

SUPPLEMENTARY MATERIALS**Functionalized C₆₀ Fullerenes as Inorganic Redox Nanostructures:
A Quantum Chemical Approach**

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Table S1

Final Single Point energies (a.u.) of the optimized structures (PBE0-D4 \ def2-TZVPD \ SMD(Water)) for calculating the electron capture energy ΔE from a superoxide ion

$C_{60}X_n$	n = 2		n = 4		n = 6	
	Neutral	Anionic	Neutral	Anionic	Neutral	Anionic
CH ₃	-2364,371112	-2364,504528	-2444,137233	-2444,270031	-2523,924751	-2759,601776
C ₂ H ₅	-2442,92192	-2443,055088	-2601,26276	-2601,394686	-2524,042797	-2759,719091
C ₃ H ₇	-2521,484266	-2521,617224	-2758,382319	-2758,513746	-2523,924751	-2759,601776
F	-2484,179112	-2484,317573	-2683,746473	-2683,906694	-2524,042797	-2759,719091
Cl	-3204,730472	-3204,868458	-4124,867197	-4125,026305	-2523,924751	-2759,601776
Br	-7432,325412	-7432,462593	-12580,06531	-12580,22389	-2524,042797	-2759,719091
OH	-2436,167336	-2436,303487	-2587,719923	-2587,86798	-2523,924751	-2759,601776
OCH ₃	-2514,682842	-2514,81861	-2744,765049	-2744,91315	-2524,042797	-2759,719091
OC ₂ H ₅	-2593,254522	-2593,390029	-2901,90446	-2902,050667	-2523,924751	-2759,601776
SH	-3081,943755	-3082,079843	-3879,28766	-3879,426218	-2524,042797	-2759,719091
SCH ₃	-3160,506822	-3160,641708	-4036,416973	-4036,560733	-2523,924751	-2759,601776
SC ₂ H ₅	-3239,06883	-3239,203633	-4193,542462	-4193,685829	-2524,042797	-2759,719091
NH ₂	-2396,444209	-2396,57867	-2508,280909	-2508,420217	-2523,924751	-2759,601776
COOH	-2662,732799	-2662,870514	-3040,874107	-3041,020477	-2524,042797	-2759,719091
COCl	-2623,027086	-2623,163202	-2961,457389	-2961,60221	-2523,924751	-2759,601776
CONH ₂	-3431,259145	-3431,397917	-4577,921572	-4578,075725	-2524,042797	-2759,719091
CN	-2470,132092	-2470,271702	-2655,656649	-2655,812932	-2523,924751	-2759,601776
NO ₂	-2694,564631	-2694,704902	-3104,533977	-3104,699025	-2524,042797	-2759,719091
C_{60}	Neutral			Anionic		
	-2284,590284			-2284,738545		
O ₂	-150,237466			-150,3722957		

Table S2

Final Single Point energies (a.u.) of the calculated structures (PBE0-D4 \ def2-TZVPD) for calculating the electronic chemical potential μ using CDFT

$C_{60}X_n$	n = 2		n = 4		n = 6	
	Neutral	Anionic	Neutral	Anionic	Neutral	Anionic
CH ₃	-2364,354422	-2364,44705	-2444,123029	-2444,212279	-2523,909734	-2523,980156
C ₂ H ₅	-2442,906351	-2442,998465	-2601,250607	-2601,339151	-2759,589568	-2759,658595
C ₃ H ₇	-2521,469305	-2521,561192	-2758,371095	-2758,459598	-2995,272944	-2995,342070
F	-2484,160101	-2484,263002	-2683,734204	-2683,838980	-2883,315738	-2883,418081
Cl	-3204,712423	-3204,814671	-4124,848050	-4124,953236	-5044,991864	-5045,091887
Br	-7432,306175	-7432,407900	-12580,03922	-12580,14435	-17727,78145	-17727,88469
OH	-2436,139015	-2436,237100	-2587,672414	-2587,773623	-2739,250091	-2739,335511
OCH ₃	-2514,663788	-2514,760052	-2744,743582	-2744,845802	-2974,836854	-2974,918639
OC ₂ H ₅	-2593,235246	-2593,330882	-2901,882275	-2901,982892	-3210,552928	-3210,633181
SH	-3081,924879	-3082,023573	-3879,270989	-3879,369035	-4676,625299	-4676,713080
SCH ₃	-3160,489419	-3160,585626	-4036,394967	-4036,495549	-4912,314951	-4912,396832
SC ₂ H ₅	-3239,051516	-3239,147692	-4193,520570	-4193,620267	-5148,003900	-5148,084397
NH ₂	-2396,416573	-2396,510712	-2508,250627	-2508,338401	-2620,094281	-2620,170063
COOH	-2662,705195	-2662,803073	-3040,821798	-3040,923720	-3418,964600	-3419,049200
COCl	-3431,239959	-3431,345537	-4577,900842	-4578,012475	-5724,572519	-5724,676841
CONH ₂	-2622,981430	-2623,079791	-2961,397985	-2961,502292	-3299,827053	-3299,913029
CN	-2470,105974	-2470,217213	-2655,620344	-2655,752846	-2841,152701	-2841,272903
NO ₂	-2694,545314	-2694,654964	-3104,504980	-3104,638203	-3514,477704	-3514,597501
$C_{60}X_n$	n = 2		n = 4		n = 6	
	Cationic		Cationic		Cationic	
CH ₃	-2364,085557		-2443,857763		-2523,648327	
C ₂ H ₅	-2442,639265		-2600,983513		-2759,331752	
C ₃ H ₇	-2521,203331		-2758,110264		-2995,016927	
F	-2483,877466		-2683,447989		-2883,021843	
Cl	-3204,432458		-4124,565903		-5044,702368	

Br	-7432,028061	-12579,75985	-17727,49524
OH	-2435,862699	-2587,397253	-2738,974011
OCH ₃	-2514,390263	-2744,471185	-2974,567486
OC ₂ H ₅	-2592,963146	-2901,607402	-3210,287688
SH	-3081,650553	-3878,998486	-4676,349837
SCH ₃	-3160,219516	-4036,125702	-4912,048436
SC ₂ H ₅	-3238,783421	-4193,254426	-5147,742179
NH ₂	-2396,145074	-2507,985539	-2619,829882
COOH	-2662,430581	-3040,545371	-3418,689600
COCl	-3430,957578	-4577,614935	-5724,279287
CONH ₂	-2622,708024	-2961,123671	-3299,554784
CN	-2469,816711	-2655,315447	-2840,840200
NO ₂	-2694,256916	-3104,204056	-3514,169100
C ₆₀	Neutral	Anionic	Cationic
	-2284,586269	-2284,683714	-2284,302306

Cartesian coordinates of the calculated structures C₆₀X₂

C₆₀(CH₃)₂

C	0.17983084394518	1.53028782423454	3.20653157859165
C	-1.06419356307142	0.75078360399206	3.64121159553498
C	-0.56372291934657	-0.67146827364115	3.37433165385393
C	0.86528446733388	-0.69134060076310	3.29606255472353
C	1.32601177517009	0.67334148516060	3.19189237924869
C	2.45057926051167	0.97486758865599	2.42132919455714
C	3.13858296360858	-0.08012713893949	1.70710735107770
C	2.69418516117339	-1.39420897089032	1.80674363275072
C	1.54301412146971	-1.71134784231320	2.62564335214270
C	0.78964590685781	-2.74115977408578	1.96663326175829
C	-0.60493219886856	-2.69861117643982	2.01468529296987
C	-1.28166241911207	-1.65480919043027	2.74010623119947
C	-2.49489842849956	-1.30246642625634	1.98494974791675
C	-2.90053041162698	0.00742832472797	1.91934046923633
C	-2.38586746671862	1.13467669532905	2.81847163362883
C	-2.15719545903993	2.20940952898993	1.75224822744046
C	-2.89484515325523	1.89956413047122	0.56547237933459
C	-3.35605967608963	0.53491757204855	0.66915363184592
C	-3.43581095257891	-0.26536035941792	-0.47223113058659
C	-3.01440121810203	-1.63645851269107	-0.40020609941245
C	-2.53636494594043	-2.13683660363243	0.81230572267346
C	-1.37514934815567	-2.99778678368036	0.82816041834239
C	-0.73020486976574	-3.32467103219832	-0.36105325188902
C	0.71656765140547	-3.35212390579178	-0.41324163725916
C	1.46073597034021	-3.06470055698967	0.72904838617198
C	2.64179049964793	-2.23309700369908	0.63026411553378
C	3.03283075000265	-1.72218891982750	-0.60482695793042
C	3.49516942978331	-0.35436120936664	-0.70892708022664
C	3.54958168563486	0.45086654578811	0.42629872507689
C	3.11556627895522	1.83054565854872	0.35696846228810
C	2.64274407614735	2.34928884034194	-0.84664218061656
C	2.58957273312999	1.51516941746164	-2.02328595190070
C	3.00731669645230	0.18786777378937	-1.95707755375877
C	2.24463965374424	-0.84381591223232	-2.62536812872292
C	2.25999640814174	-2.02366796707892	-1.78875833019033

C	1.12367794282349	-2.82407738542336	-1.69328171825067
C	-0.07104533213017	-2.47677906864524	-2.43664331462682
C	-1.21629335608399	-2.79063006786148	-1.61606156668315
C	-2.33609805825280	-1.96173515543883	-1.63366038852167
C	-2.34800017109412	-0.78351741185646	-2.47481384199739
C	-3.03100392972020	0.26880806865454	-1.75583814582366
C	-2.58659319385931	1.58288352392939	-1.85542473845665
C	-2.52738881985397	2.42103178805867	-0.67634296216530
C	-1.36144854443904	3.25387938039240	-0.77196249390751
C	-0.68218751044563	2.93331967520565	-2.00589626092185
C	-1.44129361394262	1.90035014617697	-2.67900643334482
C	-0.78000245234469	0.88756546546871	-3.36948179257248
C	-1.24184504601884	-0.48035182758764	-3.26485144037546
C	-0.08207444363471	-1.34295091553619	-3.24625940308167
C	1.09664697556656	-0.51014496681810	-3.33927882207496
C	0.66486970271456	0.86829562712868	-3.41476670028068
C	1.39475341097931	1.86211583436891	-2.76673439561673
C	0.71023149794468	2.91121426641129	-2.04950664877324
C	1.47701707803146	3.20783999307090	-0.85760032285627
C	0.82106776756055	3.50222899399328	0.33401863003012
C	-0.62385211755523	3.52468809653595	0.38197646688366
C	-1.04079338052851	3.00303776254656	1.65762428917356
C	0.17247603084554	2.65032527483246	2.41243975246244
C	1.30801703374307	2.96342622185288	1.58418104762853
C	2.44189378197630	2.14899636949690	1.59479452511359
C	-3.54677161134422	1.59245796961265	3.72365869762350
C	-1.23244426855917	0.92246397677789	5.16383905330911
H	-1.45613629367228	1.96404933350763	5.42991992798700
H	-0.29436938546031	0.64297414357373	5.66416460753208
H	-2.02707247318386	0.27427026815225	5.55639952275677
H	-4.41636063937405	1.83905377559622	3.09805329365575
H	-3.28182660775333	2.49042870880498	4.29750424630699
H	-3.84912303511871	0.79916805304356	4.41989611536330

C₆₀(C₂H₅)₂

C	0.05409721917437	1.29594611463631	3.37818643679586
C	-1.17750858323991	0.46034602488382	3.74221047607993
C	-0.63876260173338	-0.92603985898273	3.36736244082579
C	0.79122782673395	-0.91004286434063	3.31864251840773
C	1.22160766491443	0.46803748145148	3.32079283223699
C	2.35079042808560	0.84571955226646	2.59085790412585
C	3.07442188433206	-0.14272298500619	1.81853554230868
C	2.66081006865199	-1.47045123258398	1.82152409479038
C	1.50465869392467	-1.86790710554330	2.59598029972140
C	0.78875604896045	-2.87055127162726	1.85817810615702
C	-0.60679012787359	-2.86366568461286	1.88468268204729
C	-1.32017326245968	-1.88622900927090	2.66453290602625
C	-2.52975627093088	-1.51381040781470	1.91732602025361
C	-2.95998093091371	-0.21134382493565	1.93613883515770
C	-2.50260550365426	0.87123591438262	2.92315645928258
C	-2.26875401994965	2.00642455381790	1.92377255418013
C	-2.98293976727450	1.76370522004853	0.70823533586612

C	-3.41175888884477	0.38585529564509	0.71464488570631
C	-3.45606822279716	-0.33694544581911	-0.47871064013721
C	-3.00486346876642	-1.70050643961118	-0.49337889127452
C	-2.53385947796444	-2.26935145221269	0.69099234550690
C	-1.35175981710541	-3.10157837599908	0.66888200974664
C	-0.68012175330759	-3.33223979247004	-0.52844905925712
C	0.76758223234180	-3.32207973522371	-0.55752516082506
C	1.48700150842415	-3.09478324372215	0.61389498840934
C	2.64884149929423	-2.23068586281185	0.59139397926757
C	3.04571798413107	-1.62847095183266	-0.59993535692180
C	3.47499584577331	-0.24597963128980	-0.60388637823535
C	3.49147744399401	0.48212975567857	0.58310847558772
C	3.02629609729232	1.85309393228628	0.59883117290810
C	2.56017449062288	2.44058363542693	-0.57563530809095
C	2.54468152876046	1.68565680858158	-1.80568028057446
C	2.99351354182231	0.36698856125470	-1.82119769306781
C	2.26719601447652	-0.63489241387480	-2.57042511684490
C	2.29884631253054	-1.86765656045366	-1.81454925416893
C	1.18125105619586	-2.69907227360500	-1.79208881166937
C	-0.01013615446728	-2.33092616301372	-2.53078609769915
C	-1.15966688078822	-2.72642187829870	-1.75279972628452
C	-2.29943042912149	-1.92496194286216	-1.73369405352205
C	-2.32727067670025	-0.69313936906423	-2.49412319649961
C	-3.04586631706041	0.29197965643249	-1.71687927560461
C	-2.63258175811476	1.61998951166088	-1.72187108386567
C	-2.61203868650383	2.37822983539080	-0.48912433270113
C	-1.46605859996350	3.24346843397768	-0.50885214514762
C	-0.76046513749078	3.02260834302007	-1.74973838558285
C	-1.48347029344019	2.01930353804003	-2.50295497015072
C	-0.78690595533804	1.07095954160289	-3.24829556816709
C	-1.21683256618743	-0.31145145313293	-3.24345111832223
C	-0.03654974567929	-1.14613467036442	-3.26324409079754
C	1.12260351971949	-0.28114184514398	-3.28040383745896
C	0.65842900985790	1.08900314460045	-3.27071988985618
C	1.35342435504676	2.05364022586443	-2.54430350053071
C	0.63270419857658	3.03593082388880	-1.77088357640634
C	1.37383903052388	3.27018063341083	-0.54918680894287
C	0.69246154373119	3.46677842647055	0.64833386069806
C	-0.75259768253769	3.45071898255903	0.67281452242601
C	-1.17532093542578	2.83516559594739	1.90368390868350
C	0.03360699125097	2.46397432443693	2.65591396129228
C	1.17299502914394	2.85734368706547	1.86818794921735
C	2.32652343190116	2.07171313797140	1.84379044497548
C	-3.74735510657684	1.23880054564235	3.80612620350555
C	-1.31054277400670	0.43354777551391	5.29422204782155
C	-4.01998929129106	2.72638840921888	3.98467389663011
H	-3.66702532943096	0.73581966275010	4.77841541484946
H	-4.63137984825468	0.78935953196399	3.32807025825571
H	-3.13499141502622	3.28537664279311	4.31997815805303
H	-4.81895787248162	2.87912766030868	4.72623540916227
H	-4.35053848008789	3.18763512610311	3.04269620441265
C	-1.38307069355125	1.76390458984614	6.02323495878482
H	-0.41405688575346	-0.09700336614058	5.65281545229301

H	-2.15355496382836	-0.22068990657220	5.56760774583336
H	-0.56533363658987	2.43303388228763	5.71428719580510
H	-1.28149880809062	1.59820652101803	7.10614487619593
H	-2.32827704338496	2.29586790619051	5.86441722861614

C₆₀(C₃H₇)₂

C	0.16585640979009	1.47274090970527	3.30149372733168
C	-1.09142438424203	0.70367248043464	3.71913920210469
C	-0.61007786803171	-0.71890453592011	3.40995778833810
C	0.81896920857459	-0.75934849822156	3.34476031069326
C	1.30046511886805	0.59974335446726	3.27394163144192
C	2.43455116367345	0.89889599822388	2.51574825930473
C	3.11209360259823	-0.15249198651290	1.78609026802245
C	2.64873617325887	-1.46188556839280	1.85811299659840
C	1.48750181540933	-1.77735816236568	2.66267272423900
C	0.72551945188127	-2.78613297963758	1.98138672114720
C	-0.66842609224471	-2.72522757335005	2.02157818791747
C	-1.33529301301020	-1.68469705035522	2.76036081572987
C	-2.53834975635678	-1.30296258257658	2.00698020507387
C	-2.91806107371465	0.01444344440439	1.96489809337118
C	-2.41242309264724	1.12424827859035	2.89531261670763
C	-2.14781324547611	2.20243404508009	1.84058332413063
C	-2.88280980026265	1.92756615132115	0.64400627408748
C	-3.36300680620906	0.56918397095280	0.72132501437568
C	-3.44905311920740	-0.20874423078659	-0.43487567155372
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C	2.59291850763931	-2.27900059144283	0.66638754027921
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C	3.47990553630049	-0.38793742519688	-0.63253055239334
C	3.53825803707341	0.39567123775707	0.51760478801870
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C	2.66603409811854	2.32930283535801	-0.72593669888477
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C	-2.31407343814516	-0.77327163096033	-2.53960378167336
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C	2.41635739244386	0.80956154754210	2.48262357164595
C	3.12326742833936	-0.20440552001953	1.72852213821926
C	2.69188458186555	-1.52593516756284	1.76349164590284
C	1.53582986238073	-1.89106272557105	2.55458098243113
C	0.79969316232667	-2.89792137825321	1.84060245184979
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C	-2.19935188198026	2.03113095155388	1.81150823966219
C	-2.92380546126604	1.76366239955211	0.60636589874938
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C	3.09300611998989	1.76514936054840	0.46564224130806
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C	2.30207106292063	-1.99625188749270	-1.86090371095832
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C	-2.29576126538256	-1.98877036560651	-1.75527836511315
C	-2.31199948752212	-0.77412170059570	-2.54295563302914
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C	-0.66392457887990	3.41973004997211	0.52383355108700
C	-1.08673264149719	2.83327684061756	1.76829297010763
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C	1.27936875480043	0.46764737298763	3.24212755806227
C	2.40643836269189	0.81339558601331	2.49490503660726
C	3.11383328365243	-0.20044547210005	1.74127975523715
C	2.68196716315525	-1.52191344102531	1.77626077652078
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C	0.79120035786051	-2.89438639232580	1.85278182269481
C	-0.60374974739930	-2.86953242695329	1.88497232432278
C	-1.29778867758274	-1.86527094041815	2.64772546539319
C	-2.50420204663624	-1.48995377553356	1.89141850026976
C	-2.94160787124019	-0.18883431453606	1.88308800492636
C	-2.42322649193711	0.90202579637457	2.82335355720779
C	-2.21376567426919	2.03914113688057	1.82219256034851
C	-2.93374630869635	1.76901535651235	0.61491253479205
C	-3.38224952089396	0.39228813122827	0.65241958860391
C	-3.43469170603842	-0.35472773632761	-0.52507599700743
C	-2.99558508798828	-1.72278759278206	-0.50843978595334
C	-2.52737770528831	-2.27477838036767	0.68526240344238
C	-1.35667155281955	-3.12341378135626	0.67672354545525
C	-0.69508852732250	-3.38968019506988	-0.51749658601987
C	0.75235262724718	-3.39926197243254	-0.55315643591299
C	1.47978558829660	-3.15476002452487	0.61006393293308
C	2.65301776233771	-2.30787782866799	0.56305092080172
C	3.05278486161659	-1.73839781215531	-0.64355657214413
C	3.50081406943237	-0.36260897234401	-0.68051562984638
C	3.53274645299457	0.39113704091060	0.49023387408782
C	3.08499828727627	1.76786809964812	0.47731679880867
C	2.62208486193543	2.33621619956329	-0.70808576388981
C	2.59015865675301	1.55421794799359	-1.92041829265700
C	3.02180621809032	0.22990768548539	-1.90880032006125
C	2.27749178512184	-0.77818944301512	-2.63161364668600
C	2.29704102095712	-1.99437315271154	-1.84885356051128
C	1.16816782995902	-2.80940068433895	-1.80271899413921
C	-0.02163252916752	-2.44159972953454	-2.54462231055116
C	-1.17245818224880	-2.80284996232217	-1.75256367862134
C	-2.30149931683383	-1.98639442777170	-1.74786417998998

C	-2.31703938752690	-0.77241992343032	-2.53588885128480
C	-3.01964885482023	0.23956521723599	-1.77903465036295
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C	-1.43719914319825	1.92691783907123	-2.60830003279884
C	-0.75666641356762	0.95294810988504	-3.33554075253970
C	-1.20474778186147	-0.42268005400950	-3.29805936666080
C	-0.03579285689907	-1.27324685338693	-3.30333761094431
C	1.13492162148341	-0.42516332545327	-3.34504209428814
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C	1.40029865430372	1.92148332819375	-2.66209791027384
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C	1.44754112965806	3.18235776783236	-0.69474630952226
C	0.77580727782818	3.41667453747452	0.50038763089345
C	-0.67013642585577	3.42127938553516	0.53139891860395
C	-1.09336752648703	2.83210647230063	1.77410278913440
C	0.11413436631212	2.46382544109825	2.53171562524113
C	1.25414513911248	2.82797777858342	1.73168578863345
C	2.39472895429407	2.02403215205319	1.72003561273681
O	-3.38572819759786	1.24344647558720	3.80505902186739
H	-4.09349506823907	1.75101873952498	3.39324113714892
O	-1.36753317622271	0.60612345359948	5.02976311265144
H	-2.24847937779212	1.00690884212902	5.11638734475134

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C	-1.50225233821717	1.60496523764380	5.63592879415016
C	-4.79102325108481	1.51764973080651	3.22592437162085
C	2.32046532865815	1.95131401576099	1.82107053032591
C	1.18129942560471	2.75710731916866	1.80638542784216
C	0.01025881813158	2.37721493247434	2.55196287557485
C	-1.17078758374987	2.77225737421741	1.76437868595478
C	-0.69495112144500	3.38446513138574	0.55080485373416
C	0.75094191847049	3.37571069536471	0.57317326685363
C	1.46888334330059	3.16922015126968	-0.60005796980986
C	0.76492913804589	2.94697179263194	-1.84572534853963
C	1.49543782170281	1.95459581190408	-2.59620376930315
C	0.80912586517292	1.00205401797578	-3.34635556587652
C	1.25101339679277	-0.37529897662195	-3.34204801518094
C	0.07756769065414	-1.22070665991122	-3.36494541174883
C	-1.08864995487139	-0.36669283034801	-3.38520676836282
C	-0.63623270219160	1.00822046104192	-3.37371680106103
C	-1.34178317424810	1.96697284510396	-2.64996319871004
C	-0.62809215708018	2.95701258080365	-1.87175472136663
C	-1.37107490590635	3.18658482480792	-0.65382203806491
C	-2.53406480820592	2.34335298111787	-0.67459222261283
C	-2.52381637773777	1.58717631230462	-1.90958380931386
C	-2.95825303213215	0.26640809268004	-1.92063171771769
C	-2.22973929991200	-0.73015659279404	-2.67360260635439
C	-2.24671632266984	-1.96172720247986	-1.91317011545401

C	-1.12025308440276	-2.78149045593778	-1.89349010061150
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C	1.22037128775445	-2.79405603298493	-1.85469075264281
C	2.35196135471521	-1.98184029350719	-1.83916948328726
C	2.36501979992186	-0.74827046391178	-2.59419969611394
C	3.08296542172776	0.24072238620954	-1.82035702471688
C	2.65461659034895	1.56616773087282	-1.81794053408873
C	2.64135891030119	2.31977051698111	-0.58752084599059
C	3.05869475230120	1.72302168151091	0.60072277119217
C	3.50297879777889	0.34526048042392	0.59924602226331
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C	3.06217862519173	-1.75626813549393	-0.60036083137440
C	2.61564698720160	-2.35201149408400	0.57700770526778
C	1.43946163381982	-3.19601823940385	0.56003353070766
C	0.75594758121084	-3.41066677142412	-0.63536146493668
C	-0.69155752040610	-3.39726550913672	-0.65474021155215
C	-1.39726540183554	-3.15418142795321	0.51908105952089
C	-2.56496384992363	-2.30196490401907	0.50271989602543
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C	-3.42080777845390	-0.35424567155107	-0.69716985439729
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C	-2.58832613046199	-1.54452630177903	1.72642494203373
C	-1.41187532080869	-1.94126997061269	2.51784728914969
C	-0.69078688448985	-2.93074428633277	1.76021019588341
C	0.70411659220443	-2.96064334519947	1.78089727389888
C	1.41432466833288	-1.97298237004412	2.54644870786586
C	2.60093829697968	-1.59435771628578	1.80854936787072
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C	2.30379326282360	0.72447729137602	2.56989335915031
C	1.14916534292569	0.36469242412821	3.26622639829831
C	0.69527205917380	-1.00915453384401	3.25431095044761
C	-0.73470497304695	-1.00643781525452	3.25678104392751
C	-1.25869511079935	0.39045236865463	3.59504719240433
C	-0.00285605337174	1.21299614208128	3.27684797406837
H	-2.14659025006187	2.36055878877637	5.16014219159543
H	-1.87435734184201	1.41554495546776	6.65160343313834
H	-0.47094709768274	1.99581846172316	5.70259450781504
H	-4.75188488347535	2.44005861231383	2.61837274031288
H	-5.27745544049661	0.72607161726138	2.62865453091952
H	-5.40482161895882	1.71000514089289	4.11593763638311
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C	-4.83224712977690	1.70634711207563	3.07844839002479
C	2.32295969343460	1.94397249046109	1.83713423998192
C	1.20244383694830	2.77362383882184	1.77807305547917
C	0.00431522167184	2.43226883682714	2.49974607701123

C	-1.14709056510029	2.83590350863514	1.67317569093489
C	-0.62700471631109	3.41501531198000	0.46154854276743
C	0.81730281137973	3.37677515034088	0.52239982843867
C	1.56059274354180	3.13179393528851	-0.62767227707849
C	0.88471679929268	2.90093931894294	-1.88715819209875
C	1.61286130731366	1.87931611467262	-2.59974859644263
C	0.92582295919351	0.92704026352187	-3.34961744096746
C	1.33744291702322	-0.45889214219890	-3.30775534980464
C	0.14701416785466	-1.27963074244572	-3.34574581481301
C	-0.99950144757901	-0.40184897727509	-3.41263754271232
C	-0.51788354085117	0.96311164943827	-3.41493054450990
C	-1.22108769711915	1.95026082124123	-2.72836204832940
C	-0.50660089060734	2.93979466963906	-1.95008461688535
C	-1.27586031716089	3.20824380813468	-0.75665426727774
C	-2.45567523839467	2.38930271570066	-0.79230356040776
C	-2.43013649685989	1.60987015361986	-2.01243860960460
C	-2.89247427818198	0.29844715016936	-2.00997311960634
C	-2.16608897033350	-0.72749277828035	-2.72455422874579
C	-2.22906018954888	-1.94370551369180	-1.94199340958406
C	-1.12153700473016	-2.78673624386184	-1.87773295917454
C	0.08577217579049	-2.45017536889679	-2.59259862202436
C	1.21650762798789	-2.84771886334279	-1.77732215122894
C	2.36434528614688	-2.05899503025351	-1.74697654998476
C	2.42351793878130	-0.84063279846187	-2.52416140521522
C	3.14238560295311	0.14770139943407	-1.75051126960519
C	2.74269908519370	1.48149152854119	-1.78393804101751
C	2.71376904126753	2.25874581433606	-0.56856888113881
C	3.08702918247826	1.67624454188787	0.64118582829764
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C	3.52806054191251	-0.45974540164036	-0.49651367637755
C	3.04706718342848	-1.82480489304787	-0.49440039203239
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C	1.36432646204694	-3.20765720628448	0.64960622993447
C	0.70755151847031	-3.43079547195173	-0.55914650292162
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C	-1.46886892247877	-3.10609709099422	0.53319724220630
C	-2.61727394767695	-2.23033981989920	0.47034352324717
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C	-2.92541043849072	1.81907182979603	0.39175954294649
C	-2.28606607912177	2.06819704658919	1.64754978443336
C	-2.59432485729524	0.93745562556243	2.64236877417075
C	-3.06426758649010	-0.13882081094864	1.65074298384037
C	-2.65667402361634	-1.44942622377366	1.67882410844263
C	-1.50935798673531	-1.85521023415628	2.50795607070436
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C	1.31436414430103	-1.94683237523683	2.61166036174348
C	2.52780194113964	-1.60746107939328	1.89843493530087
C	2.99116984878168	-0.29589894298903	1.89622192560540
C	2.26036878550200	0.73169264226693	2.60769889228869
C	1.08052239128961	0.40921425575246	3.27873277603885

C	0.59800780188917	-0.95431331697796	3.28146324267080
C	-0.83081165405689	-0.92122135595766	3.24685370143398
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H	-5.82334591944029	1.14559014371020	4.90820850727246
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H	-5.26614997104143	2.83792136464125	4.86452267705726
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H	-2.65601762400986	1.77798988467732	6.12328487249692
H	-1.77551825208055	2.58345947558522	4.82438257235135
H	-0.45921903667102	1.10237583945354	7.18551623077938
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C	0.81812493453075	-0.90623879194584	3.26715766515051
C	1.26169262000287	0.46583719499332	3.23037006955076
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C	3.10584465990872	-0.19514041240960	1.74317045857680
C	2.67752407869570	-1.51773412779768	1.77705686791612
C	1.51826581734773	-1.88563033496818	2.56206942722628
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C	-2.51611185500617	-1.50389636652091	1.87108402570001
C	-2.93991232563226	-0.19830618071666	1.85377508643713
C	-2.43279702129033	0.88898660361945	2.78814262896735
C	-2.22416442528591	2.02502498858908	1.79776737125344
C	-2.93877035280936	1.75560945008349	0.58653697546036
C	-3.38209757996718	0.38096688555649	0.62161849811115
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C	-2.99228831189187	-1.73782751309618	-0.53463143357872
C	-2.52803518723437	-2.28580725800977	0.66289951469146
C	-1.35420628215761	-3.13035624069759	0.66006350030060
C	-0.68532269724047	-3.39452221590421	-0.53114515552100
C	0.76242189225500	-3.39993541106458	-0.55993372390569
C	1.48458096286889	-3.15458437047166	0.60584527826852
C	2.65584995686934	-2.30458433401111	0.56408323060986
C	3.05926430866960	-1.73388353791642	-0.64046632074093
C	3.50367945748716	-0.35683840617799	-0.67606184492518
C	3.52858187979073	0.39774044177226	0.49397856664957
C	3.07671858699001	1.77342027534928	0.47850510425906
C	2.61690599516838	2.33938208200848	-0.70889891563862
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C	-2.30359269663355	-0.78406460338843	-2.55835282663426
C	-3.01189303039348	0.22644233184950	-1.80519497531886
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C	-0.01762264052050	-1.27891034129276	-3.31540890511204
C	1.15066340226852	-0.42723616795148	-3.35169826073966
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C	1.40646729756490	1.92061600853615	-2.66871302398387
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C	0.76102409280288	3.41577719736560	0.49076457595387
C	-0.68495893125207	3.41695634008855	0.51488909702925
C	-1.11395914489138	2.83245732530719	1.75821628815730
C	0.09045372962764	2.46338397837468	2.51671424837562
C	1.23561146236300	2.82848863689740	1.72398885111605
C	2.37932717150151	2.02789124964664	1.71742560258297
S	-3.79846591660103	1.34639556453618	3.96256551726471
S	-1.33392302503152	0.54818929274433	5.44848523318754
H	-4.61685198003259	1.74484818199498	2.95855398907033
H	-1.32445725439983	1.89547609184720	5.55802428728206

C₆₀(SCH₃)₂

C	0.11555389385763	1.25270010229566	3.24096128992640
C	-1.11580363434737	0.43605754223850	3.58900033185190
C	-0.59442164468889	-0.96819153290671	3.29362426748387
C	0.83649003820171	-0.95778822347893	3.23981399403584
C	1.27558914047061	0.41566455500050	3.21272939055560
C	2.40601365682975	0.77826433405085	2.48085906340130
C	3.12559265308273	-0.22576787042939	1.72565456405155
C	2.70035082513110	-1.54974361746007	1.74798045687774
C	1.54129624863964	-1.92857458306302	2.52860424583294
C	0.81616873865379	-2.93361877208603	1.80155257787032
C	-0.57927121162739	-2.91694458117068	1.82595710386582
C	-1.28692693109960	-1.92190876921375	2.59004875943314
C	-2.49200043849783	-1.55283747443756	1.83370617868198
C	-2.91839638707289	-0.24659141483239	1.82545860261142
C	-2.42229376022995	0.83198222763936	2.77270976035454
C	-2.21880294577444	1.97937394494446	1.79450000876921
C	-2.92137338917137	1.71498478494705	0.57511094752801
C	-3.36037491515109	0.33845692046042	0.59751812829951
C	-3.40578062825885	-0.40270813637135	-0.58394746427530
C	-2.96418038270667	-1.76843489498581	-0.57490097444792
C	-2.50002134356302	-2.32435515161733	0.61995857434470
C	-1.32340064767049	-3.16562823263823	0.61171692500930

C	-0.65201605878525	-3.41806937030295	-0.58072159446076
C	0.79535491740016	-3.41919597648549	-0.60749263020990
C	1.51465812513298	-3.18100597642654	0.56175566659660
C	2.68321026871706	-2.32666749754396	0.52861588578493
C	3.08685192699318	-1.74477533436107	-0.67059188096873
C	3.52695533880990	-0.36610968602383	-0.69428769859855
C	3.54756934322174	0.37890431170519	0.48193159143568
C	3.09107092433438	1.75317695707543	0.47689547147668
C	2.63116792811998	2.32764721023797	-0.70652787223475
C	2.61260150778084	1.55498665275482	-1.92560441350056
C	3.05165320365699	0.23303025833657	-1.92112513751172
C	2.31929516979130	-0.77409377427370	-2.65708212596187
C	2.33999110752593	-1.99563305396042	-1.88293465789365
C	1.21608295780481	-2.81793781327481	-1.85056084786223
C	0.02914892048087	-2.45181625142206	-2.59716950733001
C	-1.12470318986446	-2.82665425383995	-1.81539363403290
C	-2.25809279005951	-2.01668445905652	-1.81076160889229
C	-2.27555515149355	-0.79683531621718	-2.59072808390813
C	-2.98838972965533	0.20508149075365	-1.83068423731506
C	-2.56429419080989	1.52907164005954	-1.85205428317851
C	-2.54124064986055	2.30623247382504	-0.62972882306642
C	-1.38850027687192	3.16133799254425	-0.65900363987010
C	-0.68218599480204	2.91695702985151	-1.89556067589260
C	-1.41105927488935	1.90851449028847	-2.63599685777553
C	-0.72038881433773	0.94425440333492	-3.36666151536501
C	-1.16054683763798	-0.43443686384902	-3.34298129394632
C	0.01332842358687	-1.27802148710354	-3.34764436794340
C	1.17899074082246	-0.42231516853858	-3.37501030012862
C	0.72511872507423	0.95105801959731	-3.38602803114685
C	1.42577674308151	1.92080298726378	-2.67207032474649
C	0.71068459324134	2.91894294559615	-1.91380322069908
C	1.45113324124521	3.16597829366743	-0.69397243024620
C	0.76913778300843	3.38755535752794	0.49876224571866
C	-0.67720113007345	3.38425356355779	0.52187352644682
C	-1.10787378234728	2.78939884160111	1.76028254198538
C	0.09902333217145	2.41755212572166	2.51524216687622
C	1.24410788106359	2.79197889576554	1.72730451263398
C	2.39041174781114	1.99495620623305	1.71626564117295
S	-3.78580883015621	1.20219406542361	3.98709872738424
S	-1.30272995007112	0.46483958644971	5.43079258520565
C	-5.07462726773192	1.84896722336837	2.90178443653404
C	-1.14908071497867	2.22130663508216	5.81251980350317
H	-5.91769125367810	2.05911019110569	3.57605563220636
H	-5.40503351610960	1.11279819748886	2.15452774723459
H	-4.78011432586829	2.78400861237433	2.40471078628227
H	-1.27570729464476	2.29140178098784	6.90266353237479
H	-1.94692517722972	2.79718617395871	5.32190785931237
H	-0.15819143622674	2.61128937255567	5.54128873505893

C₆₀(SC₂H₅)₂

C	0.10586513544636	1.23319059386977	3.24962610230909
C	-1.15777660211067	0.45405010238685	3.56164445765682
C	-0.67712386969261	-0.96251724907345	3.25920204776127

C	0.75405787606739	-0.99891329403979	3.23597060964026
C	1.23834615481521	0.35882573991455	3.23528957858348
C	2.39623389297799	0.69362254670758	2.53455120047745
C	3.09966538807165	-0.32417089380751	1.78288220900656
C	2.63129599866605	-1.63408897104478	1.77915146898559
C	1.44290358460990	-1.98394433574708	2.52846840335400
C	0.70167433866878	-2.95533514679518	1.77301652804993
C	-0.69281795630037	-2.89265635247833	1.76715775906480
C	-1.38489923265293	-1.88502195856013	2.52898497734015
C	-2.55948171455521	-1.46708242074926	1.75068552166614
C	-2.94286731785882	-0.14799032907620	1.75066854678974
C	-2.43659827434682	0.90284431828290	2.72283883518791
C	-2.17006544694378	2.05250042057850	1.76340065931507
C	-2.85329959191210	1.82856417491322	0.52468322325027
C	-3.33300701248176	0.46651222900716	0.51883111245230
C	-3.37912042574705	-0.25731765161026	-0.67181423415051
C	-2.98345814775444	-1.63783468695385	-0.67088090230338
C	-2.56497365031216	-2.22305224808164	0.52635411870173
C	-1.41678054567659	-3.10185617748650	0.53334577964488
C	-0.72721402360082	-3.36198391719654	-0.64715670201318
C	0.71956014990358	-3.41030848558504	-0.64204100231799
C	1.41978940670977	-3.21096209147152	0.54588287823311
C	2.61597082526419	-2.39487374484331	0.54954029512829
C	3.06496980464585	-1.81163566132456	-0.63285831742945
C	3.54984895102073	-0.44789232743080	-0.62895354052613
C	3.56879219493070	0.28152840213063	0.55685588829854
C	3.15737786087954	1.67029245315457	0.55977953318720
C	2.74320969304553	2.27412035908558	-0.62596587249714
C	2.72628166335290	1.51701940165883	-1.85485613318806
C	3.12213187608941	0.18167694658591	-1.85828570680504
C	2.37424797707179	-0.79174472033581	-2.62321591743015
C	2.33776616330957	-2.02263158743693	-1.86458314643194
C	1.18733713661386	-2.80795802835089	-1.86768198302372
C	0.03000004222679	-2.39413481943935	-2.63547878555381
C	-1.15248095750861	-2.74057072201200	-1.88409144217570
C	-2.25898523684277	-1.89404941100162	-1.89399462013614
C	-2.21901241575352	-0.66437067175549	-2.65815501661598
C	-2.91519281141710	0.35129922701264	-1.90125978509857
C	-2.44863563844758	1.66140917104498	-1.89667983017843
C	-2.42760653085738	2.42257900682299	-0.66449828520295
C	-1.24783867502809	3.23984730512657	-0.65692674863986
C	-0.52155052107682	2.98670228601204	-1.88034152572858
C	-1.26606380580474	2.01192323791002	-2.64982367261081
C	-0.59107206621661	1.03426940021657	-3.37739089715375
C	-1.07643010184529	-0.32955086079181	-3.38129225608744
C	0.06895241616092	-1.21134598237144	-3.37080572867957
C	1.26228078138812	-0.39407335826426	-3.36144586862353
C	0.85390108265807	0.99344740607533	-3.36457277017088
C	1.56958713668925	1.93101660218017	-2.62285078175429
C	0.87064996624267	2.94270849983872	-1.86761966336159
C	1.59087799313101	3.14976912619423	-0.62840497784456
C	0.88967194107758	3.37927734835943	0.55170605278835
C	-0.55620749684435	3.42300522060613	0.54282125875047

C	-1.03304496118019	2.82648397410303	1.76309962144259
C	0.14342057853504	2.40695575898858	2.53957492623406
C	1.31767497328083	2.75378326708272	1.78253015752692
C	2.43809193176606	1.92040321989710	1.78650597826856
S	-3.78966272229218	1.33926683523599	3.93062844956290
S	-1.38111871990643	0.46681701835761	5.39911963521693
C	-5.15288735248714	1.90030906252405	2.85977457133768
C	-1.20049628421605	2.23237440364234	5.81965240928060
C	-6.14112465172026	0.81728087124070	2.46850969942437
H	-4.74905905168566	2.43502195078479	1.98607943221441
H	-5.64620451096020	2.66832645829084	3.47699802736678
H	-5.67642848847341	0.04615713462547	1.83862879603036
H	-6.98193941720868	1.25233710900981	1.90456794517167
H	-6.54882523067257	0.31863892384467	3.36025205880924
C	0.17985614750264	2.61526202929555	6.31362917637474
H	-1.96885033654033	2.40883169621611	6.58933660258224
H	-1.51665381645382	2.81862095805420	4.94363707899082
H	0.46730342632097	2.02055330274358	7.19343780705407
H	0.19869327025823	3.67896463988565	6.60096426415085
H	0.94361499178702	2.45993000781664	5.53836765606989

C₆₀(NH₂)₂

C	0.17003561944949	1.54259466866125	3.20902390988547
C	-1.07613453260435	0.77248169075597	3.64771676975611
C	-0.58457421382748	-0.65711562605786	3.38301761617534
C	0.84494709868828	-0.68104531234064	3.31342312180044
C	1.31173863554501	0.68210484447395	3.20540960899310
C	2.43705442240931	0.97920869868443	2.43525963022360
C	3.12518618846024	-0.07814103978687	1.72561625110486
C	2.67551352583749	-1.39035755750581	1.82700793238835
C	1.52076158435550	-1.70173430788396	2.64344358698071
C	0.76663204099046	-2.73134189067667	1.98215195651386
C	-0.62749512866624	-2.68392159641110	2.02343935281003
C	-1.30264425681957	-1.63471824530190	2.74331126225976
C	-2.51007127170180	-1.28010640294443	1.97848017538406
C	-2.92576198936988	0.02581839537042	1.90941788663851
C	-2.40663675625176	1.15198910617569	2.80646302497062
C	-2.17447317274589	2.22951287486950	1.73998895741969
C	-2.90800039386358	1.91866039789149	0.55045857091323
C	-3.37344446095376	0.55292585669884	0.65643146241968
C	-3.44493990917554	-0.25015579701167	-0.48379385676537
C	-3.02396331039965	-1.62096820724825	-0.40504211079930
C	-2.55114949486369	-2.11944876078561	0.81026404711047
C	-1.39301182226205	-2.98422152644564	0.83426124349273
C	-0.74480336790261	-3.31712847025823	-0.35119550461019
C	0.70148962189193	-3.34871580658686	-0.39713428699122
C	1.44107619471747	-3.05913208310026	0.74804559267577
C	2.62485559126343	-2.23118512947227	0.65192987612819
C	3.02294497763262	-1.72529649118628	-0.58305821774767
C	3.48944371717262	-0.35920848004340	-0.68894704692059
C	3.54127183321769	0.44847542550547	0.44469300974714
C	3.11015106720816	1.82865545321903	0.36978253072261
C	2.64354877768343	2.34600306586013	-0.83710471672636

C	2.59349865256563	1.50941572779709	-2.01181080338324
C	3.00772475872491	0.18125357680250	-1.94020227505329
C	2.24496944419130	-0.85002869100855	-2.60897692667685
C	2.25422037750227	-2.02781069966053	-1.76951299288009
C	1.11530722627412	-2.82469432730809	-1.67658142690126
C	-0.07523160147621	-2.47590294507212	-2.42617427299793
C	-1.22451133835581	-2.78397366879034	-1.60956086274083
C	-2.34240382054042	-1.95281792818478	-1.63526765807263
C	-2.34809824352050	-0.77736885983161	-2.47987387004362
C	-3.03164446857452	0.27867892972955	-1.76698205385477
C	-2.58385237050199	1.59134116702244	-1.86834954199940
C	-2.52923048401610	2.43239465654987	-0.69069242645532
C	-1.35904388985769	3.26138049760391	-0.78256346235633
C	-0.67500138536283	2.93600389612854	-2.01252835756859
C	-1.43362282100673	1.90345496956074	-2.68673220514729
C	-0.77167488800039	0.88725403098978	-3.37177486835998
C	-1.23743271283407	-0.47905735582511	-3.26570082354282
C	-0.08003079423115	-1.34444618112000	-3.23931979301327
C	1.10124823674100	-0.51511301821483	-3.32933473575595
C	0.67336633144956	0.86408196443665	-3.41046257097918
C	1.40282896436765	1.85765026582212	-2.76153915890750
C	0.71773283118033	2.90997348438867	-2.04995746481939
C	1.48035195896003	3.20773460235109	-0.85565733357674
C	0.81996716205153	3.50636750547847	0.33214760109347
C	-0.62550636523985	3.53366530646062	0.37393258114844
C	-1.05016297143951	3.01348276506332	1.64748022485877
C	0.16074422006012	2.65637490221426	2.40749306755118
C	1.30056145248084	2.96856225873226	1.58489118295177
C	2.43167844341233	2.15098619275476	1.60370286047766
N	-3.45893360150259	1.50200546261951	3.75762166575353
H	-4.35770984744914	1.52315021459894	3.28009708044550
H	-3.30371984627818	2.44022702587897	4.12251933149284
N	-1.22828599265140	0.94036641051102	5.07940339319571
H	-2.14730674283503	0.59935475721726	5.35776526294425
H	-1.18599958330275	1.92504167008511	5.33228370041948

C₆₀(COOH)₂

C	2.7048659116	-1.1733532664	-0.9746129019
C	1.4479383416	-1.9805006770	-0.6273166183
C	1.9549727547	-3.3916714208	-0.9135634302
C	3.3866233449	-3.3978960074	-0.9761311490
C	3.8470152843	-2.0300654902	-0.9996968017
C	4.9855964376	-1.6799761098	-1.7273139570
C	5.6941016756	-2.6907604947	-2.4829541736
C	5.2494362399	-4.0083174356	-2.4663973343
C	4.0821810132	-4.3738403003	-1.6906522168
C	3.3463035158	-5.3652830133	-2.4246360564
C	1.9515951817	-5.3288555748	-2.4044881929
C	1.2558791370	-4.3282641749	-1.6359836718
C	0.0629720331	-3.9380438150	-2.4012071459
C	-0.3422759571	-2.6283508792	-2.4164526805
C	0.1592051520	-1.5527126378	-1.4501007479
C	0.3752303748	-0.4007627058	-2.4253853274

C	-0.3269368206	-0.6539187245	-3.6474330600
C	-0.7787841414	-2.0252580004	-3.6353263490
C	-0.8301950623	-2.7638258109	-4.8180872896
C	-0.4046325770	-4.1357502464	-4.8105561968
C	0.0466872370	-4.7052394674	-3.6183524996
C	1.2097560901	-5.5630853073	-3.6236920151
C	1.8812843279	-5.8210685774	-4.8145248845
C	3.3286904922	-5.8421313955	-4.8359285759
C	4.0464782456	-5.6188997744	-3.6629800349
C	5.2265248634	-4.7806982708	-3.6885295921
C	5.6431130502	-4.2004547731	-4.8844367719
C	6.1027944903	-2.8280720513	-4.9018853023
C	6.1296425178	-2.0875521571	-3.7228989424
C	5.6918512907	-0.7074916611	-3.7249550293
C	5.2438361753	-0.1226587781	-4.9072741477
C	5.2196549494	-0.8899502359	-6.1294130695
C	5.6404836796	-2.2178595189	-6.1280029136
C	4.8968125209	-3.2119103081	-6.8705036475
C	4.8975598736	-4.4363658582	-6.1004785114
C	3.7622732225	-5.2430112915	-6.0754901971
C	2.5832269658	-4.8573818047	-6.8249304970
C	1.4213937144	-5.2179995919	-6.0483677070
C	0.2998656895	-4.3915315673	-6.0456794282
C	0.3014091487	-3.1689511214	-6.8211524003
C	-0.4015604344	-2.1592818443	-6.0611962436
C	0.0414297614	-0.8410271344	-6.0745222188
C	0.0683114446	-0.0672293958	-4.8502201137
C	1.2356318198	0.7698290770	-4.8724527460
C	1.9440212847	0.5190752933	-6.1066368909
C	1.2039165031	-0.4764563334	-6.8527091166
C	1.8837281919	-1.4476186204	-7.5843737924
C	1.4242059923	-2.8201626051	-7.5677981000
C	2.5860113416	-3.6803557485	-7.5703108684
C	3.7640086516	-2.8411521608	-7.5903420987
C	3.3293170343	-1.4614233261	-7.5983831180
C	4.0409688522	-0.5042959742	-6.8787809651
C	3.3370108106	0.5016503149	-6.1200562486
C	4.0756755016	0.7335210492	-4.8969969257
C	3.3914376992	0.9594450531	-3.7070127806
C	1.9455883075	0.9775657773	-3.6893792039
C	1.4999734841	0.3849654653	-2.4543672069
C	2.6984356642	-0.0086087949	-1.6985458139
C	3.8523852997	0.3518456498	-2.4790778384
C	4.9869211635	-0.4619041115	-2.4877395845
C	1.2655809291	-1.6727408654	0.8662267069
O	0.7534509033	-0.6657465823	1.2702086048
O	1.8220365946	-2.5913147784	1.6467101794
H	1.7411318760	-2.2750535170	2.5605159099
C	-1.0565047659	-1.2654090426	-0.5525857804
O	-1.7616813916	-0.3048530571	-0.6438872663
O	-1.2983679594	-2.3058271094	0.2520949123
H	-2.0776289886	-2.0809670273	0.7834769047

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C	2.0769613230	-3.3220804309	-0.8803193858
C	3.5046876794	-3.3559938551	-0.9784579476
C	3.9867608155	-1.9963757370	-1.0273639718
C	5.1081188896	-1.6711196539	-1.7916030537
C	5.7785682984	-2.6999858885	-2.5572707178
C	5.3111203284	-4.0094525575	-2.5162875188
C	4.1634253466	-4.3506891698	-1.7022062934
C	3.3895628395	-5.3359306552	-2.4046631256
C	1.9967532117	-5.2733586439	-2.3443458395
C	1.3409448209	-4.2553774434	-1.5645748296
C	0.1310831639	-3.8519345716	-2.2953908119
C	-0.2562670020	-2.5367335083	-2.3075351078
C	0.2944653222	-1.4659276442	-1.3656222625
C	0.5064943029	-0.3292053436	-2.3624170039
C	-0.2377737672	-0.5786871056	-3.5632806840
C	-0.7164454794	-1.9402929981	-3.5210930661
C	-0.8145427709	-2.6857202625	-4.6973077973
C	-0.4121092040	-4.0636539359	-4.6904356843
C	0.0671555959	-4.6274409273	-3.5058452634
C	1.2152128369	-5.5052105175	-3.5385641608
C	1.8459568592	-5.7856190661	-4.7467334688
C	3.2910726497	-5.8319236836	-4.8111196345
C	4.0464125997	-5.6093494646	-3.6616706626
C	5.2392589378	-4.7914819745	-3.7304369093
C	5.6299589241	-4.2289668241	-4.9431170270
C	6.1121984953	-2.8648321249	-4.9865645192
C	6.1865174728	-2.1152212538	-3.8152379623
C	5.7720512348	-0.7276298958	-3.8172419810
C	5.3005823307	-0.1449813145	-4.9921201254
C	5.2267364595	-0.9223831438	-6.2058717302
C	5.6240630622	-2.2574192957	-6.2039613989
C	4.8415882259	-3.2453369090	-6.9145853376
C	4.8455123398	-4.4632746565	-6.1345882691
C	3.6976132368	-5.2496524656	-6.0676548368
C	2.5035766998	-4.8506312659	-6.7855581232
C	1.3594125334	-5.1854659985	-5.9717715492
C	0.2518385817	-4.3413834542	-5.9435985152
C	0.2516553466	-3.1256381196	-6.7295830469
C	-0.4106065499	-2.0978611505	-5.9574783644
C	0.0517813851	-0.7869167258	-5.9987359122
C	0.1306922730	-0.0056957092	-4.7815448970
C	1.3112484975	0.8103945633	-4.8451958409
C	1.9760097098	0.5408609200	-6.0994276341
C	1.1965816992	-0.4477974860	-6.8138790901
C	1.8385461046	-1.4370921985	-7.5552885437
C	1.3571407637	-2.8014480134	-7.5123212500
C	2.5042115735	-3.6809783835	-7.5424258243
C	3.6947375463	-2.8622442058	-7.6051501005
C	3.2827980483	-1.4755522853	-7.6112167511
C	4.0323780054	-0.5240516198	-6.9234499785

C	3.3675210518	0.4987889969	-6.1522979970
C	4.1475550360	0.7295228413	-4.9539459705
C	3.5048702613	0.9793181354	-3.7453841459
C	2.0604788938	1.0198488831	-3.6862495361
C	1.6449963130	0.4409055860	-2.4345811183
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C	5.1113640643	-0.4576347849	-2.5614771292
C	-0.8776596631	-1.2309165710	-0.3674743371
O	-1.1739433644	-2.0850545474	0.4325239714
N	-1.5211946808	-0.0472958062	-0.4903176332
H	-1.3239517402	0.5838138426	-1.2551696407
H	-2.3660694044	0.0841054978	0.0517275838
C	1.4964831786	-1.7468849809	0.9711952956
O	1.7200307921	-2.6691976782	1.7141472511
N	1.2607827235	-0.4786080276	1.3868722619
H	1.0242407422	0.2676460555	0.7490398304
H	1.1087065010	-0.3317803264	2.3761381282

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C	0.82555008506690	-0.91274128098103	3.28265815047785
C	1.26343706905334	0.46167625234791	3.25912219079537
C	2.39006231837972	0.81388681689180	2.51729171999141
C	3.10218401603791	-0.19453448829772	1.75921362835247
C	2.67990402284325	-1.51901502473753	1.78711806386707
C	1.52243870527570	-1.89008140338299	2.57163595833012
C	0.78981113606321	-2.89437102342338	1.85276421132270
C	-0.60580752835125	-2.87865371565096	1.88355355663662
C	-1.30907448750807	-1.88130368099405	2.64577394454311
C	-2.51888761855041	-1.51011422896220	1.89818893281184
C	-2.96172398757806	-0.21113929513221	1.89539230783895
C	-2.43440201105477	0.87583012095744	2.82969142906920
C	-2.22118038161881	2.01093592099387	1.82601268625167
C	-2.94961463036084	1.74616769703260	0.62718365269374
C	-3.39694126743709	0.37381487201015	0.66256189846361
C	-3.44326984811807	-0.36827276682588	-0.51756728684231
C	-2.99847603067108	-1.73442384487327	-0.50641588578949
C	-2.53176215002913	-2.28859480284932	0.68584223032099
C	-1.35676959954010	-3.13119138328397	0.67443722295102
C	-0.69046636011539	-3.38873924522062	-0.51907020942573
C	0.75776464250254	-3.39156352244494	-0.55232996925055
C	1.48377467393602	-3.15092929857074	0.61167927161060
C	2.65444242133891	-2.30008198736121	0.57057847241590
C	3.05259316927465	-1.72255131456822	-0.63244020293055
C	3.49381141427549	-0.34435356884559	-0.66185510713308
C	3.52077113968001	0.40488378982653	0.51196485249684
C	3.06740228385215	1.77955438650324	0.50444862486956
C	2.60231461214077	2.34969654171460	-0.67854780420328
C	2.57687646350910	1.57383947883410	-1.89534291055432
C	3.01378195554298	0.25139935942369	-1.88841257760267

C	2.27610916749402	-0.75676781696153	-2.61767994723635
C	2.29874254423469	-1.97586643347566	-1.83958926078405
C	1.17362527832479	-2.79636640659494	-1.79961391471130
C	-0.01645433115892	-2.43056790624723	-2.54128883311511
C	-1.16740574073387	-2.80019506999940	-1.75255506579277
C	-2.29965567062883	-1.98869001891269	-1.74538068371356
C	-2.31897894170044	-0.77130361965042	-2.52800549684375
C	-3.02759952242038	0.23394440026187	-1.76794143967542
C	-2.60217743124664	1.55741731396982	-1.79911787596651
C	-2.57089295447236	2.33538111579688	-0.57935761213323
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C	-0.71569164904192	2.94043473178379	-1.85472234192255
C	-1.45052020018838	1.93207337582707	-2.58881209736011
C	-0.76462029497201	0.96432690769343	-3.31862250045543
C	-1.20714685051904	-0.41341689500508	-3.28700710036326
C	-0.03445836322517	-1.25891143656208	-3.29435528865779
C	1.13267771144221	-0.40545093821713	-3.33030370185480
C	0.68075175933227	0.96867209358739	-3.34394624544552
C	1.38693726859281	1.93940750355663	-2.63703495183540
C	0.67701443644977	2.94094934855084	-1.87841812700003
C	1.42457057902857	3.19095397393917	-0.66301437489762
C	0.75013573110351	3.41621694860230	0.53242676208767
C	-0.69478904718923	3.41410621502966	0.55974333379334
C	-1.11636286754520	2.82165554318949	1.80034011268148
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C	1.22752403842963	2.82396926902627	1.76256189573918
C	2.37141629834943	2.02592831163873	1.74660511599040
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C	3.4493453754	-3.3451964666	-0.9806138371
C	3.8965660776	-1.9726732374	-1.0178074764
C	5.0215581108	-1.6249528698	-1.7662560573
C	5.7288810908	-2.6386794955	-2.5200898816
C	5.2974797983	-3.9598610650	-2.4850710124
C	4.1412310939	-4.3244040991	-1.6941640408
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C	2.0087979223	-5.3055968968	-2.3745833577
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C	0.1049429379	-3.9288407562	-2.3639364715
C	-0.3311979470	-2.6288870057	-2.3816054084
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C	0.3978981575	-0.3925646368	-2.4419271366
C	-0.3225257191	-0.6683225560	-3.6452842761
C	-0.7697609695	-2.0408565996	-3.6084456563

C	-0.8211593323	-2.7906791246	-4.7837671725
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C	1.2549599308	-5.5590605320	-3.5817426609
C	1.9164976275	-5.8243910814	-4.7760301138
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C	6.1468673137	-2.0458661891	-3.7708566376
C	5.6982443357	-0.6696342813	-3.7831894533
C	5.2327026317	-0.1019924213	-4.9670187813
C	5.2017334991	-0.8824322125	-6.1805852825
C	5.6329736491	-2.2067508962	-6.1689949062
C	4.8892339204	-3.2147545889	-6.8922999314
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C	0.0590448081	-0.0905826197	-4.8565133741
C	1.2193035029	0.7549160521	-4.8982789676
C	1.9150675057	0.4995208949	-6.1386226260
C	1.1747508345	-0.5089801402	-6.8666653959
C	1.8547562927	-1.4829033909	-7.5938756862
C	1.4064680125	-2.8587038243	-7.5564337518
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C	1.9918293737	-5.3117973155	-2.3839075305
C	1.3040916580	-4.3033273308	-1.6202805615
C	0.1035503460	-3.9212265609	-2.3766522098
C	-0.3115334762	-2.6156501306	-2.3988667251
C	0.2235590707	-1.5382773683	-1.4669736809
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N	1.3030227377	-1.7022529152	0.8573464808
O	1.5868268026	-2.5928435050	1.6059682244
O	0.9544905288	-0.5851672087	1.1422969095

Cartesian coordinates of the calculated structures C₆₀X₄

C₆₀(CH₃)₄

C	0.21171245218024	1.14570964041527	3.17033308456366
C	-0.97202645709485	0.29957664321122	3.22661438881178
C	-0.53722803522963	-0.99069410541403	3.15278441618049
C	0.92899768601019	-0.99956429311025	3.07203820611766
C	1.38447807406258	0.28533751270931	3.09673589231252
C	2.70706952576357	0.74731211298259	2.53961495633214
C	3.16732557837171	-0.30365675249314	1.52438090466000
C	2.72090099888724	-1.60417367400782	1.52325737688237
C	1.71425751282326	-2.16514326067973	2.53578070911213
C	0.78942973733230	-2.95538426217796	1.60415551719934
C	-0.58416397400367	-2.94694974264354	1.68004034784447
C	-1.39051230752155	-2.14652399873779	2.70767492607605
C	-2.49639240452418	-1.57321135480429	1.81163833631294
C	-2.92404273924519	-0.26715846483466	1.86041263267983
C	-2.34236174791754	0.77746970593454	2.81833789191944
C	-2.18187375292030	1.96278211844473	1.85833111408508
C	-2.93294550665628	1.74744224099406	0.66794321153703
C	-3.38454045275598	0.37094925365398	0.66349818005186
C	-3.47454665144346	-0.32495510106636	-0.54308063785901
C	-3.03722082202808	-1.68884134888630	-0.59342847005940
C	-2.52451000369494	-2.27621341655670	0.56526987712987
C	-1.35620053287248	-3.12226118357173	0.48660003632664
C	-0.74959840783658	-3.36224073295340	-0.74701988313993
C	0.68115252934535	-3.37083537444231	-0.82611859563316
C	1.42259543918595	-3.13837492748433	0.33289936402215
C	2.60230263213624	-2.30635540181257	0.28180917152098
C	2.99151655815880	-1.72460049756737	-0.92636749576355
C	3.44801682428755	-0.36624181633909	-0.92514749351628
C	3.50111721588281	0.32995611235146	0.28346966067822
C	3.06935833895381	1.71189801902834	0.33662796423041
C	2.58690087589887	2.33882868254732	-0.82048676209878
C	2.51535753638754	1.60625639460097	-2.06403051665406
C	2.93582097963582	0.28001345173323	-2.11455269702331
C	2.16744853632716	-0.69321685331506	-2.85692517636724
C	2.19951022654079	-1.93487109281786	-2.11896760322143
C	1.06906306258038	-2.74463500493399	-2.07092947017300
C	-0.13687546010876	-2.34512067422110	-2.76038932194115
C	-1.26433309867194	-2.73048438283573	-1.94202863782796
C	-2.38350907029765	-1.90737481792212	-1.86578670250115
C	-2.41804117576665	-0.66563934737826	-2.60358818133030
C	-3.08899763399121	0.31622523547586	-1.78234987353388

C	-2.64865166945526	1.63700639005168	-1.77843498944323
C	-2.57389082685708	2.36992496432239	-0.53533948919779
C	-1.40864081081008	3.20783747941496	-0.58205414741948
C	-0.75215766183449	2.99915728108862	-1.85662754675000
C	-1.52237816354788	2.02693326733352	-2.59667242669679
C	-0.87453470370861	1.07998476867278	-3.39105828345547
C	-1.33039648528791	-0.29148533944428	-3.39391483207190
C	-0.16909155682542	-1.14772620092827	-3.47636016571182
C	1.00414997048879	-0.30562191140337	-3.52321250818324
C	0.56755836897152	1.07143356606749	-3.47121940753636
C	1.30993889423671	2.00954438255635	-2.75287735557896
C	0.63784748661723	2.99055840190294	-1.93336542162125
C	1.43378967297763	3.19067125794571	-0.73919723353434
C	0.80403219890292	3.36096115098006	0.49300442408545
C	-0.64493216609486	3.36971939789867	0.57310043857325
C	-1.04523189539798	2.74836344996355	1.80458238582291
C	0.18124551457692	2.32556298137851	2.48987609303638
C	1.32972410161691	2.73397530725342	1.67343009059100
C	2.45603493375420	1.93513717480454	1.60233520356531
C	-3.26105308250581	1.10708291401056	4.00493415406645
C	-1.91900768795053	-3.00186595031221	3.86651649585656
H	-4.24691956425675	1.44621505461855	3.65409187718590
H	-2.81466557161036	1.90048196958750	4.62173768556906
H	-3.39852108745380	0.21533329253112	4.63317370823285
H	-2.52635801091338	-3.83607378628333	3.48479190013608
H	-2.54060671983554	-2.39283851120292	4.53876151977639
H	-1.08413329622799	-3.41710729930264	4.44993474338221
C	2.35680095850026	-3.02797145767205	3.62950016038132
H	2.90603780360759	-3.87062262440896	3.18357325042749
H	1.58698608791902	-3.43251999734001	4.30295800108240
H	3.05794723891062	-2.42914532585598	4.22876991412651
C	3.75574667598646	1.06570024390037	3.61639957449282
H	4.69924251335603	1.39572162388575	3.15711822100803
H	3.95483421107864	0.17171822837183	4.22480751313744
H	3.39037656040105	1.86272198683778	4.28022601042133

C₆₀(C₂H₅)₄

C	0.20234301261887	1.17976874648754	3.25847236097344
C	-1.01229754644578	0.37692733120933	3.31835771968204
C	-0.61855805936856	-0.92997573432860	3.29275870102811
C	0.85027473685372	-0.99230823759159	3.24844608636247
C	1.34734786750317	0.27874792421908	3.23854286264853
C	2.69626121791023	0.68425734398306	2.69814383896471
C	3.14951909967266	-0.41807412364583	1.73198338574546
C	2.65719749789297	-1.70347956276020	1.76060199508561
C	1.60186669521350	-2.20115552144819	2.75946534007668
C	0.67265146996313	-2.97360881624809	1.82329575587324
C	-0.69928982571177	-2.91985437285688	1.86845943614199
C	-1.49827770816828	-2.07141404926228	2.85939142561364
C	-2.56862921749425	-1.48825067251288	1.92375819464589
C	-2.95258409379474	-0.16651008869349	1.92283254902130
C	-2.35228648429638	0.89303666643837	2.85438528232745
C	-2.12241234796932	2.02987537257692	1.85584601510637

C	-2.85926855043350	1.80622584599043	0.65991825332041
C	-3.36058881217340	0.44790592428704	0.69178950165685
C	-3.44728506457568	-0.28097566851013	-0.49544419219666
C	-3.05599322061906	-1.65959734597948	-0.49377008018175
C	-2.59078976212595	-2.22552051550771	0.69470973503167
C	-1.44997398064765	-3.11047253079926	0.66583925436862
C	-0.82403444448202	-3.41241621291636	-0.54403563325019
C	0.60710656925592	-3.47143859272368	-0.58894866453641
C	1.32995873878920	-3.22424235787820	0.57854513367414
C	2.54013459796862	-2.43740391879714	0.53448359447123
C	2.97503885003578	-1.90957694346261	-0.68259379136991
C	3.47749160870807	-0.56819307229379	-0.71284561311043
C	3.52737833540039	0.16244873400259	0.47530323601841
C	3.13974580356669	1.55807316876474	0.47163206441435
C	2.70699120982500	2.16532351456310	-0.71477931634933
C	2.63902806796616	1.39717513503490	-1.93620403428621
C	3.01492022926884	0.05678415561677	-1.93415514856239
C	2.23034387064561	-0.91298898808362	-2.66382666248017
C	2.20314502878949	-2.13070981224836	-1.88718967070052
C	1.04432545403990	-2.89973511751170	-1.84279477544727
C	-0.13153818067629	-2.48219769479491	-2.57272874237648
C	-1.28992933296077	-2.80295801426966	-1.76948106913399
C	-2.38172949514212	-1.94072456082353	-1.74348051707122
C	-2.35635531544874	-0.72248293276822	-2.51942701795241
C	-3.01139992894049	0.30688396152059	-1.74491609688407
C	-2.52616191407037	1.61158940010835	-1.77360726147775
C	-2.45329111752213	2.37981354506398	-0.55244649693162
C	-1.25958500913682	3.17727179440258	-0.59768920382782
C	-0.58212114134076	2.90594881419919	-1.84918103204076
C	-1.36874512405168	1.93703081191579	-2.57648150466603
C	-0.73635061291805	0.94407303205495	-3.32564706459716
C	-1.23928258212178	-0.41047595696184	-3.29601084465147
C	-0.10646903363898	-1.30720078874932	-3.32485820638589
C	1.09616951939799	-0.50765987284026	-3.36940655101054
C	0.70621140037933	0.88399794866308	-3.37099578839904
C	1.46437380813258	1.81915072695992	-2.66565816074271
C	0.80829328699992	2.84851683246419	-1.89322885258606
C	1.58326318585816	3.05870429313191	-0.68705279282251
C	0.93229529119752	3.28957099791023	0.52396913913119
C	-0.51633687566197	3.34959541756947	0.56923151459725
C	-0.96342807915179	2.77948759080443	1.80900969819153
C	0.22936402978500	2.33655817850168	2.53780681308489
C	1.40775251441242	2.68124403444388	1.73512291313957
C	2.50363548443085	1.84025354217010	1.71267528520616
C	-3.29614774110759	1.37353217845409	3.98151707185558
C	-2.04622029917027	-2.89648649391715	4.04393881686465
C	2.15002510398500	-3.12447140951095	3.86962515125341
C	3.70978357556668	1.04915407888650	3.80956150341541
C	5.09373796596505	1.42229831328060	3.30946397275031
H	3.77157047203078	0.19410341054220	4.49736303447149
H	3.27192249595939	1.88024016178379	4.38660225853309
H	5.55455631911926	0.59824242060964	2.74293234336472
H	5.75780004202726	1.65708522071477	4.15455959483753

H	5.06887580061864	2.30460233527395	2.65179352365052
C	3.14870691781816	-2.47517619858265	4.80601539523203
H	2.60341678018876	-4.00007075666861	3.37543769303311
H	1.28648711876320	-3.50572684977046	4.43946308941020
H	4.03241160388291	-2.11316431584355	4.25804481794593
H	3.49757041869446	-3.19391948633456	5.56214210174728
H	2.70128573622752	-1.62047371605360	5.33578989551702
C	-2.94248832184910	-4.05259700159088	3.63822945301977
H	-2.58549553855356	-2.20974717920159	4.71185881701792
H	-1.17976838487943	-3.26723981083352	4.61662678498644
H	-3.82805953576125	-3.70121099379458	3.08641312389200
H	-3.29725982339436	-4.59742644613919	4.52568214389026
H	-2.41347030682901	-4.77188329987663	2.99443641622682
C	-3.67032643091378	0.30743210169629	4.99105267854210
H	-4.20294333068903	1.78390833400702	3.50713330897784
H	-2.79889380084131	2.21815805274193	4.48622311433546
H	-4.19852965761769	-0.53167660219445	4.51194165289647
H	-4.33603790383291	0.72138663118007	5.76288496960634
H	-2.77849026260043	-0.09248343294876	5.49718459125172

C₆₀(C₃H₇)₄

C	0.25092662791275	1.10965647198790	3.24651530782248
C	-0.98247167339855	0.33613206232897	3.29988218352056
C	-0.61959567311745	-0.97896127485349	3.25962613237448
C	0.84649541315429	-1.07787477459974	3.21380122437515
C	1.37350936969562	0.18097575954300	3.21317483826235
C	2.73311584118925	0.55976131015998	2.67823023257646
C	3.15496419431873	-0.54437038551777	1.69925855481417
C	2.63282021957122	-1.81884890223420	1.71705004962692
C	1.56622906412973	-2.30085678760523	2.71240050499272
C	0.61625839825820	-3.03953184144746	1.76990278602212
C	-0.75405548792431	-2.95478393103624	1.82002094771516
C	-1.52899390787951	-2.09321244765649	2.81920077795630
C	-2.58340426657329	-1.47411136672529	1.88978931855435
C	-2.93904109565368	-0.14425816436265	1.90614514418790
C	-2.31234275421257	0.89006676853208	2.84985165659610
C	-2.05505132421638	2.02909292011849	1.85847375057659
C	-2.79945397401030	1.83628542953467	0.66217405235699
C	-3.33431082204048	0.49091749324986	0.68199547568304
C	-3.44045614530434	-0.22405637523949	-0.51265545006702
C	-3.08295778884181	-1.61130251411308	-0.52607428943884
C	-2.62740900214099	-2.19891925223281	0.65546866721023
C	-1.51046697915727	-3.11328155135621	0.61628600560677
C	-0.89475727520036	-3.41826382966826	-0.59791218073888
C	0.53432164727649	-3.51157108564245	-0.64652167036468
C	1.26526884828055	-3.29396703078093	0.52188362222313
C	2.49444226475792	-2.53655390590814	0.48334925175325
C	2.93952451009764	-2.00780138759859	-0.72985227756536
C	3.47447545011615	-0.67918444194913	-0.74832722457014
C	3.54342258747220	0.03820759410843	0.44729626761996
C	3.18859552836968	1.44154961199031	0.45819337613979
C	2.77035560633081	2.07198147176571	-0.72067151412358
C	2.68178284009788	1.31834934159762	-1.94965578920037

C	3.02512388854600	-0.03078080135219	-1.96209780136155
C	2.21573512013132	-0.97367711108700	-2.69983345788093
C	2.16021205602278	-2.19801689104922	-1.93509393166671
C	0.98285445063832	-2.93843111689811	-1.89563285720489
C	-0.18383068806614	-2.48490192939123	-2.61877029940923
C	-1.34804886253962	-2.78522273192033	-1.81632808220465
C	-2.41851780778426	-1.89697198036740	-1.77997108252020
C	-2.36497238915236	-0.67200633781953	-2.54377810626623
C	-2.99288689402848	0.36533493690083	-1.75718243029632
C	-2.47622854463998	1.65815184989823	-1.77426691407402
C	-2.38177936011772	2.41183388480953	-0.54550238638195
C	-1.16927677380137	3.18040381025213	-0.58564875683430
C	-0.50103526166442	2.90523134789863	-1.84125606054659
C	-1.31248845570756	1.96304065394020	-2.57630896121700
C	-0.70594354444776	0.96238031964945	-3.33650525119490
C	-1.24199845589162	-0.37966331055214	-3.31946675335415
C	-0.13156818939993	-1.30361579250711	-3.35952073796333
C	1.09035447709488	-0.53349160041200	-3.39865288788628
C	0.73459667211161	0.86726634894594	-3.38532814529365
C	1.51683117041414	1.77662505087293	-2.67260677671382
C	0.88758083313039	2.81426047109521	-1.88878569968211
C	1.66942769017338	2.99342400779033	-0.68220439562662
C	1.02663883600806	3.22734838296773	0.53234082612597
C	-0.41990752997614	3.32246153507091	0.58154907263386
C	-0.87835556611911	2.75135220901893	1.81666057222385
C	0.30503538381607	2.27282505029348	2.53802344970936
C	1.48950547978784	2.59629520165563	1.73675577388747
C	2.56481616912704	1.72928414989002	1.70509496829091
C	-3.21094590672486	1.41881245419834	3.99702141992552
C	-2.09343869935800	-2.90407199918244	4.00337809048278
C	2.08487637395219	-3.25437963118342	3.80934005761310
C	3.74858417723302	0.85276588254675	3.81161140476232
C	5.15186305829028	1.27102003565015	3.37777307663653
H	3.80404304929570	-0.06009038781903	4.41980349308068
H	3.30638496925846	1.62694609774649	4.46148728569244
C	3.10817662714542	-2.66030554281082	4.75959558243105
H	2.51022870498818	-4.14052718123591	3.30703508396096
H	1.21112823517199	-3.61488202770724	4.37905874937944
C	-3.04425322365879	-4.02430208948526	3.61283804940916
H	-2.59885903584531	-2.20526495791356	4.68724256103152
H	-1.23721474500088	-3.31606367692577	4.56488604801156
C	-3.63423834353993	0.41043894491362	5.05857859382532
H	-4.10197317263921	1.88860561954551	3.54623944622015
H	-2.64213834502122	2.23316003689793	4.47432353986124
C	-3.58182207398704	-4.77637683765030	4.81932425952429
H	-2.53030995120742	-4.72507891331592	2.93310497770788
H	-3.88425321548689	-3.60514356652036	3.03253660912230
H	-2.76687808740381	-5.23416425927816	5.40295452558293
H	-4.26844807741659	-5.58199139513454	4.51924411052157
H	-4.13342699873759	-4.10377764848372	5.49599805516698
C	-4.79801557781983	-0.48886065716344	4.66735953196783
H	-3.91363753349243	0.97418573960152	5.96400933021711
H	-2.75649200401717	-0.19131881083429	5.35149030842694

H	-5.69655718007963	0.10713480953664	4.44134080348454
H	-5.05691787324687	-1.18003628310509	5.48451104694582
H	-4.57935024761164	-1.09582872491837	3.77726910286425
C	5.31770138636242	2.75011786074775	3.05979555092585
H	5.47126972179899	0.65807245786978	2.51692410520036
H	5.84646085977646	1.00857867858373	4.19313034116709
H	4.68291603029143	3.07302929504720	2.22214884392578
H	6.35941625751968	2.98183894647759	2.79038123605012
H	5.05337608661728	3.37201664436391	3.93025975021730
C	3.57519324412746	-3.65144967766711	5.81324828678634
H	2.67303615802957	-1.77273809812913	5.24897123727939
H	3.97368713905945	-2.30052351015156	4.17718174353048
H	2.73401589473430	-4.00494237241162	6.43091292978459
H	4.31646462749901	-3.20029258941859	6.48973893134977
H	4.04088369312059	-4.53774596056441	5.35342308813648

C₆₀F₄

C	0.21290934143805	1.15009113014089	3.19513027480402
C	-0.96580899396847	0.30246398524086	3.23954111916052
C	-0.53300244137179	-0.99040423237090	3.16521576787347
C	0.92588418601765	-0.99921351568806	3.08485942282062
C	1.37930528655785	0.28834641337435	3.10992428211131
C	2.69050886551058	0.73781225728249	2.53427837156055
C	3.17429780298036	-0.30995167679524	1.52892624650414
C	2.73059361322723	-1.60895380272912	1.52706412066252
C	1.70486096918127	-2.15065669916227	2.52663312054023
C	0.78903130412691	-2.95595814688051	1.60679029399431
C	-0.58315860428489	-2.94727109295724	1.68250068472254
C	-1.38209758529131	-2.13234220267444	2.69763243791772
C	-2.50608036697955	-1.57816321828591	1.81699668253646
C	-2.93083433454196	-0.27357408106985	1.86617087997792
C	-2.32665588118673	0.76794959620789	2.81106289215244
C	-2.18176610608008	1.96491557732134	1.86315023153281
C	-2.93478131863640	1.74662638477592	0.67712106945905
C	-3.39131281284450	0.36866099725806	0.67312994422916
C	-3.47490477910166	-0.32670247290461	-0.53275111958260
C	-3.03860618197981	-1.69299355932762	-0.58368422292890
C	-2.53315176033043	-2.28507251394082	0.57388437395642
C	-1.36021075458494	-3.12926675862876	0.49449532233327
C	-0.75052242154718	-3.36262700808483	-0.73629066064951
C	0.68325334333808	-3.37128959766017	-0.81562139573844
C	1.42746979837055	-3.14564792715419	0.34021375318147
C	2.61171017448549	-2.31530856793321	0.28922708231283
C	2.99399225230807	-1.72868519094144	-0.91702392738692
C	3.44953855140538	-0.36786074748851	-0.91508265668096
C	3.50886701337816	0.32778341296047	0.29214808411104
C	3.07224856454724	1.71129077568189	0.34559437208128
C	2.58907759557429	2.33611218946197	-0.81110506522616
C	2.51642518483690	1.60369571856771	-2.05341840853111
C	2.93729500309351	0.27733675182715	-2.10425965321117
C	2.16829024765765	-0.69549965112737	-2.84540028524372
C	2.20114457354151	-1.93738675360386	-2.10885579692254
C	1.07020585792322	-2.74678767605213	-2.06057783569013

C	-0.13621388711447	-2.34648966359107	-2.74796015120585
C	-1.26433732043613	-2.73260410230860	-1.93155114830994
C	-2.38399478999227	-1.90989960064822	-1.85541114734910
C	-2.41761633751164	-0.66799675574573	-2.59187397916541
C	-3.08928603768640	0.31343618800171	-1.77177942890532
C	-2.64863699665139	1.63436563218275	-1.76774068718577
C	-2.57509056817542	2.36713489937712	-0.52578835363079
C	-1.40839017145020	3.20520669530669	-0.57236056813581
C	-0.75193830136714	2.99621725897483	-1.84630113310898
C	-1.52166618354717	2.02395193594024	-2.58533296542232
C	-0.87385317183674	1.07719246910711	-3.37981280585778
C	-1.32965464583530	-0.29384133866311	-3.38214386922747
C	-0.16847739549941	-1.14948688715417	-3.46468095140993
C	1.00462249024296	-0.30793528562710	-3.51151674587651
C	0.56800201355837	1.06866632149142	-3.45995926701456
C	1.31036546162156	2.00661666276926	-2.74153000672940
C	0.63864460334191	2.98764747558333	-1.92306990632070
C	1.43452489050809	3.18803494550896	-0.72950604224141
C	0.80515498539141	3.36200840584918	0.50109182319675
C	-0.64509787032614	3.37076004127622	0.58120100492431
C	-1.04461424059024	2.74649366493976	1.81029157175257
C	0.18141669836854	2.31983432013449	2.49297352862156
C	1.32988743267690	2.73216938953855	1.67928569847746
C	2.45698405146284	1.93768180965839	1.60749890793121
F	-3.14894799385702	1.06462947284912	3.87356645761024
F	-1.84698586481934	-2.90104924723170	3.73779557423448
F	2.27408662711967	-2.92501069704711	3.50921696094543
F	3.62841148833393	1.02071665398774	3.50017368805910

C₆₀Cl₄

C	0.21222580992267	1.15579248496785	3.17963255983244
C	-0.96518859101672	0.30686890259124	3.22406351985655
C	-0.53295403025023	-0.98712580839296	3.15008763391725
C	0.92443398138281	-0.99593470512677	3.06980307005935
C	1.37735711033785	0.29271720309678	3.09472089393182
C	2.66991546786299	0.73751533640952	2.49923414527750
C	3.16711869407825	-0.30458815966461	1.51018017291158
C	2.72350685420966	-1.60385759936769	1.50829961139102
C	1.69193958947869	-2.13431676060791	2.49293411883349
C	0.78766779604626	-2.95212033143833	1.58693941205964
C	-0.58395639788975	-2.94360993861274	1.66273917654026
C	-1.37269089667973	-2.11600730241337	2.66265108284504
C	-2.50065947866080	-1.57292324690176	1.79733068338647
C	-2.92511256566836	-0.26807502922889	1.84640037691591
C	-2.30992686522834	0.76742591021115	2.77411695237527
C	-2.17892800329984	1.96709628005572	1.84411456479228
C	-2.93625221590155	1.75025791842290	0.65937768906143
C	-3.39049400334345	0.37368527848136	0.65483095215919
C	-3.47627828636557	-0.32318299107480	-0.55022484566754
C	-3.03974404034439	-1.68919314253778	-0.60132498666549
C	-2.53217242338167	-2.28196694510959	0.55533348057566
C	-1.36160473735718	-3.12702307026165	0.47568807027307
C	-0.75124572117116	-3.36155559537780	-0.75540753369187

C	0.68180920116610	-3.37020586712372	-0.83470821949997
C	1.42675502041908	-3.14328918103228	0.32133472842410
C	2.60881108199461	-2.31226132401265	0.27093446489120
C	2.99322615619185	-1.72502686587427	-0.93469717576953
C	3.44905617425362	-0.36450233379247	-0.93261654196253
C	3.50626451862222	0.33258426409118	0.27405819174925
C	3.07182840970475	1.71464864797354	0.32760787879213
C	2.58737572678723	2.34056927351746	-0.82760731603004
C	2.51542661064478	1.60810155347685	-2.07030652706961
C	2.93616675863752	0.28164420720591	-2.12122457987510
C	2.16737463588244	-0.69130963748175	-2.86284771215381
C	2.19999066394665	-1.93370901127311	-2.12650026927902
C	1.06920386903788	-2.74336132145762	-2.07872718877583
C	-0.13725658990637	-2.34266559722595	-2.76631621303749
C	-1.26539465282984	-2.72915073261890	-1.94968554612486
C	-2.38480607535570	-1.90613558338073	-1.87307163510215
C	-2.41863791458979	-0.66371018117953	-2.60931786340936
C	-3.09001502631114	0.31787510488142	-1.78877321888251
C	-2.64941769659131	1.63888141791614	-1.78454146485811
C	-2.57508941600391	2.37171035129417	-0.54226324272975
C	-1.40889322698554	3.21089561123781	-0.58882396975786
C	-0.75262352249675	3.00152790685435	-1.86290345353461
C	-1.52254440356296	2.02882788685953	-2.60203569773573
C	-0.87481117703223	1.08202331644435	-3.39610995802990
C	-1.33063314727134	-0.28919840493065	-3.39878494858950
C	-0.16942862268773	-1.14506116174850	-3.48151630903841
C	1.00375202339117	-0.30334324657549	-3.52816169374786
C	0.56718302333672	1.07345971672932	-3.47628703276515
C	1.30947430215760	2.01142998492522	-2.75829099824734
C	0.63762875163385	2.99291361545692	-1.93968235448461
C	1.43337776299454	3.19367093143426	-0.74600314126154
C	0.80413900408437	3.36796572297038	0.48484628908951
C	-0.64573927462358	3.37678145544618	0.56501972722666
C	-1.04358275334732	2.75212756497269	1.79536479670794
C	0.18064665109189	2.32585480691202	2.47740087911767
C	1.32726563892394	2.73765029010331	1.66436539568961
C	2.45178684305487	1.93943427617166	1.58842270407443
Cl	-3.41106327273040	1.16647490039318	4.16320660730927
Cl	-1.99022122094820	-3.13516730612742	4.02852094368528
Cl	2.44435546108681	-3.16176221287502	3.78294266101771
Cl	3.92161681016916	1.12284723442239	3.75865406440716

C₆₀Br₄

C	0.21187371730908	1.15833495744080	3.17282131903046
C	-0.96509967484452	0.30959334150124	3.21747090172744
C	-0.53274263859559	-0.98675278686542	3.14404827336589
C	0.92355271091979	-0.99556264362805	3.06382048065171
C	1.37658427395800	0.29542527186967	3.08818128065881
C	2.65910737143629	0.73678571015569	2.48334903383320
C	3.16445655504727	-0.30201658710747	1.50336588827186
C	2.72090548852457	-1.60237858436321	1.50160429685202
C	1.68569537451385	-2.12624174640055	2.47784434262034
C	0.78779392592051	-2.95168237661337	1.58050106295747

C	-0.58483723056488	-2.94318574646602	1.65635722295475
C	-1.36805387406839	-2.10797588595355	2.64694855793223
C	-2.49881292363669	-1.57145797378689	1.79042941783577
C	-2.92314777424163	-0.26549797147175	1.83930864857756
C	-2.30096889452303	0.76661102961031	2.75717243102617
C	-2.17878860621388	1.96887029364281	1.83847261862405
C	-2.93674824943952	1.75202653232704	0.65270169762826
C	-3.39016102407990	0.37581356262677	0.64782425280964
C	-3.47690300215202	-0.32169596748819	-0.55681587091438
C	-3.04032185427538	-1.68781719399666	-0.60791758222410
C	-2.53202913915151	-2.28091440039979	0.54833546611881
C	-1.36224621642791	-3.12651203473532	0.46874899875805
C	-0.75165904372028	-3.36129077779989	-0.76242873545880
C	0.68139123157066	-3.36995399053679	-0.84172429364694
C	1.42657161857309	-3.14278752575475	0.31437370950857
C	2.60786545771894	-2.31123211860604	0.26397790343396
C	2.99307541876720	-1.72369951534028	-0.94132279911599
C	3.44897589953416	-0.36306759363505	-0.93923606981927
C	3.50522379076711	0.33466623564002	0.26713028832556
C	3.07162845210662	1.71635755310990	0.32090163057613
C	2.58697930885971	2.34241529963180	-0.83379190173387
C	2.51510901097573	1.60977420346568	-2.07658907453976
C	2.93579680862737	0.28326271092642	-2.12757241067655
C	2.16703103358154	-0.68977979263460	-2.86929680091475
C	2.19963474644705	-1.93231718138784	-2.13300578567201
C	1.06885524986572	-2.74209825953308	-2.08527974525968
C	-0.13762702437963	-2.34116575528129	-2.77287910028370
C	-1.26579734425100	-2.72787371938528	-1.95623913074800
C	-2.38517608448705	-1.90470982890429	-1.87957148001934
C	-2.41899773980133	-0.66214864111143	-2.61576756377525
C	-3.09032259364306	0.31953700361447	-1.79513078579580
C	-2.64975633331271	1.64059370534607	-1.79082248976406
C	-2.57532289135570	2.37359277139368	-0.54845161048790
C	-1.40908489166025	3.21313911202766	-0.59516749347586
C	-0.75292653263461	3.00346575782043	-1.86916021777924
C	-1.52288455537792	2.03056400564565	-2.60823412786789
C	-0.87514947417973	1.08372441617072	-3.40216971071005
C	-1.33097168434159	-0.28753342063477	-3.40495526302507
C	-0.16976830143063	-1.14347975890272	-3.48774167502671
C	1.00342961535764	-0.30169221091996	-3.53433819262025
C	0.56688394797868	1.07515316305351	-3.48235268272709
C	1.30917608234467	2.01314244432155	-2.76449106013728
C	0.63730687417374	2.99483947431704	-1.94594016092369
C	1.43293871222174	3.19589639784963	-0.75233363968071
C	0.80381449723677	3.37088808110256	0.47852021201603
C	-0.64603935009255	3.37971669683482	0.55869594923493
C	-1.04336486407106	2.75529035120902	1.78949960008164
C	0.18032237039474	2.32943603798438	2.47095564540587
C	1.32645396503302	2.74077579031828	1.65854149761159
C	2.45102931758268	1.94112698041308	1.58279058556599
Br	-3.51009188705594	1.19886769723962	4.27393971930240
Br	-2.04500313410442	-3.22136661794645	4.13949259905764
Br	2.51020112905582	-3.24850514139318	3.88722833489706

Br	4.03245502841051	1.15462592147357	3.85776944897207
C₆₀(OH)₄			
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C	-1.02833663697169	0.39591518395673	3.23956654521086
C	-0.59941161001447	-0.89517884945471	3.18609829459428
C	0.86499417645619	-0.91080786728168	3.12127277049837
C	1.32395904887087	0.37088400864540	3.13493894461364
C	2.65630299005070	0.81638387258063	2.59875493827907
C	3.13360238525787	-0.25019323407780	1.59583197409784
C	2.68387755741206	-1.54900300370808	1.60625501743513
C	1.65312068162698	-2.08588138415772	2.61925618644472
C	0.73477372126592	-2.88725266432796	1.68155109263228
C	-0.63951201144237	-2.87261161867804	1.74268684214056
C	-1.45342847406693	-2.05293337132438	2.75766407454054
C	-2.55896034166117	-1.49379170127575	1.83946583124728
C	-2.97947283148123	-0.18537715400178	1.86703122368912
C	-2.39307137703251	0.86989256936318	2.82278386051364
C	-2.21913539274551	2.04940024669088	1.84352075162584
C	-2.95728090170892	1.81939851949342	0.65067631188997
C	-3.41949515951115	0.44241124245844	0.65922599887461
C	-3.49551550510827	-0.26690582433092	-0.54051203516510
C	-3.06435695008772	-1.63419386442397	-0.56928532252602
C	-2.57234789547064	-2.21142612477062	0.60304578172721
C	-1.40138656210781	-3.06157293811608	0.54665048233119
C	-0.78140874270762	-3.31529505176690	-0.67649854171881
C	0.65154593211973	-3.33048284720360	-0.74027803674974
C	1.38263575714769	-3.09047816664775	0.42265854547875
C	2.57152263798022	-2.26526898614796	0.37419726669325
C	2.97012871650246	-1.69782057834276	-0.83739454811032
C	3.43108951678320	-0.34020408366204	-0.84807069000865
C	3.47828084741395	0.36941207298394	0.35302399905252
C	3.04641509991520	1.75605611444242	0.38413814938552
C	2.58036028546711	2.36912238820518	-0.78689902768091
C	2.51806061982404	1.62039841305440	-2.02092825136823
C	2.93455961383805	0.29237810953297	-2.05108660108426
C	2.16967690614356	-0.68677937449518	-2.78873011944788
C	2.18909013262057	-1.91895630835212	-2.03535106812997
C	1.05464445251841	-2.72327372266091	-1.98930165792949
C	-0.14241713870270	-2.32796184171226	-2.69580792392745
C	-1.28033516464668	-2.69838428897468	-1.88554944914230
C	-2.39707093260458	-1.87026555619731	-1.83151468482042
C	-2.41819360313549	-0.63798582606315	-2.58465631247365
C	-3.09432384652502	0.35639090504207	-1.78357160686782
C	-2.64788432192279	1.67498856606116	-1.79096487102206
C	-2.58454372246973	2.42411396028871	-0.55734415016041
C	-1.41521797409082	3.25644843410008	-0.60205388598578
C	-0.74561528218825	3.02850557817968	-1.86619565801376
C	-1.51125621854036	2.04994384581560	-2.60180834011300
C	-0.85933559577973	1.09105288365318	-3.37828603846419
C	-1.32067538095391	-0.27828087543634	-3.36831792275953
C	-0.16210351308850	-1.13966373001491	-3.42742587997289
C	1.01491947764754	-0.30320014167159	-3.47241277446848

C	0.58337418981275	1.07575587176734	-3.44270594165072
C	1.32158654912444	2.01951435676317	-2.72755702605548
C	0.64539171862540	3.01364305799426	-1.92808350131510
C	1.42971100196752	3.22611462086677	-0.72856099615361
C	0.78773146511290	3.41739316977628	0.49434996607353
C	-0.66331233110024	3.43284045386244	0.55886176117617
C	-1.07892910074166	2.82867870868678	1.79237237544662
C	0.13869951313546	2.40856932100765	2.49580138185521
C	1.29786621403622	2.80326716135638	1.68682116380838
C	2.42147173022066	2.00023215595627	1.63752193498785
O	3.54409792867865	1.10110401743847	3.64621154059777
H	4.37839943633059	1.39342981015548	3.25984559026073
O	2.18163563016494	-2.81149632473493	3.69352053867805
H	2.64714633088216	-3.57739004668462	3.33656555772789
O	-1.89962310300252	-2.76808237912178	3.87550061658707
H	-2.41184338670521	-3.52311769493781	3.56202041680840
O	-3.17890585744952	1.17232816070688	3.94416013645308
H	-4.03920821731028	1.47820754630787	3.63251498830405

C₆₀(OCH₃)₄

C	1.09787865718207	1.58365365571716	2.97856833508961
C	-0.14357744718055	0.86958201507744	3.23108153687804
C	0.19826419219593	-0.38978109113255	3.63194584340488
C	1.65457755842036	-0.50001556809661	3.65927855650448
C	2.20456829188453	0.68971942158297	3.28290705124890
C	3.58842377553309	0.84259809856836	2.69862529944515
C	4.01904701325747	-0.51632775960779	2.14000289805846
C	3.48771463786592	-1.71067321858712	2.56202910920400
C	2.37686244690132	-1.81373159049631	3.62960327889875
C	1.44547779805642	-2.84315060132563	2.96040028617523
C	0.07407025905945	-2.73835123832903	2.93361885068599
C	-0.72547960637129	-1.57766901596069	3.55261139539983
C	-1.74117046272894	-1.30483294433501	2.43983171186110
C	-2.07119576165255	-0.04484579255570	2.00899234851319
C	-1.45638047344076	1.24424193636247	2.58603159423087
C	-1.16542775104109	2.01035045560450	1.28756772453708
C	-1.87263794597375	1.43060104619172	0.19871344446796
C	-2.42701386713090	0.16366778860075	0.63817931838811
C	-2.50369524814589	-0.90400674227574	-0.25671677752355
C	-2.16630723450636	-2.22255900893401	0.19735039409993
C	-1.76018101875261	-2.39879684922348	1.52035576306928
C	-0.65322145461135	-3.27878076184069	1.82382587169219
C	-0.00382210239674	-3.95836451173556	0.79420856095639
C	1.42674722943954	-4.06739580644280	0.82394491444049
C	2.12738443701865	-3.48926523083552	1.88110689689372
C	3.36989724981361	-2.79102716939355	1.63181036271435
C	3.85392942345309	-2.68669602557856	0.32707127963233
C	4.40711098210017	-1.43737065866247	-0.10877715427352
C	4.45602286470169	-0.36794836818670	0.78598179399322
C	4.12322519024078	0.96770083004553	0.32783519782975
C	3.74437523423701	1.17384753245882	-1.00510177741140
C	3.67846057298090	0.05864440185947	-1.92062427158792
C	4.00329037289774	-1.22217230502800	-1.48145524420397

C	3.20169415788708	-2.35109274989721	-1.89373207681116
C	3.10709561031065	-3.25736597461242	-0.77296075546098
C	1.91880250767411	-3.93917175676647	-0.52920261633468
C	0.77980504249235	-3.74229918181732	-1.39693395794297
C	-0.41157094840866	-3.75988879471431	-0.57907525894219
C	-1.46921773300747	-2.90406098959244	-0.87125095868310
C	-1.37618241387659	-1.99748815769679	-1.99182335320140
C	-2.01235825671099	-0.75771075321150	-1.60996094783460
C	-1.47742453778412	0.45656086985258	-2.03198337285409
C	-1.40975412883513	1.57138635726174	-1.11629499873135
C	-0.18505759370748	2.27909998805337	-1.36732575915207
C	0.51597565369814	1.60454636587726	-2.44065327381888
C	-0.28624314881953	0.47651870463364	-2.85154045855211
C	0.32775302347600	-0.72035533631371	-3.22253389726510
C	-0.22720082437166	-1.98034218811518	-2.78376015759375
C	0.87040049702803	-2.87030495038806	-2.48283431133873
C	2.10323913270249	-2.16027326752326	-2.73337628239039
C	1.76728619884591	-0.83147964328557	-3.19097297017332
C	2.54098426884410	0.25851691874608	-2.79053941353841
C	1.90432028405230	1.49753022499451	-2.41112559003672
C	2.65353735117463	2.05986902127151	-1.30628428229674
C	1.97900269402711	2.68457780335162	-0.25947972412657
C	0.53170194282573	2.79541954759958	-0.28960968740334
C	0.02743239049668	2.66364180754483	1.04827669984008
C	1.18544566044928	2.44098811839062	1.92165264436381
C	2.39967100082189	2.47977131515632	1.09816645789436
C	3.46741437645951	1.65233443892989	1.38849036228777
O	-2.32885191286752	2.00667982503291	3.37545599307554
O	-1.40263523821524	-1.88292922629864	4.74315837144896
O	4.57679147244554	1.32750076481753	3.56727530881843
C	4.26513394137005	2.54239939557255	4.19257656362715
C	-0.56763140444078	-2.18776185442860	5.83034870870868
C	-2.66714973067389	1.41718496821175	4.60455946989847
C	3.50478164571903	-3.33413517350990	5.05217446076901
O	2.79065030870592	-2.13361836320093	4.92983812704901
H	5.13394009982409	2.81900790572345	4.80427626560047
H	3.38051997114728	2.45240310129140	4.84894459162018
H	4.07779162896058	3.35110982189631	3.46148661225756
H	3.75726561604698	-3.44768704794180	6.11462080251702
H	4.44141517737393	-3.31850363652490	4.46575280254433
H	2.90724207153804	-4.20843241111939	4.73420765335282
H	-1.22273867121565	-2.37828497270438	6.69052113820499
H	0.11879574278216	-1.35774069589540	6.07458229161870
H	0.04419492227823	-3.08769710227100	5.63966829018967
H	-3.41903910822294	2.06766817973840	5.07038042974202
H	-1.79332540666349	1.33646734344417	5.27560417137065
H	-3.09163388814372	0.40504878933150	4.47910596456999
C₆₀(OC₂H₅)₄			
C	1.29882303354893	1.54052250130288	2.82361665747230
C	0.05391592169490	0.85285007603149	3.12712035441192
C	0.38457857242591	-0.42092008196985	3.48681239222213
C	1.83707492843539	-0.56913474048507	3.43795417057776

C	2.39648894746070	0.61196564152735	3.05301558365132
C	3.75575297131556	0.74482124266540	2.41130803126564
C	4.12350624038215	-0.61533363425961	1.80961524677699
C	3.58593426702959	-1.80429928714186	2.23929769623811
C	2.52487039008483	-1.89713423696210	3.35652172591031
C	1.53761795513316	-2.89361357277852	2.72020030464236
C	0.16971568498157	-2.75311607174540	2.76285067481072
C	-0.56709321572123	-1.58601093573356	3.44191519942763
C	-1.63094562878396	-1.26695465819931	2.38599557221648
C	-1.95142902545010	0.00802097256798	1.99055903255720
C	-1.27869721670047	1.27212881919807	2.55743410031546
C	-1.03062921356610	2.05006275136936	1.25691480366524
C	-1.80532731995472	1.50700983615958	0.19577054254780
C	-2.36948273414282	0.24711088830824	0.64222001969543
C	-2.51724057074364	-0.80319197441889	-0.26399827544501
C	-2.19063954616682	-2.13664926919912	0.15232335611735
C	-1.72377359824210	-2.34434096420179	1.45071671671958
C	-0.62556749430142	-3.25635173051776	1.68338078693380
C	-0.04559008699638	-3.93475132366431	0.61238982409307
C	1.38158019141958	-4.07992627703013	0.56857636190584
C	2.14871110975586	-3.53801042266878	1.59851565955296
C	3.39424205278410	-2.86535796405103	1.29871091672534
C	3.81480785576035	-2.74999688704929	-0.02690677034675
C	4.37671499902099	-1.50702874012023	-0.46986811064338
C	4.49671034841769	-0.45438412849459	0.43804914164245
C	4.17509358933918	0.89644342336530	0.01845479212789
C	3.73613638219116	1.13460111230875	-1.29049056871279
C	3.59737973110925	0.03691804188671	-2.21898802939146
C	3.91128673969929	-1.25878820429918	-1.81718473606655
C	3.06228940800478	-2.36088171596256	-2.20710881167734
C	3.00015481368049	-3.28320202996523	-1.09717537915390
C	1.80871464369898	-3.94037039510452	-0.80532478536850
C	0.63334247806125	-3.70063735984106	-1.61143395441919
C	-0.51591783524751	-3.70298902265742	-0.73528164446950
C	-1.56451887895753	-2.81651457552762	-0.96043297341184
C	-1.50467799562833	-1.89391033134062	-2.07018208887157
C	-2.09000681640550	-0.64578564509133	-1.63764585729899
C	-1.54629018472367	0.56217173738222	-2.06673083067069
C	-1.40503137334163	1.65937466079131	-1.13837286231328
C	-0.17698311915484	2.34130162095981	-1.43953439110565
C	0.45283132272793	1.66780265287105	-2.55682901600740
C	-0.39705330720544	0.56673081753469	-2.94437931107686
C	0.16775759339438	-0.63817154546305	-3.36435252445632
C	-0.39621425080670	-1.89144797266895	-2.91802321395253
C	0.69199398605376	-2.81322253584192	-2.68700205221540
C	1.92848123493666	-2.12897539388067	-2.98729512427583
C	1.60385412325764	-0.78475787778224	-3.40663552820404
C	2.42381013933017	0.27897130216413	-3.02805745013440
C	1.83784564206073	1.52659614748664	-2.59810180961111
C	2.65445530905590	2.05184052784215	-1.52334832559049
C	2.04880069742084	2.67518837192648	-0.43434960284073
C	0.60484491237098	2.82159570588450	-0.39065295963616
C	0.16410406366624	2.68000004383114	0.96856561079170

C	1.35759627528916	2.41472470458801	1.77915196983019
C	2.53080000237374	2.43665644661838	0.89720769756230
C	3.59029212756040	1.57869557061408	1.12127498794549
O	-2.07129791966670	2.06057630956492	3.40397771888347
O	-1.19563368975689	-1.90509539536213	4.65807007021255
O	4.80410884910062	1.18768743971471	3.23116179385757
C	-0.35758118698097	-2.34365516616433	5.71387368051611
C	-2.58396172975589	1.40893417023974	4.55476402122119
C	4.57790832832182	2.39039197671633	3.94166304814878
C	4.06059647744102	2.14339274337188	5.34359373651810
C	0.16499048062356	-1.22139239629367	6.58642361768016
C	-4.04193282231205	1.04413833156798	4.37866005306773
H	4.74346593996272	1.47434168872681	5.88765100279400
H	3.06540775621523	1.67568789263168	5.33354244438289
H	3.98827145259076	3.09243999428847	5.89711300499145
H	0.48351769796928	-2.93636367442071	5.31293539230134
H	-0.98133156522639	-3.02765553296435	6.31055690804623
H	0.86602760356804	-0.57033999281462	6.04589511362830
H	0.70632142379355	-1.64461309892328	7.44679572436200
H	-0.66240835426695	-0.60587113792560	6.97048552130032
H	-2.46126856393636	2.11476814488232	5.39273677411405
H	-1.98871701535089	0.51177871885455	4.79791546596917
H	-4.63755424504742	1.93589934837907	4.13295684468448
H	-4.44135842166140	0.60309428770295	5.30506022964889
H	-4.17382268648401	0.30861207904462	3.57128201165013
H	5.55253524407568	2.90275855745595	3.98121016784694
H	3.89669117420433	3.05402046416519	3.37755279515873
H	4.72854307553767	-2.80730768482563	6.50450275631971
C	4.12043463405240	-3.65343108649787	6.15247626828767
H	4.70968777252919	-4.57586831729656	6.25964018496810
H	3.23386888966139	-3.73070216174746	6.79945180908856
C	3.71681566035950	-3.44821930551504	4.71420587588909
H	4.60919633953988	-3.39408783087221	4.06167491944112
H	3.10162333502845	-4.29570603229279	4.35390429612127
O	2.98753739437744	-2.24349327715900	4.63326704181463

C₆₀(SH)₄

C	0.21171535319104	1.14589731776890	3.17714046904737
C	-0.96595692709359	0.29722995532480	3.22570722081696
C	-0.53340241173679	-0.99607865190868	3.15108434586402
C	0.92420846877006	-1.00500667009784	3.07105621959121
C	1.37749508248702	0.28300568288361	3.09640594166334
C	2.68142116115855	0.73468171053707	2.51327808834325
C	3.16573904243226	-0.30978612325676	1.51907193821609
C	2.72081940640902	-1.60995715257876	1.51695579244958
C	1.70067808158729	-2.15425191245152	2.50919543867873
C	0.78861554049911	-2.96316502857842	1.59726088281912
C	-0.58459344033404	-2.95458131130893	1.67301268545455
C	-1.38047609718489	-2.13567717836431	2.67950351315770
C	-2.49786445172729	-1.57908990028149	1.80539762196541
C	-2.92345574789923	-0.27324732520347	1.85470616537112
C	-2.32042270544751	0.76471934623274	2.78894188440990
C	-2.17795774873443	1.96064944728211	1.85479489686535

C	-2.93416904459732	1.74520934787840	0.66726992196569
C	-3.38605629630420	0.36764226015265	0.66153643225926
C	-3.47553116582716	-0.32794598047813	-0.54482633206045
C	-3.03863110181919	-1.69266472260341	-0.59635206170183
C	-2.52810909628281	-2.28358375248612	0.56112067124444
C	-1.35853926970713	-3.13062358463665	0.48197941611917
C	-0.75037685285783	-3.36688322064001	-0.75142801313056
C	0.68088278198882	-3.37553253301588	-0.83053716370234
C	1.42376988331769	-3.14688288008937	0.32813208580783
C	2.60474851321123	-2.31380336120714	0.27746385439772
C	2.99225068087005	-1.72854222285188	-0.92923321058413
C	3.44855657379270	-0.36934296102435	-0.92671432638173
C	3.50210622667220	0.32651589137828	0.28167166636017
C	3.07023048653105	1.70956513626618	0.33608587888978
C	2.58610921519649	2.33635232549119	-0.81925254011259
C	2.51488640524605	1.60458305841592	-2.06321684317091
C	2.93516073417816	0.27820076048940	-2.11468602803717
C	2.16719401697799	-0.69435537022459	-2.85804870372358
C	2.19918589059952	-1.93683524820482	-2.12146224086579
C	1.06874915973398	-2.74673442502452	-2.07416720814254
C	-0.13714533468898	-2.34590691230388	-2.76266462189371
C	-1.26474809004232	-2.73252032100238	-1.94534702465465
C	-2.38372801956159	-1.90921690982148	-1.86841931751740
C	-2.41805332180274	-0.66669674433470	-2.60483631238774
C	-3.08849203812048	0.31450422294615	-1.78274031615256
C	-2.64825073289964	1.63543310289230	-1.77787095829957
C	-2.57317029210910	2.36753479910399	-0.53440135968334
C	-1.40833302873424	3.20792915666671	-0.58107233680601
C	-0.75213670135412	2.99884686465151	-1.85552236604503
C	-1.52199546701237	2.02620129971460	-2.59552932071517
C	-0.87447384404723	1.07996721979117	-3.39060758508602
C	-1.33022605326072	-0.29156901543473	-3.39417338800350
C	-0.16921982572071	-1.14772138075094	-3.47743589468453
C	1.00386703923048	-0.30575009615759	-3.52340679608317
C	0.56752144285170	1.07138846074315	-3.47070882602481
C	1.30964923192725	2.00876510976498	-2.75158744281282
C	0.63789792106227	2.99021350232954	-1.93220433013426
C	1.43348132273757	3.19068227292036	-0.73806355619920
C	0.80431649912628	3.36362834308255	0.49357012990141
C	-0.64531361944102	3.37246622788603	0.57364550661135
C	-1.04326738501661	2.74887950787217	1.80483648057233
C	0.18075414486682	2.32151504734571	2.48482086351497
C	1.32750473450214	2.73435920373389	1.67397038534790
C	2.45149646208237	1.93297111289149	1.59949816673842
S	-3.35622831078195	1.14699534555255	4.26845409625118
S	-1.96355162675118	-3.10284377121097	4.13601840215280
S	2.43087364372381	-3.12940237160762	3.89208948901968
S	3.87701257891739	1.10378651990086	3.87044334044757
H	4.87744841999345	1.51206191884939	3.05682174955770
H	2.96171408133500	-4.09139993687930	3.10313760768028
H	-2.58109491924414	-4.06420754913203	3.41206793877679
H	-4.43127892006425	1.57624620161231	3.56873417246696

C₆₀(SCH₃)₄

C	0.21317908912352	1.19530517729204	3.16914614074348
C	-0.96419079971688	0.34552495870725	3.22594947872076
C	-0.52913748198343	-0.94626450989459	3.15942766103048
C	0.92913841828681	-0.95352384197015	3.07840631096970
C	1.38126826157771	0.33381995713992	3.09515878133660
C	2.68572758196487	0.78296793912980	2.51276437838244
C	3.17044024615577	-0.26765394428756	1.52390315485274
C	2.72625931805024	-1.56935639244756	1.53144999262221
C	1.70739794452027	-2.10648440370855	2.53009128675800
C	0.79604695773422	-2.92386582447616	1.62314293937656
C	-0.57822505133692	-2.91681575325267	1.69959697140320
C	-1.37460317176541	-2.09131748631670	2.70209698901739
C	-2.49341412140746	-1.54390552422379	1.82235208996282
C	-2.92169498975931	-0.23736749421519	1.86236145810202
C	-2.32049599106095	0.80778363340852	2.79109687333326
C	-2.17970143195499	1.99604739145125	1.84670791954412
C	-2.93383427586119	1.77173189801754	0.65998459168297
C	-3.38435188237625	0.39309052758786	0.66429628650625
C	-3.47319064067737	-0.31114828238165	-0.53764859441443
C	-3.03432526473337	-1.67457374607529	-0.57929976762169
C	-2.52240340763419	-2.25588429816200	0.58304524273062
C	-1.35083676041072	-3.10142253868582	0.50951980040456
C	-0.74359216347940	-3.34594152026521	-0.72295698123683
C	0.68674174652067	-3.35313198265061	-0.80263935787548
C	1.42919206818334	-3.11461273982338	0.35456489544196
C	2.60985649488255	-2.28077093539638	0.29707815269365
C	2.99578445579788	-1.70418219461728	-0.91488839763074
C	3.45016307678156	-0.34537949529625	-0.92265248834722
C	3.50371018704636	0.35905804691884	0.28135213322782
C	3.06936575194661	1.74236013339678	0.32614699126778
C	2.58436236724656	2.35995000230732	-0.83398447190082
C	2.51354674656872	1.61882293042161	-2.07306028487790
C	2.93596097794842	0.29301692716285	-2.11569814301890
C	2.16871261716569	-0.68593338601666	-2.85150039055699
C	2.20268952257393	-1.92286245516406	-2.10566613032882
C	1.07341590136372	-2.73371091260726	-2.05173139320554
C	-0.13333979116415	-2.34018317951049	-2.74304579781797
C	-1.25990464375754	-2.72194949895410	-1.92191559845636
C	-2.38005620772402	-1.89998122643098	-1.85056077196262
C	-2.41663904210251	-0.66300450326341	-2.59618251413606
C	-3.08842795265924	0.32308463542035	-1.78099469525598
C	-2.64967716164137	1.64425522865785	-1.78529774791172
C	-2.57507843975286	2.38577194635289	-0.54676889017137
C	-1.41138500342691	3.22585038488882	-0.59943619737167
C	-0.75535752533601	3.00895682322503	-1.87283402383785
C	-1.52436541731975	2.03060823450854	-2.60623814139334
C	-0.87594640641813	1.07983037987039	-3.39534269784825
C	-1.32978272680465	-0.29221755183467	-3.38910800763471
C	-0.16743845798127	-1.14724086490031	-3.46651042291879
C	1.00449153731101	-0.30395862175727	-3.51937783267129
C	0.56613139700155	1.07272914535767	-3.47602952152403
C	1.30729739307755	2.01609644729810	-2.76361309169479

C	0.63445388549141	3.00180674826622	-1.95015653297808
C	1.43053377546242	3.21160812610507	-0.75771400380437
C	0.80181195200508	3.39194797644090	0.47369129962355
C	-0.64805394110354	3.39927697212575	0.55440533115683
C	-1.04531808521900	2.78558527169877	1.79020885602874
C	0.18070442214383	2.36820549519629	2.47494810329155
C	1.32730580112854	2.77357354984365	1.65823866781569
C	2.45333682425333	1.97317899247843	1.58909421941851
S	-3.33579371384696	1.18297439499039	4.28138688171433
S	-1.94820856022795	-3.02741770930391	4.17637158805404
S	2.43337350403287	-3.04773728774880	3.93227982419998
S	3.86121224812449	1.14882629420694	3.88284354005205
C	5.32827037541624	1.63862794950072	2.95595722711604
C	3.20460010448720	-4.41392976559706	3.04439108142939
C	-2.85446050230354	-4.36677172448327	3.37958122712770
C	-4.88663869204793	1.69911332010793	3.51959446704454
H	-5.56459974909655	1.93381005995015	4.35256037647428
H	-5.33352989914811	0.89208958844067	2.92055587520681
H	-4.76377550418196	2.60095332842395	2.90230707219365
H	-3.25230417455921	-4.98687943379246	4.19543471597216
H	-2.19925092100993	-4.98925088704505	2.75256317186946
H	-3.69788670732926	-3.99015306041111	2.78209461415410
H	3.68405260682662	-5.03788719029207	3.81204410446385
H	3.97780350737765	-4.06339956475836	2.34465401058186
H	2.46262957424766	-5.02395105424160	2.50843521795320
H	6.09337245596013	1.87126965195122	3.71035543872717
H	5.15175013886507	2.53737788411178	2.34718464286639
H	5.69970763266814	0.82114286919964	2.32078004055731

C₆₀(SC₂H₅)₄

C	0.21374062863636	1.15435560006701	3.11335453687058
C	-0.95733733398722	0.29556566265862	3.16499490615782
C	-0.51203480461142	-0.99226553347973	3.09515520085932
C	0.94613105559927	-0.98837722450553	3.01831430758027
C	1.38857401946135	0.30204879487105	3.04025221337691
C	2.69192275236241	0.76288575568257	2.46478224981807
C	3.18502193136736	-0.28138332928292	1.47384252012039
C	2.75071248964830	-1.58608272494910	1.47829863604811
C	1.73542307766542	-2.13592634931494	2.47342298078447
C	0.83277725774076	-2.95777458566868	1.56269599211426
C	-0.54247135498248	-2.96118628045010	1.63559716283346
C	-1.34783620116481	-2.14477518528007	2.63761317552658
C	-2.46734435027896	-1.60186048131202	1.75639757437862
C	-2.90586331818490	-0.29888441296509	1.79719638025981
C	-2.31664287258088	0.74861356142669	2.73049432249622
C	-2.18263374583766	1.94072660124985	1.78891094767510
C	-2.93113109807415	1.71237410633110	0.59913288302252
C	-3.37025529760699	0.33027162423320	0.59906905323330
C	-3.45130869417108	-0.37206029454714	-0.60419826323684
C	-3.00080545351456	-1.73194850092448	-0.64714138467882
C	-2.48628005438608	-2.31086028515400	0.51460237092728
C	-1.30964120920065	-3.14899295870761	0.44275289775067
C	-0.69803696654771	-3.38724606790135	-0.78957852460214

C	0.73198214942431	-3.38334110352932	-0.86564011727988
C	1.46932166682090	-3.14089532117027	0.29487647741340
C	2.64158372763927	-2.29556223561592	0.24159254837546
C	3.02741707018010	-1.71444115651259	-0.96752580064954
C	3.47242308781077	-0.35216207122591	-0.97186089373616
C	3.51672073851668	0.35018986217131	0.23331748190020
C	3.07280087214009	1.73008253117987	0.28036094241074
C	2.58599307822489	2.34602813579466	-0.87981159396296
C	2.52393703800812	1.60690550219958	-2.12065207933518
C	2.95659832637457	0.28439083969377	-2.16496623717627
C	2.19857568717961	-0.69901448249389	-2.90451042186504
C	2.23973555156137	-1.93709471147122	-2.16108203993387
C	1.11705143092188	-2.75735636346821	-2.11200077365633
C	-0.09074771086889	-2.37158786887816	-2.80576991119749
C	-1.21615420247874	-2.76376652173722	-1.98805365982002
C	-2.34228051058446	-1.94994153723923	-1.91745753539562
C	-2.38698920890262	-0.71188169953406	-2.66067410387397
C	-3.06849141180819	0.26742591339629	-1.84525245469836
C	-2.63993419779576	1.59198131609505	-1.84581049016105
C	-2.57410022744884	2.33140520687891	-0.60547993379913
C	-1.41678346726571	3.18048085370290	-0.65351481453671
C	-0.75598728054937	2.97126534641716	-1.92564838293392
C	-1.51560151964266	1.98852645292899	-2.66306354286338
C	-0.85795427208048	1.04445978100352	-3.45263371005527
C	-1.30113926221727	-0.33108644952879	-3.45028741111695
C	-0.13218439349279	-1.17707161071423	-3.52645306094745
C	1.03321982467417	-0.32457493105868	-3.57471582578867
C	0.58433865160957	1.04867022076459	-3.52974629315142
C	1.31643093616035	1.99619184983743	-2.81334753445021
C	0.63399017627695	2.97500412478559	-1.99947514750517
C	1.42545598668250	3.18862549552049	-0.80471927887261
C	0.79229054464276	3.36138552613689	0.42557102675499
C	-0.65768146025660	3.35737542793931	0.50262657721858
C	-1.05365557924571	2.73843804950046	1.73639198687349
C	0.17413013714688	2.32919995628917	2.42325624249184
C	1.31995687974765	2.74493665654586	1.61034968831176
C	2.45301559996815	1.95418885249156	1.54302759888192
S	-3.33814120537099	1.10411793548927	4.21985142711253
S	-1.87884079328409	-3.08483181702431	4.12807842871061
S	2.43031929932286	-3.07462351861887	3.89636395868699
S	3.86079725224032	1.12412346190877	3.84004081606947
C	5.33771952956651	1.64558448813547	2.91927244136792
C	3.40677102647618	-4.35660492676637	3.05494283057635
C	-2.91020430184972	-4.39247618476455	3.39924022953441
C	-4.89569401983841	1.64529424817244	3.45631726332413
C	-5.91833883131199	1.90053294443639	4.54865734968345
H	-5.24856623790723	0.86091676334944	2.76790974545305
H	-4.71729349970572	2.55838831835960	2.86671397231242
H	-6.11360316075935	0.98883700419599	5.13325334020234
H	-6.86998819133266	2.23306385568945	4.10735773803090
H	-5.57612664422056	2.68302743647918	5.24301194369893
C	-4.36871753184136	-4.01913344777364	3.20978523617945
H	-2.80874800655267	-5.23399876389711	4.10297679994158

H	-2.44119005707457	-4.72522473145392	2.45906774240438
H	-4.82156924198306	-3.71276015924872	4.16422408534105
H	-4.93796261137170	-4.87779091266576	2.81797794293997
H	-4.48603532209957	-3.18553181103005	2.50285597530602
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H	5.10171643890140	2.54233267514557	2.32469157018933
H	5.62767194460189	0.84307098266113	2.2252798839194
H	6.17747477603533	2.73592723885425	4.60333965794714
H	7.36292742420659	2.25031517418740	3.36786719528249
H	6.70648171041475	1.03904519557488	4.49628436502739
C	4.83055825095071	-3.95107082739364	2.72147986229357
H	2.85097649774231	-4.69168269528003	2.16411760733325
H	3.39423809178819	-5.20509317912438	3.75748689536564
H	4.85676793057368	-3.10994562970425	2.01417623904849
H	5.37439619291054	-4.79422081045083	2.26528308322417
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C₆₀(NH₂)₄

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C	-0.53808907662698	-0.99504468329768	3.15392765402635
C	0.92307198864138	-1.00831221737621	3.07701862897537
C	1.37888714386643	0.27349983301919	3.10746897708828
C	2.71108984386131	0.72899258613946	2.57409173681320
C	3.16530995139186	-0.32650668632506	1.54688429871767
C	2.72535989037178	-1.62920866970193	1.54592168805579
C	1.71115325336857	-2.17981890532392	2.56226305442181
C	0.77979677849981	-2.96924516322760	1.62266416929864
C	-0.59413040946789	-2.96149800295308	1.69850315235292
C	-1.39328519343180	-2.15524360134044	2.73203019046728
C	-2.50895093379131	-1.58161469234259	1.83233883005849
C	-2.93362767490017	-0.27467495838199	1.88049044188582
C	-2.34743218630421	0.76330845348080	2.84777041163274
C	-2.17957375828440	1.96024809222440	1.88399617638601
C	-2.92977661562863	1.74714076354621	0.69388523013963
C	-3.38728670606164	0.36964022473314	0.68693099436785
C	-3.47596156297766	-0.32392737321076	-0.52140452418516
C	-3.04284395651518	-1.68967454662086	-0.57290135636249
C	-2.53666104441041	-2.28227121251877	0.58592318176121
C	-1.36729343593868	-3.13093568305662	0.50662565804114
C	-0.76014955475678	-3.36821737143094	-0.72715451127777
C	0.67137472979237	-3.38019376611924	-0.80558493111054
C	1.41391442536915	-3.15501617884596	0.35354438936339
C	2.59977225529018	-2.32705744554800	0.30445246813362
C	2.98738488575854	-1.74275732144886	-0.90343624760532
C	3.44539081147114	-0.38447409421913	-0.89954434981728
C	3.50166156658853	0.30924987296167	0.31025658216600
C	3.07230922559914	1.69474065329280	0.36628627839815
C	2.59260637666126	2.32279204563491	-0.79171012741296
C	2.51906200147237	1.59142692433446	-2.03577312146925
C	2.93640208483450	0.26447062088898	-2.08882827507447
C	2.16548920952126	-0.70532016098955	-2.83249843593359
C	2.19384773271349	-1.94778179607126	-2.09588234951548

C	1.06136161016909	-2.75482911608144	-2.05034346018475
C	-0.14310246746905	-2.35049687574254	-2.73889977604487
C	-1.27203770168534	-2.73355990712666	-1.92164154901316
C	-2.38934609499757	-1.90800271529666	-1.84559326052867
C	-2.41955026128173	-0.66525435554480	-2.58141064330541
C	-3.08779102943180	0.31732758612111	-1.75909173001320
C	-2.64370015903647	1.63698408658319	-1.75295505507501
C	-2.56807733620121	2.36848541983176	-0.50928423104383
C	-1.40036198537425	3.20406758291851	-0.55515286453033
C	-0.74366862429410	2.99389015509832	-1.82927828631988
C	-1.51596326445323	2.02450586323923	-2.57038795897040
C	-0.87087677593066	1.07706576644657	-3.36640785244313
C	-1.33062992314195	-0.29310491697743	-3.37107117675022
C	-0.17187420621484	-1.15237559143504	-3.45421150973265
C	1.00370954588191	-0.31372075511166	-3.49944430707440
C	0.57114115162159	1.06441566971570	-3.44601036304530
C	1.31564359589727	1.99923282999976	-2.72539197486565
C	0.64645305931993	2.98153613954236	-1.90559837087151
C	1.44247402626044	3.17791565849189	-0.71079841267381
C	0.81332484968240	3.35087544848585	0.52124874422001
C	-0.63707136139946	3.36502563395050	0.60029056949536
C	-1.04089908911436	2.74461705050341	1.83066601206375
C	0.18597621838040	2.31848634655856	2.51431952390178
C	1.33828402892629	2.72304792292433	1.70083801020814
C	2.46523506985512	1.92388405470246	1.63223860194734
N	-3.20229040844049	0.97187368483407	4.00708254926890
N	-1.77509329333852	-2.95223122424826	3.88458490644425
N	2.33808025665609	-2.90802905060831	3.65258716446217
N	3.63317985896815	1.05832396689610	3.64694748493328
H	4.55137840238879	1.27888430933100	3.26482399401367
H	3.74428827846177	0.24063953240967	4.24479658164712
H	2.80616029840127	-3.73806178494066	3.29106593714448
H	1.61382515368423	-3.23229226056553	4.29280988323712
H	-2.37801811684997	-3.72131047926900	3.59586195143816
H	-2.31261594814453	-2.37081817258143	4.52648256702521
H	-4.09635170721271	1.36627176708738	3.71798693997516
H	-2.76926386189201	1.64388681661836	4.63821636484200

C₆₀(COOH)₄

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C	-0.52933845209184	-0.96997054544331	3.20621345048104
C	0.92892850296571	-0.97867443521568	3.12547694332134
C	1.37787100736205	0.30688578957051	3.12676470656258
C	2.69280328688549	0.76120729490170	2.54966404985285
C	3.17000235877939	-0.29918848661100	1.55730414236540
C	2.72590508416627	-1.59805579266990	1.56952473942340
C	1.70994208601433	-2.13417814313958	2.58366495767901
C	0.79375816011300	-2.95551049186772	1.66784622452900
C	-0.57955237647841	-2.94702067408401	1.74404334667553
C	-1.37866529821718	-2.11614205216255	2.75565941495697
C	-2.49486697453817	-1.56750944540485	1.85957263514503
C	-2.92142743774489	-0.26305573509104	1.89501016638971

C	-2.32534707337511	0.79109092215415	2.82785154968859
C	-2.18497579641921	1.98090677863405	1.87932160954411
C	-2.93229656997504	1.74613404243730	0.69056480227854
C	-3.38244502718377	0.36851960285671	0.69685431384694
C	-3.47055154475413	-0.34051834760836	-0.50154392969019
C	-3.03288313548432	-1.70506127135450	-0.53895781114532
C	-2.52110481200509	-2.28474224032312	0.62331125047236
C	-1.35434160638581	-3.13150344378370	0.55346896330015
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C	1.42909272177807	-3.14751770120222	0.39875315335828
C	2.60600455758170	-2.31442548700831	0.33844306348404
C	2.99330710252503	-1.74040230992117	-0.87336307545517
C	3.44862418811534	-0.38133061422935	-0.88527214748945
C	3.50356198035801	0.32794823625106	0.31503067405654
C	3.07183690704554	1.71096546096730	0.35764502225400
C	2.58758524879290	2.32414428961624	-0.80537961395632
C	2.51553907563953	1.57887275612269	-2.04150112980946
C	2.93733754889831	0.25282060573144	-2.08109273039015
C	2.16941532983059	-0.72809192690970	-2.81356278650234
C	2.20197434653956	-1.96265502486540	-2.06382504337636
C	1.07241740329762	-2.77302287661701	-2.00753678713528
C	-0.13407304763257	-2.38075992995439	-2.70007722831811
C	-1.26120714430617	-2.75899954442023	-1.87805023143311
C	-2.38037908477964	-1.93539775698551	-1.80948112298879
C	-2.41615943104492	-0.70076148565970	-2.55891374859529
C	-3.08730067684719	0.28864094015890	-1.74723876718329
C	-2.64704634848911	1.60923442727894	-1.75457597819125
C	-2.57300942570673	2.35493929887629	-0.51894841117056
C	-1.40798973957026	3.19248429944665	-0.57400337972351
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C	-1.52166311198485	1.99204921330083	-2.57697099105015
C	-0.87384509120109	1.03794398461026	-3.36276094683337
C	-1.32881501344895	-0.33366344066882	-3.35259511967045
C	-0.16711378690308	-1.19007418143099	-3.42705415021147
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C	1.33220203373995	2.74574040240808	1.68475839291321
C	2.46295134019327	1.95345287751618	1.62171918793849
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O	4.01938843135340	2.13899933115424	4.04006500428607
O	4.12094297946735	-0.09185561367104	4.21492722222563
H	4.68850616440369	0.13835839453426	4.96659302980064
C	2.34929179430614	-2.98614000527567	3.68316563442683
O	2.17058359913715	-2.83562890339166	4.85647473765088
O	3.12548565519371	-3.93651264654644	3.15833536350887

H	3.48908817247024	-4.44822643975830	3.89732244735455
C	-1.90370636957537	-2.96108792197738	3.91913408595873
O	-1.60728166106889	-2.80452017673239	5.06748910870338
O	-2.73099823344439	-3.91211759897853	3.48053993760287
H	-3.02104711986788	-4.41795234010304	4.25524173724618
C	-3.19062290412283	1.08969411640918	4.05322838939316
O	-3.45853735752750	2.18475554316886	4.45644257403974
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C	0.99959142305773	-0.91390623101179	3.14980193484653
C	1.44843957449013	0.37250956891091	3.14266815293651
C	2.75204962911935	0.82852404035029	2.55012544030267
C	3.21865117454933	-0.24001990999603	1.55159946202029
C	2.76557899515793	-1.53728197149466	1.57706335986389
C	1.76131620755911	-2.07910679288483	2.59952680251258
C	0.83185279466236	-2.88098985641321	1.69853369598654
C	-0.53584763983787	-2.87076529919883	1.79385462320843
C	-1.31898802907545	-2.05653750402284	2.81484724348100
C	-2.44824393046865	-1.49991706095526	1.94086261066716
C	-2.88038311108915	-0.19570093963628	1.97613393923325
C	-2.26474132395321	0.86484880268956	2.89940918545051
C	-2.13200510797527	2.04133271313092	1.93189456335117
C	-2.89962295329324	1.80372435952595	0.75450008365201
C	-3.35610186319795	0.42937366520515	0.77844209097804
C	-3.45892105452345	-0.28363766715824	-0.41625484018742
C	-3.02239270404218	-1.64846180078896	-0.45338621694129
C	-2.49337260027300	-2.22216517413229	0.70479314381686
C	-1.32623716723705	-3.06769055724801	0.61993523595475
C	-0.73857715354871	-3.32747957569267	-0.61834896214570
C	0.69059853317024	-3.33799270482950	-0.71807189482486
C	1.44786931360534	-3.08709228228413	0.42624966888363
C	2.62736583674047	-2.25852745688846	0.34747633052572
C	2.99927478540823	-1.69184000623272	-0.87315712117694
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C	3.09783024383000	1.76058870780898	0.33664430028505
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C	2.14796362696122	-0.68801414879982	-2.80563663540918
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C	2.50423203059512	2.00810763385809	1.60906028333944
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O	2.40508194005923	-4.22004110983969	3.47398465452985
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O	-1.87129813415321	-4.18806136830525	3.77092107036184
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H	-2.43038358287752	-1.34223283706635	5.08538491142324
H	-2.72762280441550	-2.93058597936154	5.75282042998258
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H	-3.94498479715843	2.82184327944776	3.25360662251391
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O	3.94257092959438	0.30214212420286	4.57567363139246
N	4.60790548382709	2.14352185943495	3.46129109331624
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H	5.34607197900734	2.31944241866837	4.13072961007897

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C	1.37587513651442	0.29475419565312	3.14555413181364
C	2.69507375412317	0.71919880663936	2.56339668673473
C	3.15936419259995	-0.34308022861807	1.57062024575046
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C	2.48194338540980	1.92088150121747	1.63367896261355
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C	0.78965558306541	-2.96603348779478	1.63253540798222
C	-0.58094244910051	-2.95745739639685	1.70827415887359
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C	2.60677695328726	-2.31254832285870	0.31265556647088
C	2.99118918592639	-1.72729941622583	-0.89423589097864
C	3.44740868138228	-0.36883656722927	-0.89549861162534
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C	-1.52093743844922	2.02041144172341	-2.57137772371789
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C	-1.32885375359939	-0.29945381938079	-3.36343641841463
C	-0.16750830884040	-1.15555204538386	-3.44433051469922
C	1.00559841427977	-0.31358759369015	-3.49288317141731
C	0.56883182797013	1.06334031363599	-3.44335465286421
C	1.31104108906027	2.00301779034803	-2.72772597533558
C	0.63883872817006	2.98519217369211	-1.91039533867985
C	1.43425572130221	3.18662068122105	-0.71620089500596
C	0.80558952895042	3.36291133738999	0.51432297977328
C	-0.64388103311603	3.37170811799388	0.59450376700691
C	-1.04290043382965	2.75308917574410	1.82689252394438
C	0.18254751385460	2.32812921863025	2.50966981639167
C	1.33026195174570	2.73862978054485	1.69574340399619
C	2.45981894781353	1.94791007838243	1.62075855563393
C	-1.89168950804524	-2.95525336981786	3.84050395603357
N	-2.29100070941072	-3.59889823968758	4.71444474504043
C	-3.21072646987313	1.09386673081120	3.96652829989780
N	-3.90470343728821	1.34552089622566	4.85678289422456
C	2.32811076701626	-2.98007331781775	3.60698191519127
N	2.81367061963562	-3.62837737798394	4.43247348770543
C	3.69974588449341	1.05253853524489	3.58560956356652
N	4.48944722146088	1.29530209530303	4.39487336255012

C₆₀(NO₂)₄

C	0.20313534992843	1.18875849752063	3.19451351998220
C	-0.96954124908341	0.34008535224067	3.24511058163791
C	-0.53855466177457	-0.95441457580475	3.19147408319529
C	0.91615639379765	-0.96739883781784	3.12135391260007
C	1.36348298442127	0.32280507662018	3.12576280774839
C	2.65741062790290	0.76231721207290	2.52279366925486
C	3.16131755825323	-0.29019595945391	1.55010240553980
C	2.71936544054299	-1.58897264423897	1.56051024704949
C	1.68083350700827	-2.10459276894183	2.54890576687741
C	0.78471361010426	-2.93909016018047	1.64887149930504
C	-0.58713701588415	-2.92539255301873	1.71622651083903
C	-1.38140112667555	-2.08058557859137	2.70248508397716
C	-2.51341629747753	-1.55629838676445	1.83806285237251
C	-2.93031584982742	-0.24931935348929	1.86505929205369
C	-2.31094679204128	0.79677181563869	2.78123484246306
C	-2.19132308050999	1.99755887478445	1.85624443981240
C	-2.93847071393875	1.76462369692372	0.66703072556413
C	-3.39232414649349	0.38718410944421	0.67086719873673
C	-3.47326803920588	-0.32181007243376	-0.52685026972376
C	-3.03776372391160	-1.68872167087865	-0.56322975273360
C	-2.53637170099688	-2.27315527878956	0.59983615333883
C	-1.36487268637602	-3.11810896339948	0.53081192934826
C	-0.74945461151217	-3.36177784786034	-0.69545166843665
C	0.68354556586106	-3.37340305705149	-0.76975746956854
C	1.42676551695076	-3.14050795901597	0.38580951144056
C	2.60759407321319	-2.31001074589120	0.33081187826311
C	2.99411741711477	-1.73053677795217	-0.87763015252942
C	3.44921440914909	-0.36991064437685	-0.88697084034943

C	3.50436350422268	0.33895465950210	0.31190418775335
C	3.07163226977025	1.72313021772160	0.35392455385474
C	2.59097478865831	2.33671015801409	-0.80865665725102
C	2.52184987559926	1.59226347109755	-2.04485252393009
C	2.94225289676098	0.26552045839380	-2.08376306620477
C	2.17565709966864	-0.71393822404408	-2.81834716624915
C	2.20546499821485	-1.94966058447630	-2.07052821388682
C	1.07460688848675	-2.75847022800371	-2.01872308319393
C	-0.12946135974701	-2.36342039545305	-2.71374502763019
C	-1.26032538013038	-2.74149837083477	-1.89724487824735
C	-2.37946474895153	-1.91745287100605	-1.83117915836951
C	-2.41082980878571	-0.68201137983142	-2.57887235700684
C	-3.08460831211723	0.30743486659652	-1.77022125270938
C	-2.64272904798532	1.62791547426770	-1.77491690893423
C	-2.57311078749407	2.37300451227442	-0.53961287838662
C	-1.40554472950590	3.20991471686031	-0.59002325367764
C	-0.74556719154694	2.98878269074270	-1.86018127871215
C	-1.51355344247325	2.00996636531062	-2.59267079150871
C	-0.86392588146592	1.05571870157266	-3.37610166431370
C	-1.32010998972078	-0.31531054645091	-3.36802280732012
C	-0.15909632118521	-1.17226092283008	-3.43964552182301
C	1.01437714298979	-0.33147991886597	-3.49072414544210
C	0.57827222785774	1.04566914056733	-3.45186166069475
C	1.31867033981754	1.98997604882808	-2.74022003824628
C	0.64467223362128	2.97892853038707	-1.93276157439178
C	1.43644746686353	3.18985445222684	-0.73819700139557
C	0.80420414935909	3.37760623438434	0.48859144836095
C	-0.64667418859039	3.38773417650503	0.56425653195295
C	-1.04976044218399	2.77510353161111	1.79832129804949
C	0.17406050349124	2.35588097932555	2.48586008443476
C	1.32498417007325	2.75916134091158	1.67477566723014
C	2.45462002953504	1.96565637081693	1.61424608910181
N	2.34967462715151	-2.98271109051084	3.63000085550823
O	2.88629232111001	-3.97693757522370	3.21377368259893
O	2.29051429891471	-2.59879625432448	4.76265263578844
N	-1.85042213750918	-2.95909124920583	3.87492777875904
O	-3.02499471561719	-3.18682881056637	3.96250979321500
O	-0.96535132959304	-3.35785052885565	4.58678460795568
N	-3.24942179720421	1.05380079110736	3.98139452730604
O	-3.36892140910602	0.12871445454519	4.73870033297729
O	-3.78078875619390	2.12999189190988	4.04509945052946
N	3.69054174678136	1.02793456754921	3.63899433223996
O	4.16252654703165	0.04597843406064	4.14531376926128
O	3.90026827258851	2.17653962009863	3.92452446658950

Cartesian coordinates of the calculated structures C₆₀X₆

C₆₀(CH₃)₆

C	0.04858193911703	1.18175318678360	3.12198161836612
C	-1.13679051652341	0.32529142158581	3.12436154195329
C	-0.75631500557389	-0.96393996577392	3.22156676598097
C	0.73775825747987	-1.01976839797477	3.54454284352648
C	1.15246767592538	0.41500995130702	3.21580606675130

C	2.51317871828178	0.85453254236061	2.75267555516433
C	2.99292973710193	-0.22341165264748	1.77794145086658
C	2.53708203807008	-1.51588377095671	1.77951293242846
C	1.53457787986310	-2.12364983061498	2.76150936267049
C	0.64221286194235	-2.88556689566022	1.78077551079649
C	-0.72806784296163	-2.91135668820026	1.77979631907231
C	-1.60073406720978	-2.11685880979829	2.75486715827440
C	-2.64420907340375	-1.55473089351859	1.77338283140235
C	-3.05763124916535	-0.24355957655030	1.75901559670294
C	-2.49600172715365	0.81276244251418	2.70843635810314
C	-2.28282685201459	1.98451722373331	1.74882127328966
C	-2.97613876953732	1.73927807458985	0.52239797921056
C	-3.44189085748254	0.37094005909397	0.52407104397056
C	-3.47427005815583	-0.35065041729492	-0.66980432139916
C	-3.03834137562088	-1.71580102477779	-0.66269130714219
C	-2.59993290621608	-2.28136829905707	0.53876765739176
C	-1.42565520422580	-3.12051220336197	0.54384726273466
C	-0.74543840901354	-3.38176844787889	-0.64583478595465
C	0.68825123979376	-3.37742677370280	-0.63873339295114
C	1.35176768406904	-3.10215771847435	0.55516669520771
C	2.52006373973663	-2.25865699438697	0.55483914657697
C	2.98942853138474	-1.71527863659076	-0.63945860387820
C	3.44370553223385	-0.35561362236587	-0.64710634836777
C	3.41054316330249	0.37280428133842	0.54209155057117
C	2.98347672626829	1.75173244981429	0.53719814117905
C	2.58345904351210	2.34509928050499	-0.66428915882989
C	2.58477608925609	1.57774115317877	-1.89160370187718
C	3.01018935348942	0.25335831429236	-1.88509188380398
C	2.28837538996041	-0.74339047756368	-2.64444825373235
C	2.27741788830879	-1.96477538723619	-1.87284483681963
C	1.14865440493659	-2.78043425738640	-1.87259468188173
C	-0.01494849604548	-2.40698091370165	-2.64336904378379
C	-1.18789976616532	-2.77893370707451	-1.88380427771289
C	-2.31178154820824	-1.95903482243508	-1.89064626433775
C	-2.30478142871898	-0.73429204728105	-2.65831440990851
C	-3.02341214514267	0.26356911763188	-1.90054597690754
C	-2.58609214038219	1.58479841932809	-1.90217477570972
C	-2.57733324332178	2.34420829413614	-0.67097746568855
C	-1.41584963717098	3.18303797636874	-0.67130311517220
C	-0.69291569065630	2.95311044039265	-1.90303361031138
C	-1.41796768712910	1.96174978699592	-2.66435243454577
C	-0.72308271796176	0.99936481398065	-3.39842526556365
C	-1.17437858445300	-0.37349369023379	-3.39410568561107
C	-0.00758967687419	-1.22579549365202	-3.38648511757900
C	1.16425392171300	-0.37932977258919	-3.38696961183869
C	0.72196082423248	0.99633987455494	-3.39477034264430
C	1.41965292903411	1.95583758737095	-2.65852381625079
C	0.69889398512994	2.95249368000545	-1.90141007025222
C	1.42461750377535	3.18821968644347	-0.67115784522861
C	0.72979228403413	3.38439958085718	0.52316620726139
C	-0.71577873747656	3.37140540363027	0.52158951897514
C	-1.16649622941862	2.79065505442528	1.74812164198289
C	0.01329789854220	2.62538166444872	2.70723196031617

C	1.19296488456708	2.82672183553403	1.75795170177349
C	2.30878359478045	2.02296631289260	1.77236430303638
C	-3.40905624821684	1.14417142398760	3.89475159194641
C	-2.20854287044226	-2.98119136122981	3.86640229874135
C	0.85945345504094	-1.17274444925713	5.08250628556533
C	2.26992833642799	-3.13967587542795	3.65527941720701
C	-0.01675566536936	3.59623363077725	3.89352287748331
C	3.52437911296600	1.15699236297161	3.86559180194855
H	-0.05449404659842	4.63760159836727	3.54090098533735
H	0.88089020451441	3.46788993665026	4.51571257286420
H	-0.90105957896254	3.41144877216572	4.52117322854441
H	4.49021800166169	1.46220436396260	3.43648159752670
H	3.69497758085684	0.26632055133449	4.48798433916781
H	3.15706772825258	1.96712716513779	4.51222684601840
H	1.90289137085681	-1.09323569390225	5.41605459062081
H	0.46710196928203	-2.13803905832362	5.42998913933229
H	0.28277489102210	-0.37380227412259	5.56780594821029
H	2.79463883561747	-3.86690443188148	3.01924732972344
H	1.57143370337799	-3.69714534342585	4.29426451366049
H	3.01912533679097	-2.65006927847507	4.29233669896947
H	-4.38608435007642	1.50663503152714	3.54244770642735
H	-2.95691443900622	1.92468718637163	4.52424937408663
H	-3.56836415036736	0.25014962002196	4.51494957673399
H	-2.79710524774149	-3.80516336797852	3.43646960559526
H	-2.86712596903569	-2.37746969665710	4.50772312810529
H	-1.41820330881045	-3.41831012344759	4.49421025683087

C₆₀(C₂H₅)₆

C	0.07559055851591	1.04246529954175	3.27805767905376
C	-1.12172836944230	0.19739379206840	3.22119994355095
C	-0.74841411556740	-1.09723655328992	3.24470476048530
C	0.73646071276395	-1.19017140263206	3.61216225502314
C	1.17936075094166	0.26335462753115	3.36544901975891
C	2.53599509187994	0.69969429975373	2.85657388203673
C	2.97082150108234	-0.35309754223393	1.83754171594050
C	2.51162373226991	-1.64193904829785	1.80338413174717
C	1.51897935900505	-2.27972487017121	2.77526826283390
C	0.61037681111712	-2.99001595126659	1.76470205046866
C	-0.75968971384632	-3.00851791198591	1.76500384756438
C	-1.61308840997755	-2.22885141756099	2.76545435603832
C	-2.65532800164620	-1.63132668905204	1.80753851535867
C	-3.04454781436200	-0.31540525331106	1.83364195747241
C	-2.48557808139609	0.69641568344190	2.82585393811517
C	-2.26874599042207	1.90763298469302	1.91679010406903
C	-2.96474314179263	1.70997144843532	0.67941596885838
C	-3.43848500618745	0.34604211476726	0.62983445033177
C	-3.48783665844974	-0.33451352870809	-0.58693441427605
C	-3.06663971258390	-1.70377932441691	-0.62892400280785
C	-2.62740631705618	-2.31540971860317	0.54958571874646
C	-1.46270469909324	-3.16627428226690	0.52276869940501
C	-0.79165581118390	-3.39117884474575	-0.67853896380723
C	0.64135323257084	-3.39802667492010	-0.67538600970066
C	1.30849006063130	-3.16666592549862	0.52541356489531

C	2.48250727786269	-2.33545337852703	0.54898686014295
C	2.95596804998961	-1.76052734596995	-0.62795082037980
C	3.42388317280328	-0.40658184177996	-0.59153989275181
C	3.39731253632996	0.27881333559378	0.62167764147824
C	2.98922223569004	1.66109989606848	0.66468053984294
C	2.59397916564766	2.30113564342684	-0.51381722708580
C	2.58298747979284	1.57696048287157	-1.76681024466618
C	2.99504586637866	0.24863573164141	-1.80714003320558
C	2.26062119021084	-0.71458110832113	-2.59719503519664
C	2.23963617563383	-1.96131393941877	-1.86721425618500
C	1.10328947785707	-2.76552843506128	-1.89054894316661
C	-0.05912717971412	-2.35488717434419	-2.64382501584976
C	-1.23296950534396	-2.74206382411817	-1.89346803800583
C	-2.34876144849459	-1.91140525132114	-1.86805177243724
C	-2.33271758644401	-0.66061208352708	-2.59275990744271
C	-3.03816371829355	0.31751207160413	-1.79755869489130
C	-2.58788666733404	1.63388784079107	-1.75257993658708
C	-2.56685664162210	2.35017219903311	-0.49514564001898
C	-1.39669248149421	3.17620023881197	-0.47143791089201
C	-0.68152166647371	2.98298122294176	-1.71425045523842
C	-1.41924521067833	2.02568817639454	-2.50620639971440
C	-0.73676625505871	1.08265954577285	-3.27701250454570
C	-1.20121685073450	-0.28528470063515	-3.31950076708611
C	-0.04289066445836	-1.14902567414931	-3.34637106744807
C	1.13722868578434	-0.31416494239667	-3.32232416580424
C	0.70823950311549	1.06530721852825	-3.28023314397091
C	1.41851848860888	1.99261273466355	-2.51522407231552
C	0.71033700534442	2.96924318362329	-1.72084975005497
C	1.44288203902976	3.15476921722891	-0.48691935059387
C	0.75359048834281	3.31193987919337	0.71560116891707
C	-0.69075045184728	3.31340555972299	0.72458453384613
C	-1.14004719981618	2.69746503381725	1.93686120692743
C	0.04714246384999	2.49727966267130	2.88497702112670
C	1.21535830747485	2.70652101706827	1.92694299956561
C	2.32188943621444	1.89447022179292	1.91156336333555
C	-3.47150537127821	0.90693747705661	3.99369986082656
C	-2.21675524128272	-3.09323131773542	3.89188565244456
C	0.70344659780975	-1.43812914191549	5.16546769039050
C	2.24163763553960	-3.34382929865226	3.64699094159824
C	0.06821190904831	3.46263034185377	4.08889835053726
C	3.67368397430556	0.95533020607850	3.87053499650268
C	-0.01894662792079	4.92996818349063	3.70946028737045
H	0.99507891977615	3.26708180332394	4.64639961090154
H	-0.75834677115528	3.19552429244541	4.76117015299036
H	0.80417244381784	5.22651128164936	3.04101923055794
H	0.03434121022205	5.56545311626073	4.60597772538679
H	-0.96342364553236	5.16091903265601	3.19290041430316
C	-3.04411103289676	1.91604403906107	5.03925910504755
H	-3.62964112309631	-0.07802045397546	4.46306211186183
H	-4.44110112023867	1.20100265984870	3.55849824321670
H	-2.09659780452855	1.62274186270462	5.51745018121626
H	-3.80318046884023	2.00024563529025	5.83120681097132
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C	2.60599616908803	0.58154821860214	2.76745211400490
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C	1.17088071127130	-0.38135212301242	-3.36548776193869
C	0.72840969681974	0.99402032213997	-3.37600489549021
C	1.42465215714541	1.95486417849684	-2.64055939996446
C	0.70242338795921	2.95246685234141	-1.88703583777587
C	1.42641253742795	3.19230216493837	-0.65655446274220
C	0.73080586803873	3.39686371328999	0.53418055830619
C	-0.71605830174992	3.37959666405144	0.52900673189067
C	-1.16848073336802	2.78943214910490	1.74885363076019
C	0.00976216283661	2.60008545446990	2.68386392385946
C	1.19435913366445	2.83626061616405	1.76691952990279
C	2.30657108320877	2.03115121382643	1.78426908481861
Cl	-3.53917493429074	1.21431842585011	4.08489491790587
Cl	-2.28958141466064	-3.10117824718362	4.05932041340477
Cl	0.87175788887042	-1.20872404863017	5.33518580429499
Cl	2.37874567181153	-3.29749078345921	3.79958790671652
Cl	-0.04596124891641	3.73719730588302	4.08810829377251
Cl	3.65642934110226	1.19446105693234	4.06688495839258

C₆₀Br₆

C	0.03652884645910	1.18676324978793	3.13234562514647
C	-1.14490949085556	0.33340528289946	3.13130844591289
C	-0.76518937410164	-0.95756547604605	3.22902414016801
C	0.72507212283959	-1.01140114988883	3.53038796284408
C	1.14240390826269	0.42035764689298	3.23020410045022
C	2.46527061656329	0.84622376995822	2.72295532892304
C	2.98610795479887	-0.22063375790674	1.78745036093568
C	2.53618372109367	-1.51497206693257	1.78992480615190
C	1.51316695798283	-2.10024461063924	2.74289119757816
C	0.63860115701468	-2.88728899867612	1.78725037491747
C	-0.73156372421790	-2.90682899837765	1.78121253613680
C	-1.58332073079996	-2.07864655777425	2.71634509650115
C	-2.65056490914417	-1.55045723304568	1.76657308667430
C	-3.06831629506739	-0.24176475695947	1.74996982238940
C	-2.46915489605948	0.80466799167285	2.66082029869967
C	-2.28651135502157	1.98602223440238	1.73582903678423
C	-2.98610807487867	1.74302697954598	0.51391131719312
C	-3.45459406671403	0.37431274505748	0.51677273259043
C	-3.47613133851034	-0.35025010668958	-0.67392845430359
C	-3.03853448843753	-1.71680890647378	-0.66345268314945
C	-2.60621420440441	-2.28514061070858	0.53767388773951
C	-1.43122651252737	-3.12356353456091	0.54733770003557
C	-0.74491711637689	-3.38139494037073	-0.63723461913376
C	0.69096321010417	-3.37658729825327	-0.62613680118003
C	1.35477286614243	-3.10539986289977	0.56650685703098
C	2.52212380681039	-2.26216907675764	0.56856255088281
C	2.99086887325557	-1.71486417526012	-0.62209768987907
C	3.44606445966697	-0.35318263787914	-0.62979029008231
C	3.41462984689945	0.37752621209736	0.55565768229233
C	2.98813654867360	1.75672114844951	0.54749229169702
C	2.58678490366383	2.34758338012704	-0.65355615215671
C	2.59044255071716	1.57808794299249	-1.87890436363754
C	3.01613980280035	0.25376561079562	-1.86947248396876
C	2.29602911737012	-0.74429347862971	-2.62859927032211

C	2.28294210449533	-1.96497693756373	-1.85618846088033
C	1.15384313210670	-2.78107414962635	-1.85825335504943
C	-0.00774327383555	-2.40864336234738	-2.63231262661945
C	-1.18338111754936	-2.78030916965172	-1.87686836187191
C	-2.30728831721636	-1.96039290617121	-1.88799498500325
C	-2.29759735907434	-0.73618081105224	-2.65636169592726
C	-3.01894521891521	0.26251598440643	-1.90302259863443
C	-2.58173006624591	1.58405020650789	-1.90564616366084
C	-2.57731683182658	2.34486450176545	-0.67592649606491
C	-1.41420723928448	3.18513911835712	-0.67380179006724
C	-0.68795376852830	2.95314639384794	-1.90260657890996
C	-1.41068729701471	1.96000648950345	-2.66351789272132
C	-0.71339122603299	0.99653836869929	-3.39309890085972
C	-1.16460771088013	-0.37607504124723	-3.38791053343339
C	0.00205246975562	-1.22820415420470	-3.37558069724231
C	1.17382452227860	-0.38160687732517	-3.37368413654134
C	0.73137769513021	0.99381357457421	-3.38472950430094
C	1.42700946602955	1.95473949657859	-2.64899580912417
C	0.70409982667889	2.95268665596000	-1.89635859461030
C	1.42706486836712	3.19261245767218	-0.66534549511907
C	0.72957001864747	3.39752677003571	0.52431957367328
C	-0.71718148745042	3.38191361396849	0.51787880027810
C	-1.17078888607543	2.79218926810380	1.73781675609284
C	0.00641233412209	2.59289539086980	2.66474468270850
C	1.19033972688793	2.83476227250531	1.75730985065108
C	2.30229690037711	2.02777772930334	1.77545306397722
Br	-3.63357206836787	1.24786182789501	4.19352546543780
Br	-2.37136696586514	-3.18883805402270	4.15455273870609
Br	0.84514172742837	-1.18034911837628	5.49725092116141
Br	2.47634942554797	-3.43056002554035	3.84502075325221
Br	-0.05075549865464	3.83423577833928	4.19978042701515
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C₆₀(OH)₆

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C	0.85682493478444	-1.03397231351096	3.72149656970479
C	1.27052521354807	0.40829042609924	3.39637868046199
C	2.61551377059149	0.84558417237645	2.89582635583251
C	3.07186812523382	-0.22790438458703	1.90761134876815
C	2.63034499825633	-1.52455777400294	1.92251630300526
C	1.65190878167892	-2.13893376530028	2.92853270942892
C	0.73982840452925	-2.91440529677507	1.97232394334407
C	-0.63116779583028	-2.93428042395534	2.00340672322342
C	-1.47592503053432	-2.13477171775773	3.00150810901944
C	-2.57493201679971	-1.59395840083126	2.05387959959829
C	-2.99001799314418	-0.28194717119578	2.04716071393257
C	-2.39311715634581	0.78324145509519	2.98019877051838
C	-2.20795017998846	1.95591665765819	2.01037212946843
C	-2.93421446651745	1.70524554880392	0.80620594032107
C	-3.40065535042942	0.33355802106095	0.82252703360604
C	-3.45472667601389	-0.38702467339630	-0.37051037844888

C	-3.01398084922904	-1.75145617094025	-0.37413740380239
C	-2.54901361926597	-2.31728876304018	0.81688632481872
C	-1.36532931912737	-3.14806377408936	0.79050093142293
C	-0.71294145008390	-3.40381018227020	-0.41416613926175
C	0.72211785011051	-3.39367313848961	-0.44374071867237
C	1.41881940368112	-3.12284974573508	0.73209505686463
C	2.58379774336328	-2.26974413985917	0.70209701978995
C	3.01323281839572	-1.72167704574089	-0.50362071812628
C	3.46157386769039	-0.35868870550672	-0.52428292395775
C	3.45827953112542	0.37092164852082	0.66275419949459
C	3.03262546432116	1.75147007844683	0.66548337599264
C	2.59426653045898	2.33796851888901	-0.52555834878689
C	2.56549772248807	1.56913467737190	-1.75138038391564
C	2.99428435344996	0.24593569106892	-1.75180773427832
C	2.25714553647678	-0.75465031334436	-2.49072014042417
C	2.27129117332669	-1.97461904600906	-1.71740521213052
C	1.14650109661686	-2.79634731153876	-1.68870948789056
C	-0.03740617935941	-2.42829630187724	-2.43005409859275
C	-1.18917089793602	-2.80478884502944	-1.64149465229552
C	-2.31672291296515	-1.99074686612802	-1.62016938099685
C	-2.33404617000895	-0.76683243416088	-2.38816948909044
C	-3.03629837031082	0.22804453146124	-1.61280498634497
C	-2.60430458975764	1.55084686070467	-1.62715055987926
C	-2.56512990991932	2.30830414630103	-0.39597291428135
C	-1.40693719248516	3.15343975332769	-0.42730204146528
C	-0.71838980993469	2.92831903259359	-1.67883049565928
C	-1.45891185528898	1.93335162853396	-2.41973433690495
C	-0.77911863561314	0.97319773695495	-3.17062543915716
C	-1.22410416233309	-0.40140798754769	-3.15283009859427
C	-0.05388910050192	-1.24836995994671	-3.17503622901973
C	1.11358073679741	-0.39695697431971	-3.20629585562370
C	0.66537958696119	0.97653930936021	-3.20456596026715
C	1.37810733170620	1.93942787176562	-2.48720672308731
C	0.67312846053613	2.93348703730963	-1.71298706198480
C	1.43103514491804	3.17734314562666	-0.50368174915060
C	0.77018136953603	3.37670724624097	0.70788560082259
C	-0.67762319321389	3.35141747464435	0.74529439514292
C	-1.09433401305097	2.76785423072814	1.98174535265202
C	0.11585849835470	2.60750803154812	2.91131973083760
C	1.27272430618008	2.82485197776892	1.92866560159654
C	2.38782385027355	2.02301016923593	1.91544212454763
O	3.58478733822929	1.05814005497909	3.88416246538895
H	3.19802188462307	1.64304562999888	4.54721764620690
O	2.29393305768659	-3.00147592865398	3.81132360811454
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O	-1.89775148104308	-2.85075547823178	4.13441774780767
H	-2.28715491402137	-3.68427777218146	3.84329802174902
O	1.04463318323228	-1.27060364462821	5.11208049410046
H	0.23339061721656	-1.66582575969660	5.45679249318992
O	0.11869750579042	3.42134860248839	4.05419379215766
H	0.01274590814063	4.33650154983283	3.76766484595186
O	-3.11653304820323	1.07007407861589	4.14404080029163
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C₆₀(OCH₃)₆

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C	-1.09754495346372	0.21068425740578	3.05078551011180
C	-0.57115226797348	-1.01542099913253	3.20234838164700
C	0.94393104179839	-0.86572873382537	3.47546748800213
C	1.15944296600171	0.58935528057670	3.03869542043990
C	2.44146961684837	1.17335420769525	2.54099067836826
C	3.02713380622098	0.11998183523182	1.58396211828529
C	2.74292137703935	-1.22087082421755	1.65458101371238
C	1.83956576507586	-1.90380547692235	2.69503297585113
C	1.01675143152100	-2.80816800147532	1.77012648255199
C	-0.34108642091441	-2.99095695141099	1.81376083607821
C	-1.27786062638875	-2.27715137591725	2.78580930425857
C	-2.42045838252711	-1.88677237281004	1.81741254851809
C	-2.99295237912890	-0.63951105156455	1.76859226233935
C	-2.51401636534837	0.51379097936333	2.66330625266377
C	-2.48235542482299	1.67040017852157	1.65092401355539
C	-3.17458170864688	1.29020845478469	0.45899925084892
C	-3.47766899037448	-0.12347349826230	0.52602175382760
C	-3.45182171807575	-0.89078829995342	-0.63833748946971
C	-2.85184914738306	-2.19255515562129	-0.59414913414039
C	-2.31808982596235	-2.65399444066817	0.61227177007619
C	-1.04606308680332	-3.33778738349684	0.61239543329208
C	-0.37373489841797	-3.55985691782244	-0.58764022244292
C	1.04908360627307	-3.38197324059899	-0.63028235210446
C	1.70813099934345	-2.98212436702633	0.52851903770725
C	2.76774769711538	-2.00480763988901	0.45703497267096
C	3.12634473584419	-1.45871240423404	-0.77291265182919
C	3.41087958067353	-0.05507908272435	-0.84813686841664
C	3.32578809028551	0.71172831571366	0.31234182462871
C	2.73787570097238	2.03148643184545	0.26844359014688
C	2.23191355468886	2.51679435260489	-0.94090192922687
C	2.29123720883356	1.70567700401211	-2.13813590240892
C	2.87421354304222	0.44349764943000	-2.09488614676272
C	2.25732056082782	-0.66438607229822	-2.78935021391059
C	2.41777885518482	-1.84428596194422	-1.97136006258646
C	1.39666310809261	-2.78930601116621	-1.90107501075813
C	0.17494167427968	-2.59272220180650	-2.64599305737222
C	-0.92119298263958	-3.07139102406410	-1.83379954506612
C	-2.13735185712923	-2.39637295263083	-1.83597502947627
C	-2.30091911212913	-1.21217793119540	-2.64846271332690
C	-3.11347427779387	-0.27823793031787	-1.90522746694493
C	-2.84106451139766	1.08510222727234	-1.97151800306671
C	-2.88505112469341	1.88610473777587	-0.76824620543438
C	-1.83373283615831	2.85795340693355	-0.83975696012035
C	-1.12904621974078	2.67042394791122	-2.08818188704215
C	-1.75026951408109	1.56877170794602	-2.78656587487086
C	-0.96463449529699	0.66753471076082	-3.50622625222772
C	-1.24446920088265	-0.74800013115263	-3.43434601805639
C	0.01720505174657	-1.45189192208019	-3.43401266675771
C	1.07636372598218	-0.47093354653362	-3.50728683732323
C	0.46920019839511	0.83943705000931	-3.55162113702481

C	1.06617381369250	1.90707130037411	-2.87815875867816
C	0.25170589006286	2.83891784421296	-2.13439218409384
C	0.97885158720732	3.21255670374728	-0.93969631721797
C	0.30452919001295	3.37647656581699	0.27071321226638
C	-1.12932521890377	3.18201185635712	0.31918683572876
C	-1.47165253955001	2.60446912494791	1.58038954651347
C	-0.24800971141815	2.61634662543511	2.51050623303141
C	0.87418969563875	2.94358439408218	1.50934250968585
C	2.07969289064913	2.28109959826877	1.51526229306849
O	3.25817606189123	1.55675609619448	3.60418926128564
O	2.55851877792105	-2.61297992896502	3.66672120561404
O	-1.65218536740048	-3.14967882002420	3.81855556325326
O	-3.25094090777943	0.73659654032957	3.83456624103191
O	-0.34580198619522	3.43688513896064	3.63694193957679
O	1.24827520478777	-0.86822623916604	4.83883076295219
C	-0.57419458713043	4.79130991282375	3.36321619884569
C	4.52144440743293	2.04209906366250	3.24522053551925
H	-0.61207715045260	5.31055377379655	4.32983557222068
H	-1.53261164512741	4.95478484343765	2.83596750130355
H	0.23698703550078	5.23283421171722	2.75489972895728
H	5.04098743123564	2.29761927413994	4.17807345390808
H	4.45594939104290	2.94967280188526	2.61631218675780
H	5.12031204428574	1.28635163410910	2.70382393490599
C	3.43356616398960	-3.60706232887131	3.21536747202715
H	3.89578565382852	-4.04404255157587	4.11069286452652
H	4.23391230820027	-3.20041224226054	2.57079927439250
H	2.91381610397366	-4.40939282636010	2.66054119599947
C	-2.70459853930073	-2.67597173585543	4.61987044082690
C	0.65096110498645	-1.85987439161117	5.63478312722738
H	1.23913191054787	-1.91439508085098	6.56131047382350
H	0.65597517674838	-2.84879574653409	5.15405516648417
H	-0.38823319141298	-1.58932506420467	5.89113434412510
H	-3.66889808531113	-2.70723216111087	4.08055433480667
H	-2.53834590925461	-1.63763664981450	4.95777021192176
H	-2.76547456685692	-3.33740819943873	5.49439816614106
C	-4.59313733182874	1.08635760275348	3.63107959439413
H	-5.04267132714278	1.21952021212757	4.62379498222165
H	-5.14900988541872	0.29780180211485	3.09064178179010
H	-4.69248157956089	2.03170593228644	3.06724157163477

C₆₀(OCH₃)₆

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C	-1.02485980871532	0.50709543003642	3.25356565542082
C	-0.49112175120089	-0.70161836021318	3.49555178372754
C	1.02852710457650	-0.52484461512351	3.72389700912936
C	1.22881807073317	0.88906402135019	3.16750267605535
C	2.50093028177263	1.43590898207271	2.60821323485523
C	3.07837715984682	0.31194018234428	1.72877278690413
C	2.80059952539094	-1.02053787599150	1.90942807400179
C	1.91500673868082	-1.62054780106465	3.01538394350097
C	1.07944098881419	-2.59664826145866	2.17815105620558
C	-0.27687160320155	-2.77888319649521	2.25941155257044
C	-1.20013577252618	-1.99414356666737	3.18931235704753

C	-2.35927982447907	-1.68231702529498	2.21239791519787
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C	-3.44606258916108	-0.02874029563180	0.80590640290605
C	-3.43818517936821	-0.88508960709638	-0.29478727987689
C	-2.83237574335429	-2.17787176774144	-0.15923465237946
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C	1.74957181456033	-2.86507003057319	0.94167935270981
C	2.80479962277574	-1.89476454189820	0.77549577798477
C	3.13965221967280	-1.44590714349691	-0.49990988136231
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C	3.34980551426895	0.80282051624280	0.40864421120606
C	2.75427438478408	2.11283890858403	0.27158844887220
C	2.22620772411995	2.50202620086613	-0.96291163151865
C	2.26745081423750	1.59979955133644	-2.09346263646528
C	2.85619721505948	0.34655051488540	-1.96190749851692
C	2.23171771772800	-0.81360599386507	-2.55672403791582
C	2.41115117507903	-1.92508054807750	-1.65171562650337
C	1.39524379544676	-2.86405346674827	-1.48977863894262
C	0.16009948701904	-2.72981649795273	-2.22649947188895
C	-0.91976943005388	-3.14617117080056	-1.36013926597053
C	-2.13829171029754	-2.47611649837487	-1.39343795121968
C	-2.32102637314257	-1.36024570692789	-2.29365016684844
C	-3.12461283332740	-0.37313034206952	-1.61166853370746
C	-2.85889902903962	0.98167901545697	-1.78906171366921
C	-2.88480361069641	1.87472630579078	-0.65166154399813
C	-1.83916480828637	2.84065496169119	-0.81820701729743
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C	-1.78430320416335	1.40232920545305	-2.65871330717350
C	-1.00733411371175	0.44969388585288	-3.31974072520455
C	-1.28049744564404	-0.95679455569220	-3.13274235277162
C	-0.01613810430212	-1.65553136058346	-3.09959321650902
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C	1.02959381708423	1.73970839910986	-2.82610733412200
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O	-3.16483322213193	1.08373062308136	4.03368906679080
O	-0.29414824884279	3.75759188251099	3.58743261625716

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C	-0.46067468236482	5.12423266634217	3.26855336516671
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C	3.50602109563459	-3.30115772889055	3.65532023789015
C	-2.58370091899680	-2.24631853092241	5.09384881721260
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C	-4.52183960480872	1.41028836219587	3.83764772166630
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C	4.19072508397300	-3.80629790698099	4.90130223214065
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H	-4.61310630823509	2.50628008844266	5.69045934568127
H	-5.07581115825149	0.79198027641901	5.82948756122663
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H	-4.60843706842986	2.29788313098335	3.18155106010340
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H	-2.36806134694712	-1.18850030329528	5.33371817042299
H	-2.89241487196976	-4.13299097307029	6.09073773947059
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H	-1.76302465975877	-3.03980993882647	6.92789425035269
H	0.68906615331171	-2.33592868075693	5.49241637617772
H	-0.22542616991085	-1.00988648343367	6.24936434036805
H	2.67310430297323	-1.79720082220014	6.89930020522930
H	1.24719569459744	-2.10532490182799	7.93646149509936
H	1.79728047391940	-0.43287598234763	7.63930349591283
H	4.25433778808846	-2.94954925323333	2.91955572440159
H	2.93467565807885	-4.11559334499710	3.17022070645252
H	4.77033323995594	-3.00168658074258	5.37724866891107
H	4.87584148975516	-4.63068232845764	4.65462756891676
H	3.45216889868629	-4.17465491880545	5.62857899859485
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H	1.46237216451617	5.50835682433957	2.31772602479143
H	1.44590039481032	5.71343723556796	4.08538430082458
H	0.68545004263402	6.94048381352889	3.03355348520596
H	-1.06634473883829	5.54681596984747	4.08583297205542
H	-1.05372323436929	5.24049119197848	2.34232029070349
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H	4.47095616085908	3.21449186680834	2.49751915786268
H	5.15145082782779	1.58192914825591	2.69800926953395
H	4.77937140963713	3.64372272106471	4.95549426971125
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C	-0.54773226416171	-1.03849229766305	3.45866651553105
C	0.95844616565751	-1.01905752396471	3.68532115690357
C	1.27999075242259	0.43106896784508	3.37774077951352
C	2.58392817079655	0.93462455275639	2.85935865550529
C	3.10832374450317	-0.10253748869109	1.87735766747880
C	2.72132925731212	-1.41834385074992	1.88045914066891

C	1.76880657732891	-2.06825343521231	2.86954044077152
C	0.89272288575617	-2.88049586130770	1.93375760895674
C	-0.47384013574784	-2.96980894543289	1.98493826447556
C	-1.33855223619860	-2.21284331656458	2.98205415073840
C	-2.45877611072620	-1.71140156460386	2.06712323153667
C	-2.93865650983242	-0.42314308205648	2.08181253495906
C	-2.37730034914973	0.64757945099831	2.99969708520568
C	-2.27515187815298	1.84590310932577	2.06892589950554
C	-3.00278246088459	1.57678994610637	0.86920992527243
C	-3.40040411514926	0.18497354270402	0.87211115993377
C	-3.43824048395899	-0.52538651258113	-0.32763802003879
C	-2.93404797448891	-1.86710918080452	-0.35222471729010
C	-2.42488906922864	-2.42379930693928	0.82516801714286
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C	-0.56229609066001	-3.41637645961736	-0.44078481604708
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C	3.44833177873591	0.53096945907864	0.63613105088724
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C	2.25983480335867	-0.60815036062833	-2.51915189088165
C	2.33855496844395	-1.83671082067311	-1.76334497039626
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C	-2.24264171805515	-2.06069386413246	-1.60885965536707
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C	1.15657572498139	2.86086312882267	1.95805306664617
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S	-1.90558311374483	-3.23061267699665	4.40964030708766

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S	-0.00141860733272	3.62661773685533	4.43533514825136
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S	3.73667945849158	1.30614020365036	4.25609277038042
H	4.87284280569498	1.19755564158777	3.53208591511870
S	2.69932322630807	-3.21040992626341	3.99522168311360
H	3.30947501268040	-3.83453582936114	2.95747035290028
S	1.14882120188739	-1.17623282051715	5.52755421485636
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C	0.97539316865849	-0.83780475147933	3.46698306946254
C	1.15542879261575	0.61976656337539	3.06467715852457
C	2.41195657235896	1.23157032788808	2.54482010099481
C	3.04745667582213	0.20936373666464	1.61462556211349
C	2.78891239963223	-1.13733260750645	1.67685636586942
C	1.89493310970006	-1.83342189306267	2.69200702284077
C	1.11128086639034	-2.75983621115153	1.78207987139635
C	-0.24110503003867	-2.97452133126180	1.81879091380008
C	-1.19234675203877	-2.27723232460912	2.78145570195402
C	-2.33370235417268	-1.91378833391634	1.82995430916725
C	-2.94681003729021	-0.68486817969825	1.79176594946069
C	-2.49714332905677	0.47423138051224	2.66626644151291
C	-2.49417780200876	1.62741710239035	1.67460384474089
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C	-3.44958825742195	-0.17890967370730	0.54864409548760
C	-3.40296862979995	-0.94034437848280	-0.61942331183425
C	-2.76913062452038	-2.22591090616789	-0.58066516043249
C	-2.21993376320733	-2.67607221924302	0.62234384733966
C	-0.93721579481408	-3.33391627702495	0.61835219258953
C	-0.25873358356959	-3.53824503793836	-0.58192530068098
C	1.15822422160150	-3.32534437753167	-0.62099956248767
C	1.80683555080842	-2.91345100326633	0.53909011632683
C	2.84372640262452	-1.91469513020122	0.47604031845007
C	3.19316961614505	-1.35175028249360	-0.75052278633973
C	3.44470995199619	0.05679199645680	-0.81755432877584
C	3.33787877208479	0.81458689654524	0.34911357919603
C	2.71224431413462	2.11753990317159	0.31060479306149
C	2.19726291963429	2.60191594185442	-0.89627107381490
C	2.27910525275246	1.79886485510726	-2.09825076794863
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C	2.49197619932585	-1.74778349440045	-1.95164327878516
C	1.49406311066528	-2.71673966916948	-1.88856141891522
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C	-1.75790002613324	1.57006879287628	-2.75542560747226
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C	-1.19530777847006	-0.73123245173476	-3.41192975346511
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C	0.21220316259453	2.88408895411056	-2.09273223291323
C	0.92920246791297	3.26828503984815	-0.89445355926635
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C	-0.29492533382127	2.60612967969830	2.52066684924208
C	0.81523803797438	2.96592069420872	1.54829319770593
C	2.03628212125329	2.33219142960623	1.55300725876415
C	-0.82778885909744	5.25978982093285	3.17700113112668
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C	-3.04458076477979	-2.68242017628839	4.85928585468991
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C	-5.11496510947243	1.13718623826209	3.38544439205471
S	-3.51846098356315	0.81553111109000	4.15766689737654
H	-5.81284697377002	1.34862269768791	4.20784129524008
H	-5.48009638680382	0.26274982119400	2.82678953008487
H	-5.07475270286083	2.01421039245059	2.72315804545566
S	-1.72507897887987	-3.55337840155779	3.99985163617209
H	-3.40822478815205	-3.37131587772324	5.63510997358272
H	-3.87263250761631	-2.43377241306517	4.18018779156214
H	-2.68613357206076	-1.75766746898914	5.33350914071582
S	1.35833763188427	-0.69264009453761	5.28752126998207
H	-0.57416931165590	-1.91562874777291	6.11870277187802
H	0.91234578602910	-2.07423429237540	7.10565368304309
H	0.75090352044480	-3.02378905877685	5.59598022177230
S	-0.43309013160184	3.69970303208955	3.98912428763437
H	-0.90358803878982	6.00845556762344	3.97816948521624
H	-1.79003965681802	5.21259309260488	2.64615091149365
H	-0.03178474704201	5.56742486636246	2.48276586887676
S	3.48227820796130	1.79283197760248	3.93114676247705
H	5.69809336502428	2.57126750447043	3.78315220814145
H	4.81931490961880	2.99571121019717	2.28724411746115
H	5.42337984087826	1.31713625413506	2.54047194618646
S	2.95924873460441	-2.77281781281743	3.89231534515006
H	4.28308496949616	-4.65729420681673	3.49406103690311
H	4.19529531473779	-3.69655891370911	1.99439495151940
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O	-2.80527910101917	-2.36868865569008	4.84552079264579
O	-2.18036305432616	-4.24538310103379	3.79875163982899
H	-2.68805688352943	-4.63555245648261	4.52761414645946

C	-3.26539477029808	1.11395043474136	4.03388049153625
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O	-4.49162387514113	0.60783300246166	4.03698705594755
H	-4.92073217831456	0.90117952161642	4.85657834879384
C	-0.01241996373400	3.57048256031476	3.95137712883132
O	-0.43277376857806	4.68684769730414	3.83765253192625
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C	1.31351538835231	0.51497652877512	3.23293354525316
C	2.66439241665646	0.89612271728716	2.70171184899951
C	3.09608930639145	-0.21865965291403	1.75750090340824
C	2.59384989004370	-1.49051082524340	1.81006339854920
C	1.60607775744015	-2.03370834519513	2.83355370155789
C	0.67205548599590	-2.81961804682962	1.92504855539037
C	-0.69542150802708	-2.79896279641618	1.96254108976514
C	-1.50782641653031	-1.93822959529911	2.91962487411852
C	-2.57090079936995	-1.37965066048939	1.96311180178488
C	-2.96481325664271	-0.06279242591690	1.92114366847825
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C	-3.04475181006211	-1.61001131356534	-0.44914277854710
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C	-0.80249620631290	-3.34553880805317	-0.44367898392042
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