Supplementary material (ESI) for Journal of Materials Chemistry

Electronic Supplementary Information

First Hyperpolarizability of some Nonconjugated Donor–Acceptor 3D Molecules: Noncentrosymmetric Crystal through Conformational Flexibility.

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Optimized Geometric Parameters for the two most stable Conformations of Molecule 1-4 at HF/6-31G level.

Molecule1- Conformation 1 (C_3)

ATOM NUMBER (I)	CHEMICAL SYMBOL	BOND LENGTH (ANGSTROMS) NA:I	BOND ANGLE (DEGREES) NB:NA:I	TWIST ANGLE (DEGREES) NC:NB:NA:I	NA	NB	NC
1	N	0.00000	0.00000	0.00000	0	0	0
2	C	1.33387	0.00000	0.00000	1	0	0
3	N	1.34749	124.29644	0.00000	2	1	0
4	C	1.33387	115.70252	-.45068	3	2	1
5	N	1.34749	124.29647	.44917	4	3	2
6	C	1.33387	115.70250	-.45068	5	4	3
7	N	1.34021	118.98564	179.97813	2	1	3
8	N	1.34021	118.98559	-179.57271	4	3	2
9	N	1.34021	118.98555	-179.57271	6	5	4
10	C	1.45537	124.44809	-1.85643	7	2	1
11	C	1.45537	124.44814	-1.85643	8	4	3
12	C	1.45537	124.44811	-1.85643	9	6	5
13	H	1.08026	108.10119	37.11307	10	7	2
14	H	1.08026	108.10110	37.11305	11	8	4
15	H	1.08026	108.10118	37.11308	12	9	6
16	H	1.08447	110.44171	-79.41831	10	7	2
17	H	1.08447	110.44167	-79.41823	11	8	4
18	H	1.08447	110.44167	-79.41832	12	9	6
19	C	1.51278	110.81847	158.64397	10	7	2
20	C	1.51278	110.81848	158.64395	11	8	4
21	C	1.51278	110.81846	158.64398	12	9	6
22	C	1.38922	120.76376	121.41542	19	10	7
23	C	1.38922	120.76376	121.41543	20	11	8
24	C	1.38922	120.76377	121.41538	21	12	9
25	C	1.39419	120.49934	-59.41036	19	10	7
26	C	1.39419	120.49937	-59.41033	20	11	8
27	C	1.39419	120.49932	-59.41035	21	12	9
28	C	1.38959	120.76324	179.04454	22	19	10
29	C	1.38959	120.76325	179.04455	23	20	11
30	C	1.38959	120.76324	179.04455	24	21	12
31	C	1.38526	120.65902	-179.19716	25	19	10
32	C	1.38526	120.65902	-179.19715	26	20	11
33	C	1.38526	120.65901	-179.19719	27	21	12
34	C	1.38532	120.06592	.18807	28	22	19
35	C	1.38532	120.06591	.18805	29	23	20
36	C	1.38532	120.06593	.18807	30	24	21
37	H	1.07402	119.60596	-1.05364	22	19	10
38	H	1.07402	119.60595	-1.05369	23	20	11
39	H	1.07402	119.60591	-1.05364	24	21	12
40	H	1.07373	119.42994	.84691	25	19	10
41	H	1.07373	119.42995	.84691	26	20	11
42	H	1.07373	119.42996	.84692	27	21	12
43	H	1.07318	119.79695	179.98623	28	22	19
44	H	1.07318	119.79697	179.98622	29	23	20
45	H	1.07318	119.79695	179.98621	30	24	21
46	H	1.07323	119.83617	179.93514	31	25	19
47	H	1.07323	119.83617	179.93513	32	26	20
48	H	1.07323	119.83616	179.93507	33	27	21
49	H	1.07305	120.22252	179.89427	34	28	22
50	H	1.07305	120.22251	179.89427	35	29	23
51	H	1.07305	120.22253	179.89427	36	30	24
52	H	.99236	116.15501	-177.19291	7	2	1
53	H	.99236	116.15500	-177.19291	8	4	3

54	H	.99236	116.15493	-177.19291	9	6	5

Molecule1-Conformation 2 (C_1)

ATOM NUMBER (I)	CHEMICAL SYMBOL	BOND LENGTH (ANGSTROMS) NA:I	BOND ANGLE (DEGREES) NB:NA:I	TWIST ANGLE (DEGREES) NC:NB:NA:I	NA	NB	NC
1	N	0.00000	0.00000	0.00000	0	0	0
2	C	1.33389	0.00000	0.00000	1	0	0
3	N	1.34751	124.29663	0.00000	2	1	0
4	C	1.33387	115.70055	-.06411	3	2	1
5	N	1.34749	124.29770	.63501	4	3	2
6	C	1.33388	115.70224	-.69578	5	4	3
7	N	1.34018	118.98646	179.76673	2	1	3
8	N	1.34020	118.98281	-179.41755	4	3	2
9	N	1.34020	118.98791	-179.54410	6	5	4
10	C	1.45540	124.46172	1.72541	7	2	1
11	C	1.45540	124.44507	-1.79846	8	4	3
12	C	1.45536	124.46268	-1.78294	9	6	5
13	H	1.08025	108.10756	-36.94749	10	7	2
14	H	1.08026	108.11381	37.24743	11	8	4
15	H	1.08025	108.09661	36.84375	12	9	6
16	H	1.08446	110.43666	79.58739	10	7	2
17	H	1.08446	110.43901	-79.28642	11	8	4
18	H	1.08447	110.43960	-79.68877	12	9	6
19	C	1.51278	110.81552	-158.47865	10	7	2
20	C	1.51277	110.80795	158.77559	11	8	4
21	C	1.51280	110.82464	158.37718	12	9	6
22	C	1.39420	120.49205	59.57870	19	10	7
23	C	1.38922	120.76888	121.23225	20	11	8
24	C	1.38922	120.76560	121.39718	21	12	9
25	C	1.38922	120.76926	-121.23596	19	10	7
26	C	1.39420	120.49344	-59.58092	20	11	8
27	C	1.39420	120.49659	-59.42867	21	12	9
28	C	1.38526	120.65737	179.20662	22	19	10
29	C	1.38959	120.76266	179.05998	23	20	11
30	C	1.38959	120.76323	179.04375	24	21	12
31	C	1.38959	120.76274	-179.05723	25	19	10
32	C	1.38526	120.65888	-179.21051	26	20	11
33	C	1.38526	120.65780	-179.19516	27	21	12
34	C	1.38532	120.06487	-.18490	31	25	19
35	C	1.38532	120.06549	.18461	29	23	20
36	C	1.38532	120.06544	.18762	30	24	21
37	H	1.07374	119.43136	-.83199	22	19	10
38	H	1.07402	119.60570	-1.03679	23	20	11
39	H	1.07402	119.60607	-1.05424	24	21	12
40	H	1.07403	119.60588	1.03903	25	19	10
41	H	1.07373	119.43075	.82827	26	20	11
42	H	1.07373	119.43025	.84909	27	21	12
43	H	1.07323	119.83537	-179.92755	28	22	19
44	H	1.07318	119.79761	179.98769	29	23	20
45	H	1.07318	119.79725	179.98558	30	24	21
46	H	1.07318	119.79797	-179.98694	31	25	19
47	H	1.07323	119.83621	179.93118	32	26	20
48	H	1.07323	119.83566	179.93135	33	27	21
49	H	1.07305	120.22165	-179.89994	34	31	25
50	H	1.07305	120.22220	179.89878	35	29	23
51	H	1.07305	120.22202	179.89619	36	30	24
52	H	.99234	116.16253	177.45272	7	2	1
53	H	.99235	116.16036	-177.18822	8	4	3
54	H	.99235	116.15891	-177.45593	9	6	5

Molecule2-Conformation 1 (C_3)

ATOM NUMBER (I)	CHEMICAL SYMBOL	BOND LENGTH (ANGSTROMS) NA:I	BOND ANGLE (DEGREES) NB:NA:I	TWIST ANGLE (DEGREES) NC:NB:NA:I	NA	NB	NC
1	N	0.00000	0.00000	0.00000	0	0	0
2	C	1.33394	0.00000	0.00000	1	0	0
3	N	1.34769	124.31000	0.00000	2	1	0
4	C	1.33394	115.68910	-.42471	3	2	1
5	N	1.34769	124.30998	.42327	4	3	2
6	C	1.33394	115.68916	-.42471	5	4	3
7	N	1.33990	118.91955	179.96308	2	1	3
8	N	1.33990	118.91950	-179.61365	4	3	2
9	N	1.33990	118.91958	-179.61365	6	5	4
10	C	1.45626	124.36756	-1.67238	7	2	1
11	C	1.45626	124.36759	-1.67238	8	4	3
12	C	1.45626	124.36753	-1.67238	9	6	5
13	H	1.08047	108.20857	39.82300	10	7	2
14	H	1.08047	108.20862	39.82302	11	8	4
15	H	1.08047	108.20857	39.82305	12	9	6
16	H	1.08436	110.37821	-76.69281	10	7	2
17	H	1.08436	110.37823	-76.69287	11	8	4
18	H	1.08436	110.37818	-76.69285	12	9	6
19	C	1.51174	110.66246	161.43088	10	7	2
20	C	1.51174	110.66245	161.43089	11	8	4
21	C	1.51174	110.66242	161.43089	12	9	6
22	C	1.38633	121.15677	117.95660	19	10	7
23	C	1.38633	121.15680	117.95654	20	11	8
24	C	1.38633	121.15676	117.95656	21	12	9
25	C	1.39501	120.64479	-62.62270	19	10	7
26	C	1.39501	120.64481	-62.62270	20	11	8
27	C	1.39501	120.64480	-62.62269	21	12	9
28	C	1.39062	120.93887	179.31457	22	19	10
29	C	1.39062	120.93889	179.31457	23	20	11
30	C	1.39062	120.93886	179.31457	24	21	12
31	C	1.38255	120.83702	-179.46528	25	19	10
32	C	1.38255	120.83706	-179.46531	26	20	11
33	C	1.38255	120.83704	-179.46528	27	21	12
34	C	1.38766	120.98748	.17435	28	22	19
35	C	1.38766	120.98748	.17442	29	23	20
36	C	1.38766	120.98747	.17438	30	24	21
37	H	1.07421	119.67454	-.73927	22	19	10
38	H	1.07421	119.67455	-.73916	23	20	11
39	H	1.07421	119.67455	-.73925	24	21	12
40	H	1.07405	119.43298	.57136	25	19	10
41	H	1.07405	119.43296	.57137	26	20	11
42	H	1.07405	119.43294	.57129	27	21	12
43	H	1.07397	119.35504	-179.98633	28	22	19
44	H	1.07397	119.35505	-179.98626	29	23	20
45	H	1.07397	119.35504	-179.98624	30	24	21
46	H	1.07461	119.46701	179.92566	31	25	19
47	H	1.07461	119.46696	179.92564	32	26	20
48	H	1.07461	119.46696	179.92563	33	27	21
49	C	1.50982	121.46831	179.92917	34	28	22
50	C	1.50982	121.46832	179.92916	35	29	23
51	C	1.50982	121.46829	179.92919	36	30	24
52	H	.99221	116.25107	-177.30211	7	2	1
53	H	.99222	116.25099	-177.30211	8	4	3
54	H	.99221	116.25103	-177.30211	9	6	5
55	H	1.08256	111.28452	.05910	49	34	28
56	H	1.08498	111.18712	120.20191	49	34	28
57	H	1.08499	111.20426	-120.09945	49	34	28
58	H	1.08256	111.28453	.05910	50	35	29
59	H	1.08498	111.18710	120.20191	50	35	29
60	H	1.08499	111.20424	-120.09948	50	35	29
61	H	1.08256	111.28454	.05905	51	36	30
62	H	1.08498	111.18718	120.20191	51	36	30
63	H	1.08499	111.20426	-120.09948	51	36	30

Molecule2-Conformation 2 (C_1)

ATOM NUMBER (I)	CHEMICAL SYMBOL	BOND LENGTH (ANGSTROMS) NA:I	BOND ANGLE (DEGREES) NB:NA:I	TWIST ANGLE (DEGREES) NC:NB:NA:I	NA	NB	NC
1	N	0.00000	0.00000	0.00000	0	0	0
2	C	1.33395	0.00000	0.00000	1	0	0
3	N	1.34772	124.31131	0.00000	2	1	0
4	C	1.33393	115.68742	-.05563	3	2	1
5	N	1.34770	124.31036	.59802	4	3	2
6	C	1.33394	115.68910	-.65895	5	4	3
7	N	1.33985	118.91583	179.79722	2	1	3
8	N	1.33990	118.92045	-179.46518	4	3	2
9	N	1.33987	118.91603	-179.58389	6	5	4
10	C	1.45632	124.37009	1.52611	7	2	1
11	C	1.45628	124.36918	-1.62052	8	4	3
12	C	1.45630	124.36949	-1.58060	9	6	5
13	H	1.08048	108.22465	-39.84856	10	7	2
14	H	1.08046	108.21493	39.85007	11	8	4
15	H	1.08048	108.21554	39.79738	12	9	6
16	H	1.08432	110.36856	76.67041	10	7	2
17	H	1.08435	110.37557	-76.66556	11	8	4
18	H	1.08433	110.37207	-76.71984	12	9	6
19	C	1.51170	110.65350	-161.45664	10	7	2
20	C	1.51171	110.65917	161.45675	11	8	4
21	C	1.51171	110.65838	161.40838	12	9	6
22	C	1.39502	120.63639	62.87562	19	10	7
23	C	1.38633	121.15957	117.85707	20	11	8
24	C	1.38634	121.16136	117.78410	21	12	9
25	C	1.38633	121.16439	-117.67942	19	10	7
26	C	1.39501	120.64222	-62.70905	20	11	8
27	C	1.39501	120.64016	-62.77618	21	12	9
28	C	1.38255	120.83634	179.48846	22	19	10
29	C	1.39062	120.93936	179.32874	23	20	11
30	C	1.39062	120.93894	179.33393	24	21	12
31	C	1.39062	120.93865	-179.34050	25	19	10
32	C	1.38255	120.83689	-179.47513	26	20	11
33	C	1.38255	120.83678	-179.48103	27	21	12
34	C	1.38766	120.98656	-.16550	31	25	19
35	C	1.38765	120.98674	.16443	29	23	20
36	C	1.38766	120.98703	.16512	30	24	21
37	H	1.07406	119.43447	-.54627	22	19	10
38	H	1.07421	119.67387	-.73141	23	20	11
39	H	1.07421	119.67376	-.72545	24	21	12
40	H	1.07421	119.67389	.71580	25	19	10
41	H	1.07405	119.43372	.56035	26	20	11
42	H	1.07406	119.43369	.55698	27	21	12
43	H	1.07461	119.46636	-179.92456	28	22	19
44	H	1.07397	119.35589	-179.99132	29	23	20
45	H	1.07397	119.35556	-179.99121	30	24	21
46	H	1.07397	119.35612	179.98955	31	25	19
47	H	1.07461	119.46625	179.92730	32	26	20
48	H	1.07461	119.46660	179.92751	33	27	21
49	C	1.50983	121.46771	-179.96879	34	31	25
50	C	1.50982	121.46839	179.97432	35	29	23
51	C	1.50983	121.46773	179.97233	36	30	24
52	H	.99219	116.26510	177.55814	7	2	1
53	H	.99221	116.25294	-177.30035	8	4	3
54	H	.99220	116.26261	-177.55926	9	6	5
55	H	1.08501	111.18247	-119.70880	49	34	31
56	H	1.08256	111.28457	.42641	49	34	31
57	H	1.08496	111.20830	120.59275	49	34	31
58	H	1.08256	111.28487	-.56150	50	35	29
59	H	1.08501	111.18193	119.57236	50	35	29
60	H	1.08495	111.20860	-120.72968	50	35	29
61	H	1.08256	111.28463	-.53622	51	36	30
62	H	1.08501	111.18254	119.59795	51	36	30

63	H	1.08495	111.20859	-120.70333	51	36	30

Molecule3-Conformation 1 (C_3)

ATOM NUMBER (I)	CHEMICAL SYMBOL	BOND LENGTH (ANGSTROMS) NA:I	BOND ANGLE (DEGREES) NB:NA:I	TWIST ANGLE (DEGREES) NC:NB:NA:I	NA	NB	NC
1	N	0.00000	0.00000	0.00000	0	0	0
2	C	1.33396	0.00000	0.00000	1	0	0
3	N	1.34774	124.32111	0.00000	2	1	0
4	C	1.33396	115.67789	-.45260	3	2	1
5	N	1.34774	124.32108	.45106	4	3	2
6	C	1.33396	115.67788	-.45260	5	4	3
7	N	1.33975	118.85916	179.94511	2	1	3
8	N	1.33975	118.85917	-179.60383	4	3	2
9	N	1.33975	118.85916	-179.60383	6	5	4
10	C	1.45698	124.28638	-1.39735	7	2	1
11	C	1.45698	124.28640	-1.39735	8	4	3
12	C	1.45698	124.28641	-1.39735	9	6	5
13	H	1.08055	108.28784	41.65832	10	7	2
14	H	1.08055	108.28780	41.65831	11	8	4
15	H	1.08055	108.28778	41.65831	12	9	6
16	H	1.08428	110.30513	-74.79957	10	7	2
17	H	1.08428	110.30508	-74.79960	11	8	4
18	H	1.08428	110.30511	-74.79957	12	9	6
19	C	1.51073	110.57841	163.35783	10	7	2
20	C	1.51073	110.57838	163.35783	11	8	4
21	C	1.51073	110.57839	163.35783	12	9	6
22	C	1.38386	121.31268	114.48093	19	10	7
23	C	1.38386	121.31265	114.48095	20	11	8
24	C	1.38386	121.31263	114.48098	21	12	9
25	C	1.39861	120.59408	-65.87181	19	10	7
26	C	1.39861	120.59409	-65.87182	20	11	8
27	C	1.39861	120.59409	-65.87186	21	12	9
28	C	1.39328	121.50013	179.54765	22	19	10
29	C	1.39328	121.50012	179.54763	23	20	11
30	C	1.39328	121.50011	179.54759	24	21	12
31	C	1.37825	121.13633	-179.69027	25	19	10
32	C	1.37825	121.13632	-179.69026	26	20	11
33	C	1.37825	121.13633	-179.69026	27	21	12
34	C	1.38306	119.38590	.15490	28	22	19
35	C	1.38306	119.38589	.15493	29	23	20
36	C	1.38306	119.38585	.15492	30	24	21
37	H	1.07398	119.64936	-.45110	22	19	10
38	H	1.07398	119.64943	-.45113	23	20	11
39	H	1.07398	119.64946	-.45115	24	21	12
40	H	1.07372	119.40445	.32639	25	19	10
41	H	1.07372	119.40445	.32638	26	20	11
42	H	1.07372	119.40443	.32647	27	21	12
43	H	1.07088	119.40887	-179.94874	28	22	19
44	H	1.07088	119.40887	-179.94876	29	23	20
45	H	1.07088	119.40884	-179.94876	30	24	21
46	H	1.07107	121.63339	179.88786	31	25	19
47	H	1.07107	121.63334	179.88788	32	26	20
48	H	1.07106	121.63337	179.88786	33	27	21
49	O	1.37277	124.18278	179.94097	34	28	22
50	O	1.37277	124.18279	179.94099	35	29	23
51	O	1.37277	124.18275	179.94098	36	30	24
52	H	.99214	116.33005	-177.50303	7	2	1
53	H	.99214	116.33002	-177.50303	8	4	3
54	H	.99214	116.33007	-177.50303	9	6	5
55	C	1.42786	121.58803	.26880	49	34	28
56	C	1.42786	121.58802	.26877	50	35	29
57	C	1.42786	121.58804	.26876	51	36	30
58	H	1.08241	111.08697	-61.38303	55	49	34
59	H	1.08240	111.08264	61.02695	55	49	34
60	H	1.07616	105.58118	179.82623	55	49	34
61	H	1.08241	111.08697	-61.38304	56	50	35
62	H	1.08240	111.08271	61.02697	56	50	35

63	H	1.07616	105.58119	179.82625	56	50	35
64	H	1.08241	111.08696	-61.38304	57	51	36
65	H	1.08240	111.08263	61.02695	57	51	36
66	H	1.07616	105.58115	179.82628	57	51	36

Molecule3-Conformation 2 (C_1)

ATOM NUMBER (I)	CHEMICAL SYMBOL	BOND LENGTH (ANGSTROMS) NA:I	BOND ANGLE (DEGREES) NB:NA:I	TWIST ANGLE (DEGREES) NC:NB:NA:I	NA	NB	NC
1	N	0.00000	0.00000	0.00000	0	0	0
2	C	1.33526	0.00000	0.00000	1	0	0
3	N	1.34732	124.10327	0.00000	2	1	0
4	C	1.33439	115.82420	-.60267	3	2	1
5	N	1.34757	124.31371	.30330	4	3	2
6	C	1.33397	115.62780	-.23049	5	4	3
7	N	1.34098	119.51127	179.79806	2	1	3
8	N	1.33907	118.82011	-179.70544	4	3	2
9	N	1.33966	118.81079	-179.65201	6	5	4
10	C	1.45570	125.54099	.29735	7	2	1
11	C	1.45735	124.29142	-1.32795	8	4	3
12	C	1.45738	124.27136	-1.16556	9	6	5
13	H	1.07803	107.22785	15.63310	10	7	2
14	H	1.08058	108.31141	42.20605	11	8	4
15	H	1.08056	108.31405	41.84728	12	9	6
16	H	1.08362	108.27623	131.53671	10	7	2
17	H	1.08414	110.26792	-74.25650	11	8	4
18	H	1.08418	110.27436	-74.61384	12	9	6
19	C	1.51464	113.45328	-106.74758	10	7	2
20	C	1.51064	110.55274	163.90198	11	8	4
21	C	1.51066	110.55003	163.55297	12	9	6
22	C	1.38906	120.76019	68.09722	19	10	7
23	C	1.38389	121.30984	114.06312	20	11	8
24	C	1.38388	121.31849	114.08108	21	12	9
25	C	1.39260	121.12343	-111.87566	19	10	7
26	C	1.39860	120.59196	-66.26779	20	11	8
27	C	1.39862	120.58577	-66.25133	21	12	9
28	C	1.38830	121.31603	-179.81708	22	19	10
29	C	1.39323	121.49554	179.57705	23	20	11
30	C	1.39324	121.49847	179.58073	24	21	12
31	C	1.38340	121.27975	179.89323	25	19	10
32	C	1.37825	121.13495	-179.72164	26	20	11
33	C	1.37823	121.13507	-179.72492	27	21	12
34	C	1.38727	119.74902	-.05934	31	25	19
35	C	1.38311	119.38795	.15279	29	23	20
36	C	1.38311	119.38684	.15112	30	24	21
37	H	1.07347	119.34775	.36037	22	19	10
38	H	1.07397	119.65208	-.41261	23	20	11
39	H	1.07399	119.65206	-.39941	24	21	12
40	H	1.07447	119.65355	-.20077	25	19	10
41	H	1.07375	119.41254	.28282	26	20	11
42	H	1.07375	119.41356	.27230	27	21	12
43	H	1.07105	119.40165	-179.93234	28	22	19
44	H	1.07087	119.40831	-179.94052	29	23	20
45	H	1.07087	119.41190	-179.93881	30	24	21
46	H	1.07113	121.59688	-179.99716	31	25	19
47	H	1.07106	121.63564	179.88637	32	26	20
48	H	1.07105	121.63456	179.88472	33	27	21
49	O	1.37457	116.02293	-179.94475	34	31	25
50	O	1.37262	124.18423	179.94443	35	29	23
51	O	1.37256	124.18638	179.94188	36	30	24
52	H	.99265	115.36252	-176.95523	7	2	1
53	H	.99216	116.34957	-177.62961	8	4	3
54	H	.99209	116.41372	-177.99954	9	6	5
55	C	1.42736	121.57616	179.89014	49	34	31
56	C	1.42796	121.59748	.28530	50	35	29
57	C	1.42796	121.60362	.28987	51	36	30
58	H	1.08247	111.13143	-61.04357	55	49	34
59	H	1.08247	111.13334	61.38014	55	49	34
60	H	1.07632	105.59022	-179.83742	55	49	34
61	H	1.08240	111.08363	-61.39025	56	50	35

62	H	1.08239	111.07919	61.02146	56	50	35
63	H	1.07615	105.57791	179.81984	56	50	35
64	H	1.08240	111.08290	-61.39959	57	51	36
65	H	1.08239	111.07852	61.01443	57	51	36
66	H	1.07614	105.57706	179.81287	57	51	36

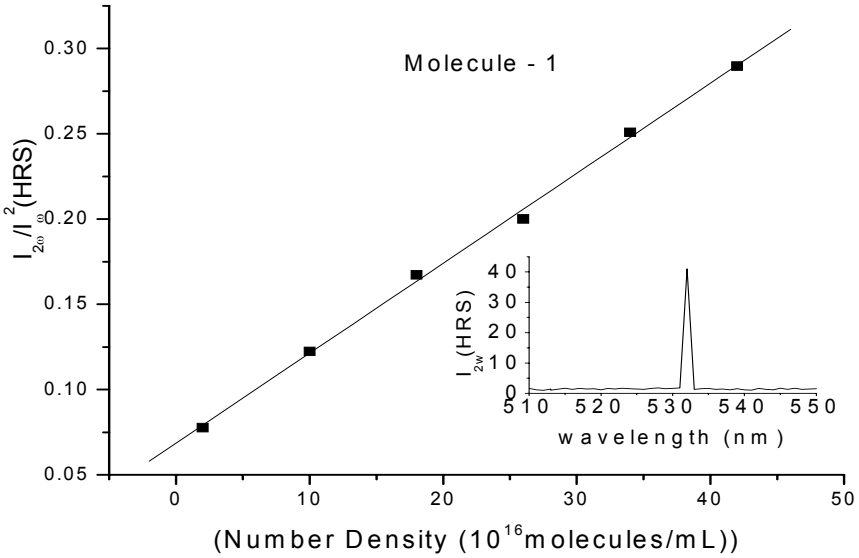
Molecule4-Conformation 1 (C_3)

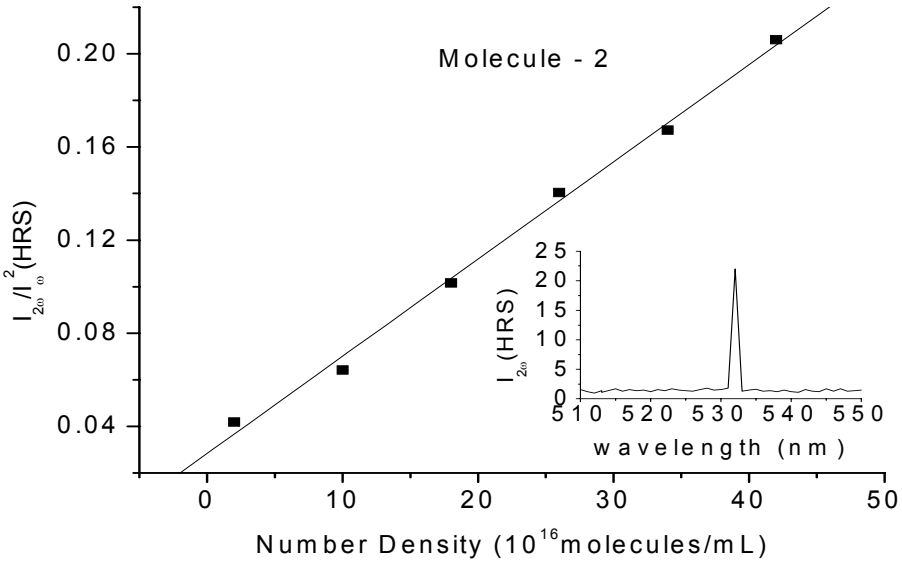
ATOM NUMBER (I)	CHEMICAL SYMBOL	BOND LENGTH (ANGSTROMS) NA:I	BOND ANGLE (DEGREES) NB:NA:I	TWIST ANGLE (DEGREES) NC:NB:NA:I	NA	NB	NC
1	N	0.00000	0.00000	0.00000	0	0	0
2	C	1.33386	0.00000	0.00000	1	0	0
3	N	1.34688	124.24937	0.00000	2	1	0
4	C	1.33386	115.74972	-.41446	3	2	1
5	N	1.34688	124.24940	.41312	4	3	2
6	C	1.33386	115.74980	-.41446	5	4	3
7	N	1.34117	119.17156	-179.93592	2	1	3
8	N	1.34117	119.17149	-179.52280	4	3	2
9	N	1.34117	119.17155	-179.52280	6	5	4
10	C	1.45422	124.75684	-2.46599	7	2	1
11	C	1.45422	124.75689	-2.46599	8	4	3
12	C	1.45422	124.75686	-2.46599	9	6	5
13	H	1.07950	107.73617	28.95963	10	7	2
14	H	1.07950	107.73610	28.95959	11	8	4
15	H	1.07950	107.73616	28.95961	12	9	6
16	H	1.08487	110.47379	-87.49326	10	7	2
17	H	1.08487	110.47373	-87.49324	11	8	4
18	H	1.08487	110.47373	-87.49326	12	9	6
19	C	1.51315	111.18934	150.56469	10	7	2
20	C	1.51315	111.18937	150.56466	11	8	4
21	C	1.51315	111.18930	150.56471	12	9	6
22	C	1.38962	120.70978	124.81514	19	10	7
23	C	1.38962	120.70977	124.81513	20	11	8
24	C	1.38962	120.70975	124.81519	21	12	9
25	C	1.39475	120.55224	-56.27836	19	10	7
26	C	1.39475	120.55227	-56.27833	20	11	8
27	C	1.39475	120.55227	-56.27842	21	12	9
28	C	1.38931	121.08625	178.72740	22	19	10
29	C	1.38930	121.08626	178.72739	23	20	11
30	C	1.38931	121.08625	178.72734	24	21	12
31	C	1.38466	120.96398	-178.87379	25	19	10
32	C	1.38466	120.96400	-178.87381	26	20	11
33	C	1.38466	120.96400	-178.87375	27	21	12
34	C	1.37425	118.26317	.19226	28	22	19
35	C	1.37425	118.26317	.19230	29	23	20
36	C	1.37425	118.26316	.19224	30	24	21
37	H	1.07321	119.74624	-1.37116	22	19	10
38	H	1.07321	119.74626	-1.37109	23	20	11
39	H	1.07321	119.74628	-1.37125	24	21	12
40	H	1.07271	119.51702	1.26381	25	19	10
41	H	1.07271	119.51700	1.26387	26	20	11
42	H	1.07271	119.51699	1.26391	27	21	12
43	H	1.07068	121.71926	179.95234	28	22	19
44	H	1.07068	121.71927	179.95239	29	23	20
45	H	1.07068	121.71929	179.95229	30	24	21
46	H	1.07077	121.76045	179.93555	31	25	19
47	H	1.07077	121.76048	179.93549	32	26	20
48	H	1.07077	121.76046	179.93556	33	27	21
49	F	1.37503	118.80503	179.82939	34	28	22
50	F	1.37503	118.80503	179.82934	35	29	23
51	F	1.37503	118.80505	179.82934	36	30	24
52	H	.99277	115.88710	-177.02362	7	2	1
53	H	.99277	115.88711	-177.02362	8	4	3
54	H	.99277	115.88708	-177.02362	9	6	5

Molecule4-Conformation 2 (C_1)

ATOM NUMBER (I)	CHEMICAL SYMBOL	BOND LENGTH (ANGSTROMS) NA:I	BOND ANGLE (DEGREES) NB:NA:I	TWIST ANGLE (DEGREES) NC:NB:NA:I	NA	NB	NC
1	N	0.00000	0.00000	0.00000	0	0	0
2	C	1.33530	0.00000	0.00000	1	0	0
3	N	1.34637	124.12365	0.00000	2	1	0
4	C	1.33419	115.83393	-.64148	3	2	1
5	N	1.34687	124.24445	.25003	4	3	2
6	C	1.33378	115.74654	-.12629	5	4	3
7	N	1.34113	119.43177	179.72759	2	1	3
8	N	1.34068	119.16913	-179.60765	4	3	2
9	N	1.34118	119.18687	-179.59077	6	5	4
10	C	1.45451	125.47871	1.06498	7	2	1
11	C	1.45438	124.80054	-2.46968	8	4	3
12	C	1.45437	124.83383	-2.33046	9	6	5
13	H	1.07815	107.40611	16.37156	10	7	2
14	H	1.07942	107.70929	28.32969	11	8	4
15	H	1.07937	107.68056	27.24338	12	9	6
16	H	1.08315	108.32345	132.44314	10	7	2
17	H	1.08482	110.44453	-88.11877	11	8	4
18	H	1.08487	110.43686	-89.20304	12	9	6
19	C	1.51546	113.36302	-105.82660	10	7	2
20	C	1.51316	111.20716	149.93793	11	8	4
21	C	1.51326	111.24715	148.86265	12	9	6
22	C	1.39517	120.35659	66.00115	19	10	7
23	C	1.38960	120.70741	124.74316	20	11	8
24	C	1.38960	120.70301	125.00620	21	12	9
25	C	1.38905	120.86700	-114.14460	19	10	7
26	C	1.39476	120.54831	-56.35133	20	11	8
27	C	1.39474	120.55244	-56.10051	21	12	9
28	C	1.38420	120.87931	-179.99496	22	19	10
29	C	1.38932	121.08250	178.72486	23	20	11
30	C	1.38932	121.08400	178.71226	24	21	12
31	C	1.39002	121.11478	-179.92543	25	19	10
32	C	1.38465	120.96031	-178.87044	26	20	11
33	C	1.38464	120.95863	-178.85630	27	21	12
34	C	1.37369	118.19718	-.06827	31	25	19
35	C	1.37424	118.26246	.19164	29	23	20
36	C	1.37424	118.26154	.19155	30	24	21
37	H	1.07258	119.39068	.29120	22	19	10
38	H	1.07322	119.75015	-1.37167	23	20	11
39	H	1.07323	119.75363	-1.38143	24	21	12
40	H	1.07369	119.80782	.00000	25	19	10
41	H	1.07272	119.52099	1.26408	26	20	11
42	H	1.07271	119.52470	1.27875	27	21	12
43	H	1.07084	121.75361	-179.90176	28	22	19
44	H	1.07068	121.71836	179.94992	29	23	20
45	H	1.07067	121.71919	179.94751	30	24	21
46	H	1.07075	121.76159	-179.97943	31	25	19
47	H	1.07076	121.76063	179.93710	32	26	20
48	H	1.07076	121.75928	179.93356	33	27	21
49	F	1.37581	118.80170	-179.94033	34	31	25
50	F	1.37501	118.80556	179.83352	35	29	23
51	F	1.37498	118.80712	179.82738	36	30	24
52	H	.99273	115.41433	-177.18602	7	2	1
53	H	.99281	115.88074	-177.18682	8	4	3
54	H	.99278	115.91971	-177.65666	9	6	5

Plots of $I_{2\omega}/I_{\omega}^2$ vs number density for Molecule **1**-**4** in chloroform at 1064nm. The solid lines represent the linear least squares fit through the experimental data. Inset: HRS spectra obtained by averaging 150 laser pulses in the range of 510–550 nm.





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