chalconeSupporting Information for

Synthesis, Structural Characterization and Computational Study of a Novel Amino Chalcone: a Potential Nonlinear Optical Material

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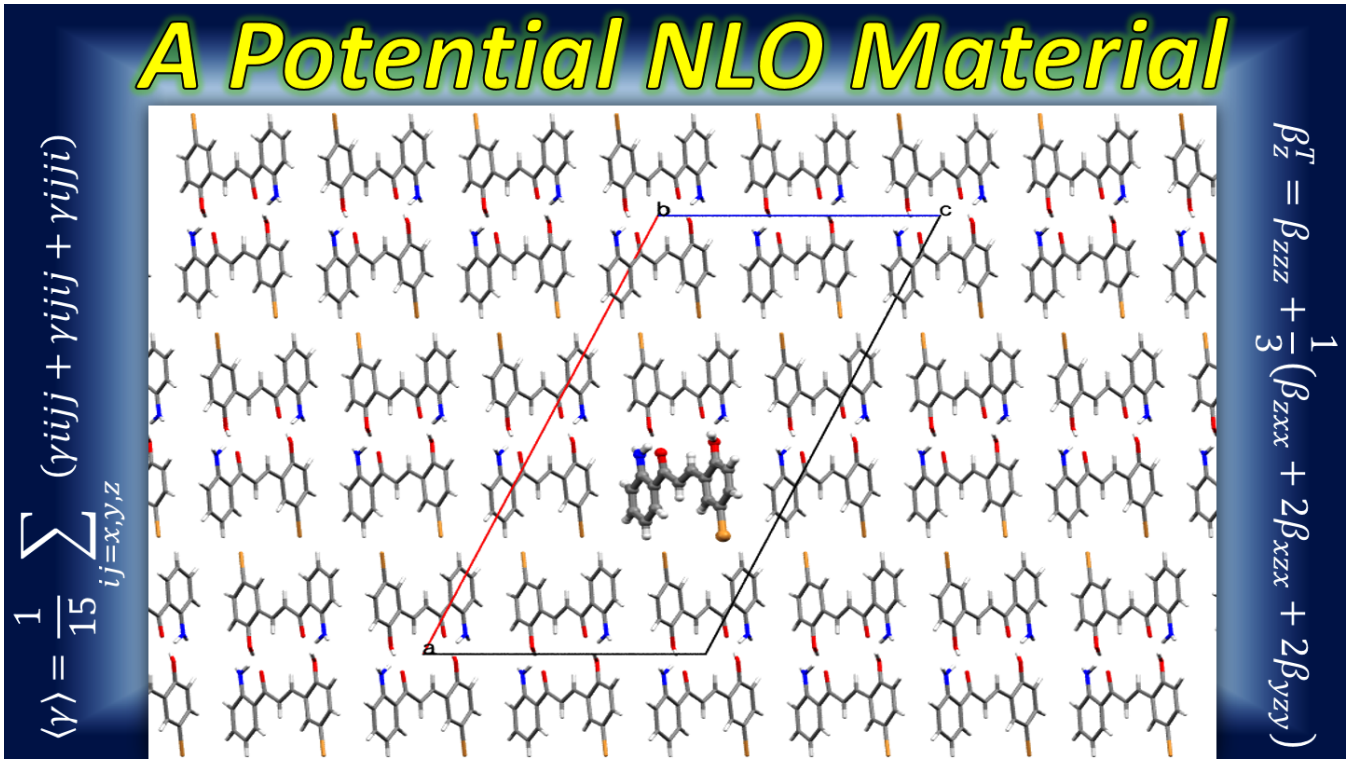

Summary

FIGURE S1:

TABLE S1: CAM-B3LYP/6-311+G(d) results for the components of the dipole moment (D), static linear polarizability (in 10^{-24} esu) and second hyperpolarizability (in 10^{-36} esu) as a function of the iterative process.

0	**1**	**2**	**3**	**4**	**5**
1.39	1.80	1.98	2.01	2.03	2.03
32.42	32.71	32.82	32.85	32.86	32.86
64.05	67.71	68.81	69.14	69.29	69.29

TABLE S2: PCM-CAM-B3LYP/6-311+G(d) results for the components of the dipole moment (D), static linear polarizability (in 10^{-24} esu), first hyperpolarizability (in 10^{-30} esu) and second hyperpolarizability (in 10^{-36} esu) calculated in gas-phase and in different solvents.

Gas	**Chloroform**	**THF**	**Acetone**	**Ethanol**	**Methanol**	**DMSO**
1.58	2.07	2.12	2.19	2.20	2.21	2.22
33.93	42.14	43.58	45.48	45.69	45.93	46.17
0.71	2.24	2.83	3.70	3.78	3.84	4.01
66.32	136.13	151.14	172.08	174.48	177.23	180.00

TABLE S3: PCM-CAM-B3LYP 6-311+G(d) results for the CHELPG atomic charges of 2-amino-chalcone calculated in gas-phase and in different solvents.

Atomic Charge	Gas	Chloroform	THF	Acetone	Ethanol	Methanol	DMSO
Br1	-0.109761	-0.122586	-0.123493	-0.124040	-0.124300	-0.124587	-0.125212
C2	0.390260	0.394905	0.396404	0.393580	0.391981	0.393726	0.392265
C3	-0.367544	-0.361367	-0.358387	-0.359732	-0.360074	-0.354066	-0.353416
C4	0.670209	0.647785	0.646229	0.642585	0.642775	0.639115	0.637859
C5	0.733478	0.738332	0.739081	0.742220	0.742482	0.734164	0.733935
C6	0.093904	0.104471	0.105006	0.109764	0.109275	0.111754	0.112139
H7	0.127524	0.116764	0.114996	0.112110	0.111934	0.109194	0.108692
C8	-0.052573	-0.071166	-0.073534	-0.080046	-0.078868	-0.080108	-0.079149
C9	0.035356	0.027164	0.024380	0.018613	0.019443	0.019432	0.021618
C10	-0.033769	-0.038404	-0.034283	-0.037236	-0.038244	-0.035308	-0.034834
H11	0.097798	0.107322	0.107158	0.110062	0.110278	0.109758	0.109079
C12	-0.326421	-0.310326	-0.313119	-0.305710	-0.303823	-0.308452	-0.307516
H13	0.155797	0.169354	0.173555	0.175862	0.176006	0.177775	0.178143
C14	-0.353086	-0.351823	-0.351709	-0.353444	-0.354006	-0.350274	-0.349842
H15	0.137315	0.150403	0.153483	0.157179	0.157541	0.157283	0.157693
C16	-0.459362	-0.472532	-0.476986	-0.483538	-0.483464	-0.479448	-0.480036
H17	0.197968	0.212535	0.217018	0.221783	0.221750	0.222892	0.223954
C18	-0.078551	-0.077081	-0.076171	-0.070811	-0.072350	-0.072501	-0.075435
H19	0.087212	0.095477	0.096160	0.096951	0.097539	0.096510	0.097104
C20	0.013842	0.000920	-0.006632	-0.007025	-0.006554	-0.010574	-0.011535
H21	0.090070	0.101330	0.104523	0.105996	0.106205	0.107142	0.107537
C22	0.002113	-0.013800	-0.023508	-0.026778	-0.026625	-0.030572	-0.031920
H23	0.063215	0.074890	0.078679	0.081290	0.081772	0.081951	0.082483
C24	-0.233120	-0.232717	-0.222783	-0.217669	-0.218568	-0.215755	-0.214495
H25	0.114498	0.121899	0.120403	0.119398	0.119864	0.119996	0.119869
O26	-0.621654	-0.653942	-0.658877	-0.666990	-0.667851	-0.665734	-0.666722
O27	-0.647171	-0.670157	-0.673407	-0.676161	-0.676183	-0.676397	-0.676400
H28	0.450801	0.476909	0.480667	0.485101	0.485426	0.486050	0.486447
N29	-1.094810	-1.081130	-1.083534	-1.083556	-1.084128	-1.083106	-1.082349
H30	0.427728	0.437795	0.440253	0.441902	0.442378	0.442372	0.442179
H31	0.488733	0.478774	0.478428	0.478334	0.478390	0.477768	0.477866

TABLE S4: CAM-B3LYP 6-311+G(d) results for the CHELPG atomic charges of 2-amino-chalcone as function of the iterative process.

Atomic Charge	0	1	2	3	4	5
Br1	-0.11112	-0.14924	-0.15072	-0.15521	-0.1525	-0.15524
C2	0.36169	0.3997	0.40981	0.41168	0.41226	0.41263
C3	-0.25155	-0.28168	-0.29548	-0.29691	-0.29959	-0.29827
C4	0.44018	0.46724	0.48379	0.48663	0.48849	0.48818
C5	0.65293	0.7347	0.75145	0.75389	0.75641	0.75511
C6	0.11457	0.15307	0.15574	0.15729	0.15773	0.15763
H7	0.09114	0.08408	0.08204	0.08263	0.08167	0.08262
C8	-0.04405	-0.08334	-0.09522	-0.09564	-0.09813	-0.0969
C9	0.03099	0.06062	0.06274	0.06466	0.06324	0.06456
C10	-0.00453	-0.04345	-0.04652	-0.04891	-0.04644	-0.04838
H11	0.09073	0.11406	0.11596	0.11659	0.11647	0.11663
C12	-0.34569	-0.3469	-0.34101	-0.33592	-0.33779	-0.33515
H13	0.19034	0.22446	0.22824	0.22993	0.22976	0.23027
C14	-0.32886	-0.3392	-0.34694	-0.34504	-0.34672	-0.34515
H15	0.16799	0.18212	0.18563	0.18616	0.18626	0.18638
C16	-0.49164	-0.51686	-0.52305	-0.52436	-0.52596	-0.52525
H17	0.21736	0.22196	0.22532	0.2241	0.2257	0.22432
C18	-0.12341	-0.1291	-0.12989	-0.1346	-0.13184	-0.13494
H19	0.12584	0.13954	0.14234	0.14322	0.14293	0.14332
C20	0.00548	-0.0101	-0.00752	-0.00917	-0.00688	-0.00866
H21	0.09216	0.09874	0.10126	0.10069	0.10148	0.10086
C22	-0.06211	-0.06528	-0.06497	-0.06615	-0.06514	-0.06627
H23	0.09272	0.1005	0.10374	0.10366	0.10416	0.10385
C24	-0.19287	-0.18349	-0.17854	-0.17921	-0.1777	-0.17876
H25	0.11568	0.11519	0.11651	0.11566	0.11636	0.11569
O26	-0.55505	-0.70731	-0.74053	-0.74759	-0.75255	-0.75084
O27	-0.61428	-0.67727	-0.70078	-0.70335	-0.70571	-0.70538
H28	0.43756	0.49268	0.51216	0.51626	0.51718	0.51801
N29	-0.77849	-0.8568	-0.89615	-0.90116	-0.90623	-0.90486
H30	0.33026	0.37445	0.38726	0.39101	0.39154	0.39226
H31	0.34605	0.42691	0.45336	0.45917	0.46151	0.46175

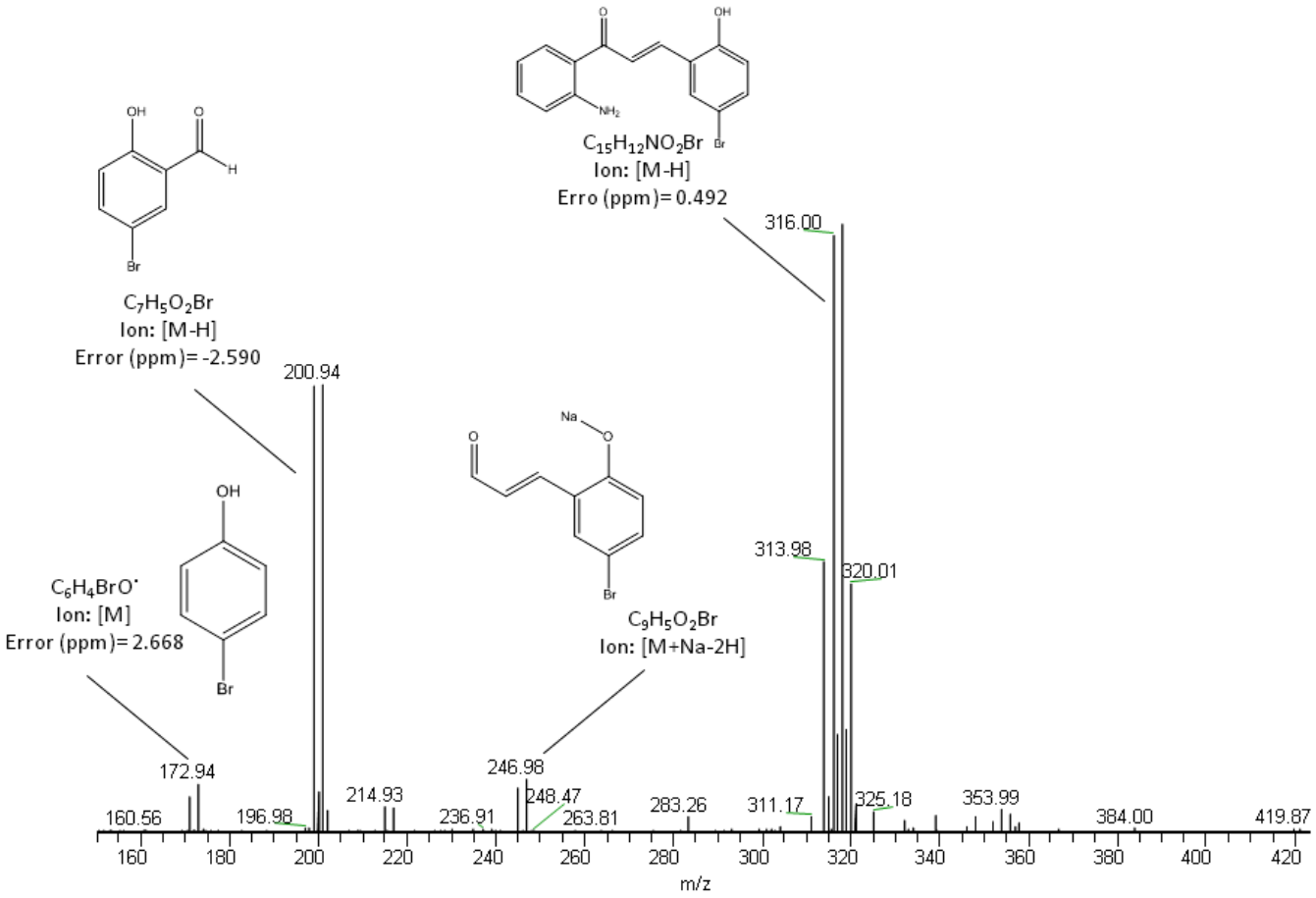

Figure S1. Mass Spectra of 2-amino-chalcone ($C_{15}H_{12}BrNO_2$).

Cartesian coordinates (Angstroms and Degrees), the calculated 2-amino-chalcone at CAM-B3LYP/6-311+G(d) level

1) Gas-Phase

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	-4.128883	-1.925197	0.331812
2	6	0	-2.216428	2.268712	-0.406948
3	6	0	3.473040	-0.176417	-0.046300
4	6	0	4.817002	0.054357	0.355760
5	6	0	2.424361	0.824858	0.231017
6	6	0	0.053716	1.406869	0.072881
7	1	0	0.378238	2.432364	0.209707
8	6	0	-1.387860	1.191461	-0.063692
9	6	0	-3.351362	-0.216754	0.020059
10	6	0	-4.162872	0.852105	-0.327261
11	1	0	-5.232613	0.721354	-0.428176
12	6	0	-3.588458	2.094402	-0.538459
13	1	0	-4.217324	2.936794	-0.811290
14	6	0	5.780607	-0.935525	0.078692
15	1	0	6.804024	-0.766835	0.399207
16	6	0	0.996301	0.462453	0.030516
17	1	0	0.735505	-0.573167	-0.139974
18	6	0	-1.986342	-0.050946	0.154166
19	1	0	-1.374351	-0.891146	0.455431
20	6	0	5.449678	-2.089008	-0.590031
21	1	0	6.219715	-2.825852	-0.792635
22	6	0	3.180557	-1.365930	-0.735234
23	1	0	2.171467	-1.541205	-1.083350
24	6	0	4.138309	-2.313958	-1.014977
25	1	0	3.878655	-3.215775	-1.555561
26	8	0	2.701449	1.949782	0.639005
27	8	0	-1.622576	3.473399	-0.614267
28	1	0	-2.278497	4.152383	-0.801053
29	7	0	5.195109	1.178201	1.017885
30	1	0	6.169114	1.338863	1.203627
31	1	0	4.538713	1.941178	1.086408

1) Chloroform

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	-4.120799	-1.930667	0.333036
2	6	0	-2.220786	2.271305	-0.406283
3	6	0	3.470998	-0.169759	-0.045809
4	6	0	4.815228	0.048290	0.364267
5	6	0	2.425489	0.833350	0.229390
6	6	0	0.053237	1.410515	0.056429
7	1	0	0.374032	2.440558	0.163489
8	6	0	-1.388013	1.193496	-0.071564
9	6	0	-3.346427	-0.217143	0.022437
10	6	0	-4.164199	0.851905	-0.313892
11	1	0	-5.234766	0.722227	-0.406509
12	6	0	-3.594703	2.095520	-0.526139
13	1	0	-4.225584	2.938047	-0.789706
14	6	0	5.773904	-0.945989	0.081955
15	1	0	6.796730	-0.786354	0.407531
16	6	0	0.999124	0.466952	0.041578
17	1	0	0.741491	-0.573886	-0.096638
18	6	0	-1.981258	-0.052889	0.145952
19	1	0	-1.365047	-0.894358	0.434643
20	6	0	5.437141	-2.091688	-0.597897
21	1	0	6.202960	-2.831601	-0.804540
22	6	0	3.171456	-1.353329	-0.745279
23	1	0	2.162500	-1.519697	-1.097799
24	6	0	4.124486	-2.304636	-1.029386
25	1	0	3.860901	-3.200232	-1.578341
26	8	0	2.708398	1.964619	0.626035
27	8	0	-1.633904	3.476953	-0.616841
28	1	0	-2.292085	4.153514	-0.811764
29	7	0	5.201369	1.159517	1.045792
30	1	0	6.181101	1.319581	1.206888
31	1	0	4.566126	1.940952	1.087830

2) Tetrahydrofuran (THF)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	-4.121325	-1.931016	0.331160
2	6	0	-2.221012	2.271943	-0.403761
3	6	0	3.471338	-0.169634	-0.045470
4	6	0	4.815829	0.048897	0.363839
5	6	0	2.425885	0.833955	0.226750
6	6	0	0.053382	1.409323	0.052188
7	1	0	0.374011	2.440029	0.152790

8	6	0	-1.387982	1.192871	-0.073091
9	6	0	-3.346504	-0.216819	0.022926
10	6	0	-4.164871	0.853602	-0.308490
11	1	0	-5.235802	0.725062	-0.398304
12	6	0	-3.595603	2.097387	-0.519723
13	1	0	-4.226741	2.940864	-0.779135
14	6	0	5.774229	-0.946277	0.083347
15	1	0	6.797158	-0.786158	0.408138
16	6	0	0.999822	0.465957	0.042556
17	1	0	0.742850	-0.575866	-0.088730
18	6	0	-1.981016	-0.054102	0.143058
19	1	0	-1.364360	-0.896829	0.427040
20	6	0	5.436835	-2.093358	-0.594027
21	1	0	6.202413	-2.833798	-0.799504
22	6	0	3.170905	-1.355031	-0.742075
23	1	0	2.161730	-1.522269	-1.093472
24	6	0	4.123730	-2.307019	-1.024466
25	1	0	3.859722	-3.203803	-1.571249
26	8	0	2.709369	1.967570	0.618160
27	8	0	-1.634163	3.477458	-0.614037
28	1	0	-2.292043	4.154175	-0.810334
29	7	0	5.203021	1.160859	1.044416
30	1	0	6.183870	1.322583	1.198248
31	1	0	4.570993	1.945150	1.078637

3) Acetone

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	-4.122726	-1.931364	0.327190
2	6	0	-2.221230	2.273074	-0.398503
3	6	0	3.472067	-0.170053	-0.044758
4	6	0	4.817103	0.050617	0.361983
5	6	0	2.426569	0.834581	0.221581
6	6	0	0.053727	1.406951	0.045207
7	1	0	0.374449	2.438592	0.134643
8	6	0	-1.387924	1.191663	-0.075199
9	6	0	-3.347023	-0.216204	0.023597
10	6	0	-4.166034	0.856700	-0.299301
11	1	0	-5.237542	0.730080	-0.384634
12	6	0	-3.596858	2.100806	-0.508224
13	1	0	-4.228390	2.945978	-0.760574
14	6	0	5.775258	-0.946036	0.085717
15	1	0	6.798541	-0.784114	0.408212
16	6	0	1.000849	0.463834	0.044138
17	1	0	0.744804	-0.579562	-0.075185
18	6	0	-1.980960	-0.056105	0.138160
19	1	0	-1.363815	-0.901134	0.414026

20	6	0	5.436981	-2.096738	-0.585316
21	1	0	6.202392	-2.838046	-0.788020
22	6	0	3.170371	-1.359679	-0.734366
23	1	0	2.160690	-1.529273	-1.083058
24	6	0	4.123078	-2.312902	-1.012835
25	1	0	3.858464	-3.212695	-1.554310
26	8	0	2.710825	1.972320	0.602827
27	8	0	-1.633992	3.478466	-0.607316
28	1	0	-2.291081	4.155690	-0.805444
29	7	0	5.205751	1.165557	1.038258
30	1	0	6.188179	1.330397	1.180182
31	1	0	4.577939	1.953564	1.059311

4) Ethanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	-4.123011	-1.931307	0.326793
2	6	0	-2.221166	2.273170	-0.398042
3	6	0	3.472159	-0.170161	-0.044618
4	6	0	4.817287	0.050834	0.361705
5	6	0	2.426625	0.834504	0.221218
6	6	0	0.053770	1.406614	0.044638
7	1	0	0.374524	2.438324	0.133084
8	6	0	-1.387909	1.191500	-0.075372
9	6	0	-3.347119	-0.216101	0.023639
10	6	0	-4.166124	0.857075	-0.298513
11	1	0	-5.237688	0.730685	-0.383470
12	6	0	-3.596901	2.101183	-0.507227
13	1	0	-4.228426	2.946529	-0.758968
14	6	0	5.775465	-0.945901	0.085774
15	1	0	6.798814	-0.783701	0.407890
16	6	0	1.000942	0.463504	0.044354
17	1	0	0.744964	-0.580016	-0.073944
18	6	0	-1.981001	-0.056318	0.137729
19	1	0	-1.363847	-0.901579	0.412856
20	6	0	5.437105	-2.097012	-0.584541
21	1	0	6.202532	-2.838351	-0.787040
22	6	0	3.170344	-1.360267	-0.733439
23	1	0	2.160583	-1.530211	-1.081714
24	6	0	4.123078	-2.313549	-1.011586
25	1	0	3.858404	-3.213690	-1.552446
26	8	0	2.710923	1.972621	0.601594
27	8	0	-1.633796	3.478503	-0.606724
28	1	0	-2.290741	4.155826	-0.805085
29	7	0	5.206089	1.166111	1.037477
30	1	0	6.188673	1.331310	1.178123

31	1	0	4.578632	1.954419	1.057336

5) Methanol

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	-4.123371	-1.931202	0.326423
2	6	0	-2.221051	2.273264	-0.397654
3	6	0	3.472257	-0.170285	-0.044489
4	6	0	4.817503	0.051089	0.361330
5	6	0	2.426676	0.834358	0.220947
6	6	0	0.053806	1.406243	0.044212
7	1	0	0.374597	2.437993	0.131946
8	6	0	-1.387895	1.191329	-0.075497
9	6	0	-3.347228	-0.215975	0.023678
10	6	0	-4.166191	0.857480	-0.297834
11	1	0	-5.237808	0.731338	-0.382476
12	6	0	-3.596895	2.101571	-0.506377
13	1	0	-4.228391	2.947083	-0.757599
14	6	0	5.775722	-0.945713	0.085709
15	1	0	6.799148	-0.783199	0.407392
16	6	0	1.001027	0.463130	0.044507
17	1	0	0.745094	-0.580467	-0.073085
18	6	0	-1.981060	-0.056530	0.137377
19	1	0	-1.363905	-0.902000	0.411852
20	6	0	5.437269	-2.097245	-0.583860
21	1	0	6.202722	-2.838595	-0.786186
22	6	0	3.170306	-1.360894	-0.732479
23	1	0	2.160449	-1.531272	-1.080240
24	6	0	4.123092	-2.314201	-1.010344
25	1	0	3.858336	-3.214711	-1.550546
26	8	0	2.711024	1.972795	0.600665
27	8	0	-1.633491	3.478491	-0.606253
28	1	0	-2.290269	4.155940	-0.804864
29	7	0	5.206459	1.166649	1.036661
30	1	0	6.189187	1.332182	1.176149
31	1	0	4.579305	1.955206	1.055581

6) Dimethyl sulfoxide (DMSO)

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	35	0	-4.123729	-1.931123	0.325942
2	6	0	-2.220966	2.273376	-0.397099
3	6	0	3.472371	-0.170429	-0.044317
4	6	0	4.817729	0.051361	0.360977
5	6	0	2.426740	0.834247	0.220517
6	6	0	0.053859	1.405830	0.043553
7	1	0	0.374699	2.437654	0.130126
8	6	0	-1.387877	1.191130	-0.075689
9	6	0	-3.347353	-0.215850	0.023723
10	6	0	-4.166297	0.857930	-0.296918
11	1	0	-5.237978	0.732062	-0.381128
12	6	0	-3.596933	2.102022	-0.505206
13	1	0	-4.228419	2.947739	-0.755721
14	6	0	5.775985	-0.945529	0.085762
15	1	0	6.799494	-0.782660	0.406967
16	6	0	1.001132	0.462721	0.044761
17	1	0	0.745272	-0.581017	-0.071631
18	6	0	-1.981120	-0.056782	0.136874
19	1	0	-1.363962	-0.902527	0.410482
20	6	0	5.437441	-2.097567	-0.582917
21	1	0	6.202922	-2.838948	-0.784995
22	6	0	3.170288	-1.361627	-0.731337
23	1	0	2.160335	-1.532439	-1.078584
24	6	0	4.123116	-2.314997	-1.008809
25	1	0	3.858294	-3.215936	-1.548256
26	8	0	2.711130	1.973128	0.599199
27	8	0	-1.633233	3.478530	-0.605524
28	1	0	-2.289828	4.156107	-0.804405
29	7	0	5.206856	1.167349	1.035664
30	1	0	6.189756	1.333304	1.173683
31	1	0	4.580087	1.956231	1.053198