

Electronic Supplementary Information (ESI)

What is the role of defect in single-walled carbon nanotubes for Nonlinear optical property?

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1. The selection of the basis set

In order to select the proper basis set to calculating the β_0 in this work, we calculated the β_0 of the **SW5577-xz** structure at the LC-BLYP level using the 6-31G(d) and the larger basis set 6-311G(d). From the Table S1, the number of basis set increase 21% from 1104 for 6-31G(d) to 1332 for 6-311G(d), the β_0 increase only 7.3% from 38043 to 39393 a.u., so the basis set 6-31G(d) is proper in this work.

Table S1: The selection of the basis set.

basis set	6-31G(d)	6-311G(d)
Number of Basis	1104	1332
β_0 (a.u.)	32565	34948

2. The selection of the applied electric field used in the β_0 calculation

In order to select the proper applied electric field, we calculated the β_0 of the **SW5577-xz** structure at the LC-BLYP/6-31G(d) level using the applied electric field from 0.0005 to 0.0015 a.u.. It showed in Table S2 that the applied electric field of 0.0010 a.u. is proper in this work.

Table S2: The selection of the applied electric field.

electric field(a.u.)	0.0005	0.0008	0.0010	0.0012	0.0015
β_0 (a.u.)	32871	32691	32565	32447	32292

3. The β_0 values at the LC-BLYP and HF level using basis set 6-31G(d).

Table S3: The β_0 values at the LC-BLYP and HF level.

structure	β_0 (a.u.)	
	LC-BLYP	HF
Perfect	0	0
DV585-z	5.0×10^2	6.6×10^2
SW5577-z	5.3×10^2	9.2×10^2
DV585-xz	4.6×10^3	6.6×10^3
DV555777	6.0×10^3	6.8×10^3
SV-xz	7.3×10^3	6.4×10^3
SV-z	1.1×10^4	6.0×10^3
SW5577-xz	3.3×10^4	3.8×10^4
SW57-75	2.2×10^5	1.5×10^5

4. The coordinates of the nine CNTs structures

For nine CNTs of perfect and defective molecules, the ground state optimized structures with all real frequencies are obtained at the UB3LYP/6-31G(d) level.

The coordinate of the **Perfect** structure:

C	-2.84594300	-2.09177600	1.20968200
C	-3.55896100	-2.42239100	0.00287000
C	-2.84594000	-2.09463500	-1.20472500
C	-1.42602800	-2.09700100	-1.20623700
C	-0.70850600	-2.41990200	0.00286600
C	-1.42602800	-2.09414100	1.21120300
C	-3.55905500	-1.21147800	-2.09057900
C	-0.70878700	-1.21065200	-2.08982500
C	-1.42586700	-0.00286500	-2.41584100
C	-2.84651300	-0.00286100	-2.41262000
C	-0.70878700	1.20568400	-2.09266900
C	0.70878800	1.20568400	-2.09266900
C	1.42586800	-0.00286500	-2.41583900
C	0.70878800	-1.21065300	-2.08982500
C	1.42602700	-2.09700100	-1.20623700
C	0.70850300	-2.41990500	0.00286600
C	-4.99121200	-2.41525100	0.00285700
C	-5.69162700	-2.05656400	-1.18212500
C	-4.99187400	-1.20785800	-2.08393800

C	-5.69179100	-0.00280900	-2.36729900
C	-4.99187500	1.20289900	-2.08677000
C	-3.55905500	1.20650600	-2.09342100
C	-1.42602700	2.09413900	-1.21120200
C	-2.84594100	2.09177700	-1.20968200
C	2.84594100	-2.09178200	1.20968200
C	3.55905600	-1.20650800	2.09341600
C	1.42602600	-2.09414100	1.21120200
C	2.84651500	0.00286100	2.41261500
C	4.99187500	-1.20290300	2.08676200
C	0.70878800	-1.20568600	2.09266900
C	1.42586900	0.00286500	2.41583900
C	5.69179700	0.00280900	2.36727900
C	-0.70878600	-1.20568500	2.09267000
C	-1.42586500	0.00286500	2.41584300
C	3.55895900	-2.42240900	0.00286700
C	4.99120400	-2.41527500	0.00285600
C	2.84593900	-2.09463900	-1.20472500
C	5.69162000	-2.05375300	1.18697000
C	5.69162200	-2.05656900	-1.18211600
C	3.55905500	-1.21147800	-2.09057200
C	4.99187600	-1.20785900	-2.08392800
C	2.84651500	-0.00286100	-2.41261400

C	5.69179600	-0.00280900	-2.36728200
C	3.55905500	1.20650600	-2.09341300
C	4.99187700	1.20290000	-2.08675800
C	5.69162100	2.05375700	-1.18697200
C	2.84594000	2.09178200	-1.20968300
C	1.42602600	2.09414000	-1.21120200
C	3.55895900	2.42241200	-0.00286700
C	0.70850100	2.41990600	-0.00286600
C	2.84593700	2.09464000	1.20472500
C	4.99120000	2.41528000	-0.00285700
C	1.42602800	2.09700200	1.20623800
C	-0.70850400	2.41990300	-0.00286500
C	3.55905600	1.21147700	2.09057000
C	5.69161900	2.05656500	1.18210900
C	0.70878800	1.21065100	2.08982400
C	-1.42602900	2.09700200	1.20624000
C	4.99187500	1.20785700	2.08392500
C	-0.70878500	1.21065100	2.08982500
C	-3.55896100	2.42239300	-0.00286500
C	-4.99120900	2.41525400	-0.00285700
C	-2.84593900	2.09463400	1.20472500
C	-5.69161700	2.05654800	1.18211000
C	-5.69162700	2.05375200	-1.18698100

C	-3.55905400	1.21147900	2.09058500
C	-4.99186800	1.20785900	2.08394200
C	-2.84651100	0.00286100	2.41262700
C	-5.69179600	0.00280900	2.36729400
C	-3.55905400	-1.20650800	2.09343000
C	-4.99186900	-1.20290400	2.08677800
C	-5.69161800	-2.05373600	1.18697000
H	-6.77895300	0.00282200	2.37923900
H	-6.77873900	-2.06501500	1.19338300
H	-6.77873800	2.06784600	1.18849900
H	-6.77874800	-2.06786900	-1.18850900
H	-6.77874700	2.06504500	-1.19339100
H	-6.77895000	-0.00282200	-2.37923100
H	6.77873900	2.06787500	1.18849300
H	6.77895500	0.00282100	2.37921000
H	6.77874200	2.06505500	-1.19338000
H	6.77895400	-0.00282300	-2.37921000
H	6.77874100	-2.06504300	1.19337900
H	6.77874300	-2.06787800	-1.18849900

The coordinate of the **DV585-z** structure:

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.43420999

C	1.39354295	0.00000000	1.77332012
C	2.17092957	0.42220868	0.61678127
C	1.30755344	0.42220846	-0.48188777
C	1.81835235	-1.10277986	2.54393970
C	3.61579494	0.12621960	0.59864959
C	3.86203482	-1.21225165	1.10983070
C	2.93697561	-1.85317164	1.98592475
C	4.69268589	-1.99629360	0.25201300
C	5.68476270	-1.35422079	-0.52759901
C	5.83360426	0.06374948	-0.43950418
C	4.58390727	0.75278259	-0.16213021
C	4.38392841	1.85446239	-1.12227746
C	-0.95567883	-0.72488797	2.18521917
C	-0.50789053	-1.35814415	3.38417493
C	0.85367215	-1.78795684	3.38179647
C	1.07318307	-3.16487223	3.68445584
C	1.75237395	-3.91768147	2.68033802
C	2.73039177	-3.25329719	1.85840572
C	4.05368295	-3.19718357	-0.23539507
C	3.04932127	-3.80211536	0.55582052
C	4.13745572	2.67776592	-3.25137056
C	4.36762884	2.14355338	-4.53670174
C	3.52055161	1.85446386	-2.22094597

C	4.12199072	0.71209854	-4.66471531
C	5.35503431	2.77193340	-5.39241685
C	2.63491120	0.75278558	-2.64227612
C	3.19990333	0.06375267	-3.79095535
C	6.00606786	1.97310367	-6.37918549
C	1.66679870	0.12622300	-1.88149620
C	1.22833311	-1.21224788	-2.24161986
C	5.24436176	3.39415539	-2.68700947
C	6.26765372	3.95005874	-3.49115150
C	5.53099918	2.67776465	-1.47805085
C	6.09664344	3.89156565	-4.90761075
C	7.60351544	3.89156352	-2.99007821
C	6.83430797	2.14354983	-1.39779052
C	7.89922512	2.77193077	-2.15486921
C	6.90061023	0.71209547	-1.12885133
C	9.01194585	1.97310032	-2.55412935
C	7.68845914	-0.04443249	-2.03783377
C	8.72763061	0.59670981	-2.80108808
C	9.01010901	0.10865642	-4.10634939
C	7.03768699	-1.22084226	-2.57839022
C	6.06048187	-1.89838077	-1.81241463
C	6.92579264	-1.18916242	-4.00834541
C	4.95670190	-2.56591217	-2.46095828

C	5.56284035	-1.22084147	-4.45517076
C	7.91401766	-0.49806728	-4.78493219
C	4.58753002	-1.89838087	-3.68678474
C	3.95771142	-3.21245952	-1.67591325
C	5.19148136	-0.04442920	-5.21530104
C	7.51383996	0.10865900	-6.01039086
C	3.25030686	-1.35421834	-3.62550617
C	2.58073074	-3.19718278	-2.10976490
C	6.17879793	0.59671333	-6.04454190
C	2.25823005	-1.99629115	-2.84589416
C	1.92356253	-4.42661039	-0.07740115
C	0.90259307	-5.03586824	0.72491703
C	1.57447463	-3.80211457	-1.32096002
C	-0.43600856	-5.03649136	0.23690761
C	1.06026065	-5.03649211	2.14094895
C	0.23341502	-3.25329638	-1.31906048
C	-0.79645746	-3.91768116	-0.56311682
C	0.15835742	-1.85317073	-1.54993934
C	-1.93269382	-3.16487161	-0.14060117
C	-0.64832587	-1.10277856	-0.59497224
C	-1.69051879	-1.78795609	0.14424893
C	-2.01476197	-1.35814340	1.46664196
H	-2.68853532	-3.67834490	0.44896503

H	-2.75156073	-1.93362191	2.02216506
H	-1.20716397	-5.49852698	0.84880471
H	-1.22187366	-1.93362352	3.96873082
H	0.28337969	-5.49852863	2.74555940
H	0.32162014	-3.67834640	4.27946590
H	8.26598932	0.63250842	-6.59556504
H	6.77395192	2.44578665	-6.98702129
H	9.75653521	0.63250273	-4.69881084
H	9.78410848	2.44578240	-3.15652129
H	6.87800622	4.29864239	-5.54511728
H	8.40769349	4.29864027	-3.59855168

The coordinate of the **SW5577-z** structure:

C	1.20564200	2.12068500	1.46401500
C	0.70671700	1.04477700	2.25679000
C	1.43806200	-0.14624500	2.37746200
C	2.84840300	-0.05859800	2.20527900
C	3.43789700	1.17833100	1.79931500
C	2.56976600	2.19203900	1.21723900
C	0.71822100	-1.35863000	2.06835300
C	3.58603800	-1.25729000	1.94609000
C	2.86375300	-2.23703800	1.19060100
C	1.43039900	-2.24824300	1.20331600

C	3.57503400	-2.64253500	0.00032500
C	5.00280500	-2.63031600	0.00028400
C	5.70539400	-2.18731300	1.16715100
C	5.01473700	-1.19202000	1.88071000
C	5.63643400	0.11100800	1.90371100
C	4.87436400	1.22465500	1.61598500
C	-0.70671700	1.04477700	2.25679000
C	-1.43806200	-0.14624500	2.37746200
C	-0.71822100	-1.35863000	2.06835300
C	-1.43039900	-2.24824300	1.20331600
C	-0.70927100	-2.60038600	0.00035500
C	0.70927100	-2.60038600	0.00035500
C	2.86374600	-2.23744700	-1.18996400
C	1.43033600	-2.24859100	-1.20264000
C	5.44251500	2.37719800	0.84514400
C	4.48627000	3.07223300	-0.00039300
C	5.44251500	2.37653700	-0.84539900
C	3.16607800	2.80100500	-0.00041300
C	2.56978200	2.19171200	-1.21797200
C	5.70535400	-2.18798600	-1.16688900
C	5.01468800	-1.19269700	-1.88045400
C	5.63639400	0.11028600	-1.90359700
C	3.58599700	-1.25793300	-1.94576400

C	4.87436900	1.22406700	-1.61603000
C	2.84835900	-0.05923400	-2.20524500
C	3.43792600	1.17774500	-1.79964500
C	0.71821100	-1.35922700	-2.06802000
C	-0.71821100	-1.35922700	-2.06802000
C	1.43806400	-0.14690400	-2.37744200
C	-1.43806400	-0.14690400	-2.37744200
C	-1.43033600	-2.24859100	-1.20264000
C	0.70669000	1.04415800	-2.25713000
C	-2.84835900	-0.05923400	-2.20524500
C	-0.70669000	1.04415800	-2.25713000
C	-2.86374600	-2.23744700	-1.18996400
C	-3.58599700	-1.25793300	-1.94576400
C	-3.43792600	1.17774500	-1.79964500
C	-5.01468800	-1.19269600	-1.88045400
C	-4.87436900	1.22406700	-1.61603000
C	-5.63639400	0.11028600	-1.90359700
C	-3.43789700	1.17833100	1.79931500
C	-4.87436400	1.22465500	1.61598500
C	-2.84840300	-0.05859800	2.20527900
C	-5.63643300	0.11100800	1.90371100
C	-5.44251500	2.37719800	0.84514400
C	-3.58603800	-1.25729000	1.94609000

C	-5.01473700	-1.19202000	1.88071000
C	-2.86375300	-2.23703900	1.19060100
C	-5.70539400	-2.18731300	1.16715100
C	-3.57503400	-2.64253500	0.00032500
C	-5.00280500	-2.63031600	0.00028400
C	-5.70535400	-2.18798600	-1.16688900
C	1.20569700	2.12030000	-1.46473000
C	-1.20569700	2.12030000	-1.46473000
C	0.00000000	2.58959500	-0.69366600
C	-2.56978200	2.19171200	-1.21797200
C	0.00000000	2.58970300	0.69275700
C	-3.16607800	2.80100500	-0.00041300
C	-5.44251500	2.37653700	-0.84539900
C	-1.20564200	2.12068500	1.46401500
C	-4.48627000	3.07223300	-0.00039300
C	-2.56976600	2.19203900	1.21723900
H	-6.71452500	0.15931300	-1.76727600
H	-6.79006300	-2.13298200	-1.11831700
H	-6.35590700	2.84917000	-1.20390100
H	-6.79010600	-2.13220000	1.11849000
H	-6.35560800	2.85016500	1.20396800
H	-6.71456400	0.16002400	1.76739300
H	6.79010600	-2.13220000	1.11849000

H	6.35560700	2.85016600	1.20396900
H	6.71456400	0.16002400	1.76739300
H	6.35590700	2.84916900	-1.20390100
H	6.79006200	-2.13298200	-1.11831700
H	6.71452500	0.15931300	-1.76727700

The coordinate of the **SV-z** structure:

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.42846173
C	1.29215977	0.00000000	2.05752617
C	2.39846254	0.55195773	1.37783498
C	2.22888613	1.05873018	0.04139607
C	1.16219799	0.46252359	-0.69377671
C	1.49229808	-1.12723234	2.95730618
C	3.73800729	-0.00468217	1.58526943
C	3.65789453	-1.45206698	1.79963216
C	2.55181261	-2.00436172	2.47938831
C	4.26957402	-2.18845944	0.72481364
C	5.37493173	-1.62856333	0.01483537
C	5.88233302	-0.34561669	0.39567776
C	4.82399262	0.53337713	0.89904424
C	4.62637833	1.65286661	-0.02494305
C	3.34704426	1.59825167	-0.66429426

C	-1.13436581	-0.54515974	2.13066528
C	-0.92967405	-1.15906735	3.39993544
C	0.38054895	-1.68547641	3.62454102
C	0.29040374	-3.10048781	3.80853348
C	0.96749108	-3.88965943	2.83457433
C	2.08443925	-3.31679279	2.12654123
C	3.40277122	-3.10271955	0.05658823
C	2.34698319	-3.73455919	0.78600171
C	4.43769214	2.22745620	-2.78547035
C	4.74100837	1.84446309	-4.13609100
C	3.34992209	1.59703390	-2.09259411
C	4.33487227	0.52074654	-4.48964785
C	5.87685922	2.42698246	-4.80676017
C	2.59575164	0.53539800	-2.70773256
C	3.22020855	-0.09405052	-3.83785975
C	6.59279335	1.66133186	-5.76897108
C	1.57643764	-0.12144182	-1.94995572
C	1.14995832	-1.50042786	-2.02773812
C	5.52932179	2.76787219	-2.02792875
C	6.65993101	3.34317482	-2.71416000
C	5.72476941	2.19382287	-0.72503129
C	6.67331662	3.38301776	-4.12753961
C	7.95166569	3.27266069	-2.11574370

C	7.05030957	1.63437243	-0.51746933
C	8.15047553	2.17811178	-1.21905618
C	6.97898546	0.19809103	-0.30499039
C	9.18145876	1.31578349	-1.70389832
C	7.63158858	-0.57730382	-1.32389126
C	8.77023078	-0.01478629	-2.00743253
C	9.07083830	-0.43197925	-3.32462242
C	6.80635917	-1.54162208	-1.99221485
C	5.63768298	-2.04330172	-1.32643133
C	6.85698122	-1.52252794	-3.42746379
C	4.48334890	-2.46818915	-2.07558130
C	5.58271881	-1.46485609	-4.07175101
C	8.00142906	-0.95369675	-4.09525037
C	4.42310608	-2.00813066	-3.43501107
C	3.31055945	-2.88081791	-1.36920259
C	5.40807840	-0.33092959	-4.95170811
C	7.83264644	-0.31155109	-5.35374279
C	3.14134182	-1.51081531	-3.78934387
C	1.92817328	-2.73872225	-1.76710492
C	6.54055960	0.24725427	-5.58613052
C	1.24649353	-4.29814584	0.05469528
C	0.13844254	-4.88358211	0.77847258
C	0.99517982	-3.67703260	-1.20165331

C	-1.18452503	-4.81707082	0.24786871
C	0.16531575	-4.86564326	2.19703173
C	-0.34796926	-3.19240960	-1.36014905
C	-1.43550857	-3.72259724	-0.63190620
C	-0.19433832	-1.78425499	-1.60004172
C	-2.43980046	-2.81967798	-0.17253428
C	-0.85428527	-0.95534933	-0.64885729
C	-1.99850347	-1.48323488	0.06281034
C	-2.23144002	-1.05188161	1.39435992
H	-3.29252474	-3.20032669	0.38453727
H	-3.07443323	-1.47266862	1.93836982
H	-2.00406278	-5.25051389	0.81606440
H	-1.77840371	-1.55032790	3.95502234
H	-0.68248283	-5.27877994	2.73943545
H	-0.53622921	-3.52690271	4.37102350
H	8.69908832	0.11628436	-5.85210093
H	7.44893993	2.10554604	-6.27077971
H	9.92479689	0.00610158	-3.83636958
H	10.05183464	1.73523554	-2.20199338
H	7.53523691	3.80843297	-4.63661993
H	8.80221619	3.72365562	-2.62047908

The coordinate of the **SV-xz** structure:

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.43494053
C	1.28844055	0.00000000	2.07053941
C	2.43776379	0.48405982	1.36147423
C	2.27274649	0.94709642	0.02075524
C	1.13163724	0.49083073	-0.69955721
C	1.47203392	-1.01958663	3.07358286
C	3.75948170	-0.02553447	1.64602026
C	3.74817398	-1.38275515	2.11681121
C	2.58049311	-1.88923571	2.77316181
C	4.55132459	-2.26819627	1.30064822
C	5.70522107	-1.79371953	0.62531843
C	6.03189941	-0.38935685	0.67154685
C	4.89487052	0.46478927	0.91343854
C	4.69684017	1.45579297	-0.11135238
C	3.40025834	1.42263757	-0.71195374
C	-1.14275952	-0.54765800	2.13595200
C	-0.96842263	-1.03471517	3.45013607
C	0.32331727	-1.55540722	3.74534417
C	0.24381061	-2.95101535	4.02755219
C	0.95624517	-3.75989983	3.10964800
C	2.13716832	-3.23416312	2.50545212
C	3.70762942	-3.24121452	0.64703615

C	2.48264037	-3.65594613	1.19151279
C	4.51780482	1.70440491	-2.89704445
C	4.78262855	1.05126345	-4.14752158
C	3.41992451	1.26515251	-2.13483985
C	4.43140479	-0.36449668	-4.15237492
C	5.87259800	1.55228620	-4.92066782
C	2.58503002	0.23740996	-2.66815456
C	3.30393592	-0.85631083	-3.34972725
C	6.65594668	0.66177867	-5.70091061
C	1.34288635	0.02023672	-2.06798947
C	0.60965556	-1.05553927	-2.56331538
C	5.61008367	2.33867593	-2.24276330
C	6.71600313	2.81460825	-3.02873019
C	5.80742638	1.92747659	-0.88027702
C	6.66553934	2.64026286	-4.43621192
C	8.00409674	2.86164013	-2.43823509
C	7.12411314	1.43380269	-0.61030785
C	8.23520897	1.92737711	-1.39428053
C	7.14954389	0.09751235	-0.08887869
C	9.34573535	1.07584680	-1.63739164
C	7.93646459	-0.81203495	-0.89666452
C	9.02811006	-0.31055097	-1.67784868
C	9.32133385	-0.90056101	-2.93908305

C	7.17803314	-1.91630187	-1.40475951
C	6.08469315	-2.41414646	-0.63264104
C	7.15052108	-2.06077669	-2.83320787
C	5.02365136	-3.00205147	-1.34371935
C	5.84377931	-2.13858891	-3.44356177
C	8.24747961	-1.54362971	-3.60513436
C	4.77223790	-2.62050115	-2.68464273
C	3.79091336	-3.27222964	-0.74444689
C	5.57829445	-1.17463648	-4.46265673
C	8.00950142	-1.11167068	-4.93941682
C	3.37334142	-2.22277853	-2.76107432
C	2.66687193	-2.99502008	-1.61592178
C	6.68504855	-0.67296713	-5.22869090
C	1.43396963	-4.02869363	0.29464713
C	0.27941905	-4.63486934	0.94270404
C	1.38944816	-3.45890144	-1.05388833
C	-0.94317732	-4.73057162	0.22397987
C	0.18604600	-4.68680619	2.34837257
C	-0.01375060	-3.13683908	-1.42345567
C	-1.10136164	-3.74839227	-0.79427732
C	-0.21689928	-1.71071518	-1.70092549
C	-2.21471382	-2.97377060	-0.27795970
C	-0.83294186	-0.99995164	-0.62205074

C	-1.89647782	-1.62622473	0.10447419
C	-2.19514269	-1.18597064	1.40561606
H	-3.10398244	-3.46955950	0.10037177
H	-2.99051917	-1.67135074	1.96708497
H	-1.79021621	-5.27172498	0.63590226
H	-1.82769569	-1.45470098	3.96772617
H	-0.71241536	-5.11281487	2.78958404
H	-0.65101760	-3.34257175	4.50543576
H	8.83644391	-0.72559746	-5.53044245
H	7.47523114	1.04407797	-6.30507710
H	10.14985418	-0.50924136	-3.52505453
H	10.17984999	1.44819572	-2.22714409
H	7.48736110	3.00548792	-5.04721909
H	8.84726150	3.21356244	-3.02803313

The coordinate of the **DV585-xz** structure:

C	2.41405100	1.95202400	-1.27082900
C	3.06014600	2.60568500	-0.16377200
C	2.40685600	2.26507000	1.10389600
C	0.97109800	2.03780700	1.16177600
C	0.20343900	2.20214800	-0.11430100
C	1.01464400	1.77420400	-1.24466700
C	3.33166400	1.53533100	1.94140600

C	0.46215900	1.08897400	2.11339200
C	1.46428000	0.10897200	2.48368900
C	2.84367400	0.26828900	2.36388500
C	0.90614000	-1.16639900	2.22964500
C	-0.48301300	-1.00176400	2.13418100
C	-0.84679900	0.37198000	2.15593300
C	-1.18128900	2.24771700	-0.36772400
C	4.46146700	2.80614800	-0.23949500
C	5.27991800	2.64833500	0.92593100
C	4.76059100	1.69921000	1.84256300
C	5.61264000	0.58760600	2.08781600
C	5.06536600	-0.70939500	1.92307900
C	3.63805200	-0.88337200	2.03152900
C	1.57468900	-2.09953000	1.42406300
C	2.99316500	-1.96800500	1.34823800
C	-3.02282400	1.82982100	-1.75719700
C	-3.76353200	0.72324200	-2.21344600
C	-1.63283900	1.74195400	-1.63915400
C	-3.04511400	-0.54592600	-2.24286400
C	-5.18972000	0.76708500	-1.99269900
C	-0.91898600	0.68551800	-2.24013900
C	-1.60327300	-0.56390700	-2.32915500
C	-5.88590700	-0.45945900	-1.87859800

C	0.46350500	0.76455200	-2.10329400
C	1.25762200	-0.40383100	-2.28611100
C	-3.51493500	2.59288600	-0.64975600
C	-4.89228800	2.59302300	-0.39360200
C	-2.46760000	2.46495500	0.36607300
C	-5.75896500	1.86525200	-1.27715500
C	-5.28935900	2.56842300	0.96601500
C	-2.93655400	1.83274600	1.54855300
C	-4.37314500	1.93259800	1.84824000
C	-2.24421600	0.64321300	2.07513500
C	-5.06737400	0.87322700	2.49941200
C	-3.10443700	-0.52194600	2.12609800
C	-4.52223100	-0.41304200	2.33511100
C	-5.37988900	-1.46089400	1.89541700
C	-2.63267300	-1.76604900	1.58702100
C	-1.26538400	-1.98341600	1.50889000
C	-3.50496400	-2.43237000	0.65234000
C	-0.62153500	-2.64289800	0.37453900
C	-2.89145800	-2.40865700	-0.68172100
C	-4.88748400	-2.29599100	0.83718800
C	-1.47407400	-2.46050300	-0.81631400
C	0.78214000	-2.64483300	0.30271700
C	-3.69959500	-1.62669700	-1.59651500

C	-5.74744600	-2.20351500	-0.29900200
C	-0.82399400	-1.67542300	-1.83892100
C	1.45278500	-2.40973800	-0.98037400
C	-5.14655700	-1.57748800	-1.42742800
C	0.62023800	-1.61253700	-1.87861600
C	3.68225500	-2.47312200	0.17861300
C	5.08298300	-2.33136000	0.11865900
C	2.86482600	-2.30177400	-1.03594600
C	5.73276100	-1.97337600	-1.11051400
C	5.79879500	-1.65821800	1.16050300
C	3.49117700	-1.35928300	-1.93926100
C	4.91982300	-1.18347100	-1.97557000
C	2.66826800	-0.24805800	-2.27461600
C	5.46505600	0.08727600	-2.28078900
C	3.21855000	1.05323500	-2.03652500
C	4.64613200	1.22861300	-2.07228900
C	5.20470900	2.32031400	-1.36057300
H	6.88260300	-1.58852900	1.11039800
H	6.81622100	-1.92832100	-1.17478300
H	6.68783100	0.72150600	1.99334400
H	6.34964900	2.83237000	0.87202000
H	6.27758200	2.49147000	-1.40138100
H	6.54605900	0.20790900	-2.29686900

H	-6.96039300	-0.44483000	-1.71016700
H	-6.83206300	1.87807600	-1.10179800
H	-6.34257200	2.60582800	1.23347300
H	-6.12652000	0.98827900	2.71484100
H	-6.44853000	-1.39344400	2.08329400
H	-6.82716100	-2.17743400	-0.17805100

The coordinate of the **DV555777** structure:

C	1.42807500	0.39545400	-2.45125700
C	0.69810400	1.54424900	-2.04805700
C	1.18905900	2.27280400	-0.90825000
C	2.56638300	2.28766700	-0.67406500
C	3.40174100	1.61616700	-1.65177000
C	2.82760500	0.46089400	-2.29586200
C	0.00000000	2.37387800	-0.02660400
C	3.21706400	2.38469200	0.64057100
C	2.59573500	1.70814500	1.72757600
C	1.24419000	1.09818800	1.72524000
C	3.47659600	0.81701800	2.43843500
C	4.88666800	0.89201000	2.39925800
C	5.45983600	1.98337800	1.70107900
C	4.66549700	2.53672000	0.65853400
C	5.40900300	2.50811900	-0.56121900

C	4.82356500	1.72157000	-1.59054600
C	-0.69810500	1.54424900	-2.04805700
C	-1.18905900	2.27280400	-0.90825000
C	-1.24419000	1.09818800	1.72524000
C	0.00000000	1.64659500	1.17883100
C	2.83054000	-0.44689500	2.37680700
C	1.44331300	-0.24788600	2.08689100
C	5.62240300	0.63679800	-2.04004200
C	5.01632000	-0.64544000	-2.06862000
C	5.72512400	-1.66977400	-1.38577000
C	3.58511100	-0.74278200	-2.16749800
C	2.87273500	-1.82162700	-1.55593600
C	5.62629900	-0.32656800	2.35023300
C	4.97206200	-1.49300300	1.86874300
C	5.69808400	-2.21381300	0.87239000
C	3.53153300	-1.55251900	1.85823100
C	5.00122600	-2.36006400	-0.37730500
C	2.82422500	-2.30735400	0.81167700
C	3.57883600	-2.40047900	-0.41885800
C	0.68459800	-1.40358600	1.64269700
C	-0.68459900	-1.40358600	1.64269700
C	1.42651500	-2.29122700	0.76016200
C	-1.42651500	-2.29122700	0.76016200

C	-1.44331300	-0.24788600	2.08689000
C	0.70072300	-2.44918700	-0.51080100
C	-2.82422600	-2.30735400	0.81167700
C	-0.70072300	-2.44918700	-0.51080100
C	-2.83054100	-0.44689500	2.37680600
C	-3.53153400	-1.55251800	1.85823000
C	-3.57883600	-2.40048000	-0.41885800
C	-4.97206300	-1.49300200	1.86874200
C	-5.00122600	-2.36006500	-0.37730500
C	-5.69808400	-2.21381400	0.87238900
C	-3.40174100	1.61616700	-1.65176900
C	-4.82356500	1.72157000	-1.59054500
C	-2.56638300	2.28766700	-0.67406500
C	-5.40900300	2.50811900	-0.56121900
C	-5.62240200	0.63679800	-2.04004200
C	-3.21706400	2.38469300	0.64057100
C	-4.66549700	2.53672100	0.65853400
C	-2.59573500	1.70814600	1.72757600
C	-5.45983600	1.98337800	1.70107900
C	-3.47659700	0.81701800	2.43843500
C	-4.88666800	0.89201100	2.39925800
C	-5.62629900	-0.32656700	2.35023200
C	1.44334200	-1.86300300	-1.61675000

C	-1.44334200	-1.86300300	-1.61675000
C	0.71939700	-0.85577900	-2.34100400
C	-2.87273500	-1.82162700	-1.55593600
C	-0.71939700	-0.85577900	-2.34100400
C	-3.58511100	-0.74278200	-2.16749800
C	-5.72512300	-1.66977500	-1.38576900
C	-1.42807500	0.39545400	-2.45125700
C	-5.01632000	-0.64544000	-2.06862000
C	-2.82760600	0.46089400	-2.29586100
H	6.71340400	-0.28717600	2.32664200
H	6.54003300	2.10248700	1.66381500
H	6.48633700	2.64608500	-0.53230800
H	6.70590900	0.71341600	-1.98511400
H	6.81150200	-1.64431000	-1.35083800
H	6.78400800	-2.22926100	0.89163900
H	-6.48633600	2.64608500	-0.53230800
H	-6.70590900	0.71341600	-1.98511300
H	-6.81150200	-1.64431100	-1.35083800
H	-6.78400800	-2.22926200	0.89163900
H	-6.71340400	-0.28717500	2.32664100
H	-6.54003300	2.10248900	1.66381500

The coordinate of the **SW5577-xz** structure:

C	2.66963300	1.89866100	-1.33982600
C	3.47670300	0.93601200	-2.12529300
C	3.02414500	-0.40384300	-2.32867500
C	1.68944000	-0.92462900	-2.05980300
C	0.36960600	1.18878300	-2.11347900
C	1.25156600	1.98719900	-1.30854900
C	3.93909700	-1.44979100	-1.99501900
C	0.50793000	-0.22436100	-2.26459300
C	1.82000400	-2.06160200	-1.22219900
C	3.22582300	-2.28854500	-1.07579200
C	0.90002600	-2.31759600	-0.13149100
C	-0.50966900	-2.26495700	-0.23044900
C	-1.31680700	-1.86607100	-1.42411300
C	-0.82099100	-0.81128400	-2.26213500
C	-1.72429300	0.26301700	-2.51716500
C	-1.03215900	1.45829100	-2.13947300
C	4.92447800	1.11439500	-2.13977800
C	5.82667600	0.01381500	-2.26083400
C	5.33365100	-1.26549400	-1.90062200
C	6.03156000	-1.97534300	-0.88124100
C	5.27625700	-2.35180600	0.26481800
C	3.83801200	-2.47524900	0.18155300
C	1.57002500	-2.04942100	1.15410300

C	2.99153800	-2.04526100	1.28831200
C	-3.11090200	2.19528700	-1.08725600
C	-3.75832000	2.47751100	0.17701900
C	-1.67945500	2.26757200	-1.18088300
C	-2.94366800	2.06064000	1.30877800
C	-5.17310900	2.38921700	0.26452800
C	-0.85704300	2.52492600	-0.00029500
C	-1.52416700	2.11608500	1.23147900
C	-5.79678500	1.87201900	1.44374100
C	0.55548500	2.46461600	-0.09192800
C	1.32190200	2.14403500	1.09805200
C	-3.84337700	1.28368300	-1.92294000
C	-5.27169500	1.15685500	-1.80101800
C	-3.10565600	0.14735800	-2.39015400
C	-5.94750600	1.97834300	-0.86267800
C	-5.88171400	-0.09132000	-2.09676700
C	-3.64121900	-1.14023000	-2.08688700
C	-5.07234300	-1.25529900	-1.98305700
C	-2.75467300	-2.02331400	-1.36292600
C	-5.62204300	-2.28358900	-1.17650500
C	-3.38615200	-2.55881500	-0.16458900
C	-4.79540000	-2.69834900	-0.08965600
C	-5.49276600	-2.40574500	1.12802700

C	-2.66619000	-2.18538600	1.03277200
C	-1.26166300	-2.06883500	0.99544800
C	-3.42148100	-1.37154200	1.94497300
C	-0.60764400	-1.20631300	1.94483000
C	-2.79717100	-0.13915400	2.31169200
C	-4.85493700	-1.47235600	1.98774500
C	-1.38017100	-0.05253200	2.30368000
C	0.79901700	-1.15867100	1.98515100
C	-3.57447900	1.04387300	2.11223800
C	-5.61303200	-0.33145400	2.35467000
C	-0.74896400	1.19684100	2.02890700
C	1.43799200	0.07691800	2.32580700
C	-5.00959900	0.93901700	2.17157200
C	0.66738600	1.24926600	2.00616800
C	3.62227300	-1.05809400	2.12901800
C	5.05788700	-0.97381300	2.20532700
C	2.85547900	0.13930800	2.34199300
C	5.67457300	0.29455400	2.35334000
C	5.86868600	-1.89772800	1.47996200
C	3.49547400	1.35443700	1.95806700
C	4.93027600	1.42728200	1.93917100
C	2.72913500	2.17120300	1.06135000
C	5.55587400	2.28308400	0.99223300

C	3.39746400	2.40739300	-0.19884900
C	4.81050200	2.52702400	-0.20151900
C	5.53156000	2.13662800	-1.35939700
H	-6.57029100	-2.53912600	1.17640400
H	-6.69803100	-0.40217800	2.38266200
H	-6.69928400	-2.41925800	-1.12456000
H	-6.88078400	1.84079600	1.51536100
H	-6.96064600	-0.18879900	-2.00241700
H	-7.03093300	1.93287200	-0.78451300
H	6.95062600	-1.82382200	1.55119200
H	7.10913900	-1.86137200	-0.78807700
H	6.76051700	0.35224500	2.37172700
H	6.89577900	0.21116500	-2.24181000
H	6.63815900	2.38506000	0.98315600
H	6.60639100	2.28828600	-1.41127400

The coordinate of the **SW57-75** structure:

C	-3.25268900	-1.22751900	-2.11924900
C	-3.66000000	0.11065300	-2.27036600
C	-2.68854200	1.11934700	-1.87815700
C	-1.29753800	0.77371800	-1.98529700
C	-0.85221900	-0.60193100	-1.98872100
C	-1.89883200	-1.53517200	-1.70975200

C	-3.19353700	2.17085000	-1.02352400
C	-0.26141800	1.71407100	-1.71730100
C	-1.11362800	2.41741700	0.49247300
C	-2.49542700	2.36625200	0.29247700
C	-0.16565800	2.58369800	-0.60132900
C	1.22590000	2.78530100	-0.35293500
C	1.98027700	2.29821500	-1.48967800
C	1.07650700	1.41050300	-2.14888100
C	1.49541500	0.07147700	-2.30717000
C	0.53888700	-0.94473300	-1.89575800
C	-5.07896900	0.39565600	-2.25000200
C	-5.48948000	1.70397800	-1.88532100
C	-4.59320400	2.42972600	-1.03766800
C	-5.31401400	2.66290100	0.17958500
C	-4.74135500	2.06146400	1.33657900
C	-3.32160100	1.89390900	1.36978500
C	-1.34556900	0.74039300	2.21002700
C	-2.74820000	0.85688900	2.15708200
C	2.47367100	-2.22180500	-1.04855500
C	3.17608800	-2.54074200	0.19403700
C	1.07674200	-1.98963800	-1.03909800
C	2.57196200	-1.92755800	1.34473900
C	4.58063200	-2.77076300	0.21472000

C	0.35711400	-2.19523600	0.27235500
C	1.17797200	-1.74191200	1.36893300
C	5.35405000	-2.35515600	1.33728300
C	-1.01679700	-2.25357600	0.48170700
C	-1.98203400	-2.39644600	-0.60277900
C	3.35711800	-1.51641700	-1.96556000
C	4.76164700	-1.77818700	-1.95681300
C	2.90487500	-0.20210400	-2.32035600
C	5.32161700	-2.67952200	-1.00014300
C	5.68865400	-0.74240500	-2.25350300
C	3.84275700	0.86683400	-2.11534100
C	5.25302800	0.59137500	-2.05937700
C	3.34045800	2.01770500	-1.41831400
C	6.09191500	1.42355900	-1.26634800
C	4.05517700	2.34762100	-0.21148300
C	5.45615900	2.07518900	-0.16627000
C	6.06022500	1.74181800	1.07555600
C	3.23360800	2.25038600	0.98266900
C	1.81166000	2.45386900	0.90702900
C	3.77725200	1.32998800	1.95179800
C	0.91661300	1.68720200	1.77873700
C	2.88607000	0.26680900	2.31787000
C	5.19415400	1.09297900	2.00218300

C	1.47206100	0.47064000	2.27254400
C	-0.51147400	1.77518800	1.64401600
C	3.40774000	-1.05370200	2.10465000
C	5.69125300	-0.19308700	2.34147100
C	0.61638100	-0.69199400	2.14916800
C	-1.60924900	-1.61304200	1.64639900
C	4.82567100	-1.29072400	2.12047200
C	-0.78144800	-0.57388000	2.20899400
C	-3.58864600	-0.31330100	2.28770800
C	-5.01575400	-0.11838600	2.34598600
C	-3.03253600	-1.52885600	1.79671900
C	-5.87708700	-1.18321800	1.98460700
C	-5.55343600	1.17119700	2.07444300
C	-3.92787500	-2.30212200	0.93351900
C	-5.35476000	-2.10820600	1.03805800
C	-3.37871100	-2.60679000	-0.33988700
C	-6.18457800	-2.13711500	-0.12526900
C	-4.15316200	-2.11996300	-1.45997200
C	-5.52659900	-1.82432900	-1.35284500
C	-6.01086500	-0.64579100	-1.98640700
H	-7.25460000	-1.97626600	-0.02085500
H	-7.06857400	-0.39802800	-1.92649500
H	-6.95300700	-1.04201500	2.04992200

H	-6.54380300	1.96608600	-1.90477000
H	-6.63201900	1.30946900	2.08799600
H	-6.37220700	2.90752700	0.15124400
H	6.76603200	-0.35647300	2.37093500
H	6.42382900	-2.54856200	1.35120100
H	7.13226300	1.57040600	1.13054700
H	7.16004500	1.22597500	-1.22717900
H	6.38201500	-2.91496100	-1.02131800
H	6.75353200	-0.96387600	-2.24293300