350612
C	2.435832	1.140707	0.800488
H	0.810005	2.530064	0.737642
C	2.807057	-0.177252	0.596568
H	2.235499	-2.166437	0.040204
H	3.170364	1.865712	1.126345
O	4.129350	-0.556477	0.859735
C	4.990202	-0.466684	-0.171966
F	4.628304	-1.232630	-1.205817
F	6.178811	-0.866754	0.250426
F	5.104158	0.782361	-0.634479

s13-ts

Symbol	X	Y	Z
C	-0.400179	2.552909	1.018062
C	-0.315388	3.910617	0.767271
C	-0.891381	4.412932	-0.396191
C	-1.522036	3.542714	-1.275603
C	-1.559073	2.191609	-0.965335
N	-1.015837	1.734122	0.160514
H	-0.843731	5.472385	-0.614961
H	0.023203	2.096285	1.904613
H	0.192120	4.555052	1.471785
H	-1.979231	3.893880	-2.190374
Cl	-1.634222	-0.077726	2.122165
C	-1.048654	-0.058149	0.381897
N	-1.807567	-0.622712	-0.533515
S	-4.215224	-1.433549	-0.512173
O	-3.179486	-0.218484	-0.276030
O	-5.502487	-0.845450	-0.206361
O	-4.002265	-2.014884	-1.820493
C	-3.751525	-2.601083	0.738830
H	-4.385724	-3.474856	0.599384
H	-2.701953	-2.846575	0.589559
H	-3.921004	-2.135421	1.706929
H	-2.015639	1.445045	-1.605053
C	0.404171	-0.418298	0.217232
C	0.960529	-0.276837	-1.057889
C	1.186480	-0.897456	1.263904
C	2.284601	-0.617150	-1.287671
H	0.350328	0.095031	-1.871277
C	2.516624	-1.242057	1.042421
H	0.767873	-1.016496	2.253529

C	3.042125	-1.091103	-0.227384
H	2.730274	-0.520668	-2.269557
H	3.135544	-1.627296	1.842566
O	4.367050	-1.482591	-0.471093
C	5.311773	-0.554192	-0.239755
F	5.346074	-0.165093	1.039938
F	6.488077	-1.078477	-0.546999
F	5.136093	0.549438	-0.974598

s13-ts-p

Symbol	X	Y	Z
C	-0.872244	2.227457	0.848827
C	-1.298215	3.514155	1.102204
C	-2.185572	4.122293	0.222757
C	-2.633471	3.432166	-0.901815
C	-2.191123	2.149054	-1.118122
N	-1.326355	1.578793	-0.246436
H	-2.526997	5.132784	0.408567
H	-0.207597	1.666637	1.491816
H	-0.934421	4.021766	1.983959
H	-3.318921	3.878683	-1.607585
Cl	-1.253501	-0.393082	2.688612
C	-0.870114	0.223079	-0.490600
N	-1.683528	-0.739068	-0.625819
S	-4.013050	-1.687260	-0.406569
O	-2.993842	-0.365953	-0.396145
O	-5.275137	-1.080608	-0.070136
O	-3.844399	-2.369969	-1.665106
C	-3.362928	-2.643395	0.930493
H	-4.084862	-3.438262	1.114151
H	-2.403238	-3.044191	0.611007
H	-3.239610	-1.978712	1.785724
H	-2.488757	1.545076	-1.963379
C	0.580783	-0.000347	-0.577136
C	1.423989	0.991892	-1.081252
C	1.098257	-1.229073	-0.160097
C	2.785969	0.749010	-1.192934
H	1.027037	1.947971	-1.403492
C	2.457201	-1.476980	-0.271709
H	0.433445	-1.968986	0.266484
C	3.275463	-0.481704	-0.785798
H	3.460665	1.494141	-1.593733
H	2.886304	-2.419512	0.043066
O	4.639246	-0.749814	-0.947428

C	5.439560	-0.418952	0.085073
F	5.112888	-1.062235	1.209004
F	6.680360	-0.743221	-0.239793
F	5.401698	0.889021	0.358838

s13-ts-r

Symbol	X	Y	Z
C	0.066421	2.204590	1.353437
C	0.981335	2.677407	0.417605
C	0.550684	2.864379	-0.890498
C	-0.767927	2.560345	-1.206850
C	-1.601728	2.081518	-0.199784
N	-1.203220	1.909784	1.063321
H	1.233015	3.229361	-1.649449
H	0.371030	2.048096	2.384336
H	2.001478	2.890293	0.712598
H	-1.148989	2.682775	-2.213013
Cl	-1.537652	-1.270831	2.732754
C	-1.199140	-1.156454	1.040739
N	-2.111096	-1.225053	0.161199
S	-4.539039	-1.174973	-0.468967
O	-3.382678	-1.387926	0.695432
O	-5.756669	-1.416060	0.261737
O	-4.309585	0.094785	-1.114364
C	-4.186958	-2.504792	-1.583410
H	-4.933059	-2.447119	-2.374509
H	-3.184098	-2.355381	-1.976940
H	-4.273364	-3.435783	-1.027614
H	-2.630112	1.811349	-0.420397
C	0.201463	-0.941664	0.609284
C	0.451504	-0.630955	-0.731857
C	1.258399	-1.000985	1.517653
C	1.742179	-0.362371	-1.155787
H	-0.369969	-0.576599	-1.433864
C	2.555220	-0.730911	1.099483
H	1.077831	-1.245003	2.555614
C	2.770736	-0.402920	-0.227211
H	1.953358	-0.104932	-2.185990
H	3.387326	-0.766612	1.790764
O	4.080054	-0.144628	-0.656994
C	4.470730	1.141692	-0.606734
F	4.427061	1.642011	0.633452
F	5.718236	1.210995	-1.042077
F	3.711781	1.938002	-1.369699

s14Cl-ts
 Symbol X Y Z
 Cl 1.524512 -0.622936 -0.047705
 C 0.000017 0.754749 0.433905
 C 0.000067 1.912752 -0.230600
 H 0.000013 2.823774 0.356779
 H 0.000036 1.977982 -1.309703
 H -0.000065 0.667476 1.508259
 Cl -1.524567 -0.622732 -0.048309

s14Cl-ts-sgm
 Symbol X Y Z
 Cl 2.376451 -0.350255 0.000343
 C 0.000067 0.099627 -0.001207
 H 0.000036 -0.961895 -0.003953
 C -0.001398 1.400130 -0.000103
 H -0.938377 1.939708 0.001289
 H 0.934696 1.941341 -0.000448
 Cl -2.375767 -0.350786 0.000303

s14
 Symbol X Y Z
 Cl -1.060284 -0.099103 0.000147
 C 0.577158 0.508337 0.000059
 C 1.630057 -0.288581 0.000231
 H 2.621385 0.147487 0.000066
 H 1.537475 -1.367336 0.000273
 H 0.616903 1.588452 -0.000092

s14-ts
 Symbol X Y Z
 C -0.876681 1.170512 -0.253807
 C -2.236081 1.042119 -0.498418
 C -2.859320 -0.157809 -0.182368
 C -2.105974 -1.196457 0.359345
 C -0.749141 -1.004887 0.547299
 N -0.171754 0.159693 0.238316
 H -3.921822 -0.283907 -0.349315
 H -0.310603 2.081245 -0.426240
 H -2.787523 1.873348 -0.916240
 H -2.556774 -2.142265 0.627227
 Cl 2.144186 -1.006341 -0.559413
 C 1.526625 0.466433 0.592005

H -0.096803 -1.775672 0.939823
 C 1.996232 1.708924 0.321823
 H 2.373243 2.296497 1.147489
 H 2.089433 2.091859 -0.685592
 H 1.569997 0.072131 1.599309

s14-ts-sgm
 Symbol X Y Z
 C -1.374447 1.086534 -0.298108
 C -2.754997 1.030701 -0.431543
 C -3.398637 -0.174457 -0.174165
 C -2.643701 -1.279156 0.202630
 C -1.266869 -1.135800 0.307972
 N -0.656704 0.024604 0.067895
 H -4.474790 -0.252217 -0.268256
 H -0.821795 2.000814 -0.489305
 H -3.304743 1.912131 -0.733501
 H -3.105462 -2.234616 0.412656
 Cl 3.692818 -0.368290 -0.359770
 C 1.444794 0.074839 0.142448
 H -0.630553 -1.966955 0.595207
 H 1.332111 -0.779483 -0.481214
 C 1.574860 1.084786 0.961840
 H 0.704752 1.565735 1.388542
 H 2.556821 1.450258 1.224325

s15
 Symbol X Y Z
 C -0.274604 0.456479 0.000038
 C -1.455744 1.372844 -0.000054
 H -1.117892 2.409498 0.000935
 H -2.075638 1.202435 -0.883028
 H -2.076842 1.201133 0.881807
 Cl -0.731562 -1.252513 -0.000212
 C 1.004169 0.813551 0.000097
 C 2.212478 -0.067437 -0.000013
 H 2.829783 0.138183 0.878189
 H 1.948903 -1.123624 0.000694
 H 2.828910 0.137196 -0.879066
 H 1.181313 1.886498 0.000225

s15-ts
 Symbol X Y Z
 C -1.165988 1.141141 0.240906

C	-2.537776	1.233213	0.053502	Cl	-0.378299	-1.611662	1.594520
C	-3.254374	0.069247	-0.193109	C	-0.523849	-0.564392	-0.013666
C	-2.577234	-1.144838	-0.248198	H	1.929716	-1.864440	0.398846
C	-1.202627	-1.150532	-0.071049	C	-1.443678	0.449814	0.009286
N	-0.529178	-0.022707	0.164525	Cl	-0.584739	-1.652052	-1.387132
H	-4.327268	0.105108	-0.336565	Cl	-1.579961	1.433725	1.439996
H	-0.536122	1.997117	0.465154	Cl	-2.676898	0.700096	-1.186404
H	-3.024908	2.197398	0.107887				
H	-3.098168	-2.075096	-0.430529				
Cl	1.771874	-1.319360	-0.890030				
C	1.366174	-0.688539	1.894171				
H	2.395168	-0.997898	2.081426				
H	1.016832	-0.057329	2.714661				
H	0.747550	-1.583626	1.858914				
C	1.300444	0.081697	0.613193				
H	-0.614502	-2.057914	-0.123631				
C	1.797400	1.299699	0.383589				
C	1.808551	1.985161	-0.952546				
H	1.688317	3.066574	-0.852458				
H	2.746205	1.805098	-1.490390				
H	1.000893	1.611682	-1.587604				
H	2.323811	1.743580	1.223420				

s16

Symbol	X	Y	Z
Cl	1.589238	-1.450033	-0.000194
C	0.667964	0.000311	0.000193
C	-0.667921	-0.000411	0.000214
Cl	1.588676	1.450242	-0.000195
Cl	-1.589162	-1.450053	-0.000205
Cl	-1.588703	1.450212	-0.000204

s16-ts

Symbol	X	Y	Z
C	1.290041	1.255917	-0.391570
C	2.561267	1.791352	-0.518065
C	3.657981	0.967381	-0.305632
C	3.453786	-0.370319	0.021898
C	2.159863	-0.838081	0.146616
N	1.118423	-0.019784	-0.050967
H	4.663137	1.358241	-0.401654
H	0.378840	1.817186	-0.567010
H	2.675941	2.833083	-0.783302
H	4.281473	-1.047747	0.180123