

Supporting Information for:

A Continuous Symmetry Measure of $[4\text{Fe}-4\text{S}]^+$ core distortions and analysis of supramolecular synthons in crystal structures of $(\text{Et}_4\text{N})_3[\text{Fe}_4\text{S}_4\text{Cl}_4]\cdot\text{Et}_4\text{NCl}$ at 100 & 295 K and high resolution protein structures

Karl S. Hagen and Mohammad Uddin*

Department of Chemistry, Emory University, Atlanta, GA 30322

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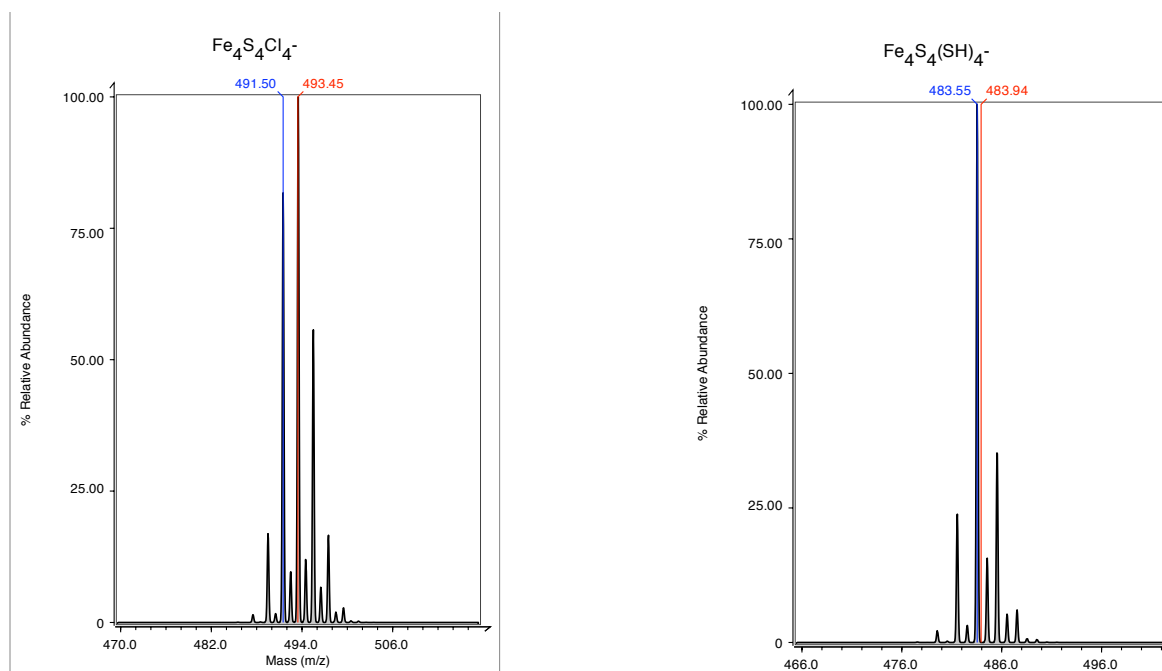


Figure S1a Calculated Mass Spectra (blue - Monoisotopic Mass, red -Average Mass)

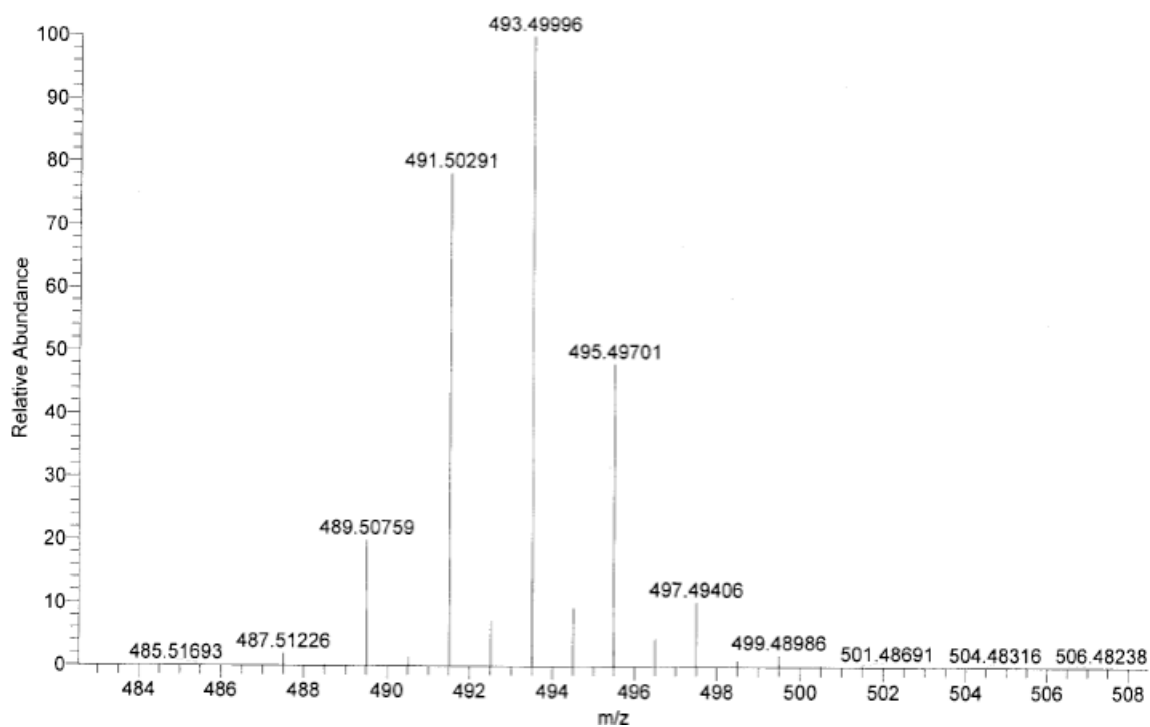


Figure S1b Observed ESI-MS for a solution containing $(\text{Et}_4\text{N})_3[\text{Fe}_4\text{S}_4\text{Cl}_4] \cdot \text{Et}_4\text{NCl}$.

Table S1 MOLSYM search and CSM for 1aLT_MU12fnls; (Et₄N)₃[Fe₄S₄Cl₄]•Et₄NCl at 100 K

For Details on the Molecular Symmetry Determination see: T. Pilati & A. Forni, J.Appl.Cryst. (1998), 31, 503-504 & (2000), 33, 417.

For CSM (i.e. Continuous Symmetry Measure), see: H. Zabrodsky et al. (1993) JACS, 115, 8278-8289

Resd	Inertial Moments			Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄ Cl ₄] ³⁻	1600.	1600.	1495.	2	D _{2d}	0.0006	0.0024	0.10
Symmetry element	CSM and Max.Diff.			Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [S ₄]	y,-x,-z	0.0000	0.0000	
3 [C ₂]	-x,-y,z	0.0000	0.0000	4 [C _s]	y,x,z	0.0006	0.0040	
5 [C ₂]	-x,y,-z	0.0006	0.0040	6 [C ₂]	x,-y,-z	0.0006	0.0040	
7 [S ₄]	-y,x,-z	0.0000	0.0000	8 [C _s]	-y,-x,z	0.0006	0.0040	
Resd	Inertial Moments			Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄ Cl ₄] ³⁻	2400.	2400.	2304.	3	T _d	0.6121	0.0782	0.30
Symmetry element	CSM and Max.Diff.			Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C ₃]	y,z,x	0.6113	0.1355	
3 [C ₂]	-x,-y,z	0.0008	0.0041	4 [S ₄]	-x,-z,y	0.4586	0.1161	
5 [C ₂]	x,-y,-z	0.0007	0.0035	6 [C ₂]	-x,y,-z	0.0015	0.0066	
7 [C ₃]	z,x,y	0.6113	0.1355	8 [C ₃]	-y,z,-x	0.6118	0.1356	
9 [C _s]	-z,y,-x	0.4583	0.1145	10 [C ₃]	-y,-z,x	0.6113	0.1355	
11 [C ₃]	y,-z,-x	0.6118	0.1356	12 [C ₃]	z,-x,-y	0.6113	0.1355	
13 [S ₄]	y,-x,-z	0.0008	0.0041	14 [C ₃]	-z,x,-y	0.6118	0.1356	
15 [C ₃]	-z,-x,y	0.6118	0.1356	16 [C _s]	x,z,y	0.4591	0.1184	
17 [C _s]	z,y,x	0.4590	0.1180	18 [C _s]	y,x,z	0.0011	0.0056	
19 [S ₄]	z,-y,-x	0.4594	0.1180	20 [C _s]	-y,-x,z	0.0011	0.0056	
21 [S ₄]	-x,z,-y	0.4586	0.1161	22 [S ₄]	-y,x,-z	0.0008	0.0041	
23 [C _s]	x,-z,-y	0.4591	0.1201	24 [S ₄]	-z,-y,x	0.4594	0.1180	

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4]+	866.	855.	855.	3	Td	0.0454	0.0213 0.10
Symmetry	element	CSM	and Max.Diff.	Symmetry	element	CSM	and Max.Diff.
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.0450	0.0318
3 [C2]	-x,-y,z	0.0004	0.0022	4 [S4]	-x,-z,y	0.0338	0.0271
5 [C2]	x,-y,-z	0.0004	0.0025	6 [C2]	-x,y,-z	0.0008	0.0041
7 [C3]	z,x,y	0.0450	0.0318	8 [C3]	-y,z,-x	0.0452	0.0319
9 [Cs]	-z,y,-x	0.0337	0.0259	10 [C3]	-y,-z,x	0.0450	0.0317
11 [C3]	y,-z,-x	0.0452	0.0321	12 [C3]	z,-x,-y	0.0450	0.0317
13 [S4]	y,-x,-z	0.0004	0.0022	14 [C3]	-z,x,-y	0.0452	0.0321
15 [C3]	-z,-x,y	0.0452	0.0319	16 [Cs]	x,z,y	0.0340	0.0293
17 [Cs]	z,y,x	0.0340	0.0282	18 [Cs]	y,x,z	0.0006	0.0036
19 [S4]	z,-y,-x	0.0342	0.0282	20 [Cs]	-y,-x,z	0.0006	0.0036
21 [S4]	-x,z,-y	0.0338	0.0271	22 [S4]	-y,x,-z	0.0004	0.0022
23 [Cs]	x,-z,-y	0.0340	0.0281	24 [S4]	-z,-y,x	0.0342	0.0282

Table S2. MOLSYM search and CSM for cpd 1aRT-mu12rt; (Et₄N)₃[Fe₄S₄Cl₄]•Et₄NCl;

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄ Cl ₄] ³⁻	1587.	1587.	1522.	2	D2d	0.0007	0.0026 0.10
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000 0.0000	2 [S ₄]	y,-x,-z	0.0000 0.0000		
3 [C ₂]	-x,-y,z	0.0000 0.0000	4 [C _s]	y,x,z	0.0007 0.0037		
5 [C ₂]	-x,y,-z	0.0007 0.0037	6 [C ₂]	x,-y,-z	0.0007 0.0037		
7 [S ₄]	-y,x,-z	0.0000 0.0000	8 [C _s]	-y,-x,z	0.0007 0.0037		
[Fe ₄ S ₄ Cl ₄] ³⁻	2389.	2389.	2328.	3	Td	0.2333	0.0483 0.20
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000 0.0000	2 [C ₃]	y,z,x	0.2328 0.0864		
3 [C ₂]	-x,-y,z	0.0014 0.0054	4 [S ₄]	-x,-z,y	0.1741 0.0710		
5 [C ₂]	x,-y,-z	0.0007 0.0039	6 [C ₂]	-x,y,-z	0.0022 0.0060		
7 [C ₃]	z,x,y	0.2328 0.0864	8 [C ₃]	-y,z,-x	0.2325 0.0864		
9 [C _s]	-z,y,-x	0.1747 0.0736	10 [C ₃]	-y,-z,x	0.2328 0.0865		
11 [C ₃]	y,-z,-x	0.2325 0.0864	12 [C ₃]	z,-x,-y	0.2328 0.0865		
13 [S ₄]	y,-x,-z	0.0014 0.0054	14 [C ₃]	-z,x,-y	0.2325 0.0864		
15 [C ₃]	-z,-x,y	0.2325 0.0864	16 [C _s]	x,z,y	0.1752 0.0762		
17 [C _s]	z,y,x	0.1742 0.0733	18 [C _s]	y,x,z	0.0014 0.0054		
19 [S ₄]	z,-y,-x	0.1755 0.0737	20 [C _s]	-y,-x,z	0.0014 0.0054		
21 [S ₄]	-x,z,-y	0.1741 0.0710	22 [S ₄]	-y,x,-z	0.0014 0.0054		
23 [C _s]	x,-z,-y	0.1752 0.0764	24 [S ₄]	-z,-y,x	0.1755 0.0737		

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4]+	863.	858.	858.	3	Td	0.0142	0.0119 0.10
Symmetry	element	CSM	and Max.Diff.	Symmetry	element	CSM	and Max.Diff.
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.0139	0.0190
3 [C2]	-x,-y,z	0.0007	0.0030	4 [S4]	-x,-z,y	0.0104	0.0159
5 [C2]	x,-y,-z	0.0011	0.0041	6 [C2]	-x,y,-z	0.0018	0.0061
7 [C3]	z,x,y	0.0139	0.0190	8 [C3]	-y,z,-x	0.0134	0.0183
9 [Cs]	-z,y,-x	0.0106	0.0170	10 [C3]	-y,-z,x	0.0139	0.0195
11 [C3]	y,-z,-x	0.0134	0.0181	12 [C3]	z,-x,-y	0.0139	0.0195
13 [S4]	y,-x,-z	0.0007	0.0030	14 [C3]	-z,x,-y	0.0134	0.0181
15 [C3]	-z,-x,y	0.0134	0.0183	16 [Cs]	x,z,y	0.0106	0.0185
17 [Cs]	z,y,x	0.0099	0.0140	18 [Cs]	y,x,z	0.0015	0.0056
19 [S4]	z,-y,-x	0.0111	0.0170	20 [Cs]	-y,-x,z	0.0015	0.0056
21 [S4]	-x,z,-y	0.0104	0.0159	22 [S4]	-y,x,-z	0.0007	0.0030
23 [Cs]	x,-z,-y	0.0106	0.0168	24 [S4]	-z,-y,x	0.0111	0.0170

Table S-3. MOLSYM search and CSM for 1b-Uddin1; (Et₄N)₃[Fe₄S₄Cl₄]•Et₄NCl; @ 100 K

Resd	Inertial Moments		Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄ Cl ₄] ³⁻	1593.	1593.	1493.	2	D2d	0.0005	0.0021 0.10
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [S4]	y,-x,-z	0.0000	0.0000
3 [C2]	-x,-y,z	0.0000	0.0000	4 [Cs]	y,x,z	0.0005	0.0037
5 [C2]	-x,y,-z	0.0005	0.0037	6 [C2]	x,-y,-z	0.0005	0.0037
7 [S4]	-y,x,-z	0.0000	0.0000	8 [Cs]	-y,-x,z	0.0005	0.0037
[Fe ₄ S ₄ Cl ₄] ³⁻	2389.	2389.	2299.	3	Td	0.5470	0.0740 0.30
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.5467	0.1265
3 [C2]	-x,-y,z	0.0002	0.0019	4 [S4]	-x,-z,y	0.4102	0.1097
5 [C2]	x,-y,-z	0.0005	0.0030	6 [C2]	-x,y,-z	0.0007	0.0043
7 [C3]	z,x,y	0.5467	0.1265	8 [C3]	-y,z,-x	0.5469	0.1272
9 [Cs]	-z,y,-x	0.4099	0.1087	10 [C3]	-y,-z,x	0.5467	0.1265
11 [C3]	y,-z,-x	0.5469	0.1271	12 [C3]	z,-x,-y	0.5467	0.1265
13 [S4]	y,-x,-z	0.0002	0.0019	14 [C3]	-z,x,-y	0.5469	0.1271
15 [C3]	-z,-x,y	0.5469	0.1272	16 [Cs]	x,z,y	0.4101	0.1101
17 [Cs]	z,y,x	0.4102	0.1105	18 [Cs]	y,x,z	0.0006	0.0040
19 [S4]	z,-y,-x	0.4104	0.1106	20 [Cs]	-y,-x,z	0.0006	0.0040
21 [S4]	-x,z,-y	0.4102	0.1097	22 [S4]	-y,x,-z	0.0002	0.0019
23 [Cs]	x,-z,-y	0.4101	0.1115	24 [S4]	-z,-y,x	0.4104	0.1106

Table S-3 (Cont.) 1b-Uddin1; (Et₄N)₃[Fe₄S₄Cl₄]•Et₄NCl; @ 100 K

Resd	Inertial Moments		Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄] ⁺	863.	852.	852.	3 Td	0.0404	0.0201	0.10
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.0402	0.0293
3 [C2]	-x,-y,z	0.0001	0.0010	4 [S4]	-x,-z,y	0.0303	0.0257
5 [C2]	x,-y,-z	0.0004	0.0024	6 [C2]	-x,y,-z	0.0005	0.0030
7 [C3]	z,x,y	0.0402	0.0293	8 [C3]	-y,z,-x	0.0403	0.0299
9 [Cs]	-z,y,-x	0.0301	0.0251	10 [C3]	-y,-z,x	0.0402	0.0294
11 [C3]	y,-z,-x	0.0403	0.0300	12 [C3]	z,-x,-y	0.0402	0.0294
13 [S4]	y,-x,-z	0.0001	0.0010	14 [C3]	-z,x,-y	0.0403	0.0300
15 [C3]	-z,-x,y	0.0403	0.0299	16 [Cs]	x,z,y	0.0302	0.0267
17 [Cs]	z,y,x	0.0302	0.0262	18 [Cs]	y,x,z	0.0004	0.0029
19 [S4]	z,-y,-x	0.0304	0.0262	20 [Cs]	-y,-x,z	0.0004	0.0029
21 [S4]	-x,z,-y	0.0303	0.0257	22 [S4]	-y,x,-z	0.0001	0.0010
23 [Cs]	x,-z,-y	0.0302	0.0256	24 [S4]	-z,-y,x	0.0304	0.0262

Table S-4. MOLSYM search and CSM for 1c-MUSPhC; (Et₄N)₃[Fe₄S₄Cl₄]•Et₄NCl;

Resd	Inertial Moments			Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄ Cl ₄] ³⁻	1590.	1590.	1491.	2	D2d	0.0004	0.0019	0.10
Symmetry element	CSM and Max.Diff.			Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [S4]	y,-x,-z	0.0000	0.0000	
3 [C2]	-x,-y,z	0.0000	0.0000	4 [Cs]	y,x,z	0.0004	0.0030	
5 [C2]	-x,y,-z	0.0004	0.0030	6 [C2]	x,-y,-z	0.0004	0.0030	
7 [S4]	-y,x,-z	0.0000	0.0000	8 [Cs]	-y,-x,z	0.0004	0.0030	
Resd #	Inertial Moments			Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄ Cl ₄] ³⁻	2386.	2386.	2295.	3	Td	0.5394	0.0734	0.30
Symmetry element	CSM and Max.Diff.			Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.5388	0.1284	
3 [C2]	-x,-y,z	0.0012	0.0049	4 [S4]	-x,-z,y	0.4037	0.1078	
5 [C2]	x,-y,-z	0.0003	0.0029	6 [C2]	-x,y,-z	0.0015	0.0052	
7 [C3]	z,x,y	0.5388	0.1284	8 [C3]	-y,z,-x	0.5390	0.1284	
9 [Cs]	-z,y,-x	0.4041	0.1101	10 [C3]	-y,-z,x	0.5388	0.1284	
11 [C3]	y,-z,-x	0.5390	0.1284	12 [C3]	z,-x,-y	0.5388	0.1284	
13 [S4]	y,-x,-z	0.0012	0.0049	14 [C3]	-z,x,-y	0.5390	0.1284	
15 [C3]	-z,-x,y	0.5390	0.1284	16 [Cs]	x,z,y	0.4048	0.1124	
17 [Cs]	z,y,x	0.4042	0.1096	18 [Cs]	y,x,z	0.0009	0.0042	
19 [S4]	z,-y,-x	0.4049	0.1102	20 [Cs]	-y,-x,z	0.0009	0.0042	
21 [S4]	-x,z,-y	0.4037	0.1078	22 [S4]	-y,x,-z	0.0012	0.0049	
23 [Cs]	x,-z,-y	0.4048	0.1127	24 [S4]	-z,-y,x	0.4049	0.1102	

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4]+	861.	851.	851.	3	Td	0.0373	0.0193 0.10
Symmetry	element	CSM	and Max.Diff.	Symmetry	element	CSM	and Max.Diff.
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.0369	0.0292
3 [C2]	-x,-y,z	0.0006	0.0027	4 [S4]	-x,-z,y	0.0277	0.0247
5 [C2]	x,-y,-z	0.0005	0.0026	6 [C2]	-x,y,-z	0.0010	0.0046
7 [C3]	z,x,y	0.0369	0.0292	8 [C3]	-y,z,-x	0.0371	0.0295
9 [Cs]	-z,y,-x	0.0275	0.0233	10 [C3]	-y,-z,x	0.0369	0.0292
11 [C3]	y,-z,-x	0.0371	0.0294	12 [C3]	z,-x,-y	0.0369	0.0292
13 [S4]	y,-x,-z	0.0006	0.0027	14 [C3]	-z,x,-y	0.0371	0.0294
15 [C3]	-z,-x,y	0.0371	0.0295	16 [Cs]	x,z,y	0.0280	0.0273
17 [Cs]	z,y,x	0.0279	0.0259	18 [Cs]	y,x,z	0.0007	0.0040
19 [S4]	z,-y,-x	0.0283	0.0259	20 [Cs]	-y,-x,z	0.0007	0.0039
21 [S4]	-x,z,-y	0.0277	0.0247	22 [S4]	-y,x,-z	0.0006	0.0027
23 [Cs]	x,-z,-y	0.0280	0.0260	24 [S4]	-z,-y,x	0.0283	0.0259

Resd	Inertial		Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4Cl4]3-	1578.	1578.	1521.	2	D2d	0.0010	0.0031	0.10
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [S4]	y,-x,-z	0.0000	0.0000	
3 [C2]	-x,-y,z	0.0000	0.0000	4 [Cs]	y,x,z	0.0010	0.0053	
5 [C2]	-x,y,-z	0.0010	0.0053	6 [C2]	x,-y,-z	0.0010	0.0053	
7 [S4]	-y,x,-z	0.0000	0.0000	8 [Cs]	-y,-x,z	0.0010	0.0053	
Resd	Inertial		Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4Cl4]3-	2378.	2378.	2324.	3	Td	0.1783	0.0422	0.20
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.1776	0.0761	
3 [C2]	-x,-y,z	0.0013	0.0052	4 [S4]	-x,-z,y	0.1329	0.0630	
5 [C2]	x,-y,-z	0.0008	0.0044	6 [C2]	-x,y,-z	0.0022	0.0064	
7 [C3]	z,x,y	0.1776	0.0761	8 [C3]	-y,z,-x	0.1775	0.0760	
9 [Cs]	-z,y,-x	0.1332	0.0655	10 [C3]	-y,-z,x	0.1776	0.0762	
11 [C3]	y,-z,-x	0.1775	0.0760	12 [C3]	z,-x,-y	0.1776	0.0762	
13 [S4]	y,-x,-z	0.0013	0.0052	14 [C3]	-z,x,-y	0.1775	0.0760	
15 [C3]	-z,-x,y	0.1775	0.0761	16 [Cs]	x,z,y	0.1338	0.0672	
17 [Cs]	z,y,x	0.1331	0.0635	18 [Cs]	y,x,z	0.0015	0.0059	
19 [S4]	z,-y,-x	0.1342	0.0656	20 [Cs]	-y,-x,z	0.0015	0.0059	
21 [S4]	-x,z,-y	0.1329	0.0630	22 [S4]	-y,x,-z	0.0013	0.0052	
23 [Cs]	x,-z,-y	0.1338	0.0682	24 [S4]	-z,-y,x	0.1342	0.0656	

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4]+	860.	856.	856.	3	Td	0.0095	0.0098 0.10
Symmetry	element	CSM	and Max.Diff.	Symmetry	element	CSM	and Max.Diff.
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.0089	0.0151
3 [C2]	-x,-y,z	0.0007	0.0029	4 [S4]	-x,-z,y	0.0069	0.0129
5 [C2]	x,-y,-z	0.0008	0.0035	6 [C2]	-x,y,-z	0.0015	0.0055
7 [C3]	z,x,y	0.0089	0.0151	8 [C3]	-y,z,-x	0.0092	0.0157
9 [Cs]	-z,y,-x	0.0065	0.0111	10 [C3]	-y,-z,x	0.0089	0.0150
11 [C3]	y,-z,-x	0.0092	0.0160	12 [C3]	z,-x,-y	0.0089	0.0150
13 [S4]	y,-x,-z	0.0007	0.0029	14 [C3]	-z,x,-y	0.0092	0.0160
15 [C3]	-z,-x,y	0.0092	0.0157	16 [Cs]	x,z,y	0.0071	0.0154
17 [Cs]	z,y,x	0.0071	0.0140	18 [Cs]	y,x,z	0.0011	0.0049
19 [S4]	z,-y,-x	0.0075	0.0140	20 [Cs]	-y,-x,z	0.0011	0.0049
21 [S4]	-x,z,-y	0.0069	0.0129	22 [S4]	-y,x,-z	0.0007	0.0029
23 [Cs]	x,-z,-y	0.0071	0.0140	24 [S4]	-z,-y,x	0.0075	0.0140

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4(SH)4]3-	1444.	1444. 1410.	2	D2d	0.0264	0.0162	0.10
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000 0.0000	2 [S4]	y,-x,-z	0.0000	0.0000	
3 [C2]	-x,-y,z	0.0000 0.0000	4 [Cs]	y,x,z	0.0264	0.0222	
5 [C2]	-x,y,-z	0.0264 0.0222	6 [C2]	x,-y,-z	0.0264	0.0222	
7 [S4]	-y,x,-z	0.0000 0.0000	8 [Cs]	-y,-x,z	0.0264	0.0222	
Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4(SH)4]3-	2241.	2241. 2211.	3	Td	0.1100	0.0332	0.20
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000 0.0000	2 [C3]	y,z,x	0.1004	0.0636	
3 [C2]	-x,-y,z	0.0005 0.0031	4 [S4]	-x,-z,y	0.0885	0.0579	
5 [C2]	x,-y,-z	0.0252 0.0242	6 [C2]	-x,y,-z	0.0257	0.0259	
7 [C3]	z,x,y	0.1004 0.0636	8 [C3]	-y,z,-x	0.1025	0.0658	
9 [Cs]	-z,y,-x	0.0746 0.0524	10 [C3]	-y,-z,x	0.1004	0.0629	
11 [C3]	y,-z,-x	0.1025 0.0651	12 [C3]	z,-x,-y	0.1004	0.0629	
13 [S4]	y,-x,-z	0.0005 0.0031	14 [C3]	-z,x,-y	0.1025	0.0651	
15 [C3]	-z,-x,y	0.1025 0.0658	16 [Cs]	x,z,y	0.0763	0.0509	
17 [Cs]	z,y,x	0.0776 0.0554	18 [Cs]	y,x,z	0.0254	0.0258	
19 [S4]	z,-y,-x	0.0889 0.0584	20 [Cs]	-y,-x,z	0.0254	0.0258	
21 [S4]	-x,z,-y	0.0885 0.0579	22 [S4]	-y,x,-z	0.0005	0.0031	
23 [Cs]	x,-z,-y	0.0763 0.0570	24 [S4]	-z,-y,x	0.0889	0.0584	

Table S-6 (Cont) 2-MU10rt; (Et₄N)₃[Fe₄S₄(SH)₄]•Et₄NCl

Resd	Inertial Moments		Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄] ⁺	856.	851.	851.	3	Td	0.0102	0.0101 0.10
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.0101	0.0155
3 [C2]	-x,-y,z	0.0002	0.0017	4 [S4]	-x,-z,y	0.0075	0.0122
5 [C2]	x,-y,-z	0.0000	0.0002	6 [C2]	-x,y,-z	0.0002	0.0018
7 [C3]	z,x,y	0.0101	0.0155	8 [C3]	-y,z,-x	0.0101	0.0155
9 [Cs]	-z,y,-x	0.0076	0.0129	10 [C3]	-y,-z,x	0.0101	0.0155
11 [C3]	y,-z,-x	0.0101	0.0155	12 [C3]	z,-x,-y	0.0101	0.0155
13 [S4]	y,-x,-z	0.0002	0.0017	14 [C3]	-z,x,-y	0.0101	0.0155
15 [C3]	-z,-x,y	0.0101	0.0155	16 [Cs]	x,z,y	0.0077	0.0139
17 [Cs]	z,y,x	0.0076	0.0131	18 [Cs]	y,x,z	0.0001	0.0015
19 [S4]	z,-y,-x	0.0077	0.0132	20 [Cs]	-y,-x,z	0.0001	0.0015
21 [S4]	-x,z,-y	0.0075	0.0122	22 [S4]	-y,x,-z	0.0002	0.0017
23 [Cs]	x,-z,-y	0.0077	0.0138	24 [S4]	-z,-y,x	0.0077	0.0132

Table S7. MOLSYM search and CSM for cpd 3-Uddin Xt13; (Et₄N)₃[Fe₄S₄Cl₄]•Et₄N(Cl-/HS-)

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4Cl4]3-	1595.	1595.	1534.	2	D2d	0.0006	0.0025 0.10
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [S4]	y,-x,-z	0.0000	0.0000
3 [C2]	-x,-y,z	0.0000	0.0000	4 [Cs]	y,x,z	0.0006	0.0042
5 [C2]	-x,y,-z	0.0006	0.0042	6 [C2]	x,-y,-z	0.0006	0.0042
7 [S4]	-y,x,-z	0.0000	0.0000	8 [Cs]	-y,-x,z	0.0006	0.0042
Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4Cl4]3-	2403.	2403.	2347.	3	Td	0.1955	0.0442 0.20
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.1951	0.0784
3 [C2]	-x,-y,z	0.0007	0.0039	4 [S4]	-x,-z,y	0.1462	0.0658
5 [C2]	x,-y,-z	0.0005	0.0036	6 [C2]	-x,y,-z	0.0013	0.0050
7 [C3]	z,x,y	0.1951	0.0784	8 [C3]	-y,z,-x	0.1951	0.0784
9 [Cs]	-z,y,-x	0.1463	0.0661	10 [C3]	-y,-z,x	0.1951	0.0783
11 [C3]	y,-z,-x	0.1951	0.0784	12 [C3]	z,-x,-y	0.1951	0.0783
13 [S4]	y,-x,-z	0.0007	0.0039	14 [C3]	-z,x,-y	0.1951	0.0784
15 [C3]	-z,-x,y	0.1951	0.0784	16 [Cs]	x,z,y	0.1467	0.0688
17 [Cs]	z,y,x	0.1463	0.0676	18 [Cs]	y,x,z	0.0009	0.0046
19 [S4]	z,-y,-x	0.1470	0.0677	20 [Cs]	-y,-x,z	0.0009	0.0046
21 [S4]	-x,z,-y	0.1462	0.0658	22 [S4]	-y,x,-z	0.0007	0.0039
23 [Cs]	x,-z,-y	0.1467	0.0696	24 [S4]	-z,-y,x	0.1470	0.0677

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4]+	869.	864.	864.	3 Td	0.0109	0.0104	0.10
Symmetry	element	CSM	and Max.Diff.	Symmetry	element	CSM	and Max.Diff.
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.0107	0.0163
3 [C2]	-x,-y,z	0.0004	0.0021	4 [S4]	-x,-z,y	0.0080	0.0137
5 [C2]	x,-y,-z	0.0005	0.0028	6 [C2]	-x,y,-z	0.0009	0.0043
7 [C3]	z,x,y	0.0107	0.0163	8 [C3]	-y,z,-x	0.0104	0.0159
9 [Cs]	-z,y,-x	0.0081	0.0146	10 [C3]	-y,-z,x	0.0107	0.0166
11 [C3]	y,-z,-x	0.0105	0.0159	12 [C3]	z,-x,-y	0.0107	0.0166
13 [S4]	y,-x,-z	0.0004	0.0021	14 [C3]	-z,x,-y	0.0105	0.0159
15 [C3]	-z,-x,y	0.0104	0.0159	16 [Cs]	x,z,y	0.0081	0.0157
17 [Cs]	z,y,x	0.0078	0.0124	18 [Cs]	y,x,z	0.0007	0.0039
19 [S4]	z,-y,-x	0.0084	0.0146	20 [Cs]	-y,-x,z	0.0007	0.0039
21 [S4]	-x,z,-y	0.0080	0.0137	22 [S4]	-y,x,-z	0.0004	0.0021
23 [Cs]	x,-z,-y	0.0081	0.0145	24 [S4]	-z,-y,x	0.0084	0.0146

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4(SH)4]3-	2232.	2225.	2225.	3 Td	0.0182	0.0135	0.10
Symmetry element	CSM	and Max.Diff.	Symmetry element	CSM	and Max.Diff.		
1 [E] x,y,z	0.0000	0.0000	2 [C3] y,z,x		0.0136	0.0250	
3 [C2] -x,-y,z	0.0001	0.0012	4 [S4] -x,-z,y		0.0173	0.0241	
5 [C2] x,-y,-z	0.0146	0.0184	6 [C2] -x,y,-z		0.0147	0.0191	
7 [C3] z,x,y	0.0136	0.0250	8 [C3] -y,z,-x		0.0130	0.0240	
9 [Cs] -z,y,-x	0.0105	0.0192	10 [C3] -y,-z,x		0.0136	0.0244	
11 [C3] y,-z,-x	0.0130	0.0233	12 [C3] z,-x,-y		0.0136	0.0244	
13 [S4] y,-x,-z	0.0001	0.0012	14 [C3] -z,x,-y		0.0130	0.0233	
15 [C3] -z,-x,y	0.0130	0.0240	16 [Cs] x,z,y		0.0100	0.0188	
17 [Cs] z,y,x	0.0095	0.0174	18 [Cs] y,x,z		0.0147	0.0190	
19 [S4] z,-y,-x	0.0173	0.0243	20 [Cs] -y,-x,z		0.0147	0.0190	
21 [S4] -x,z,-y	0.0173	0.0241	22 [S4] -y,x,-z		0.0001	0.0012	
23 [Cs] x,-z,-y	0.0100	0.0193	24 [S4] -z,-y,x		0.0173	0.0243	
[Fe4S4]+	853.	853.	853.	3 Td	0.0002	0.0013	0.10
Symmetry element	CSM	and Max.Diff.	Symmetry element	CSM	and Max.Diff.		
1 [E] x,y,z	0.0000	0.0000	2 [C3] y,z,x		0.0001	0.0021	
3 [C2] -x,-y,z	0.0000	0.0007	4 [S4] -x,-z,y		0.0001	0.0013	
5 [C2] x,-y,-z	0.0000	0.0000	6 [C2] -x,y,-z		0.0000	0.0007	
7 [C3] z,x,y	0.0001	0.0021	8 [C3] -y,z,-x		0.0001	0.0021	
9 [Cs] -z,y,-x	0.0001	0.0016	10 [C3] -y,-z,x		0.0001	0.0020	
11 [C3] y,-z,-x	0.0001	0.0020	12 [C3] z,-x,-y		0.0001	0.0020	
13 [S4] y,-x,-z	0.0000	0.0007	14 [C3] -z,x,-y		0.0001	0.0020	
15 [C3] -z,-x,y	0.0001	0.0021	16 [Cs] x,z,y		0.0001	0.0020	
17 [Cs] z,y,x	0.0001	0.0016	18 [Cs] y,x,z		0.0000	0.0006	
19 [S4] z,-y,-x	0.0001	0.0017	20 [Cs] -y,-x,z		0.0000	0.0006	
21 [S4] -x,z,-y	0.0001	0.0013	22 [S4] -y,x,-z		0.0000	0.0007	
23 [Cs] x,-z,-y	0.0001	0.0019	24 [S4] -z,-y,x		0.0001	0.0017	

Table S-9. MOLSYM search and CSM for COZXUK; (Me₄N)₃[Fe₄S₄(SEt)₄]; Hagen, K. S.; Watson, A. D.; Holm, R. H. *Inorg. Chem.* **1984**, 23, 2984-2990.

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4(SeEt)4]3-	1849.	1849.	1841.	2	S4	0.0000	0.0004 0.10
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E] x,y,z		0.0000	0.0000	2 [S4] y,-x,-z		0.0000	0.0007
3 [C2] -x,-y,z		0.0000	0.0007	4 [S4] -y,x,-z		0.0000	0.0007
Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4S4]3-	1480.	1480.	1322.	2	D2d	0.0800	0.0283 0.10
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E] x,y,z		0.0000	0.0000	2 [S4] y,-x,-z		0.0000	0.0000
3 [C2] -x,-y,z		0.0000	0.0000	4 [Cs] y,x,z		0.0800	0.0412
5 [C2] -x,y,-z		0.0800	0.0412	6 [C2] x,-y,-z		0.0800	0.0412
7 [S4] -y,x,-z		0.0000	0.0000	8 [Cs] -y,-x,z		0.0800	0.0412
Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4S4]3-	2277.	2277.	2130.	3	Td	1.6728	0.1293 0.50
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E] x,y,z		0.0000	0.0000	2 [C3] y,z,x		1.6530	0.2447
3 [C2] -x,-y,z		0.0085	0.0132	4 [S4] -x,-z,y		1.2660	0.2093
5 [C2] x,-y,-z		0.0715	0.0398	6 [C2] -x,y,-z		0.0799	0.0481
7 [C3] z,x,y		1.6530	0.2447	8 [C3] -y,z,-x		1.6391	0.2364
9 [Cs] -z,y,-x		1.2448	0.2127	10 [C3] -y,-z,x		1.6532	0.2434
11 [C3] y,-z,-x		1.6393	0.2355	12 [C3] z,-x,-y		1.6532	0.2434
13 [S4] y,-x,-z		0.0085	0.0132	14 [C3] -z,x,-y		1.6393	0.2355
15 [C3] -z,-x,y		1.6391	0.2364	16 [Cs] x,z,y		1.2388	0.2026
17 [Cs] z,y,x		1.2239	0.2002	18 [Cs] y,x,z		0.0757	0.0467
19 [S4] z,-y,-x		1.2743	0.2138	20 [Cs] -y,-x,z		0.0757	0.0468
21 [S4] -x,z,-y		1.2660	0.2093	22 [S4] -y,x,-z		0.0085	0.0132
23 [Cs] x,-z,-y		1.2386	0.2195	24 [S4] -z,-y,x		1.2743	0.2138

Table S9 (Cont.) COZXUK; (Me₄N)₃[Fe₄S₄(SEt)₄]; Hagen, K. S.; Watson, A. D.; Holm, R. H. *Inorg. Chem.* **1984**, 23, 2984-2990.

Resd	Inertial Moments		Degree Symbol		CSM	RMS	Tol
[Fe ₄ S ₄] ⁺	864.	852.	852.	3 Td	0.0751	0.0274	0.10
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.0730	0.0432
3 [C2]	-x,-y,z	0.0041	0.0072	4 [S4]	-x,-z,y	0.0535	0.0340
5 [C2]	x,-y,-z	0.0009	0.0037	6 [C2]	-x,y,-z	0.0050	0.0095
7 [C3]	z,x,y	0.0730	0.0432	8 [C3]	-y,z,-x	0.0740	0.0438
9 [Cs]	-z,y,-x	0.0544	0.0338	10 [C3]	-y,-z,x	0.0730	0.0431
11 [C3]	y,-z,-x	0.0740	0.0432	12 [C3]	z,-x,-y	0.0730	0.0431
13 [S4]	y,-x,-z	0.0041	0.0072	14 [C3]	-z,x,-y	0.0740	0.0432
15 [C3]	-z,-x,y	0.0740	0.0438	16 [Cs]	x,z,y	0.0571	0.0410
17 [Cs]	z,y,x	0.0558	0.0375	18 [Cs]	y,x,z	0.0029	0.0072
19 [S4]	z,-y,-x	0.0576	0.0376	20 [Cs]	-y,-x,z	0.0029	0.0072
21 [S4]	-x,z,-y	0.0535	0.0340	22 [S4]	-y,x,-z	0.0041	0.0072
23 [Cs]	x,-z,-y	0.0571	0.0393	24 [S4]	-z,-y,x	0.0576	0.0376

Table S-10 MOLSYM search and CSM for BZTFEA; $(\text{Et}_4\text{N})_3[\text{Fe}_4\text{S}_4(\text{SBzl})_4]$; Berg, J. M.; Hodgson, K. O.; Holm, R. H. *J. Am. Chem. Soc.* **1979**, *101*, 4586-4593.

Resd #	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4S4]3- 2275.	2204.	2158.	3	T23	1.3063	0.1143	0.60
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000 0.0000	2 [C3]	y,z,x	1.2283	0.2220	
3 [C2]	-x,-y,z	0.9965 0.2283	4 [C2]	x,-y,-z	0.4209	0.1349	
5 [C2]	-x,y,-z	0.6498 0.1577	6 [C3]	z,x,y	1.2283	0.2220	
7 [C3]	-y,z,-x	0.7522 0.1998	8 [C3]	-y,-z,x	0.7970	0.2066	
9 [C3]	y,-z,-x	1.0696 0.2692	10 [C3]	z,-x,-y	0.7970	0.2066	
11 [C3]	-z,x,-y	1.0696 0.2692	12 [C3]	-z,-x,y	0.7522	0.1998	
[Fe4S4S4]3- 2275.	2204.	2158.	3	Td	1.3463	0.1160	0.70
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000 0.0000	2 [C3]	y,z,x	1.1748	0.2370	
3 [C2]	-x,-y,z	0.8014 0.1756	4 [S4]	-x,-z,y	1.2595	0.2449	
5 [C2]	-x,y,-z	0.3370 0.1124	6 [C3]	z,x,y	1.1748	0.2370	
7 [C3]	-y,z,-x	1.1955 0.2190	8 [Cs]	-z,y,-x	0.4865	0.1469	
9 [C3]	y,-z,-x	0.7992 0.1795	10 [C3]	z,-x,-y	0.7977	0.1680	
11 [S4]	y,-x,-z	1.0097 0.1933	12 [C3]	-z,-x,y	1.1955	0.2190	
13 [C3]	-y,-z,x	0.7977 0.1680	14 [C3]	-z,x,-y	0.7992	0.1795	
15 [C2]	x,-y,-z	0.9884 0.1754	16 [Cs]	x,z,y	1.1625	0.1874	
17 [Cs]	z,y,x	0.3545 0.1640	18 [Cs]	y,x,z	0.6802	0.1663	
19 [S4]	z,-y,-x	1.0547 0.2204	20 [Cs]	-y,-x,z	0.3900	0.1405	
21 [S4]	-x,z,-y	1.2595 0.2449	22 [S4]	-y,x,-z	1.0097	0.1933	
23 [Cs]	x,-z,-y	0.4827 0.1415	24 [S4]	-z,-y,x	1.0547	0.2204	

Table S-10 (cont.) for BZTFEA; $(Et_4N)_3[Fe_4S_4(SBzl)_4]$

Resd	Inertial Moments		Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄] ⁺	864.	857.	847.	3	Td	0.0860	0.0293 0.10
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.0791	0.0434
3 [C2]	-x,-y,z	0.0299	0.0213	4 [S4]	-x,-z,y	0.0279	0.0222
5 [C2]	x,-y,-z	0.0126	0.0126	6 [C2]	-x,y,-z	0.0184	0.0177
7 [C3]	z,x,y	0.0791	0.0434	8 [C3]	-y,z,-x	0.0725	0.0410
9 [Cs]	-z,y,-x	0.0493	0.0337	10 [C3]	-y,-z,x	0.0715	0.0436
11 [C3]	y,-z,-x	0.0805	0.0402	12 [C3]	z,-x,-y	0.0715	0.0436
13 [S4]	y,-x,-z	0.0777	0.0429	14 [C3]	-z,x,-y	0.0805	0.0402
15 [C3]	-z,-x,y	0.0725	0.0410	16 [Cs]	x,z,y	0.0123	0.0186
17 [Cs]	z,y,x	0.0500	0.0346	18 [Cs]	y,x,z	0.0735	0.0417
19 [S4]	z,-y,-x	0.0583	0.0320	20 [Cs]	-y,-x,z	0.0514	0.0317
21 [S4]	-x,z,-y	0.0279	0.0222	22 [S4]	-y,x,-z	0.0777	0.0429
23 [Cs]	x,-z,-y	0.0128	0.0177	24 [S4]	-z,-y,x	0.0583	0.0320

Table S-11 MOLSYM search and CSM for COZXOE; (Et₄N)₃[Fe₄S₄(S-t-Bu)₄]; Hagen, K. S.; Watson, A. D.; Holm, R. H. *Inorg. Chem.* **1984**, *23*, 2984-2990.

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄ S ₄]- 2302.	2248.	2103.	3	Td	3.1884	0.1786	0.80
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E] x,y,z	0.0000	0.0000	2 [C3] y,z,x		3.1643	0.3281	
3 [C2] -x,-y,z	0.7773	0.1928	4 [S4] -x,-z,y		2.2812	0.3712	
5 [C2] x,-y,-z	0.6603	0.1868	6 [C2] -x,y,-z		0.7636	0.1987	
7 [C3] z,x,y	3.1643	0.3281	8 [C3] -y,z,-x		2.4975	0.3518	
9 [Cs] -z,y,-x	2.1644	0.2884	10 [C3] -y,-z,x		2.7108	0.3530	
11 [C3] y,-z,-x	2.9114	0.3915	12 [C3] z,-x,-y		2.7108	0.3530	
13 [S4] y,-x,-z	0.9404	0.2368	14 [C3] -z,x,-y		2.9114	0.3915	
15 [C3] -z,-x,y	2.4975	0.3518	16 [Cs] x,z,y		1.3077	0.2526	
17 [Cs] z,y,x	2.3929	0.3498	18 [Cs] y,x,z		1.0909	0.2266	
19 [S4] z,-y,-x	2.8630	0.3960	20 [Cs] -y,-x,z		0.4006	0.1371	
21 [S4] -x,z,-y	2.2812	0.3712	22 [S4] -y,x,-z		0.9404	0.2368	
23 [Cs] x,-z,-y	1.8001	0.2607	24 [S4] -z,-y,x		2.8630	0.3960	
Resd #	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄]+ 868.	859.	849.	3	Td	0.1363	0.0369	0.20
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E] x,y,z	0.0000	0.0000	2 [C3] y,z,x		0.1247	0.0557	
3 [C2] -x,-y,z	0.0233	0.0181	4 [S4] -x,-z,y		0.0561	0.0362	
5 [C2] x,-y,-z	0.0220	0.0200	6 [C2] -x,y,-z		0.0043	0.0089	
7 [C3] z,x,y	0.1247	0.0557	8 [C3] -y,z,-x		0.1309	0.0530	
9 [Cs] -z,y,-x	0.0434	0.0330	10 [C3] -y,-z,x		0.1329	0.0481	
11 [C3] y,-z,-x	0.1238	0.0491	12 [C3] z,-x,-y		0.1329	0.0481	
13 [S4] y,-x,-z	0.1277	0.0504	14 [C3] -z,x,-y		0.1238	0.0491	
15 [C3] -z,-x,y	0.1309	0.0530	16 [Cs] x,z,y		0.0416	0.0312	
17 [Cs] z,y,x	0.0420	0.0294	18 [Cs] y,x,z		0.1184	0.0494	
19 [S4] z,-y,-x	0.0455	0.0255	20 [Cs] -y,-x,z		0.1132	0.0524	
21 [S4] -x,z,-y	0.0561	0.0362	22 [S4] -y,x,-z		0.1277	0.0504	
23 [Cs] x,-z,-y	0.0501	0.0393	24 [S4] -z,-y,x		0.0455	0.0255	

Table S-12 MOLSYM search and CSM for $(Et_4N)_3[Fe_4S_4(S-p-C_6H_4Br)_4]$; BUTFAX; Stephan, D. W.; Papaefthymiou, G. C.; Frankel, R. B.; Holm, R. H. *Inorg. Chem.*, **1983** 22, 1550-1557.

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol		
[Fe4S4S4]3-	1488.	1295.	1396.	1	C2	0.0000	0.10		
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.				
1	[E]	x,y,z	0.0000	0.0000	2	[C2]	-x,-y,z	0.0000	0.0000
Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol		
[Fe4S4S4]3-	2291.	2206.	2105.	3	Td	1.9469	0.1395	0.60	
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.				
1	[E]	x,y,z	0.0000	0.0000	2	[C3]	y,z,x	1.8850	0.2562
3	[C2]	-x,-y,z	0.1855	0.0617	4	[S4]	-x,-z,y	1.8671	0.2345
5	[C2]	x,-y,-z	0.0000	0.0000	6	[C2]	-x,y,-z	0.1855	0.0617
7	[C3]	z,x,y	1.8850	0.2562	8	[C3]	-y,z,-x	1.8850	0.2562
9	[Cs]	-z,y,-x	0.5526	0.1686	10	[C3]	-y,-z,x	1.8850	0.2714
11	[C3]	y,-z,-x	1.8850	0.2714	12	[C3]	z,-x,-y	1.8850	0.2714
13	[S4]	y,-x,-z	0.6448	0.1655	14	[C3]	-z,x,-y	1.8850	0.2714
15	[C3]	-z,-x,y	1.8850	0.2562	16	[Cs]	x,z,y	1.7631	0.2400
17	[Cs]	z,y,x	0.5526	0.1686	18	[Cs]	y,x,z	0.5521	0.1599
19	[S4]	z,-y,-x	0.6453	0.1700	20	[Cs]	-y,-x,z	0.5521	0.1599
21	[S4]	-x,z,-y	1.8671	0.2345	22	[S4]	-y,x,-z	0.6448	0.1655
23	[Cs]	x,-z,-y	1.7631	0.2400	24	[S4]	-z,-y,x	0.6453	0.1700

Table S-12 (Cont.) BUTFAX; (Et₄N)₃[Fe₄S₄(S-p-C₆H₄Br)₄] Stephan, D. W.; Papaefthymiou, G. C.; Frankel, R. B.; Holm, R. H. *Inorg. Chem.*, **1983** 22, 1550-1557.

Resd	Inertial Moments			Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄] ⁺	855.	851.	842.	3	Td	0.1503	0.0388	0.10
Symmetry	element	CSM and Max.Diff.		Symmetry		element	CSM and Max.Diff.	
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.1270	0.0489	
3 [C2]	-x,-y,z	0.0698	0.0268	4 [S4]	-x,-z,y	0.0405	0.0261	
5 [C2]	x,-y,-z	0.0000	0.0000	6 [C2]	-x,y,-z	0.0698	0.0268	
7 [C3]	z,x,y	0.1270	0.0489	8 [C3]	-y,z,-x	0.1270	0.0489	
9 [Cs]	-z,y,-x	0.1131	0.0449	10 [C3]	-y,-z,x	0.1270	0.0485	
11 [C3]	y,-z,-x	0.1270	0.0485	12 [C3]	z,-x,-y	0.1270	0.0485	
13 [S4]	y,-x,-z	0.0898	0.0399	14 [C3]	-z,x,-y	0.1270	0.0485	
15 [C3]	-z,-x,y	0.1270	0.0489	16 [Cs]	x,z,y	0.0744	0.0384	
17 [Cs]	z,y,x	0.1131	0.0449	18 [Cs]	y,x,z	0.0549	0.0343	
19 [S4]	z,-y,-x	0.1479	0.0495	20 [Cs]	-y,-x,z	0.0549	0.0343	
21 [S4]	-x,z,-y	0.0405	0.0261	22 [S4]	-y,x,-z	0.0898	0.0399	
23 [Cs]	x,-z,-y	0.0744	0.0384	24 [S4]	-z,-y,x	0.1479	0.0495	

Table S-13 MOLSYM search and CSM for (Me₄N)₃[Fe₄S₄(SPh)₄]•2MeCN; GAPXEA; Carney, M. J. *et. al. Inorg. Chem.* **1988**, 27, 346-352.

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄ S ₄] ³⁻	1567.	1382.	1210.	1 C2	0.0000	0.0000	0.10
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C2]	-x,-y,z	0.0000	0.0000
Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄ S ₄] ³⁻	1567.	1382.	1210.	1 D2	0.8842	0.0940	0.30
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C2]	-x,-y,z	0.0000	0.0000
3 [C2]	-x,y,-z	0.8842	0.1326	4 [C2]	x,-y,-z	0.8842	0.1326
Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[4Fe-4S] ⁺	574.	553.	544.	1 D2	0.0947	0.0308	0.10
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C2]	-x,-y,z	0.0947	0.0352
3 [C2]	-x,y,-z	0.0947	0.0352	4 [C2]	x,-y,-z	0.0000	0.0000

Table S-13 (Cont.) for $(\text{Me}_4\text{N})_3[\text{Fe}_4\text{S}_4(\text{SPh})_4]\bullet 2\text{MeCN}$; GAPXEA; Carney, M. J. *et. al. Inorg. Chem.* **1988**, 27, 346-352.

Resd	Inertial Moments			Degree	Symbol	CSM	RMS	Tol
[4Fe-4S]+	859.	846.	830.	3	Td	0.3320	0.0576	0.20
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.3141	0.0969	
3 [C2]	-x,-y,z	0.0600	0.0277	4 [S4]	-x,-z,y	0.1719	0.0584	
5 [C2]	x,-y,-z	0.0017	0.0043	6 [C2]	-x,y,-z	0.0617	0.0316	
7 [C3]	z,x,y	0.3141	0.0969	8 [C3]	-y,z,-x	0.3088	0.0898	
9 [Cs]	-z,y,-x	0.2472	0.0773	10 [C3]	-y,-z,x	0.3140	0.0933	
11 [C3]	y,-z,-x	0.3088	0.0953	12 [C3]	z,-x,-y	0.3140	0.0933	
13 [S4]	y,-x,-z	0.0840	0.0367	14 [C3]	-z,x,-y	0.3088	0.0953	
15 [C3]	-z,-x,y	0.3088	0.0898	16 [Cs]	x,z,y	0.2310	0.0860	
17 [Cs]	z,y,x	0.2401	0.0816	18 [Cs]	y,x,z	0.0527	0.0277	
19 [S4]	z,-y,-x	0.2745	0.0859	20 [Cs]	-y,-x,z	0.0528	0.0302	
21 [S4]	-x,z,-y	0.1719	0.0584	22 [S4]	-y,x,-z	0.0840	0.0367	
23 [Cs]	x,-z,-y	0.2310	0.0822	24 [S4]	-z,-y,x	0.2745	0.0859	

Table S-14 MOLSYM search and CSM for (Et₄N)₃[Fe₄Se₄(SPh)₄]: SUVWUB Hauptman, R.; Schneider, J.; Chen, C.; Henkel *Acta Cryst, C55*, **1999**, 194-196

Resd	Inertial Moments			Degree Symbol		CSM	RMS	Tol	
[Fe ₄ Se ₄ (S) ₄]	2808.	3220.	2853.	2	C2	0.0000	0.0000	0.10	
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.			
1	[E]	x,y,z	0.0000	0.0000	2	[C2]	-x,-y,z	0.0000	0.0000

Resd	Inertial Moments			Degree Symbol		CSM	RMS	Tol	
[Fe ₄ Se ₄ (S) ₄]	2808.	2853.	3220.	2	D2	0.1684	0.0410	0.20	
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.			
1	[E]	x,y,z	0.0000	0.0000	2	[C2]	-x,-y,z	0.1684	0.0593
3	[C2]	-x,y,-z	0.0000	0.0000	4	[C2]	x,-y,-z	0.1684	0.0593

Resd	Inertial Moments			Degree Symbol		CSM	RMS	Tol	
[Fe ₄ Se ₄ (S) ₄]	2808.	2853.	3220.	2	D2d	0.8673	0.0931	0.30	
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.			
1	[E]	x,y,z	0.0000	0.0000	2	[S4]	y,-x,-z	0.8673	0.1291
3	[C2]	-x,-y,z	0.1684	0.0593	4	[Cs]	y,x,z	0.7830	0.1291
5	[C2]	-x,y,-z	0.0000	0.0000	6	[C2]	x,-y,-z	0.1684	0.0593
7	[S4]	-y,x,-z	0.8673	0.1291	8	[Cs]	-y,-x,z	0.7830	0.1291

Table S-14 (Cont.) for (Et₄N)₃[Fe₄Se₄(SPh)₄]: SUVWUB

Resd	Inertial Moments			Degree Symbol		CSM	RMS	Tol
[Fe ₄ Se ₄]+	1388.	1189.	1303.	1	C2	0.0000	0.0000	0.10
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C2]	-x,-y,z	0.0000	0.0000	
Resd	Inertial Moments			Degree Symbol		CSM	RMS	Tol
[Fe ₄ Se ₄]+	1726.	1663.	1551.	3	Td	2.0603	0.1435	0.60
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	1.9230	0.2491	
3 [C2]	-x,-y,z	0.5470	0.0878	4 [S4]	-x,-z,y	0.4195	0.0917	
5 [C2]	x,-y,-z	0.0346	0.0201	6 [C2]	-x,y,-z	0.5816	0.0919	
7 [C3]	z,x,y	1.9230	0.2491	8 [C3]	-y,z,-x	1.8095	0.2261	
9 [Cs]	-z,y,-x	0.7703	0.1321	10 [C3]	-y,-z,x	1.9229	0.2272	
11 [C3]	y,-z,-x	1.8096	0.2156	12 [C3]	z,-x,-y	1.9229	0.2272	
13 [S4]	y,-x,-z	2.0091	0.2213	14 [C3]	-z,x,-y	1.8096	0.2156	
15 [C3]	-z,-x,y	1.8095	0.2261	16 [Cs]	x,z,y	0.9484	0.1769	
17 [Cs]	z,y,x	0.5875	0.1087	18 [Cs]	y,x,z	1.7353	0.1946	
19 [S4]	z,-y,-x	0.9698	0.1505	20 [Cs]	-y,-x,z	1.7355	0.2141	
21 [S4]	-x,z,-y	0.4195	0.0917	22 [S4]	-y,x,-z	2.0091	0.2213	
23 [Cs]	x,-z,-y	0.9487	0.1775	24 [S4]	-z,-y,x	0.9698	0.1505	

Table S-15 M0LSYM search and CSM for (Me₄N)₃[Fe₄Se₄(SPh)₄]•2MeCN; GAPXIE; Carney, M. J.; Papaefthymiou, G. C.; Whitener, M. A.; Spartalian, K.; Frankel, R. B.; Holm, R. H. *Inorg. Chem.* **1988**, 27, 346-352.

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe ₄ Se ₄ (S) ₄]	1744.	1396.	1252.	2 C2	0.0000	0.0000	0.10
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.	
1 [E]	x,y,z	0.0000	0.0000	2 [C2]	-x,-y,z	0.0000	0.0000
Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe ₄ Se ₄ (S) ₄]	1252.	1396.	1744.	2 D2	5.4598	0.2337	0.60
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.	
1 [E]	x,y,z	0.0000	0.0000	2 [C2]	-x,-y,z	5.4598	0.2750
3 [C2]	-x,y,-z	5.4598	0.2750	4 [C2]	x,-y,-z	0.0000	0.0000
Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe ₄ Se ₄ (S) ₄]	1252.	1396.	1744.	2 S4	6.6286	0.2575	0.70
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.	
1 [E]	x,y,z	0.0000	0.0000	2 [S4]	y,-x,-z	6.6286	0.4067
3 [C2]	-x,-y,z	5.4598	0.2750	4 [S4]	-y,x,-z	6.6286	0.4067

Table S-15 (Cont.) (Me₄N)₃[Fe₄Se₄(SPh)₄]•2MeCN; GAPXIE;

Resd	Inertial Moments			Degree Symbol		CSM	RMS	Tol
[Fe ₄ Se ₄]+	1099.	1179.	1223.	1	C2	0.0000	0.0000	0.10
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C2]	-x,-y,z	0.0000	0.0000	
Resd	Inertial Moments			Degree Symbol		CSM	RMS	Tol
[Fe ₄ Se ₄]+	1688.	1651.	1573.	3	Td	0.7064	0.0840	0.30
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.6322	0.1390	
3 [C2]	-x,-y,z	0.2225	0.0525	4 [S4]	-x,-z,y	0.1689	0.0525	
5 [C2]	x,-y,-z	0.0000	0.0000	6 [C2]	-x,y,-z	0.2225	0.0525	
7 [C3]	z,x,y	0.6322	0.1390	8 [C3]	-y,z,-x	0.6322	0.1390	
9 [Cs]	-z,y,-x	0.2440	0.0665	10 [C3]	-y,-z,x	0.6322	0.1317	
11 [C3]	y,-z,-x	0.6322	0.1317	12 [C3]	z,-x,-y	0.6322	0.1317	
13 [S4]	y,-x,-z	0.6836	0.1316	14 [C3]	-z,x,-y	0.6322	0.1317	
15 [C3]	-z,-x,y	0.6322	0.1390	16 [Cs]	x,z,y	0.3173	0.0995	
17 [Cs]	z,y,x	0.2440	0.0665	18 [Cs]	y,x,z	0.5724	0.1245	
19 [S4]	z,-y,-x	0.3552	0.0821	20 [Cs]	-y,-x,z	0.5724	0.1245	
21 [S4]	-x,z,-y	0.1689	0.0525	22 [S4]	-y,x,-z	0.6836	0.1316	
23 [Cs]	x,-z,-y	0.3173	0.0995	24 [S4]	-z,-y,x	0.3552	0.0821	

Table S-16 MOLSYM search and CSM for (Bu₄N)₃[Fe₄S₄(CN)₄]: JAHXEW Scott, T. A; Zhou; H.-C. *Angew. Chem. Intl. Ed.* **2004**, 43, 5628-5631.

Resd	Inertial Moments			Degree	Symbol	CSM	RMS	Tol	
[Fe ₄ S ₄ (CN) ₄] ³⁻	2162.	2162.	2061.	3	T23	2.8592	0.1691	1.00	
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.			
1	[E]	x,y,z	0.0000	0.0000	2	[C3]	y,z,x	2.1839	0.3134
3	[C2]	-x,-y,z	1.7821	0.3138	4	[C3]	z,x,y	2.1839	0.3134
5	[C3]	-y,z,-x	2.5967	0.3412	6	[C3]	z,-x,-y	0.2308	0.0851
7	[C3]	-y,-z,x	0.2308	0.0851	8	[C3]	-z,x,-y	2.6132	0.4071
9	[C2]	x,-y,-z	1.8346	0.2396	10	[C3]	-z,-x,y	2.5967	0.3412
11	[C2]	-x,y,-z	2.1008	0.3215	12	[C3]	y,-z,-x	2.6132	0.4071
Resd	Inertial Moments			Degree	Symbol	CSM	RMS	Tol	
[Fe ₄ S ₄ C ₄]	1277.	1277.	1245.	3	T23	0.8345	0.0914	0.40	
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.			
1	[E]	x,y,z	0.0000	0.0000	2	[C3]	y,z,x	0.6711	0.1618
3	[C2]	-x,-y,z	0.5211	0.1599	4	[C3]	z,x,y	0.6711	0.1618
5	[C3]	-y,z,-x	0.7527	0.1715	6	[C3]	z,-x,-y	0.0459	0.0364
7	[C3]	-y,-z,x	0.0459	0.0364	8	[C3]	-z,x,-y	0.7558	0.2067
9	[C2]	x,-y,-z	0.5500	0.1295	10	[C3]	-z,-x,y	0.7527	0.1715
11	[C2]	-x,y,-z	0.5979	0.1646	12	[C3]	y,-z,-x	0.7558	0.2067

Table S-16 (Cont.) for $(\text{Bu}_4\text{N})_3[\text{Fe}_4\text{S}_4(\text{CN})_4]$: JAHXEW

Resd	Inertial Moments			Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄ C ₄]	1277.	1277.	1245.	3	Td	0.8345	0.0914	0.60
Symmetry element	CSM and Max.Diff.			Symmetry element	CSM and Max.Diff.			
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x		0.6711	0.1618
3 [C2]	-x,-y,z	0.5211	0.1599	4 [S4]	-x,-z,y		0.7660	0.1950
5 [C2]	x,-y,-z	0.5500	0.1295	6 [C2]	-x,y,-z		0.5979	0.1646
7 [C3]	z,x,y	0.6711	0.1618	8 [C3]	-y,z,-x		0.7527	0.1715
9 [Cs]	-z,y,-x	0.4527	0.1548	10 [C3]	-y,-z,x		0.0459	0.0364
11 [C3]	y,-z,-x	0.7558	0.2067	12 [C3]	z,-x,-y		0.0459	0.0364
13 [S4]	y,-x,-z	0.7340	0.1999	14 [C3]	-z,x,-y		0.7558	0.2067
15 [C3]	-z,-x,y	0.7527	0.1715	16 [Cs]	x,z,y		0.5379	0.1605
17 [Cs]	z,y,x	0.1885	0.0877	18 [Cs]	y,x,z		0.5564	0.2051
19 [S4]	z,-y,-x	0.8128	0.2164	20 [Cs]	-y,-x,z		0.1658	0.0848
21 [S4]	-x,z,-y	0.7660	0.1950	22 [S4]	-y,x,-z		0.7340	0.1999
23 [Cs]	x,-z,-y	0.1490	0.0797	24 [S4]	-z,-y,x		0.8128	0.2164
Resd	Inertial Moments			Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄] ⁺	834.	834.	827.	3	Td	0.0213	0.0146	0.10
Symmetry element	CSM and Max.Diff.			Symmetry element	CSM and Max.Diff.			
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x		0.0140	0.0226
3 [C2]	-x,-y,z	0.0126	0.0168	4 [S4]	-x,-z,y		0.0208	0.0260
5 [C2]	x,-y,-z	0.0162	0.0199	6 [C2]	-x,y,-z		0.0139	0.0165
7 [C3]	z,x,y	0.0140	0.0226	8 [C3]	-y,z,-x		0.0166	0.0230
9 [Cs]	-z,y,-x	0.0131	0.0174	10 [C3]	-y,-z,x		0.0065	0.0112
11 [C3]	y,-z,-x	0.0197	0.0228	12 [C3]	z,-x,-y		0.0065	0.0112
13 [S4]	y,-x,-z	0.0173	0.0253	14 [C3]	-z,x,-y		0.0197	0.0228
15 [C3]	-z,-x,y	0.0166	0.0230	16 [Cs]	x,z,y		0.0162	0.0199
17 [Cs]	z,y,x	0.0063	0.0108	18 [Cs]	y,x,z		0.0157	0.0170
19 [S4]	z,-y,-x	0.0185	0.0249	20 [Cs]	-y,-x,z		0.0050	0.0090
21 [S4]	-x,z,-y	0.0208	0.0260	22 [S4]	-y,x,-z		0.0173	0.0253
23 [Cs]	x,-z,-y	0.0009	0.0048	24 [S4]	-z,-y,x		0.0185	0.0249

Table S17 M0LSYM search and CSM for VAMJOI; (Et4N)3[Fe4S4(S-o-C6H4S-t-Bu)4]
M.J.Carney, G.C.Papaefthymiou, R.B.Frankel, R.H.Holm (1989) Inorg.Chem. 28:1497-1503

:: Resd [Fe₄S₄(S)₄], No Molecular Symmetry Within Tolerance = 1.00 Ang.

Resd	Inertial Moments			Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄]+	856.	835.	833.	3	Td	0.2946	0.0543	0.20
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.2764	0.0790	
3 [C2]	-x,-y,z	0.0196	0.0225	4 [S4]	-x,-z,y	0.1780	0.0657	
5 [C2]	x,-y,-z	0.0119	0.0153	6 [C2]	-x,y,-z	0.0156	0.0194	
7 [C3]	z,x,y	0.2764	0.0790	8 [C3]	-y,z,-x	0.2929	0.0801	
9 [Cs]	-z,y,-x	0.2500	0.0717	10 [C3]	-y,-z,x	0.2932	0.0821	
11 [C3]	y,-z,-x	0.2846	0.0775	12 [C3]	z,-x,-y	0.2932	0.0821	
13 [S4]	y,-x,-z	0.0337	0.0296	14 [C3]	-z,x,-y	0.2846	0.0775	
15 [C3]	-z,-x,y	0.2929	0.0801	16 [Cs]	x,z,y	0.1651	0.0632	
17 [Cs]	z,y,x	0.2456	0.0727	18 [Cs]	y,x,z	0.0157	0.0149	
19 [S4]	z,-y,-x	0.2600	0.0809	20 [Cs]	-y,-x,z	0.0244	0.0250	
21 [S4]	-x,z,-y	0.1780	0.0657	22 [S4]	-y,x,-z	0.0337	0.0296	
23 [Cs]	x,-z,-y	0.1706	0.0613	24 [S4]	-z,-y,x	0.2600	0.0809	

Table S18 MOLSYM search and CSM for RAPSEG; (Et₄N)₃[Fe₄S₄(SBzl)₄] Gloux, J.; Gloux, P.; Laugier, J. *J. Am. Chem. Soc.* **1996**, *118*, 11644-11653.

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄ (S) ₄]	2282.	2172.	2154.	3	Td	1.5161	0.1231 0.60
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	1.1034	0.2665
3 [C2]	-x,-y,z	0.7840	0.1615	4 [S4]	-x,-z,y	1.2660	0.2332
5 [C2]	x,-y,-z	0.0943	0.0647	6 [C2]	-x,y,-z	0.8402	0.1787
7 [C3]	z,x,y	1.1034	0.2665	8 [C3]	-y,z,-x	1.3737	0.2505
9 [Cs]	-z,y,-x	0.5647	0.1532	10 [C3]	-y,-z,x	1.1254	0.2420
11 [C3]	y,-z,-x	1.3163	0.2665	12 [C3]	z,-x,-y	1.1254	0.2420
13 [S4]	y,-x,-z	1.3519	0.2742	14 [C3]	-z,x,-y	1.3163	0.2665
15 [C3]	-z,-x,y	1.3737	0.2505	16 [Cs]	x,z,y	0.5151	0.1449
17 [Cs]	z,y,x	0.3118	0.1091	18 [Cs]	y,x,z	0.8960	0.2665
19 [S4]	z,-y,-x	0.8490	0.1807	20 [Cs]	-y,-x,z	1.0199	0.2394
21 [S4]	-x,z,-y	1.2660	0.2332	22 [S4]	-y,x,-z	1.3519	0.2742
23 [Cs]	x,-z,-y	0.5733	0.1502	24 [S4]	-z,-y,x	0.8490	0.1807
Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄] ⁺	853.	851.	842.	3	Td	0.0991	0.0315 0.20
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	0.0945	0.0485
3 [C2]	-x,-y,z	0.0144	0.0162	4 [S4]	-x,-z,y	0.0227	0.0264
5 [C2]	x,-y,-z	0.0171	0.0206	6 [C2]	-x,y,-z	0.0103	0.0125
7 [C3]	z,x,y	0.0945	0.0485	8 [C3]	-y,z,-x	0.0945	0.0479
9 [Cs]	-z,y,-x	0.0772	0.0421	10 [C3]	-y,-z,x	0.0919	0.0502
11 [C3]	y,-z,-x	0.0876	0.0402	12 [C3]	z,-x,-y	0.0919	0.0502
13 [S4]	y,-x,-z	0.0620	0.0381	14 [C3]	-z,x,-y	0.0876	0.0402
15 [C3]	-z,-x,y	0.0945	0.0479	16 [Cs]	x,z,y	0.0169	0.0193
17 [Cs]	z,y,x	0.0769	0.0415	18 [Cs]	y,x,z	0.0508	0.0369
19 [S4]	z,-y,-x	0.0880	0.0465	20 [Cs]	-y,-x,z	0.0606	0.0452
21 [S4]	-x,z,-y	0.0227	0.0264	22 [S4]	-y,x,-z	0.0620	0.0381
23 [Cs]	x,-z,-y	0.0085	0.0146	24 [S4]	-z,-y,x	0.0880	0.0465

Table S19 M0LSYM search and CSM for PSFEEA; $(\text{Et}_3\text{MeN})_3[\text{Fe}_4\text{S}_4(\text{SPh})_4]$ Laskowski, E. J.; Frankel, R. B.; Gillum, W. O.; Papaefthymiou, G. C.; Renaud, J.; Ibers, J. A.; Holm, R. H. *J. Am. Chem. Soc.* **1978**, *100*, 5322-5337.

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4(SPh)4]-A	2072.	2112. 2363.	2	D2d	14.5414	0.3813	0.90
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E] x,y,z	0.0000 0.0000		2 [S4] y,-x,-z		14.4844 0.5474		
3 [C2] -x,y,-z	0.6255 0.1749		4 [C2] -x,-y,z		14.2888 0.4955		
5 [Cs] y,x,z	8.1112 0.4379		6 [S4] -y,x,-z		14.4844 0.5474		
7 [C2] x,-y,-z	14.0973 0.5030		8 [Cs] -y,-x,z		6.3320 0.3250		
Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4(SPh)4]-B	2081.	2118. 2363.	2	D2d	0.6330	0.0796	0.30
Symmetry element	CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.		
1 [E] x,y,z	0.0000 0.0000		2 [S4] y,-x,-z		0.5573 0.1538		
3 [C2] -x,-y,z	0.4603 0.1058		4 [Cs] y,x,z		0.1156 0.0825		
5 [C2] -x,y,-z	0.4480 0.1270		6 [C2] x,-y,-z		0.3190 0.1012		
7 [S4] -y,x,-z	0.5573 0.1538		8 [Cs] -y,-x,z		0.5347 0.1270		

Table S19 MOLSYM search and CSM for PSFEEA; (Et₃MeN)₃[Fe₄S₄(SPh)₄] (Cont.)

Resd	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄]-A	862.	854.	831.	3	Td	0.1841	0.0429 0.20
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.	
1 [E]	x,y,z	0.0000 0.0000	2 [C ₃]	y,z,x	0.1785	0.0671	
3 [C ₂]	-x,-y,z	0.0146 0.0160	4 [S ₄]	-x,-z,y	0.1059	0.0484	
5 [C ₂]	x,-y,-z	0.0034 0.0082	6 [C ₂]	-x,y,-z	0.0139	0.0130	
7 [C ₃]	z,x,y	0.1785 0.0671	8 [C ₃]	-y,z,-x	0.1786	0.0686	
9 [C _s]	-z,y,-x	0.0121 0.0184	10 [C ₃]	-y,-z,x	0.1810	0.0639	
11 [C ₃]	y,-z,-x	0.1771 0.0706	12 [C ₃]	z,-x,-y	0.1810	0.0639	
13 [S ₄]	y,-x,-z	0.1633 0.0643	14 [C ₃]	-z,x,-y	0.1771	0.0706	
15 [C ₃]	-z,-x,y	0.1786 0.0686	16 [C _s]	x,z,y	0.1072	0.0561	
17 [C _s]	z,y,x	0.0155 0.0152	18 [C _s]	y,x,z	0.1559	0.0620	
19 [S ₄]	z,-y,-x	0.0223 0.0216	20 [C _s]	-y,-x,z	0.1562	0.0545	
21 [S ₄]	-x,z,-y	0.1059 0.0484	22 [S ₄]	-y,x,-z	0.1633	0.0643	
23 [C _s]	x,-z,-y	0.1065 0.0602	24 [S ₄]	-z,-y,x	0.0223	0.0216	
Resd #	Inertial	Moments	Degree	Symbol	CSM	RMS	Tol
[Fe ₄ S ₄]-B	860.	855.	834.	3	Td	0.1028	0.0321 0.10
Symmetry element		CSM and Max.Diff.		Symmetry element		CSM and Max.Diff.	
1 [E]	x,y,z	0.0000 0.0000	2 [C ₃]	y,z,x	0.0965	0.0535	
3 [C ₂]	-x,-y,z	0.0218 0.0176	4 [S ₄]	-x,-z,y	0.0624	0.0372	
5 [C ₂]	x,-y,-z	0.0075 0.0119	6 [C ₂]	-x,y,-z	0.0221	0.0195	
7 [C ₃]	z,x,y	0.0965 0.0535	8 [C ₃]	-y,z,-x	0.0923	0.0479	
9 [C _s]	-z,y,-x	0.0176 0.0198	10 [C ₃]	-y,-z,x	0.1008	0.0555	
11 [C ₃]	y,-z,-x	0.0872 0.0420	12 [C ₃]	z,-x,-y	0.1008	0.0555	
13 [S ₄]	y,-x,-z	0.0850 0.0431	14 [C ₃]	-z,x,-y	0.0872	0.0420	
15 [C ₃]	-z,-x,y	0.0923 0.0479	16 [C _s]	x,z,y	0.0691	0.0439	
17 [C _s]	z,y,x	0.0100 0.0157	18 [C _s]	y,x,z	0.0827	0.0420	
19 [S ₄]	z,-y,-x	0.0249 0.0201	20 [C _s]	-y,-x,z	0.0685	0.0457	
21 [S ₄]	-x,z,-y	0.0624 0.0372	22 [S ₄]	-y,x,-z	0.0850	0.0431	
23 [C _s]	x,-z,-y	0.0754 0.0502	24 [S ₄]	-z,-y,x	0.0249	0.0201	

Table S16 MOLSYM search and CSM for K1190 (Et₄N)₃[Fe₄S₄(OPh)₄] Hagen, K. S. *unpublished results*

Resd	Inertial Moments			Degree	Symbol	CSM	RMS	Tol
Fe4S404	677.	668.	572.	2	D2d	0.1065	0.0326	0.10
	Symmetry element	CSM and Max.Diff.			Symmetry element		CSM and Max.Diff.	
1 [E]	x,y,z	0.0000	0.0000	2 [S4]	y,-x,-z	0.0987	0.0414	
3 [C2]	-x,-y,z	0.0000	0.0000	4 [C2]	-x,y,-z	0.0178	0.0200	
5 [C2]	x,-y,-z	0.0178	0.0200	6 [S4]	-y,x,-z	0.0987	0.0414	
7 [Cs]	y,x,z	0.0965	0.0523	8 [Cs]	-y,-x,z	0.0965	0.0523	
Fe4S404	1446.	1439.	1351.	3	Td	3.9624	0.1991	0.70
	Symmetry element	CSM and Max.Diff.			Symmetry element		CSM and Max.Diff.	
1 [E]	x,y,z	0.0000	0.0000	2 [C3]	y,z,x	3.8364	0.3821	
3 [C2]	-x,-y,z	0.3870	0.0895	4 [S4]	-x,-z,y	3.0365	0.2909	
5 [C2]	x,-y,-z	0.0160	0.0171	6 [C2]	-x,y,-z	0.3710	0.0842	
7 [C3]	z,x,y	3.8364	0.3821	8 [C3]	-y,z,-x	3.8306	0.3885	
9 [Cs]	-z,y,-x	0.2815	0.0798	10 [C3]	-y,-z,x	3.8307	0.3804	
11 [C3]	y,-z,-x	3.8368	0.3985	12 [C3]	z,-x,-y	3.8307	0.3804	
13 [S4]	y,-x,-z	2.6397	0.3133	14 [C3]	-z,x,-y	3.8368	0.3985	
15 [C3]	-z,-x,y	3.8306	0.3885	16 [Cs]	x,z,y	3.3971	0.3692	
17 [Cs]	z,y,x	0.2816	0.0834	18 [Cs]	y,x,z	2.4377	0.3045	
19 [S4]	z,-y,-x	0.4691	0.1115	20 [Cs]	-y,-x,z	2.4544	0.2794	
21 [S4]	-x,z,-y	3.0365	0.2909	22 [S4]	-y,x,-z	2.6397	0.3133	
23 [Cs]	x,-z,-y	3.3973	0.3747	24 [S4]	-z,-y,x	0.4691	0.1115	

Table S16 (Cont.) K1190_(Et4N)3[Fe4S4(OPh)4]

Resd	Inertial		Moments	Degree	Symbol	CSM	RMS	Tol
[Fe4S4]+	575.	560.	538.	3	Td	0.5128	0.0716	0.20
Symmetry	element	CSM and Max.Diff.		Symmetry		element	CSM and Max.Diff.	

1	[E]	x,y,z	0.0000	0.0000				
2	[C3]	y,z,x	0.4976	0.1092				
3	[C2]	-x,-y,z	0.0454	0.0217				
4	[S4]	-x,-z,y	0.1091	0.0418				
5	[C2]	x,-y,-z	0.0000	0.0000				
6	[C2]	-x,y,-z	0.0454	0.0217				
7	[C3]	z,x,y	0.4976	0.1092				
8	[C3]	-y,z,-x	0.4976	0.1092				
9	[Cs]	-z,y,-x	0.1719	0.0551				
10	[C3]	-y,-z,x	0.4976	0.1065				
11	[C3]	y,-z,-x	0.4976	0.1065				
12	[C3]	z,-x,-y	0.4976	0.1065				
13	[S4]	y,-x,-z	0.5099	0.1093				
14	[C3]	-z,x,-y	0.4976	0.1065				
15	[C3]	-z,-x,y	0.4976	0.1092				
16	[Cs]	x,z,y	0.1109	0.0541				
17	[Cs]	z,y,x	0.1719	0.0551				
18	[Cs]	y,x,z	0.4872	0.1092				
19	[S4]	z,-y,-x	0.1946	0.0589				
20	[Cs]	-y,-x,z	0.4872	0.1092				
21	[S4]	-x,z,-y	0.1091	0.0418				
22	[S4]	-y,x,-z	0.5099	0.1093				
23	[Cs]	x,-z,-y	0.1109	0.0541				
24	[S4]	-z,-y,x	0.1946	0.0589				