

Molecular mechanics results

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FeCl3 bis tetraethyl malonamide

REMARK This PDB file was created by CS Chem3D.

HETATM	1	N	1	0.438	-2.610	0.325	N
HETATM	2	O	1	0.078	-0.456	-0.153	O
HETATM	3	O	1	-2.895	0.114	-1.067	O
HETATM	4	C	1	-5.339	-1.008	-1.543	C
HETATM	5	N	1	-4.108	-1.768	-1.293	N
HETATM	6	C	1	-2.919	-1.116	-0.981	C
HETATM	7	C	1	-0.395	-1.588	-0.115	C
HETATM	8	C	1	-1.788	-2.044	-0.536	C
HETATM	9	C	1	1.821	-2.329	0.731	C
HETATM	10	C	1	0.072	-4.033	0.379	C
HETATM	11	C	1	2.743	-2.041	-0.464	C
HETATM	12	C	1	0.472	-4.781	-0.900	C
HETATM	13	C	1	-4.261	-3.226	-1.420	C
HETATM	14	C	1	-4.674	-3.936	-0.124	C
HETATM	15	C	1	-6.044	-0.638	-0.231	C
HETATM	16	Fe	1	-1.200	0.762	-0.678	FE
HETATM	17	O	1	-1.942	0.203	0.926	O
HETATM	18	O	1	-1.909	2.280	-1.442	O
HETATM	19	Cl	1	-0.396	2.124	0.846	CL
HETATM	20	Cl	1	0.604	1.652	-1.579	CL
HETATM	21	Cl	1	-1.051	-0.113	-2.687	CL
HETATM	22	C	1	-2.932	2.619	-0.854	C
HETATM	23	C	1	-2.807	0.999	1.303	C
HETATM	24	C	1	-3.391	2.187	0.536	C
HETATM	25	N	1	-3.358	0.806	2.562	N
HETATM	26	N	1	-3.742	3.565	-1.466	N
HETATM	27	C	1	-4.984	4.105	-0.903	C
HETATM	28	C	1	-3.406	4.110	-2.784	C
HETATM	29	C	1	-2.992	-0.351	3.383	C
HETATM	30	C	1	-4.316	1.707	3.211	C
HETATM	31	C	1	-3.590	2.783	4.031	C
HETATM	32	C	1	-6.202	3.299	-1.373	C
HETATM	33	C	1	-2.355	5.221	-2.665	C
HETATM	34	C	1	-3.868	-1.554	3.012	C
HETATM	35	H	1	-2.214	-2.553	0.356	H
HETATM	36	H	1	-1.598	-2.757	-1.369	H
HETATM	37	H	1	-5.118	-0.085	-2.129	H
HETATM	38	H	1	-6.055	-1.573	-2.182	H
HETATM	39	H	1	1.838	-1.470	1.442	H
HETATM	40	H	1	2.259	-3.179	1.303	H
HETATM	41	H	1	0.556	-4.529	1.252	H
HETATM	42	H	1	-1.008	-4.193	0.583	H
HETATM	43	H	1	3.787	-1.858	-0.119	H
HETATM	44	H	1	2.774	-2.895	-1.175	H
HETATM	45	H	1	2.431	-1.142	-1.039	H
HETATM	46	H	1	0.093	-5.829	-0.883	H
HETATM	47	H	1	0.064	-4.290	-1.811	H
HETATM	48	H	1	1.578	-4.838	-1.009	H

HETATM	49	H	1	-5.026	-3.465	-2.195	H	
HETATM	50	H	1	-3.350	-3.702	-1.841	H	
HETATM	51	H	1	-4.764	-5.034	-0.292	H	
HETATM	52	H	1	-3.937	-3.799	0.695	H	
HETATM	53	H	1	-5.662	-3.585	0.244	H	
HETATM	54	H	1	-6.916	0.029	-0.418	H	
HETATM	55	H	1	-6.433	-1.535	0.299	H	
HETATM	56	H	1	-5.360	-0.116	0.472	H	
HETATM	57	H	1	-3.250	3.090	1.174	H	
HETATM	58	H	1	-4.471	1.940	0.431	H	
HETATM	59	H	1	-4.955	4.168	0.207	H	
HETATM	60	H	1	-5.112	5.168	-1.216	H	
HETATM	61	H	1	-3.049	3.304	-3.466	H	
HETATM	62	H	1	-4.310	4.522	-3.291	H	
HETATM	63	H	1	-1.913	-0.605	3.267	H	
HETATM	64	H	1	-3.112	-0.130	4.469	H	
HETATM	65	H	1	-5.023	2.173	2.491	H	
HETATM	66	H	1	-4.985	1.129	3.890	H	
HETATM	67	H	1	-4.319	3.469	4.521	H	
HETATM	68	H	1	-2.965	2.328	4.833	H	
HETATM	69	H	1	-2.918	3.404	3.398	H	
HETATM	70	H	1	-7.142	3.701	-0.929	H	
HETATM	71	H	1	-6.311	3.333	-2.481	H	
HETATM	72	H	1	-6.124	2.229	-1.082	H	
HETATM	73	H	1	-2.115	5.651	-3.665	H	
HETATM	74	H	1	-2.721	6.050	-2.018	H	
HETATM	75	H	1	-1.403	4.844	-2.228	H	
HETATM	76	H	1	-3.574	-2.461	3.589	H	
HETATM	77	H	1	-4.943	-1.352	3.218	H	
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CONECT 73 33
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END

FeCl3 bis dimethyldipropyl malonamide

REMARK This PDB file was created by CS Chem3D.

HETATM	1	C	1	-1.599	-2.382	-0.440	C
HETATM	2	C	1	-0.172	-2.062	0.007	C
HETATM	3	C	1	-2.516	-1.381	-1.142	C
HETATM	4	N	1	-3.767	-1.877	-1.481	N
HETATM	5	C	1	-4.709	-1.047	-2.232	C
HETATM	6	O	1	-2.285	-0.208	-1.439	O
HETATM	7	O	1	0.518	-1.100	-0.319	O
HETATM	8	N	1	0.395	-3.030	0.822	N
HETATM	9	C	1	-0.299	-4.241	1.260	C
HETATM	10	C	1	1.771	-2.919	1.313	C
HETATM	11	C	1	2.756	-3.726	0.449	C
HETATM	12	C	1	-4.313	-3.177	-1.076	C
HETATM	13	C	1	-5.400	-3.030	0.006	C
HETATM	14	Fe	1	-0.530	0.233	-1.037	FE
HETATM	15	O	1	-1.379	0.022	0.597	O
HETATM	16	O	1	-0.998	1.705	-2.041	O
HETATM	17	Cl	1	0.408	1.687	0.316	CL
HETATM	18	Cl	1	1.413	0.715	-1.955	CL
HETATM	19	Cl	1	-0.441	-0.968	-2.874	CL
HETATM	20	C	1	-1.953	2.289	-1.532	C
HETATM	21	C	1	-2.170	0.943	0.796	C
HETATM	22	C	1	-2.573	2.072	-0.152	C
HETATM	23	N	1	-2.812	0.978	2.025	N
HETATM	24	N	1	-2.540	3.301	-2.279	N
HETATM	25	C	1	-2.084	3.560	-3.646	C
HETATM	26	C	1	-3.598	4.202	-1.806	C
HETATM	27	C	1	-2.516	-0.018	3.060	C
HETATM	28	C	1	-3.800	1.989	2.401	C
HETATM	29	C	1	-3.056	5.430	-1.052	C
HETATM	30	C	1	-1.189	0.265	3.785	C
HETATM	31	C	1	-2.165	6.340	-1.907	C
HETATM	32	C	1	-1.149	1.651	4.441	C
HETATM	33	C	1	-4.897	-2.340	1.280	C
HETATM	34	C	1	2.840	-3.232	-1.000	C
HETATM	35	H	1	-2.151	-2.664	0.486	H
HETATM	36	H	1	-1.493	-3.253	-1.130	H
HETATM	37	H	1	-4.235	-0.663	-3.164	H
HETATM	38	H	1	-5.618	-1.603	-2.550	H
HETATM	39	H	1	-5.038	-0.184	-1.609	H
HETATM	40	H	1	-1.109	-3.987	1.981	H
HETATM	41	H	1	-0.717	-4.803	0.396	H
HETATM	42	H	1	0.378	-4.953	1.782	H
HETATM	43	H	1	2.107	-1.860	1.378	H
HETATM	44	H	1	1.822	-3.277	2.369	H
HETATM	45	H	1	3.773	-3.663	0.908	H
HETATM	46	H	1	2.469	-4.804	0.452	H
HETATM	47	H	1	-4.748	-3.681	-1.971	H
HETATM	48	H	1	-3.545	-3.894	-0.720	H

HETATM	49	H	1	-5.790	-4.042	0.272				H
HETATM	50	H	1	-6.267	-2.455	-0.396				H
HETATM	51	H	1	-2.396	3.023	0.398				H
HETATM	52	H	1	-3.662	1.901	-0.319				H
HETATM	53	H	1	-2.286	2.671	-4.287				H
HETATM	54	H	1	-2.589	4.427	-4.124				H
HETATM	55	H	1	-0.992	3.776	-3.662				H
HETATM	56	H	1	-4.216	4.558	-2.662				H
HETATM	57	H	1	-4.343	3.669	-1.178				H
HETATM	58	H	1	-3.336	-0.083	3.811				H
HETATM	59	H	1	-2.482	-1.038	2.611				H
HETATM	60	H	1	-4.690	1.934	1.735				H
HETATM	61	H	1	-4.178	1.862	3.439				H
HETATM	62	H	1	-3.364	3.012	2.368				H
HETATM	63	H	1	-3.922	6.031	-0.682				H
HETATM	64	H	1	-2.484	5.116	-0.149				H
HETATM	65	H	1	-1.034	-0.513	4.572				H
HETATM	66	H	1	-0.331	0.171	3.079				H
HETATM	67	H	1	-1.868	7.252	-1.340				H
HETATM	68	H	1	-1.227	5.823	-2.209				H
HETATM	69	H	1	-2.695	6.675	-2.827				H
HETATM	70	H	1	-0.205	1.792	5.016				H
HETATM	71	H	1	-1.196	2.461	3.679				H
HETATM	72	H	1	-2.000	1.786	5.147				H
HETATM	73	H	1	-5.713	-2.245	2.033				H
HETATM	74	H	1	-4.525	-1.313	1.065				H
HETATM	75	H	1	-4.074	-2.921	1.755				H
HETATM	76	H	1	3.602	-3.808	-1.574				H
HETATM	77	H	1	1.868	-3.353	-1.530				H
HETATM	78	H	1	3.130	-2.157	-1.043				H
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CONECT 73 33
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CONECT 77 34
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END

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HETATM	1	N	1	0.640	-2.346	-0.548	N
HETATM	2	O	1	-0.561	-0.480	0.012	O
HETATM	3	O	1	-1.180	0.000	2.319	O
HETATM	4	C	1	-1.397	-0.613	5.045	C
HETATM	5	N	1	-0.577	-1.333	4.067	N
HETATM	6	C	1	-0.521	-0.947	2.739	C
HETATM	7	C	1	0.109	-1.451	0.365	C
HETATM	8	C	1	0.292	-1.850	1.823	C
HETATM	9	C	1	1.602	-3.398	-0.204	C
HETATM	10	C	1	0.324	-2.276	-1.973	C
HETATM	11	C	1	3.031	-2.840	-0.229	C
HETATM	12	C	1	-1.047	-2.910	-2.236	C
HETATM	13	C	1	0.152	-2.472	4.632	C
HETATM	14	C	1	-0.697	-3.751	4.629	C
HETATM	15	C	1	-0.593	0.479	5.762	C
HETATM	16	O	1	1.482	0.730	-0.119	O
HETATM	17	O	1	-1.532	1.941	0.009	O
HETATM	18	Cl	1	1.676	0.987	2.663	Cl
HETATM	19	Cl	1	-1.100	2.581	2.635	Cl
HETATM	20	Cl	1	0.903	3.240	0.675	Cl
HETATM	21	C	1	-1.389	1.656	-1.175	C
HETATM	22	C	1	1.277	1.190	-1.246	C
HETATM	23	C	1	-0.053	1.578	-1.922	C
HETATM	24	N	1	2.386	1.326	-2.075	N
HETATM	25	N	1	-2.520	1.522	-1.964	N
HETATM	26	C	1	-3.858	1.506	-1.367	C
HETATM	27	C	1	-2.525	1.456	-3.429	C
HETATM	28	C	1	2.350	1.873	-3.438	C
HETATM	29	C	1	3.732	0.973	-1.604	C
HETATM	30	C	1	4.316	2.001	-0.623	C
HETATM	31	C	1	-4.359	2.928	-1.082	C
HETATM	32	C	1	-2.542	0.012	-3.945	C
HETATM	33	C	1	2.584	3.390	-3.453	C
HETATM	34	H	1	-0.136	-2.872	1.932	H
HETATM	35	H	1	1.372	-1.831	2.090	H
HETATM	36	H	1	-2.300	-0.171	4.565	H
HETATM	37	H	1	-1.802	-1.319	5.807	H
HETATM	38	H	1	1.389	-3.869	0.779	H
HETATM	39	H	1	1.526	-4.249	-0.921	H
HETATM	40	H	1	0.353	-1.227	-2.333	H
HETATM	41	H	1	1.093	-2.798	-2.588	H
HETATM	42	H	1	3.772	-3.626	0.043	H
HETATM	43	H	1	3.296	-2.464	-1.243	H
HETATM	44	H	1	3.152	-1.998	0.489	H
HETATM	45	H	1	-1.282	-2.925	-3.325	H
HETATM	46	H	1	-1.075	-3.963	-1.873	H
HETATM	47	H	1	-1.859	-2.349	-1.719	H
HETATM	48	H	1	1.119	-2.645	4.111	H
HETATM	49	H	1	0.452	-2.250	5.683	H
HETATM	50	H	1	-0.122	-4.609	5.049	H

AuCl3 bis tetraethyl malonamide

HETATM	51	H	1	-1.617	-3.634	5.245	H
HETATM	52	H	1	-1.020	-4.038	3.604	H
HETATM	53	H	1	-1.230	1.027	6.494	H
HETATM	54	H	1	0.271	0.054	6.322	H
HETATM	55	H	1	-0.189	1.228	5.046	H
HETATM	56	H	1	0.059	2.597	-2.361	H
HETATM	57	H	1	-0.167	0.822	-2.728	H
HETATM	58	H	1	-4.585	0.992	-2.037	H
HETATM	59	H	1	-3.859	0.896	-0.433	H
HETATM	60	H	1	-3.429	1.980	-3.822	H
HETATM	61	H	1	-1.684	2.032	-3.874	H
HETATM	62	H	1	3.121	1.386	-4.079	H
HETATM	63	H	1	1.407	1.622	-3.969	H
HETATM	64	H	1	3.713	-0.034	-1.129	H
HETATM	65	H	1	4.445	0.868	-2.454	H
HETATM	66	H	1	5.359	1.727	-0.343	H
HETATM	67	H	1	4.346	3.021	-1.065	H
HETATM	68	H	1	3.738	2.064	0.324	H
HETATM	69	H	1	-5.385	2.907	-0.647	H
HETATM	70	H	1	-3.702	3.462	-0.359	H
HETATM	71	H	1	-4.400	3.535	-2.015	H
HETATM	72	H	1	-2.618	-0.012	-5.057	H
HETATM	73	H	1	-1.614	-0.532	-3.671	H
HETATM	74	H	1	-3.403	-0.561	-3.535	H
HETATM	75	H	1	2.436	3.804	-4.477	H
HETATM	76	H	1	1.888	3.924	-2.769	H
HETATM	77	H	1	3.623	3.643	-3.145	H
HETATM	78	Au	1	-0.060	1.139	1.099	AU
CONNECT	1	7	9	10			
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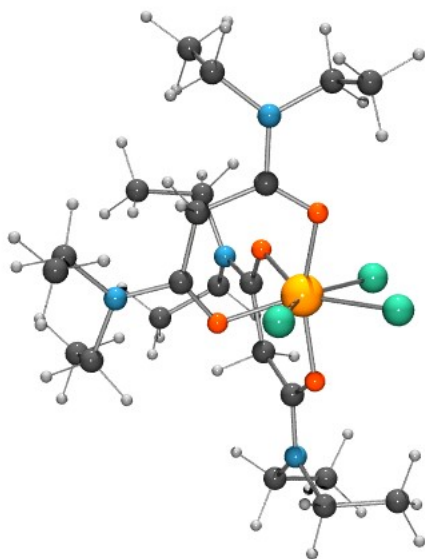
REMARK This PDB file was created by CS Chem3D.

HETATM	1	C	1	-1.575	-2.576	-0.470	C
HETATM	2	C	1	-0.044	-2.648	-0.398	C
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HETATM	5	C	1	-4.688	-0.363	-0.707	C
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HETATM	12	C	1	-4.454	-2.802	-0.595	C
HETATM	13	C	1	-5.217	-3.032	0.723	C
HETATM	14	Au	1	-0.086	0.053	-0.365	AU
HETATM	15	O	1	0.386	1.551	0.892	O
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HETATM	18	Cl	1	2.134	0.544	-0.931	CL
HETATM	19	Cl	1	-0.336	-0.650	-2.590	CL
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HETATM	21	C	1	-0.637	2.102	1.300	C
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HETATM	23	N	1	-0.754	2.469	2.630	N
HETATM	24	N	1	-2.428	2.667	-1.982	N
HETATM	25	C	1	-2.251	2.407	-3.409	C
HETATM	26	C	1	-3.663	3.384	-1.652	C
HETATM	27	C	1	-1.956	3.047	3.242	C
HETATM	28	C	1	0.343	2.238	3.569	C
HETATM	29	C	1	-3.625	4.861	-2.087	C
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HETATM	31	C	1	-2.534	5.676	-1.382	C
HETATM	32	C	1	-3.490	0.984	3.171	C
HETATM	33	C	1	-4.308	-3.034	1.960	C
HETATM	34	C	1	2.307	-3.547	-2.701	C
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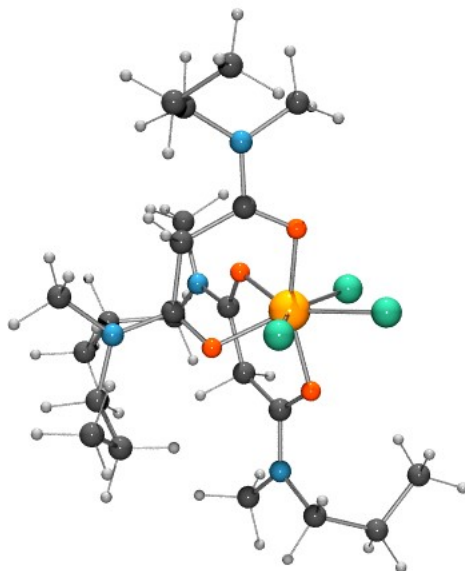
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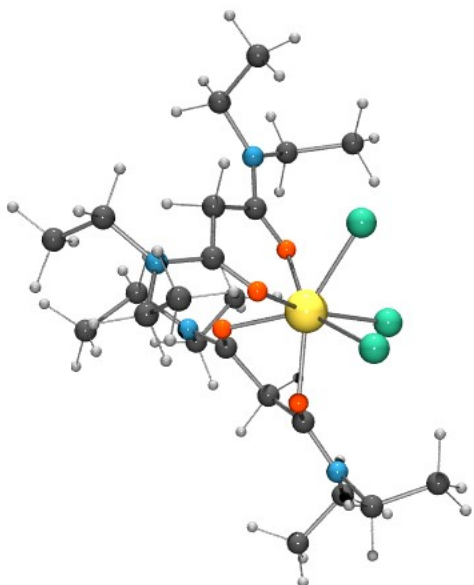
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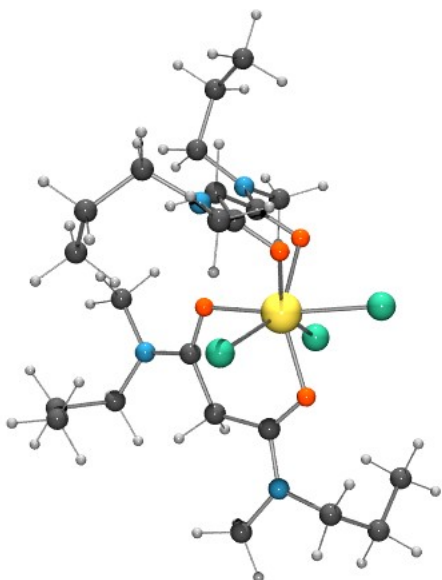
Iron trichloride *bis* tetraethyl malonamide



Iron trichloride *bis* dimethyldipropyl malonamide



Gold trichloride *bis* tetraethyl malonamide



Gold trichloride *bis* dimethyl dipropyl malonamide