A Conformationally Reliable Spacer for Molecular Tweezers

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Energy optimization of **1** and **2** was carried out with MacroModel version 6.0 on IRIX6.5.
Energy optimized coordinates (MacroModel format)

meso-(*1R,4aR,5as,6aS,10S,10aS,11as,12aR*)-1,10-Diphenyl-octadecahydronaphthacene (1):

by MM2"

3	2 1	4 1	31 1	32 1	0 0	0 0	6.727985	-4.257244	0.979973	0X	2	0.00000	0.00000	UNK
3	1 1	3 1	33 1	34 1	0 0	0 0	8.253132	-4.089715	0.937044	0X	2	0.00000	0.00000	UNK
3	2 1	6 1	35 1	36 1	0 0	0 0	8.661303	-2.710207	1.471524	0X	2	0.00000	0.00000	UNK
3	5 1	1 1	21 1	37 1	0 0	0 0	6.025742	-3.133920	0.196895	0X	2	0.04172	0.04172	UNK
3	6 1	8 1	4 1	38 1	0 0	0 0	6.441132	-1.743070	0.721757	0X	2	0.00000	0.00000	UNK
3	5 1	7 1	3 1	39 1	0 0	0 0	7.974291	-1.584607	0.679172	0X	2	0.00000	0.00000	UNK
3	6 1	10 1	40 1	41 1	0 0	0 0	8.393393	-0.202025	1.208023	0X	2	0.00000	0.00000	UNK
3	9 1	5 1	42 1	43 1	0 0	0 0	5.769743	-0.605862	-0.070266	0X	2	0.00000	0.00000	UNK
3	10 1	12 1	8 1	44 1	0 0	0 0	6.190272	0.776888	0.456821	0X	2	0.00000	0.00000	UNK
3	9 1	11 1	7 1	45 1	0 0	0 0	7.719853	0.928977	0.413130	0X	2	0.00000	0.00000	UNK
3	10 1	14 1	46 1	47 1	0 0	0 0	8.135737	2.311177	0.943469	0X	2	0.00000	0.00000	UNK
3	13 1	9 1	48 1	49 1	0 0	0 0	5.512615	1.907615	-0.336217	0X	2	0.00000	0.00000	UNK
3	14 1	18 1	12 1	50 1	0 0	0 0	5.924947	3.295023	0.189436	0X	2	0.00000	0.00000	UNK
3	13 1	15 1	11 1	51 1	0 0	0 0	7.459334	3.442166	0.149599	0X	2	0.00000	0.00000	UNK
3	14 1	16 1	52 1	53 1	0 0	0 0	7.888817	4.821415	0.678779	0X	2	0.00000	0.00000	UNK
3	15 1	17 1	54 1	55 1	0 0	0 0	7.224012	5.950618	-0.120148	0X	2	0.00000	0.00000	UNK
3	16 1	18 1	56 1	57 1	0 0	0 0	5.695683	5.813325	-0.082757	0X	2	0.00000	0.00000	UNK
3	17 1	13 1	27 1	58 1	0 0	0 0	5.251290	4.435126	-0.603577	0X	2	0.04172	0.04172	UNK
2	20 1	24 2	65 1	0 0	0 0	0 0	2.452836	-3.761388	-0.999210	0X	2	0.00000	0.00000	UNK
2	19 1	21 2	59 1	0 0	0 0	0 0	3.835250	-3.580393	-0.992291	0X	2	0.00000	0.00000	UNK
2	20 2	22 1	4 1	0 0	0 0	0 0	4.521194	-3.335015	0.201042	0X	2	-0.04172	-0.04172	UNK
2	21 1	23 2	60 1	0 0	0 0	0 0	3.788777	-3.275410	1.390044	0X	2	0.00000	0.00000	UNK
2	22 2	24 1	61 1	0 0	0 0	0 0	2.406278	-3.455498	1.389185	0X	2	0.00000	0.00000	UNK
2	23 1	19 2	66 1	0 0	0 0	0 0	1.734534	-3.699147	0.193055	0X	2	0.00000	0.00000	UNK
2	26 2	30 1	62 1	0 0	0 0	0 0	1.654294	4.072542	-1.836520	0X	2	0.00000	0.00000	UNK
2	25 2	27 1	63 1	0 0	0 0	0 0	3.044364	4.178440	-1.818171	0X	2	0.00000	0.00000	UNK
2	26 1	28 2	18 1	0 0	0 0	0 0	3.737299	4.326244	-0.612850	0X	2	-0.04172	-0.04172	UNK
2	27 2	29 1	64 1	0 0	0 0	0 0	3.003935	4.366078	0.576379	0X	2	0.00000	0.00000	UNK
2	28 1	30 2	67 1	0 0	0 0	0 0	1.613810	4.260457	0.564153	0X	2	0.00000	0.00000	UNK
2	29 2	25 1	68 1	0 0	0 0	0 0	0.935198	4.113267	-0.643789	0X	2	0.00000	0.00000	UNK
41	1 1	0 0	0 0	0 0	0 0	0 0	6.448016	-5.250350	0.553128	0X	21	0.00000	0.00000	UNK
41	1 1	0 0	0 0	0 0	0 0	0 0	6.396221	-4.252363	2.044644	0X	21	0.00000	0.00000	UNK
41	2 1	0 0	0 0	0 0	0 0	0 0	8.741680	-4.892059	1.540925	0X	21	0.00000	0.00000	UNK
41	2 1	0 0	0 0	0 0	0 0	0 0	8.614031	-4.206164	-0.112669	0X	21	0.00000	0.00000	UNK
41	3 1	0 0	0 0	0 0	0 0	0 0	8.384294	-2.633373	2.549445	0X	21	0.00000	0.00000	UNK
41	3 1	0 0	0 0	0 0	0 0	0 0	9.770287	-2.599602	1.408441	0X	21	0.00000	0.00000	UNK
41	4 1	0 0	0 0	0 0	0 0	0 0	6.385737	-3.200986	-0.857291	0X	21	0.00000	0.00000	UNK
41	5 1	0 0	0 0	0 0	0 0	0 0	6.122930	-1.655808	1.787842	0X	21	0.00000	0.00000	UNK
41	6 1	0 0	0 0	0 0	0 0	0 0	8.307357	-1.660547	-0.384573	0X	21	0.00000	0.00000	UNK
41	7 1	0 0	0 0	0 0	0 0	0 0	8.118725	-0.116098	2.285336	0X	21	0.00000	0.00000	UNK
41	7 1	0 0	0 0	0 0	0 0	0 0	9.502183	-0.095532	1.141656	0X	21	0.00000	0.00000	UNK
41	8 1	0 0	0 0	0 0	0 0	0 0	4.660172	-0.695984	-0.002584	0X	21	0.00000	0.00000	UNK
41	8 1	0 0	0 0	0 0	0 0	0 0	6.040449	-0.693736	-1.148355	0X	21	0.00000	0.00000	UNK
41	9 1	0 0	0 0	0 0	0 0	0 0	5.858614	0.855463	1.520916	0X	21	0.00000	0.00000	UNK
41	10 1	0 0	0 0	0 0	0 0	0 0	8.052185	0.851021	-0.650712	0X	21	0.00000	0.00000	UNK
41	11 1	0 0	0 0	0 0	0 0	0 0	7.860944	2.395964	2.020840	0X	21	0.00000	0.00000	UNK
41	11 1	0 0	0 0	0 0	0 0	0 0	9.244517	2.417944	0.877367	0X	21	0.00000	0.00000	UNK
41	12 1	0 0	0 0	0 0	0 0	0 0	4.406302	1.785317	-0.265818	0X	21	0.00000	0.00000	UNK
41	12 1	0 0	0 0	0 0	0 0	0 0	5.783650	1.823211	-1.414503	0X	21	0.00000	0.00000	UNK
41	13 1	0 0	0 0	0 0	0 0	0 0	5.607076	3.368091	1.256689	0X	21	0.00000	0.00000	UNK
41	14 1	0 0	0 0	0 0	0 0	0 0	7.793790	3.362584	-0.913452	0X	21	0.00000	0.00000	UNK
41	15 1	0 0	0 0	0 0	0 0	0 0	7.609141	4.914141	1.754755	0X	21	0.00000	0.00000	UNK
41	15 1	0 0	0 0	0 0	0 0	0 0	8.998553	4.925229	0.617462	0X	21	0.00000	0.00000	UNK
41	16 1	0 0	0 0	0 0	0 0	0 0	7.527794	6.941472	0.295815	0X	21	0.00000	0.00000	UNK
41	16 1	0 0	0 0	0 0	0 0	0 0	7.577774	5.918859	-1.178243	0X	21	0.00000	0.00000	UNK
41	17 1	0 0	0 0	0 0	0 0	0 0	5.347465	5.960995	0.966320	0X	21	0.00000	0.00000	UNK
41	17 1	0 0	0 0	0 0	0 0	0 0	5.231851	6.620297	-0.699590	0X	21	0.00000	0.00000	UNK
41	18 1	0 0	0 0	0 0	0 0	0 0	5.615063	4.354372	-1.655506	0X	21	0.00000	0.00000	UNK
41	20 1	0 0	0 0	0 0	0 0	0 0	4.382272	-3.632190	-1.948165	0X	21	0.00000	0.00000	UNK
41	22 1	0 0	0 0	0 0	0 0	0 0	4.296649	-3.082634	2.348779	0X	21	0.00000	0.00000	UNK
41	23 1	0 0	0 0	0 0	0 0	0 0	1.842669	-3.404659	2.336143	0X	21	0.00000	0.00000	UNK
41	25 1	0 0	0 0	0 0	0 0	0 0	1.122314	3.955725	-2.795869	0X	21	0.00000	0.00000	UNK
41	26 1	0 0	0 0	0 0	0 0	0 0	3.592193	4.141775	-2.774287	0X	21	0.00000	0.00000	UNK
41	28 1	0 0	0 0	0 0	0 0	0 0	3.517475	4.480362	1.544597	0X	21	0.00000	0.00000	UNK
41	19 1	0 0	0 0	0 0	0 0	0 0	1.926174	-3.953562	-1.949322	0X	21	0.00000	0.00000	UNK
41	24 1	0 0	0 0	0 0	0 0	0 0	0.640666	-3.841592	0.190018	0X	21	0.00000	0.00000	UNK
41	29 1	0 0	0 0	0 0	0 0	0 0	1.049687	4.292838	1.511620	0X	21	0.00000	0.00000	UNK
41	30 1	0 0	0 0	0 0	0 0	0 0	-0.164644	4.029189	-0.655759	0X	21	0.00000	0.00000	UNK

by MM3"

3	2 1	4 1	31 1	32 1	0 0	0 0	6.726881	-4.256495	0.985020	0X	2	0.00000	0.00000	UNK
3	1 1	3 1	33 1	34 1	0 0	0 0	8.252311	-4.093979	0.956881	0X	2	0.00000	0.00000	UNK
3	2 1	6 1	35 1	36 1	0 0	0 0	8.667444	-2.708648	1.468932	0X	2	0.00000	0.00000	UNK
3	5 1	1 1	21 1	37 1	0 0	0 0	6.024055	-3.135558	0.193489	0X	2	0.12501	0.12501	UNK
3	6 1	8 1	4 1	38 1	0 0	0 0	6.442191	-1.746687	0.734953	0X	2	0.00000	0.00000	UNK
3	5 1	7 1	3 1	39 1	0 0	0 0	7.978438	-1.588812	0.668672	0X	2	0.00000	0.00000	UNK
3	6 1	10 1	40 1	41 1	0 0	0 0	8.397462	-0.203575	1.194889	0X	2	0.00000	0.00000	UNK
3	9 1	5 1	42 1	43 1	0 0	0 0	5.770152	-0.604788	-0.055127	0X	2	0.00000	0.00000	UNK
3	10 1	12 1	8 1	44 1	0 0	0 0	6.191494	0.778608	0.472452	0X	2	0.00000	0.00000	UNK
3	9 1	11 1	7 1	45 1	0 0	0 0	7.722549	0.927798	0.400224	0X	2	0.00000	0.00000	UNK
3	10 1	14 1	46 1	47 1	0 0	0 0	8.139821	2.311045	0.928918	0X	2	0.00000	0.00000	UNK
3	13 1	9 1	48 1	49 1	0 0	0 0	5.512676	1.909434	-0.321329	0X	2	0.00000	0.00000	UNK
3	14 1	18 1	12 1	50 1	0 0	0 0	5.925055	3.301284	0.200649	0X	2	0.00000	0.00000	UNK
3	13 1	15 1	11 1	51 1	0 0	0 0	7.462829	3.444501	0.136250	0X	2	0.00000	0.00000	UNK
3	14 1	16 1	52 1	53 1	0 0	0 0	7.895981	4.820689	0.672618	0X	2	0.00000	0.00000	UNK
3	15 1	17 1	54 1	55 1	0 0	0 0	7.222504	5.957995	-0.106276	0X	2	0.00000	0.00000	UNK
3	16 1	18 1	56 1	57 1	0 0	0 0	5.695214	5.813411	-0.080587	0X	2	0.00000	0.00000	UNK
3	17 1	13 1	27 1	58 1	0 0	0 0	5.248800	4.435181	-0.608032	0X	2	0.12501	0.12501	UNK
2	20 1	24 2	65 1	0 0	0 0	0 0	2.457233	-3.784045	-1.006844	0X	2	-0.11346	-0.11346	UNK
2	19 1	21 2	59 1	0 0	0 0	0 0	3.840053	-3.598437	-0.996408	0X	2	-0.11346	-0.11346	UNK
2	20 2	22 1	4 1	0 0	0 0	0 0	4.521517	-3.340083	0.201203	0X	2	-0.12501	-0.12501	UNK
2	21 1	23 2	60 1	0 0	0 0	0 0	3.780388	-3.272467	1.388971	0X	2	-0.11346	-0.11346	UNK
2	22 2	24 1	61 1	0 0	0 0	0 0	2.397514	-3.457804	1.380482	0X	2	-0.11346	-0.11346	UNK
2	23 1	19 2	66 1	0 0	0 0	0 0	1.733522	-3.713937	0.182175	0X	2	-0.11346	-0.11346	UNK
2	26 2	30 1	62 1	0 0	0 0	0 0	1.649699	4.091630	-1.840988	0X	2	-0.11346	-0.11346	UNK
2	25 2	27 1	63 1	0 0	0 0	0 0	3.041124	4.193308	-1.823010	0X	2	-0.11346	-0.11346	UNK
2	26 1	28 2	18 1	0 0	0 0	0 0	3.735979	4.331066	-0.613350	0X	2	-0.12501	-0.12501	UNK
2	27 2	29 1	64 1	0 0	0 0	0 0	2.999722	4.364241	0.578994	0X	2	-0.11346	-0.11346	UNK
2	28 1	30 2	67 1	0 0	0 0	0 0	1.608236	4.262687	0.562899	0X	2	-0.11346	-0.11346	UNK
2	29 2	25 1	68 1	0 0	0 0	0 0	0.930831	4.126158	-0.647462	0X	2	-0.11346	-0.11346	UNK
41	1 1	0 0	0 0	0 0	0 0	0 0	6.450882	-5.249365	0.559912	0X	21	0.00000	0.00000	UNK
41	1 1	0 0	0 0	0 0	0 0	0 0	6.380132	-4.254261	2.043446	0X	21	0.00000	0.00000	UNK
41	2 1	0 0	0 0	0 0	0 0	0 0	8.729819	-4.886793	1.577847	0X	21	0.00000	0.00000	UNK
41	2 1	0 0	0 0	0 0	0 0	0 0	8.624335	-4.234807	-0.084095	0X	21	0.00000	0.00000	UNK
41	3 1	0 0	0 0	0 0	0 0	0 0	8.405626	-2.617321	2.547953	0X	21	0.00000	0.00000	UNK
41	3 1	0 0	0 0	0 0	0 0	0 0	9.774245	-2.601005	1.396568	0X	21	0.00000	0.00000	UNK
41	4 1	0 0	0 0	0 0	0 0	0 0	6.374619	-3.203045	-0.864403	0X	21	0.00000	0.00000	UNK
41	5 1	0 0	0 0	0 0	0 0	0 0	6.128164	-1.666723	1.802773	0X	21	0.00000	0.00000	UNK
41	6 1	0 0	0 0	0 0	0 0	0 0	8.300941	-1.670619	-0.397424	0X	21	0.00000	0.00000	UNK

41	7 1	0 0	0 0	0 0	0 0	0 0	8.134217	-0.115098	2.273440	0X	21	0.00000	0.00000	UNK
41	7 1	0 0	0 0	0 0	0 0	0 0	9.504442	-0.097744	1.124924	0X	21	0.00000	0.00000	UNK
41	8 1	0 0	0 0	0 0	0 0	0 0	4.662573	-0.697825	0.014593	0X	21	0.00000	0.00000	UNK
41	8 1	0 0	0 0	0 0	0 0	0 0	6.030947	-0.691392	-1.134404	0X	21	0.00000	0.00000	UNK
41	9 1	0 0	0 0	0 0	0 0	0 0	5.872404	0.858913	1.539698	0X	21	0.00000	0.00000	UNK
41	10 1	0 0	0 0	0 0	0 0	0 0	8.042074	0.847662	-0.666808	0X	21	0.00000	0.00000	UNK
41	11 1	0 0	0 0	0 0	0 0	0 0	7.876801	2.396854	2.007740	0X	21	0.00000	0.00000	UNK
41	11 1	0 0	0 0	0 0	0 0	0 0	9.246771	2.417205	0.858972	0X	21	0.00000	0.00000	UNK
41	12 1	0 0	0 0	0 0	0 0	0 0	4.407706	1.790840	-0.249057	0X	21	0.00000	0.00000	UNK
41	12 1	0 0	0 0	0 0	0 0	0 0	5.773812	1.821063	-1.400380	0X	21	0.00000	0.00000	UNK
41	13 1	0 0	0 0	0 0	0 0	0 0	5.610633	3.382968	1.268216	0X	21	0.00000	0.00000	UNK
41	14 1	0 0	0 0	0 0	0 0	0 0	7.785116	3.366824	-0.930218	0X	21	0.00000	0.00000	UNK
41	15 1	0 0	0 0	0 0	0 0	0 0	7.634835	4.904092	1.752442	0X	21	0.00000	0.00000	UNK
41	15 1	0 0	0 0	0 0	0 0	0 0	9.003172	4.924640	0.600799	0X	21	0.00000	0.00000	UNK
41	16 1	0 0	0 0	0 0	0 0	0 0	7.517817	6.941462	0.327036	0X	21	0.00000	0.00000	UNK
41	16 1	0 0	0 0	0 0	0 0	0 0	7.581059	5.952108	-1.161394	0X	21	0.00000	0.00000	UNK
41	17 1	0 0	0 0	0 0	0 0	0 0	5.333238	5.960863	0.962350	0X	21	0.00000	0.00000	UNK
41	17 1	0 0	0 0	0 0	0 0	0 0	5.234962	6.620750	-0.696258	0X	21	0.00000	0.00000	UNK
41	18 1	0 0	0 0	0 0	0 0	0 0	5.601975	4.351144	-1.663888	0X	21	0.00000	0.00000	UNK
41	20 1	0 0	0 0	0 0	0 0	0 0	4.396122	-3.655897	-1.946844	0X	21	0.11346	0.11346	UNK
41	22 1	0 0	0 0	0 0	0 0	0 0	4.286704	-3.069550	2.346697	0X	21	0.11346	0.11346	UNK
41	23 1	0 0	0 0	0 0	0 0	0 0	1.828610	-3.400595	2.323596	0X	21	0.11346	0.11346	UNK
41	25 1	0 0	0 0	0 0	0 0	0 0	1.117835	3.982817	-2.801018	0X	21	0.11346	0.11346	UNK
41	26 1	0 0	0 0	0 0	0 0	0 0	3.593743	4.162608	-2.776690	0X	21	0.11346	0.11346	UNK
41	28 1	0 0	0 0	0 0	0 0	0 0	3.516765	4.470184	1.546564	0X	21	0.11346	0.11346	UNK
41	19 1	0 0	0 0	0 0	0 0	0 0	1.935813	-3.985618	-1.957562	0X	21	0.11346	0.11346	UNK
41	24 1	0 0	0 0	0 0	0 0	0 0	0.640436	-3.859766	0.174759	0X	21	0.11346	0.11346	UNK
41	29 1	0 0	0 0	0 0	0 0	0 0	1.043310	4.289562	1.509750	0X	21	0.11346	0.11346	UNK
41	30 1	0 0	0 0	0 0	0 0	0 0	-0.168904	4.045101	-0.660674	0X	21	0.11346	0.11346	UNK

by OPLS"

3	2 1	4 1	31 1	32 1	0 0	0 0	6.762009	-4.209551	1.007592	0X	2	0.00000	0.00000	UNK
3	1 1	3 1	33 1	34 1	0 0	0 0	8.276518	-4.029578	0.904108	0X	2	0.00000	0.00000	UNK
3	2 1	6 1	35 1	36 1	0 0	0 0	8.672426	-2.658431	1.449155	0X	2	0.00000	0.00000	UNK
3	5 1	1 1	21 1	37 1	0 0	0 0	6.011965	-3.119614	0.228414	0X	2	0.00000	0.00000	UNK
3	6 1	8 1	4 1	38 1	0 0	0 0	6.424960	-1.727366	0.756918	0X	2	0.00000	0.00000	UNK
3	5 1	7 1	3 1	39 1	0 0	0 0	7.953426	-1.558479	0.662003	0X	2	0.00000	0.00000	UNK
3	6 1	10 1	40 1	41 1	0 0	0 0	8.383041	-0.189485	1.201538	0X	2	0.00000	0.00000	UNK
3	9 1	5 1	42 1	43 1	0 0	0 0	5.749999	-0.590864	-0.033687	0X	2	0.00000	0.00000	UNK
3	10 1	12 1	8 1	44 1	0 0	0 0	6.184017	0.780478	0.497547	0X	2	0.00000	0.00000	UNK
3	9 1	11 1	7 1	45 1	0 0	0 0	7.706126	0.926208	0.401109	0X	2	0.00000	0.00000	UNK
3	10 1	14 1	46 1	47 1	0 0	0 0	8.128325	2.295950	0.938921	0X	2	0.00000	0.00000	UNK
3	13 1	9 1	48 1	49 1	0 0	0 0	5.495274	1.896532	-0.296937	0X	2	0.00000	0.00000	UNK
3	14 1	18 1	12 1	50 1	0 0	0 0	5.911566	3.283879	0.226745	0X	2	0.00000	0.00000	UNK
3	13 1	15 1	11 1	51 1	0 0	0 0	7.444541	3.409086	0.136945	0X	2	0.00000	0.00000	UNK
3	14 1	16 1	52 1	53 1	0 0	0 0	7.911219	4.769452	0.664301	0X	2	0.00000	0.00000	UNK
3	15 1	17 1	54 1	55 1	0 0	0 0	7.260250	5.890302	-0.144280	0X	2	0.00000	0.00000	UNK
3	16 1	18 1	56 1	57 1	0 0	0 0	5.738529	5.780163	-0.048956	0X	2	0.00000	0.00000	UNK
3	17 1	13 1	27 1	58 1	0 0	0 0	5.239439	4.424778	-0.570007	0X	2	0.00000	0.00000	UNK
2	20 1	24 2	65 1	0 0	0 0	0 0	2.479002	-3.897451	-1.016144	0X	2	-0.11499	-0.11499	UNK
2	19 1	21 2	59 1	0 0	0 0	0 0	3.861658	-3.660232	-0.996261	0X	2	-0.11499	-0.11499	UNK
2	20 2	22 1	4 1	0 0	0 0	0 0	4.514305	-3.378645	0.215157	0X	2	0.00000	0.00000	UNK
2	21 1	23 2	60 1	0 0	0 0	0 0	3.770702	-3.338832	1.406814	0X	2	-0.11499	-0.11499	UNK
2	22 2	24 1	61 1	0 0	0 0	0 0	2.388214	-3.576120	1.386211	0X	2	-0.11499	-0.11499	UNK
2	23 1	19 2	66 1	0 0	0 0	0 0	1.740131	-3.855633	0.174748	0X	2	-0.11499	-0.11499	UNK
2	26 2	30 1	62 1	0 0	0 0	0 0	1.650438	4.203363	-1.876049	0X	2	-0.11499	-0.11499	UNK
2	25 2	27 1	63 1	0 0	0 0	0 0	3.051804	4.257718	-1.835781	0X	2	-0.11499	-0.11499	UNK
2	26 1	28 2	18 1	0 0	0 0	0 0	3.720915	4.369605	-0.605924	0X	2	0.00000	0.00000	UNK
2	27 2	29 1	64 1	0 0	0 0	0 0	2.974433	4.428796	0.583122	0X	2	-0.11499	-0.11499	UNK
2	28 1	30 2	67 1	0 0	0 0	0 0	1.573231	4.374387	0.542132	0X	2	-0.11499	-0.11499	UNK
2	29 2	25 1	68 1	0 0	0 0	0 0	0.909007	4.261425	-0.687433	0X	2	-0.11499	-0.11499	UNK
41	1 1	0 0	0 0	0 0	0 0	0 0	6.498559	-5.184557	0.596989	0X	21	0.00000	0.00000	UNK
41	1 1	0 0	0 0	0 0	0 0	0 0	6.472683	-4.181838	2.058501	0X	21	0.00000	0.00000	UNK
41	2 1	0 0	0 0	0 0	0 0	0 0	8.771656	-4.805434	1.488016	0X	21	0.00000	0.00000	UNK
41	2 1	0 0	0 0	0 0	0 0	0 0	8.587333	-4.115825	-0.137522	0X	21	0.00000	0.00000	UNK
41	3 1	0 0	0 0	0 0	0 0	0 0	8.405432	-2.595349	2.504632	0X	21	0.00000	0.00000	UNK
41	3 1	0 0	0 0	0 0	0 0	0 0	9.750890	-2.536763	1.346895	0X	21	0.00000	0.00000	UNK
41	4 1	0 0	0 0	0 0	0 0	0 0	6.353939	-3.181779	-0.804989	0X	21	0.00000	0.00000	UNK
41	5 1	0 0	0 0	0 0	0 0	0 0	6.128220	-1.643574	1.803007	0X	21	0.00000	0.00000	UNK
41	6 1	0 0	0 0	0 0	0 0	0 0	8.258031	-1.627732	-0.383197	0X	21	0.00000	0.00000	UNK
41	7 1	0 0	0 0	0 0	0 0	0 0	8.110291	-0.106508	2.254253	0X	21	0.00000	0.00000	UNK
41	7 1	0 0	0 0	0 0	0 0	0 0	9.464384	-0.089022	1.106074	0X	21	0.00000	0.00000	UNK
41	8 1	0 0	0 0	0 0	0 0	0 0	4.666866	-0.651984	0.066731	0X	21	0.00000	0.00000	UNK
41	8 1	0 0	0 0	0 0	0 0	0 0	6.011901	-0.675298	-1.088996	0X	21	0.00000	0.00000	UNK
41	9 1	0 0	0 0	0 0	0 0	0 0	5.878637	0.859697	1.541779	0X	21	0.00000	0.00000	UNK
41	10 1	0 0	0 0	0 0	0 0	0 0	8.014177	0.847505	-0.642360	0X	21	0.00000	0.00000	UNK
41	11 1	0 0	0 0	0 0	0 0	0 0	7.855343	2.379591	1.991523	0X	21	0.00000	0.00000	UNK
41	11 1	0 0	0 0	0 0	0 0	0 0	9.209635	2.396873	0.843576	0X	21	0.00000	0.00000	UNK
41	12 1	0 0	0 0	0 0	0 0	0 0	4.419992	1.758629	-0.188557	0X	21	0.00000	0.00000	UNK
41	12 1	0 0	0 0	0 0	0 0	0 0	5.757417	1.811378	-1.352128	0X	21	0.00000	0.00000	UNK
41	13 1	0 0	0 0	0 0	0 0	0 0	5.615170	3.360790	1.273461	0X	21	0.00000	0.00000	UNK
41	14 1	0 0	0 0	0 0	0 0	0 0	7.751479	3.320318	-0.906095	0X	21	0.00000	0.00000	UNK
41	15 1	0 0	0 0	0 0	0 0	0 0	7.639601	4.873799	1.715316	0X	21	0.00000	0.00000	UNK
41	15 1	0 0	0 0	0 0	0 0	0 0	8.994123	4.848140	0.566992	0X	21	0.00000	0.00000	UNK
41	16 1	0 0	0 0	0 0	0 0	0 0	7.576951	6.853349	0.256104	0X	21	0.00000	0.00000	UNK
41	16 1	0 0	0 0	0 0	0 0	0 0	7.569963	5.819876	-1.187427	0X	21	0.00000	0.00000	UNK
41	17 1	0 0	0 0	0 0	0 0	0 0	5.437877	5.912942	0.990691	0X	21	0.00000	0.00000	UNK
41	17 1	0 0	0 0	0 0	0 0	0 0	5.293877	6.576005	-0.646916	0X	21	0.00000	0.00000	UNK
41	18 1	0 0	0 0	0 0	0 0	0 0	5.584527	4.339081	-1.600686	0X	21	0.00000	0.00000	UNK
41	20 1	0 0	0 0	0 0	0 0	0 0	4.419422	-3.694042	-1.920610	0X	21	0.11499	0.11499	UNK
41	22 1	0 0	0 0	0 0	0 0	0 0	4.258960	-3.123235	2.345661	0X	21	0.11499	0.11499	UNK
41	23 1	0 0	0 0	0 0	0 0	0 0	1.822309	-3.542736	2.305823	0X	21	0.11499	0.11499	UNK
41	25 1	0 0	0 0	0 0	0 0	0 0	1.142041	4.116012	-2.825235	0X	21	0.11499	0.11499	UNK
41	26 1	0 0	0 0	0 0	0 0	0 0	3.611606	4.210793	-2.758323	0X	21	0.11499	0.11499	UNK
41	28 1	0 0	0 0	0 0	0 0	0 0	3.475292	4.514507	1.536069	0X	21	0.11499	0.11499	UNK
41	19 1	0 0	0 0	0 0	0 0	0 0	1.982941	-4.112208	-1.951481	0X	21	0.11499	0.11499	UNK
41	24 1	0 0	0 0	0 0	0 0	0 0	0.675221	-4.037905	0.158896	0X	21	0.11499	0.11499	UNK
41	29 1	0 0	0 0	0 0	0 0	0 0	1.005466	4.419108	1.460115	0X	21	0.11499	0.11499	UNK
41	30 1	0 0	0 0	0 0	0 0	0 0	-0.170216	4.219035	-0.718885	0X	21	0.11499	0.11499	UNK

by MMFF

3	2 1	4 1	31 1	32 1	0 0	0 0	6.759986	-4.263450	0.955288	0X	2	0.00000	0.00000	UNK
3	1 1	3 1	33 1	34 1	0 0	0 0	8.271876	-4.066347	0.943675	0X	2	0.00000	0.00000	UNK
3	2 1	6 1	35 1	36 1	0 0	0 0	8.659862	-2.691176	1.474550	0X	2	0.00000	0.00000	UNK
3	5 1	1 1	21 1	37 1	0 0	0 0	6.024483	-3.148235	0.185434	0X	2	0.14350	0.14350	UNK
3	6 1	8 1	4 1	38 1	0 0	0 0	6.425716	-1.744249	0.717757	0X	2	0.00000	0.00000	UNK
3	5 1	7 1	3 1	39 1	0 0	0 0	7.963662	-1.575440	0.686887	0X	2	0.00000	0.00000	UNK
3	6 1	10 1	40 1	41 1	0 0	0 0	8.381160	-0.196618	1.218519	0X	2	0.00000	0.00000	UNK
3	9 1	5 1	42 1	43 1	0 0	0 0	5.757942	-0.604306	-0.079026	0X	2	0.00000	0.00000	UNK
3	10 1	12 1	8 1	44 1	0 0	0 0	6.179509	0.775003	0.450251	0X	2	0.00000	0.00000	UNK
3	9 1	11 1	7 1	45 1	0 0	0 0	7.708545	0.928739	0.423021	0X	2	0.00000	0.00000	UNK
3	10 1	14 1	46 1	47 1	0 0	0 0	8.124833	2.306015	0.953549	0X	2	0.00000	0.00000	UNK
3	13 1	9 1	48 1	49 1	0 0	0 0	5.501273	1.901517	-0.344291	0X	2	0.00000	0.00000	UNK
3	14 1	18 1	12 1	50 1	0 0	0 0	5.909855	3.292047	0.184611	0X	2	0.00000	0.00000	UNK
3	13 1	15 1	11 1	51 1	0 0	0 0	7.450716	3.432381	0.156713	0X	2	0.00000	0.00000	UNK
3	14 1	16 1	52 1	53 1	0 0	0 0	7.892225	4.803548	0.681087	0X	2	0.00000	0.00000	UNK
3	15 1	17 1	54 1	55 1	0 0	0 0	7.247672	5.932531	-0.114798	0X	2	0.00000	0.00000	UNK
3	16 1	18 1	56 1	57 1	0 0	0 0	5.727073	5.820491	-0.112105	0X	2	0.00000	0.00000	UNK
3	17 1	13 1	27 1	58 1	0 0	0 0	5.246644	4.445659	-0.618424	0X	2	0.14350	0.14350	UNK

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  2    20 1    24 2    65 1     0 0     0 0     0 0    2.478111   -3.980533   -0.970524     0X    2 -0.15000 -0.15000 UNK
  2    19 1    21 2    59 1     0 0     0 0     0 0    3.853206   -3.738379   -0.972837     0X    2 -0.15000 -0.15000 UNK
  2    20 2    22 1     4 1     0 0     0 0     0 0    4.524860   -3.407483    0.214099     0X    2 -0.14350 -0.14350 UNK
  2    21 1    23 2    60 1     0 0     0 0     0 0    3.784485   -3.331160    1.403860     0X    2 -0.15000 -0.15000 UNK
  2    22 2    24 1    61 1     0 0     0 0     0 0    2.409445   -3.573766    1.404618     0X    2 -0.15000 -0.15000 UNK
  2    23 1    19 2    66 1     0 0     0 0     0 0    1.756549   -3.897637    0.217801     0X    2 -0.15000 -0.15000 UNK
  2    26 2    30 1    62 1     0 0     0 0     0 0    1.630799    4.292003   -1.846312     0X    2 -0.15000 -0.15000 UNK
  2    25 2    27 1    63 1     0 0     0 0     0 0    3.026249    4.335343   -1.827546     0X    2 -0.15000 -0.15000 UNK
  2    26 1    28 2    18 1     0 0     0 0     0 0    3.725229    4.399134   -0.612318     0X    2 -0.14350 -0.14350 UNK
  2    27 2    29 1    64 1     0 0     0 0     0 0    2.990083    4.424155    0.582859     0X    2 -0.15000 -0.15000 UNK
  2    28 1    30 2    67 1     0 0     0 0     0 0    1.594617    4.380929    0.562468     0X    2 -0.15000 -0.15000 UNK
  2    29 2    25 1    68 1     0 0     0 0     0 0    0.915418    4.314217   -0.651590     0X    2 -0.15000 -0.15000 UNK
 41     1 1     0 0     0 0     0 0     0 0     0 0    6.522067   -5.241345    0.517785     0X   21  0.00000  0.00000 UNK
 41     1 1     0 0     0 0     0 0     0 0     0 0    6.418739   -4.299126    1.998002     0X   21  0.00000  0.00000 UNK
 41     2 1     0 0     0 0     0 0     0 0     0 0    8.748696   -4.843499    1.551684     0X   21  0.00000  0.00000 UNK
 41     2 1     0 0     0 0     0 0     0 0     0 0    8.649203   -4.185596   -0.079358     0X   21  0.00000  0.00000 UNK
 41     3 1     0 0     0 0     0 0     0 0     0 0    8.396385   -2.621782    2.537543     0X   21  0.00000  0.00000 UNK
 41     3 1     0 0     0 0     0 0     0 0     0 0    9.748070   -2.574196    1.407835     0X   21  0.00000  0.00000 UNK
 41     4 1     0 0     0 0     0 0     0 0     0 0    6.358523   -3.204676   -0.860947     0X   21  0.00000  0.00000 UNK
 41     5 1     0 0     0 0     0 0     0 0     0 0    6.097587   -1.655587    1.763336     0X   21  0.00000  0.00000 UNK
 41     6 1     0 0     0 0     0 0     0 0     0 0    8.298286   -1.645586   -0.358458     0X   21  0.00000  0.00000 UNK
 41     7 1     0 0     0 0     0 0     0 0     0 0    8.119881   -0.111737    2.281429     0X   21  0.00000  0.00000 UNK
 41     7 1     0 0     0 0     0 0     0 0     0 0    9.471167   -0.091526    1.150685     0X   21  0.00000  0.00000 UNK
 41     8 1     0 0     0 0     0 0     0 0     0 0    4.666821   -0.685918   -0.013864     0X   21  0.00000  0.00000 UNK
 41     8 1     0 0     0 0     0 0     0 0     0 0    6.019808   -0.692501   -1.141512     0X   21  0.00000  0.00000 UNK
 41     9 1     0 0     0 0     0 0     0 0     0 0    5.838628    0.850482    1.493123     0X   21  0.00000  0.00000 UNK
 41    10 1     0 0     0 0     0 0     0 0     0 0    8.049498    0.853257   -0.619749     0X   21  0.00000  0.00000 UNK
 41    11 1     0 0     0 0     0 0     0 0     0 0    7.863405    2.392638    2.016278     0X   21  0.00000  0.00000 UNK
 41    11 1     0 0     0 0     0 0     0 0     0 0    9.214961    2.409885    0.885810     0X   21  0.00000  0.00000 UNK
 41    12 1     0 0     0 0     0 0     0 0     0 0    4.414809    1.774389   -0.274309     0X   21  0.00000  0.00000 UNK
 41    12 1     0 0     0 0     0 0     0 0     0 0    5.762630    1.818299   -1.407302     0X   21  0.00000  0.00000 UNK
 41    13 1     0 0     0 0     0 0     0 0     0 0    5.584067    3.358031    1.232603     0X   21  0.00000  0.00000 UNK
 41    14 1     0 0     0 0     0 0     0 0     0 0    7.786560    3.350016   -0.887350     0X   21  0.00000  0.00000 UNK
 41    15 1     0 0     0 0     0 0     0 0     0 0    7.625608    4.904536    1.740760     0X   21  0.00000  0.00000 UNK
 41    15 1     0 0     0 0     0 0     0 0     0 0    8.982950    4.895907    0.616876     0X   21  0.00000  0.00000 UNK
 41    16 1     0 0     0 0     0 0     0 0     0 0    7.545982    6.898257    0.308736     0X   21  0.00000  0.00000 UNK
 41    16 1     0 0     0 0     0 0     0 0     0 0    7.614999    5.910418   -1.148127     0X   21  0.00000  0.00000 UNK
 41    17 1     0 0     0 0     0 0     0 0     0 0    5.363598    6.002223    0.907619     0X   21  0.00000  0.00000 UNK
 41    17 1     0 0     0 0     0 0     0 0     0 0    5.307199    6.618521   -0.737527     0X   21  0.00000  0.00000 UNK
 41    18 1     0 0     0 0     0 0     0 0     0 0    5.584731    4.349888   -1.660640     0X   21  0.00000  0.00000 UNK
 41    20 1     0 0     0 0     0 0     0 0     0 0    4.397114   -3.807973   -1.912156     0X   21  0.15000  0.15000 UNK
 41    22 1     0 0     0 0     0 0     0 0     0 0    4.272361   -3.081428    2.342879     0X   21  0.15000  0.15000 UNK
 41    23 1     0 0     0 0     0 0     0 0     0 0    1.848336   -3.509270    2.333035     0X   21  0.15000  0.15000 UNK
 41    25 1     0 0     0 0     0 0     0 0     0 0    1.102818    4.240102   -2.794731     0X   21  0.15000  0.15000 UNK
 41    26 1     0 0     0 0     0 0     0 0     0 0    3.564998    4.316373   -2.772208     0X   21  0.15000  0.15000 UNK
 41    28 1     0 0     0 0     0 0     0 0     0 0    3.498055    4.477424    1.542687     0X   21  0.15000  0.15000 UNK
 41    19 1     0 0     0 0     0 0     0 0     0 0    1.970673   -4.233226   -1.897668     0X   21  0.15000  0.15000 UNK
 41    24 1     0 0     0 0     0 0     0 0     0 0    0.686335   -4.085227    0.218981     0X   21  0.15000  0.15000 UNK
 41    29 1     0 0     0 0     0 0     0 0     0 0    1.038233    4.399063    1.495784     0X   21  0.15000  0.15000 UNK
 41    30 1     0 0     0 0     0 0     0 0     0 0   -0.170452    4.279523   -0.666618     0X   21  0.15000  0.15000 UNK
by AMBER"
  3     2 1     4 1    31 1    32 1     0 0     0 0    6.744489   -4.199123    1.010505     0X    2 -0.07640 -0.07640 UNK
  3     1 1     3 1    33 1    34 1     0 0     0 0    8.261256   -4.033194    0.907055     0X    2 -0.07640 -0.07640 UNK
  3     2 1     6 1    35 1    36 1     0 0     0 0    8.672655   -2.664907    1.449970     0X    2 -0.07640 -0.07640 UNK
  3     5 1     1 1    21 1    37 1     0 0     0 0    6.016233   -3.096917    0.230016     0X    2 -0.13817 -0.13817 UNK
  3     6 1     8 1     4 1    38 1     0 0     0 0    6.443212   -1.716095    0.762482     0X    2 -0.03820 -0.03820 UNK
  3     5 1     7 1     3 1    39 1     0 0     0 0    7.967986   -1.557944    0.659970     0X    2 -0.03820 -0.03820 UNK
  3     6 1    10 1    40 1    41 1     0 0     0 0    8.398583   -0.188817    1.197110     0X    2 -0.07640 -0.07640 UNK
  3     9 1     5 1    42 1    43 1     0 0     0 0    5.764408   -0.588241   -0.029596     0X    2 -0.07640 -0.07640 UNK
  3    10 1    12 1     8 1    44 1     0 0     0 0    6.197810    0.782368    0.501966     0X    2 -0.03820 -0.03820 UNK
  3     9 1    11 1     7 1    45 1     0 0     0 0    7.718678    0.927284    0.398848     0X    2 -0.03820 -0.03820 UNK
  3    10 1    14 1    46 1    47 1     0 0     0 0    8.143719    2.297462    0.934698     0X    2 -0.07640 -0.07640 UNK
  3    13 1     9 1    48 1    49 1     0 0     0 0    5.509870    1.897837   -0.292667     0X    2 -0.07640 -0.07640 UNK
  3    14 1    18 1    12 1    50 1     0 0     0 0    5.931540    3.277930    0.234358     0X    2 -0.03820 -0.03820 UNK
  3    13 1    15 1    11 1    51 1     0 0     0 0    7.458925    3.411193    0.135255     0X    2 -0.03820 -0.03820 UNK
  3    14 1    16 1    52 1    53 1     0 0     0 0    7.909927    4.775883    0.664660     0X    2 -0.07640 -0.07640 UNK
  3    15 1    17 1    54 1    55 1     0 0     0 0    7.244362    5.891510   -0.140752     0X    2 -0.07640 -0.07640 UNK
  3    16 1    18 1    56 1    57 1     0 0     0 0    5.723233    5.767294   -0.042872     0X    2 -0.07640 -0.07640 UNK
  3    17 1    13 1    27 1    58 1     0 0     0 0    5.248278    4.404366   -0.563636     0X    2 -0.13817 -0.13817 UNK
  2    20 1    24 2    65 1     0 0     0 0     0 0    2.447712   -3.743472   -1.038372     0X    2 -0.15000 -0.15000 UNK
  2    19 1    21 2    59 1     0 0     0 0     0 0    3.840052   -3.548034   -1.012479     0X    2 -0.15000 -0.15000 UNK
  2    20 2    22 1     4 1     0 0     0 0     0 0    4.511570   -3.310938    0.203210     0X    2  0.09997  0.09997 UNK
  2    21 1    23 2    60 1     0 0     0 0     0 0    3.761153   -3.273932    1.394628     0X    2 -0.15000 -0.15000 UNK
  2    22 2    24 1    61 1     0 0     0 0     0 0    2.368772   -3.468622    1.374394     0X    2 -0.15000 -0.15000 UNK
  2    23 1    19 2    66 1     0 0     0 0     0 0    1.709906   -3.703939    0.156336     0X    2 -0.15000 -0.15000 UNK
  2    26 2    30 1    62 1     0 0     0 0     0 0    1.651890    4.045222   -1.866732     0X    2 -0.15000 -0.15000 UNK
  2    25 2    27 1    63 1     0 0     0 0     0 0    3.054204    4.142906   -1.828794     0X    2 -0.15000 -0.15000 UNK
  2    26 1    28 2    18 1     0 0     0 0     0 0    3.732243    4.301744   -0.604013     0X    2  0.09997  0.09997 UNK
  2    27 2    29 1    64 1     0 0     0 0     0 0    2.978014    4.361739    0.584056     0X    2 -0.15000 -0.15000 UNK
  2    28 1    30 2    67 1     0 0     0 0     0 0    1.575678    4.264490    0.551807     0X    2 -0.15000 -0.15000 UNK
  2    29 2    25 1    68 1     0 0     0 0     0 0    0.910440    4.106011   -0.675178     0X    2 -0.15000 -0.15000 UNK
 41     1 1     0 0     0 0     0 0     0 0     0 0    6.468204   -5.171741    0.600546     0X   21  0.03820  0.03820 UNK
 41     1 1     0 0     0 0     0 0     0 0     0 0    6.453010   -4.168163    2.060894     0X   21  0.03820  0.03820 UNK
 41     2 1     0 0     0 0     0 0     0 0     0 0    8.750977   -4.815279    1.488575     0X   21  0.03820  0.03820 UNK
 41     2 1     0 0     0 0     0 0     0 0     0 0    8.570811   -4.123280   -0.135111     0X   21  0.03820  0.03820 UNK
 41     3 1     0 0     0 0     0 0     0 0     0 0    8.404249   -2.596354    2.505038     0X   21  0.03820  0.03820 UNK
 41     3 1     0 0     0 0     0 0     0 0     0 0    9.753302   -2.553926    1.352089     0X   21  0.03820  0.03820 UNK
 41     4 1     0 0     0 0     0 0     0 0     0 0    6.373024   -3.160300   -0.798995     0X   21  0.03820  0.03820 UNK
 41     5 1     0 0     0 0     0 0     0 0     0 0    6.150049   -1.630300    1.809667     0X   21  0.03820  0.03820 UNK
 41     6 1     0 0     0 0     0 0     0 0     0 0    8.268400   -1.631131   -0.386636     0X   21  0.03820  0.03820 UNK
 41     7 1     0 0     0 0     0 0     0 0     0 0    8.127627   -0.105629    2.250473     0X   21  0.03820  0.03820 UNK
 41     7 1     0 0     0 0     0 0     0 0     0 0    9.480544   -0.088817    1.101922     0X   21  0.03820  0.03820 UNK
 41     8 1     0 0     0 0     0 0     0 0     0 0    4.681270   -0.665148    0.069251     0X   21  0.03820  0.03820 UNK
 41     8 1     0 0     0 0     0 0     0 0     0 0    6.027535   -0.672924   -1.084694     0X   21  0.03820  0.03820 UNK
 41     9 1     0 0     0 0     0 0     0 0     0 0    5.896909    0.862208    1.547901     0X   21  0.03820  0.03820 UNK
 41    10 1     0 0     0 0     0 0     0 0     0 0    8.020902    0.847879   -0.646780     0X   21  0.03820  0.03820 UNK
 41    11 1     0 0     0 0     0 0     0 0     0 0    7.872462    2.381175    1.987944     0X   21  0.03820  0.03820 UNK
 41    11 1     0 0     0 0     0 0     0 0     0 0    9.225539    2.399057    0.839595     0X   21  0.03820  0.03820 UNK
 41    12 1     0 0     0 0     0 0     0 0     0 0    4.431441    1.774681   -0.189218     0X   21  0.03820  0.03820 UNK
 41    12 1     0 0     0 0     0 0     0 0     0 0    5.773270    1.813325   -1.347712     0X   21  0.03820  0.03820 UNK
 41    13 1     0 0     0 0     0 0     0 0     0 0    5.638829    3.353770    1.282440     0X   21  0.03820  0.03820 UNK
 41    14 1     0 0     0 0     0 0     0 0     0 0    7.761157    3.325335   -0.909866     0X   21  0.03820  0.03820 UNK
 41    15 1     0 0     0 0     0 0     0 0     0 0    7.637881    4.874319    1.716425     0X   21  0.03820  0.03820 UNK
 41    15 1     0 0     0 0     0 0     0 0     0 0    8.992742    4.866240    0.569560     0X   21  0.03820  0.03820 UNK
 41    16 1     0 0     0 0     0 0     0 0     0 0    7.554372    6.858849    0.256554     0X   21  0.03820  0.03820 UNK
 41    16 1     0 0     0 0     0 0     0 0     0 0    7.552334    5.824779   -1.185090     0X   21  0.03820  0.03820 UNK
 41    17 1     0 0     0 0     0 0     0 0     0 0    5.420846    5.896082    0.996942     0X   21  0.03820  0.03820 UNK
 41    17 1     0 0     0 0     0 0     0 0     0 0    5.266545    6.558530   -0.639327     0X   21  0.03820  0.03820 UNK
 41    18 1     0 0     0 0     0 0     0 0     0 0    5.607958    4.323977   -1.590451     0X   21  0.03820  0.03820 UNK
 41    20 1     0 0     0 0     0 0     0 0     0 0    4.396971   -3.579051   -1.937543     0X   21  0.15000  0.15000 UNK
 41    22 1     0 0     0 0     0 0     0 0     0 0    4.258840   -3.091790    2.335474     0X   21  0.15000  0.15000 UNK
 41    23 1     0 0     0 0     0 0     0 0     0 0    1.806413   -3.436013    2.296834     0X   21  0.15000  0.15000 UNK
 41    25 1     0 0     0 0     0 0     0 0     0 0    1.145420    3.922470   -2.813650     0X   21  0.15000  0.15000 UNK
 41    26 1     0 0     0 0     0 0     0 0     0 0    3.614156    4.093350   -2.751217     0X   21  0.15000  0.15000 UNK
 41    28 1     0 0     0 0     0 0     0 0     0 0    3.480943    4.481540    1.532090     0X   21  0.15000  0.15000 UNK
 41    19 1     0 0     0 0     0 0     0 0     0 0    1.945919   -3.923259   -1.978646     0X   21  0.15000  0.15000 UNK
 41    24 1     0 0     0 0     0 0     0 0     0 0    0.638983   -3.853251    0.138388     0X   21  0.15000  0.15000 UNK
 41    29 1     0 0     0 0     0 0     0 0     0 0    1.010765    4.310893    1.472094     0X   21  0.15000  0.15000 UNK
```

```
 41    30 1     0 0     0 0     0 0     0 0     0 0   -0.167997    4.030308   -0.702226     0X   21  0.15000  0.15000 UNK
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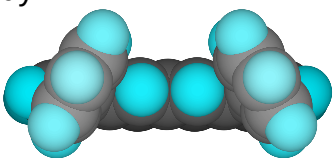
1,10-Diphenylnaphthacene (2):

by MM2"



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  2     1 2     3 1     6 1     0 0     0 0     0 0   -2.812767   -1.598121   -5.934594     0X    2  0.00000  0.00000 UNK
  2     2 1     4 2     7 1     0 0     0 0     0 0   -1.999174   -2.286744   -5.038947     0X    2  0.00000  0.00000 UNK
  2     3 2    10 1    30 1     0 0     0 0     0 0   -1.633289   -1.710043   -3.820264     0X    2  0.00000  0.00000 UNK
 41     1 1     0 0     0 0     0 0     0 0     0 0   -3.909310    0.212379   -6.330124     0X   21  0.00000  0.00000 UNK
 41     2 1     0 0     0 0     0 0     0 0     0 0   -3.092539   -2.058998   -6.897106     0X   21  0.00000  0.00000 UNK
 41     3 1     0 0     0 0     0 0     0 0     0 0   -1.635874   -3.292544   -5.309678     0X   21  0.00000  0.00000 UNK
  2    15 2     9 1    12 1     0 0     0 0     0 0   -3.385915    1.539428   -4.072365     0X    2  0.00000  0.00000 UNK
  2     8 1    10 2     1 1     0 0     0 0     0 0   -2.916293    0.262610   -4.390768     0X    2  0.00000  0.00000 UNK
  2     9 2    11 1     4 1     0 0     0 0     0 0   -2.100601   -0.430645   -3.487451     0X    2  0.00000  0.00000 UNK
  2    10 1    16 2    13 1     0 0     0 0     0 0   -1.793007    0.180661   -2.267630     0X    2  0.00000  0.00000 UNK
 41     8 1     0 0     0 0     0 0     0 0     0 0   -4.026301    2.079456   -4.790352     0X   21  0.00000  0.00000 UNK
 41    11 1     0 0     0 0     0 0     0 0     0 0   -1.172602   -0.346725   -1.526031     0X   21  0.00000  0.00000 UNK
  2    22 2    15 1    18 1     0 0     0 0     0 0   -3.532404    3.416640   -2.529785     0X    2  0.00000  0.00000 UNK
  2    14 1    16 1     8 2     0 0     0 0     0 0   -3.062090    2.143924   -2.856786     0X    2  0.00000  0.00000 UNK
  2    15 1    17 1    11 2     0 0     0 0     0 0   -2.260074    1.457460   -1.945302     0X    2  0.00000  0.00000 UNK
  2    16 1    23 2    19 1     0 0     0 0     0 0   -1.939493    2.057838   -0.725055     0X    2  0.00000  0.00000 UNK
 41    14 1     0 0     0 0     0 0     0 0     0 0   -4.172813    3.956675   -3.247755     0X   21  0.00000  0.00000 UNK
 41    17 1     0 0     0 0     0 0     0 0     0 0   -1.316005    1.490447   -0.016300     0X   21  0.00000  0.00000 UNK
  2    21 2    25 1    26 1     0 0     0 0     0 0   -3.396681    5.884620    0.214581     0X    2  0.00000  0.00000 UNK
  2    20 2    22 1    27 1     0 0     0 0     0 0   -3.704117    5.283721   -1.003253     0X    2  0.00000  0.00000 UNK
  2    21 1    23 1    14 2     0 0     0 0     0 0   -3.208955    4.013419   -1.308538     0X    2  0.00000  0.00000 UNK
  2    22 1    24 1    17 2     0 0     0 0     0 0   -2.394594    3.337499   -0.390990     0X    2  0.00000  0.00000 UNK
  2    23 1    25 2    39 1     0 0     0 0     0 0   -2.074769    3.948599    0.829762     0X    2  0.00000  0.00000 UNK
  2    24 2    20 1    28 1     0 0     0 0     0 0   -2.584565    5.215094    1.125910     0X    2  0.00000  0.00000 UNK
 41    20 1     0 0     0 0     0 0     0 0     0 0   -3.790676    6.886773    0.454466     0X   21  0.00000  0.00000 UNK
 41    21 1     0 0     0 0     0 0     0 0     0 0   -4.347315    5.826505   -1.716664     0X   21  0.00000  0.00000 UNK
 41    25 1     0 0     0 0     0 0     0 0     0 0   -2.337935    5.703955    2.083545     0X   21  0.00000  0.00000 UNK
  2    36 1    30 2    33 1     0 0     0 0     0 0   -1.146559   -3.760733   -2.453956     0X    2  0.00000  0.00000 UNK
  2    29 2    31 1     4 1     0 0     0 0     0 0   -0.733710   -2.512291   -2.924827     0X    2  0.00000  0.00000 UNK
  2    30 1    32 2    34 1     0 0     0 0     0 0    0.532110   -2.037127   -2.573811     0X    2  0.00000  0.00000 UNK
  2    31 2    37 1    35 1     0 0     0 0     0 0    1.368099   -2.791647   -1.751170     0X    2  0.00000  0.00000 UNK
 41    29 1     0 0     0 0     0 0     0 0     0 0   -2.140697   -4.153469   -2.725881     0X   21  0.00000  0.00000 UNK
 41    31 1     0 0     0 0     0 0     0 0     0 0    0.881420   -1.061261   -2.951114     0X   21  0.00000  0.00000 UNK
 41    32 1     0 0     0 0     0 0     0 0     0 0    2.365289   -2.407522   -1.477431     0X   21  0.00000  0.00000 UNK
  2    37 2    29 1    47 1     0 0     0 0     0 0   -0.312812   -4.517518   -1.631000     0X    2  0.00000  0.00000 UNK
  2    36 2    32 1    48 1     0 0     0 0     0 0    0.945564   -4.032764   -1.277029     0X    2  0.00000  0.00000 UNK
  2    46 1    39 2    42 1     0 0     0 0     0 0    0.139726    2.993093    1.559799     0X    2  0.00000  0.00000 UNK
  2    38 2    40 1    24 1     0 0     0 0     0 0   -1.187796    3.308807    1.858641     0X    2  0.00000  0.00000 UNK
  2    39 1    41 2    43 1     0 0     0 0     0 0   -1.677673    3.046828    3.140095     0X    2  0.00000  0.00000 UNK
  2    40 2    45 1    44 1     0 0     0 0     0 0   -0.857524    2.463149    4.105362     0X    2  0.00000  0.00000 UNK
 41    38 1     0 0     0 0     0 0     0 0     0 0    0.548340    3.209376    0.558327     0X   21  0.00000  0.00000 UNK
 41    40 1     0 0     0 0     0 0     0 0     0 0   -2.721804    3.294844    3.394583     0X   21  0.00000  0.00000 UNK
 41    41 1     0 0     0 0     0 0     0 0     0 0   -1.254118    2.255464    5.113574     0X   21  0.00000  0.00000 UNK
  2    46 2    41 1    50 1     0 0     0 0     0 0    0.463718    2.142030    3.797155     0X    2  0.00000  0.00000 UNK
  2    45 2    38 1    49 1     0 0     0 0     0 0    0.962310    2.409492    2.522954     0X    2  0.00000  0.00000 UNK
 41    36 1     0 0     0 0     0 0     0 0     0 0   -0.648830   -5.500500   -1.259855     0X   21  0.00000  0.00000 UNK
 41    37 1     0 0     0 0     0 0     0 0     0 0    1.606066   -4.630694   -0.626585     0X   21  0.00000  0.00000 UNK
 41    46 1     0 0     0 0     0 0     0 0     0 0    2.008807    2.161605    2.277434     0X   21  0.00000  0.00000 UNK
 41    45 1     0 0     0 0     0 0     0 0     0 0    1.113475    1.680802    4.559989     0X   21  0.00000  0.00000 UNK
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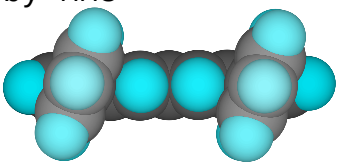
by MM3"



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  2     9 1     2 2     5 1     0 0     0 0     0 0   -3.454353   -0.419039   -5.522572     0X    2 -0.11346 -0.11346 UNK
  2     1 2     3 1     6 1     0 0     0 0     0 0   -2.989466   -1.690963   -5.848028     0X    2 -0.11346 -0.11346 UNK
  2     2 1     4 2     7 1     0 0     0 0     0 0   -2.133245   -2.357886   -4.975302     0X    2 -0.11346 -0.11346 UNK
  2     3 2    10 1    30 1     0 0     0 0     0 0   -1.734808   -1.765883   -3.771699     0X    2  0.00000  0.00000 UNK
 41     1 1     0 0     0 0     0 0     0 0     0 0   -4.132759    0.102650   -6.218215     0X   21  0.11346  0.11346 UNK
 41     2 1     0 0     0 0     0 0     0 0     0 0   -3.300728   -2.169908   -6.792061     0X   21  0.11346  0.11346 UNK
 41     3 1     0 0     0 0     0 0     0 0     0 0   -1.773457   -3.368752   -5.231554     0X   21  0.11346  0.11346 UNK
  2    15 2     9 1    12 1     0 0     0 0     0 0   -3.521919    1.477344   -4.008594     0X    2 -0.11346 -0.11346 UNK
  2     8 1    10 2     1 1     0 0     0 0     0 0   -3.061768    0.195536   -4.328774     0X    2  0.00000  0.00000 UNK
  2     9 2    11 1     4 1     0 0     0 0     0 0   -2.196268   -0.475814   -3.446904     0X    2  0.00000  0.00000 UNK
  2    10 1    16 2    13 1     0 0     0 0     0 0   -1.800584    0.171952   -2.268211     0X    2 -0.11346 -0.11346 UNK
 41     8 1     0 0     0 0     0 0     0 0     0 0   -4.203359    1.997645   -4.701575     0X   21  0.11346  0.11346 UNK
 41    11 1     0 0     0 0     0 0     0 0     0 0   -1.107733   -0.329186   -1.573213     0X   21  0.11346  0.11346 UNK
  2    22 2    15 1    18 1     0 0     0 0     0 0   -3.592052    3.390108   -2.504235     0X    2 -0.11346 -0.11346 UNK
  2    14 1    16 1     8 2     0 0     0 0     0 0   -3.130234    2.111113   -2.826336     0X    2  0.00000  0.00000 UNK
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 41    14 1     0 0     0 0     0 0     0 0     0 0   -4.280133    3.906878   -3.193248     0X   21  0.11346  0.11346 UNK
 41    17 1     0 0     0 0     0 0     0 0     0 0   -1.186256    1.552186   -0.082957     0X   21  0.11346  0.11346 UNK
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  2    23 1    25 2    39 1     0 0     0 0     0 0   -1.918014    4.014107    0.748045     0X    2  0.00000  0.00000 UNK
  2    24 2    20 1    28 1     0 0     0 0     0 0   -2.412338    5.290011    1.040928     0X    2 -0.11346 -0.11346 UNK
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 41    21 1     0 0     0 0     0 0     0 0     0 0   -4.364783    5.818801   -1.699207     0X   21  0.11346  0.11346 UNK
 41    25 1     0 0     0 0     0 0     0 0     0 0   -2.100957    5.795475    1.970756     0X   21  0.11346  0.11346 UNK
  2    36 1    30 2    33 1     0 0     0 0     0 0    0.487617   -2.750764   -3.227752     0X    2 -0.11346 -0.11346 UNK
  2    29 2    31 1     4 1     0 0     0 0     0 0   -0.846300   -2.521050   -2.873691     0X    2  0.00000  0.00000 UNK
  2    30 1    32 2    34 1     0 0     0 0     0 0   -1.324180   -3.031991   -1.661543     0X    2 -0.11346 -0.11346 UNK
  2    31 2    37 1    35 1     0 0     0 0     0 0   -0.481478   -3.752427   -0.813126     0X    2 -0.11346 -0.11346 UNK
 41    29 1     0 0     0 0     0 0     0 0     0 0    0.875497   -2.354799   -4.181192     0X   21  0.11346  0.11346 UNK
 41    31 1     0 0     0 0     0 0     0 0     0 0   -2.376388   -2.865394   -1.375585     0X   21  0.11346  0.11346 UNK
 41    32 1     0 0     0 0     0 0     0 0     0 0   -0.867766   -4.149668    0.140896     0X   21  0.11346  0.11346 UNK
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  2    36 2    32 1    48 1     0 0     0 0     0 0    0.848662   -3.971264   -1.172537     0X    2 -0.11346 -0.11346 UNK
  2    46 1    39 2    42 1     0 0     0 0     0 0   -1.443469    2.934827    2.942143     0X    2 -0.11346 -0.11346 UNK
```

```
  2    38 2    40 1    24 1     0 0     0 0     0 0   -0.987739    3.382154    1.697314     0X    2  0.00000  0.00000 UNK
  2    39 1    41 2    43 1     0 0     0 0     0 0    0.366147    3.231929    1.376333     0X    2 -0.11346 -0.11346 UNK
  2    40 2    45 1    44 1     0 0     0 0     0 0    1.248228    2.636532    2.279903     0X    2 -0.11346 -0.11346 UNK
 41    38 1     0 0     0 0     0 0     0 0     0 0   -2.507812    3.049388    3.207366     0X   21  0.11346  0.11346 UNK
 41    40 1     0 0     0 0     0 0     0 0     0 0    0.739141    3.588917    0.401613     0X   21  0.11346  0.11346 UNK
 41    41 1     0 0     0 0     0 0     0 0     0 0    2.313363    2.521430    2.016495     0X   21  0.11346  0.11346 UNK
  2    46 2    41 1    50 1     0 0     0 0     0 0    0.782971    2.188519    3.516494     0X    2 -0.11346 -0.11346 UNK
  2    45 2    38 1    49 1     0 0     0 0     0 0   -0.563881    2.338875    3.847909     0X    2 -0.11346 -0.11346 UNK
 41    36 1     0 0     0 0     0 0     0 0     0 0    2.384159   -3.643403   -2.668349     0X   21  0.11346  0.11346 UNK
 41    37 1     0 0     0 0     0 0     0 0     0 0    1.515666   -4.540333   -0.503002     0X   21  0.11346  0.11346 UNK
 41    46 1     0 0     0 0     0 0     0 0     0 0   -0.933978    1.986468    4.825666     0X   21  0.11346  0.11346 UNK
 41    45 1     0 0     0 0     0 0     0 0     0 0    1.478938    1.717804    4.231397     0X   21  0.11346  0.11346 UNK
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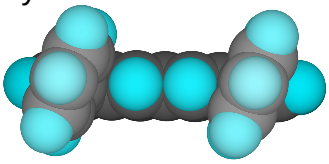
by OPLS"



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  2     2 1     4 2     7 1     0 0     0 0     0 0   -2.160089   -2.245530   -4.942658     0X    2 -0.11499 -0.11499 UNK
  2     3 2    10 1    30 1     0 0     0 0     0 0   -1.726863   -1.737343   -3.773886     0X    2  0.00000  0.00000 UNK
 41     1 1     0 0     0 0     0 0     0 0     0 0   -4.129674    0.172709   -6.111952     0X   21  0.11499  0.11499 UNK
 41     2 1     0 0     0 0     0 0     0 0     0 0   -3.322388   -2.012124   -6.672329     0X   21  0.11499  0.11499 UNK
 41     3 1     0 0     0 0     0 0     0 0     0 0   -1.830344   -3.229924   -5.242146     0X   21  0.11499  0.11499 UNK
  2    15 2     9 1    12 1     0 0     0 0     0 0   -3.541764    1.511614   -3.982443     0X    2 -0.11499 -0.11499 UNK
  2     8 1    10 2     1 1     0 0     0 0     0 0   -3.086108    0.280980   -4.289752     0X    2  0.00000  0.00000 UNK
  2     9 2    11 1     4 1     0 0     0 0     0 0   -2.178176   -0.407499   -3.382278     0X    2  0.00000  0.00000 UNK
  2    10 1    16 2    13 1     0 0     0 0     0 0   -1.791519    0.198509   -2.237923     0X    2 -0.11499 -0.11499 UNK
 41     8 1     0 0     0 0     0 0     0 0     0 0   -4.215914    2.017098   -4.657366     0X   21  0.11499  0.11499 UNK
 41    11 1     0 0     0 0     0 0     0 0     0 0   -1.112496   -0.289946   -1.556184     0X   21  0.11499  0.11499 UNK
  2    22 2    15 1    18 1     0 0     0 0     0 0   -3.616175    3.345799   -2.527934     0X    2 -0.11499 -0.11499 UNK
  2    14 1    16 1     8 2     0 0     0 0     0 0   -3.161351    2.115903   -2.839654     0X    2  0.00000  0.00000 UNK
  2    15 1    17 1    11 2     0 0     0 0     0 0   -2.245119    1.429567   -1.928154     0X    2  0.00000  0.00000 UNK
  2    16 1    23 2    19 1     0 0     0 0     0 0   -1.861483    2.033364   -0.785384     0X    2 -0.11499 -0.11499 UNK
 41    14 1     0 0     0 0     0 0     0 0     0 0   -4.293839    3.852836   -3.198183     0X   21  0.11499  0.11499 UNK
 41    17 1     0 0     0 0     0 0     0 0     0 0   -1.189283    1.510265   -0.122833     0X   21  0.11499  0.11499 UNK
  2    21 2    25 1    26 1     0 0     0 0     0 0   -3.305036    5.777480    0.083266     0X    2 -0.11499 -0.11499 UNK
  2    20 2    22 1    27 1     0 0     0 0     0 0   -3.684051    5.172429   -1.062245     0X    2 -0.11499 -0.11499 UNK
  2    21 1    23 1    14 2     0 0     0 0     0 0   -3.231799    3.946855   -1.384586     0X    2  0.00000  0.00000 UNK
  2    22 1    24 1    17 2     0 0     0 0     0 0   -2.316098    3.268120   -0.478329     0X    2  0.00000  0.00000 UNK
  2    23 1    25 2    39 1     0 0     0 0     0 0   -1.938295    3.975998    0.739005     0X    2  0.00000  0.00000 UNK
  2    24 2    20 1    28 1     0 0     0 0     0 0   -2.457456    5.198018    0.960507     0X    2 -0.11499 -0.11499 UNK
 41    20 1     0 0     0 0     0 0     0 0     0 0   -3.692159    6.761374    0.305619     0X   21  0.11499  0.11499 UNK
 41    21 1     0 0     0 0     0 0     0 0     0 0   -4.363983    5.685329   -1.726724     0X   21  0.11499  0.11499 UNK
 41    25 1     0 0     0 0     0 0     0 0     0 0   -2.184145    5.729886    1.860428     0X   21  0.11499  0.11499 UNK
  2    36 1    30 2    33 1     0 0     0 0     0 0    0.515210   -2.783115   -3.346397     0X    2 -0.11499 -0.11499 UNK
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  2    31 2    37 1    35 1     0 0     0 0     0 0   -0.380527   -3.857207   -0.915883     0X    2 -0.11499 -0.11499 UNK
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  2    37 2    29 1    47 1     0 0     0 0     0 0    1.384731   -3.548221   -2.553614     0X    2 -0.11499 -0.11499 UNK
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  2    46 1    39 2    42 1     0 0     0 0     0 0    0.366430    3.259648    1.445554     0X    2 -0.11499 -0.11499 UNK
  2    38 2    40 1    24 1     0 0     0 0     0 0   -0.998548    3.391603    1.745146     0X    2  0.00000  0.00000 UNK
  2    39 1    41 2    43 1     0 0     0 0     0 0   -1.478720    2.980351    2.997665     0X    2 -0.11499 -0.11499 UNK
  2    40 2    45 1    44 1     0 0     0 0     0 0   -0.599168    2.433571    3.944934     0X    2 -0.11499 -0.11499 UNK
 41    38 1     0 0     0 0     0 0     0 0     0 0    0.737992    3.579643    0.482661     0X   21  0.11499  0.11499 UNK
 41    40 1     0 0     0 0     0 0     0 0     0 0   -2.528958    3.082133    3.230043     0X   21  0.11499  0.11499 UNK
 41    41 1     0 0     0 0     0 0     0 0     0 0   -0.973314    2.115952    4.907536     0X   21  0.11499  0.11499 UNK
  2    46 2    41 1    50 1     0 0     0 0     0 0    0.764417    2.298437    3.643229     0X    2 -0.11499 -0.11499 UNK
  2    45 2    38 1    49 1     0 0     0 0     0 0    1.246247    2.712679    2.392309     0X    2 -0.11499 -0.11499 UNK
 41    36 1     0 0     0 0     0 0     0 0     0 0    2.399549   -3.722778   -2.880937     0X   21  0.11499  0.11499 UNK
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 41    46 1     0 0     0 0     0 0     0 0     0 0    2.295961    2.611244    2.157203     0X   21  0.11499  0.11499 UNK
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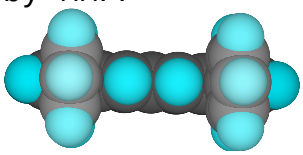
by MMFF



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  2     3 2    10 1    30 1     0 0     0 0     0 0   -1.641703   -1.765256   -3.864999     0X    2  0.00000  0.00000 UNK
 41     1 1     0 0     0 0     0 0     0 0     0 0   -3.932519    0.197497   -6.327971     0X   21  0.15000  0.15000 UNK
 41     2 1     0 0     0 0     0 0     0 0     0 0   -3.142574   -2.054014   -6.923422     0X   21  0.15000  0.15000 UNK
 41     3 1     0 0     0 0     0 0     0 0     0 0   -1.690953   -3.314435   -5.378931     0X   21  0.15000  0.15000 UNK
  2    15 2     9 1    12 1     0 0     0 0     0 0   -3.383287    1.534676   -4.077083     0X    2 -0.15000 -0.15000 UNK
  2     8 1    10 2     1 1     0 0     0 0     0 0   -2.925915    0.247112   -4.407956     0X    2  0.00000  0.00000 UNK
  2     9 2    11 1     4 1     0 0     0 0     0 0   -2.093464   -0.460491   -3.507557     0X    2  0.00000  0.00000 UNK
  2    10 1    16 2    13 1     0 0     0 0     0 0   -1.755801    0.178658   -2.290028     0X    2 -0.15000 -0.15000 UNK
 41     8 1     0 0     0 0     0 0     0 0     0 0   -4.023214    2.068528   -4.778594     0X   21  0.15000  0.15000 UNK
 41    11 1     0 0     0 0     0 0     0 0     0 0   -1.117627   -0.340115   -1.575343     0X   21  0.15000  0.15000 UNK
  2    22 2    15 1    18 1     0 0     0 0     0 0   -3.494112    3.438925   -2.534336     0X    2 -0.15000 -0.15000 UNK
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 41    14 1     0 0     0 0     0 0     0 0     0 0   -4.133937    3.969438   -3.238498     0X   21  0.15000  0.15000 UNK
 41    17 1     0 0     0 0     0 0     0 0     0 0   -1.225547    1.540440   -0.053137     0X   21  0.15000  0.15000 UNK
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  2    24 2    20 1    28 1     0 0     0 0     0 0   -2.475901    5.321031    1.090743     0X    2 -0.15000 -0.15000 UNK
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 41    25 1     0 0     0 0     0 0     0 0     0 0   -2.222349    5.822587    2.023400     0X   21  0.15000  0.15000 UNK
  2    36 1    30 2    33 1     0 0     0 0     0 0   -1.324675   -3.464027   -2.058859     0X    2 -0.15000 -0.15000 UNK
  2    29 2    31 1     4 1     0 0     0 0     0 0   -0.773273   -2.568326   -2.988288     0X    2  0.00000  0.00000 UNK
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  2    31 2    37 1    35 1     0 0     0 0     0 0    1.447953   -3.222518   -2.237609     0X    2 -0.15000 -0.15000 UNK
 41    29 1     0 0     0 0     0 0     0 0     0 0   -2.405023   -3.567394   -1.977907     0X   21  0.15000  0.15000 UNK
 41    31 1     0 0     0 0     0 0     0 0     0 0    1.075813   -1.773388   -3.782368     0X   21  0.15000  0.15000 UNK
```

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  2    37 2    29 1    47 1     0 0     0 0     0 0   -0.500610   -4.227028   -1.227770     0X    2 -0.15000 -0.15000 UNK
  2    36 2    32 1    48 1     0 0     0 0     0 0    0.885051   -4.105338   -1.317471     0X    2 -0.15000 -0.15000 UNK
  2    46 1    39 2    42 1     0 0     0 0     0 0    0.272833    3.574238    1.816084     0X    2 -0.15000 -0.15000 UNK
  2    38 2    40 1    24 1     0 0     0 0     0 0   -1.119704    3.400526    1.846602     0X    2  0.00000  0.00000 UNK
  2    39 1    41 2    43 1     0 0     0 0     0 0   -1.676636    2.619109    2.870989     0X    2 -0.15000 -0.15000 UNK
  2    40 2    45 1    44 1     0 0     0 0     0 0   -0.861852    2.022411    3.836401     0X    2 -0.15000 -0.15000 UNK
 41    38 1     0 0     0 0     0 0     0 0     0 0    0.728794    4.176739    1.032800     0X   21  0.15000  0.15000 UNK
 41    40 1     0 0     0 0     0 0     0 0     0 0   -2.753737    2.470392    2.917281     0X   21  0.15000  0.15000 UNK
 41    41 1     0 0     0 0     0 0     0 0     0 0   -1.306396    1.418073    4.623175     0X   21  0.15000  0.15000 UNK
  2    46 2    41 1    50 1     0 0     0 0     0 0    0.519686    2.201710    3.790624     0X    2 -0.15000 -0.15000 UNK
  2    45 2    38 1    49 1     0 0     0 0     0 0    1.087635    2.977542    2.781476     0X    2 -0.15000 -0.15000 UNK
 41    36 1     0 0     0 0     0 0     0 0     0 0   -0.941163   -4.915494   -0.510965     0X   21  0.15000  0.15000 UNK
 41    37 1     0 0     0 0     0 0     0 0     0 0    1.526297   -4.698890   -0.670557     0X   21  0.15000  0.15000 UNK
 41    46 1     0 0     0 0     0 0     0 0     0 0    2.164919    3.118845    2.744721     0X   21  0.15000  0.15000 UNK
 41    45 1     0 0     0 0     0 0     0 0     0 0    1.153743    1.737167    4.541731     0X   21  0.15000  0.15000 UNK
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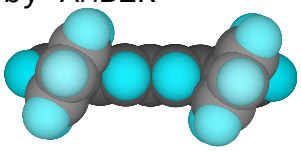
by AMBER"



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  2     1 2     3 1     6 1     0 0     0 0     0 0   -3.003172   -1.574232   -5.756087     0X    2 -0.15000 -0.15000 UNK
  2     2 1     4 2     7 1     0 0     0 0     0 0   -2.181755   -2.263479   -4.935328     0X    2 -0.15000 -0.15000 UNK
  2     3 2    10 1    30 1     0 0     0 0     0 0   -1.754580   -1.756074   -3.761074     0X    2  0.00000  0.00000 UNK
 41     1 1     0 0     0 0     0 0     0 0     0 0   -4.106565    0.158662   -6.157983     0X   21  0.15000  0.15000 UNK
 41     2 1     0 0     0 0     0 0     0 0     0 0   -3.318329   -2.032438   -6.683515     0X   21  0.15000  0.15000 UNK
 41     3 1     0 0     0 0     0 0     0 0     0 0   -1.865474   -3.256727   -5.222982     0X   21  0.15000  0.15000 UNK
  2    15 2     9 1    12 1     0 0     0 0     0 0   -3.525177    1.526772   -4.010738     0X    2 -0.15000 -0.15000 UNK
  2     8 1    10 2     1 1     0 0     0 0     0 0   -3.087304    0.287091   -4.314507     0X    2  0.00000  0.00000 UNK
  2     9 2    11 1     4 1     0 0     0 0     0 0   -2.194495   -0.410831   -3.389914     0X    2  0.00000  0.00000 UNK
  2    10 1    16 2    13 1     0 0     0 0     0 0   -1.809353    0.203817   -2.250976     0X    2 -0.15000 -0.15000 UNK
 41     8 1     0 0     0 0     0 0     0 0     0 0   -4.187676    2.037028   -4.695278     0X   21  0.15000  0.15000 UNK
 41    11 1     0 0     0 0     0 0     0 0     0 0   -1.134646   -0.299593   -1.574893     0X   21  0.15000  0.15000 UNK
  2    22 2    15 1    18 1     0 0     0 0     0 0   -3.587436    3.377691   -2.558901     0X    2 -0.15000 -0.15000 UNK
  2    14 1    16 1     8 2     0 0     0 0     0 0   -3.148227    2.138925   -2.868208     0X    2  0.00000  0.00000 UNK
  2    15 1    17 1    11 2     0 0     0 0     0 0   -2.243984    1.444576   -1.944978     0X    2  0.00000  0.00000 UNK
  2    16 1    23 2    19 1     0 0     0 0     0 0   -1.861581    2.057875   -0.804663     0X    2 -0.15000 -0.15000 UNK
 41    14 1     0 0     0 0     0 0     0 0     0 0   -4.257131    3.890343   -3.234595     0X   21  0.15000  0.15000 UNK
 41    17 1     0 0     0 0     0 0     0 0     0 0   -1.205334    1.539532   -0.121764     0X   21  0.15000  0.15000 UNK
  2    21 2    25 1    26 1     0 0     0 0     0 0   -3.258412    5.823162    0.057018     0X    2 -0.15000 -0.15000 UNK
  2    20 2    22 1    27 1     0 0     0 0     0 0   -3.641513    5.221139   -1.089028     0X    2 -0.15000 -0.15000 UNK
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  2    22 1    24 1    17 2     0 0     0 0     0 0   -2.295302    3.300009   -0.502013     0X    2  0.00000  0.00000 UNK
  2    23 1    25 2    39 1     0 0     0 0     0 0   -1.904315    4.006264    0.718423     0X    2  0.00000  0.00000 UNK
  2    24 2    20 1    28 1     0 0     0 0     0 0   -2.416847    5.234944    0.934090     0X    2 -0.15000 -0.15000 UNK
 41    20 1     0 0     0 0     0 0     0 0     0 0   -3.635216    6.812254    0.278734     0X   21  0.15000  0.15000 UNK
 41    21 1     0 0     0 0     0 0     0 0     0 0   -4.315833    5.750454   -1.748194     0X   21  0.15000  0.15000 UNK
 41    25 1     0 0     0 0     0 0     0 0     0 0   -2.136748    5.769404    1.831429     0X   21  0.15000  0.15000 UNK
  2    36 1    30 2    33 1     0 0     0 0     0 0    0.434084   -2.937027   -3.316069     0X    2 -0.15000 -0.15000 UNK
  2    29 2    31 1     4 1     0 0     0 0     0 0   -0.856035   -2.578695   -2.880742     0X    2  0.00000  0.00000 UNK
  2    30 1    32 2    34 1     0 0     0 0     0 0   -1.293635   -3.012315   -1.614299     0X    2 -0.15000 -0.15000 UNK
  2    31 2    37 1    35 1     0 0     0 0     0 0   -0.454261   -3.784858   -0.791942     0X    2 -0.15000 -0.15000 UNK
 41    29 1     0 0     0 0     0 0     0 0     0 0    0.781010   -2.609166   -4.286090     0X   21  0.15000  0.15000 UNK
 41    31 1     0 0     0 0     0 0     0 0     0 0   -2.286084   -2.749908   -1.274317     0X   21  0.15000  0.15000 UNK
 41    32 1     0 0     0 0     0 0     0 0     0 0   -0.801022   -4.111359    0.178768     0X   21  0.15000  0.15000 UNK
  2    37 2    29 1    47 1     0 0     0 0     0 0    1.277256   -3.709781   -2.497488     0X    2 -0.15000 -0.15000 UNK
  2    36 2    32 1    48 1     0 0     0 0     0 0    0.833481   -4.133987   -1.233285     0X    2 -0.15000 -0.15000 UNK
  2    46 1    39 2    42 1     0 0     0 0     0 0   -1.397104    3.111652    3.026019     0X    2 -0.15000 -0.15000 UNK
  2    38 2    40 1    24 1     0 0     0 0     0 0   -0.957439    3.410969    1.722425     0X    2  0.00000  0.00000 UNK
  2    39 1    41 2    43 1     0 0     0 0     0 0    0.383893    3.153687    1.378874     0X    2 -0.15000 -0.15000 UNK
  2    40 2    45 1    44 1     0 0     0 0     0 0    1.270550    2.598914    2.318926     0X    2 -0.15000 -0.15000 UNK
 41    38 1     0 0     0 0     0 0     0 0     0 0   -2.424845    3.304272    3.300733     0X   21  0.15000  0.15000 UNK
 41    40 1     0 0     0 0     0 0     0 0     0 0    0.733733    3.388182    0.382883     0X   21  0.15000  0.15000 UNK
 41    41 1     0 0     0 0     0 0     0 0     0 0    2.297909    2.404893    2.043230     0X   21  0.15000  0.15000 UNK
  2    46 2    41 1    50 1     0 0     0 0     0 0    0.821363    2.299230    3.616382     0X    2 -0.15000 -0.15000 UNK
  2    45 2    38 1    49 1     0 0     0 0     0 0   -0.514182    2.557003    3.969910     0X    2 -0.15000 -0.15000 UNK
 41    36 1     0 0     0 0     0 0     0 0     0 0    2.267196   -3.976333   -2.841040     0X   21  0.15000  0.15000 UNK
 41    37 1     0 0     0 0     0 0     0 0     0 0    1.480556   -4.728318   -0.602446     0X   21  0.15000  0.15000 UNK
 41    46 1     0 0     0 0     0 0     0 0     0 0   -0.863936    2.328154    4.967097     0X   21  0.15000  0.15000 UNK
 41    45 1     0 0     0 0     0 0     0 0     0 0    1.501715    1.872586    4.340954     0X   21  0.15000  0.15000 UNK
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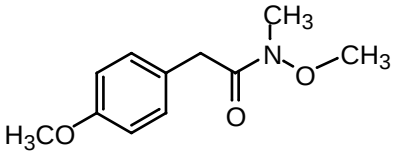
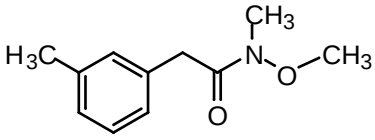
The spectra were measured with the following equipments and conditions unless otherwise noted. IR spectra were measured with PERKIN-ELMER 1720 Infrared Fourier Transfer Spectrometer indicating with cm^{-1}. ^{1}H-NMR spectra were measured with JEOL FX200 Spectrometer at 200MHz, JEOL JMN-AL300 Spectrometer at 300MHz, or JEOL GSX400 Spectrometer at 400MHz. ^{13}C-NMR spectra were measured with JEOL JMN-AL300 Spectrometer at 75MHz, or JEOL GSX400 Spectrometer at 100MHz. Both of the measurements were carried out in chloroform-d at 25˚C unless otherwise noted and indicated as δ value. High Resolution Mass Spectra (HRMS) were measured with JEOL JMS-DX303. Pyridine (Py) and triethylamine (Et_3N) were distilled over potassium hydroxide. Dichloromethane (CH_2Cl_2) and carbon tetrachloride (CCl_4) were distilled over phosphorous pentoxide. Acetonitrile and *N*,*N*-dimethylformamide (DMF) were distilled over calcium hydride. Tetrahydrofuran (THF), benzene, hexane for the reaction solvent and diethyl ether were distilled over sodium/benzophenone. All the reactions were carried out under argon atmosphere. “Room temperature” is abbreviated to “rt”.

***N*-Methoxy-*N*-methyl(4-methoxyphenyl)carboxamide:**



To a solution of 4-methoxybenzyl chloride (10.00 g, 54.17 mmol) and in CH_2Cl_2 (500 ml) was added N,O-dimethylhydroxyamine hydrochloride (5.81 g, 59.58 mmol) in one portion at rt, and the resulting mixture was stirred for 30 min at rt. To the mixture was added Py (9.64 ml, 119.16 mmol) dropwise over 10 min at 0˚C and the resulting mixture was stirred for 1 h at 0˚C. The resulting mixture was poured into 1N HClaq and extracted with three portions of CH_2Cl_2. The combined organic layers were washed with sat. $NaHCO_3$aq, brine, dried over $MgSO_4$, and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel eluted with ethyl acetate/hexane (3/2) to give the desired compound (10.20 g, 48.75 mmol, 90% yield). mp 37-38˚C; IR (KBr) 1662, 1247, 1035 cm^{-1}; ^{1}H-NMR (200MHz) 7.21 (d, J = 8.5Hz, 2H), 6.85 (d, J = 8.5Hz, 2H), 3.78 (s, 2H), 3.61 (s, 3H), 3.18 (s, 3H).; ^{13}C-NMR (100MHz) 172.7 (C), 158.4 (C), 130.3 (CH), 127.0 (C), 113.9 (CH), 61.3 (CH_3), 55.2 (CH_3), 38.4 (brd, CH_2), 32.2 (brd, CH_3), HRMS: m/z calcd. for $C_{11}H_{15}NO_3$: 209.1053. Found: 209.1035.

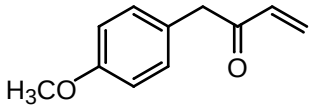
***N*-Methoxy-*N*-methyl(3-methylphenyl)carboxamide:**



A solution of 3-methylbenzoic acid (1.00 g, 6.66 mmol) in thionyl chloride (11 ml) was refluxed with stirring for 3 h. The resulting mixture was concentrated *in vacuo* to give the crude 3-methylbenzoyl chloride as a pale yellow oil, which was used in the next reaction without further purification.

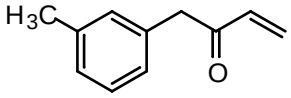
To the crude 3-methylbenzoyl chloride in CH_2Cl_2 (20 ml) was added N,O-dimethylhydroxyamine hydrochloride (714 mg, 7.32 mmol) in one portion at rt, and the resulting mixture was stirred for 30 min at rt. To the mixture was added Py (1.19 ml, 14.65 mmol) dropwise over 10 min at 0˚C and the resulting mixture was stirred for 1 h at 0˚C. The resulting mixture was poured into 1N HClaq and extracted with three portions of CH_2Cl_2. The combined organic layers were washed with sat. $NaHCO_3$aq, brine, dried over $MgSO_4$, and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel eluted with ethyl acetate/hexane (1/4) to give the desired compound (1.10 g, 5.69 mmol, 85% yield). IR (neat) 1662, 1381 cm^{-1}; ^{1}H-NMR (200MHz) 7.24-7.03 (m, 4H), 3.73 (s, 2H), 3.61 (s, 3H), 3.19 (s, 3H), 2.33 (s, 3H); ^{13}C-NMR (100MHz) 172.5 (C), 138.1 (C), 134.8 (C), 130.0 (CH), 128.4 (CH), 127.5 (CH), 126.3 (CH), 61.3 (CH_3), 39.3 (CH_2), 32.2 (brd, CH_2), 21.4 (brd, CH_3), HRMS: m/z calcd. for $C_{11}H_{15}NO_2$: 193.1104. Found: 193.1108.

1-(4-Methoxyphenyl)prop-2-en-1-one (4a):



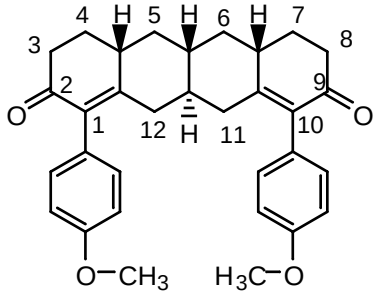
To a solution of N-methoxy-N-methyl(4-methoxyphenyl)carboxamide (37.15 g, 177.54 mmol) in THF (1635 ml) was added vinylmagnesium bromide (1.0M in THF, 213.05 ml, 213.05 mmol) dropwise over 30 min at 0˚C. The resulting mixture was stirred for 1 h, poured into 1N HClaq and extracted with three portions of ethyl acetate. The combined organic layers were washed with sat. $NaHCO_3$aq, brine, dried over $MgSO_4$, and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel eluted with ethyl acetate/hexane (1/4) to give **4a** (19.21 g, 108.30 mmol, 61% yield). IR (neat) 1695, 1250, and 1035 cm^{-1}, ^{1}H-NMR (200MHz) 7.13 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 2H), 6.42 (dd, *J* = 17.6, 9.5 Hz, 1H), 6.28 (dd, *J* = 2.2, 17.6 Hz, 1H), 5.81 (dd, *J* = 2.2, 9.5 Hz, 1H), 3.81 (s, 2H), 3.79 (s, 3H); ^{13}C-NMR (75MHz), 198.0 (C), 158.6 (C), 135.6 (CH), 130.5 (CHx2), 128.8 (CH_2), 126.0 (C), 114.2 (CHx2), 55.2 (CH_3), 46.3 (CH_2); HRMS: m/z calcd. for $C_{11}H_{12}O_2$: 176.0838. Found: 176.0844.

1-(3-Methylphenyl)prop-2-en-1-one (4b):



To a solution of N-methoxy-N-methyl(3-methylphenyl)carboxamide (40.00 g, 206.96 mmol) in THF (520 ml) was added vinylmagnesium bromide (1.0M in THF, 248.40 ml, 248.40 mmol) dropwise over 30 min at -15˚C. The resulting mixture was stirred for 30 min, poured into 2N HClaq and extracted with three portions of ethyl acetate. The combined organic layers were washed with sat, $NaHCO_3$aq, brine, dried over $MgSO_4$, and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel eluted with ethyl acetate/hexane (1/4) to give **4b** (27.50 g, 171.63 mmol, 83% yield). (19.21 g, 108.30 mmol, 61% overall yield). IR (neat) 1709, 1609, 1039 cm^{-1}, ^{1}H-NMR (300MHz) 7.21 (t, *J* = 7.5 Hz, 1H), 7.06 (d, *J* = 7.5 Hz, 1H), 7.02 (s, 1H), 7.00 (d, *J* = 7.5 Hz, 1H), 6.40 (dd, *J* = 17.5, 10.0 Hz, 1H), 6.28 (t, *J* = 17.5, 1.2 Hz, 1H), 5.80 (dd, *J* = 10.0, 1.2 Hz, 1H), 3.82 (s, 2H), 2.33 (s, 3H); ^{13}C-NMR (75MHz), 197.8 (C), 138.4 (C), 135.6 (CH), 134.0 (C), 130.2 (CH), 128.9 (CH_2), 128.6 (C), 127.8 (CH), 126.5 (CH), 47.2 (CH_2), 21.4 (CH_3); HRMS: m/z calcd. for $C_{11}H_{12}O$: 160.0889. Found: 160.0908.

***meso*-(*4aS,6aR,5ar,11ar*)-1,10-Bis(4-methoxyphenyl)-3,4,5,6,7,8,11,12,4a,5a,6a,11a-dodecahydro-naphthacene-2,9-dione (5a):**



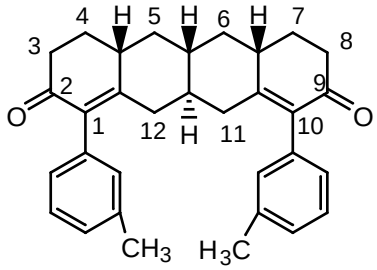
A mixture of *trans*-bicyclo[4.4.0]decane-3,9-dione (**3**) (3.59 g, 21.60 mmol) and pyrrolidine (5.41 ml, 64.79 mmol) in benzene (36 ml) was refulxed with stirring for 21 h. The resulting mixture was concentrated *in vacuo* and the residual pale yellow oil, the crude bis(enamine), was used in the next reaction without further purification.

To a solution of the crude bis(enamine) in benzene (50 ml) was added a solution of **4a** (8.20 g, 47.51 mmol) in benzene (22 ml) dropwise over 15 min at rt, and the reaction mixture was stirred for 3 h at rt. The resulting mixture was poured into water and extracted with three portions of ethyl acetate. The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated *in vacuo*. The residual pale yellow solid, the crude tetraketone was used in the next reaction without further purification.

A mixture of the crude tetraketone and *p*-toluenesulfonic acid monohydrate (1.67 g, 8.78 mmol) in benzene (200 ml) was refulxed with stirring for 5 h. The resulting mixture was poured into sat. $NaHCO_3$aq and extracted with three portions of ethyl

acetate. The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel eluted with hexane/ethyl acetate (3/7) to give **5a** (4.53 g, 9.29 mmol, 43% overall yield). The bis(enone) **5a** was purified further by recrystallization from methanol to give colorless prism. mp. 183-184˚C; IR (KBr) 1672, 1253,1032 cm^{-1}; ^{1}H-NMR (400MHz) 6.90 (d, *J* = 8.7 Hz, 2Hx2), 6.86 (d, *J* = 8.7 Hz, 2Hx2), 3.80 (s, 3Hx2), 2.59-2.40 (m, 3Hx2), 2.42 (ddd, *J* = 3.4, 14.3, 14.3 Hz, 1Hx2), 2.19 (ddd, *J* = 4.5, 9.5, 12.6 Hz, 1Hx2), 2.00 (ddd, *J* = 4.1, 4.1, 12.1 Hz, 1Hx2), 1.78-1.68 (m, 1Hx2), 1.66 (dd, *J* = 13.5, 13.5 Hz, 1Hx2), 1.61-1.53 (m, 1H), 1.28-1.18 (m, 1H), 1.17 (ddd, *J* = 12.1, 12.1, 12.1 Hz, 1Hx2); ^{13}C-NMR (100MHz) 198.5 (Cx2), 159.3 (Cx2), 158.7 (Cx2), 135.8 (Cx2), 131.0 (CHx4), 127.8 (CHx2), 113.5 (CHx4), 55.1 (CH_3x2), 44.2 (CHx2), 41.2 (CH_2x2), 41.1 (CH), 39.2 (CH_3x2), 38.5 (CH), 36.9 (CH_2x2), 28.4 (CH_2x2); HRMS: m/z calcd. for $C_{32}H_{34}O_4$: 482.2458. Found: 482.2483.

***meso*-(*4aS,6aR,5ar,11ar*)-1,10-Bis(4-methylphenyl)-3,4,5,6,7,8,11,12,11a,4a,5a,6a-dodecahydro-naphthacene-2,9-dione (5b):**

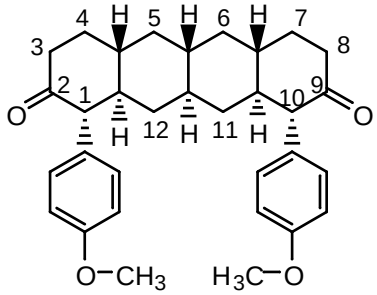


A mixture of *trans*-bicyclo[4.4.0]decane-3,9-dione (**3**) (30.25 g, 181.97 mmol) and pyrollidine (46.0 ml, 551.07 mmol) in benzene (320 ml) was refulxed with stirring for 21 h. The resulting mixture was concentrated *in vacuo* and the residual pale yellow oil, the crude bis(enamine), was used in the next reaction without further purification.

To a solution of the crude bis(enamine) in benzene (500 ml) was added a solution of **4b** (64.20 g, 400.67 mmol) in benzene (700 ml) dropwise over 15 min at rt, and the reaction mixture was stirred for 3 h at rt. The resulting mixture was poured into water and extracted with three portions of ethyl acetate. The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated *in vacuo*. The residual pale yellow solid, the crude tetraketone was used in the next reaction without further purification.

A mixture of the crude tetraketone and *p*-toluenesulfonic acid monohydrate (14.10 g, 74.12 mmol) in benzene (200 ml) was refulxed with stirring for 24 h. The resulting mixture was poured into sat. $NaHCO_3$aq and extracted with three portions of ethyl acetate. The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel eluted with hexane/ethyl acetate (2/3) to give **5b** (41.09 g, 91.18 mmol, 50% overall yield). IR (KBr) 2917, 2858, 1670, 701 cm^{-1}; ^{1}H-NMR (300MHz) 7.19 (t, *J* = 7.7 Hz, 1Hx2), 7.06 (d, *J* = 7.7 Hz, 1Hx2), 6.77 (s, 1Hx2), 6.76 (d, *J* = 7.7 Hz, 1Hx2), 2.59-2.45 (m, 3Hx2), 2.41-2.33 (m, 1Hx2), 2.29 (s, 3Hx2), 2.23-2.13 (m, 1Hx2), 2.03-1.96 (m, 1Hx2), 1.81-1.55 (m, 2Hx2+1H), 1.30-1.11 (m, 1Hx2+1H); ^{13}C-NMR (75MHz) 198.2 (Cx2), 159.3 (Cx2), 137.5 (Cx2), 136.4 (Cx2), 135.7 (Cx2), 130.4 (CHx2), 128.0 (CHx2), 127.9 (CHx2), 126.8 (CHx2), 44.2 (CHx2), 41.1 (CH_2x2), 41.1 (CH), 39.2 (CH_2x2), 38.5 (CH), 36.9 (CH_2x2), 28.4 (CH_2x2), 21.4 (CH_3x2); HRMS: m/z calcd. for $C_{32}H_{34}O_2$: 450.2560. Found: 450.2569.

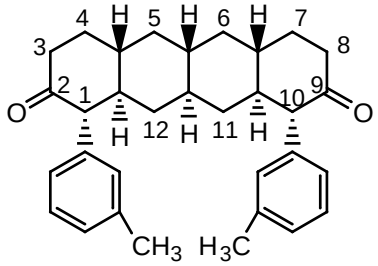
***meso*-(*1R,4aR,5as,6aS,10S,10aS,11as,12aR*)-1,10-Bis(4-methoxyphenyl)-1,3,4,5,6,7,8,10,11,12,4a,5a,6a,10a,11a,12a-hexadecahydronaphthacene-2,9-dione (101a):**



A solution of **5a** (400 mg, 0.83 mmol) in THF (10 ml) was added at -78˚C to a mixture of lithium (400 mg, 57.64 mmol)

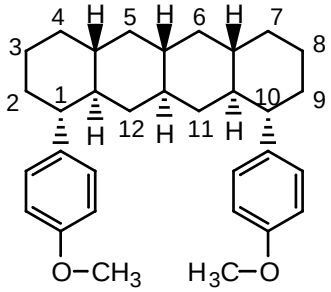
in liquid ammonia (40 ml), and the resulting mixture was stirred for 30 min at -78˚C. To the mixture was added $NaNO_2$ portionwise at -78˚C until the blue color was disappeared. After removal of ammonia at rt, water was added to the residue, and the resulting mixture was extracted with three portions of ethyl acetate. The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel eluted with hexane/ethyl acetate (3/2) to give the desired product as a colorless solid (162 mg, 0.33 mmol, 40% yield). FT-IR (KBr) 1713, 1250, 1036 cm^{-1}; ^{1}H-NMR (200MHz) 6.88 (d, *J* = 8.9 Hz, 2Hx2), 6.81 (d, *J* = 8.9 Hz, 2Hx2), 3.77 (s, 3Hx2), 3.14 (d, *J* = 11.5 Hz, 1Hx2), 2.54-2.44 (m, 4H), 2.05-2.01 (m, 1Hx2), 1.80-1.49 (m, 8H), 1.22-0.58 (m, 8H); ^{13}C-NMR (100MHz) 210.0 (Cx2), 158.3 (Cx2), 130.2 (CHx4), 129.0 (Cx2), 113.7 (CHx4), 62.5 (CHx2), 55.1 (CH_3x2), 49.1 (CHx2), 42.2 (CHx2), 42.2 (CH), 41.8 (CH_2x2), 41.2 (CH), 39.9 (CH_2x2), 38.9 (CHx2), 33.6 (CHx2); HRMS: m/z calcd. for $C_{32}H_{38}O_4$: 486.2771. Found: 486.2775.

***meso*-(*1R,4aR,5as,6aS,10S,10aS,11as,12aR*)-1,10-Bis(3-methylphenyl)-1,3,4,5,6,7,8,10,11,12, 4a,5a,6a,10a,11a,12a-hexadecahydronaphthacene-2,9-dione (101b):**



A solution of **5b** (100 mg, 0.22 mmol) in THF (2.5 ml) was added at -78˚C to a mixture of lithium (100 mg, 0.22 mmol) in liquid ammonia (10 ml), and the resulting mixture was stirred for 30 min at -78˚C. To the mixture was added $NaNO_2$ portionwise at -78˚C until the blue color was disappeared. After removal of ammonia at rt, water was added to the residue, and the resulting mixture was extracted with three portions of ethyl acetate. The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel eluted with hexane/ethyl acetate (2/1) to give the desired product as a colorless solid (54 mg, 0.12 mmol, 54% yield). FT-IR (KBr) 2900, 2856, 1709, 704 cm^{-1}; ^{1}H-NMR (300MHz) 7.15 (t, *J* = 7.6 Hz, 1Hx2), 7.01 (d, *J* =7.6 Hz, 1Hx2), 6.76 (s, 1Hx2), 6.75 (d, *J* =7.6 Hz, 1Hx2), 3.13 (d, *J* = 11.2 Hz, 1Hx2), 2.52-2.46 (m, 4H), 2.29 (s, 3Hx2), 2.04-2.00 (m, 2H), 1.78-1.50 (m, 8H), 1.13-0.56 (m, 8H); ^{13}C-NMR (75MHz) 209.6 (Cx2), 137.6 (Cx2), 137.0 (Cx2), 130.2 (CHx2), 128.0 (CHx2), 127.7 (CHx2), 126.3 (CHx2), 63.3 (CHx2), 48.8 (CH_2x2), 42.1 (CHx2), 42.1 (CH), 41.8 (CH_2x2), 41.1 (CH), 39.9 (CH_2x2), 38.9 (CH_2x2), 33.5 (CHx2), 21.5 (CH_3x2); HRMS: m/z calcd. for $C_{32}H_{38}O_2$: 454.2873. Found: 454.2864.

***meso*-(*1R,4aR,5as,6aS,10S,10aS,11as,12aR*)-1,10-Bis(4-methoxyphenyl)-octadecahydro-naphthacene (6a):**

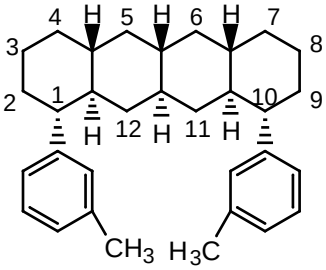


To a mixture of **101a** (729 mg, 1.50 mmol) and 1,2-ethanedithiol (0.38 ml, 4.49 mmol) in CH_2Cl_2 (15 ml) was added boron trifluoride diethyl etherate (0.18 ml, 1.50 mmol) at rt, and the mixture was stirred for 14 h at rt. The resulting mixture was poured into 2N NaOHaq, and extracted with three portions of CH_2Cl_2. The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated *in vacuo*. The pale yellow colored residual solid, the crude bis(1,3-dithiolane) **102a**, was used on the next reaction without further purification.

To a solution of **102a** in ethanol (70 ml) was added freshly prepared raney nickel (13.0 g, 221.50 mmol) in one portion and the mixture was refluxed with stirring for 24 h. The resulting suspension was filtered on celite, and the filtrate was concentrated

in vacuo. The residue was purified by recrystallization from CH_2Cl_2/ethanol to give **6a** as a colorless foam (390 mg, 0.85 mmol, 57% yield). FT-IR (KBr) 1259, 1038 cm^{-1}; ^{1}H-NMR (200MHz) 6.97 (d, *J* = 8.7 Hz, 2Hx2), 6.76 (d, *J* = 8.7 Hz, 2Hx2), 3.75 (s, 3Hx2), 2.09-2.01 (m, 1Hx2), 1.74-1.34 (m, 12H), 1.08-0.63 (m, 12H), 0.48-0.30 (m, 2H); ^{13}C-NMR (100MHz) 157.5 (Cx2), 138.6 (CHx4), 128.3 (Cx2), 113.6 (CHx4), 55.1 (CH_3x2), 50.0 (CHx2), 48.0 (CHx2), 43.3 (CHx2), 43.2 (CH), 43.1 (CH), 41.4 (CH_2x2), 38.1 (CH_2x2), 36.1 (CH_2x2), 34.0 (CH_2x2), 26.6 (CH_2x2); HRMS: m/z calcd. for $C_{32}H_{42}O_2$: 458.3187. Found: 458.3178.

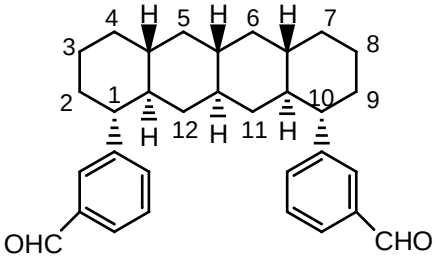
***meso*-(*1R,4aR,5as,6aS,10S,10aS,11as,12aR*)-1,10-Bis(3-methylphenyl)-octadecahydronaphthacene (6b):**



To a mixture of **101b** (3.18 g, 6.99 mmol) and 1,2-ethanedithiol (1.76 ml, 20.97 mmol) in CH_2Cl_2 (100 ml) was added boron trifluoride diethyl etherate (0.86 ml, 6.99 mmol) at rt, and the mixture was stirred for 2 h at rt. The resulting mixture was poured into 2N NaOHaq, and extracted with three portions of CH_2Cl_2. The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated *in vacuo*. The pale yellow colored residual solid, the crude bis(1,3-dithiolane) **102b**, was used on the next reaction without further purification.

To a solution of **102b** in ethanol (320 ml) was added freshly prepared raney nickel (54.0 g, 920.09 mmol) in one portion and the mixture was refluxed with stirring for 24 h. The resulting suspension was filtered on celite, and the filtrate was concentrated *in vacuo*. The residue was purified by recrystallization from CH_2Cl_2/methanol to give **6b** as a colorless foam (1.67 g, 3.91 mmol, 56% yield). FT-IR (KBr) 2916, 2848, 1607, 1445, 779, 703 cm^{-1}; ^{1}H-NMR (300MHz) 7.09 (t, *J* = 7.3 Hz, 1Hx2), 6.92 (d, *J* = 7.3 Hz, 1Hx2), 6.86 (s, 1Hx2), 6.85 (d, *J* = 7.3 Hz, 1Hx2), 2.28 (s, 3Hx2), 2.08-2.03 (m, 1Hx2), 1.77-1.38 (m, 12H), 1.12-0.69 (m, 12H), 0.46-0.35 (m, 2H); ^{13}C-NMR (100MHz) 146.5 (Cx2), 137.6 (CHx2), 128.4 (Cx2), 128.1 (CHx2), 126.6 (CHx2), 124.6 (CHx2), 51.2 (CHx2), 47.8 (CHx2), 43.5 (CHx2), 43.5 (CH), 43.2 (CH), 41.6 (CH_2x2), 38.1 (CH_2x2), 36.3 (CH_2x2), 34.1 (CH_2x2), 26.7 (CH_2x2), 21.5 (CH_3x2); HRMS: m/z calcd. for $C_{32}H_{42}$: 426.3289. Found: 426.3275.

***meso*-(*1R,4aR,5as,6aS,10S,10aS,11as,12aR*)-1,10-Bis(3-formylphenyl)-octadecahydronaphthacene (7):**

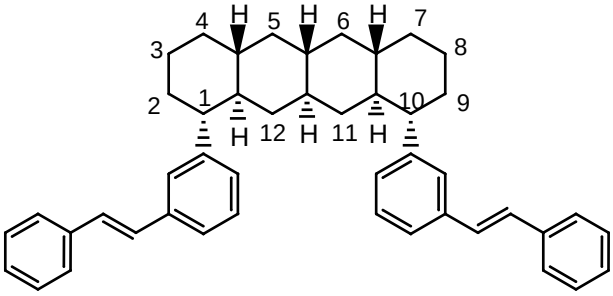


To a solution of **6b** (750 mg, 1.76 mmol) in CCl_4 (150 ml) was added *N*-bromosuccinimide (688 mg, 3.87 mmol) at rt. Then to the mixture was added α,α-azobisisobutyronitrile (29 mg, 0.18 mmol) at rt and the mixture was refluxed with stirring for 10 min. The resulting suspension was filtered, and the filtrate was concentrated *in vacuo*. The colorless residual solid, the crude dibromide, was used in the next reaction without further purification.

To the crude dibromide in 1,4-dioxane/water (60 ml/60 ml) was added calcium carbonate (1.76 g, 17.56 mmol) at rt, and the mixture was refulxed with stirring for 19 h. The resulting mixture was poured into 1N HClaq, and extracted with three portions of benzene. The combined organic layers were washed with sat. $NaHCO_3$aq, brine, dried over $MgSO_4$, and concentrated *in vacuo*. The colorless residual solid, the crude diol, was used in the next reaction without further purification.

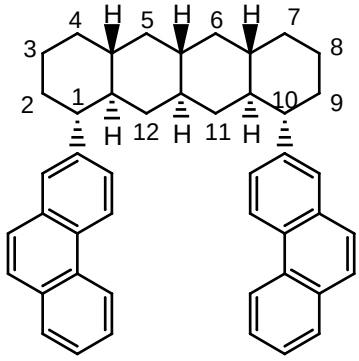
To a solution of the crude diol in CH_2Cl_2 (50 ml) was added pyridinium chlorochromate (1.52 g, 7.03 mmol) in one portion at rt and the mixture was stirred for 2 h at rt. The resulting suspension was filtered on celite, and the filtrate was concentrated *in vacuo*. The residue was purified by column chromatography on silica gel eluted with CH_2Cl_2 to give **7** as a colorless foam (491 mg, 1.08 mmol, 61% yield). FT-IR (KBr): 2919, 2852, 1697, 697 cm^{-1}; ^{1}H-NMR (300MHz) 9.93 (s, 1Hx2), 7.63-7.31 (m, 2Hx2), 2.24-2.18 (m, 1Hx2), 1.81-1.42 (m, 12H), 1.15-0.68 (m, 12H), 0.48-0.37 (m, 2H); ^{13}C-NMR (100MHz) 192.4 (CHx2), 147.6 (Cx2), 136.8 (Cx2), 133.9 (CHx2), 129.0 (CHx2), 128.3 (CHx2), 127.8 (CHx2), 50.9 (CHx2), 47.7 (CHx2), 43.3 (CHx2), 43.2 (CH), 43.0 (CH), 41.4 (CH_2x2), 38.2 (CH_2x2), 36.0 (CH_2x2), 33.9 (CH_2x2), 26.5 (CH_2x2); HRMS: m/z calcd. for $C_{32}H_{38}O_2$: 454.2873. Found: 454.2871.

***meso*-(1*R*,4a*R*,5a*s*,6a*S*,10*S*,10a*S*,11a*s*,12a*R*)-1,10-bis(3-(2-phenylethenyl)phenyl)-octadecahydro-naphthacene (103):**



After sodium hydride (60% in mineral oil, 111 mg, 2.78 mmol) was washed with three portions of hexane (10 mlx3) at rt and suspended in DME (10 ml), diethyl benzylphosphonate (0.61 ml, 2.93 mmol) was added to the suspension and the mixture was stirred for 3 h at rt. To the resulting solution was added a solution of **7** (443 mg, 0.97 mmol) in DME (30 ml) dropwise over 15 min at rt, and the mixture was stirred for 20 h at rt. The resulting mixture was poured into water, and extracted with three portions of ethyl acetate. The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated *in vacuo* to give a mixture of the mono- and the bis-styrene derivative **103**. After the same operations mentioned above were carried out, the residue was purified by column chromatography on silica gel eluted with hexane/benzene (17/3) to give **103** as a colorless foam (414 mg, 0.96 mmol, 70% yield). FT-IR (KBr) 2918, 2849, 960, 697 cm^{-1}; ^{1}H-NMR (300MHz) 7.42-6.93 (m, 11Hx2), 2.15-2.09 (m, 2H), 1.79-1.42 (m, 12H), 1.26-0.71 (m, 12H), 0.49-0.38 (m, 2H); ^{13}C-NMR (100MHz) 146.9 (Cx2), 137.7 (Cx2), 137.3 (Cx2), 129.3 (CHx2), 128.60 (CHx6), 128.5 (CHx2), 127.4 (CHx2), 127.0 (CHx2), 126.5 (CHx4), 126.0 (CHx2), 124.1 (CHx2), 51.2 (CHx2), 47.8 (CHx2), 43.4 (CHx2), 43.4 (CH), 43.2 (CH), 41.6 (CH_2x2), 38.3 (CH_2x2), 36.1 (CH_2x2), 34.1 (CH_2x2), 26.7 (CH_2x2); HRMS: m/z calcd. for $C_{46}H_{50}$: 602.3915. Found: 602.3921.

***meso*-(1*R*,4a*R*,5a*s*,6a*S*,10*S*,10a*S*,11a*s*,12a*R*)-1,10-Bis(2-phenanthryl)-octadecahydronaphthacene (8):**



To a solution of **103** (36 mg, 0.060 mmol) in benzene (170 ml, babbled with argon gas for 30 min) were added iodine (30 mg, 0.12 mmol) and 1-butene oxide (1.3 ml, 14.93 mmol) at rt. The resulting solution was irradiated with 400W high-pressured Hg-vapor lump with stirring for 10 h, and then concentrated *in vacuo*. The residue was isolated by column chromatography on silica gel eluted with hexane/chloroform (17/3) to give **8** as a colorless solid (23 mg, 0.038 mmol, 64%

yield). The colorless solid was further purified for the binding study by recrystallization from benzene/methanol to give a colorless foam. FT-IR (KBr): 2917, 2850, 810, 745, 717 cm^{-1}; ^{1}H-NMR (400MHz) 8.47 (d, *J* = 8.2 Hz, 1Hx2), 8.43 (d, *J* = 8.2 Hz, 1Hx2), 7.72 (d, *J* = 7.7 Hz, 1Hx2), 7.57 (d, *J* = 10.5 Hz, 1Hx2), 7.55 (d, *J* = 10.5 Hz, 1Hx2), 7.50-7.41 (m, 3Hx2), 7.31 (d, *J* = 8.2 Hz, 1Hx2), 2.27 (ddd, *J* = 10.9, 10.9, 2.7 Hz, 1Hx2), 1.83-1.43 (m, 12H), 1.25-0.62 (m, 12H), 0.43-0.34 (m, 2H); ^{13}C-NMR (100MHz at 55˚C) 144.9 (Cx2), 132.2 (Cx2), 131.8 (Cx2), 130.4 (Cx2), 128.6 (Cx2), 128.4 (CHx2), 127.0 (CHx2), 126.9 (CHx2), 126.7 (CHx2), 126.5 (CHx2), 126.3 (CHx2), 126.0 (CHx2), 122.6 (CHx2), 122.4 (CHx2), 51.1 (CHx2), 48.0 (CHx2), 43.5 (CHx3), 43.2 (CH), 41.6 (CH_2x2), 38.3 (CH_2x2), 36.2 (CH_2x2), 34.1 (CH_2x2), 26.7 (CH_2x2); HRMS: m/z calcd. for $C_{46}H_{46}$: 598.3602. Found: 598.3618.

X ray analysis of 5a: Crystal size 0.5x0.6x0.8 mm. All data were obtained Rigaku AFC-5S automated four circle diffractometer with graphite-monochromated Mo $K\alpha$ radiation. Final lattice parameters were obtained from a least-squares refinement using 21 reflections. Crystal data: $C_{32}H_{34}O_4$, Mr=482.6, triclinic, space group P1, a=13.37(1)Å, b=17.319(9)Å, c=12.999(6)Å, α=100.21(5)°, β=118.28(4)°, γ=71.91(6)°, V=2518(3)Å^3, Z=4.0, Dx=1.273g/cm^3, F(000)=1032, and μ(Mo$K\alpha$)= 0.823 cm^{-1}. The intensities were measured using $\omega/2\theta$ scan up to 45°. Three standard reflections were monitored every 150 measurements. The data were corrected for Lorentz and polarization factors. Absorption correction was applied and decay corrected was not applied. Of the 9332 independent reflections which collected, 4834 reflections with $I>3.0\sigma(I)$ were used for structure determination and refinement. The structure was solved by direct method using TEXSAN crystallographic software package.[1] All non-H atoms were found in Fourier map. All H atoms were calculated at geometrical positions and not refined. The refinement of atomic parameters were carried out by the full matrix least-squares refinement, using isotropically temperature factors for all non-H atoms. The final refinement converged with R=0.087 and Rw=0.086 for 574 parameters. The minimum and maximum peaks in the final difference Fourier map were -0.51 and 0.53eÅ^{-3}. Atomic scattering factors were taken from "International Tables for X-ray Crystallography".[2] The final positional parameters of non-H atoms of **5a** are given in Table 1. Although the ***R*** factor the measured crystal was not small enough, further refinement was impossible for the measured data. However, no further experiment was made since the skeleton and the stereochemistry of **5a** was determined unambiguously at this point.

References and Notes

1) "*TEXSAN, TEXRAY Structure Analysis Package*," Molecular Structure Corporation, 3200 Research Forest Drive, The Woodlands, TX 77381, USA., 1985.

2) "*International Tables for X-ray Crystallography*," Vol. **IV**. Kynoch Press, Birmingham, England, 1964, Table 2.2A.

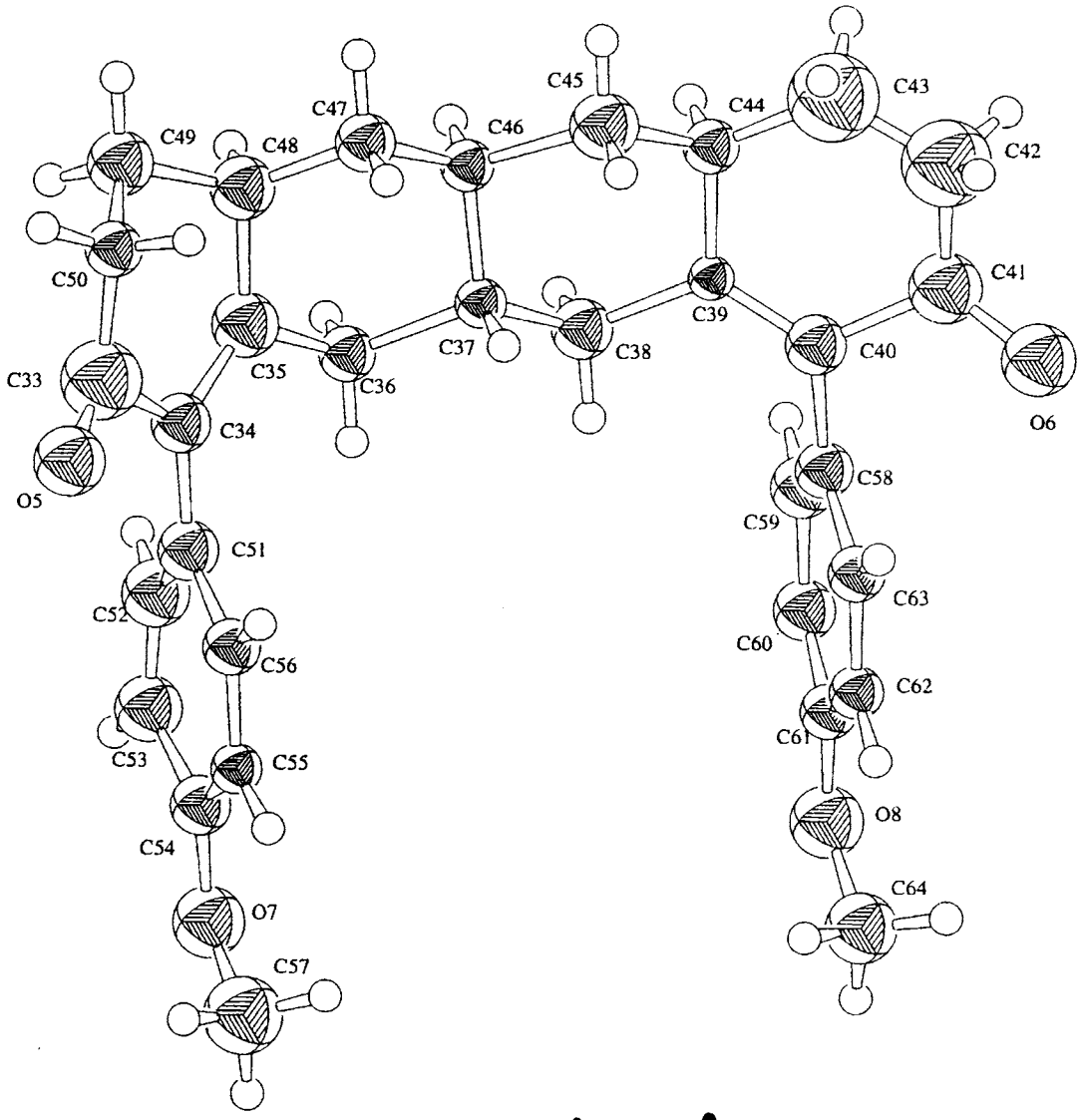
Table 1. Fractional Atomic Coordinates and Equivalent Isotropic Thermal Parameters of non-H atoms with e.s.d's in Parentheses. **5a**. The equivalent isotropic parameters *B*eq(Å^2) is taken as follows:

	atom	*x*	*y*	*z*	*Beq*
Mol1					
	O(1)	0.7262(7)	0.5639(5)	0.9713(7)	4.7(2)
	O(2)	0.3683(7)	0.7403(5)	0.0827(7)	5.6(2)
	O(3)	0.3304(8)	0.8820(5)	0.8213(7)	5.6(2)
	O(4)	0.1902(8)	0.9969(6)	0.4080(8)	6.2(2)
	C(1)	0.7799(8)	0.5644(6)	0.9131(8)	2.6(2)
	C(2)	0.7238(8)	0.6288(6)	0.8256(8)	2.0(2)
	C(3)	0.7697(9)	0.6245(6)	0.7534(9)	3.2(2)
	C(4)	0.7391(8)	0.6968(6)	0.6822(8)	2.1(2)
	C(5)	0.6933(9)	0.6831(6)	0.5484(9)	3.1(2)
	C(6)	0.6688(8)	0.7505(6)	0.4841(8)	2.6(2)
	C(7)	0.6250(9)	0.7251(6)	0.3545(8)	2.5(2)
	C(8)	0.5102(9)	0.7588(6)	0.2769(8)	2.8(2)
	C(9)	0.4711(10)	0.7238(7)	0.1554(10)	3.7(2)
	C(10)	0.5585(9)	0.6417(6)	0.1371(9)	3.9(2)
	C(11)	0.671(1)	0.6412(8)	0.197(1)	7.5(3)
	C(12)	0.7124(10)	0.6599(7)	0.3305(10)	3.9(2)
	C(13)	0.7371(10)	0.5828(7)	0.3957(10)	4.1(2)
	C(14)	0.7840(9)	0.6111(6)	0.5312(9)	3.0(2)
	C(15)	0.8002(8)	0.5314(6)	0.5937(8)	2.7(2)
	C(16)	0.8482(8)	0.5477(6)	0.7205(8)	2.7(2)
	C(17)	0.8523(8)	0.4758(6)	0.7797(8)	3.2(2)
	C(18)	0.8658(9)	0.4974(6)	0.9054(9)	3.7(2)
	C(19)	0.6313(9)	0.6957(6)	0.8333(8)	3.2(2)
	C(20)	0.627(1)	0.7452(7)	0.9281(10)	4.1(2)
	C(21)	0.537(1)	0.8017(8)	0.937(1)	5.3(3)
	C(22)	0.4309(10)	0.8201(7)	0.8370(9)	3.5(2)
	C(23)	0.4269(9)	0.7739(7)	0.7279(9)	3.8(2)
	C(24)	0.5186(10)	0.7179(7)	0.7284(9)	3.3(2)
	C(25)	0.331(1)	0.9217(8)	0.924(1)	6.6(3)
	C(26)	0.4168(8)	0.8211(6)	0.3066(8)	2.4(2)
	C(27)	0.369(1)	0.7972(7)	0.3677(10)	4.8(2)
	C(28)	0.303(1)	0.8567(8)	0.412(1)	5.0(3)
	C(29)	0.2679(9)	0.9322(6)	0.3833(9)	3.4(2)
	C(30)	0.303(1)	0.9561(7)	0.3097(10)	4.0(2)
	C(31)	0.3773(9)	0.8999(6)	0.2747(9)	3.1(2)
	C(32)	0.138(1)	0.9784(9)	0.468(1)	8.2(4)

	atom	*x*	*y*	*z*	*Beq*
Mol2					
	O(5)	0.5105(7)	0.2097(5)	1.0076(7)	4.8(1)
	O(6)	0.1762(6)	0.4230(3)	0.1484(5)	5.0(1)
	O(7)	0.6631(7)	-0.0796(5)	0.6998(7)	4.8(2)
	O(8)	0.3946(7)	0.0523(5)	0.1190(7)	5.0(2)
	C(33)	0.404(1)	0.2261(8)	0.940(1)	6.1(3)
	C(34)	0.3710(9)	0.1908(6)	0.8189(9)	3.4(2)
	C(35)	0.2509(10)	0.2270(7)	0.7313(10)	4.1(2)
	C(36)	0.2149(9)	0.2104(6)	0.6060(9)	3.0(2)
	C(37)	0.1863(9)	0.2878(6)	0.5388(8)	2.5(2)
	C(38)	0.1451(9)	0.2701(7)	0.4106(9)	3.5(2)
	C(39)	0.1165(8)	0.3464(6)	0.3461(8)	2.0(2)
	C(40)	0.1525(10)	0.3434(7)	0.2667(9)	3.5(2)
	C(41)	0.1080(10)	0.4135(7)	0.1892(9)	4.9(2)
	C(42)	0.047(1)	0.4930(7)	0.229(1)	7.3(3)
	C(43)	0.013(1)	0.4931(8)	0.315(1)	7.8(3)
	C(44)	0.0388(9)	0.4198(6)	0.3731(9)	2.9(2)
	C(45)	0.086(1)	0.4335(7)	0.507(1)	4.4(2)
	C(46)	0.1001(8)	0.3563(6)	0.5690(8)	2.6(2)
	C(47)	0.1431(10)	0.3716(7)	0.6970(9)	3.3(2)
	C(48)	0.1696(9)	0.3022(6)	0.7600(9)	3.8(2)
	C(49)	0.1989(10)	0.3017(6)	0.8867(10)	4.0(2)
	C(50)	0.3298(8)	0.3071(6)	0.9626(8)	3.0(2)
	C(51)	0.446(1)	0.1219(7)	0.7889(10)	3.5(2)
	C(52)	0.416(1)	0.0476(7)	0.7370(10)	4.4(2)
	C(53)	0.486(1)	-0.0176(7)	0.7204(10)	4.3(2)
	C(54)	0.6036(9)	-0.0111(7)	0.7380(9)	3.5(2)
	C(55)	0.6317(8)	0.0563(6)	0.7791(8)	2.4(2)
	C(56)	0.5588(9)	0.1217(6)	0.8051(8)	3.1(2)
	C(57)	0.777(1)	-0.0794(8)	0.726(1)	5.8(3)
	C(58)	0.2143(9)	0.2677(7)	0.2225(9)	3.1(2)
	C(59)	0.1639(9)	0.2088(7)	0.1645(9)	3.8(2)
	C(60)	0.2299(10)	0.1355(7)	0.1307(9)	3.6(2)
	C(61)	0.3448(9)	0.1249(6)	0.1572(8)	3.0(2)
	C(62)	0.3978(9)	0.1899(6)	0.2162(9)	2.7(2)
	C(63)	0.3324(9)	0.2593(6)	0.2452(9)	3.0(2)
	C(64)	0.5095(10)	0.0407(6)	0.1355(9)	4.7(2)

	atom	*x*	*y*	*z*	*Beq*
Mol3					
	O(9)	0.8709(7)	0.2956(5)	1.1508(7)	5.4(1)
	O(10)	0.5021(7)	0.4880(5)	0.2441(7)	5.4(2)
	O(11)	1.0485(8)	0.0587(6)	0.8112(8)	5.3(2)
	O(12)	0.9189(7)	0.1839(5)	0.3984(7)	4.9(2)
	C(65)	0.777(1)	0.3371(8)	1.072(1)	5.0(3)
	C(66)	0.7366(9)	0.3031(6)	0.9526(9)	3.3(2)
	C(67)	0.6284(9)	0.3241(6)	0.8699(9)	3.6(2)
	C(68)	0.5838(9)	0.2997(7)	0.7458(10)	3.9(2)
	C(69)	0.5463(8)	0.3798(6)	0.6708(8)	2.3(2)
	C(70)	0.502(1)	0.3528(7)	0.544(1)	4.0(2)
	C(71)	0.4792(8)	0.4244(6)	0.4771(8)	2.5(2)
	C(72)	0.5258(10)	0.4199(7)	0.4022(10)	3.8(2)
	C(73)	0.4829(9)	0.4901(7)	0.3264(9)	4.7(2)
	C(74)	0.3607(10)	0.5538(7)	0.3152(10)	4.8(2)
	C(75)	0.3722(10)	0.5745(7)	0.4335(10)	5.0(2)
	C(76)	0.3956(9)	0.4978(6)	0.4913(8)	3.3(2)
	C(77)	0.4323(9)	0.5153(6)	0.6292(9)	3.7(2)
	C(78)	0.4619(9)	0.4517(6)	0.7002(9)	3.0(2)
	C(79)	0.4985(8)	0.4649(6)	0.8271(8)	2.7(2)
	C(80)	0.5343(9)	0.3904(6)	0.8963(9)	3.3(2)
	C(81)	0.5667(9)	0.4048(6)	1.0240(9)	3.4(2)
	C(82)	0.701(1)	0.4021(7)	1.1008(10)	5.5(3)
	C(83)	0.8203(9)	0.2417(6)	0.9225(9)	3.7(2)
	C(84)	0.858(1)	0.1601(7)	0.9539(10)	4.1(2)
	C(85)	0.935(1)	0.1002(7)	0.9166(10)	4.1(2)
	C(86)	0.979(1)	0.1176(7)	0.856(1)	5.0(2)
	C(87)	0.949(1)	0.2012(7)	0.8212(10)	4.0(2)
	C(88)	0.8612(9)	0.2574(6)	0.8518(9)	3.9(2)
	C(89)	1.086(1)	0.0784(8)	0.735(1)	6.7(3)
	C(90)	0.6279(8)	0.3532(6)	0.4000(8)	2.7(2)
	C(91)	0.6123(10)	0.3136(7)	0.2915(9)	3.4(2)
	C(92)	0.7131(10)	0.2484(6)	0.2944(9)	3.4(2)
	C(93)	0.816(1)	0.2358(7)	0.396(1)	4.4(2)
	C(94)	0.8280(10)	0.2736(7)	0.4928(9)	4.0(2)
	C(95)	0.730(1)	0.3362(7)	0.4977(10)	4.1(2)
	C(96)	0.917(1)	0.1422(9)	0.289(1)	8.6(4)

	atom	*x*	*y*	*z*	*Beq*
Mol4					
	O(13)	0.1039	0.6410	1.1087	4.8(1)
	O(14)	-0.2579(7)	0.8586(5)	0.2153(7)	5.1(2)
	O(15)	-0.1649(7)	1.0071(5)	1.0837(7)	4.9(2)
	O(16)	-0.4256(7)	1.1401(5)	0.5118(7)	4.0(1)
	C(97)	0.1188(9)	0.6356(6)	1.0188(8)	3.1(2)
	C(98)	0.0933(8)	0.7109(6)	0.9649(8)	2.4(2)
	C(99)	0.129(1)	0.7114(7)	0.8823(10)	4.0(2)
	C(100)	0.1045(9)	0.7816(6)	0.8206(9)	3.0(2)
	C(101)	0.0551(9)	0.7693(7)	0.6847(9)	3.3(2)
	C(102)	0.0320(9)	0.8462(6)	0.6294(9)	3.1(2)
	C(103)	-0.0153(8)	0.8264(6)	0.4943(8)	1.9(2)
	C(104)	-0.1133(8)	0.8605(6)	0.4166(8)	2.6(2)
	C(105)	-0.1614(8)	0.8260(5)	0.2943(8)	2.2(1)
	C(106)	-0.075(1)	0.7571(8)	0.268(1)	6.6(3)
	C(107)	0.042(1)	0.7423(7)	0.335(1)	5.8(3)
	C(108)	0.0788(9)	0.7643(6)	0.4697(9)	3.3(2)
	C(109)	0.098(1)	0.6818(7)	0.528(1)	4.6(3)
	C(110)	0.1382(9)	0.6938(6)	0.6614(9)	3.6(2)
	C(111)	0.1607(9)	0.6230(7)	0.7172(9)	3.0(2)
	C(112)	0.201(1)	0.6315(7)	0.8453(10)	4.0(2)
	C(113)	0.1996(7)	0.5554(5)	0.8906(7)	2.4(1)
	C(114)	0.2305(8)	0.5692(5)	1.0220(7)	3.2(1)
	C(115)	0.0195(9)	0.7873(6)	0.9957(9)	3.0(2)
	C(116)	0.0737(9)	0.8523(7)	1.0575(9)	3.4(2)
	C(117)	0.014(1)	0.9220(7)	1.0884(10)	4.2(2)
	C(118)	-0.103(1)	0.9285(7)	1.060(1)	4.1(2)
	C(119)	-0.156(1)	0.8721(7)	1.009(1)	4.6(2)
	C(120)	-0.091(1)	0.7976(7)	0.9731(10)	3.9(2)
	C(121)	-0.282(1)	1.0150(7)	1.0664(10)	5.5(3)
	C(122)	-0.2036(9)	0.9342(6)	0.4370(9)	2.5(2)
	C(123)	-0.1722(10)	1.0060(7)	0.4754(9)	3.9(2)
	C(124)	-0.250(1)	1.0742(7)	0.5117(10)	4.6(2)
	C(125)	-0.3509(9)	1.0711(6)	0.4887(9)	3.4(2)
	C(126)	-0.388(1)	0.9971(8)	0.436(1)	5.3(3)
	C(127)	-0.3117(10)	0.9312(7)	0.4108(9)	3.5(2)
	C(128)	-0.5393(10)	1.1366(7)	0.4970(9)	3.8(2)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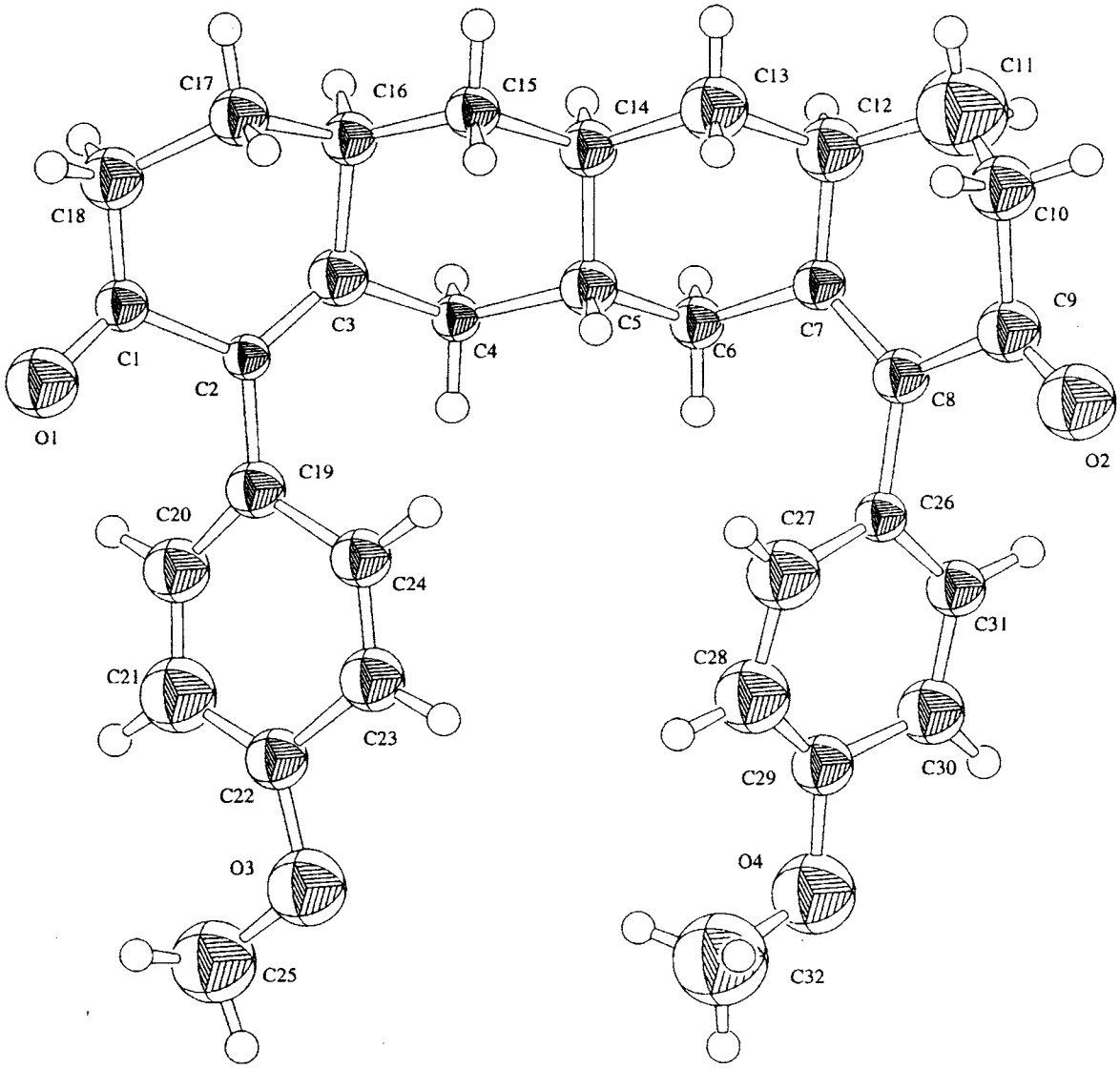
Mol-1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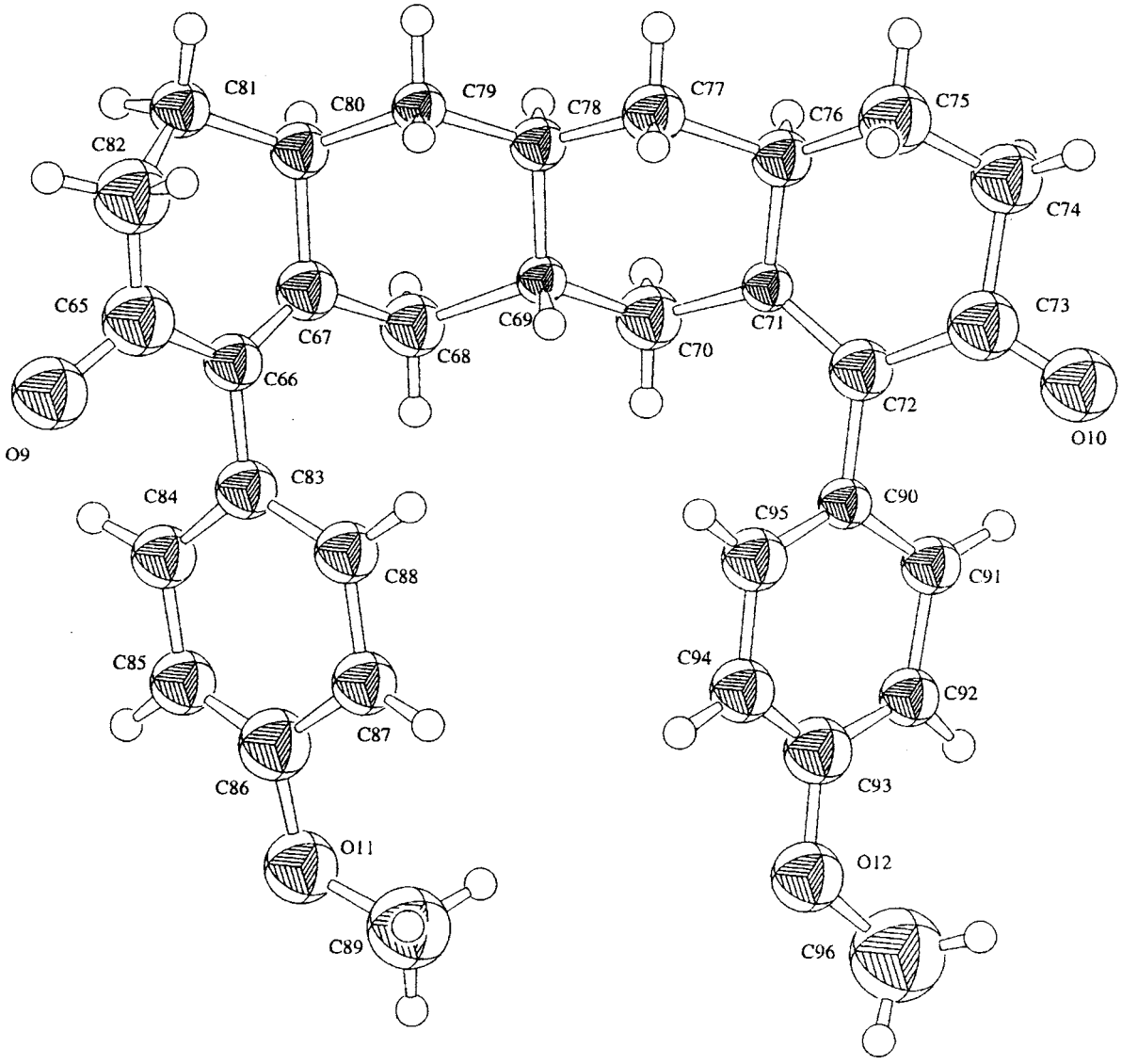
C32

Mol-2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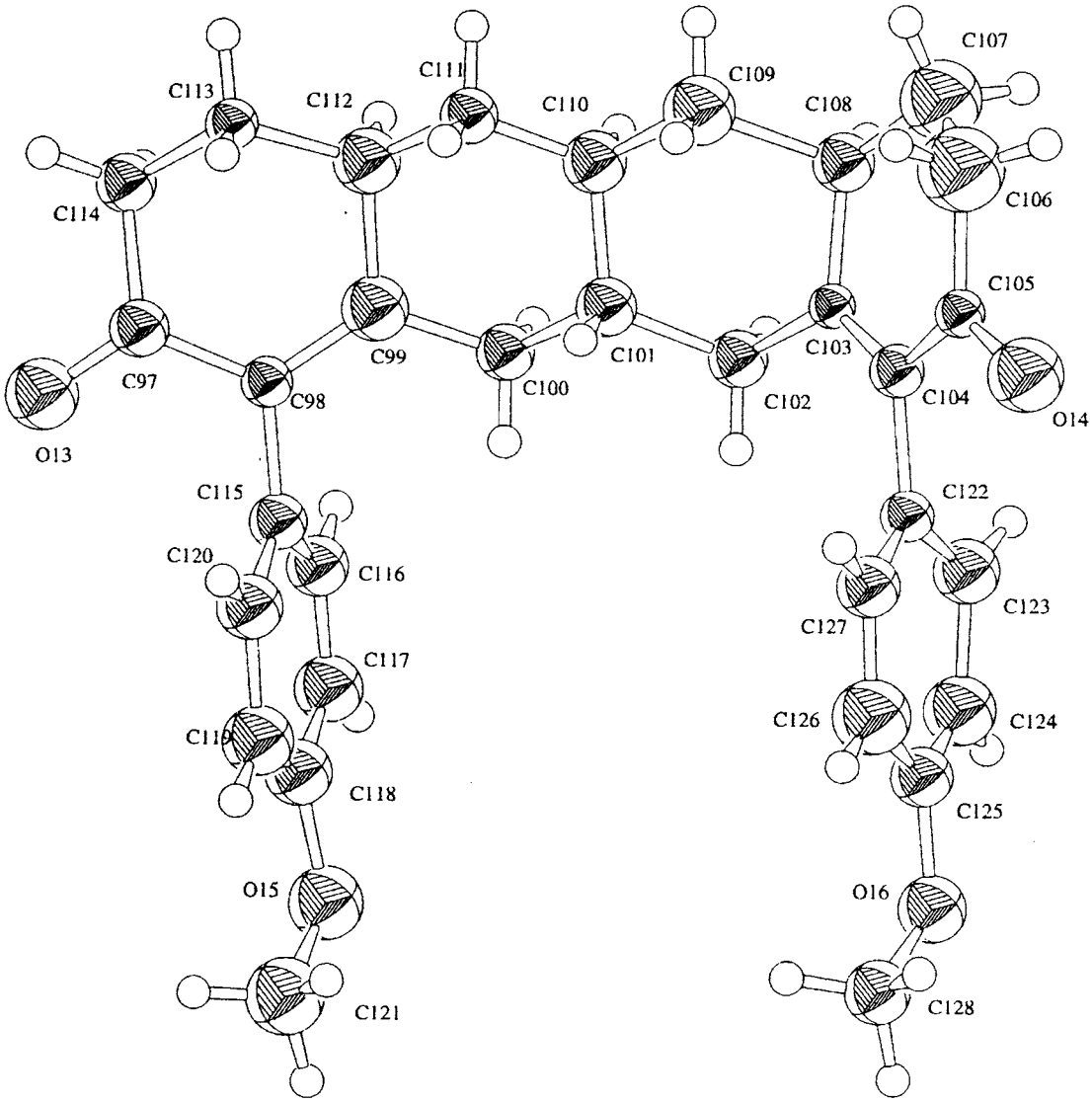
C96

Mol-3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Mol-4