Electronic Supplementary Information (ESI)

Tautomerism and stereodynamics in Schiff bases from gossypol and hemigossypol with *N*-aminoheterocycles

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Experimental Section

General. Gossypol was supplied by the Russian Academy of Sciences (Moscow). Melting points were determined on Gallenkamp and Electrothermal IA 9000 apparatuses and are uncorrected. IR spectra were recorded in the range of 4000-600 cm^{1} on an FT-IR THERMO spectrophotometer. Solid samples were recorded on KBr (Merck) pellets. Dispersive Raman spectra were recorded in the range of 4000-400 cm^{-1} on a Nicolet Almega XR THERMO spectrophotometer equipped with a 780 nm laser (with fluorescence correction). NMR spectra were recorded on Bruker 400 and 500 AC/PC instruments, in different solvent systems. Assignments were facilitated by one- and two-dimensional COSY and HMQC spectra, isotopic exchange after addition of D_2O, and DEPT (distortionless enhancement by polarization transfer) experiments. TMS was used as the internal standard (δ = 0.00 ppm) and all *J* values are given in hertz. Microanalyses were determined on a Leco® CHNS-932 analyser. HR-MS and ESI spectra were performed in a 6520 Accurate-Mass Q-TOF LC/MS from Agilent Technologies in positive mode.

Calculations. The computational DFT study has been performed using the M06-2X[1] hybrid density functional in conjunction with the 6-311G(d,p) basis set[2] as implemented in the Gaussian09 package.[3] The M06-2X method was chosen on the basis of previous studies showing its accuracy in estimating conformational energies related to non-covalent interactions.[4] In all cases, frequency calculations were also carried out to confirm the existence of true stationary points on the potential energy surface. All thermal corrections were calculated at the standard values of 1 atm at 298.15 K. Solvent effects were modeled through the method of density-based, self-consistent reaction field (SCRF) theory of bulk electrostatics, namely, the solvation model density (SMD) method[5] as implemented in the Gaussian09 suite of programs. This solvation method accounts for long-range electrostatic polarization (bulk solvent)[6] as well as for short-range effects associated with cavitation, dispersion, and solvent structural effects.[7]

Natural Bond Orbital (NBO) Approach. Intramolecular interaction of the stabilization energies were performed by using second order perturbation theory. For each donor NBO(*i*) and acceptor NBO(*j*), the stabilization energy E_2 associated with electron delocalization between donor and acceptor is estimated as:

$$E_2 = \Delta E_{ij} = - q_i (F_{ij})^2 / (\varepsilon_i - \varepsilon_j)$$

where q_i is the donor orbital occupancy, ε_i, ε_j are diagonal elements (orbital energies), and F_{ij} is the off-diagonal NBO Fock matrix element.[8]

In the natural bond orbital (NBO) approach, a hydrogen bond is viewed as an interaction between an occupied nonbonded natural orbital n_A of the acceptor atom A and the unoccupied antibonding orbital of the DH bond σ_{DH}^*.

Pseudo-aromaticity and Molecular Geometry Index. Geometrical parameters of the rings and quasi-rings (C-C, C-N, and C-O bond lengths) were used to calculate the aromaticity index HOMA (harmonic oscillator model of aromaticity)[9] as a geometry-based indicator of local aromaticity. According to its definition, HOMA can be expressed by the following equation:

$$HOMA = 1 - \frac{1}{n}\sum_{j=1}^{n} \alpha_i \, (R_{\mathrm{opt},i} - R_j)^2$$

$$HOMA = 1 - \frac{1}{n}\sum_{j=1}^{n} \alpha \, (R_{opt} - R_i)^2$$

Where R_{opt} and α_i are obtained as follows:

$$R_{opt} = (R_s + 2R_d)/3$$

$$\alpha = 2/[(R_{opt} - R_s)^2 + (R_{opt} - R_d)^2]$$

where n represents the total number of bonds taken into the summation and α_i is a normalization constant fixed to give HOMA = 0 for a model nonaromatic system, e.g., the Kekulé structure of benzene and HOMA = 1 for the system with all bonds equal to the optimal value $R_{opt,i}$, assumed to be realized for fully aromatic systems. The higher the HOMA value, the more "aromatic" is the ring in question and hence the more delocalized are the π-electrons of the system. HOMA may be estimated for the set of bonds forming the ring but also for any part of that ring or other sequence of bonds for which delocalization can be considered. In the case of quasi-rings the HOMA was estimated for the sequence of (H)O-C=C-C=C-N bonds.

Constants R_s and R_d denote specific bonds and can be obtained from model compounds; herein ethane and ethene (for C-C and C=C bonds), methylamine and methylenimine (for C-N and C=N bonds), and formic acid (for C-O and C=O bonds). Table S1 shows the R_{opt} and α values used for the calculation of the HOMA index.

Table S1. R_{opt} and α parameters used for the calculation of HOMA indices.

	Gas phase			$CHCl_3$			DMSO		
Parameter	-C	-N	-O	-C	-N	-O	-C	-N	-O
R_{opt}	1.392	1.329	1.241	1.392	1.331	1.242	1.392	1.332	1.243
α	87.55	89.68	168.68	89.55	89.48	194.84	90.30	89.35	194.95

General Synthetic Procedures. To a solution of gossypol (0.10 g, 0.193 mmol) in diethyl ether/isopropanol 5:3 (2.5 mL:1.5 ml) was added the corresponding amino derivative (0.386 mmol). The reaction mixture was warmed at 50 °C for 5 min and then left at room temperature. The resulting solid was collected by filtration, washed with diethyl ether and recrystallized from ethanol or methanol.

5,5'-Diisopropyl-1,1',6,6',7,7'-hexahydroxyl-3,3'-dimethyl-8,8´-di(*N*-piperidylazomethino)-2,2'-binaphthalene (**13**). 88 %; mp 225-227 ºC (lit.[10] mp. 230-232 ºC); ^{1}H NMR (400 MHz, DMSO-d_6) δ 14.52 (s, 2H, 2 x OH), 9.65 (s, 2H, 2 x CH=N), 8.55 (s, 2H, 2 x OH), 7.92 (s, 2H, 2 x OH), 7.56 (s, 2H, 2 x H-arom), 3.86 (m, 2H, 2 x H-^{i}Pr), 3.02 (t, J = 5.2 Hz, 8H, 4 x CH_2), 1.95 (s, 6H, 2 x CH_3-arom), 1.67 (m, 8H, 4 x CH_2), 1.46 (t, J = 6.4 Hz, 16H, 2 x CH_2, 4 x CH_3-^{i}Pr); ^{13}C NMR (100 MHz, DMSO-d_6) δ 151.3 (C-OH), 151.1 (C-arom), 147.5 (C=N), 144.5, 132.5, 129.0, 126.3, 118.8, 116.3, 108.2 (C-arom), 53.3 (2C, CH_2), 27.0 (CH-^{i}Pr), 24.9 (2C, CH_2), 23.8 ($ArCH_3$), 21.1, 21.0 (CH_3-^{i}Pr); IR (KBr) $\bar{\nu}_{max}$/cm^{-1} 3484, 3395 (OH), 2937, 1607 (C=N), 1428, 1332, 1302, 1243, 1165, 858; IR ($CHCl_3$) $\bar{\nu}_{max}$/cm^{-1} 3685, 3628, 3497, 3338 (OH), 3026, 3013, 2946, 2864, 2819, 2398, 1607 (C=N), 1524, 1499, 1429, 1328, 1227, 1205; Raman $\bar{\nu}_{max}$/cm^{-1} 2933, 1619, 1545, 1433, 1329, 1258, 1160, 1085, 858, 372; LC-MS-TOF in HPLC-acetonitrile solution, *m*/*z* (%) calculated for $C_{40}H_{50}N_4O_6$: 683.3764 (100); found: 683.3770 (100).

2,2'-bis{1,6-Dihydroxy-5-isopropyl-3-methyl-8-[(2,6-dimethyl-*N*-piperidinamino)methylidene]naphthalen-7-one} (17). 63%; mp 156-159 ºC; ^{1}H NMR (500 MHz, DMSO-d_6) δ13.59 (d, J = 9.0 Hz, 2H, 2 x NH), 9.83 (d, J = 9.0 Hz, 2H, 2 x CHN), 8.43 (s, 2H, 2 x OH), 7.94 (s, 2H, 2 x OH), 7.45 (s, 2H, 2 x H-arom), 3.73 (m, J = 7.0 Hz, 2H, 2 x H-^{i}Pr), 2.78 (sa, 4H, 4 x CH), 1.93 (s, 6H, 2 x CH_3-arom), 1.72-1.63 (m, 6H, 3 x CH_2), 1.44 (t, J = 7.0 Hz, 12H, 4 x CH_3-^{i}Pr), 1.40-1.24 (m, 6H, 3 x CH_2), 0.97 (t, J = 6.5 Hz, 12H, 4 x CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ 170.3 (C=O), 163.1 (C=NH), 149.8, 145.9, 131.4, 127.3, 127.1, 119.8, 166.4, 115.6, 101.5 (C-arom), 60.0, 59.9 (CH), 32.4, 32.4 (CH_2), 26.4 (CH-^{i}Pr), 23.1 (CH_2), 20.4, 20.4, 20.2 (CH_3); IR (KBr) $\bar{\nu}_{max}$/cm^{-1} 3493, 3283 (OH), 3109, 2965, 2932, 2871, 1604 (C=N), 1534, 1490, 1333, 1307, 1242, 1174, 1097, 763; IR ($CHCl_3$) $\bar{\nu}_{max}$/cm^{-1} 3684, 3621, 3497, 3324 (OH), 3109, 3025, 3014, 2973, 2938, 2874, 2400, 1607 (C=N), 1517, 1493, 1452, 1336, 1318, 1228, 1205; Raman $\bar{\nu}_{max}$/cm^{-1} 1617, 1524, 1426, 1332, 422, 378; HPLC-acetonitrile solution, *m*/*z* (%) calculated for $C_{44}H_{58}N_4O_6$: 739.4390 (100); found: 739.4406 (100). Elemental analysis

calcd (%) for $C_{44}H_{58}N_4O_6$: C 71.52; H 7.91; N 7.58; found: C 71.72; H 7.71; N 7.40. LC-MS-TOF in HPLC-acetonitrile solution, *m*/*z* (%) calculated for $C_{44}H_{58}N_4O_6$: 739.4390 (100); found: 739.4406 (100).

2,2'-bis{1,6-Dihydroxy-5-isopropyl-3-methyl-8-[(2-hydroxymethyl-1,3-dihydroxy-2-propylamino)methylidene]naphthalen-7-one} (18). 23%; mp 288-290 ºC (described[11] m.p. 295-297 ºC); ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.38 (d, *J* = 14.0 Hz, 2H, 2 x NH), 10.02 (d, *J* = 14.0 Hz, 2H, 2 x CHN), 8.43 (s, 2H, 2 x OH), 7.40 (s, 2H, 2 x H-arom), 4.99 (s, 6H, 6 x OH), 3.69 (m, *J* = 7.0 Hz, 2H, 2 x H-^{i}Pr), 3.60 (s, 12H, 6 x CH_2), 1.95 (s, 6H, 2 x CH_3-arom), 1.43 (d, *J* = 7.0 Hz, 6H, 2 x CH_3-^{i}Pr), 1.42 (d, *J* = 6.5 Hz, 6H, 2 x CH_3-^{i}Pr); ^{13}C NMR (125 MHz, DMSO-d_6) δ 171.14 (C=O), 160.54 (CH=N), 146.35, 130.63 126.66, 125.61, 116.30, 103.25 (C-arom), 63.85, 60.85, 26.38 (CH-^{i}Pr), 25.37 (CH_2), 20.26, 20.11 (CH_3); IR (KBr) $\tilde{\nu}_{max}$/cm^{-1} 3500-3200 (OH), 2957, 2925, 2868, 1611 (C=N), 1507, 1490, 1360, 1310, 1239, 1171, 1049, 839, 771; Raman $\tilde{\nu}_{max}$/cm^{-1} 1628, 1496, 1427, 1376, 1327, 1138, 532, 380; LC-MS-TOF in HPLC-acetonitrile solution, *m*/*z* (%) calculated for $C_{38}H_{48}N_2O_{12}$: 725.3241 (100); found: 725.3257 (100).

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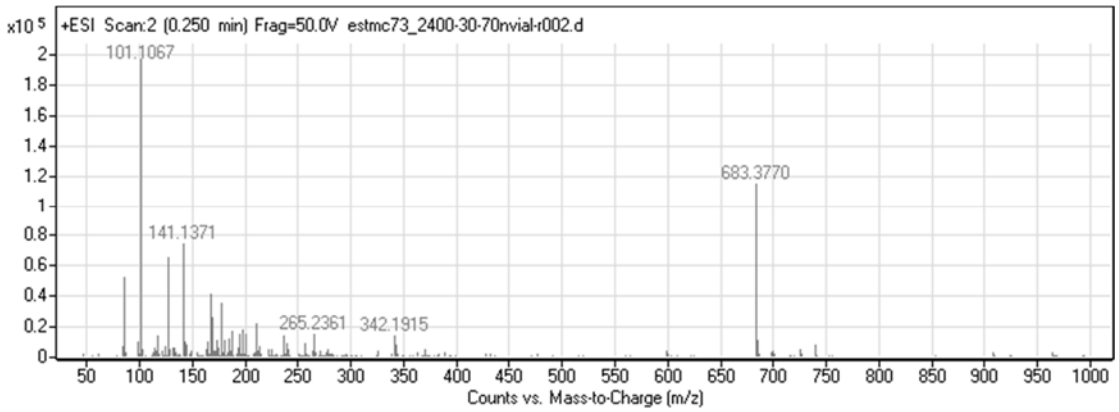


Figure S1 Mass spectrum of 5,5'-diisopropyl-1,1',6,6',7,7'-hexahydroxyl-3,3'-dimethyl-8,8´-di(*N*-piperidylazomethino)-2,2'-binaphthalene (**13**).

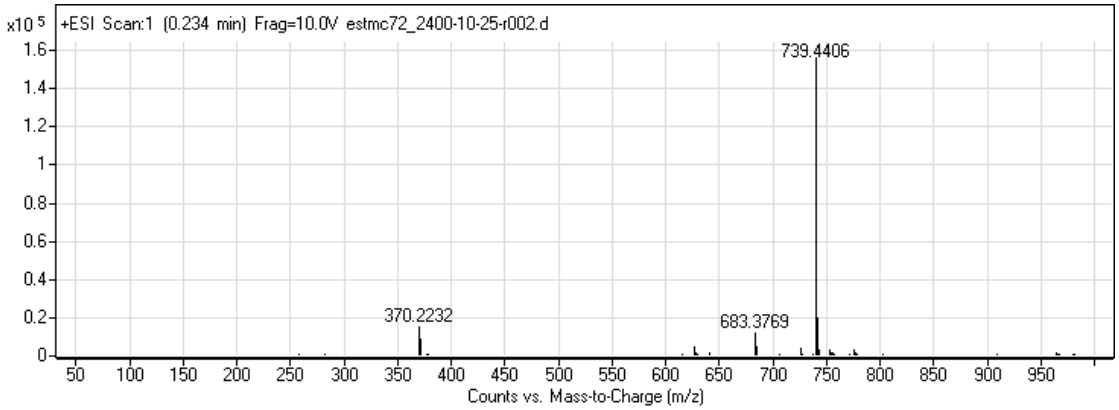


Figure S2 Mass spectrum of 2,2'-bis{1,6-dihydroxy-5-isopropyl-3-methyl-8-[(2,6-dimethyl-*N*-piperidinamino) methylidene]naphthalen-7-one} (**17**).

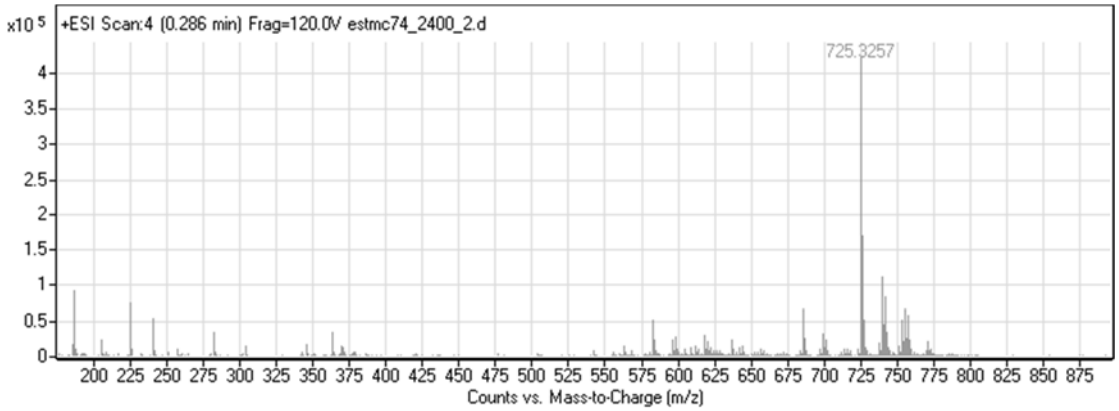
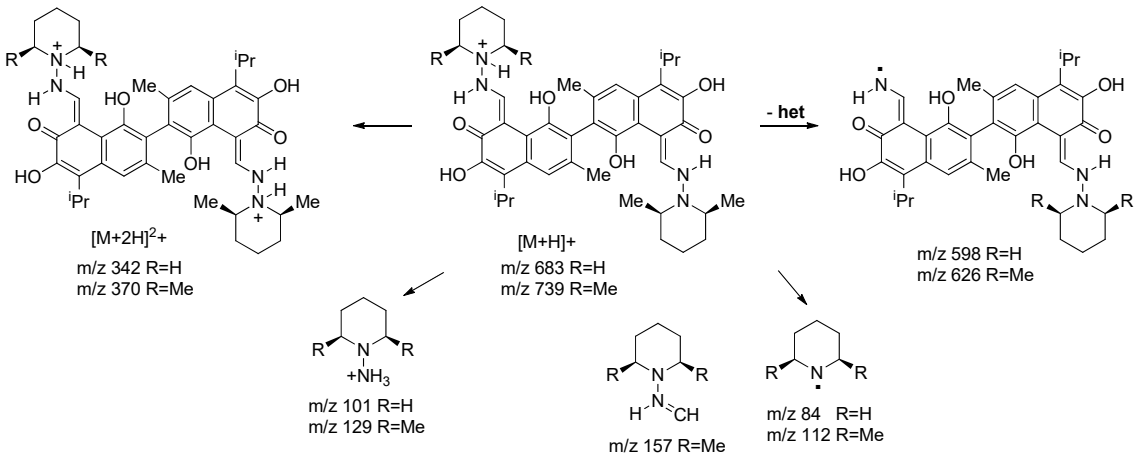


Figure S3 Mass spectrum of 2,2'-bis{1,6-Dihydroxy-5-isopropyl-3-methyl-8-[(2-hydroxymethyl-1,3-dihydroxy-2-propylamino)methylidene]naphthalen-7-one} (**18**).

Electrospray ionization mass spectrometry (ESI-MS).

High-resolution mass spectrometry (HRMS) was performed using electrospray ionization (ESI) and time-of-flight (TOF) mass analysis. Neutral compounds can be converted to their ionic form in solution by either protonation or cationisation. The ESI mass spectra of **16** and **17** show signals corresponding to both monoprotonated $[M + H]^+$ and diprotonated $[M + 2H]^{2+}$ molecular ions. In the spectrum of **17** the molecular peak is not observed, although a very weak signal at m/z 626 ($[M-112]^+$) emerges, which corresponds to the loss of 2,6-dimethylpiperidyl (**het**, $C_7H_{14}N$, m/z = 112) by breaking an N-N bond. In addition, the region of low masses shows the presence of heterocyclic fragments at m/z 157 and 129 (Scheme S1).



Scheme S1.

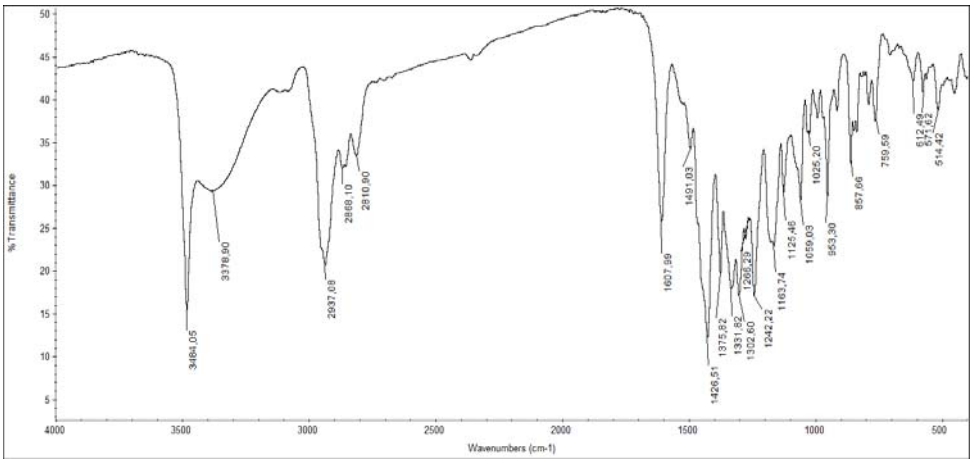


Figure S4 IR spectrum of 5,5'-diisopropyl-1,1',6,6',7,7'-hexahydroxyl-3,3'-dimethyl-8,8´-di(*N*-piperidylazomethino)-2,2'-binaphthalene (**13**).

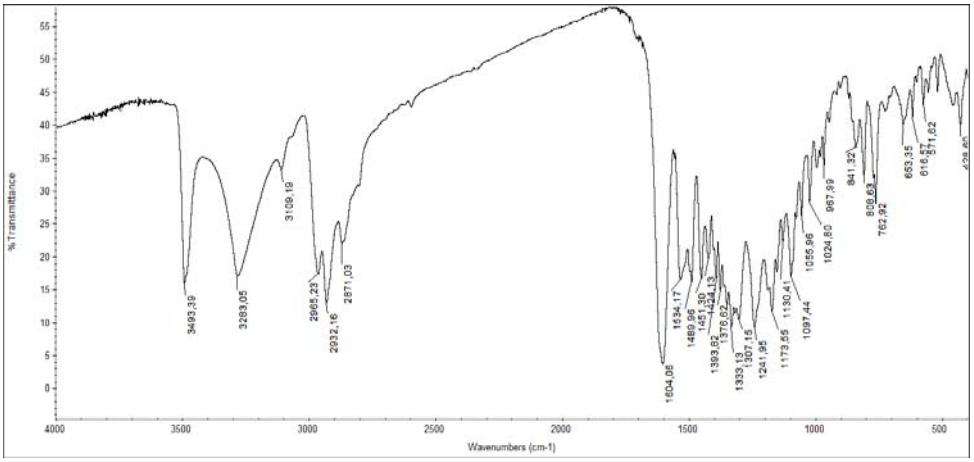


Figure S5 IR spectrum of 2,2'-bis{1,6-dihydroxy-5-isopropyl-3-methyl-8-[(2,6-dimethyl-*N*-piperidinamino) methylidene]naphthalen-7-one} (**17**).

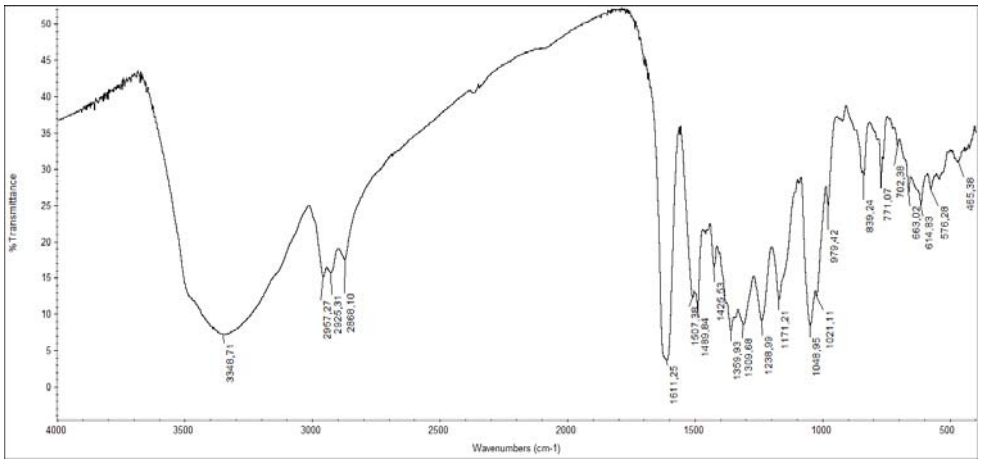


Figure S6 IR spectrum of 2,2'-bis{1,6-Dihydroxy-5-isopropyl-3-methyl-8-[(2-hydroxymethyl-1,3-dihydroxy-2-propylamino)methylidene]naphthalen-7-one} (**18**).

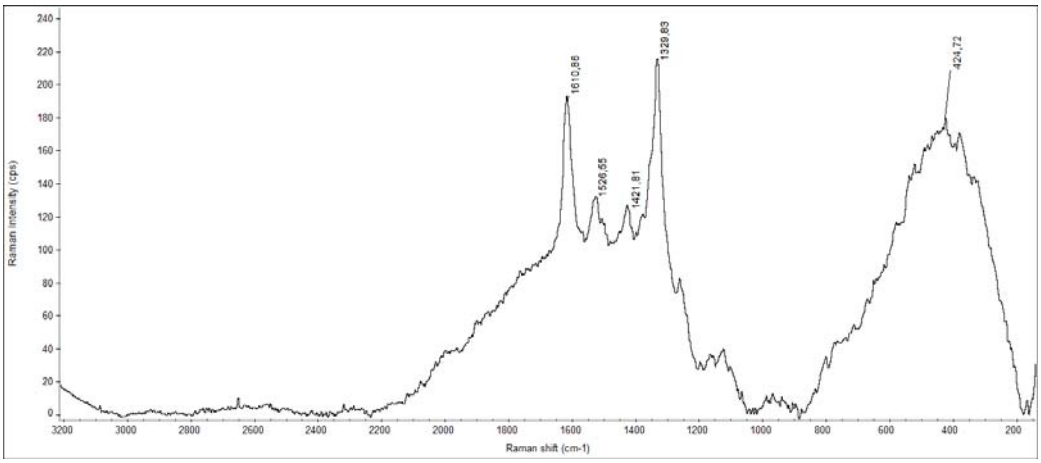


Figure S7 Raman spectrum of 5,5'-diisopropyl-1,1',6,6',7,7'-hexahydroxyl-3,3'-dimethyl-8,8´-di(*N*-piperidylazomethino)-2,2'-binaphthalene (**13**).

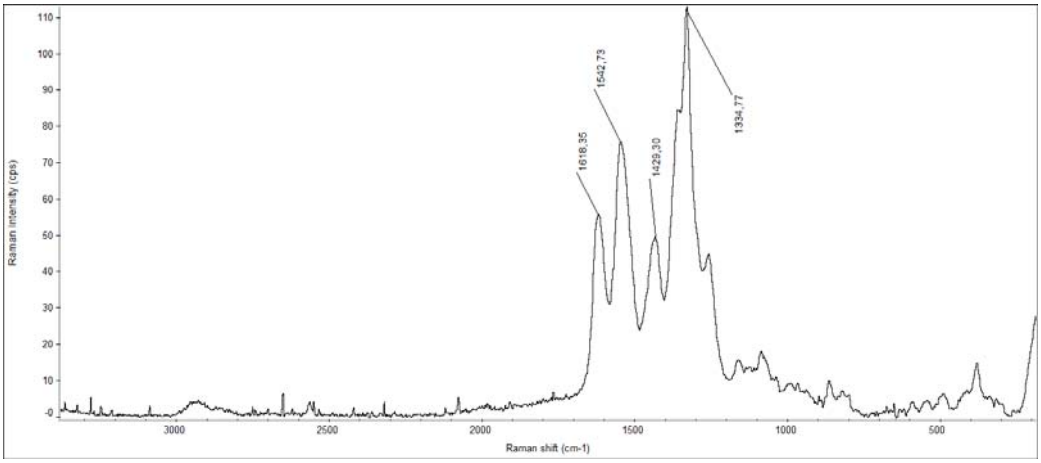


Figure S8 Raman spectrum of 2,2'-bis{1,6-dihydroxy-5-isopropyl-3-methyl-8-[(2,6-dimethyl-*N*-piperidinamino) methylidene]naphthalen-7-one} (**17**).

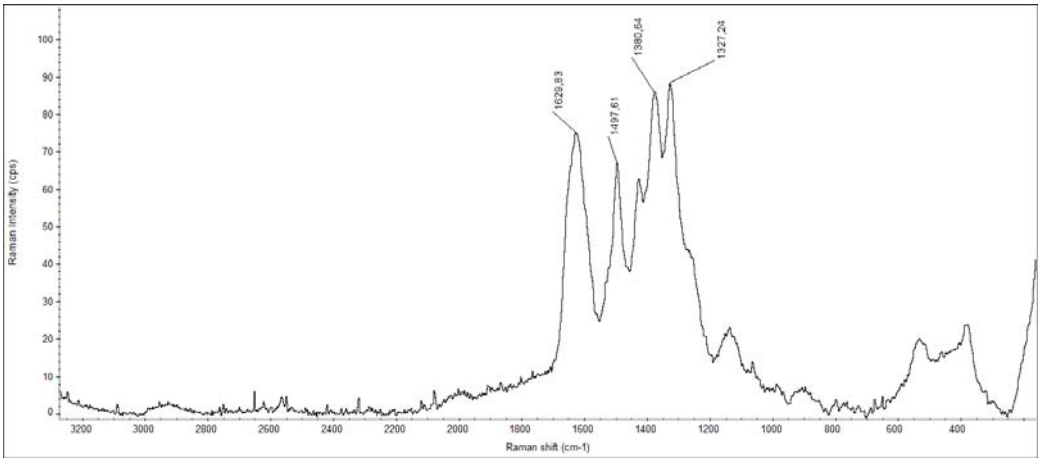


Figure S9 Raman spectrum of 2,2'-bis{1,6-Dihydroxy-5-isopropyl-3-methyl-8-[(2-hydroxymethyl-1,3-dihydroxy-2-propylamino)methylidene]naphthalen-7-one} (**18**).

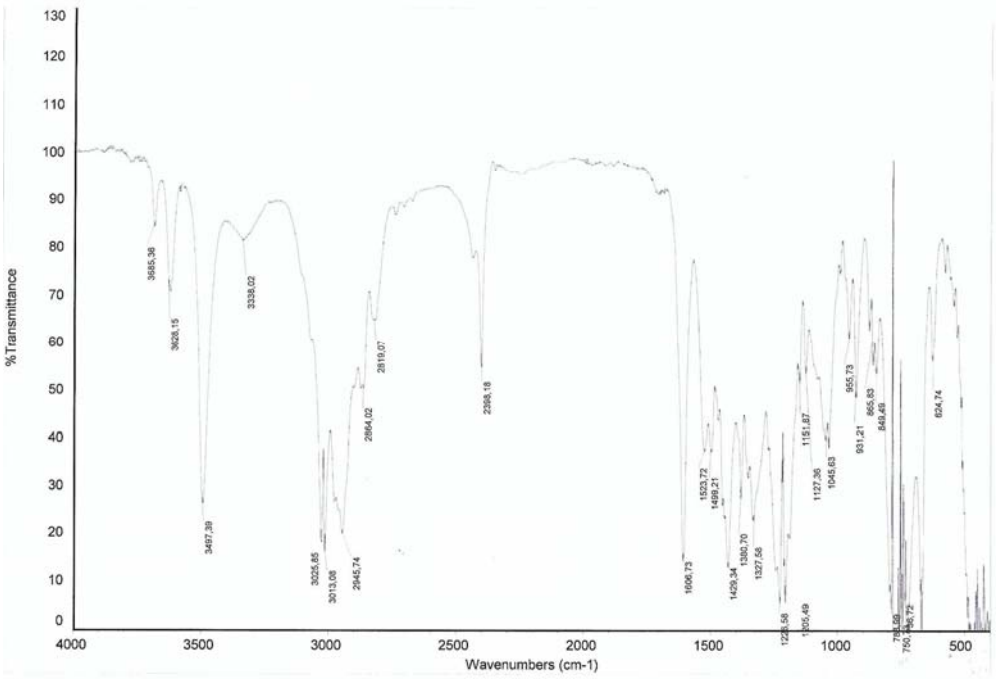


Figure S10 IR spectrum of 5,5'-diisopropyl-1,1',6,6',7,7'-hexahydroxyl-3,3'-dimethyl-8,8´-di(*N*-piperidylazomethino)-2,2'-binaphthalene (**13**), recorded in $CHCl_3$.

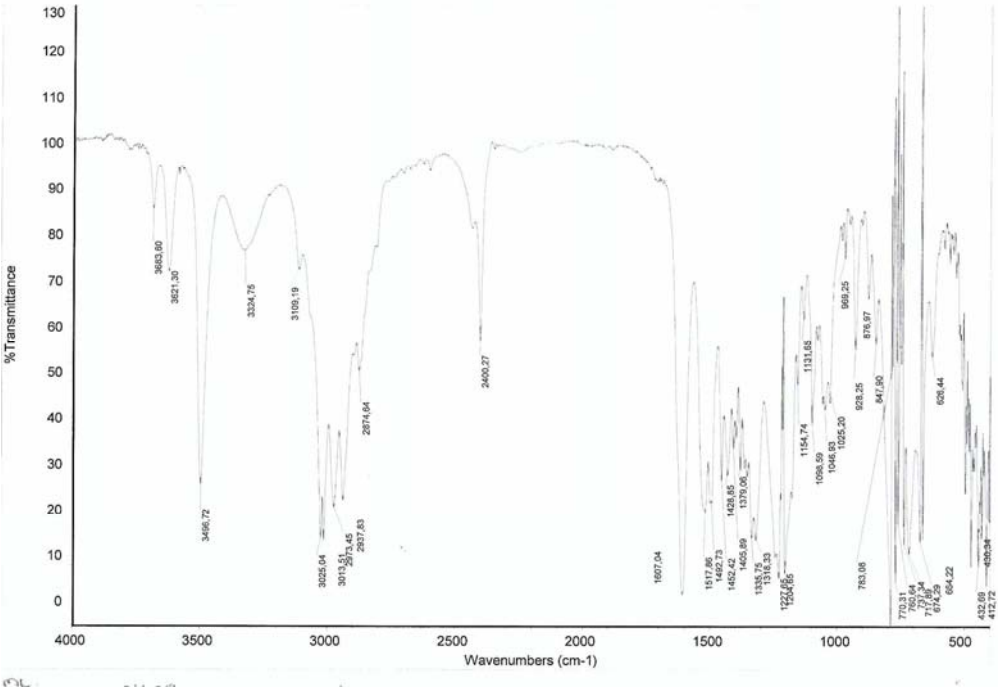


Figure S11 IR spectrum of 2,2'-bis{1,6-dihydroxy-5-isopropyl-3-methyl-8-[(2,6-dimethyl-*N*-piperidinamino) methylidene]naphthalen-7-one} (**17**), recorded in $CHCl_3$.

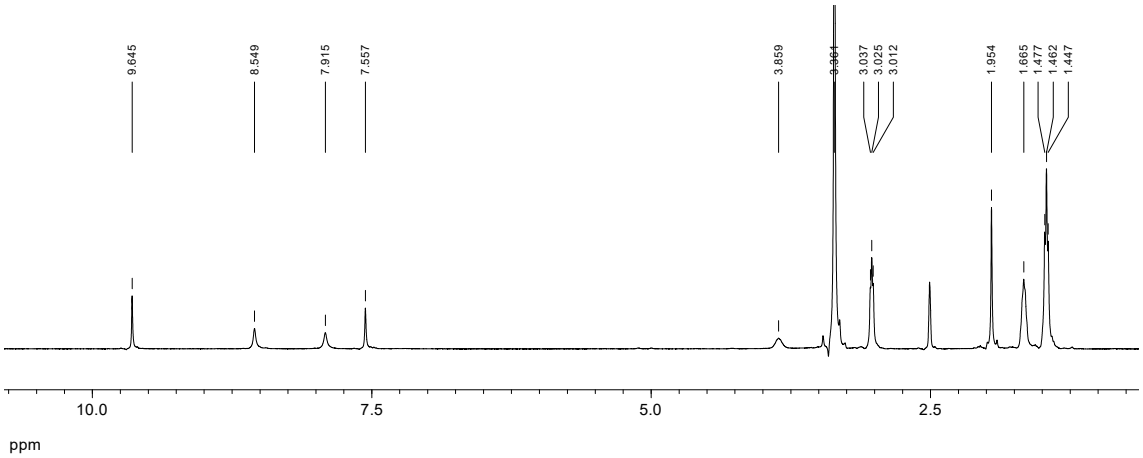


Figure S12 ^{1}H NMR spectrum of 5,5'-diisopropyl-1,1',6,6',7,7'-hexahydroxyl-3,3'-dimethyl-8,8´-di(*N*-piperidylazomethino)-2,2'-binaphthalene (**13**), recorded in DMSO-d_6.

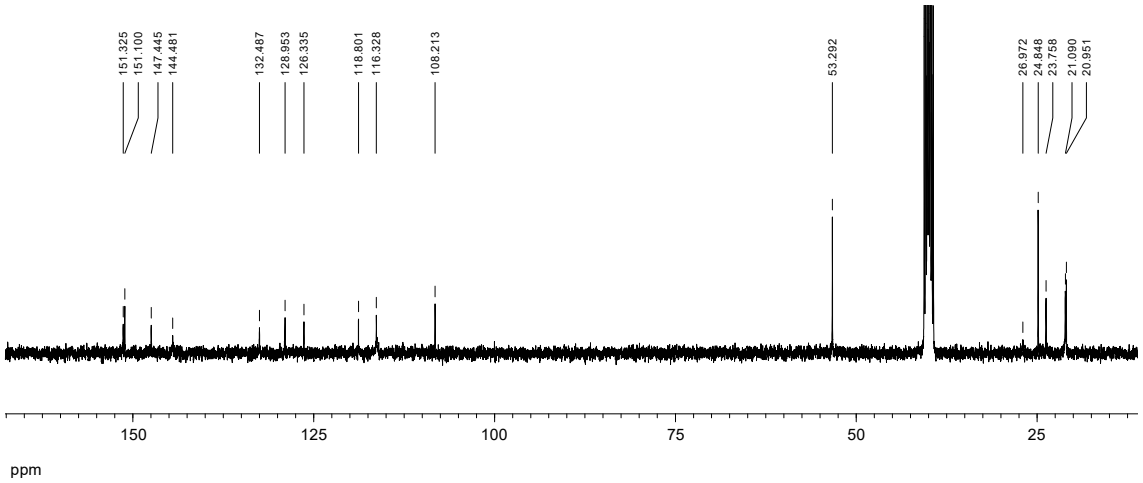


Figure S13 ^{13}C NMR spectrum of 5,5'-diisopropyl-1,1',6,6',7,7'-hexahydroxyl-3,3'-dimethyl-8,8´-di(*N*-piperidylazomethino)-2,2'-binaphthalene (**13**), recorded in DMSO-d_6.

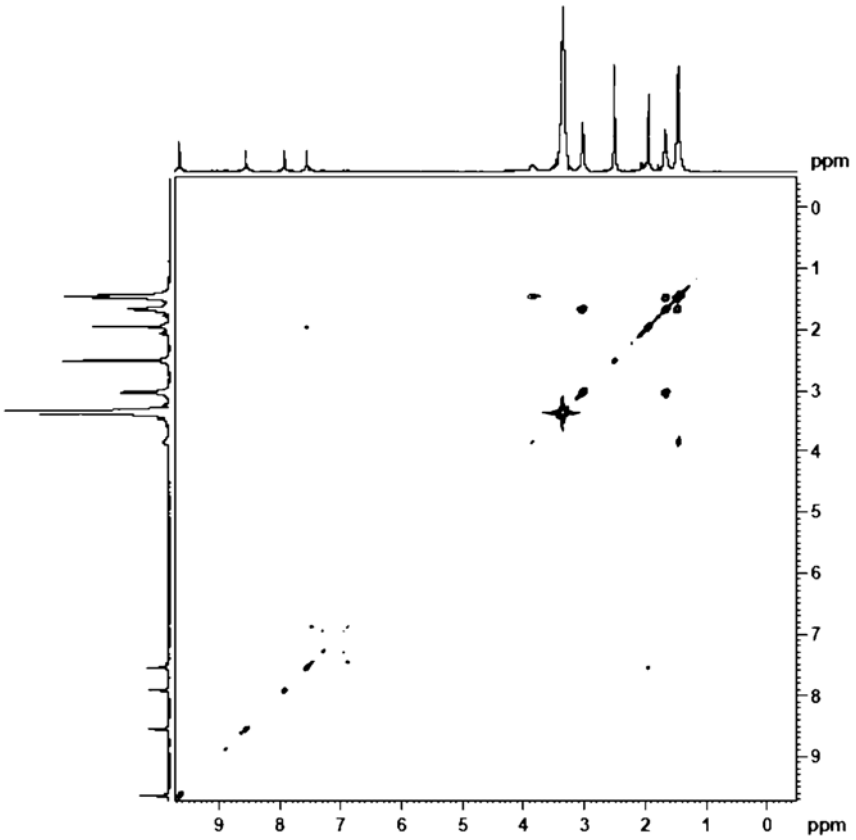


Figure S14 ^{1}H-^{1}H COSY spectrum of 5,5'-diisopropyl-1,1',6,6',7,7'-hexahydroxyl-3,3'-dimethyl-8,8´-di(*N*-piperidylazomethino)-2,2'-binaphthalene (**13**), recorded in DMSO-d_6.

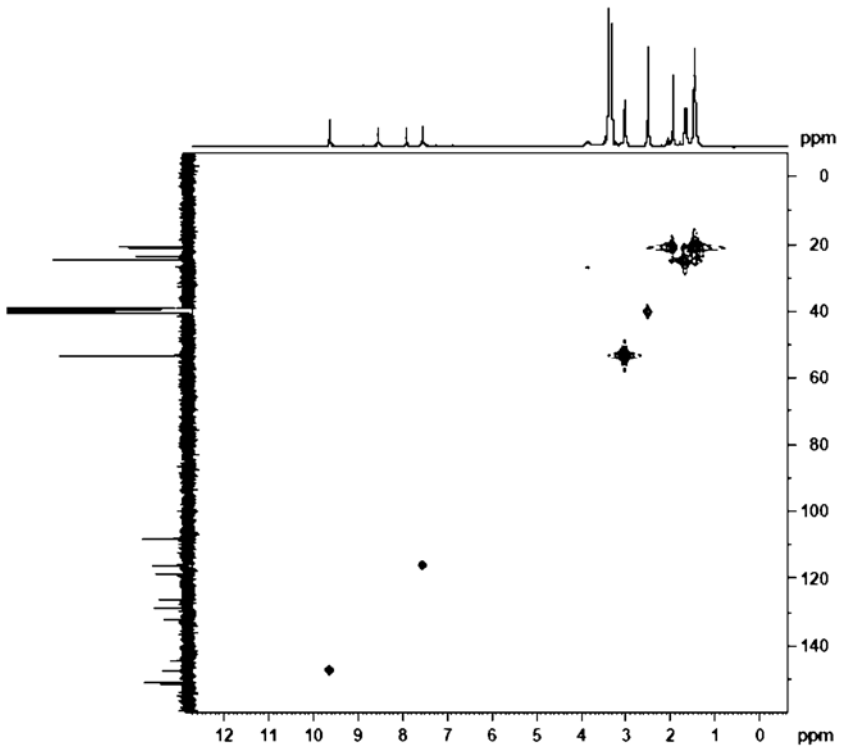


Figure S15 HMQC spectrum of 5,5'-diisopropyl-1,1',6,6',7,7'-hexahydroxyl-3,3'-dimethyl-8,8´-di(*N*-piperidylazomethino)-2,2'-binaphthalene (**13**), recorded in DMSO-d_6.

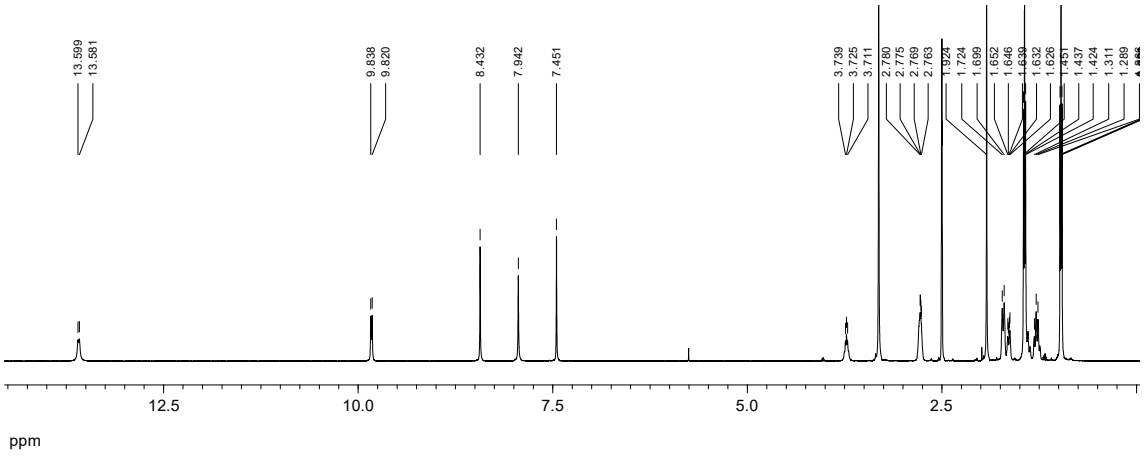


Figure S16 ^{1}H NMR spectrum of 2,2'-bis{1,6-dihydroxy-5-isopropyl-3-methyl-8-[(2,6-dimethyl-*N*-piperidinamino) methylidene]naphthalen-7-one} (**17**), recorded in DMSO-d_6.

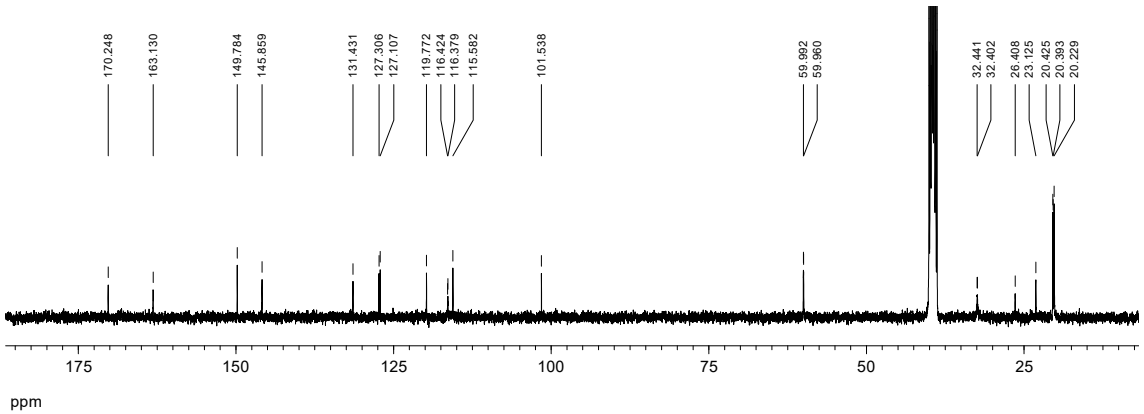


Figure S17 ^{13}C NMR spectrum of 2,2'-bis{1,6-dihydroxy-5-isopropyl-3-methyl-8-[(2,6-dimethyl-*N*-piperidinamino) methylidene]naphthalen-7-one} (**17**), recorded in DMSO-d_6.

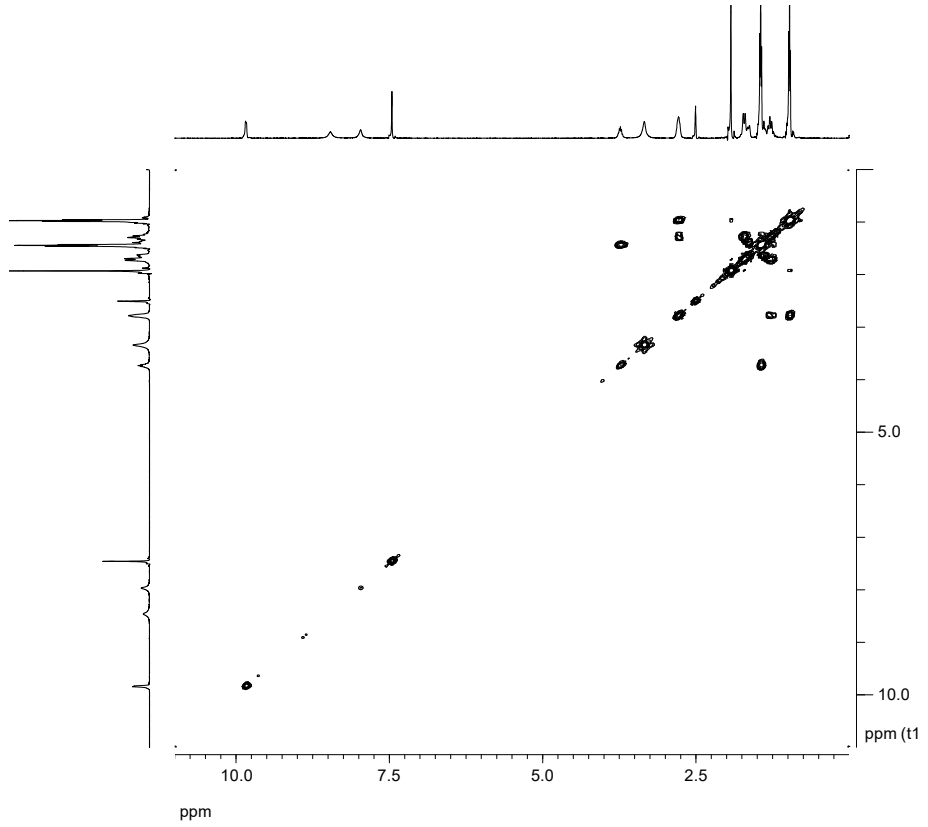


Figure S18 ^{1}H-^{1}H COSY spectrum of 2,2'-bis{1,6-dihydroxy-5-isopropyl-3-methyl-8-[(2,6-dimethyl-*N*-piperidinamino) methylidene]naphthalen-7-one} (**17**), recorded in DMSO-d_6.

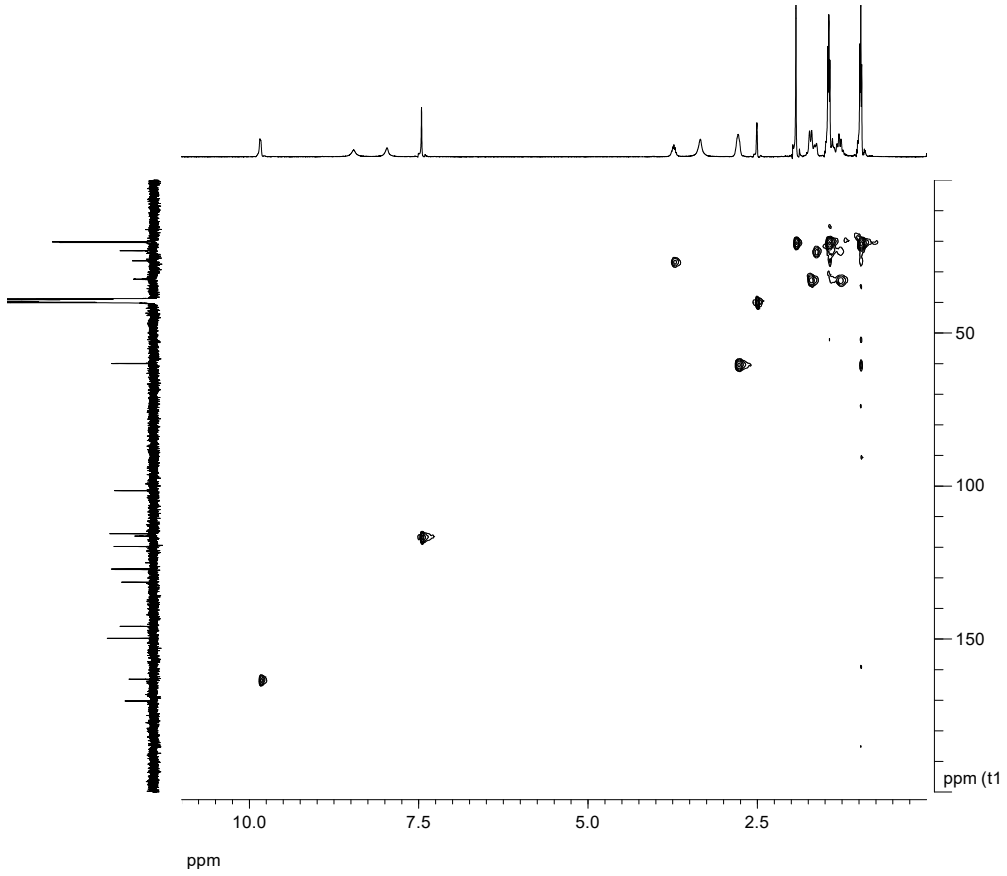


Figure S19 HMQC spectrum of 2,2'-bis{1,6-dihydroxy-5-isopropyl-3-methyl-8-[(2,6-dimethyl-*N*-piperidinamino) methylidene]naphthalen-7-one} (**17**), recorded in DMSO-d_6.

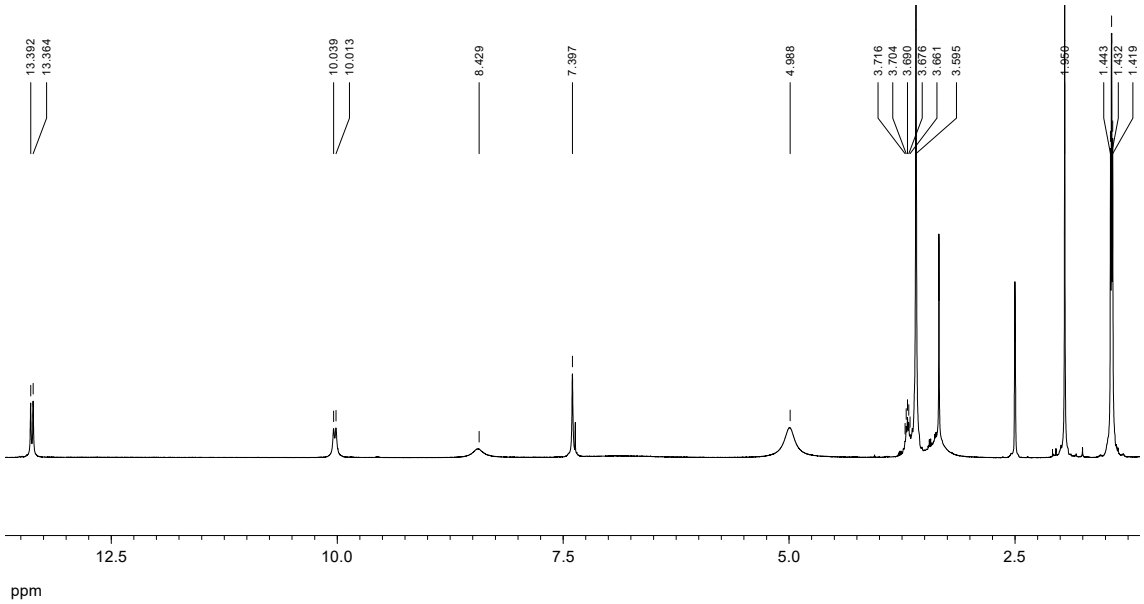


Figure S20 ^{1}H NMR spectrum of 2,2'-bis{1,6-Dihydroxy-5-isopropyl-3-methyl-8-[(2-hydroxymethyl-1,3-dihydroxy-2-propylamino)methylidene]naphthalen-7-one} (**18**), recorded in DMSO-d_6.

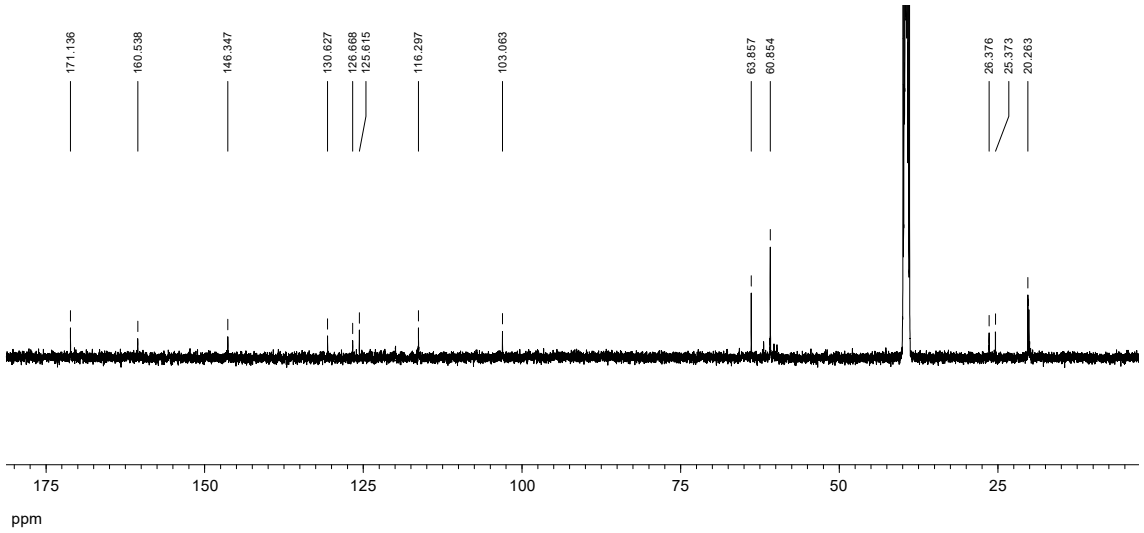


Figure S21 ^{13}C NMR spectrum of 2,2'-bis{1,6-dihydroxy-5-isopropyl-3-methyl-8-[(2-hydroxymethyl-1,3-dihydroxy-2-propylamino)methylidene]naphthalen-7-one}(**18**), recorded in DMSO-d_6.

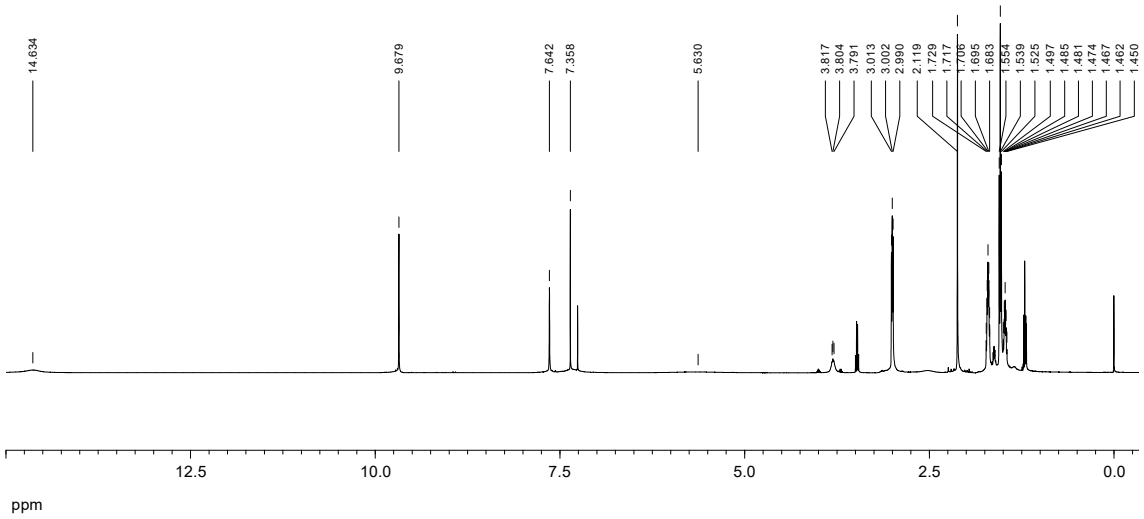


Figure S22 ^{1}H NMR spectrum of 5,5'-diisopropyl-1,1',6,6',7,7'-hexahydroxyl-3,3'-dimethyl-8,8´-di(*N*-piperidylazomethino)-2,2'-binaphthalene (**13**), recorded in $CDCl_3$.

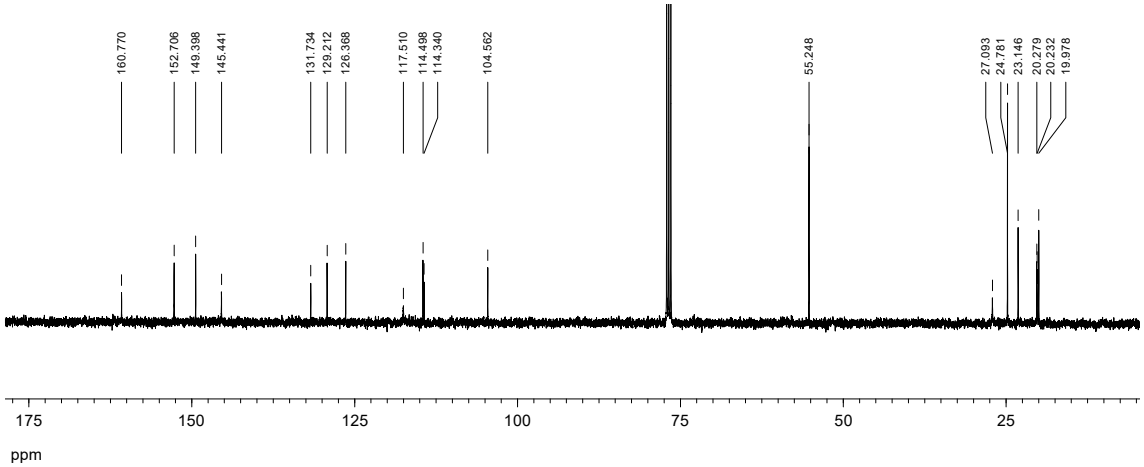


Figure S23 ^{13}C NMR spectrum of 5,5'-diisopropyl-1,1',6,6',7,7'-hexahydroxyl-3,3'-dimethyl-8,8´-di(*N*-piperidylazomethino)-2,2'-binaphthalene (**13**), recorded in $CDCl_3$.

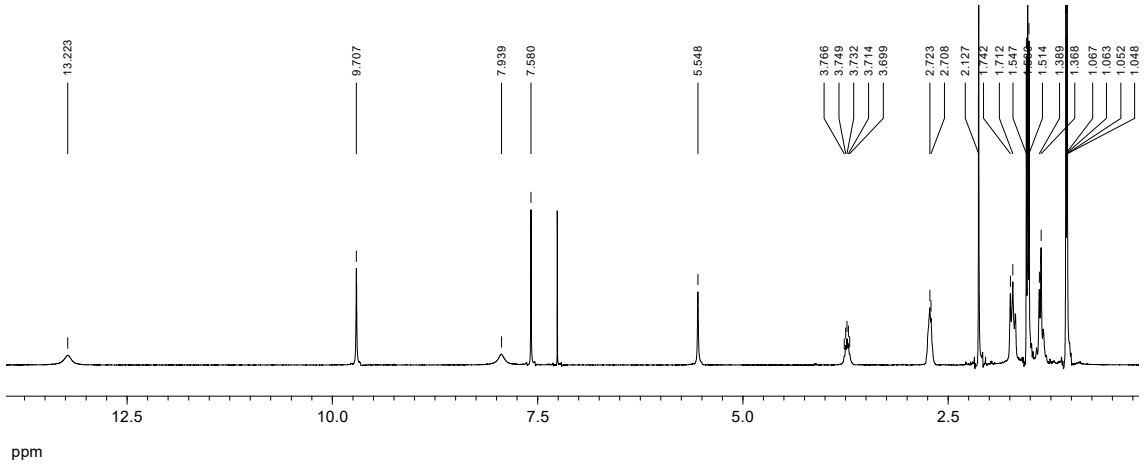


Figure S24 ^{1}H NMR spectrum of 2,2'-bis{1,6-dihydroxy-5-isopropyl-3-methyl-8-[(2,6-dimethyl-*N*-piperidinamino) methylidene]naphthalen-7-one} (**17**), recorded in $CDCl_3$.

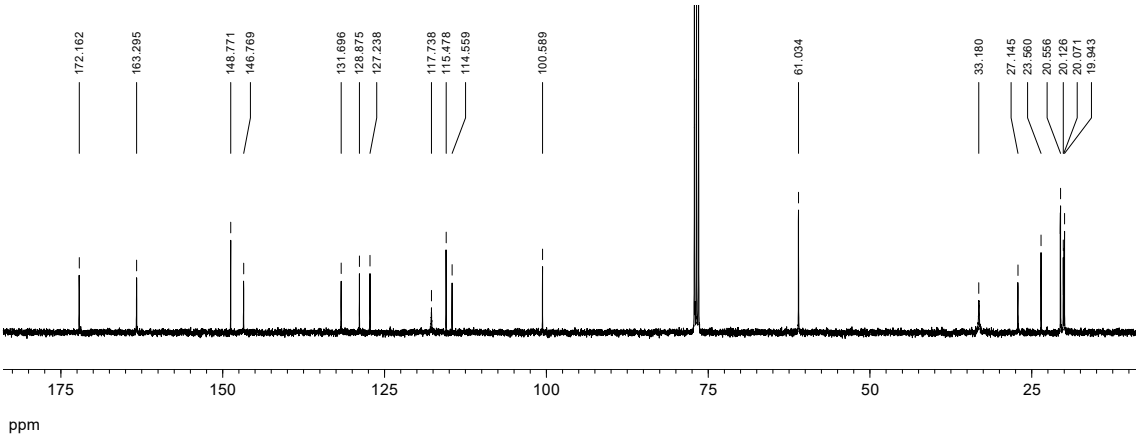


Figure S25 ^{13}C NMR spectrum of 2,2'-Bis{1,6-dihydroxy-5-isopropyl-3-methyl-8-[(2,6-dimethyl-*N*-piperidinamino) methylidene]naphthalen-7-one} (**17**), recorded in $CDCl_3$.

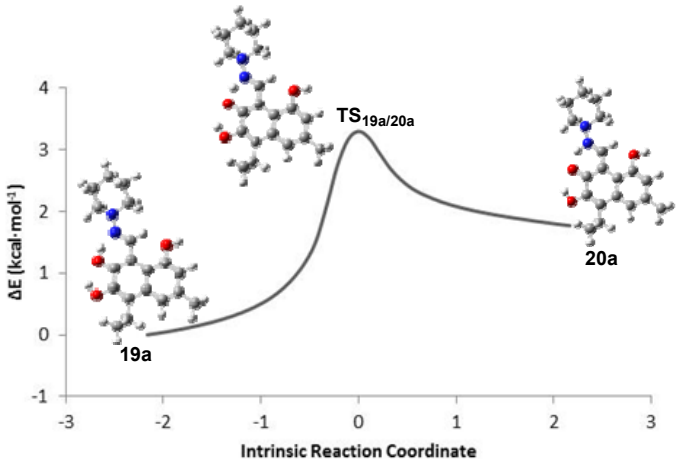


Figure S26 IRC for $\mathbf{TS_{19a/20a}}$.

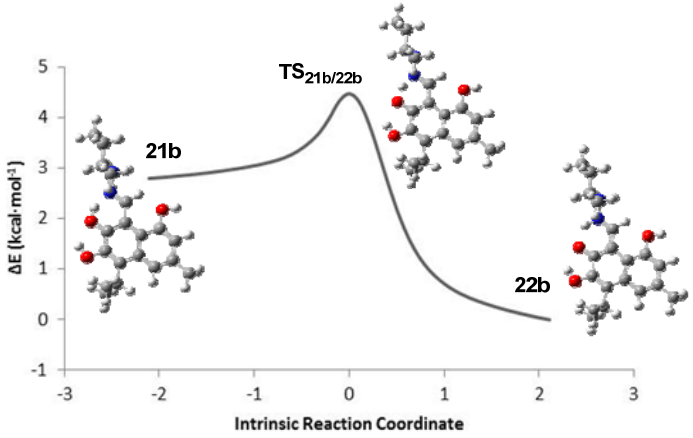


Figure S27 IRC for $\mathbf{TS_{21b/22b}}$.

Table S2 Selected IR and Raman data of compounds **13/16**, **14/17** and **15/18**.[a,b]

	$\overline{\nu}_{C1OH}$[c]	$\overline{\nu}_{C6OH}$[c]	$\overline{\nu}_{C7OH}$[c]	$\overline{\nu}_{C7OH}$[c,e]	$\overline{\nu}_{C=N}$[c]	$\overline{\nu}_{C=N}$[d]	$\overline{\nu}_{C-N}$[d]
13/16	3484	3379	2937	2798	1608w	1610w	1329s
14/17	3493	3283	3109	2901	1604s	1618s	1335s
15/18		3500 - 3200		2922	1611s	1629s	1327s

[a]In cm^{-1}; b w (=weak), s (=strong); [c]In solid (KBr); [d]Raman; [e]Calculated from equation 1.

Table S3 Selected ^{1}H NMR peaks for compounds **13**, **17** and **18**.[a]

	$\delta_{OH/NH}$	δ_{C6OH}	δ_{C1OH}	$\delta_{CH=N}$	$\delta_{C4-H.}$	J_{CHNH}[b]
13/16[c]	14.52s	8.55s	7.92s	9.65s	7.56s	0.0
13/16[d]	14.63s	7.64s	5.63s	9.68s	7.36s	0.0
14/17[c]	13.59d	8.43s	7.94s	9.83d	7.45s	9.0
14/17[d]	13.23bs	7.94bs	5.55s	9.71s	7.58s	-
15/18[c]	13.38d	8.43bs	[e]	10.03d	7.40s	14.0

[a]In ppm. [b]In Hz. [c]In DMSO-d_6. [d]In $CDCl_3$. [e]Not observed.

Table S4 Selected ^{13}C NMR peaks, and equilibrium data for compounds **13**, **17** and **18**.[a]

	δ_{C7}	$\delta_{CH=N}$	δ_{C4}	δ_{C8}	K_T	n_e(%)
13/16[c]	151.33	147.45	116.33	108.21	0.0	0.0
13/16[d]	160.77	152.78	117.71	104.89	0.5	33
14/17[c]	170.25	163.13	116.38	101.54	1.9	66
14/17[d]	172.16	163.30	117.74	100.59	2.6	72
15/18[c]	171.13	160.59	116.40	103.25	2.2	69

[a]In ppm. [b]In DMSO-d_6. [c]In $CDCl_3$.

Table S5 Conformational data of **19**/**20** (angles in degrees and energies in kcal/mol).[a]

Conformer	Minima		Maxima		Minima		Maxima	
	19a	**19c**	**19b**	**19d**	**20b**	**20d**	**20a**	**20c**
θ^{c}	13.7	215.5	122.5	294.8	116.0	296.5	39.7	196.3
$\Delta E_r^{b,c}$	0.00	-0.08	1.52	7.13	0.00	2.34	5.43	5.47
$\Delta G_r^{b,c}$	0.00	0.46	2.31	8.19	0.24	2.77	6.44	5.50
$\tilde{\nu}^{c,f}$			-20.4	-47.0			-59.6	-59.3
θ^{d}	14.3	215.0	122.2	294.3	116.1	296.3	42.9	194.9
$\Delta E_r^{b,d}$	0.00	-0.03	2.08	7.37	-1.00	1.63	3.73	3.74
$\Delta G_r^{b,d}$	0.00	0.82	1.71	7.87	-1.06	2.80	4.88	4.92
$\tilde{\nu}^{d,f}$			-21.9	-77.6			-70.0	-68.1
θ^{e}	14.6	214.8	123.9	296.0	116.6	295.3	42.8	194.8
$\Delta E_r^{b,e}$	0.00	-0.01	2.51	7.44	-1.25	1.28	3.06	3.14
$\Delta G_r^{b,e}$	0.00	0.95	2.96	7.83	-1.05	3.14	4.30	4.11
$\tilde{\nu}^{e,f}$			-27.4	-28.7			-64.9	-68.5

[a]At the M06-2X/6-311G(d,p) level. [b]Relative energy with respect to that of **19a**. [c]In the gas phase. [d]Including the solvent effect (SMD model, $CHCl_3$ as solvent). [e]Including the solvent effect (SMD model, DMSO as solvent. [f]Imaginary frequency of the transition state in cm^{-1}.

Table S6 Conformational data of **21** (angles in degrees and energies in kcal/mol).[a]

Conformer	Minima			Maxima		
	21a	**21b**	**21c**	**21e**	**21f**	**21d**
θ^{c}	347.5	105.6	239.7	42.3	186.3	304.8
$\Delta E_r^{b,c}$	4.99	1.45	4.99	8.81	8.81	8.22
$\Delta G_r^{b,c}$	4.65	1.82	4.65	9.07	9.07	8.62
$\tilde{\nu}^{c,f}$				-152.0	-152.0	-24.3
θ^{d}	348.1	106.1	239.6	43.7	185.4	307.0
$\Delta E_r^{b,d}$	6.37	2.98	6.37	10.18	10.18	9.38
$\Delta G_r^{b,d}$	6.83	3.55	6.82	10.67	10.63	10.63
$\tilde{\nu}^{d,f}$				-152.5	-161.6	-36.2
θ^{e}	348.3	107.6	239.6	44.1	185.3	307.9
$\Delta E_r^{b,e}$	6.92	3.74	6.92	10.73	10.73	9.67
$\Delta G_r^{b,e}$	7.04	3.69	7.04	10.83	10.83	10.15
$\tilde{\nu}^{e,f}$				-152.9	-152.9	-37.0

[a]At the M06-2X/6-311G(d,p) level. [b]Relative energy with respect to that of **26b**. [c]In the gas phase. [d]Including the solvent effect (SMD model, $CHCl_3$ as solvent). [e]Including the solvent effect (SMD model, DMSO as solvent). [f]Imaginary frequency of the transition structure in cm^{-1}.

Table S7 Conformational data of **22** (angles in degrees and energies in kcal/mol).[a]

Conformer	Minima		Maxima	
	22b	**22d**	**22a**	**22c**
θ^{c}	116.6	308.2	35.6	196.2
$\Delta E_r^{b,c}$	0.00	2.54	12.26	12.26
$\Delta G_r^{b,c}$	0.00	3.08	12.30	12.31
$\tilde{\nu}^{c,f}$			-115.5	-115.4
θ^{d}	115.1	312.1	36.8	194.7
$\Delta E_r^{b,d}$	0.00	2.80	12.24	12.24
$\Delta G_r^{b,d}$	0.00	4.53	12.52	12.51
$\tilde{\nu}^{d,f}$			-110.9	-110.9
θ^{e}	114.8	293.9	37.4	194.2
$\Delta E_r^{b,e}$	0.00	2.78	12.28	12.28
$\Delta G_r^{b,e}$	0.00	4.29	12.41	12.41
$\tilde{\nu}^{e,f}$			-104.1	-104.1

[a]At the M06-2X/6-311G(d,p) level. [b]Relative free energy with respect to that of **22b**. [c]In the gas phase. [d]Including the solvent effect (SMD model, $CHCl_3$ as solvent). [e]Including the solvent effect (SMD model, DMSO as solvent). [f]Imaginary frequency of the transition structure in cm^{-1}.

Table S8 NBO data of **19**/**20**.[a,b]

Donor	Acceptor	19a	19b	19c	19d	20d	20a	20b	20c
LP(1) O25	BD*(1) C1 - C6	6.59	6.66	6.57	6.63	6.21	6.18	6.18	6.18
LP(2) O25	BD*(2) C1 - C2	34.25	34.38	34.25	34.70	38.44	37.71	38.04	37.74
LP(1) O27	BD*(1) C5 - C6	8.22	8.61	8.25	8.81	2.94	5.44	3.32	5.33
LP(1) O27	BD*(1) O25 - H26	2.86	2.79	2.88	2.82	1.08	2.07	1.24	2.00
LP(1) O27	BD*(1) N34 - H28					3.65	7.60	4.72	7.45
LP(2) O27	BD*(2) C5 - C6	40.81	45.27	40.96	47.98				
LP(2) O27	BD*(1) C1 - C6					18.32	17.23	18.25	17.36
LP(2) O27	BD*(1) C5 - C6					16.30	10.76	15.40	11.00
LP(2) O27	BD*(1) O25 - H26					5.82	4.58	5.73	4.60
LP(2) O27	BD*(1) N34 - H28					6.79	26.02	8.92	24.83
LP(3) O27	BD*(2) C5 - C6								
LP(1) N34	BD*(1) C15 - H16	9.78	7.56	9.76	9.02				
LP(1) N34	BD*(1) O27 - H28	37.18	43.60	36.34					
LP(1) N34	BD*(1) C35 - N50	10.25			2.75	4.61		4.04	
LP(1) N34	BD*(1) C36 - N50			10.12	3.15	4.90		3.54	
LP(1) N34	BD*(2) C5 - C15					86.34		86.77	
LP(1) N50	BD*(1) C15 - N34			2.10	6.87	9.32	0.78	1.09	0.78
LP(1) N50	BD*(2) C15 - N34	28.13		27.84			13.32		13.14
LP(1) N50	BD*(1) C35 - H38	8.58	7.33	7.84	9.11	8.49	7.50	7.48	7.36
LP(1) N50	BD*(1) C36 - H41	7.96	7.30	8.53	9.23	8.52	7.37	7.51	7.47
LP(1) N50	BD*(1) N34 - H28					3.94		8.86	
LP(1) O32	BD*(1) C8 - C9	5.52	5.76	5.51	5.58	5.45	5.40	5.60	5.40
LP(1) O32	BD*(1) C15 - H16	1.98	1.29	2.04	2.43	2.52	2.85	1.63	2.47
LP(2) O32	BD*(2) C8 - C9	30.75	31.79	30.81	30.76	29.19	29.01	29.98	28.97
BD(1) O32 - H33	BD*(1) C4 - C8	5.07	5.09	5.07	5.03	4.88	4.88	4.92	4.87

[a]At the M06-2X/6-311G(d,p) level in gas phase. [b]In kcal/mol

Table S9 NBO data of **19**/**20**.[a,b,c]

Donor	Acceptor	19a	19b	19c	19d	20d	20a	20b	20c
LP(1) O25	BD*(1) C1 - C6	6.64	6.74	6.63	6.70	6.18	6.09	6.11	6.12
LP(2) O25	BD*(2) C1 - C2	34.14	34.24	34.12	34.41	37.60	37.08	37.33	37.15
LP(1) O27	BD*(1) C5 - C6	8.22	8.60	8.24	8.74	2.88	4.59	3.08	4.59
LP(1) O27	BD*(1) O25 - H26	2.58	2.44	2.60	2.47	1.01	1.77	1.14	1.76
LP(1) O27	BD*(1) N34 - H28					3.35	6.69	4.09	6.66
LP(2) O27	BD*(2) C5 - C6	40.66	45.07	40.77	47.43				
LP(2) O27	BD*(1) C1 - C6					18.06	17.45	18.00	17.48
LP(2) O27	BD*(1) C5 - C6					16.08	12.07	15.55	12.11
LP(2) O27	BD*(1) O25 - H26					5.73	5.15	5.85	5.14
LP(2) O27	BD*(1) N34 - H28					6.27	18.23	7.37	18.23
LP(3) O27	BD*(2) C5 - C6						105.05		105.31
LP(1) N34	BD*(1) C15 - H16	9.72	7.69	9.70	8.92				
LP(1) N34	BD*(1) O27 - H28	39.28	44.95	38.31	57.18				
LP(1) N34	BD*(1) C35 - N50	10.08			2.61				
LP(1) N34	BD*(1) C36 - N50			9.94	3.21				
LP(1) N34	BD*(2) C5 - C15								
LP(1) N50	BD*(1) C15 - N34				7.05	9.39	0.54	0.99	0.66
LP(1) N50	BD*(2) C15 - N34	29.73		29.32			13.84		13.89
LP(1) N50	BD*(1) C35 - H38	8.09	7.04	7.45	8.55	8.02	7.00	7.03	6.96
LP(1) N50	BD*(1) C36 - H41	7.56	7.01	8.06	8.69	8.06	7.01	7.07	6.96
LP(1) N50	BD*(1) N34 - H28					3.86	0.69	8.71	
LP(1) O32	BD*(1) C8 - C9	5.84	6.02	5.83	5.88	5.74	5.76	5.87	5.73
LP(1) O32	BD*(1) C15 - H16	1.57	1.06	1.66	2.01	2.41	2.26	1.51	2.27
LP(2) O32	BD*(2) C8 - C9	32.58	33.11	32.60	32.31	30.83	30.83	31.40	30.86
BD(1) O32 - H33	BD*(1) C4 - C8	5.25	5.25	5.25	5.20	5.06	5.05	5.09	5.06

[a]At the M06-2X/6-311G(d,p) level. [b]Including the solvent effect (SMD model, $CHCl_3$ as solvent). [c]In kcal/mol.

Table S10 NBO data of **19**/**20**.[a,b,c]

Donor	Acceptor	19a	19b	19c	19d	20d	20a	20b	20c
LP(1) O25	BD*(1) C1 - C6	6.64	6.71	6.62	6.67	6.13	6.05	6.08	6.07
LP(2) O25	BD*(2) C1 - C2	34.30	34.36	34.23	34.36	37.79	37.38	37.62	37.38
LP(1) O27	BD*(1) C5 - C6	8.25	8.62	8.27	8.75	2.76	4.24	2.90	4.21
LP(1) O27	BD*(1) O25 - H26	2.70	2.53	2.70	2.63	1.09	1.81	1.19	1.80
LP(1) O27	BD*(1) N34 - H28					3.28	6.53	3.90	6.45
LP(2) O27	BD*(2) C5 - C6	41.27	45.40	41.17	48.04				
LP(2) O27	BD*(1) C1 - C6					17.93	17.53	17.94	17.56
LP(2) O27	BD*(1) C5 - C6					16.19	12.70	15.87	12.78
LP(2) O27	BD*(1) O25 - H26					6.32	5.83	6.39	5.86
LP(2) O27	BD*(1) N34 - H28					5.94	15.98	6.63	15.80
LP(3) O27	BD*(2) C5 - C6						106.40		106.72
LP(1) N34	BD*(1) C15 - H16	9.62	7.73	9.60	8.68				
LP(1) N34	BD*(1) O27 - H28	42.27	46.35	40.92	62.71				
LP(1) N34	BD*(1) C35 - N50	10.04			2.78				
LP(1) N34	BD*(1) C36 - N50			9.89	2.97				
LP(1) N34	BD*(2) C5 - C15								
LP(1) N50	BD*(1) C15 - N34	2.09		2.12	7.20	9.40	0.56	0.95	0.65
LP(1) N50	BD*(2) C15 - N34	30.63		30.20			14.38		14.42
LP(1) N50	BD*(1) C35 - H38	7.85	6.90	7.29	8.29	7.76	6.83	6.84	6.82
LP(1) N50	BD*(1) C36 - H41	7.37	6.90	7.85	8.37	7.83	6.88	6.87	6.78
LP(1) N50	BD*(1) N34 - H28					3.81	0.67	8.62	
LP(1) O32	BD*(1) C8 - C9	5.90	6.04	5.87	5.89	5.80	5.81	5.88	5.79
LP(1) O32	BD*(1) C15 - H16	1.48	0.94	1.60	2.43	2.38	2.30	1.63	2.25
LP(2) O32	BD*(2) C8 - C9	33.19	33.33	33.11	32.68	31.44	31.55	31.77	31.46
BD(1) O32 - H33	BD*(1) C4 - C8	5.34	5.32	5.34	5.29	5.15	5.15	5.18	5.15

[a]At the M06-2X/6-311G(d,p) level. [b]Including the solvent effect (SMD model, DMSO as solvent). [c]In kcal/mol

Table S11 NBO data of **21**/**22**.[a,b]

Donor	Acceptor	21a	21e	21b	21f	21c	21d	22d	22b	22a	22c
LP(1) O25	BD*(1) C1 - C6	6.58	6.58	6.64	6.58	6.58	6.61	6.16	6.17	6.18	6.17
LP(2) O25	BD*(2) C1 - C2	34.39	34.32	34.28	34.32	34.39	34.69	38.26	37.53	37.97	37.54
LP(1) O27	BD*(1) C5 - C6	8.30	8.22	8.41	8.22	8.30	8.79	2.95	6.23	3.40	6.23
LP(1) O27	BD*(1) O25 - H26	2.75	2.89	2.61	2.89	2.75	2.75	1.01	2.33	1.27	2.33
LP(1) O27	BD*(1) N34 - H28							3.32	8.50	4.88	8.50
LP(2) O27	BD*(2) C5 - C6	42.27	41.57	43.31	41.57	42.27	47.88				
LP(2) O27	BD*(1) C1 - C6							18.38	16.41	18.17	16.41
LP(2) O27	BD*(1) C5 - C6							16.29	9.01	15.19	9.01
LP(2) O27	BD*(1) O25 - H26							5.67	4.00	5.69	4.01
LP(2) O27	BD*(1) N34 - H28							6.57	33.84	9.34	33.83
LP(3) O27	BD*(2) C5 - C6								99.11		99.12
LP(1) N34	BD*(1) C15 - H16	10.04	9.37	8.12	9.37	10.04	9.23				
LP(1) N34	BD*(1) O27 - H28	46.06	48.03	38.55	48.03	46.03					
LP(1) N34	BD*(1) C35 - N50	9.25	6.93	0.64			3.84	3.15		3.65	
LP(1) N34	BD*(1) C36 - N50				6.93	9.25	1.91	5.80		3.63	
LP(1) N34	BD*(2) C5 - C15							87.58		86.93	
LP(1) N50	BD*(1) C15 - N34	4.38				4.38	6.71	9.06	0.74	1.07	0.74
LP(1) N50	BD*(2) C15 - N34	17.34	23.90	0.79	23.89	17.34	0.41		14.55		14.55
LP(1) N50	BD*(1) C35 - H38	8.84	6.50	7.18	6.92	7.79	9.35	8.65	6.53	7.40	6.75
LP(1) N50	BD*(1) C36 - H41	7.79	6.92	7.26	6.50	8.84	8.79	8.05	6.75	7.38	6.53
LP(1) N50	BD*(1) N34 - H28							3.49	0.67	8.81	0.67
LP(1) O32	BD*(1) C8 - C9	5.48	5.37	5.83	5.37	5.48	5.61	5.51	5.33	5.58	5.33
LP(1) O32	BD*(1) C15 - H16	2.19	4.16	0.50	4.16	2.20	2.05	1.38	3.76	1.48	3.76
LP(2) O32	BD*(2) C8 - C9	30.37	30.29	31.73	30.29	30.37	30.84	29.15	28.56	29.93	28.56
BD(1) O32 - H33	BD*(1) C4 - C8	5.00	5.07	5.05	5.07	5.00	5.02	4.86	4.83	4.93	4.83

[a]At the M06-2X/6-311G(d,p) level in gas phase. [b]In kcal/mol

Table S12 NBO data of **21**/**22**.[a,b,c]

Donor	Acceptor	21a	21e	21b	21f	21c	21d	22d	22b	22a	22c
LP(1) O25	BD*(1) C1 - C6	6.64	6.64	6.72	6.65	6.64	6.67	6.13	6.11	6.11	6.11
LP(2) O25	BD*(2) C1 - C2	34.25	34.15	34.14	34.17	34.25	34.42	37.43	36.96	37.28	36.96
LP(1) O27	BD*(1) C5 - C6	8.30	8.24	8.42	8.25	8.30	8.70	2.93	5.66	3.12	5.66
LP(1) O27	BD*(1) O25 - H26	2.45	2.55	2.30	2.58	2.45	2.41	0.98	2.14	1.15	2.14
LP(1) O27	BD*(1) N34 - H28							3.18	8.14	4.15	8.14
LP(2) O27	BD*(2) C5 - C6	42.36	41.66	43.41	41.75	42.36	47.08				
LP(2) O27	BD*(1) C1 - C6							18.08	16.74	17.93	16.74
LP(2) O27	BD*(1) C5 - C6							15.95	9.85	15.43	9.85
LP(2) O27	BD*(1) O25 - H26							5.60	4.41	5.83	4.41
LP(2) O27	BD*(1) N34 - H28							6.37	27.33	7.58	27.33
LP(3) O27	BD*(2) C5 - C6								98.20		98.20
LP(1) N34	BD*(1) C15 - H16	9.93	9.40	8.11	9.32	9.93	9.15				
LP(1) N34	BD*(1) O27 - H28	48.87	50.15	40.27	50.90	48.87	56.93				
LP(1) N34	BD*(1) C35 - N50	9.06	6.70	0.60			3.99				
LP(1) N34	BD*(1) C36 - N50				6.70	9.06	1.75				
LP(1) N34	BD*(2) C5 - C15										
LP(1) N50	BD*(1) C15 - N34	4.45				4.45	6.81	8.99	0.64	0.97	0.64
LP(1) N50	BD*(2) C15 - N34	17.62	24.23	0.73	24.42	17.62	0.82	0.86	15.55		15.55
LP(1) N50	BD*(1) C35 - H38	8.31	6.20	6.88	6.65	7.40	8.86	8.21	6.06	7.00	6.39
LP(1) N50	BD*(1) C36 - H41	7.40	6.68	6.98	6.14	8.31	8.30	7.58	6.39	7.02	6.06
LP(1) N50	BD*(1) N34 - H28							3.37	0.79	7.73	0.79
LP(1) O32	BD*(1) C8 - C9	5.77	5.74	6.07	5.70	5.77	5.92	5.78	5.68	5.85	5.68
LP(1) O32	BD*(1) C15 - H16	2.08	3.69	0.50	4.03	2.08	1.55	1.48	3.59	1.34	3.59
LP(2) O32	BD*(2) C8 - C9	32.04	32.14	33.17	32.04	5.18	32.41	30.81	30.52	31.39	30.52
BD(1) O32 - H33	BD*(1) C4 - C8	5.18	5.21	5.22	5.22	32.04	5.18	5.04	5.01	5.09	5.01

[a]At the M06-2X/6-311G(d,p) level. [b]The solvent effect (SMD model, $CHCl_3$ as solvent). [c]In kcal/mol.

Table S13 NBO data of **21**/**22.**[a,b,c]

Donor	Aceptor	21a	21e	21b	21f	21c	21d	22d	22b	22a	22c
LP(1) O25	BD*(1) C1 - C6	6.62	6.62	6.71	6.62	6.62	6.65	6.12	6.08	6.06	6.08
LP(2) O25	BD*(2) C1 - C2	34.35	34.31	34.31	34.31	34.35	34.44	37.76	37.25	37.58	37.25
LP(1) O27	BD*(1) C5 - C6	8.35	8.27	8.49	8.27	8.35	8.67	2.78	5.35	2.94	5.35
LP(1) O27	BD*(1) O25 - H26	2.56	2.66	2.45	2.66	2.56	2.50	1.09	2.21	1.19	2.21
LP(1) O27	BD*(1) N34 - H28							3.26	8.13	3.93	8.13
LP(2) O27	BD*(2) C5 - C6	42.93	41.96	44.21	41.96	42.93	47.20				
LP(2) O27	BD*(1) C1 - C6							17.94	16.93	17.90	16.93
LP(2) O27	BD*(1) C5 - C6							16.15	10.41	15.78	10.41
LP(2) O27	BD*(1) O25 - H26							6.31	4.94	6.39	4.94
LP(2) O27	BD*(1) N34 - H28							5.93	24.81	6.77	24.81
LP(3) O27	BD*(2) C5 - C6								99.43		99.43
LP(1) N34	BD*(1) C15 - H16	9.76	9.43	8.09	9.43	9.76	9.00				
LP(1) N34	BD*(1) O27 - H28			43.41			59.66				
LP(1) N34	BD*(1) C35 - N50	8.97	6.68	0.56			4.06				
LP(1) N34	BD*(1) C36 - N50				6.68	8.97	1.68				
LP(1) N34	BD*(2) C5 - C15										
LP(1) N50	BD*(1) C15 - N34	4.50				4.50	6.89	9.25	0.61	0.93	0.61
LP(1) N50	BD*(2) C15 - N34	17.82	24.59	0.59	24.59	17.82	0.92		15.85		15.85
LP(1) N50	BD*(1) C35 - H38	8.05	6.13	6.71	6.57	7.22	8.51	7.66	5.88	6.80	6.26
LP(1) N50	BD*(1) C36 - H41	7.22	6.57	6.81	6.13	8.05	7.99	7.78	6.23	6.82	5.88
LP(1) N50	BD*(1) N34 - H28							3.75	0.85	8.63	0.85
LP(1) O32	BD*(1) C8 - C9	5.80	5.76	6.07	5.76	5.80	5.96	5.79	5.74	5.86	5.74
LP(1) O32	BD*(1) C15 - H16	2.20	3.55	0.56	3.55	2.20	1.45	2.39	3.38	1.35	3.38
LP(2) O32	BD*(2) C8 - C9	32.41	32.58	33.36	32.58	32.41	32.87	31.44	31.18	31.71	31.18
BD(1) O32 - H33	BD*(1) C4 - C8	5.27	5.31	5.30	5.31	5.27	5.28	5.15	5.12	5.18	5.12

[a]At the M06-2X/6-311G(d,p) level. [b]Including the solvent effect (SMD model, DMSO as solvent). [c]In kcal/mol.

Table S14 NBO data of **23/24**.[a,b]

Donor	Acceptor	23[c]	$TS_{23/24}$[c]	24[c]	23[d]	$TS_{23/24}$[d]	24[d]	23[e]	$TS_{23/24}$[e]	24[e]
LP(1) O25	BD*(1) C1 - C6	6.67	6.43	6.25	6.68	6.41	6.14	6.70	6.44	6.14
LP(2) O25	BD*(2) C1 - C2	34.48	35.80	38.06	34.41	35.27	37.65	34.31	35.22	37.25
LP(1) O27	BD*(1) C5 - C6	8.57	9.10	3.67	8.59	9.00	3.21	8.54	9.02	3.37
LP(1) O27	BD*(1) O25 - H26	2.56	2.77	1.24	2.47	2.79	1.23	2.35	2.66	1.14
LP(1) O27	BD*(1) N34 - H28			5.18			4.47			4.52
LP(2) O27	BD*(2) C5 - C6	46.21			47.10	57.87		46.15	64.95	
LP(2) O27	BD*(1) C1 - C6		9.99	18.40			18.17			18.21
LP(2) O27	BD*(1) C5 - C6		2.72	14.91			15.34			15.13
LP(2) O27	BD*(1) O25 - H26		1.47	5.17			5.96			5.36
LP(2) O27	BD*(1) N34 - H28			11.21			8.70			9.19
LP(3) O27	BD*(1) C1 - C6	5.79				8.63			9.31	
LP(3) O27	BD*(2) C5 - C6		70.72			4.00			2.37	
LP(1) N34	BD*(1) C15 - H16	10.72	8.60		10.42	8.78		10.57	8.71	
LP(1) N34	BD*(1) O27 - H28				56.43			50.75		
LP(1) N34	BD*(1) C36 - C37	1.96	1.80	6.06	1.90	1.80		1.94	2.95	
LP(1) N34	BD*(1) C36 - C40	2.38	2.14	7.02	2.29	2.05		2.27	1.91	
LP(1) N34	BD*(1) C36 - C43	2.77	3.05		2.75	2.93		2.73	1.95	
LP(1) N34	BD*(2) C5 - C15			84.09						
LP(1) O32	BD*(1) C8 - C9	5.60	5.55	5.47	5.97	5.94	5.87	5.92	5.84	5.79
LP(1) O32	BD*(1) C15 - H16	1.97	2.61	2.24	1.46	1.99	1.57	1.52	2.51	1.73
LP(2) O32	BD*(2) C8 - C9	30.64	29.98	29.20	32.90	32.43	31.60	32.34	31.80	30.83
BD(1) O32 - H33	BD*(1) C4 - C8	5.02	4.94	4.88	5.29	5.22	5.16	5.19	5.15	5.06

[a]At the M06-2X/6-311G(d,p) level. [b]In kcal/mol. [c]In gas phase. [d]Including the solvent effect (SMD model, $CHCl_3$ as solvent). [e]Including the solvent effect (SMD model, DMSO as solvent).

Table S15 NBO data of **13**/**16** and **14**/**17**.[a,b]

Donor	Aceptor	13cc	13aa	16dd	16bb	14aa	14bb	17dd	17bb
LP(1) O25	BD*(1) C1 - C6	6.62	6.61	6.24	6.23	6.63	6.66	6.26	6.21
LP(2) O25	BD*(1) C1 - C2	34.71	34.70	38.97	38.62	34.95	34.81	38.97	38.52
LP(1) O27	BD*(1) C5 - C6	8.28	8.30	2.87	3.21	8.40	8.52	2.97	3.25
LP(1) O27	BD*(1) O25- H26	2.94	3.00	1.04	1.20	2.87	2.70	1.07	1.16
LP(1) O27	BD*(1) N34 - H28			3.42	4.45			3.65	4.34
LP(2) O27	BD*(1) C1 -C6			18.42	18.31			18.44	18.37
LP(2) O27	BD*(2) C5 - C6	41.45	41.53	16.47	15.61	43.04	44.45	16.28	15.54
LP(2) O27	BD*(1) O25- H26			5.81	5.78			5.77	5.64
LP(2) O27	BD*(1) N34 - H28			6.34	8.22			6.82	8.22
LP(1) N34	BD*(1) C15 - H16	9.65	9.50			9.76	7.90		
LP(1) N34	BD*(1) O27 - H28	39.58	40.53			49.79			
LP(1) N34	BD*(1) C35 - N50	10.27	10.30	4.41	4.02	9.29		4.58	3.39
LP(1) N34	BD*(1) C36 - N50			4.98	3.56		0.61	4.75	3.80
LP(1) N34	BD*(2) C5 - C15			87.70	87.92			88.15	87.48
LP(1) N50	BD*(1) C15 - N34	2.11	2.05	9.31	1.09	4.51		9.23	1.07
LP(1) N50	BD*(2) C15 - N34	28.67	29.16			17.76	0.68		
LP(1) N50	BD*(1) C35 - H38	8.55	8.53	8.44	7.50	8.80	7.27	8.27	7.44
LP(1) N50	BD*(1) C36 - H41	7.91	7.94	8.48	7.52	7.80	7.13	8.44	7.41
LP(1) N50	BD*(1) N34 - H28			3.96	8.88			3.88	8.70
LP(1) O32	BD*(1) C8 - C9	6.22	6.20	6.20	6.33	6.18	6.47	6.23	6.40
LP(1) O32	BD*(1) C15 - H16	2.20	2.76	2.41	1.81	2.78	0.94	2.48	0.97
LP(2) O32	BD*(2) C8 - C9	33.55	33.33	31.65	32.35	33.02	34.09	31.81	32.39
BD(1) O32 - H33	BD*(1) C4 - C8	5.21	5.20	5.00	5.04	5.15	5.18	5.00	5.02
BD(2) C58 - C59	BD*(1) O32 - H33	1.21	1.14	0.98	0.96	1.21	0.96	0.96	0.86

[a]At the M06-2X/6-311G(d,p) level in gas phase. [b]In kcal/mol.

Table S16 NBO data of **13**/**16** and **14**/**17**.[a,b,c]

Donor	Aceptor	13cc	13aa	16dd	16bb	14aa	14bb	17dd	17bb
LP(1) O25	BD*(1) C1 - C6	6.69	6.71	6.22	6.20	6.72	6.79	6.25	6.18
LP(2) O25	BD*(1) C1 - C2	34.50	34.58	38.06	37.87	34.76	34.63	38.15	37.83
LP(1) O27	BD*(1) C5 - C6	8.25	8.28	2.83	3.04	8.42	8.52	2.95	3.06
LP(1) O27	BD*(1) O25- H26	2.58	2.61	0.96	1.07	2.49	2.31	1.02	1.05
LP(1) O27	BD*(1) N34 - H28			3.16	3.91			3.46	3.77
LP(2) O27	BD*(1) C1 -C6			18.19	18.10			18.18	18.16
LP(2) O27	BD*(2) C5 - C6	41.41	41.53	16.23	15.70	43.23	44.50	16.02	15.66
LP(2) O27	BD*(1) O25- H26			5.61	5.67			5.64	5.62
LP(2) O27	BD*(1) N34 - H28			5.91	6.97			6.50	6.95
LP(1) N34	BD*(1) C15 - H16	9.70	9.49			9.64	7.98		
LP(1) N34	BD*(1) O27 - H28	41.90	42.97						
LP(1) N34	BD*(1) C35 - N50	10.12	10.20			9.20	0.62		
LP(1) N34	BD*(1) C36 - N50								
LP(1) N34	BD*(2) C5 - C15								
LP(1) N50	BD*(1) C15 - N34	2.09	2.09	9.34	0.99	4.56		9.26	0.94
LP(1) N50	BD*(2) C15 - N34	30.17	30.55			18.42	0.86		
LP(1) N50	BD*(1) C35 - H38	8.07	7.05	8.00	7.07	8.30	6.96	7.88	7.01
LP(1) N50	BD*(1) C36 - H41	7.51	7.53	8.05	7.07	7.43	6.82	8.02	6.95
LP(1) N50	BD*(1) N34 - H28			3.86	8.70			3.79	8.66
LP(1) O32	BD*(1) C8 - C9	6.51	6.44	6.43	6.51	6.39	6.64	6.42	6.58
LP(1) O32	BD*(1) C15 - H16	1.43	2.17	2.09	1.70	2.72	0.83	2.35	0.81
LP(2) O32	BD*(2) C8 - C9	34.59	34.16	32.42	32.90	33.64	34.51	32.43	32.89
BD(1) O32 - H33	BD*(1) C4 - C8	5.23	5.19	5.00	5.04	5.13	5.17	5.00	5.00
BD(2) C58 - C59	BD*(1) O32 - H33	1.06	0.92	0.81	0.80	0.91	0.69	0.74	0.66

[a]At the M06-2X/6-311G(d,p) level. [b]Including the solvent effect (SMD model, $CHCl_3$ as solvent). [c]In kcal/mol.

Table S17 NBO data of **13**/**16** and **14**/**17**.[a,b,c]

Donor	Aceptor	13cc	13aa	16dd	16bb	14aa	14bb	17dd	17bb
LP(1) O25	BD*(1) C1 - C6	6.66	6.67	6.15	6.14	6.67	6.72	6.17	6.11
LP(2) O25	BD*(1) C1 - C2	34.62	34.70	38.19	38.14	34.79	34.75	38.22	38.10
LP(1) O27	BD*(1) C5 - C6	8.28	8.31	2.73	2.84	8.42	8.54	2.84	2.84
LP(1) O27	BD*(1) O25- H26	2.70	2.81	1.08	1.14	2.69	2.45	1.12	1.10
LP(1) O27	BD*(1) N34 - H28			3.19	3.71			3.45	3.51
LP(2) O27	BD*(1) C1 -C6			18.00	18.01			18.03	18.12
LP(2) O27	BD*(2) C5 - C6	41.66	41.95	16.28	16.03	43.60	45.08	16.09	16.04
LP(2) O27	BD*(1) O25- H26			6.32	6.36			6.27	6.25
LP(2) O27	BD*(1) N34 - H28			5.79	6.21			6.31	6.10
LP(1) N34	BD*(1) C15 - H16	9.68	9.45			9.61	8.02		
LP(1) N34	BD*(1) O27 - H28	43.00	45.11			55.35			
LP(1) N34	BD*(1) C35 - N50	10.07	10.11			9.07			
LP(1) N34	BD*(1) C36 - N50								
LP(1) N34	BD*(2) C5 - C15								
LP(1) N50	BD*(1) C15 - N34	2.12	2.12	9.43	0.94	4.63		9.30	0.90
LP(1) N50	BD*(2) C15 - N34	30.72	30.98			18.19			
LP(1) N50	BD*(1) C35 - H38	7.83	7.82	7.80	6.83	8.06	6.81	7.68	6.80
LP(1) N50	BD*(1) C36 - H41	7.31	7.32	7.87	6.86	7.22	6.74	7.81	6.75
LP(1) N50	BD*(1) N34 - H28			3.86	8.59			3.76	8.58
LP(1) O32	BD*(1) C8 - C9	6.57	6.48	6.48	6.52	6.42	6.73	6.48	6.60
LP(1) O32	BD*(1) C15 - H16	1.23	1.97	1.95	1.53	2.44	0.52	2.15	0.73
LP(2) O32	BD*(2) C8 - C9	35.02	34.79	33.07	33.29	34.23	34.96	33.10	33.33
BD(1) O32 - H33	BD*(1) C4 - C8	5.29	5.27	5.09	5.12	5.22	5.20	5.07	5.08
BD(2) C58 - C59	BD*(1) O32 - H33	1.13	1.02	0.85	0.87	1.04	0.69	0.80	0.72

[a]At the M06-2X/6-311G(d,p) level. [b]Including the solvent effect (SMD model, DMSO as solvent). [c]In kcal/mol.

Table S18 Geometry (Å and °) and energy (kcal/mol) data for intramolecular hydrogen bonds in compounds **13**/**16** and **14**/**17**.[a]

		D-H···*A*	*d*(*D*-H)	*d*(H···*A*)	*d*(*D*···*A*)	∠(*D*H*A*)	E_{HB}[b]
	Vacuum	N-H···O	1.017	1.849	2.596	127.359	-12.6
16dd	$CHCl_3$	N-H···O	1.017	1.865	2.606	126.918	-12.1
	DMSO	N-H···O	1.017	1.866	2.609	127.161	-11.9
	Vacuum	N-H···O	1.025	1.815	2.583	128.702	-13.3
16bb	$CHCl_3$	N-H···O	1.024	1.847	2.599	127.362	-12.4
	DMSO	N-H···O	1.024	1.864	2.608	126.636	-12.0
	Vacuum	N-H···O	1.017	1.832	2.586	128.065	-13.1
17dd	$CHCl_3$	N-H···O	1.017	1.843	2.594	127.837	-12.7
	DMSO	N-H···O	1.017	1.846	2.599	127.943	-12.5
	Vacuum	N-H···O	1.026	1.820	2.588	128.613	-13.0
17bb	$CHCl_3$	N-H···O	1.024	1.855	2.606	127.255	-12.1
	DMSO	N-H···O	1.024	1.876	2.618	126.463	-11.5

[a]At the M06-2X/6-311G(d,p) level. [b]Estimated as described in Ref.1 .

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Table S19 Relative stability and conformational data of the most stable conformers for theatropisomeric pathways of (*S*)-**13aa** (angles in degrees and energies in kcal/mol)[a,b]

	(*S*)-13aa	**(*S*)-13aa´**[f]	**(*R*)-13aa**	**(*R*)-13aa´**[f]	**(*R*)-13aa**[g]
Configuration	***S***	***S***	***R***	***R***	***R***
$\chi_{C9\text{-}C1\text{-}O\text{-}H}$[c]	175.5	35.4	180.2	326.7	184.5
θ[c]	13.9	13.8	13.2	13.9	346.1
Φ[c]	103.8	106.5	259.3	253.0	256.2
ΔE_r[c]	0.00	6.10	0.35	5.95	0.00
ΔG_r[c]	0.00	3.61	-1.18	3.98	0.00
$\chi_{C9\text{-}C1\text{-}O\text{-}H}$[d]	174.6	35.9	179.3	325.7	185.4
θ[d]	14.5	13.1	14.2	14.3	345.5
φ[d]	103.1	104.6	264.0	254.0	256.9
ΔE_r[d]	0.00	4.38	0.50	4.32	0.00
ΔG_r[d]	0.00	2.31	-2.05	2.52	0.00
$\chi_{C9\text{-}C1\text{-}O\text{-}H}$[e]	177.1	29.8	178.4	331.5	182.9
θ[e]	14.4	12.4	14.3	14.1	345.6
φ[e]	100.4	104.7	266.5	254.8	259.6
ΔE_r[e]	0.00	3.88	0.22	3.78	0.00
ΔG_r[e]	0.00	2.83	-2.88	2.49	0.00

[a]At the M06-2X/6-311G(d,p) level. [b]Relative energy with respect to that of **13aa**. [c]In the gas phase. [d]Including the solvent effect (SMD model, $CHCl_3$ as solvent). [e]Including the solvent effect (SMD model, DMSO as solvent). [f]OH rotated ~140°. [g]True enantiomer of **(*S*)-13aa.**

Cartesian Coordinates and Calculated Energies at the M06-2x/6-311G(d,p) level in Gas Phase, $CHCl_3$, and DMSO (SMD Model)

Structure 13aa ((*S*)-13aa) (vacuum)

Energy (Hartrees): = -2224.3849204
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.140635	2.545977	0.590114
2	6	0	-4.073715	2.911759	1.367748
3	6	0	-2.922713	2.047038	1.377163
4	6	0	-2.918321	0.828361	0.624245
5	6	0	-4.086314	0.452619	-0.138768
6	6	0	-5.153518	1.333515	-0.150127
7	6	0	4.280764	-5.432609	1.247457
8	6	0	-0.564255	-2.023249	2.979089
9	6	0	-4.156221	4.206155	2.162747
10	6	0	-1.710858	0.066087	0.649828
11	6	0	-0.604953	0.437668	1.394538
12	6	0	-0.636298	1.629387	2.158993
13	6	0	-1.770144	2.396614	2.131327
14	6	0	-5.280727	4.158623	3.207564
15	6	0	-4.280866	5.432638	1.247305
16	6	0	0.564218	2.023509	2.978965
17	6	0	-4.238263	-0.830753	-0.843456
18	6	0	4.238285	0.830728	-0.843460
19	6	0	0.604937	-0.437527	1.394564
20	6	0	0.636266	-1.629200	2.159089
21	6	0	1.770091	-2.396462	2.131445
22	6	0	2.922656	-2.046953	1.377245
23	6	0	2.918286	-0.828308	0.624277
24	6	0	1.710838	-0.066015	0.649810
25	6	0	4.156088	-4.206100	2.162861
26	6	0	5.280537	-4.158549	3.207738
27	6	0	4.073630	-2.911713	1.367840
28	6	0	5.140566	-2.545974	0.590205
29	6	0	5.153472	-1.333534	-0.150069
30	6	0	4.086291	-0.452618	-0.138742
31	1	0	3.468851	1.572405	-0.713678
32	1	0	1.767489	-3.304110	2.715023
33	1	0	-3.468847	-1.572419	-0.713576
34	1	0	-1.767554	3.304295	2.714851
35	1	0	6.869165	-2.853898	-0.081136
36	1	0	4.262825	-6.345888	1.847922
37	1	0	-3.231015	4.333712	2.719409
38	8	0	1.637893	1.079510	-0.088708
39	1	0	-5.268159	5.072745	3.806919
40	1	0	-5.145916	3.308410	3.879927
41	1	0	-6.256990	4.072414	2.731780
42	1	0	-4.263009	6.345934	1.847747
43	1	0	-3.448474	5.471830	0.541010
44	1	0	-5.212586	5.409268	0.683272
45	1	0	-0.853327	-1.216826	3.657943
46	1	0	-0.352749	-2.917063	3.566100
47	1	0	-1.428467	-2.225193	2.339407
48	8	0	-6.255617	3.314343	0.506873
49	1	0	-6.869233	2.853854	-0.081250
50	8	0	-6.296684	1.131280	-0.828200
51	1	0	-6.190466	0.270885	-1.326479
52	1	0	0.352710	2.917381	3.565887
53	1	0	1.428437	2.225389	2.339275
54	1	0	0.853280	1.217152	3.657902
55	8	0	-1.637905	-1.079504	-0.088585
56	8	0	6.296637	-1.131332	-0.828161
57	1	0	3.448424	-5.471789	0.541099
58	1	0	5.212527	-5.409291	0.683495
59	8	0	6.255535	-3.314363	0.506989
60	1	0	3.230847	-4.333646	2.719469
61	1	0	5.267947	-5.072662	3.807107
62	1	0	5.145684	-3.308326	3.880082
63	1	0	6.256823	-4.072340	2.732003
64	1	0	6.190438	-0.270961	-1.326454
65	1	0	-0.737934	-1.425063	-0.012599
66	1	0	0.737927	1.425088	-0.012745
67	7	0	-5.271787	-1.046410	-1.578356
68	6	0	-4.577158	-3.333120	-1.965027
69	6	0	-6.867264	-2.534309	-2.351055
70	6	0	-4.816935	-4.487831	-2.934513
71	1	0	-4.744587	-3.655582	-0.921534
72	1	0	-3.537386	-3.012330	-2.051398
73	6	0	-7.125870	-3.651109	-3.351612

74	1	0	-7.226351	-2.836120	-1.352652
75	1	0	-7.394600	-1.622198	-2.633890
76	6	0	-6.291097	-4.879053	-2.995243
77	1	0	-4.197629	-5.334713	-2.629981
78	1	0	-4.483162	-4.178089	-3.929544
79	1	0	-8.192452	-3.887462	-3.356009
80	1	0	-6.857261	-3.300440	-4.352862
81	1	0	-6.444010	-5.678146	-3.723900
82	1	0	-6.610277	-5.263935	-2.019499
83	7	0	-5.441772	-2.204508	-2.289061
84	7	0	5.271836	1.046321	-1.578328
85	7	0	5.441898	2.204382	-2.289068
86	6	0	4.577252	3.333000	-1.965164
87	6	0	6.867393	2.534168	-2.350953
88	6	0	4.817121	4.487686	-2.934657
89	1	0	4.744563	3.655503	-0.921663
90	1	0	3.537486	3.012208	-2.051629
91	6	0	7.126087	3.650928	-3.351532
92	1	0	7.226409	2.836015	-1.352533
93	1	0	7.394743	1.622039	-2.633708
94	6	0	6.291294	4.878894	-2.995266
95	1	0	4.197795	5.334580	-2.630198
96	1	0	4.483434	4.177932	-3.929712
97	1	0	8.192669	3.887268	-3.355859
98	1	0	6.857543	3.300227	-4.352789
99	1	0	6.444277	5.677971	-3.723925
100	1	0	6.610392	5.263793	-2.019502

Structure 13aa ((*S*)-13aa) ($CHCl_3$)

Energy (Hartrees): = -2224.4282452
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.156420	-2.526193	-0.607514
2	6	0	-4.109877	-2.867708	-1.424483
3	6	0	-2.946518	-2.018271	-1.413580
4	6	0	-2.928310	-0.814245	-0.638107
5	6	0	-4.088650	-0.445043	0.141182
6	6	0	-5.154432	-1.329319	0.158961
7	6	0	4.230686	5.390803	-1.393197
8	6	0	-0.556214	2.033755	-2.972252
9	6	0	-4.211565	-4.129667	-2.269321
10	6	0	-1.712006	-0.063011	-0.646556
11	6	0	-0.608250	-0.433778	-1.394850
12	6	0	-0.646562	-1.621901	-2.166779
13	6	0	-1.790603	-2.376222	-2.160039
14	6	0	-5.407612	-4.092369	-3.232000
15	6	0	-4.230485	-5.390605	-1.394698
16	6	0	0.556592	-2.033196	-2.972544
17	6	0	-4.244221	0.841362	0.843642
18	6	0	4.244137	-0.841496	0.843996
19	6	0	0.608435	0.434056	-1.394699
20	6	0	0.646844	1.622312	-2.166416
21	6	0	1.790892	2.376620	-2.159422
22	6	0	2.946726	2.018525	-1.412905
23	6	0	2.928421	0.814366	-0.637644
24	6	0	1.712105	0.063153	-0.646344
25	6	0	4.211883	4.130071	-2.268123
26	6	0	5.408036	4.093027	-3.230679
27	6	0	4.110113	2.867929	-1.423569
28	6	0	5.156572	2.526247	-0.606561
29	6	0	5.154482	1.329252	0.159722
30	6	0	4.088675	0.445011	0.141703
31	1	0	3.507106	-1.608542	0.674583
32	1	0	1.787392	3.286095	-2.741387
33	1	0	-3.507205	1.608456	0.674389
34	1	0	-1.787031	-3.285597	-2.742161
35	1	0	6.877945	2.869993	0.094043
36	1	0	4.238182	6.285210	-2.022500
37	1	0	-3.328593	-4.195605	-2.900325
38	8	0	1.641122	-1.062082	0.116667
39	1	0	-5.371182	-4.961111	-3.895320
40	1	0	-5.380164	-3.193764	-3.853635
41	1	0	-6.356018	-4.111608	-2.696290
42	1	0	-4.237915	-6.284861	-2.024216
43	1	0	-3.344958	-5.433528	-0.755142
44	1	0	-5.116563	-5.412826	-0.758419
45	1	0	-0.850916	1.243220	-3.667820
46	1	0	-0.344793	2.938216	-3.543555
47	1	0	-1.416397	2.229554	-2.324774
48	8	0	-6.262625	-3.305859	-0.514428

49	1	0	-6.877848	-2.870110	0.092876
50	8	0	-6.283182	-1.137759	0.863527
51	1	0	-6.162766	-0.283394	1.376078
52	1	0	0.345260	-2.937592	-3.543981
53	1	0	1.416715	-2.229042	-2.325000
54	1	0	0.851335	-1.242561	-3.667980
55	8	0	-1.641115	1.062087	0.116666
56	8	0	6.283145	1.137556	0.864388
57	1	0	3.345083	5.433562	-0.753736
58	1	0	5.116688	5.412879	-0.756806
59	8	0	6.262785	3.305873	-0.513231
60	1	0	3.328983	4.196142	-2.899214
61	1	0	5.371690	4.961962	-3.893751
62	1	0	5.380644	3.194601	-3.852575
63	1	0	6.356385	4.112101	-2.694863
64	1	0	6.162620	0.283138	1.376830
65	1	0	-0.739066	1.411100	0.075952
66	1	0	0.739064	-1.411057	0.075833
67	7	0	-5.253079	1.026591	1.620324
68	6	0	-4.652631	3.347887	1.955836
69	6	0	-6.884294	2.440296	2.455086
70	6	0	-4.905272	4.497138	2.927878
71	1	0	-4.889648	3.648425	0.920473
72	1	0	-3.594806	3.082118	1.995069
73	6	0	-7.151489	3.554630	3.455221
74	1	0	-7.297803	2.713375	1.470547
75	1	0	-7.354099	1.507526	2.771545
76	6	0	-6.392285	4.817068	3.054881
77	1	0	-4.342666	5.369320	2.586618
78	1	0	-4.509476	4.214810	3.908709
79	1	0	-8.227429	3.739139	3.499092
80	1	0	-6.827899	3.227810	4.448862
81	1	0	-6.548653	5.611633	3.788233
82	1	0	-6.772829	5.180504	2.092911
83	7	0	-5.445270	2.178863	2.329832
84	7	0	5.252924	-1.026875	1.620734
85	7	0	5.444977	-2.179253	2.330103
86	6	0	4.652255	-3.348156	1.955911
87	6	0	6.883969	-2.440833	2.455415
88	6	0	4.904714	-4.497539	2.927844
89	1	0	4.889326	-3.648603	0.920534
90	1	0	3.594453	-3.082286	1.995088
91	6	0	7.150999	-3.555315	3.455428
92	1	0	7.297514	-2.713823	1.470866
93	1	0	7.353839	-1.508145	2.772021
94	6	0	6.391688	-4.817630	3.054906
95	1	0	4.342047	-5.369630	2.586448
96	1	0	4.508879	-4.215280	3.908679
97	1	0	8.226918	-3.739941	3.499330
98	1	0	6.827397	-3.228578	4.449093
99	1	0	6.547933	-5.612286	3.788185
100	1	0	6.772252	-5.181008	2.092922

Structure 13aa ((*S*)-13aa) (DMSO)

Energy (Hartrees): = -2224.4174605
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.157727	-2.507521	-0.599556
2	6	0	-4.124038	-2.845967	-1.434342
3	6	0	-2.957155	-2.000510	-1.431760
4	6	0	-2.923017	-0.804955	-0.643324
5	6	0	-4.073434	-0.434094	0.149881
6	6	0	-5.142978	-1.314297	0.173362
7	6	0	4.238697	5.367302	-1.420025
8	6	0	-0.519331	2.007465	-3.047267
9	6	0	-4.238285	-4.101585	-2.286448
10	6	0	-1.701183	-0.062543	-0.654775
11	6	0	-0.611740	-0.429078	-1.425749
12	6	0	-0.668454	-1.603617	-2.216522
13	6	0	-1.814975	-2.354533	-2.201304
14	6	0	-5.450859	-4.061243	-3.227054
15	6	0	-4.238550	-5.367335	-1.419681
16	6	0	0.519319	-2.007478	-3.047200
17	6	0	-4.217598	0.850325	0.859937
18	6	0	4.217610	-0.850279	0.859841
19	6	0	0.611744	0.429115	-1.425775
20	6	0	0.668453	1.603624	-2.216594
21	6	0	1.814986	2.354524	-2.201435
22	6	0	2.957182	2.000512	-1.431910
23	6	0	2.923045	0.804991	-0.643426

24	6	0	1.701203	0.062595	-0.654816
25	6	0	4.238342	4.101514	-2.286737
26	6	0	5.450866	4.061086	-3.227403
27	6	0	4.124088	2.845939	-1.434568
28	6	0	5.157798	2.507496	-0.599805
29	6	0	5.143045	1.314303	0.173161
30	6	0	4.073476	0.434127	0.149752
31	1	0	3.479634	-1.617170	0.691550
32	1	0	1.823414	3.255848	-2.796037
33	1	0	-3.479671	1.617252	0.691594
34	1	0	-1.823403	-3.255883	-2.795865
35	1	0	6.866486	2.838778	0.123498
36	1	0	4.256061	6.257138	-2.055468
37	1	0	-3.366842	-4.162949	-2.933331
38	8	0	1.609201	-1.043778	0.130790
39	1	0	-5.420637	-4.923735	-3.898617
40	1	0	-5.438017	-3.157434	-3.842005
41	1	0	-6.390487	-4.089933	-2.676239
42	1	0	-4.255910	-6.257200	-2.055083
43	1	0	-3.339913	-5.413470	-0.798643
44	1	0	-5.112164	-5.396032	-0.766282
45	1	0	-0.812873	1.202745	-3.727169
46	1	0	-0.290680	2.895488	-3.637319
47	1	0	-1.385821	2.229648	-2.416803
48	8	0	-6.266818	-3.281264	-0.493876
49	1	0	-6.866381	-2.838824	0.123819
50	8	0	-6.263370	-1.121223	0.889049
51	1	0	-6.133737	-0.263688	1.398298
52	1	0	0.290670	-2.895529	-3.637211
53	1	0	1.385824	-2.229625	-2.416743
54	1	0	0.812840	-1.202783	-3.727141
55	8	0	-1.609162	1.043852	0.130797
56	8	0	6.263456	1.121236	0.888821
57	1	0	3.340092	5.413500	-0.798947
58	1	0	5.112344	5.395994	-0.766671
59	8	0	6.266914	3.281212	-0.494193
60	1	0	3.366870	4.162882	-2.933579
61	1	0	5.420639	4.923547	-3.899005
62	1	0	5.437960	3.157248	-3.842311
63	1	0	6.390524	4.089769	-2.676639
64	1	0	6.133818	0.263731	1.398119
65	1	0	-0.715158	1.407372	0.048990
66	1	0	0.715193	-1.407297	0.049018
67	7	0	-5.222882	1.032240	1.642707
68	6	0	-4.623766	3.351165	1.986145
69	6	0	-6.857476	2.438680	2.480126
70	6	0	-4.885191	4.502117	2.953399
71	1	0	-4.857551	3.647332	0.949447
72	1	0	-3.565441	3.088803	2.032018
73	6	0	-7.129789	3.555896	3.475070
74	1	0	-7.266515	2.709288	1.493624
75	1	0	-7.327043	1.506149	2.798204
76	6	0	-6.373282	4.818320	3.071542
77	1	0	-4.323155	5.373859	2.610406
78	1	0	-4.493388	4.226247	3.937896
79	1	0	-8.206561	3.736274	3.513927
80	1	0	-6.809294	3.235045	4.471850
81	1	0	-6.535203	5.616283	3.800020
82	1	0	-6.750004	5.174664	2.105577
83	7	0	-5.415920	2.179664	2.358054
84	7	0	5.222905	-1.032224	1.642588
85	7	0	5.415889	-2.179624	2.357990
86	6	0	4.623612	-3.351078	1.986199
87	6	0	6.857431	-2.438757	2.479988
88	6	0	4.884998	-4.501997	2.953503
89	1	0	4.857307	-3.647323	0.949503
90	1	0	3.565313	-3.088623	2.032123
91	6	0	7.129710	-3.555940	3.474978
92	1	0	7.266386	-2.709455	1.493475
93	1	0	7.327099	-1.506249	2.797985
94	6	0	6.373068	-4.818322	3.071569
95	1	0	4.322865	-5.373709	2.610595
96	1	0	4.493282	-4.226035	3.938009
97	1	0	8.206469	-3.736410	3.513777
98	1	0	6.809306	-3.235005	4.471760
99	1	0	6.534966	-5.616258	3.800082
100	1	0	6.749697	-5.174753	2.105600

Structure (S)-13aa' (vacuum)

Energy (Hartrees): = -2224.3751986
No imaginary frequencies

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	4.953019	-2.918263	0.254082
2	6	0	3.838419	-3.284867	0.960218
3	6	0	2.755699	-2.339199	1.046667
4	6	0	2.877595	-1.035572	0.468792
5	6	0	4.106697	-0.658396	-0.190829
6	6	0	5.095348	-1.619755	-0.304005
7	6	0	-3.590590	5.758531	0.736791
8	6	0	0.638944	1.765012	2.956362
9	6	0	3.782461	-4.674333	1.575722
10	6	0	1.726126	-0.195190	0.536905
11	6	0	0.561210	-0.570504	1.175943
12	6	0	0.463917	-1.851427	1.763583
13	6	0	1.540475	-2.694197	1.688652
14	6	0	4.916588	-4.909941	2.584035
15	6	0	3.749262	-5.762221	0.493067
16	6	0	-0.812632	-2.275048	2.439825
17	6	0	4.402264	0.700249	-0.670906
18	6	0	-4.412540	-0.654362	-0.646459
19	6	0	-0.584480	0.383279	1.222717
20	6	0	-0.542616	1.538274	2.049428
21	6	0	-1.565791	2.451026	1.977725
22	6	0	-2.716314	2.255170	1.169897
23	6	0	-2.834954	1.023035	0.461127
24	6	0	-1.696493	0.165798	0.434872
25	6	0	-3.659747	4.607181	1.750972
26	6	0	-4.800490	4.806286	2.758712
27	6	0	-3.745078	3.256479	1.059214
28	6	0	-4.829929	2.978256	0.266022
29	6	0	-4.999017	1.712869	-0.359885
30	6	0	-4.053338	0.713864	-0.241381
31	1	0	-3.845352	-1.466851	-0.207763
32	1	0	-1.482305	3.341562	2.583057
33	1	0	3.700333	1.481286	-0.431616
34	1	0	1.432255	-3.675130	2.125988
35	1	0	-6.500162	3.461995	-0.462048
36	1	0	-3.445919	6.706391	1.261337
37	1	0	2.858377	-4.765633	2.141650
38	8	0	-1.652622	-0.929368	-0.391164
39	1	0	4.780417	-5.880409	3.068772
40	1	0	4.909320	-4.138606	3.357448
41	1	0	5.889826	-4.901810	2.095748
42	1	0	3.645285	-6.748067	0.954276
43	1	0	2.903687	-5.607919	-0.181204
44	1	0	4.667082	-5.751137	-0.095400
45	1	0	0.819217	0.887975	3.582567
46	1	0	0.469464	2.628559	3.599645
47	1	0	1.551546	1.936016	2.378540
48	8	0	5.995491	-3.771003	0.074786
49	1	0	6.663713	-3.290376	-0.431691
50	8	0	6.277662	-1.424046	-0.916674
51	1	0	6.265079	-0.493890	-1.280158
52	1	0	-1.138360	-1.532142	3.172727
53	1	0	-0.680600	-3.230639	2.948080
54	1	0	-1.615952	-2.382084	1.705278
55	8	0	1.776339	1.033305	-0.067704
56	8	0	-6.171481	1.572397	-1.007926
57	1	0	-2.753424	5.617477	0.049512
58	1	0	-4.509423	5.823222	0.154570
59	8	0	-5.826974	3.882293	0.088593
60	1	0	-2.732577	4.644155	2.318916
61	1	0	-4.662744	5.750232	3.292124
62	1	0	-4.813509	3.997348	3.492449
63	1	0	-5.766216	4.833225	2.254732
64	1	0	-6.176765	0.672354	-1.416497
65	1	0	0.888289	1.411015	-0.045793
66	1	0	-2.107176	-0.719027	-1.213279
67	7	0	5.476050	0.932925	-1.339609
68	6	0	5.013624	3.308835	-1.334670
69	6	0	7.231905	2.367285	-1.796894
70	6	0	5.401686	4.588046	-2.072040
71	1	0	5.165694	3.423517	-0.246033
72	1	0	3.953003	3.113031	-1.503298
73	6	0	7.639608	3.612977	-2.569767
74	1	0	7.572617	2.448104	-0.750639
75	1	0	7.683909	1.472093	-2.226311
76	6	0	6.907191	4.834856	-2.020738
77	1	0	4.851755	5.424404	-1.633921
78	1	0	5.084197	4.496440	-3.115277
79	1	0	8.722643	3.738878	-2.499747
80	1	0	7.387727	3.474283	-3.625804
81	1	0	7.167374	5.731994	-2.586899
82	1	0	7.215088	5.005974	-0.982306
83	7	0	5.780781	2.175363	-1.835720
84	7	0	-5.407681	-0.860466	-1.434530
85	7	0	-5.788017	-2.108227	-1.831844
86	6	0	-5.226684	-3.254517	-1.126628

87	6	0	-7.240715	-2.149687	-2.016508
88	6	0	-5.651602	-4.559884	-1.794254
89	1	0	-5.534329	-3.236790	-0.065894
90	1	0	-4.137291	-3.185122	-1.157968
91	6	0	-7.666966	-3.427944	-2.722779
92	1	0	-7.742818	-2.078014	-1.037306
93	1	0	-7.512402	-1.267884	-2.598479
94	6	0	-7.167003	-4.647562	-1.952072
95	1	0	-5.268260	-5.394020	-1.202397
96	1	0	-5.180844	-4.614275	-2.780611
97	1	0	-8.755469	-3.438168	-2.813712
98	1	0	-7.248587	-3.432930	-3.734064
99	1	0	-7.443694	-5.571051	-2.464909
100	1	0	-7.639326	-4.671945	-0.962849

Structure (S)-13aa' ($CHCl_3$)

Energy (Hartrees): = -2224.4212726
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.919871	-2.932419	0.225127
2	6	0	3.817199	-3.286842	0.959216
3	6	0	2.752648	-2.323598	1.083536
4	6	0	2.866086	-1.032768	0.476109
5	6	0	4.082487	-0.667961	-0.211729
6	6	0	5.061536	-1.637591	-0.342854
7	6	0	-3.585954	5.760016	0.679080
8	6	0	0.667558	1.890532	2.898580
9	6	0	3.757460	-4.676095	1.577258
10	6	0	1.714236	-0.189505	0.533824
11	6	0	0.570412	-0.533245	1.226932
12	6	0	0.497279	-1.785599	1.880738
13	6	0	1.563783	-2.642486	1.793932
14	6	0	4.875391	-4.893792	2.606213
15	6	0	3.746988	-5.776359	0.506954
16	6	0	-0.744498	-2.166308	2.640747
17	6	0	4.389769	0.697707	-0.669186
18	6	0	-4.407224	-0.684160	-0.616019
19	6	0	-0.579754	0.418172	1.254612
20	6	0	-0.531013	1.606167	2.032684
21	6	0	-1.564946	2.505740	1.944804
22	6	0	-2.725622	2.269714	1.161119
23	6	0	-2.840035	1.017412	0.483721
24	6	0	-1.695305	0.164685	0.480285
25	6	0	-3.688819	4.624258	1.706373
26	6	0	-4.851510	4.845354	2.683430
27	6	0	-3.761138	3.263131	1.031370
28	6	0	-4.839871	2.964852	0.235995
29	6	0	-5.001321	1.686027	-0.365206
30	6	0	-4.055221	0.689817	-0.217642
31	1	0	-3.851185	-1.498473	-0.166945
32	1	0	-1.473808	3.422828	2.508250
33	1	0	3.724682	1.492805	-0.373383
34	1	0	1.469386	-3.600565	2.283062
35	1	0	-6.507940	3.446614	-0.521436
36	1	0	-3.452201	6.716104	1.192513
37	1	0	2.821718	-4.772803	2.121825
38	8	0	-1.643202	-0.958963	-0.300113
39	1	0	4.754710	-5.869849	3.084716
40	1	0	4.837324	-4.128513	3.385766
41	1	0	5.859550	-4.860484	2.138498
42	1	0	3.618567	-6.754102	0.979819
43	1	0	2.920708	-5.627807	-0.192871
44	1	0	4.678517	-5.789609	-0.059537
45	1	0	0.833671	1.083214	3.616755
46	1	0	0.530192	2.821784	3.449053
47	1	0	1.577632	1.978011	2.297906
48	8	0	5.951583	-3.795927	0.036464
49	1	0	6.622041	-3.338545	-0.490808
50	8	0	6.232790	-1.446788	-0.977228
51	1	0	6.215540	-0.514056	-1.342481
52	1	0	-0.991889	-1.414423	3.395370
53	1	0	-0.610958	-3.126153	3.141402
54	1	0	-1.602654	-2.246728	1.967335
55	8	0	1.752000	0.996425	-0.142174
56	8	0	-6.165092	1.530290	-1.023183
57	1	0	-2.728878	5.607621	0.018153
58	1	0	-4.486518	5.822729	0.067200
59	8	0	-5.833755	3.865856	0.031875
60	1	0	-2.779791	4.664794	2.302011
61	1	0	-4.715026	5.793026	3.211645

62	1	0	-4.889676	4.045966	3.427718
63	1	0	-5.808624	4.879147	2.162910
64	1	0	-6.159870	0.619467	-1.419369
65	1	0	0.867530	1.387442	-0.129380
66	1	0	-2.094821	-0.795497	-1.137211
67	7	0	5.442018	0.915791	-1.375941
68	6	0	5.076192	3.306366	-1.280597
69	6	0	7.237878	2.291608	-1.861935
70	6	0	5.485470	4.589642	-1.997856
71	1	0	5.283965	3.378659	-0.198816
72	1	0	4.002062	3.159910	-1.408262
73	6	0	7.663029	3.544198	-2.612934
74	1	0	7.615184	2.329423	-0.826801
75	1	0	7.639652	1.393627	-2.334317
76	6	0	7.000023	4.776892	-2.002767
77	1	0	4.986575	5.431450	-1.511740
78	1	0	5.121432	4.542538	-3.029123
79	1	0	8.752124	3.624830	-2.578281
80	1	0	7.369082	3.448188	-3.663236
81	1	0	7.270599	5.677356	-2.559070
82	1	0	7.356671	4.908936	-0.974497
83	7	0	5.776305	2.156798	-1.848337
84	7	0	-5.393633	-0.885447	-1.416791
85	7	0	-5.780687	-2.123953	-1.825773
86	6	0	-5.240988	-3.282004	-1.117661
87	6	0	-7.233571	-2.148887	-2.033441
88	6	0	-5.669696	-4.577350	-1.801124
89	1	0	-5.568670	-3.264839	-0.064104
90	1	0	-4.150898	-3.222740	-1.130964
91	6	0	-7.660275	-3.418947	-2.752842
92	1	0	-7.745934	-2.078529	-1.060389
93	1	0	-7.488906	-1.261635	-2.615034
94	6	0	-7.183150	-4.648348	-1.983370
95	1	0	-5.305003	-5.417557	-1.205856
96	1	0	-5.183131	-4.632816	-2.780285
97	1	0	-8.747783	-3.416311	-2.857254
98	1	0	-7.229303	-3.422361	-3.759366
99	1	0	-7.459439	-5.564891	-2.509502
100	1	0	-7.671128	-4.674798	-1.001696

Structure (S)-13aa' (DMSO)

Energy (Hartrees): = -2224.4112781
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.920148	-2.950901	0.229374
2	6	0	3.800035	-3.306728	0.936627
3	6	0	2.734806	-2.341280	1.040852
4	6	0	2.861423	-1.051143	0.433711
5	6	0	4.091681	-0.686330	-0.228990
6	6	0	5.073918	-1.656068	-0.337150
7	6	0	-3.650795	5.798526	0.601460
8	6	0	0.667890	1.857645	2.863448
9	6	0	3.724307	-4.694370	1.555792
10	6	0	1.711662	-0.203423	0.472555
11	6	0	0.561822	-0.537725	1.160390
12	6	0	0.477147	-1.786662	1.819659
13	6	0	1.536993	-2.653720	1.740241
14	6	0	4.803647	-4.898694	2.627067
15	6	0	3.763430	-5.801229	0.493480
16	6	0	-0.768055	-2.150270	2.581467
17	6	0	4.413363	0.681308	-0.673074
18	6	0	-4.435856	-0.664663	-0.619824
19	6	0	-0.579391	0.423795	1.186382
20	6	0	-0.523045	1.601912	1.978980
21	6	0	-1.545902	2.514250	1.894687
22	6	0	-2.707257	2.292407	1.107161
23	6	0	-2.838576	1.040556	0.431516
24	6	0	-1.695738	0.184428	0.408592
25	6	0	-3.630102	4.665057	1.636448
26	6	0	-4.703559	4.863319	2.714348
27	6	0	-3.736111	3.293584	0.987590
28	6	0	-4.847083	2.985245	0.241642
29	6	0	-5.027489	1.703394	-0.347927
30	6	0	-4.072563	0.710681	-0.234810
31	1	0	-3.869529	-1.482200	-0.188712
32	1	0	-1.452607	3.421892	2.473351
33	1	0	3.754164	1.482485	-0.379088
34	1	0	1.432791	-3.609024	2.233324
35	1	0	-6.546095	3.443293	-0.445053
36	1	0	-3.471152	6.754300	1.101193

37	1	0	2.768385	-4.797029	2.062520
38	8	0	-1.644144	-0.922635	-0.390565
39	1	0	4.675349	-5.875677	3.101436
40	1	0	4.727569	-4.134253	3.404928
41	1	0	5.804940	-4.854600	2.197432
42	1	0	3.620460	-6.775321	0.969461
43	1	0	2.964455	-5.664909	-0.240173
44	1	0	4.716685	-5.815567	-0.035427
45	1	0	0.807865	1.040632	3.576835
46	1	0	0.538179	2.786543	3.419463
47	1	0	1.589050	1.935352	2.278332
48	8	0	5.959886	-3.809156	0.066890
49	1	0	6.640706	-3.341189	-0.436955
50	8	0	6.258689	-1.465342	-0.943718
51	1	0	6.247508	-0.529712	-1.306942
52	1	0	-0.993714	-1.398786	3.343791
53	1	0	-0.650311	-3.116571	3.073443
54	1	0	-1.632939	-2.206498	1.914147
55	8	0	1.758759	0.972229	-0.216450
56	8	0	-6.215038	1.541542	-0.958837
57	1	0	-2.865910	5.657644	-0.146354
58	1	0	-4.609877	5.856901	0.086534
59	8	0	-5.857013	3.876137	0.078168
60	1	0	-2.667294	4.736753	2.136788
61	1	0	-4.567412	5.832175	3.202822
62	1	0	-4.633703	4.086343	3.480232
63	1	0	-5.705669	4.834173	2.284020
64	1	0	-6.218932	0.626156	-1.349378
65	1	0	0.882732	1.381755	-0.183635
66	1	0	-2.175372	-0.777838	-1.183552
67	7	0	5.477922	0.891341	-1.364363
68	6	0	5.161506	3.284807	-1.231856
69	6	0	7.306147	2.231588	-1.821926
70	6	0	5.608834	4.573697	-1.914468
71	1	0	5.361411	3.324926	-0.147549
72	1	0	4.085582	3.168636	-1.373365
73	6	0	7.764402	3.492279	-2.538234
74	1	0	7.675425	2.236930	-0.783972
75	1	0	7.690501	1.336384	-2.314096
76	6	0	7.126863	4.724206	-1.900838
77	1	0	5.124054	5.413985	-1.412061
78	1	0	5.254570	4.561902	-2.950338
79	1	0	8.854839	3.544681	-2.494191
80	1	0	7.476510	3.431757	-3.593129
81	1	0	7.424201	5.631696	-2.431562
82	1	0	7.477421	4.819576	-0.866531
83	7	0	5.840003	2.129695	-1.818503
84	7	0	-5.451766	-0.862335	-1.384645
85	7	0	-5.859017	-2.095153	-1.781891
86	6	0	-5.287644	-3.259600	-1.108732
87	6	0	-7.320204	-2.116556	-1.930808
88	6	0	-5.747378	-4.547955	-1.784237
89	1	0	-5.569832	-3.251250	-0.042529
90	1	0	-4.199296	-3.198455	-1.170567
91	6	0	-7.778298	-3.382264	-2.637812
92	1	0	-7.790153	-2.051481	-0.936853
93	1	0	-7.598013	-1.225715	-2.496821
94	6	0	-7.267098	-4.616725	-1.899560
95	1	0	-5.357130	-5.393041	-1.212556
96	1	0	-5.304583	-4.596134	-2.784435
97	1	0	-8.869497	-3.378066	-2.690872
98	1	0	-7.395277	-3.379815	-3.663693
99	1	0	-7.567529	-5.529057	-2.419995
100	1	0	-7.709906	-4.649985	-0.897097

Structure (R)-13aa (vacuum)

Energy (Hartrees): = -2224.3843705
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.549143	-1.164956	-1.556803
2	6	0	-4.527729	-1.878320	-2.126525
3	6	0	-3.222293	-1.774371	-1.528225
4	6	0	-2.997863	-0.904632	-0.413048
5	6	0	-4.082667	-0.100528	0.098452
6	6	0	-5.332158	-0.276501	-0.469191
7	6	0	5.756594	-3.924060	2.951991
8	6	0	-0.236156	-3.362885	2.017854
9	6	0	-4.827790	-2.761392	-3.327713
10	6	0	-1.693109	-0.928509	0.165573
11	6	0	-0.662615	-1.697926	-0.344525

12	6	0	-0.888269	-2.520932	-1.474670
13	6	0	-2.140459	-2.547749	-2.028395
14	6	0	-5.376624	-1.957168	-4.515616
15	6	0	-5.757016	-3.924154	-2.951459
16	6	0	0.236053	-3.363226	-2.017448
17	6	0	-3.922215	0.947671	1.118163
18	6	0	3.922272	0.947393	-1.118387
19	6	0	0.662587	-1.697898	0.344660
20	6	0	0.888202	-2.520723	1.474944
21	6	0	2.140384	-2.547490	2.028688
22	6	0	3.222253	-1.774233	1.528401
23	6	0	2.997864	-0.904677	0.413072
24	6	0	1.693113	-0.928602	-0.165556
25	6	0	4.827727	-2.760958	3.328090
26	6	0	5.376996	-1.956532	4.515652
27	6	0	4.527682	-1.878119	2.126730
28	6	0	5.549111	-1.164833	1.556940
29	6	0	5.332163	-0.276557	0.469173
30	6	0	4.082691	-0.100672	-0.098534
31	1	0	2.922361	1.192266	-1.435848
32	1	0	2.296902	-3.207737	2.867747
33	1	0	-2.922290	1.192620	1.435521
34	1	0	-2.297015	-3.208137	-2.867337
35	1	0	7.354408	-0.644103	1.490144
36	1	0	5.906902	-4.576744	3.815859
37	1	0	-3.897052	-3.204338	-3.674022
38	8	0	1.458746	-0.191666	-1.290411
39	1	0	-5.477827	-2.611580	-5.385363
40	1	0	-4.695865	-1.144608	-4.779097
41	1	0	-6.353135	-1.531365	-4.289630
42	1	0	-5.907360	-4.577024	-3.815180
43	1	0	-5.322394	-4.518317	-2.144418
44	1	0	-6.729353	-3.555000	-2.624940
45	1	0	-1.075446	-2.740091	2.340723
46	1	0	0.100073	-3.955977	2.868321
47	1	0	-0.622825	-4.039434	1.250615
48	8	0	-6.819527	-1.245501	-2.025566
49	1	0	-7.354463	-0.644319	-1.489922
50	8	0	-6.440515	0.378146	-0.080583
51	1	0	-6.178365	0.962421	0.686287
52	1	0	-0.100207	-3.956452	-2.867811
53	1	0	0.622707	-4.039659	-1.250099
54	1	0	1.075361	-2.740517	-2.340433
55	8	0	-1.458710	-0.191408	1.290313
56	8	0	6.440540	0.377989	0.080454
57	1	0	5.321686	-4.518321	2.145177
58	1	0	6.728976	-3.555252	2.625221
59	8	0	6.819456	-1.245233	2.025831
60	1	0	3.896947	-3.203588	3.674685
61	1	0	5.478270	-2.610730	5.385551
62	1	0	4.696468	-1.143759	4.779069
63	1	0	6.353545	-1.530992	4.289316
64	1	0	6.178434	0.962046	-0.686598
65	1	0	-0.533791	-0.321183	1.540936
66	1	0	0.533823	-0.321444	-1.541017
67	7	0	-4.954291	1.554959	1.587546
68	6	0	-3.545526	3.063235	2.850353
69	6	0	-5.898335	3.532231	2.324801
70	6	0	-3.614343	4.037256	4.024540
71	1	0	-3.128665	3.558580	1.954717
72	1	0	-2.881381	2.237890	3.113972
73	6	0	-6.010498	4.480052	3.509779
74	1	0	-5.663489	4.103193	1.410618
75	1	0	-6.835846	3.000879	2.155221
76	6	0	-4.656877	5.127344	3.792881
77	1	0	-2.622370	4.468001	4.179646
78	1	0	-3.873062	3.473992	4.926321
79	1	0	-6.770975	5.234330	3.294712
80	1	0	-6.339845	3.915112	4.387467
81	1	0	-4.714885	5.790158	4.659013
82	1	0	-4.361438	5.741317	2.933798
83	7	0	-4.866025	2.519655	2.556512
84	7	0	4.954354	1.554737	-1.587685
85	7	0	4.866127	2.519347	-2.556739
86	6	0	3.545614	3.062766	-2.850816
87	6	0	5.898299	3.532049	-2.324962
88	6	0	3.614501	4.036698	-4.025073
89	1	0	3.128571	3.558139	-1.955281
90	1	0	2.881593	2.237331	-3.114466
91	6	0	6.010534	4.479786	-3.510000
92	1	0	5.663262	4.103060	-1.410859
93	1	0	6.835841	3.000807	-2.155205
94	6	0	4.656886	5.126914	-3.793351
95	1	0	2.622505	4.467326	-4.180360
96	1	0	3.873412	3.473387	-4.926770
97	1	0	6.770901	5.234161	-3.294884
98	1	0	6.340067	3.914810	-4.387594
99	1	0	4.714951	5.789664	-4.659527

100	1	0	4.361258	5.740925	-2.934360

Structure (R)-13aa ($CHCl_3$)

Energy (Hartrees): = -2224.4274525
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.607797	-1.246465	1.316938
2	6	0	4.624007	-1.990931	1.915396
3	6	0	3.286979	-1.879676	1.390128
4	6	0	2.995739	-0.962278	0.330638
5	6	0	4.038038	-0.107601	-0.186884
6	6	0	5.321709	-0.303306	0.292432
7	6	0	-5.872595	-4.083203	-2.569160
8	6	0	0.126143	-3.530943	-1.970117
9	6	0	4.992749	-2.924438	3.059174
10	6	0	1.671481	-0.993430	-0.204790
11	6	0	0.675953	-1.798977	0.317304
12	6	0	0.962477	-2.658626	1.406466
13	6	0	2.239410	-2.692793	1.903381
14	6	0	5.638318	-2.182895	4.238829
15	6	0	5.871910	-4.083172	2.570106
16	6	0	-0.126737	-3.530429	1.970584
17	6	0	3.801534	1.018512	-1.106749
18	6	0	-3.801359	1.019164	1.106283
19	6	0	-0.676287	-1.798967	-0.317256
20	6	0	-0.962948	-2.658861	-1.406190
21	6	0	-2.239904	-2.693013	-1.903052
22	6	0	-3.287363	-1.879649	-1.389966
23	6	0	-2.995971	-0.962005	-0.330735
24	6	0	-1.671705	-0.993167	0.204658
25	6	0	-4.993356	-2.924689	-3.058611
26	6	0	-5.638942	-2.183404	-4.238419
27	6	0	-4.624436	-1.990904	-1.915117
28	6	0	-5.608103	-1.246156	-1.316807
29	6	0	-5.321854	-0.302742	-0.292578
30	6	0	-4.038131	-0.107077	0.186637
31	1	0	-2.781701	1.303186	1.312678
32	1	0	-2.440214	-3.387263	-2.705244
33	1	0	2.781950	1.302655	-1.313334
34	1	0	2.439612	-3.386856	2.705763
35	1	0	-7.414534	-0.707234	-1.187151
36	1	0	-6.076994	-4.774311	-3.391619
37	1	0	4.080526	-3.365779	3.453319
38	8	0	-1.400336	-0.227482	1.296983
39	1	0	5.769749	-2.873729	5.076147
40	1	0	5.002418	-1.360751	4.576980
41	1	0	6.614243	-1.777568	3.973920
42	1	0	6.076191	-4.774068	3.392773
43	1	0	5.371049	-4.640354	1.774138
44	1	0	6.825163	-3.716116	2.186216
45	1	0	0.962570	-2.927269	-2.335391
46	1	0	-0.249063	-4.133985	-2.797455
47	1	0	0.529539	-4.201934	-1.205766
48	8	0	6.903792	-1.345692	1.706412
49	1	0	7.414308	-0.707816	1.187218
50	8	0	6.396985	0.387880	-0.124287
51	1	0	6.078178	1.013098	-0.840875
52	1	0	0.248382	-4.133340	2.798057
53	1	0	-0.530226	-4.201532	1.206381
54	1	0	-0.963078	-2.926553	2.335723
55	8	0	1.400214	-0.228015	-1.297330
56	8	0	-6.397033	0.388722	0.123923
57	1	0	-5.371734	-4.640207	-1.773068
58	1	0	-6.825788	-3.715951	-2.185310
59	8	0	-6.904128	-1.345324	-1.706192
60	1	0	-4.081207	-3.366230	-3.452702
61	1	0	-5.770510	-2.874453	-5.075539
62	1	0	-5.002987	-1.361415	-4.576846
63	1	0	-6.614805	-1.777905	-3.973543
64	1	0	-6.078106	1.014237	0.840204
65	1	0	0.474573	-0.361621	-1.548300
66	1	0	-0.474705	-0.361115	1.547970
67	7	0	4.802803	1.648886	-1.611085
68	6	0	3.345366	3.310740	-2.592358
69	6	0	5.761431	3.650069	-2.255934
70	6	0	3.345960	4.395740	-3.665902
71	1	0	3.036788	3.726070	-1.617142
72	1	0	2.626145	2.538745	-2.872005
73	6	0	5.795547	4.709647	-3.346327
74	1	0	5.638746	4.129694	-1.271293

75	1	0	6.688449	3.074683	-2.237384
76	6	0	4.448969	5.423479	-3.430421
77	1	0	2.361603	4.869572	-3.678016
78	1	0	3.493894	3.921280	-4.641244
79	1	0	6.602934	5.413067	-3.130102
80	1	0	6.019143	4.229581	-4.304553
81	1	0	4.453576	6.167147	-4.230774
82	1	0	4.260461	5.955749	-2.490564
83	7	0	4.666636	2.697303	-2.478365
84	7	0	-4.802445	1.649617	1.610888
85	7	0	-4.665967	2.698047	2.478106
86	6	0	-3.344636	3.311429	2.591672
87	6	0	-5.760791	3.650856	2.255995
88	6	0	-3.344847	4.396449	3.665195
89	1	0	-3.036344	3.726727	1.616352
90	1	0	-2.625361	2.539408	2.871109
91	6	0	-5.794521	4.710455	3.346380
92	1	0	-5.638391	4.130456	1.271308
93	1	0	-6.687840	3.075511	2.237744
94	6	0	-4.447886	5.424231	3.430041
95	1	0	-2.360466	4.870240	3.676992
96	1	0	-3.492496	3.922013	4.640592
97	1	0	-6.601946	5.413905	3.130392
98	1	0	-6.017840	4.230416	4.304685
99	1	0	-4.452213	6.167913	4.230383
100	1	0	-4.259651	5.956477	2.490116

Structure (R)-13aa (DMSO)

Energy (Hartrees): = -2224.4171088
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.620924	-1.258874	1.241243
2	6	0	4.653821	-2.023760	1.842158
3	6	0	3.307630	-1.916602	1.339669
4	6	0	2.991349	-0.982541	0.302167
5	6	0	4.016085	-0.107425	-0.215487
6	6	0	5.309570	-0.299688	0.238773
7	6	0	-5.935200	-4.110661	-2.445560
8	6	0	0.078288	-3.614825	-1.936048
9	6	0	5.047675	-2.972337	2.964589
10	6	0	1.660067	-1.016885	-0.215967
11	6	0	0.681129	-1.842754	0.306295
12	6	0	0.992589	-2.720163	1.374108
13	6	0	2.276433	-2.750606	1.853604
14	6	0	5.697781	-2.241873	4.147964
15	6	0	5.935342	-4.110575	2.445534
16	6	0	-0.078229	-3.614851	1.936012
17	6	0	3.751623	1.041146	-1.100029
18	6	0	-3.751623	1.041106	1.100042
19	6	0	-0.681086	-1.842756	-0.306309
20	6	0	-0.992538	-2.720154	-1.374133
21	6	0	-2.276382	-2.750603	-1.853630
22	6	0	-3.307588	-1.916616	-1.339682
23	6	0	-2.991314	-0.982564	-0.302169
24	6	0	-1.660031	-1.016903	0.215965
25	6	0	-5.047629	-2.972346	-2.964612
26	6	0	-5.697843	-2.241872	-4.147920
27	6	0	-4.653780	-2.023786	-1.842166
28	6	0	-5.620889	-1.258911	-1.241248
29	6	0	-5.309542	-0.299730	-0.238771
30	6	0	-4.016061	-0.107462	0.215493
31	1	0	-2.726982	1.334108	1.267193
32	1	0	-2.492981	-3.455461	-2.642584
33	1	0	2.726974	1.334121	-1.267179
34	1	0	2.493040	-3.455472	2.642550
35	1	0	-7.414876	-0.699406	-1.084016
36	1	0	-6.160030	-4.810418	-3.255177
37	1	0	4.146826	-3.433082	3.361985
38	8	0	-1.367655	-0.235529	1.289973
39	1	0	5.852135	-2.946050	4.970088
40	1	0	5.052795	-1.437526	4.511209
41	1	0	6.663123	-1.815159	3.877170
42	1	0	6.160178	-4.810350	3.255133
43	1	0	5.430200	-4.664285	1.649541
44	1	0	6.878151	-3.725860	2.052936
45	1	0	0.920832	-3.028172	-2.314973
46	1	0	-0.314217	-4.220565	-2.753252
47	1	0	0.474625	-4.283924	-1.165862
48	8	0	6.924210	-1.349253	1.606740
49	1	0	7.414910	-0.699377	1.083986

50	8	0	6.370525	0.410399	-0.180969
51	1	0	6.030504	1.045569	-0.880792
52	1	0	0.314280	-4.220595	2.753210
53	1	0	-0.474560	-4.283946	1.165819
54	1	0	-0.920779	-3.028209	2.314942
55	8	0	1.367685	-0.235494	-1.289963
56	8	0	-6.370497	0.410358	0.180970
57	1	0	-5.429984	-4.664372	-1.649615
58	1	0	-6.878015	-3.726024	-2.052901
59	8	0	-6.924169	-1.349280	-1.606767
60	1	0	-4.146773	-3.433023	-3.362071
61	1	0	-5.852214	-2.946026	-4.970061
62	1	0	-5.052920	-1.437479	-4.511175
63	1	0	-6.663189	-1.815215	-3.877049
64	1	0	-6.030475	1.045531	0.880789
65	1	0	0.443597	-0.386340	-1.538017
66	1	0	-0.443565	-0.386372	1.538025
67	7	0	4.741094	1.679799	-1.617653
68	6	0	3.269312	3.378982	-2.509735
69	6	0	5.697224	3.691927	-2.232290
70	6	0	3.249784	4.491307	-3.554441
71	1	0	2.996598	3.771276	-1.515226
72	1	0	2.533944	2.621885	-2.787755
73	6	0	5.709819	4.779069	-3.295200
74	1	0	5.599166	4.147280	-1.234021
75	1	0	6.620899	3.110925	-2.251138
76	6	0	4.367211	5.504044	-3.323350
77	1	0	2.269345	4.972145	-3.524512
78	1	0	3.365991	4.042289	-4.546243
79	1	0	6.528080	5.470394	-3.080827
80	1	0	5.904632	4.324660	-4.272313
81	1	0	4.355626	6.268012	-4.104317
82	1	0	4.209454	6.011421	-2.364429
83	7	0	4.589011	2.751483	-2.451313
84	7	0	-4.741114	1.679730	1.617665
85	7	0	-4.589065	2.751418	2.451327
86	6	0	-3.269386	3.378959	2.509753
87	6	0	-5.697308	3.691827	2.232304
88	6	0	-3.249896	4.491280	3.554464
89	1	0	-2.996683	3.771266	1.515246
90	1	0	-2.533993	2.621885	2.787770
91	6	0	-5.709940	4.778964	3.295218
92	1	0	-5.599262	4.147186	1.234036
93	1	0	-6.620963	3.110795	2.251148
94	6	0	-4.367355	5.503982	3.323375
95	1	0	-2.269472	4.972150	3.524540
96	1	0	-3.366091	4.042254	4.546264
97	1	0	-6.528222	5.470264	3.080846
98	1	0	-5.904741	4.324545	4.272328
99	1	0	-4.355796	6.267947	4.104346
100	1	0	-4.209612	6.011369	2.364457

Structure (*R*)-13aa' (vacuum)

Energy (Hartrees): = -2224.3754405
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.925863	2.842290	-0.370817
2	6	0	-3.847458	3.156187	-1.159347
3	6	0	-2.789532	2.185848	-1.273214
4	6	0	-2.870270	0.951518	-0.564264
5	6	0	-4.078554	0.604508	0.138512
6	6	0	-5.054188	1.573836	0.259709
7	6	0	5.047444	-4.761288	-2.706635
8	6	0	-0.769267	-2.302823	-2.524255
9	6	0	-3.802494	4.509992	-1.848545
10	6	0	-1.707821	0.127532	-0.540682
11	6	0	-0.605856	0.375337	-1.334179
12	6	0	-0.601484	1.529215	-2.163501
13	6	0	-1.649173	2.413699	-2.086921
14	6	0	-3.793983	5.663970	-0.834953
15	6	0	-4.933884	4.663069	-2.874603
16	6	0	0.566326	1.786592	-3.080097
17	6	0	-4.395818	-0.776624	0.533305
18	6	0	4.387886	0.855858	0.492766
19	6	0	0.566794	-0.544932	-1.291762
20	6	0	0.500963	-1.833919	-1.866076
21	6	0	1.602090	-2.644983	-1.794347
22	6	0	2.813551	-2.248508	-1.169918
23	6	0	2.902230	-0.937555	-0.604447
24	6	0	1.726953	-0.130903	-0.667876

25	6	0	3.907969	-4.551796	-1.698609
26	6	0	3.903325	-5.636796	-0.612665
27	6	0	3.925861	-3.159825	-1.086979
28	6	0	5.032641	-2.756578	-0.388629
29	6	0	5.137484	-1.453038	0.166875
30	6	0	4.124783	-0.518819	0.041856
31	1	0	3.680335	1.618554	0.212908
32	1	0	1.516975	-3.633372	-2.219791
33	1	0	-3.813154	-1.567524	0.075155
34	1	0	-1.595515	3.304504	-2.695389
35	1	0	6.760687	-3.072821	0.282840
36	1	0	4.933707	-5.735260	-3.190097
37	1	0	-2.867211	4.583608	-2.399553
38	8	0	1.749779	1.101786	-0.070970
39	1	0	-3.673254	6.615287	-1.359303
40	1	0	-2.964541	5.554309	-0.132674
41	1	0	-4.724378	5.697716	-0.268992
42	1	0	-4.833287	5.616786	-3.398859
43	1	0	-4.895109	3.860206	-3.614162
44	1	0	-5.907990	4.638674	-2.386543
45	1	0	-0.611016	-3.254292	-3.032753
46	1	0	-1.130769	-1.573592	-3.253991
47	1	0	-1.557868	-2.436674	-1.778217
48	8	0	-5.953933	3.712126	-0.199614
49	1	0	-6.617824	3.267832	0.343415
50	8	0	-6.220979	1.398439	0.908137
51	1	0	-6.213286	0.487637	1.291786
52	1	0	0.365490	2.640203	-3.727629
53	1	0	0.769760	0.911408	-3.701642
54	1	0	1.476999	1.989968	-2.509876
55	8	0	-1.628632	-0.963783	0.286295
56	8	0	6.313658	-1.220627	0.778017
57	1	0	5.021019	-3.991372	-3.481025
58	1	0	6.020460	-4.729149	-2.219082
59	8	0	6.100793	-3.577353	-0.211040
60	1	0	2.986890	-4.668574	-2.264839
61	1	0	3.823395	-6.626468	-1.070471
62	1	0	3.055311	-5.501845	0.062752
63	1	0	4.821722	-5.600957	-0.026003
64	1	0	6.288657	-0.278659	1.107578
65	1	0	-2.112657	-0.779314	1.097578
66	1	0	0.851780	1.455580	-0.085044
67	7	0	-5.388007	-1.022543	1.314016
68	6	0	-4.945096	-3.398569	1.208354
69	6	0	-6.340403	-2.358606	2.947009
70	6	0	-5.634235	-4.737888	1.458708
71	1	0	-3.992120	-3.337004	1.764774
72	1	0	-4.713965	-3.320210	0.144476
73	6	0	-7.074839	-3.669181	3.187034
74	1	0	-5.512021	-2.258512	3.667860
75	1	0	-7.001940	-1.501807	3.078888
76	6	0	-6.153346	-4.849448	2.889395
77	1	0	-4.927743	-5.539622	1.232536
78	1	0	-6.471223	-4.831276	0.760029
79	1	0	-7.426792	-3.695313	4.220836
80	1	0	-7.953139	-3.710345	2.535307
81	1	0	-6.675624	-5.797660	3.032371
82	1	0	-5.308556	-4.836477	3.588144
83	7	0	-5.817318	-2.290796	1.579512
84	7	0	5.451687	1.128830	1.161955
85	7	0	5.795067	2.414180	1.504307
86	6	0	4.776845	3.446321	1.350684
87	6	0	6.438706	2.405617	2.820116
88	6	0	5.357752	4.822919	1.663756
89	1	0	3.908032	3.227563	1.997252
90	1	0	4.428909	3.441542	0.316177
91	6	0	7.067247	3.756935	3.128034
92	1	0	5.698643	2.151758	3.597946
93	1	0	7.189210	1.614269	2.804236
94	6	0	6.014163	4.859237	3.041040
95	1	0	4.559985	5.565532	1.587398
96	1	0	6.104509	5.063121	0.900499
97	1	0	7.520431	3.722459	4.121571
98	1	0	7.864665	3.950222	2.403708
99	1	0	6.459968	5.839155	3.226127
100	1	0	5.253273	4.697392	3.813680

Structure (*R*)-13aa' ($CHCl_3$)

Energy (Hartrees): = -2224.4213604
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-4.921495	2.872715	-0.324824
2	6	0	-3.831659	3.205749	-1.090926
3	6	0	-2.775470	2.234168	-1.219038
4	6	0	-2.873198	0.975113	-0.553477
5	6	0	-4.091991	0.613934	0.124151
6	6	0	-5.062109	1.586914	0.267639
7	6	0	4.918069	-4.805860	-2.710132
8	6	0	-0.734947	-2.176149	-2.681299
9	6	0	-3.776089	4.576250	-1.748058
10	6	0	-1.713407	0.143643	-0.543146
11	6	0	-0.597658	0.419501	-1.309725
12	6	0	-0.566405	1.611271	-2.083597
13	6	0	-1.614692	2.494313	-1.994848
14	6	0	-3.771647	5.709870	-0.712757
15	6	0	-4.895532	4.756809	-2.782425
16	6	0	0.626896	1.917102	-2.949808
17	6	0	-4.418466	-0.774026	0.491426
18	6	0	4.399391	0.810241	0.494956
19	6	0	0.566551	-0.514346	-1.286543
20	6	0	0.507307	-1.770810	-1.934614
21	6	0	1.587694	-2.611178	-1.854472
22	6	0	2.780872	-2.268229	-1.162887
23	6	0	2.880790	-0.970857	-0.568900
24	6	0	1.713191	-0.149190	-0.609202
25	6	0	3.822312	-4.604263	-1.654278
26	6	0	3.864802	-5.697353	-0.577265
27	6	0	3.866841	-3.208771	-1.049427
28	6	0	4.977061	-2.824590	-0.341956
29	6	0	5.102831	-1.522315	0.213468
30	6	0	4.105529	-0.571921	0.083261
31	1	0	3.724529	1.586794	0.171919
32	1	0	1.502790	-3.572970	-2.338161
33	1	0	-3.845301	-1.565432	0.023543
34	1	0	-1.538696	3.414056	-2.556228
35	1	0	6.707096	-3.185105	0.331382
36	1	0	4.806150	-5.787751	-3.178699
37	1	0	-2.837545	4.659209	-2.291223
38	8	0	1.740645	1.036065	0.068381
39	1	0	-3.635476	6.670383	-1.217130
40	1	0	-2.952125	5.583403	-0.000698
41	1	0	-4.708011	5.745888	-0.155561
42	1	0	-4.785661	5.722229	-3.284087
43	1	0	-4.850990	3.973143	-3.543025
44	1	0	-5.878551	4.724694	-2.311541
45	1	0	-0.579342	-3.120985	-3.203590
46	1	0	-1.020713	-1.417874	-3.415401
47	1	0	-1.577732	-2.299273	-1.995035
48	8	0	-5.944552	3.745219	-0.141728
49	1	0	-6.622635	3.304400	0.389554
50	8	0	-6.232129	1.398639	0.905019
51	1	0	-6.225135	0.475813	1.270535
52	1	0	0.469517	2.842066	-3.505531
53	1	0	0.810790	1.109775	-3.663522
54	1	0	1.534839	2.028013	-2.349834
55	8	0	-1.647411	-0.979517	0.236093
56	8	0	6.281422	-1.300893	0.823430
57	1	0	4.844809	-4.047335	-3.493723
58	1	0	5.912592	-4.748150	-2.267262
59	8	0	6.030772	-3.664493	-0.168136
60	1	0	2.874391	-4.726604	-2.172075
61	1	0	3.740466	-6.680005	-1.040984
62	1	0	3.057661	-5.560823	0.146965
63	1	0	4.813046	-5.690410	-0.039609
64	1	0	6.267488	-0.353073	1.146051
65	1	0	-2.129072	-0.834200	1.059604
66	1	0	0.849994	1.412902	0.067006
67	7	0	-5.416272	-1.018696	1.265418
68	6	0	-4.995293	-3.397464	1.149634
69	6	0	-6.397564	-2.350977	2.884992
70	6	0	-5.701206	-4.729723	1.386690
71	1	0	-4.051800	-3.346173	1.720975
72	1	0	-4.750234	-3.315196	0.089271
73	6	0	-7.142114	-3.657083	3.114090
74	1	0	-5.571855	-2.260885	3.608806
75	1	0	-7.055703	-1.491150	3.016888
76	6	0	-6.231060	-4.844427	2.812988
77	1	0	-4.999434	-5.535944	1.161375
78	1	0	-6.533756	-4.812494	0.680784
79	1	0	-7.495385	-3.683698	4.147581
80	1	0	-8.020440	-3.688197	2.461253
81	1	0	-6.766161	-5.787474	2.945253
82	1	0	-5.390297	-4.844964	3.516847
83	7	0	-5.862339	-2.281297	1.519190
84	7	0	5.466455	1.069978	1.164524
85	7	0	5.862313	2.349006	1.457001
86	6	0	4.880538	3.415066	1.271735
87	6	0	6.522846	2.364321	2.768023

88	6	0	5.512848	4.778865	1.535310
89	1	0	4.012848	3.248216	1.933417
90	1	0	4.525546	3.388029	0.240056
91	6	0	7.198009	3.703817	3.021667
92	1	0	5.781575	2.164404	3.558611
93	1	0	7.247912	1.549095	2.772722
94	6	0	6.181144	4.836979	2.905895
95	1	0	4.737893	5.543319	1.440756
96	1	0	6.260379	4.970534	0.758722
97	1	0	7.658109	3.686045	4.012495
98	1	0	7.995737	3.846998	2.285512
99	1	0	6.661879	5.806624	3.054878
100	1	0	5.421810	4.724378	3.688815

Structure (*R*)-13aa' (DMSO)

Energy (Hartrees): = -2224.4114316
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.918758	2.873117	-0.338255
2	6	0	-3.824110	3.203186	-1.099199
3	6	0	-2.769738	2.228486	-1.220693
4	6	0	-2.868476	0.975352	-0.543602
5	6	0	-4.090078	0.617531	0.130065
6	6	0	-5.061734	1.590751	0.261485
7	6	0	4.910457	-4.796651	-2.723859
8	6	0	-0.733930	-2.183286	-2.668451
9	6	0	-3.759750	4.570711	-1.761242
10	6	0	-1.707818	0.144527	-0.522870
11	6	0	-0.597548	0.410323	-1.301109
12	6	0	-0.570348	1.589449	-2.093851
13	6	0	-1.614807	2.477513	-2.009485
14	6	0	-3.786674	5.711432	-0.734653
15	6	0	-4.855305	4.737814	-2.822236
16	6	0	0.612687	1.873845	-2.980390
17	6	0	-4.421008	-0.768833	0.500725
18	6	0	4.401167	0.811471	0.499715
19	6	0	0.566608	-0.522734	-1.274453
20	6	0	0.507268	-1.780563	-1.919697
21	6	0	1.587480	-2.622044	-1.838202
22	6	0	2.783022	-2.273679	-1.152059
23	6	0	2.882534	-0.974618	-0.560238
24	6	0	1.712851	-0.154631	-0.597787
25	6	0	3.828286	-4.604949	-1.653012
26	6	0	3.892506	-5.700401	-0.580160
27	6	0	3.873491	-3.210631	-1.046281
28	6	0	4.988115	-2.820754	-0.348270
29	6	0	5.111878	-1.518116	0.208032
30	6	0	4.109554	-0.571142	0.085423
31	1	0	3.723030	1.589711	0.187744
32	1	0	1.501088	-3.585198	-2.319288
33	1	0	-3.853642	-1.567199	0.036162
34	1	0	-1.542545	3.387619	-2.587219
35	1	0	6.722401	-3.161915	0.310214
36	1	0	4.797477	-5.778108	-3.192823
37	1	0	-2.808095	4.657645	-2.279987
38	8	0	1.737294	1.026866	0.082745
39	1	0	-3.639682	6.667670	-1.243996
40	1	0	-2.984377	5.594486	-0.001338
41	1	0	-4.736636	5.750373	-0.201233
42	1	0	-4.743756	5.703653	-3.322672
43	1	0	-4.784432	3.954273	-3.581263
44	1	0	-5.849261	4.695479	-2.374745
45	1	0	-0.592627	-3.147410	-3.158542
46	1	0	-0.989388	-1.441625	-3.430855
47	1	0	-1.590072	-2.263724	-1.992458
48	8	0	-5.947430	3.741121	-0.167056
49	1	0	-6.622751	3.293372	0.361460
50	8	0	-6.234970	1.404171	0.892205
51	1	0	-6.222829	0.481094	1.262661
52	1	0	0.452520	2.790898	-3.548069
53	1	0	0.780715	1.053313	-3.683457
54	1	0	1.530204	1.989903	-2.395910
55	8	0	-1.631197	-0.960729	0.276027
56	8	0	6.291719	-1.292936	0.812105
57	1	0	4.821102	-4.037874	-3.505826
58	1	0	5.911141	-4.733584	-2.295318
59	8	0	6.049220	-3.652121	-0.182557
60	1	0	2.874419	-4.732928	-2.157840
61	1	0	3.768175	-6.681895	-1.046098
62	1	0	3.092806	-5.573203	0.154355

63	1	0	4.847286	-5.689426	-0.054023
64	1	0	6.271532	-0.342608	1.134836
65	1	0	-2.179778	-0.836766	1.060683
66	1	0	0.851223	1.414538	0.055045
67	7	0	-5.425952	-1.002703	1.269446
68	6	0	-5.029728	-3.384543	1.162782
69	6	0	-6.435267	-2.316335	2.887517
70	6	0	-5.754753	-4.706407	1.397945
71	1	0	-4.090929	-3.341891	1.741374
72	1	0	-4.777088	-3.306099	0.103884
73	6	0	-7.197460	-3.612688	3.110997
74	1	0	-5.613819	-2.236966	3.616646
75	1	0	-7.083620	-1.447609	3.010913
76	6	0	-6.298043	-4.810915	2.819761
77	1	0	-5.060438	-5.521226	1.180641
78	1	0	-6.582711	-4.782324	0.685571
79	1	0	-7.559073	-3.632812	4.141723
80	1	0	-8.071180	-3.635024	2.451218
81	1	0	-6.845828	-5.747194	2.948998
82	1	0	-5.463295	-4.818653	3.530529
83	7	0	-5.885606	-2.256805	1.525963
84	7	0	5.475016	1.067120	1.161025
85	7	0	5.875558	2.341041	1.459294
86	6	0	4.893883	3.410994	1.289913
87	6	0	6.552120	2.346386	2.763558
88	6	0	5.533416	4.770382	1.555678
89	1	0	4.035262	3.241724	1.961968
90	1	0	4.527152	3.390216	0.262251
91	6	0	7.230802	3.683410	3.018683
92	1	0	5.818092	2.144263	3.559797
93	1	0	7.276249	1.530032	2.754582
94	6	0	6.214106	4.817971	2.920116
95	1	0	4.759240	5.536768	1.472752
96	1	0	6.274215	4.965720	0.773284
97	1	0	7.699367	3.656691	4.005269
98	1	0	8.022922	3.831342	2.277094
99	1	0	6.697162	5.786248	3.070769
100	1	0	5.461503	4.700311	3.708628

Structure (*R*)-13aa enantiomer of (*S*)-13aa (vacuum)

Energy (Hartrees): = -2224.3849204
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.140635	-2.545977	-0.590114
2	6	0	4.073715	-2.911759	-1.367748
3	6	0	2.922713	-2.047038	-1.377163
4	6	0	2.918321	-0.828361	-0.624245
5	6	0	4.086314	-0.452619	0.138768
6	6	0	5.153518	-1.333515	0.150127
7	6	0	-4.280764	5.432609	-1.247457
8	6	0	0.564255	2.023249	-2.979089
9	6	0	4.156221	-4.206155	-2.162747
10	6	0	1.710858	-0.066087	-0.649828
11	6	0	0.604953	-0.437668	-1.394538
12	6	0	0.636298	-1.629387	-2.158993
13	6	0	1.770144	-2.396614	-2.131327
14	6	0	5.280727	-4.158623	-3.207564
15	6	0	4.280866	-5.432638	-1.247305
16	6	0	-0.564218	-2.023509	-2.978965
17	6	0	4.238263	0.830753	0.843456
18	6	0	-4.238285	-0.830728	0.843460
19	6	0	-0.604937	0.437527	-1.394564
20	6	0	-0.636266	1.629200	-2.159089
21	6	0	-1.770091	2.396462	-2.131445
22	6	0	-2.922656	2.046953	-1.377245
23	6	0	-2.918286	0.828308	-0.624277
24	6	0	-1.710838	0.066015	-0.649810
25	6	0	-4.156088	4.206100	-2.162861
26	6	0	-5.280537	4.158549	-3.207738
27	6	0	-4.073630	2.911713	-1.367840
28	6	0	-5.140566	2.545974	-0.590205
29	6	0	-5.153472	1.333534	0.150069
30	6	0	-4.086291	0.452618	0.138742
31	1	0	-3.468851	-1.572405	0.713678
32	1	0	-1.767489	3.304110	-2.715023
33	1	0	3.468847	1.572419	0.713576
34	1	0	1.767554	-3.304295	-2.714851
35	1	0	-6.869165	2.853898	0.081136
36	1	0	-4.262825	6.345888	-1.847922
37	1	0	3.231015	-4.333712	-2.719409

38	8	0	-1.637893	-1.079510	0.088708
39	1	0	5.268159	-5.072745	-3.806919
40	1	0	5.145916	-3.308410	-3.879927
41	1	0	6.256990	-4.072414	-2.731780
42	1	0	4.263009	-6.345934	-1.847747
43	1	0	3.448474	-5.471830	-0.541010
44	1	0	5.212586	-5.409268	-0.683272
45	1	0	0.853327	1.216826	-3.657943
46	1	0	0.352749	2.917063	-3.566100
47	1	0	1.428467	2.225193	-2.339407
48	8	0	6.255617	-3.314343	-0.506873
49	1	0	6.869233	-2.853854	0.081250
50	8	0	6.296684	-1.131280	0.828200
51	1	0	6.190466	-0.270885	1.326479
52	1	0	-0.352710	-2.917381	-3.565887
53	1	0	-1.428437	-2.225389	-2.339275
54	1	0	-0.853280	-1.217152	-3.657902
55	8	0	1.637905	1.079504	0.088585
56	8	0	-6.296637	1.131332	0.828161
57	1	0	-3.448424	5.471789	-0.541099
58	1	0	-5.212527	5.409291	-0.683495
59	8	0	-6.255535	3.314363	-0.506989
60	1	0	-3.230847	4.333646	-2.719469
61	1	0	-5.267947	5.072662	-3.807107
62	1	0	-5.145684	3.308326	-3.880082
63	1	0	-6.256823	4.072340	-2.732003
64	1	0	-6.190438	0.270961	1.326454
65	1	0	0.737934	1.425063	0.012599
66	1	0	-0.737927	-1.425088	0.012745
67	7	0	5.271787	1.046410	1.578356
68	6	0	4.577158	3.333120	1.965027
69	6	0	6.867264	2.534309	2.351055
70	6	0	4.816935	4.487831	2.934513
71	1	0	4.744587	3.655582	0.921534
72	1	0	3.537386	3.012330	2.051398
73	6	0	7.125870	3.651109	3.351612
74	1	0	7.226351	2.836120	1.352652
75	1	0	7.394600	1.622198	2.633890
76	6	0	6.291097	4.879053	2.995243
77	1	0	4.197629	5.334713	2.629981
78	1	0	4.483162	4.178089	3.929544
79	1	0	8.192452	3.887462	3.356009
80	1	0	6.857261	3.300440	4.352862
81	1	0	6.444010	5.678146	3.723900
82	1	0	6.610277	5.263935	2.019499
83	7	0	5.441772	2.204508	2.289061
84	7	0	-5.271836	-1.046321	1.578328
85	7	0	-5.441898	-2.204382	2.289068
86	6	0	-4.577252	-3.333000	1.965164
87	6	0	-6.867393	-2.534168	2.350953
88	6	0	-4.817121	-4.487686	2.934657
89	1	0	-4.744563	-3.655503	0.921663
90	1	0	-3.537486	-3.012208	2.051629
91	6	0	-7.126087	-3.650928	3.351532
92	1	0	-7.226409	-2.836015	1.352533
93	1	0	-7.394743	-1.622039	2.633708
94	6	0	-6.291294	-4.878894	2.995266
95	1	0	-4.197795	-5.334580	2.630198
96	1	0	-4.483434	-4.177932	3.929712
97	1	0	-8.192669	-3.887268	3.355859
98	1	0	-6.857543	-3.300227	4.352789
99	1	0	-6.444277	-5.677971	3.723925
100	1	0	-6.610392	-5.263793	2.019502

Structure (*R*)-13aa enantiomer of (*S*)-13aa ($CHCl_3$)

Energy (Hartrees): = -2224.4282452
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.156420	2.526193	-0.607514
2	6	0	-4.109877	2.867708	-1.424483
3	6	0	-2.946518	2.018271	-1.413580
4	6	0	-2.928310	0.814245	-0.638107
5	6	0	-4.088650	0.445043	0.141182
6	6	0	-5.154432	1.329319	0.158961
7	6	0	4.230686	-5.390803	-1.393197
8	6	0	-0.556214	-2.033755	-2.972252
9	6	0	-4.211565	4.129667	-2.269321
10	6	0	-1.712006	0.063011	-0.646556
11	6	0	-0.608250	0.433778	-1.394850
12	6	0	-0.646562	1.621901	-2.166779

13	6	0	-1.790603	2.376222	-2.160039
14	6	0	-5.407612	4.092369	-3.232000
15	6	0	-4.230485	5.390605	-1.394698
16	6	0	0.556592	2.033196	-2.972544
17	6	0	-4.244221	-0.841362	0.843642
18	6	0	4.244137	0.841496	0.843996
19	6	0	0.608435	-0.434056	-1.394699
20	6	0	0.646844	-1.622312	-2.166416
21	6	0	1.790892	-2.376620	-2.159422
22	6	0	2.946726	-2.018525	-1.412905
23	6	0	2.928421	-0.814366	-0.637644
24	6	0	1.712105	-0.063153	-0.646344
25	6	0	4.211883	-4.130071	-2.268123
26	6	0	5.408036	-4.093027	-3.230679
27	6	0	4.110113	-2.867929	-1.423569
28	6	0	5.156572	-2.526247	-0.606561
29	6	0	5.154482	-1.329252	0.159722
30	6	0	4.088675	-0.445011	0.141703
31	1	0	3.507106	1.608542	0.674583
32	1	0	1.787392	-3.286095	-2.741387
33	1	0	-3.507205	-1.608456	0.674389
34	1	0	-1.787031	3.285597	-2.742161
35	1	0	6.877945	-2.869993	0.094043
36	1	0	4.238182	-6.285210	-2.022500
37	1	0	-3.328593	4.195605	-2.900325
38	8	0	1.641122	1.062082	0.116667
39	1	0	-5.371182	4.961111	-3.895320
40	1	0	-5.380164	3.193764	-3.853635
41	1	0	-6.356018	4.111608	-2.696290
42	1	0	-4.237915	6.284861	-2.024216
43	1	0	-3.344958	5.433528	-0.755142
44	1	0	-5.116563	5.412826	-0.758419
45	1	0	-0.850916	-1.243220	-3.667820
46	1	0	-0.344793	-2.938216	-3.543555
47	1	0	-1.416397	-2.229554	-2.324774
48	8	0	-6.262625	3.305859	-0.514428
49	1	0	-6.877848	2.870110	0.092876
50	8	0	-6.283182	1.137759	0.863527
51	1	0	-6.162766	0.283394	1.376078
52	1	0	0.345260	2.937592	-3.543981
53	1	0	1.416715	2.229042	-2.325000
54	1	0	0.851335	1.242561	-3.667980
55	8	0	-1.641115	-1.062087	0.116666
56	8	0	6.283145	-1.137556	0.864388
57	1	0	3.345083	-5.433562	-0.753736
58	1	0	5.116688	-5.412879	-0.756806
59	8	0	6.262785	-3.305873	-0.513231
60	1	0	3.328983	-4.196142	-2.899214
61	1	0	5.371690	-4.961962	-3.893751
62	1	0	5.380644	-3.194601	-3.852575
63	1	0	6.356385	-4.112101	-2.694863
64	1	0	6.162620	-0.283138	1.376830
65	1	0	-0.739066	-1.411100	0.075952
66	1	0	0.739064	1.411057	0.075833
67	7	0	-5.253079	-1.026591	1.620324
68	6	0	-4.652631	-3.347887	1.955836
69	6	0	-6.884294	-2.440296	2.455086
70	6	0	-4.905272	-4.497138	2.927878
71	1	0	-4.889648	-3.648425	0.920473
72	1	0	-3.594806	-3.082118	1.995069
73	6	0	-7.151489	-3.554630	3.455221
74	1	0	-7.297803	-2.713375	1.470547
75	1	0	-7.354099	-1.507526	2.771545
76	6	0	-6.392285	-4.817068	3.054881
77	1	0	-4.342666	-5.369320	2.586618
78	1	0	-4.509476	-4.214810	3.908709
79	1	0	-8.227429	-3.739139	3.499092
80	1	0	-6.827899	-3.227810	4.448862
81	1	0	-6.548653	-5.611633	3.788233
82	1	0	-6.772829	-5.180504	2.092911
83	7	0	-5.445270	-2.178863	2.329832
84	7	0	5.252924	1.026875	1.620734
85	7	0	5.444977	2.179253	2.330103
86	6	0	4.652255	3.348156	1.955911
87	6	0	6.883969	2.440833	2.455415
88	6	0	4.904714	4.497539	2.927844
89	1	0	4.889326	3.648603	0.920534
90	1	0	3.594453	3.082286	1.995088
91	6	0	7.150999	3.555315	3.455428
92	1	0	7.297514	2.713823	1.470866
93	1	0	7.353839	1.508145	2.772021
94	6	0	6.391688	4.817630	3.054906
95	1	0	4.342047	5.369630	2.586448
96	1	0	4.508879	4.215280	3.908679
97	1	0	8.226918	3.739941	3.499330
98	1	0	6.827397	3.228578	4.449093
99	1	0	6.547933	5.612286	3.788185
100	1	0	6.772252	5.181008	2.092922

Structure (*R*)-13aa enantiomer of (*S*)-13aa (DMSO)

Energy (Hartrees): = -2224.4174604
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.157848	2.507348	-0.599793
2	6	0	-4.124147	2.845784	-1.434568
3	6	0	-2.957242	2.000373	-1.431917
4	6	0	-2.923057	0.804880	-0.643400
5	6	0	-4.073467	0.434020	0.149812
6	6	0	-5.143051	1.314176	0.173216
7	6	0	4.238594	-5.367129	-1.420511
8	6	0	-0.519325	-2.007382	-3.047280
9	6	0	-4.238381	4.101321	-2.286789
10	6	0	-1.701191	0.062534	-0.654783
11	6	0	-0.611746	0.429103	-1.425740
12	6	0	-0.668497	1.603608	-2.216571
13	6	0	-1.815071	2.354444	-2.201442
14	6	0	-5.450979	4.060904	-3.227359
15	6	0	-4.238564	5.367165	-1.420160
16	6	0	0.519309	2.007489	-3.047188
17	6	0	-4.217554	-0.850343	0.859992
18	6	0	4.217566	0.850280	0.859948
19	6	0	0.611755	-0.429077	-1.425771
20	6	0	0.668495	-1.603542	-2.216662
21	6	0	1.815070	-2.354378	-2.201592
22	6	0	2.957254	-2.000343	-1.432070
23	6	0	2.923079	-0.804891	-0.643489
24	6	0	1.701213	-0.062546	-0.654814
25	6	0	4.238391	-4.101238	-2.287072
26	6	0	5.450973	-4.060764	-3.227658
27	6	0	4.124163	-2.845747	-1.434782
28	6	0	5.157874	-2.507350	-0.600004
29	6	0	5.143084	-1.314220	0.173070
30	6	0	4.073496	-0.434063	0.149724
31	1	0	3.479561	1.617163	0.691722
32	1	0	1.823554	-3.255656	-2.796268
33	1	0	-3.479577	-1.617244	0.691730
34	1	0	-1.823563	3.255753	-2.796072
35	1	0	6.866593	-2.838640	0.123201
36	1	0	4.255874	-6.256889	-2.056062
37	1	0	-3.366939	4.162574	-2.933689
38	8	0	1.609160	1.043751	0.130894
39	1	0	-5.420762	4.923332	-3.899005
40	1	0	-5.438156	3.157033	-3.842221
41	1	0	-6.390596	4.089660	-2.676528
42	1	0	-4.255843	6.256960	-2.055662
43	1	0	-3.339931	5.413294	-0.799117
44	1	0	-5.112183	5.396009	-0.766774
45	1	0	-0.812944	-1.202600	-3.727074
46	1	0	-0.290677	-2.895333	-3.637442
47	1	0	-1.385751	-2.229668	-2.416758
48	8	0	-6.266983	3.281043	-0.494235
49	1	0	-6.866558	2.838606	0.123450
50	8	0	-6.263417	1.121089	0.888942
51	1	0	-6.133675	0.263641	1.398301
52	1	0	0.290651	2.895468	-3.637304
53	1	0	1.385744	2.229748	-2.416668
54	1	0	0.812920	1.202741	-3.727025
55	8	0	-1.609119	-1.043804	0.130865
56	8	0	6.263456	-1.121188	0.888800
57	1	0	3.339968	-5.413299	-0.799461
58	1	0	5.112220	-5.396000	-0.767137
59	8	0	6.267011	-3.281048	-0.494499
60	1	0	3.366939	-4.162461	-2.933962
61	1	0	5.420745	-4.923150	-3.899357
62	1	0	5.438142	-3.156855	-3.842464
63	1	0	6.390599	-4.089555	-2.676843
64	1	0	6.133715	-0.263783	1.398234
65	1	0	-0.715090	-1.407269	0.049085
66	1	0	0.715131	1.407225	0.049150
67	7	0	-5.222813	-1.032231	1.642802
68	6	0	-4.623665	-3.351128	1.986417
69	6	0	-6.857355	-2.438601	2.480464
70	6	0	-4.885034	-4.501988	2.953793
71	1	0	-4.857490	-3.647402	0.949759
72	1	0	-3.565343	-3.088729	2.032212
73	6	0	-7.129601	-3.555734	3.475516
74	1	0	-7.266477	-2.709288	1.494018
75	1	0	-7.326893	-1.506042	2.798502

76	6	0	-6.373117	-4.818191	3.072042
77	1	0	-4.323006	-5.373753	2.610844
78	1	0	-4.493183	-4.226028	3.938245
79	1	0	-8.206370	-3.736110	3.514467
80	1	0	-6.809033	-3.234803	4.472247
81	1	0	-6.535003	-5.616100	3.800588
82	1	0	-6.749892	-5.174601	2.106122
83	7	0	-5.415807	-2.179598	2.358255
84	7	0	5.222837	1.032188	1.642739
85	7	0	5.415803	2.179548	2.358212
86	6	0	4.623604	3.351053	1.986418
87	6	0	6.857343	2.438608	2.480389
88	6	0	4.884952	4.501906	2.953809
89	1	0	4.857391	3.647357	0.949759
90	1	0	3.565294	3.088612	2.032235
91	6	0	7.129570	3.555732	3.475456
92	1	0	7.266429	2.709331	1.493937
93	1	0	7.326929	1.506061	2.798396
94	6	0	6.373025	4.818166	3.072025
95	1	0	4.322879	5.373654	2.610892
96	1	0	4.493138	4.225910	3.938266
97	1	0	8.206333	3.736150	3.514384
98	1	0	6.809039	3.234768	4.472189
99	1	0	6.534898	5.616069	3.800582
100	1	0	6.749761	5.174608	2.106102

Structure 13cc (vacuum)

Energy (Hartrees): = -2224.3843705
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.549155	-1.164974	1.556861
2	6	0	-4.527650	-1.878100	2.126709
3	6	0	-3.222226	-1.774103	1.528373
4	6	0	-2.997910	-0.904535	0.413036
5	6	0	-4.082823	-0.100662	-0.098609
6	6	0	-5.332289	-0.276691	0.469082
7	6	0	5.756508	-3.923713	-2.952421
8	6	0	-0.236318	-3.362342	-2.018081
9	6	0	-4.827664	-2.760965	3.328062
10	6	0	-1.693163	-0.928391	-0.165616
11	6	0	-0.662564	-1.697599	0.344589
12	6	0	-0.888125	-2.520452	1.474863
13	6	0	-2.140290	-2.547285	2.028638
14	6	0	-5.376816	-1.956538	4.515679
15	6	0	-5.756617	-3.923982	2.951954
16	6	0	0.236285	-3.362591	2.017709
17	6	0	-3.922507	0.947384	-1.118511
18	6	0	3.922526	0.947214	1.118647
19	6	0	0.662553	-1.697565	-0.344760
20	6	0	0.888102	-2.520280	-1.475136
21	6	0	2.140264	-2.547056	-2.028919
22	6	0	3.222210	-1.773946	-1.528564
23	6	0	2.997906	-0.904515	-0.413116
24	6	0	1.693161	-0.928429	0.165537
25	6	0	4.827634	-2.760588	-3.328389
26	6	0	5.376873	-1.956014	-4.515866
27	6	0	4.527630	-1.877877	-2.126921
28	6	0	5.549140	-1.164817	-1.557000
29	6	0	5.332287	-0.276669	-0.469108
30	6	0	4.082828	-0.100709	0.098619
31	1	0	2.922637	1.192203	1.436088
32	1	0	2.296720	-3.207245	-2.868036
33	1	0	-2.922612	1.192424	-1.435893
34	1	0	-2.296755	-3.207578	2.867671
35	1	0	7.354519	-0.644397	-1.490068
36	1	0	5.906837	-4.576277	-3.816379
37	1	0	-3.896893	-3.203660	3.674595
38	8	0	1.458904	-0.191740	1.290578
39	1	0	-5.478034	-2.610732	5.385588
40	1	0	-4.696227	-1.143794	4.779031
41	1	0	-6.353366	-1.530965	4.289427
42	1	0	-5.906961	-4.576661	3.815822
43	1	0	-5.321763	-4.518265	2.145126
44	1	0	-6.728971	-3.555087	2.625202
45	1	0	-1.075544	-2.739428	-2.340880
46	1	0	0.099853	-3.955394	-2.868599
47	1	0	-0.623062	-4.038926	-1.250911
48	8	0	-6.819523	-1.245631	2.025649
49	1	0	-7.354539	-0.644570	1.489950
50	8	0	-6.440733	0.377751	0.080381

51	1	0	-6.178655	0.961956	-0.686579
52	1	0	-0.099895	-3.955745	2.868152
53	1	0	0.623026	-4.039084	1.250456
54	1	0	1.075516	-2.739724	2.340588
55	8	0	-1.458898	-0.191569	-1.290568
56	8	0	6.440737	0.377717	-0.080330
57	1	0	5.321596	-4.518086	-2.145692
58	1	0	6.728875	-3.554924	-2.625590
59	8	0	6.819498	-1.245400	-2.025828
60	1	0	3.896851	-3.203183	-3.675016
61	1	0	5.478102	-2.610088	-5.385865
62	1	0	4.696333	-1.143202	-4.779130
63	1	0	6.353433	-1.530519	-4.289507
64	1	0	6.178672	0.961805	0.686724
65	1	0	-0.533978	-0.321328	-1.541202
66	1	0	0.533983	-0.321520	1.541196
67	7	0	-4.954622	1.554641	-1.587843
68	6	0	-3.545868	3.062939	-2.850588
69	6	0	-5.898732	3.531846	-2.325250
70	6	0	-3.614639	4.036883	-4.024836
71	1	0	-3.129112	3.558339	-1.954937
72	1	0	-2.881650	2.237626	-3.114125
73	6	0	-6.010861	4.479583	-3.510303
74	1	0	-5.663970	4.102883	-1.411094
75	1	0	-6.836231	3.000464	-2.155694
76	6	0	-4.657256	5.126928	-3.793361
77	1	0	-2.622679	4.467683	-4.179872
78	1	0	-3.873228	3.473547	-4.926612
79	1	0	-6.771389	5.233840	-3.295345
80	1	0	-6.340123	3.914558	-4.387969
81	1	0	-4.715245	5.789650	-4.659566
82	1	0	-4.361920	5.741004	-2.934318
83	7	0	-4.866364	2.519303	-2.556839
84	7	0	4.954645	1.554448	1.588002
85	7	0	4.866404	2.519003	2.557106
86	6	0	3.545907	3.062569	2.850975
87	6	0	5.898733	3.531599	2.325580
88	6	0	3.614703	4.036389	4.025325
89	1	0	3.129095	3.558053	1.955397
90	1	0	2.881723	2.237209	3.114455
91	6	0	6.010890	4.479211	3.510730
92	1	0	5.663915	4.102728	1.411496
93	1	0	6.836239	3.000261	2.155925
94	6	0	4.657280	5.126488	3.793919
95	1	0	2.622738	4.467145	4.180453
96	1	0	3.873350	3.472964	4.927028
97	1	0	6.771388	5.233513	3.295819
98	1	0	6.340207	3.914101	4.388321
99	1	0	4.715289	5.789119	4.660192
100	1	0	4.361888	5.740647	2.934954

Structure 13cc ($CHCl_3$)

Energy (Hartrees): = -2224.4274525
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.607955	-1.246247	1.316995
2	6	0	-4.624190	-1.990796	1.915397
3	6	0	-3.287157	-1.879539	1.390156
4	6	0	-2.995883	-0.962082	0.330732
5	6	0	-4.038144	-0.107349	-0.186758
6	6	0	-5.321831	-0.303013	0.292563
7	6	0	5.872361	-4.083300	-2.569254
8	6	0	-0.126482	-3.530602	-1.970194
9	6	0	-4.992994	-2.924403	3.059077
10	6	0	-1.671624	-0.993229	-0.204703
11	6	0	-0.676115	-1.798832	0.317383
12	6	0	-0.962677	-2.658531	1.406498
13	6	0	-2.239609	-2.692692	1.903394
14	6	0	-5.638463	-2.182910	4.238820
15	6	0	-5.872287	-4.082984	2.569876
16	6	0	0.126526	-3.530383	1.970566
17	6	0	-3.801562	1.018748	-1.106620
18	6	0	3.801528	1.018936	1.106475
19	6	0	0.676129	-1.798860	-0.317196
20	6	0	0.962710	-2.658682	-1.406208
21	6	0	2.239652	-2.692904	-1.903076
22	6	0	3.287191	-1.879694	-1.389911
23	6	0	2.995892	-0.962101	-0.330612
24	6	0	1.671627	-0.993191	0.204809
25	6	0	4.993074	-2.924792	-3.058638

26	6	0	5.638568	-2.183463	-4.238471
27	6	0	4.624239	-1.991025	-1.915098
28	6	0	5.607989	-1.246397	-1.316770
29	6	0	5.321838	-0.303022	-0.292475
30	6	0	4.038139	-0.107296	0.186786
31	1	0	2.781916	1.303071	1.312954
32	1	0	2.439904	-3.387107	-2.705324
33	1	0	-2.781956	1.302845	-1.313180
34	1	0	-2.439847	-3.386801	2.705727
35	1	0	7.414482	-0.707648	-1.187103
36	1	0	6.076724	-4.774398	-3.391725
37	1	0	-4.080805	-3.365882	3.453154
38	8	0	1.400323	-0.227606	1.297235
39	1	0	-5.770037	-2.873832	5.076041
40	1	0	-5.002425	-1.360923	4.577088
41	1	0	-6.614310	-1.777381	3.973930
42	1	0	-6.076632	-4.773965	3.392450
43	1	0	-5.371492	-4.640100	1.773824
44	1	0	-6.825504	-3.715766	2.186051
45	1	0	-0.962892	-2.926822	-2.335334
46	1	0	0.248627	-4.133569	-2.797627
47	1	0	-0.529888	-4.201643	-1.205894
48	8	0	-6.903963	-1.345449	1.706454
49	1	0	-7.414452	-0.707520	1.187300
50	8	0	-6.397104	0.388267	-0.124035
51	1	0	-6.078353	1.013605	-0.840560
52	1	0	-0.248578	-4.133285	2.798049
53	1	0	0.529948	-4.201485	1.206326
54	1	0	0.962923	-2.926557	2.335659
55	8	0	-1.400334	-0.227768	-1.297219
56	8	0	6.397097	0.388324	0.124049
57	1	0	5.371551	-4.640304	-1.773132
58	1	0	6.825569	-3.716025	-2.185462
59	8	0	6.904008	-1.345652	-1.706180
60	1	0	4.080896	-3.366332	-3.452672
61	1	0	5.770165	-2.874502	-5.075591
62	1	0	5.002534	-1.361526	-4.576870
63	1	0	6.614407	-1.777892	-3.973614
64	1	0	6.078324	1.013772	0.840466
65	1	0	-0.474698	-0.361399	-1.548200
66	1	0	0.474686	-0.361216	1.548224
67	7	0	-4.802767	1.649087	-1.611115
68	6	0	-3.345181	3.310788	-2.592387
69	6	0	-5.761290	3.650214	-2.256287
70	6	0	-3.345625	4.395653	-3.666061
71	1	0	-3.036724	3.726221	-1.617175
72	1	0	-2.625941	2.538741	-2.871845
73	6	0	-5.795234	4.709685	-3.346785
74	1	0	-5.638725	4.129909	-1.271666
75	1	0	-6.688331	3.074858	-2.237812
76	6	0	-4.448621	5.423460	-3.430816
77	1	0	-2.361249	4.869445	-3.678148
78	1	0	-3.493480	3.921076	-4.641359
79	1	0	-6.602621	5.413155	-3.130723
80	1	0	-6.018743	4.229530	-4.304986
81	1	0	-4.453120	6.167038	-4.231253
82	1	0	-4.260189	5.955834	-2.491004
83	7	0	-4.666488	2.697399	-2.478495
84	7	0	4.802719	1.649336	1.610922
85	7	0	4.666416	2.697780	2.478139
86	6	0	3.345112	3.311205	2.591876
87	6	0	5.761239	3.650548	2.255828
88	6	0	3.345522	4.396240	3.665378
89	1	0	3.036702	3.726486	1.616586
90	1	0	2.625850	2.539210	2.871425
91	6	0	5.795148	4.710192	3.346158
92	1	0	5.638721	4.130088	1.271126
93	1	0	6.688274	3.075179	2.237484
94	6	0	4.448541	5.423997	3.430016
95	1	0	2.361151	4.870046	3.677345
96	1	0	3.493328	3.921818	4.640758
97	1	0	6.602553	5.413618	3.130020
98	1	0	6.018610	4.230187	4.304446
99	1	0	4.453012	6.167703	4.230334
100	1	0	4.260157	5.956222	2.490110

Structure 13cc (DMSO)

Energy (Hartrees): = -2224.4171088
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-5.620825	-1.258819	1.241149
2	6	0	-4.653829	-2.023763	1.842145
3	6	0	-3.307637	-1.916877	1.339596
4	6	0	-2.991190	-0.982775	0.302156
5	6	0	-4.015818	-0.107507	-0.215518
6	6	0	-5.309366	-0.299733	0.238600
7	6	0	5.935278	-4.110527	-2.445729
8	6	0	-0.077805	-3.616021	-1.935594
9	6	0	-5.047767	-2.972151	2.964702
10	6	0	-1.659893	-1.017263	-0.215876
11	6	0	-0.681118	-1.843416	0.306216
12	6	0	-0.992776	-2.721007	1.373813
13	6	0	-2.276625	-2.751219	1.853360
14	6	0	-5.698141	-2.241575	4.147872
15	6	0	-5.935287	-4.110535	2.445718
16	6	0	0.077840	-3.616033	1.935560
17	6	0	-3.751203	1.041146	-1.099926
18	6	0	3.751197	1.041160	1.099926
19	6	0	0.681142	-1.843410	-0.306238
20	6	0	0.992806	-2.720993	-1.373840
21	6	0	2.276656	-2.751195	-1.853383
22	6	0	3.307663	-1.916852	-1.339614
23	6	0	2.991209	-0.982756	-0.302171
24	6	0	1.659912	-1.017254	0.215858
25	6	0	5.047810	-2.972106	-2.964720
26	6	0	5.698250	-2.241518	-4.147846
27	6	0	4.653858	-2.023729	-1.842157
28	6	0	5.620847	-1.258776	-1.241160
29	6	0	5.309379	-0.299696	-0.238609
30	6	0	4.015828	-0.107485	0.215510
31	1	0	2.726520	1.334010	1.267120
32	1	0	2.493383	-3.456106	-2.642259
33	1	0	-2.726531	1.334013	-1.267119
34	1	0	-2.493346	-3.456134	2.642231
35	1	0	7.414757	-0.698999	-1.083978
36	1	0	6.160192	-4.810138	-3.255454
37	1	0	-4.146942	-3.432740	3.362323
38	8	0	1.367393	-0.235805	1.289767
39	1	0	-5.852319	-2.945623	4.970141
40	1	0	-5.053420	-1.436951	4.510979
41	1	0	-6.663599	-1.815219	3.876928
42	1	0	-6.160194	-4.810157	3.255435
43	1	0	-5.430000	-4.664389	1.649914
44	1	0	-6.878067	-3.725950	2.052906
45	1	0	-0.920413	-3.029625	-2.314772
46	1	0	0.314894	-4.221947	-2.752567
47	1	0	-0.474044	-4.284959	-1.165205
48	8	0	-6.924128	-1.349104	1.606604
49	1	0	-7.414745	-0.699072	1.083951
50	8	0	-6.370204	0.410403	-0.181279
51	1	0	-6.029995	1.045805	-0.880845
52	1	0	-0.314854	-4.221968	2.752528
53	1	0	0.474081	-4.284962	1.165164
54	1	0	0.920447	-3.029637	2.314741
55	8	0	-1.367380	-0.235812	-1.289782
56	8	0	6.370211	0.410449	0.181269
57	1	0	5.429946	-4.664382	-1.649955
58	1	0	6.878056	-3.725979	-2.052876
59	8	0	6.924149	-1.349039	-1.606627
60	1	0	4.146987	-3.432660	-3.362384
61	1	0	5.852451	-2.945551	-4.970122
62	1	0	5.053562	-1.436872	-4.510965
63	1	0	6.663705	-1.815187	-3.876850
64	1	0	6.029998	1.045849	0.880835
65	1	0	-0.443387	-0.386967	-1.538033
66	1	0	0.443401	-0.386965	1.538015
67	7	0	-4.740656	1.680083	-1.617260
68	6	0	-3.268645	3.378989	-2.509433
69	6	0	-5.696390	3.692603	-2.231354
70	6	0	-3.249034	4.491551	-3.553894
71	1	0	-2.995457	3.770942	-1.514923
72	1	0	-2.533592	2.621734	-2.787886
73	6	0	-5.708977	4.779828	-3.294197
74	1	0	-5.597917	4.147941	-1.233109
75	1	0	-6.620227	3.111854	-2.249910
76	6	0	-4.366193	5.504511	-3.322419
77	1	0	-2.268478	4.972144	-3.523922
78	1	0	-3.365511	4.042789	-4.545774
79	1	0	-6.527056	5.471299	-3.079645
80	1	0	-5.903997	4.325530	-4.271324
81	1	0	-4.354500	6.268651	-4.103212
82	1	0	-4.208194	6.011606	-2.363381
83	7	0	-4.588494	2.751894	-2.450730
84	7	0	4.740637	1.680105	1.617275
85	7	0	4.588454	2.751904	2.450755
86	6	0	3.268595	3.378977	2.509456
87	6	0	5.696335	3.692634	2.231392
88	6	0	3.248959	4.491531	3.553926

89	1	0	2.995405	3.770934	1.514948
90	1	0	2.533553	2.621707	2.787900
91	6	0	5.708899	4.779852	3.294243
92	1	0	5.597860	4.147977	1.233151
93	1	0	6.620183	3.111900	2.249950
94	6	0	4.366102	5.504511	3.322463
95	1	0	2.268395	4.972107	3.523952
96	1	0	3.365438	4.042764	4.545802
97	1	0	6.526967	5.471338	3.079700
98	1	0	5.903921	4.325550	4.271369
99	1	0	4.354392	6.268645	4.103261
100	1	0	4.208100	6.011611	2.363428

Structure 14aa (vacuum)

Energy (Hartrees): = -2381.6007179
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.052277	-2.699947	0.837436
2	6	0	4.012495	-2.996517	1.678720
3	6	0	2.877428	-2.109223	1.684566
4	6	0	2.880836	-0.915544	0.894494
5	6	0	4.034160	-0.596738	0.086532
6	6	0	5.073827	-1.510558	0.058752
7	6	0	-4.063236	5.521581	1.667743
8	6	0	0.590906	1.981232	3.321928
9	6	0	4.092397	-4.252318	2.533271
10	6	0	1.694257	-0.123708	0.924233
11	6	0	0.594680	-0.451503	1.697354
12	6	0	0.610675	-1.628020	2.485291
13	6	0	1.728704	-2.419056	2.461087
14	6	0	5.306141	-4.234348	3.474465
15	6	0	4.061674	-5.521102	1.669525
16	6	0	-0.591307	-1.981979	3.320988
17	6	0	4.197138	0.646427	-0.681141
18	6	0	-4.197146	-0.646457	-0.681028
19	6	0	-0.594680	0.451421	1.697382
20	6	0	-0.610815	1.627692	2.485685
21	6	0	-1.728739	2.418868	2.461334
22	6	0	-2.877289	2.109369	1.684416
23	6	0	-2.880750	0.915651	0.894383
24	6	0	-1.694165	0.123816	0.924061
25	6	0	-4.091800	4.253183	2.532154
26	6	0	-5.304265	4.234693	3.474984
27	6	0	-4.012207	2.996854	1.678324
28	6	0	-5.052407	2.699796	0.837714
29	6	0	-5.074098	1.510254	0.059279
30	6	0	-4.034205	0.596680	0.086686
31	1	0	-3.459339	-1.420208	-0.558683
32	1	0	-1.712031	3.319070	3.056527
33	1	0	3.459691	1.420448	-0.558277
34	1	0	1.711844	-3.319575	3.055805
35	1	0	-6.732108	3.093508	0.093004
36	1	0	-4.059295	6.409317	2.305454
37	1	0	3.218173	-4.288201	3.179143
38	8	0	-1.636215	-1.004335	0.156279
39	1	0	5.266238	-5.100553	4.140021
40	1	0	5.303152	-3.332058	4.090047
41	1	0	6.241237	-4.271181	2.917991
42	1	0	4.058265	-6.408604	2.307564
43	1	0	3.164146	-5.542568	1.046983
44	1	0	4.935430	-5.567157	1.019268
45	1	0	0.854761	1.159098	3.992300
46	1	0	0.396227	2.871942	3.919294
47	1	0	1.466138	2.170329	2.693283
48	8	0	6.132005	-3.512399	0.725119
49	1	0	6.731522	-3.094207	0.091988
50	8	0	6.184751	-1.363913	-0.678178
51	1	0	6.056179	-0.519662	-1.223092
52	1	0	-0.396889	-2.873116	3.917801
53	1	0	-1.466401	-2.170544	2.691991
54	1	0	-0.855228	-1.160270	3.991855
55	8	0	1.636395	1.004596	0.156679
56	8	0	-6.185291	1.363292	-0.677182
57	1	0	-3.166666	5.543297	1.043836
58	1	0	-4.938004	5.566951	1.018824
59	8	0	-6.132409	3.511944	0.725803
60	1	0	-3.216634	4.290275	3.176670
61	1	0	-5.264542	5.101500	4.139768
62	1	0	-5.299553	3.332905	4.091289
63	1	0	-6.240074	4.270036	2.919588

64	1	0	-6.056713	0.519086	-1.222172
65	1	0	0.754665	1.389556	0.257126
66	1	0	-0.754518	-1.389349	0.256820
67	7	0	5.208494	0.790373	-1.460809
68	6	0	4.245707	2.840386	-2.381791
69	6	0	6.679122	2.546178	-1.857771
70	6	0	4.629280	3.995914	-3.311397
71	1	0	3.971377	3.268155	-1.400531
72	6	0	7.030603	3.676958	-2.817225
73	1	0	6.563768	2.975031	-0.845891
74	6	0	5.908782	4.701857	-2.890551
75	1	0	3.787810	4.692498	-3.342856
76	1	0	4.754392	3.589083	-4.321280
77	1	0	7.963235	4.136009	-2.479538
78	1	0	7.211902	3.247828	-3.809332
79	1	0	6.153430	5.501270	-3.593801
80	1	0	5.771290	5.166196	-1.906995
81	7	0	5.391631	1.923104	-2.244975
82	7	0	-5.208722	-0.790568	-1.460381
83	7	0	-5.391746	-1.923138	-2.244823
84	6	0	-4.245583	-2.840031	-2.382318
85	6	0	-6.678961	-2.546671	-1.857489
86	6	0	-4.629098	-3.995319	-3.312237
87	1	0	-3.970840	-3.268085	-1.401302
88	6	0	-7.030392	-3.677192	-2.817266
89	1	0	-6.563248	-2.975849	-0.845788
90	6	0	-5.908301	-4.701747	-2.891294
91	1	0	-3.787461	-4.691684	-3.344150
92	1	0	-4.754559	-3.588157	-4.321944
93	1	0	-7.962798	-4.136639	-2.479493
94	1	0	-7.212094	-3.247743	-3.809162
95	1	0	-6.152931	-5.500972	-3.594763
96	1	0	-5.770406	-5.166407	-1.907945
97	6	0	3.044791	2.120884	-3.009527
98	1	0	3.389924	1.564915	-3.884127
99	1	0	2.528413	1.430684	-2.345804
100	1	0	2.318657	2.865779	-3.341359
101	6	0	7.797871	1.507915	-1.830775
102	1	0	7.708455	0.815438	-0.995252
103	1	0	7.791401	0.936419	-2.762549
104	1	0	8.759207	2.017921	-1.743768
105	6	0	-7.797957	-1.508684	-1.829857
106	1	0	-7.708512	-0.816484	-0.994109
107	1	0	-7.791819	-0.936854	-2.761430
108	1	0	-8.759155	-2.018944	-1.742825
109	6	0	-3.045078	-2.119876	-3.010129
110	1	0	-3.390791	-1.563169	-3.884032
111	1	0	-2.528361	-1.430232	-2.346086
112	1	0	-2.319066	-2.864390	-3.343076

Structure 14aa ($CHCl_3$)

Energy (Hartrees): = -2381.6438267
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.054369	-2.735388	-0.857133
2	6	0	-3.993682	-3.029309	-1.673897
3	6	0	-2.861057	-2.137571	-1.653529
4	6	0	-2.887507	-0.939996	-0.869143
5	6	0	-4.061775	-0.624453	-0.087790
6	6	0	-5.098396	-1.543841	-0.081985
7	6	0	3.989528	5.552157	-1.651583
8	6	0	-0.637197	2.003543	-3.216991
9	6	0	-4.040490	-4.290886	-2.523989
10	6	0	-1.705057	-0.138174	-0.878483
11	6	0	-0.589170	-0.459549	-1.631239
12	6	0	-0.580119	-1.645697	-2.406981
13	6	0	-1.691968	-2.447334	-2.400135
14	6	0	-5.242824	-4.312273	-3.478936
15	6	0	-3.989690	-5.552193	-1.651331
16	6	0	0.637154	-2.003648	-3.216913
17	6	0	-4.252822	0.621902	0.671632
18	6	0	4.252808	-0.621867	0.671613
19	6	0	0.589133	0.459509	-1.631260
20	6	0	0.580080	1.645624	-2.407050
21	6	0	1.691929	2.447261	-2.400241
22	6	0	2.861022	2.137529	-1.653627
23	6	0	2.887473	0.939985	-0.869194
24	6	0	1.705023	0.138163	-0.878497
25	6	0	4.040483	4.290807	-2.524171
26	6	0	5.242936	4.312196	-3.478966

27	6	0	3.993648	3.029268	-1.674027
28	6	0	5.054351	2.735361	-0.857279
29	6	0	5.098379	1.543842	-0.082088
30	6	0	4.061748	0.624465	-0.087843
31	1	0	3.523033	-1.404728	0.561668
32	1	0	1.652240	3.353884	-2.985300
33	1	0	-3.523059	1.404767	0.561634
34	1	0	-1.652284	-3.353983	-2.985155
35	1	0	6.758596	3.152261	-0.154952
36	1	0	3.968768	6.445310	-2.282330
37	1	0	-3.160052	-4.310937	-3.161631
38	8	0	1.680946	-0.989523	-0.113959
39	1	0	-5.160472	-5.171869	-4.149827
40	1	0	-5.268175	-3.408656	-4.093438
41	1	0	-6.186406	-4.388785	-2.940045
42	1	0	-3.968911	-6.445381	-2.282030
43	1	0	-3.093049	-5.557423	-1.026025
44	1	0	-4.863761	-5.612829	-1.001141
45	1	0	-0.892579	1.201595	-3.915134
46	1	0	-0.464709	2.917700	-3.785733
47	1	0	-1.508555	2.158896	-2.573568
48	8	0	-6.128372	-3.558333	-0.767782
49	1	0	-6.758570	-3.152303	-0.154706
50	8	0	-6.223555	-1.398703	0.632412
51	1	0	-6.107507	-0.545702	1.174654
52	1	0	0.464664	-2.917828	-3.785617
53	1	0	1.508516	-2.158974	-2.573488
54	1	0	0.892531	-1.201729	-3.915090
55	8	0	-1.680976	0.989541	-0.113989
56	8	0	6.223543	1.398717	0.632302
57	1	0	3.092820	5.557372	-1.026372
58	1	0	4.863526	5.612875	-1.001303
59	8	0	6.128382	3.558279	-0.768018
60	1	0	3.160119	4.310793	-3.161915
61	1	0	5.160655	5.171775	-4.149887
62	1	0	5.268389	3.408565	-4.093442
63	1	0	6.186446	4.388740	-2.939949
64	1	0	6.107480	0.545751	1.174594
65	1	0	-0.796516	1.381196	-0.159048
66	1	0	0.796487	-1.381182	-0.159002
67	7	0	-5.281631	0.755141	1.430582
68	6	0	-4.370282	2.823063	2.363208
69	6	0	-6.796798	2.478221	1.813795
70	6	0	-4.788037	3.978557	3.278049
71	1	0	-4.092406	3.244822	1.381987
72	6	0	-7.177429	3.607689	2.763584
73	1	0	-6.677738	2.902995	0.801943
74	6	0	-6.076891	4.654805	2.838680
75	1	0	-3.960404	4.691411	3.309538
76	1	0	-4.915160	3.580651	4.291535
77	1	0	-8.115399	4.044764	2.411829
78	1	0	-7.360238	3.183515	3.757955
79	1	0	-6.344735	5.453240	3.534869
80	1	0	-5.939510	5.114320	1.852794
81	7	0	-5.497701	1.880165	2.216249
82	7	0	5.281654	-0.755097	1.430515
83	7	0	5.497744	-1.880109	2.216195
84	6	0	4.370331	-2.823013	2.363168
85	6	0	6.796840	-2.478164	1.813742
86	6	0	4.788094	-3.978481	3.278038
87	1	0	4.092466	-3.244796	1.381955
88	6	0	7.177483	-3.607610	2.763554
89	1	0	6.677777	-2.902960	0.801900
90	6	0	6.076951	-4.654730	2.838680
91	1	0	3.960465	-4.691338	3.309546
92	1	0	4.915216	-3.580548	4.291514
93	1	0	8.115453	-4.044688	2.411803
94	1	0	7.360295	-3.183413	3.757914
95	1	0	6.344803	-5.453147	3.534888
96	1	0	5.939568	-5.114270	1.852807
97	6	0	-3.166344	2.132252	3.014726
98	1	0	-3.504565	1.593836	3.903766
99	1	0	-2.635608	1.431427	2.372696
100	1	0	-2.449745	2.893970	3.330341
101	6	0	-7.894940	1.419759	1.780624
102	1	0	-7.790892	0.730180	0.943578
103	1	0	-7.891565	0.845719	2.711602
104	1	0	-8.864464	1.913286	1.684447
105	6	0	7.894978	-1.419698	1.780543
106	1	0	7.790925	-0.730140	0.943479
107	1	0	7.891602	-0.845634	2.711506
108	1	0	8.864503	-1.913222	1.684376
109	6	0	3.166384	-2.132191	3.014656
110	1	0	3.504595	-1.593743	3.903681
111	1	0	2.635648	-1.431392	2.372598
112	1	0	2.449789	-2.893904	3.330291

Structure 14aa (DMSO)

Energy (Hartrees): = -2381.6307347
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.060375	-2.693200	-0.841097
2	6	0	-4.026309	-2.983319	-1.693152
3	6	0	-2.886525	-2.099638	-1.693462
4	6	0	-2.880705	-0.915501	-0.888387
5	6	0	-4.032785	-0.597370	-0.075916
6	6	0	-5.074846	-1.510313	-0.051199
7	6	0	4.060431	5.507135	-1.716332
8	6	0	-0.564179	1.959906	-3.357435
9	6	0	-4.108784	-4.229102	-2.562994
10	6	0	-1.687741	-0.129396	-0.907663
11	6	0	-0.597398	-0.448591	-1.697282
12	6	0	-0.624997	-1.612911	-2.504084
13	6	0	-1.743938	-2.404626	-2.482578
14	6	0	-5.331149	-4.211493	-3.491237
15	6	0	-4.060169	-5.507106	-1.715906
16	6	0	0.564243	-1.959864	-3.357395
17	6	0	-4.198770	0.647949	0.692162
18	6	0	4.198855	-0.647863	0.691979
19	6	0	0.597527	0.448681	-1.697323
20	6	0	0.625100	1.612972	-2.504170
21	6	0	1.744053	2.404675	-2.482753
22	6	0	2.886676	2.099702	-1.693683
23	6	0	2.880873	0.915602	-0.888557
24	6	0	1.687906	0.129508	-0.907745
25	6	0	4.108954	4.229094	-2.563367
26	6	0	5.331265	4.211402	-3.491679
27	6	0	4.026484	2.983350	-1.693467
28	6	0	5.060578	2.693238	-0.841444
29	6	0	5.075061	1.510387	-0.051490
30	6	0	4.032970	0.597463	-0.076123
31	1	0	3.470579	-1.430287	0.565145
32	1	0	1.729951	3.297761	-3.089691
33	1	0	-3.470598	1.430464	0.565306
34	1	0	-1.729854	-3.297739	-3.089478
35	1	0	6.742923	3.094813	-0.093461
36	1	0	4.057594	6.386829	-2.365813
37	1	0	-3.241747	-4.253643	-3.218089
38	8	0	1.626027	-0.973307	-0.111727
39	1	0	-5.283028	-5.064039	-4.174260
40	1	0	-5.349088	-3.300008	-4.094594
41	1	0	-6.264496	-4.273387	-2.932442
42	1	0	-4.057332	-6.386827	-2.365350
43	1	0	-3.153472	-5.535192	-1.105656
44	1	0	-4.924800	-5.573201	-1.053675
45	1	0	-0.814376	1.136289	-4.032274
46	1	0	-0.361913	2.849980	-3.953876
47	1	0	-1.448753	2.152764	-2.742544
48	8	0	-6.141265	-3.504707	-0.731365
49	1	0	-6.742681	-3.094788	-0.093026
50	8	0	-6.179652	-1.364080	0.693280
51	1	0	-6.046984	-0.507077	1.228611
52	1	0	0.361970	-2.849984	-3.953766
53	1	0	1.448860	-2.152652	-2.742544
54	1	0	0.814373	-1.136283	-4.032304
55	8	0	-1.625806	0.973445	-0.111686
56	8	0	6.179904	1.364209	0.692942
57	1	0	3.153767	5.535282	-1.106036
58	1	0	4.925100	5.573226	-1.054148
59	8	0	6.141491	3.504724	-0.731791
60	1	0	3.241881	4.253637	-3.218416
61	1	0	5.283133	5.063917	-4.174738
62	1	0	5.349140	3.299889	-4.094995
63	1	0	6.264646	4.273291	-2.932940
64	1	0	6.047264	0.507244	1.228349
65	1	0	-0.752508	1.380779	-0.212254
66	1	0	0.752728	-1.380654	-0.212230
67	7	0	-5.209725	0.780930	1.474927
68	6	0	-4.277183	2.848130	2.387684
69	6	0	-6.713158	2.509024	1.879647
70	6	0	-4.675381	4.009093	3.303580
71	1	0	-4.017930	3.263512	1.399571
72	6	0	-7.073839	3.645130	2.828455
73	1	0	-6.604497	2.927370	0.864640
74	6	0	-5.967993	4.687759	2.879621
75	1	0	-3.843771	4.717804	3.317124
76	1	0	-4.788454	3.617883	4.321492
77	1	0	-8.015334	4.082960	2.487499

78	1	0	-7.243626	3.228551	3.828582
79	1	0	-6.221520	5.491718	3.574834
80	1	0	-5.843646	5.139335	1.888527
81	7	0	-5.409777	1.905864	2.266375
82	7	0	5.209773	-0.780983	1.474768
83	7	0	5.409619	-1.905934	2.266245
84	6	0	4.276852	-2.847993	2.387535
85	6	0	6.712898	-2.509338	1.879552
86	6	0	4.674811	-4.009017	3.303456
87	1	0	4.017556	-3.263342	1.399419
88	6	0	7.073346	-3.645504	2.828379
89	1	0	6.604182	-2.927673	0.864547
90	6	0	5.967306	-4.687928	2.879532
91	1	0	3.843069	-4.717574	3.316990
92	1	0	4.787934	-3.617815	4.321365
93	1	0	8.014767	-4.083513	2.487448
94	1	0	7.243190	-3.228948	3.828506
95	1	0	6.220668	-5.491927	3.574759
96	1	0	5.842897	-5.139492	1.888441
97	6	0	-3.063840	2.158000	3.020036
98	1	0	-3.376570	1.662302	3.942865
99	1	0	-2.572434	1.421535	2.386534
100	1	0	-2.320954	2.916826	3.276074
101	6	0	-7.817474	1.456848	1.869629
102	1	0	-7.734726	0.764364	1.032342
103	1	0	-7.802587	0.885051	2.802204
104	1	0	-8.784836	1.957349	1.789284
105	6	0	7.817414	-1.457372	1.869552
106	1	0	7.734819	-0.764880	1.032256
107	1	0	7.802615	-0.885564	2.802122
108	1	0	8.784682	-1.958057	1.789233
109	6	0	3.063613	-2.157633	3.019834
110	1	0	3.376400	-1.661979	3.942667
111	1	0	2.572364	-1.421088	2.386303
112	1	0	2.320579	-2.916320	3.275858

Structure 14bb (vacuum)

Energy (Hartrees): = -2381.6113891
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.967022	2.823980	-0.795343
2	6	0	3.924023	3.114520	-1.634822
3	6	0	2.817288	2.191031	-1.684798
4	6	0	2.861715	0.968794	-0.947780
5	6	0	4.024094	0.652492	-0.155407
6	6	0	5.024193	1.605801	-0.061054
7	6	0	-3.866014	-5.634606	-1.523952
8	6	0	0.650430	-2.007923	-3.312612
9	6	0	3.961493	4.404889	-2.438383
10	6	0	1.699907	0.145318	-0.983312
11	6	0	0.584491	0.463870	-1.738147
12	6	0	0.563779	1.663957	-2.490385
13	6	0	1.656149	2.491431	-2.445058
14	6	0	5.185652	4.476207	-3.363317
15	6	0	3.865753	5.634485	-1.524262
16	6	0	-0.650650	2.007366	-3.312767
17	6	0	4.270657	-0.641950	0.485383
18	6	0	-4.270621	0.641941	0.485527
19	6	0	-0.584567	-0.464277	-1.738048
20	6	0	-0.563899	-1.664483	-2.490104
21	6	0	-1.656337	-2.491857	-2.444726
22	6	0	-2.817484	-2.191271	-1.684542
23	6	0	-2.861831	-0.968962	-0.947637
24	6	0	-1.699976	-0.145547	-0.983282
25	6	0	-3.961910	-4.405030	-2.438082
26	6	0	-5.186206	-4.476392	-3.362833
27	6	0	-3.924315	-3.114646	-1.634543
28	6	0	-4.967268	-2.823996	-0.795043
29	6	0	-5.024314	-1.605781	-0.060800
30	6	0	-4.024175	-0.652535	-0.155257
31	1	0	-3.663871	1.502586	0.233625
32	1	0	-1.606049	-3.412159	-3.006454
33	1	0	3.664023	-1.502675	0.233477
34	1	0	1.605823	3.411641	-3.006935
35	1	0	-6.630876	-3.249124	-0.026970
36	1	0	-3.840409	-6.546586	-2.125870
37	1	0	3.093964	4.428268	-3.093988
38	8	0	-1.692055	0.991761	-0.233153
39	1	0	5.117045	5.367397	-3.992372
40	1	0	5.225675	3.601549	-4.016321

41	1	0	6.112573	4.527034	-2.794503
42	1	0	3.840058	6.546447	-2.126203
43	1	0	2.957008	5.597331	-0.919057
44	1	0	4.725479	5.686927	-0.856038
45	1	0	0.889349	-1.199201	-4.008072
46	1	0	0.484166	-2.922173	-3.882156
47	1	0	1.529138	-2.151658	-2.677089
48	8	0	6.014195	3.671471	-0.640868
49	1	0	6.630645	3.249233	-0.027374
50	8	0	6.134869	1.465164	0.674116
51	1	0	6.050537	0.593930	1.176482
52	1	0	-0.483723	2.920524	-3.883871
53	1	0	-1.528783	2.153143	-2.676893
54	1	0	-0.890944	1.197798	-4.006745
55	8	0	1.692042	-0.991885	-0.233026
56	8	0	-6.134888	-1.465036	0.674490
57	1	0	-2.957179	-5.597431	-0.918885
58	1	0	-4.725639	-5.687031	-0.855595
59	8	0	-6.014487	-3.671418	-0.640491
60	1	0	-3.094493	-4.428401	-3.093832
61	1	0	-5.117653	-5.367588	-3.991884
62	1	0	-5.226353	-3.601747	-4.015846
63	1	0	-6.113045	-4.527245	-2.793889
64	1	0	-6.050345	-0.593809	1.176856
65	1	0	0.815231	-1.393528	-0.301693
66	1	0	-0.815211	1.393323	-0.301837
67	7	0	5.229572	-0.782792	1.323261
68	6	0	6.795220	-2.457165	1.789089
69	6	0	4.844604	-2.105362	3.233446
70	6	0	6.982625	-3.865776	2.347395
71	1	0	7.363209	-1.746263	2.415960
72	6	0	5.003825	-3.509579	3.813000
73	1	0	5.442759	-1.399956	3.836635
74	6	0	6.453720	-3.976080	3.772202
75	1	0	8.044815	-4.121199	2.303949
76	1	0	6.447610	-4.565696	1.695714
77	1	0	4.623995	-3.508336	4.837990
78	1	0	4.375721	-4.191217	3.228592
79	1	0	6.540635	-5.001296	4.139756
80	1	0	7.057720	-3.343960	4.433259
81	7	0	5.360093	-2.104693	1.842048
82	7	0	-5.229571	0.782957	1.323329
83	7	0	-5.359849	2.104875	1.842100
84	6	0	-6.794871	2.457702	1.789010
85	6	0	-4.844411	2.105493	3.233523
86	6	0	-6.981971	3.866381	2.347249
87	1	0	-7.363070	1.746956	2.415858
88	6	0	-5.003369	3.509767	3.813041
89	1	0	-5.442684	1.400205	3.836734
90	6	0	-6.453152	3.976608	3.772100
91	1	0	-8.044098	4.122062	2.303706
92	1	0	-6.446735	4.566154	1.695587
93	1	0	-4.623618	3.508485	4.838066
94	1	0	-4.375073	4.191242	3.228651
95	1	0	-6.539845	5.001862	4.139607
96	1	0	-7.057353	3.344665	4.433141
97	6	0	7.300975	-2.372473	0.354165
98	1	0	6.678723	-2.996816	-0.292729
99	1	0	7.275993	-1.350314	-0.024421
100	1	0	8.330641	-2.731916	0.301175
101	6	0	3.381164	-1.680284	3.274780
102	1	0	3.243469	-0.637037	2.992428
103	1	0	2.791378	-2.301683	2.595211
104	1	0	2.993608	-1.810619	4.287250
105	6	0	-3.381062	1.680169	3.274871
106	1	0	-3.243550	0.636898	2.992529
107	1	0	-2.791158	2.301462	2.595304
108	1	0	-2.993501	1.810456	4.287350
109	6	0	-7.300528	2.373026	0.354057
110	1	0	-6.677967	2.997039	-0.292870
111	1	0	-7.275932	1.350803	-0.024399
112	1	0	-8.330046	2.732856	0.300939

Structure 14bb ($CHCl_3$)

Energy (Hartrees): = -2381.6546006
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.015963	2.782733	-0.861120
2	6	0	3.966278	3.068680	-1.694711
3	6	0	2.840410	2.166117	-1.700794

4	6	0	2.879382	0.955943	-0.943689
5	6	0	4.050540	0.638207	-0.163277
6	6	0	5.062599	1.582393	-0.096519
7	6	0	-3.914849	-5.590036	-1.654426
8	6	0	0.656892	-2.015726	-3.259007
9	6	0	4.008549	4.336065	-2.535245
10	6	0	1.706628	0.144601	-0.948091
11	6	0	0.585808	0.462936	-1.694843
12	6	0	0.565382	1.658539	-2.456466
13	6	0	1.667875	2.474945	-2.440989
14	6	0	5.229793	4.385297	-3.464635
15	6	0	3.914721	5.589793	-1.655522
16	6	0	-0.657086	2.014894	-3.259429
17	6	0	4.295056	-0.650906	0.493595
18	6	0	-4.295074	0.651074	0.493546
19	6	0	-0.585904	-0.463398	-1.694718
20	6	0	-0.565548	-1.659152	-2.456102
21	6	0	-1.668090	-2.475491	-2.440464
22	6	0	-2.840621	-2.166445	-1.700345
23	6	0	-2.879505	-0.956123	-0.943469
24	6	0	-1.706693	-0.144866	-0.948009
25	6	0	-4.009017	-4.336470	-2.534345
26	6	0	-5.230606	-4.385909	-3.463263
27	6	0	-3.966566	-3.068923	-1.694068
28	6	0	-5.016258	-2.782700	-0.860582
29	6	0	-5.062790	-1.582215	-0.096205
30	6	0	-4.050646	-0.638146	-0.163133
31	1	0	-3.690783	1.514869	0.245261
32	1	0	-1.614921	-3.392774	-3.007992
33	1	0	3.690948	-1.514819	0.245277
34	1	0	1.614667	3.392114	-3.008701
35	1	0	-6.708943	-3.216500	-0.134787
36	1	0	-3.896439	-6.487281	-2.279291
37	1	0	3.141166	4.341182	-3.191097
38	8	0	-1.705402	0.976164	-0.177832
39	1	0	5.141549	5.243795	-4.135998
40	1	0	5.286525	3.483295	-4.079407
41	1	0	6.160698	4.481294	-2.907194
42	1	0	3.896165	6.486930	-2.280537
43	1	0	3.002136	5.576545	-1.053943
44	1	0	4.770690	5.659340	-0.982474
45	1	0	0.907221	-1.218911	-3.964775
46	1	0	0.493620	-2.937144	-3.818553
47	1	0	1.527390	-2.157743	-2.611458
48	8	0	6.074408	3.622097	-0.744342
49	1	0	6.708507	3.216902	-0.135213
50	8	0	6.176217	1.441846	0.633657
51	1	0	6.082157	0.578266	1.152560
52	1	0	-0.493805	2.936123	-3.819282
53	1	0	-1.527541	2.157161	-2.611876
54	1	0	-0.907487	1.217856	-3.964918
55	8	0	1.705417	-0.976293	-0.177716
56	8	0	-6.176365	-1.441404	0.633987
57	1	0	-3.002074	-5.576635	-1.053140
58	1	0	-4.770597	-5.659518	-0.981094
59	8	0	-6.074840	-3.621887	-0.743783
60	1	0	-3.141857	-4.341690	-3.190489
61	1	0	-5.142678	-5.244619	-4.134398
62	1	0	-5.287523	-3.484088	-4.078284
63	1	0	-6.161301	-4.481679	-2.905424
64	1	0	-6.082148	-0.577768	1.152758
65	1	0	0.823738	-1.375446	-0.201735
66	1	0	-0.823697	1.375257	-0.201928
67	7	0	5.254150	-0.777919	1.332406
68	6	0	6.852645	-2.405666	1.834211
69	6	0	4.882753	-2.069803	3.263941
70	6	0	7.080564	-3.789946	2.435351
71	1	0	7.395160	-1.659894	2.441281
72	6	0	5.089253	-3.448654	3.888065
73	1	0	5.451843	-1.323697	3.844707
74	6	0	6.552671	-3.870999	3.862323
75	1	0	8.150841	-4.010435	2.401871
76	1	0	6.571713	-4.528945	1.805535
77	1	0	4.709188	-3.423106	4.912711
78	1	0	4.482930	-4.171101	3.329406
79	1	0	6.668666	-4.881661	4.261383
80	1	0	7.136666	-3.200661	4.503400
81	7	0	5.405266	-2.089450	1.871849
82	7	0	-5.254200	0.778259	1.332292
83	7	0	-5.405012	2.089803	1.871782
84	6	0	-6.852320	2.406382	1.834274
85	6	0	-4.882390	2.069905	3.263817
86	6	0	-7.079853	3.790651	2.435598
87	1	0	-7.394985	1.660674	2.441289
88	6	0	-5.088487	3.448750	3.888086
89	1	0	-5.451619	1.323885	3.844559
90	6	0	-6.551808	3.871435	3.862529
91	1	0	-8.150079	4.011405	2.402240

92	1	0	-6.570882	4.529594	1.805813
93	1	0	-4.708328	3.423018	4.912692
94	1	0	-4.482052	4.171106	3.329432
95	1	0	-6.667531	4.882081	4.261706
96	1	0	-7.135896	3.201164	4.503591
97	6	0	7.361711	-2.348348	0.399501
98	1	0	6.758576	-3.001951	-0.237631
99	1	0	7.320690	-1.336927	-0.007696
100	1	0	8.399611	-2.686896	0.360739
101	6	0	3.404541	-1.700178	3.287637
102	1	0	3.223558	-0.673523	2.968036
103	1	0	2.836150	-2.371149	2.636820
104	1	0	3.022320	-1.804912	4.305607
105	6	0	-3.404275	1.699885	3.287318
106	1	0	-3.223599	0.673223	2.967563
107	1	0	-2.835770	2.370787	2.636531
108	1	0	-3.021930	1.804384	4.305265
109	6	0	-7.361497	2.349383	0.399590
110	1	0	-6.758235	3.002917	-0.237492
111	1	0	-7.320772	1.338010	-0.007750
112	1	0	-8.399310	2.688213	0.360943

Structure 14bb (DMSO)

Energy (Hartrees): = -2381.6409022
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.749575	-3.143612	-0.526706
2	6	0	-3.664936	-3.414182	-1.320815
3	6	0	-2.646286	-2.398437	-1.448107
4	6	0	-2.798999	-1.138708	-0.794309
5	6	0	-4.006036	-0.853444	-0.059565
6	6	0	-4.931341	-1.873267	0.092199
7	6	0	3.371169	5.888493	-0.943746
8	6	0	-0.775105	2.001973	-3.124475
9	6	0	-3.552642	-4.777213	-1.986373
10	6	0	-1.694945	-0.239330	-0.839605
11	6	0	-0.554814	-0.499906	-1.580477
12	6	0	-0.447359	-1.721773	-2.292718
13	6	0	-1.466358	-2.637549	-2.202079
14	6	0	-4.728352	-5.069104	-2.928171
15	6	0	-3.371012	-5.888461	-0.944189
16	6	0	0.775169	-2.001771	-3.124570
17	6	0	-4.391363	0.478222	0.418534
18	6	0	4.391330	-0.478265	0.418624
19	6	0	0.554826	0.500007	-1.580431
20	6	0	0.447400	1.721912	-2.292610
21	6	0	1.466406	2.637674	-2.201895
22	6	0	2.646318	2.398508	-1.447914
23	6	0	2.799002	1.138742	-0.794181
24	6	0	1.694935	0.239384	-0.839542
25	6	0	3.552711	4.777312	-1.986018
26	6	0	4.728395	5.069224	-2.927842
27	6	0	3.664984	3.414230	-1.320561
28	6	0	4.749622	3.143591	-0.526471
29	6	0	4.931357	1.873212	0.092372
30	6	0	4.006030	0.853420	-0.059442
31	1	0	3.852071	-1.356464	0.082310
32	1	0	1.340927	3.570779	-2.730990
33	1	0	-3.852143	1.356439	0.082203
34	1	0	-1.340853	-3.570626	-2.731218
35	1	0	6.395427	3.651555	0.245259
36	1	0	3.226364	6.849662	-1.444331
37	1	0	-2.661402	-4.785916	-2.608408
38	8	0	1.777927	-0.898154	-0.100109
39	1	0	-4.545108	-6.006273	-3.460702
40	1	0	-4.838406	-4.276229	-3.672561
41	1	0	-5.667541	-5.163566	-2.383809
42	1	0	-3.226207	-6.849591	-1.444847
43	1	0	-2.493626	-5.695470	-0.321328
44	1	0	-4.244922	-5.967354	-0.295953
45	1	0	-0.925361	1.218295	-3.872386
46	1	0	-0.676144	2.958147	-3.638850
47	1	0	-1.678746	2.037837	-2.508689
48	8	0	-5.721381	-4.064507	-0.313393
49	1	0	-6.395361	-3.651658	0.245012
50	8	0	-6.073368	-1.755410	0.779053
51	1	0	-6.087045	-0.819057	1.167192
52	1	0	0.676244	-2.957930	-3.638981
53	1	0	1.678800	-2.037632	-2.508770
54	1	0	0.925416	-1.218062	-3.872450

55	8	0	-1.777969	0.898173	-0.100121
56	8	0	6.073373	1.755288	0.779233
57	1	0	2.493810	5.695487	-0.320851
58	1	0	4.245116	5.967317	-0.295550
59	8	0	5.721452	4.064451	-0.313117
60	1	0	2.661443	4.786094	-2.608012
61	1	0	4.545181	6.006451	-3.460282
62	1	0	4.838378	4.276411	-3.672307
63	1	0	5.667611	5.163588	-2.383509
64	1	0	6.087019	0.818917	1.167327
65	1	0	-0.935339	1.371685	-0.157565
66	1	0	0.935292	-1.371653	-0.157592
67	7	0	-5.404972	0.621912	1.187545
68	6	0	-7.160081	2.167690	1.227712
69	6	0	-5.417420	2.173486	2.956636
70	6	0	-7.550746	3.598535	1.585957
71	1	0	-7.741279	1.470633	1.855350
72	6	0	-5.786923	3.604120	3.341998
73	1	0	-6.033961	1.473207	3.544912
74	6	0	-7.250050	3.909338	3.046835
75	1	0	-8.613646	3.732277	1.368325
76	1	0	-6.991760	4.281703	0.935583
77	1	0	-5.565603	3.743511	4.403367
78	1	0	-5.141937	4.287994	2.777650
79	1	0	-7.478687	4.953631	3.274301
80	1	0	-7.886921	3.289119	3.688030
81	7	0	-5.716766	1.975812	1.514140
82	7	0	5.404957	-0.621983	1.187606
83	7	0	5.716685	-1.975887	1.514248
84	6	0	7.159953	-2.167902	1.227666
85	6	0	5.417482	-2.173420	2.956793
86	6	0	7.550560	-3.598738	1.586016
87	1	0	7.741280	-1.470820	1.855157
88	6	0	5.786936	-3.604041	3.342249
89	1	0	6.034129	-1.473128	3.544941
90	6	0	7.250013	-3.909371	3.046959
91	1	0	8.613426	-3.732577	1.368274
92	1	0	6.991451	-4.281937	0.935780
93	1	0	5.565720	-3.743319	4.403655
94	1	0	5.141849	-4.287929	2.778034
95	1	0	7.478616	-4.953653	3.274510
96	1	0	7.886989	-3.289118	3.688017
97	6	0	-7.447351	1.880434	-0.239991
98	1	0	-6.802914	2.494060	-0.877111
99	1	0	-7.283685	0.831159	-0.491083
100	1	0	-8.488481	2.122513	-0.465513
101	6	0	-3.944915	1.911555	3.244479
102	1	0	-3.666719	0.869661	3.081073
103	1	0	-3.316679	2.542428	2.607943
104	1	0	-3.730717	2.155878	4.287551
105	6	0	3.945024	-1.911370	3.244767
106	1	0	3.666874	-0.869477	3.081281
107	1	0	3.316681	-2.542274	2.608366
108	1	0	3.730923	-2.155570	4.287888
109	6	0	7.447065	-1.880830	-0.240104
110	1	0	6.802508	-2.494487	-0.877073
111	1	0	7.283438	-0.831573	-0.491295
112	1	0	8.488150	-2.123006	-0.465726

Structure 16bb χ = 175.2° (vacuum)

Energy (Hartrees): = -2224.3852161
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.100609	-2.609795	-0.597536
2	6	0	-4.124304	-2.864077	-1.501474
3	6	0	-2.940896	-2.002686	-1.506887
4	6	0	-2.908185	-0.809454	-0.735553
5	6	0	-4.055549	-0.462346	0.104348
6	6	0	-5.124098	-1.409597	0.239966
7	6	0	3.990530	5.366591	-1.648640
8	6	0	-0.549838	2.053881	-3.084979
9	6	0	-4.242767	-4.066374	-2.423565
10	6	0	-1.715091	-0.053226	-0.777783
11	6	0	-0.607212	-0.433793	-1.533086
12	6	0	-0.647332	-1.625894	-2.276320
13	6	0	-1.804237	-2.378161	-2.249415
14	6	0	-5.579041	-4.114057	-3.178865
15	6	0	-3.990512	-5.366505	-1.649058
16	6	0	0.549930	-2.053741	-3.085073
17	6	0	-4.212929	0.768273	0.747479

18	6	0	4.212927	-0.768312	0.747557
19	6	0	0.607270	0.433854	-1.533048
20	6	0	0.647404	1.625995	-2.276218
21	6	0	1.804305	2.378266	-2.249241
22	6	0	2.940946	2.002757	-1.506702
23	6	0	2.908220	0.809483	-0.735434
24	6	0	1.715130	0.053253	-0.777737
25	6	0	4.242820	4.066512	-2.423224
26	6	0	5.579112	4.114260	-3.178489
27	6	0	4.124348	2.864156	-1.501211
28	6	0	5.100634	2.609826	-0.597266
29	6	0	5.124111	1.409581	0.240167
30	6	0	4.055565	0.462335	0.104477
31	1	0	3.497337	-1.566176	0.622009
32	1	0	1.810159	3.302869	-2.808081
33	1	0	-3.497342	1.566146	0.621980
34	1	0	-1.810080	-3.302735	-2.808304
35	1	0	6.708270	2.944602	0.250074
36	1	0	4.035117	6.227582	-2.320689
37	1	0	-3.478223	-3.978183	-3.194372
38	8	0	1.642860	-1.097050	-0.046137
39	1	0	-5.535209	-4.900211	-3.937043
40	1	0	-5.771144	-3.164843	-3.683947
41	1	0	-6.411473	-4.323378	-2.510096
42	1	0	-4.035103	-6.227453	-2.321162
43	1	0	-3.008087	-5.351876	-1.170833
44	1	0	-4.749371	-5.493322	-0.874318
45	1	0	-0.858742	1.260735	-3.770651
46	1	0	-0.323312	2.948891	-3.664547
47	1	0	-1.406387	2.268020	-2.439161
48	8	0	-6.173590	-3.408458	-0.419586
49	1	0	-6.708267	-2.944612	0.249746
50	8	0	-6.124208	-1.271678	0.982239
51	1	0	0.323417	-2.948722	-3.664692
52	1	0	1.406463	-2.267912	-2.439246
53	1	0	0.858850	-1.260559	-3.770698
54	8	0	-1.642836	1.097037	-0.046121
55	8	0	6.124204	1.271623	0.982454
56	1	0	3.008097	5.351913	-1.170433
57	1	0	4.749374	5.493373	-0.873879
58	8	0	6.173605	3.408487	-0.419241
59	1	0	3.478296	3.978361	-3.194055
60	1	0	5.535288	4.900463	-3.936617
61	1	0	5.771240	3.165081	-3.683627
62	1	0	6.411525	4.323550	-2.509687
63	1	0	-0.745435	1.448152	-0.124207
64	1	0	0.745462	-1.448163	-0.124265
65	7	0	-5.226206	1.085613	1.536738
66	6	0	-6.499876	3.056499	1.572564
67	6	0	-5.316578	2.281483	3.549067
68	6	0	-6.552011	4.479109	2.118053
69	1	0	-7.410840	2.505607	1.864680
70	1	0	-6.439802	3.055132	0.483170
71	6	0	-5.334442	3.680141	4.153764
72	1	0	-6.199672	1.713004	3.889877
73	1	0	-4.423819	1.732635	3.852177
74	6	0	-6.539826	4.471244	3.646419
75	1	0	-7.446162	4.977005	1.736281
76	1	0	-5.681339	5.026985	1.745010
77	1	0	-5.350097	3.599350	5.243044
78	1	0	-4.410447	4.194232	3.872420
79	1	0	-6.520912	5.491396	4.035558
80	1	0	-7.460664	4.002515	4.012710
81	7	0	-5.304433	2.371841	2.083236
82	7	0	5.226184	-1.085695	1.536823
83	7	0	5.304378	-2.371944	2.083278
84	6	0	6.499832	-3.056598	1.572628
85	6	0	5.316467	-2.281640	3.549113
86	6	0	6.551927	-4.479229	2.118066
87	1	0	7.410792	-2.505729	1.864801
88	1	0	6.439802	-3.055189	0.483231
89	6	0	5.334286	-3.680321	4.153759
90	1	0	6.199556	-1.713186	3.889979
91	1	0	4.423703	-1.732791	3.852209
92	6	0	6.539679	-4.471422	3.646433
93	1	0	7.446087	-4.977123	1.736313
94	1	0	5.681262	-5.027080	1.744967
95	1	0	5.349899	-3.599571	5.243042
96	1	0	4.410295	-4.194388	3.872357
97	1	0	6.520734	-5.491589	4.035532
98	1	0	7.460510	-4.002721	4.012778
99	1	0	-5.955232	0.384417	1.704415
100	1	0	5.955210	-0.384513	1.704552

Structure 16bb ($CHCl_3$)

Energy (Hartrees): = -2224.4320195
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.088865	-2.640634	-0.589421
2	6	0	-4.107709	-2.893587	-1.490051
3	6	0	-2.931583	-2.022232	-1.495695
4	6	0	-2.909996	-0.828271	-0.724051
5	6	0	-4.066768	-0.484092	0.104724
6	6	0	-5.124488	-1.438184	0.244141
7	6	0	3.931236	5.395241	-1.617535
8	6	0	-0.563324	2.054824	-3.060084
9	6	0	-4.207514	-4.106376	-2.402098
10	6	0	-1.716166	-0.067393	-0.753832
11	6	0	-0.605190	-0.437801	-1.508880
12	6	0	-0.636936	-1.629272	-2.256421
13	6	0	-1.789455	-2.389010	-2.236800
14	6	0	-5.540925	-4.186864	-3.157965
15	6	0	-3.931240	-5.395165	-1.617969
16	6	0	0.563416	-2.054693	-3.060170
17	6	0	-4.240826	0.760214	0.730271
18	6	0	4.240812	-0.760252	0.730369
19	6	0	0.605241	0.437858	-1.508840
20	6	0	0.637006	1.629366	-2.256320
21	6	0	1.789520	2.389109	-2.236625
22	6	0	2.931627	2.022300	-1.495502
23	6	0	2.910023	0.828298	-0.723921
24	6	0	1.716196	0.067418	-0.753775
25	6	0	4.207560	4.106512	-2.401745
26	6	0	5.540995	4.187081	-3.157562
27	6	0	4.107748	2.893661	-1.489781
28	6	0	5.088887	2.640660	-0.589144
29	6	0	5.124494	1.438164	0.244351
30	6	0	4.066775	0.484081	0.104867
31	1	0	3.535984	-1.564245	0.584199
32	1	0	1.785546	3.312045	-2.798752
33	1	0	-3.536002	1.564219	0.584142
34	1	0	-1.785467	-3.311920	-2.798970
35	1	0	6.703013	2.995159	0.253340
36	1	0	3.960124	6.262376	-2.283117
37	1	0	-3.444236	-4.013410	-3.173102
38	8	0	1.657246	-1.071065	-0.007619
39	1	0	-5.477214	-4.971056	-3.917440
40	1	0	-5.758479	-3.243992	-3.666183
41	1	0	-6.372155	-4.419165	-2.494332
42	1	0	-3.960131	-6.262252	-2.283612
43	1	0	-2.947975	-5.362096	-1.141318
44	1	0	-4.684963	-5.534980	-0.839356
45	1	0	-0.861586	1.272360	-3.763125
46	1	0	-0.346313	2.962730	-3.623848
47	1	0	-1.423320	2.251386	-2.412676
48	8	0	-6.155834	-3.450420	-0.413281
49	1	0	-6.703014	-2.995180	0.253005
50	8	0	-6.129035	-1.305629	0.985259
51	1	0	0.346429	-2.962588	-3.623962
52	1	0	1.423402	-2.251258	-2.412749
53	1	0	0.861681	-1.272207	-3.763185
54	8	0	-1.657234	1.071052	-0.007616
55	8	0	6.129026	1.305571	0.985483
56	1	0	2.947959	5.362116	-1.140913
57	1	0	4.684935	5.535021	-0.838893
58	8	0	6.155848	3.450439	-0.412931
59	1	0	3.444309	4.013583	-3.172779
60	1	0	5.477286	4.971314	-3.916995
61	1	0	5.758595	3.244245	-3.665827
62	1	0	6.372196	4.419368	-2.493888
63	1	0	-0.760200	1.431838	-0.052228
64	1	0	0.760211	-1.431845	-0.052263
65	7	0	-5.250608	1.083338	1.511705
66	6	0	-6.548041	3.037398	1.533156
67	6	0	-5.350948	2.286636	3.514698
68	6	0	-6.628086	4.458019	2.079242
69	1	0	-7.444562	2.466396	1.827224
70	1	0	-6.487679	3.038907	0.443455
71	6	0	-5.398711	3.684468	4.118073
72	1	0	-6.224051	1.701107	3.848117
73	1	0	-4.447707	1.757064	3.821827
74	6	0	-6.617393	4.452356	3.607412
75	1	0	-7.533218	4.934111	1.695247
76	1	0	-5.769844	5.026059	1.706259
77	1	0	-5.417895	3.599208	5.207200
78	1	0	-4.483279	4.218503	3.843530
79	1	0	-6.615600	5.473871	3.994063
80	1	0	-7.529865	3.967334	3.973344

81	7	0	-5.336161	2.376496	2.045576
82	7	0	5.250577	-1.083415	1.511808
83	7	0	5.336105	-2.376593	2.045636
84	6	0	6.547981	-3.037495	1.533210
85	6	0	5.350874	-2.286782	3.514762
86	6	0	6.628000	-4.458136	2.079251
87	1	0	7.444507	-2.466515	1.827308
88	1	0	6.487634	-3.038969	0.443509
89	6	0	5.398609	-3.684635	4.118091
90	1	0	6.223981	-1.701277	3.848211
91	1	0	4.447636	-1.757207	3.821896
92	6	0	6.617286	-4.452523	3.607421
93	1	0	7.533130	-4.934227	1.695252
94	1	0	5.769756	-5.026152	1.706237
95	1	0	5.417780	-3.599411	5.207221
96	1	0	4.483173	-4.218647	3.843519
97	1	0	6.615474	-5.474051	3.994038
98	1	0	7.529762	-3.967527	3.973381
99	1	0	-5.975143	0.386746	1.708650
100	1	0	5.975116	-0.386838	1.708792

Structure 16bb (DMSO)

Energy (Hartrees): = -2224.4220489
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.070000	2.662963	-0.565567
2	6	0	4.096598	2.906920	-1.477357
3	6	0	2.924825	2.029401	-1.488614
4	6	0	2.902145	0.839804	-0.709107
5	6	0	4.054432	0.503787	0.128838
6	6	0	5.105329	1.462935	0.273016
7	6	0	-3.908122	-5.406111	-1.621637
8	6	0	0.555467	-2.035997	-3.083838
9	6	0	4.198007	4.114487	-2.395835
10	6	0	1.709375	0.076581	-0.739375
11	6	0	0.604802	0.438402	-1.507681
12	6	0	0.639596	1.622056	-2.267479
13	6	0	1.788359	2.387397	-2.243316
14	6	0	5.537829	4.197117	-3.138685
15	6	0	3.908415	5.406102	-1.622272
16	6	0	-0.555465	2.035992	-3.083922
17	6	0	4.236008	-0.744940	0.747178
18	6	0	-4.235994	0.745060	0.747377
19	6	0	-0.604722	-0.438325	-1.507622
20	6	0	-0.639548	-1.622024	-2.267345
21	6	0	-1.788294	-2.387381	-2.243048
22	6	0	-2.924710	-2.029362	-1.488284
23	6	0	-2.902016	-0.839705	-0.708864
24	6	0	-1.709248	-0.076467	-0.739266
25	6	0	-4.197847	-4.114569	-2.395275
26	6	0	-5.537713	-4.197338	-3.138030
27	6	0	-4.096445	-2.906930	-1.476891
28	6	0	-5.069796	-2.662959	-0.565051
29	6	0	-5.105110	-1.462882	0.273458
30	6	0	-4.054284	-0.503687	0.129126
31	1	0	-3.540203	1.554635	0.588277
32	1	0	-1.784996	-3.306257	-2.812121
33	1	0	3.540081	-1.554419	0.588161
34	1	0	1.785037	3.306234	-2.812448
35	1	0	-6.666915	-3.013621	0.295352
36	1	0	-3.943083	-6.269193	-2.292113
37	1	0	3.442200	4.015226	-3.173152
38	8	0	-1.642855	1.050872	0.022053
39	1	0	5.479548	4.982035	-3.897706
40	1	0	5.761653	3.255502	-3.647070
41	1	0	6.362934	4.429317	-2.467082
42	1	0	3.943391	6.269133	-2.292813
43	1	0	2.917975	5.372803	-1.160500
44	1	0	4.651184	5.553114	-0.834148
45	1	0	0.850006	-1.242416	-3.776204
46	1	0	0.333947	-2.934869	-3.660026
47	1	0	1.418633	-2.245000	-2.444290
48	8	0	6.132858	3.475005	-0.378313
49	1	0	6.667205	3.013611	0.294689
50	8	0	6.104745	1.341049	1.022276
51	1	0	-0.333978	2.934836	-3.660166
52	1	0	-1.418595	2.245024	-2.444335
53	1	0	-0.850044	1.242378	-3.776234
54	8	0	1.643072	-1.050716	0.022015
55	8	0	-6.104527	-1.340912	1.022703

56	1	0	-2.917655	-5.372714	-1.159932
57	1	0	-4.650830	-5.553115	-0.833455
58	8	0	-6.132607	-3.475032	-0.377670
59	1	0	-3.442098	-4.015317	-3.172649
60	1	0	-5.479427	-4.982296	-3.897010
61	1	0	-5.761639	-3.255769	-3.646456
62	1	0	-6.362756	-4.429557	-2.466360
63	1	0	0.754141	-1.426790	-0.055549
64	1	0	-0.753920	1.426920	-0.055609
65	7	0	5.241414	-1.067022	1.531016
66	6	0	6.545449	-3.013731	1.486624
67	6	0	5.399849	-2.297266	3.511377
68	6	0	6.651852	-4.439901	2.011960
69	1	0	7.442530	-2.437697	1.766131
70	1	0	6.454118	-3.002051	0.399083
71	6	0	5.475640	-3.702419	4.094391
72	1	0	6.279503	-1.710927	3.823401
73	1	0	4.502278	-1.778646	3.852473
74	6	0	6.685383	-4.452928	3.539514
75	1	0	7.550009	-4.902486	1.596348
76	1	0	5.788614	-5.012096	1.656471
77	1	0	5.525541	-3.629278	5.183389
78	1	0	4.557095	-4.241682	3.840632
79	1	0	6.703987	-5.479284	3.912910
80	1	0	7.603096	-3.962390	3.884021
81	7	0	5.341669	-2.369104	2.041384
82	7	0	-5.241432	1.067022	1.531223
83	7	0	-5.341900	2.369115	2.041520
84	6	0	-6.545812	3.013498	1.486763
85	6	0	-5.400020	2.297349	3.511519
86	6	0	-6.652457	4.439677	2.012025
87	1	0	-7.442781	2.437316	1.766330
88	1	0	-6.454513	3.001774	0.399219
89	6	0	-5.476046	3.702521	4.094458
90	1	0	-6.279561	1.710870	3.823602
91	1	0	-4.502346	1.778908	3.852616
92	6	0	-6.685942	4.452781	3.539579
93	1	0	-7.550711	4.902076	1.596417
94	1	0	-5.789334	5.012010	1.656476
95	1	0	-5.525900	3.629431	5.183462
96	1	0	-4.557606	4.241935	3.840642
97	1	0	-6.704718	5.479155	3.912919
98	1	0	-7.603555	3.962097	3.884142
99	1	0	5.964916	-0.373428	1.741208
100	1	0	-5.964808	0.373317	1.741482

Structure 16bb $\chi = 36.6^{o}$ (vacuum)

Energy (Hartrees): = -2224.3745815
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.702502	-3.033706	-0.270307
2	6	0	-3.763978	-3.154000	-1.241415
3	6	0	-2.705258	-2.141920	-1.318661
4	6	0	-2.773205	-0.970772	-0.523373
5	6	0	-3.949145	-0.738730	0.318008
6	6	0	-4.855443	-1.831405	0.554879
7	6	0	3.560431	5.764182	-0.719159
8	6	0	-0.768306	2.400881	-2.447589
9	6	0	-3.781172	-4.365118	-2.158161
10	6	0	-1.654586	-0.114294	-0.508984
11	6	0	-0.549662	-0.310867	-1.332810
12	6	0	-0.527942	-1.431506	-2.183741
13	6	0	-1.581098	-2.329592	-2.140200
14	6	0	-5.128751	-4.542207	-2.872606
15	6	0	-3.379372	-5.632461	-1.391466
16	6	0	0.645021	-1.661638	-3.101959
17	6	0	-4.372500	0.529054	0.704643
18	6	0	4.433809	-0.632978	0.550757
19	6	0	0.600438	0.636325	-1.272991
20	6	0	0.511571	1.927220	-1.811447
21	6	0	1.613834	2.753596	-1.729022
22	6	0	2.818081	2.358428	-1.117687
23	6	0	2.916614	1.058245	-0.555563
24	6	0	1.776259	0.231182	-0.650066
25	6	0	3.897989	4.650492	-1.719143
26	6	0	5.186144	4.966857	-2.492737
27	6	0	3.933141	3.302662	-1.018710
28	6	0	4.975334	2.986902	-0.213614
29	6	0	5.138775	1.670022	0.402661
30	6	0	4.138037	0.671764	0.154841

31	1	0	3.779329	-1.457361	0.311628
32	1	0	1.515441	3.754179	-2.125023
33	1	0	-3.864772	1.423951	0.360175
34	1	0	-1.507494	-3.211955	-2.759793
35	1	0	6.598593	3.310544	0.608168
36	1	0	3.491804	6.729198	-1.228529
37	1	0	-3.047166	-4.207151	-2.946918
38	8	0	1.833753	-1.018839	-0.092698
39	1	0	-5.045096	-5.345434	-3.609066
40	1	0	-5.410390	-3.627506	-3.398807
41	1	0	-5.921376	-4.796846	-2.171214
42	1	0	-3.354729	-6.492402	-2.065527
43	1	0	-2.390043	-5.518060	-0.942042
44	1	0	-4.099493	-5.835503	-0.597197
45	1	0	-1.135161	1.681757	-3.184612
46	1	0	-0.620640	3.360713	-2.943569
47	1	0	-1.548117	2.520776	-1.690257
48	8	0	-5.642250	-3.973636	-0.030527
49	1	0	-6.213187	-3.583307	0.653587
50	8	0	-5.834654	-1.794417	1.327574
51	1	0	0.446758	-2.492130	-3.779542
52	1	0	1.551216	-1.887540	-2.532990
53	1	0	0.854818	-0.766534	-3.692005
54	8	0	-1.601251	0.969178	0.330560
55	8	0	6.189987	1.492626	1.062482
56	1	0	2.608046	5.567060	-0.221120
57	1	0	4.340430	5.830379	0.042314
58	8	0	5.991678	3.835433	0.056083
59	1	0	3.109094	4.619115	-2.469719
60	1	0	5.027743	5.859073	-3.104291
61	1	0	5.451109	4.141337	-3.157084
62	1	0	6.022878	5.150342	-1.821821
63	1	0	-2.021651	0.731607	1.164650
64	1	0	0.949942	-1.405098	-0.127673
65	7	0	-5.431914	0.783828	1.461933
66	6	0	-7.122701	2.300747	0.871293
67	6	0	-6.045385	2.387105	3.051991
68	6	0	-7.583486	3.747068	1.002442
69	1	0	-7.904149	1.618344	1.247451
70	1	0	-6.924120	2.044870	-0.170889
71	6	0	-6.476541	3.836063	3.244615
72	1	0	-6.799545	1.708847	3.488124
73	1	0	-5.091585	2.192837	3.544753
74	6	0	-7.763766	4.122629	2.472618
75	1	0	-8.515608	3.877161	0.448190
76	1	0	-6.831508	4.396934	0.544931
77	1	0	-6.608402	4.030821	4.311236
78	1	0	-5.676369	4.489666	2.884565
79	1	0	-8.042288	5.174070	2.568742
80	1	0	-8.581940	3.531532	2.900481
81	7	0	-5.872381	2.102376	1.621749
82	7	0	5.517562	-0.995422	1.221900
83	7	0	5.726131	-2.345833	1.523180
84	6	0	6.982469	-2.802946	0.916053
85	6	0	5.726529	-2.535266	2.979454
86	6	0	7.172812	-4.292074	1.182761
87	1	0	7.835988	-2.234801	1.326174
88	1	0	6.924581	-2.599033	-0.154121
89	6	0	5.875449	-4.016381	3.305856
90	1	0	6.549524	-1.962462	3.441644
91	1	0	4.784138	-2.141070	3.362551
92	6	0	7.153485	-4.577963	2.683984
93	1	0	8.113316	-4.620617	0.734414
94	1	0	6.361889	-4.839106	0.692239
95	1	0	5.877818	-4.147820	4.390323
96	1	0	5.006422	-4.549436	2.908344
97	1	0	7.232948	-5.650980	2.871396
98	1	0	8.022687	-4.103167	3.154073
99	1	0	-5.997600	-0.008784	1.783127
100	1	0	6.193501	-0.271995	1.488745

Structure 16bb χ = 77.9º (vacuum)

Energy (Hartrees): = -2224.3736051
Imaginary frequency -310.56

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.839533	-2.941765	-0.366712
2	6	0	-3.865634	-3.127882	-1.290646
3	6	0	-2.772696	-2.154554	-1.353224
4	6	0	-2.828433	-0.950386	-0.600128
5	6	0	-4.006385	-0.672111	0.222675

6	6	0	-4.970699	-1.716238	0.425542
7	6	0	3.614035	5.667688	-1.070262
8	6	0	-0.710052	2.243014	-2.708593
9	6	0	-3.888114	-4.367524	-2.169415
10	6	0	-1.693627	-0.114463	-0.626874
11	6	0	-0.571191	-0.383775	-1.402915
12	6	0	-0.543250	-1.555443	-2.182344
13	6	0	-1.627590	-2.412737	-2.126958
14	6	0	-5.219357	-4.541486	-2.914746
15	6	0	-3.534439	-5.617027	-1.351627
16	6	0	0.649807	-1.867162	-3.049589
17	6	0	-4.335172	0.597794	0.698766
18	6	0	4.358059	-0.652274	0.634039
19	6	0	0.593471	0.547083	-1.372129
20	6	0	0.541481	1.799300	-1.999773
21	6	0	1.652054	2.615766	-1.934382
22	6	0	2.829059	2.248134	-1.255937
23	6	0	2.891592	0.986057	-0.609239
24	6	0	1.744363	0.166685	-0.690068
25	6	0	3.965465	4.478582	-1.973879
26	6	0	5.286026	4.715364	-2.720717
27	6	0	3.952757	3.184015	-1.178465
28	6	0	4.958490	2.912619	-0.312704
29	6	0	5.081386	1.637463	0.394937
30	6	0	4.082250	0.632721	0.166642
31	1	0	3.713491	-1.486920	0.402983
32	1	0	1.581322	3.589117	-2.398461
33	1	0	-3.738720	1.463927	0.445344
34	1	0	-1.565526	-3.325699	-2.702087
35	1	0	6.553705	3.274351	0.548016
36	1	0	3.586322	6.594222	-1.649973
37	1	0	-3.132332	-4.250426	-2.944765
38	8	0	1.769115	-1.047027	-0.053004
39	1	0	-5.127908	-5.361918	-3.631082
40	1	0	-5.473960	-3.634890	-3.468094
41	1	0	-6.034312	-4.768825	-2.230095
42	1	0	-3.514380	-6.500521	-1.994878
43	1	0	-2.554025	-5.510289	-0.881067
44	1	0	-4.278344	-5.776042	-0.568941
45	1	0	-1.064932	1.476411	-3.402333
46	1	0	-0.531800	3.161949	-3.267837
47	1	0	-1.509874	2.426151	-1.985925
48	8	0	-5.823549	-3.836821	-0.137921
49	1	0	-6.396908	-3.404925	0.519708
50	8	0	-5.972249	-1.636286	1.170827
51	1	0	0.449526	-2.731856	-3.682589
52	1	0	1.535546	-2.080069	-2.444268
53	1	0	0.897147	-1.014261	-3.685824
54	8	0	-1.671596	1.055475	0.112979
55	8	0	6.102689	1.493174	1.107191
56	1	0	2.638818	5.525079	-0.598385
57	1	0	4.365221	5.774066	-0.284747
58	8	0	5.974976	3.766472	-0.061393
59	1	0	3.203159	4.404341	-2.748627
60	1	0	5.169381	5.565398	-3.398081
61	1	0	5.555484	3.840634	-3.316942
62	1	0	6.102966	4.928596	-2.034382
63	1	0	-1.499295	0.841105	1.036567
64	1	0	0.894260	-1.447494	-0.130659
65	7	0	-5.390608	0.877007	1.447216
66	6	0	-6.890827	2.639094	1.038591
67	6	0	-5.852583	2.337953	3.215705
68	6	0	-7.174101	4.106802	1.336658
69	1	0	-7.755073	2.018707	1.331890
70	1	0	-6.708228	2.482401	-0.025712
71	6	0	-6.108882	3.795608	3.579740
72	1	0	-6.692923	1.710868	3.561921
73	1	0	-4.939952	1.969816	3.686698
74	6	0	-7.335851	4.328879	2.840293
75	1	0	-8.071621	4.415280	0.795909
76	1	0	-6.338422	4.706202	0.962963
77	1	0	-6.237914	3.877206	4.661414
78	1	0	-5.227933	4.383577	3.305116
79	1	0	-7.484954	5.388390	3.058228
80	1	0	-8.229124	3.798090	3.189994
81	7	0	-5.685784	2.208402	1.763201
82	7	0	5.411818	-0.983880	1.366322
83	7	0	5.626189	-2.324687	1.704571
84	6	0	6.887398	-2.790084	1.112660
85	6	0	5.624448	-2.475547	3.165207
86	6	0	7.086016	-4.270267	1.417594
87	1	0	7.735942	-2.205954	1.510194
88	1	0	6.831121	-2.614119	0.037423
89	6	0	5.782447	-3.946693	3.530528
90	1	0	6.442756	-1.885453	3.613867
91	1	0	4.678766	-2.077712	3.536144
92	6	0	7.064826	-4.517147	2.925788
93	1	0	8.029561	-4.604690	0.980138

94	1	0	6.279578	-4.834722	0.939577
95	1	0	5.783990	-4.049286	4.618141
96	1	0	4.917200	-4.495483	3.146395
97	1	0	7.149417	-5.584486	3.141239
98	1	0	7.930467	-4.025768	3.385267
99	1	0	-6.026979	0.112086	1.697389
100	1	0	6.081805	-0.250280	1.620404

Structure 16bb χ = 279.0º (vacuum)

Energy (Hartrees): = -2224.3722425
Imaginary frequency -314.00

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.467624	2.037359	-1.024180
2	6	0	4.356145	2.683231	-1.452799
3	6	0	3.081122	1.962820	-1.423392
4	6	0	2.973869	0.700657	-0.779307
5	6	0	4.148659	0.131381	-0.117561
6	6	0	5.428045	0.746972	-0.330548
7	6	0	-4.326893	-4.920618	-2.401559
8	6	0	0.370021	-1.580775	-3.529841
9	6	0	4.470509	4.081932	-2.035321
10	6	0	1.742765	0.020491	-0.885287
11	6	0	0.638173	0.555313	-1.538843
12	6	0	0.739210	1.825594	-2.134410
13	6	0	1.951684	2.487091	-2.077151
14	6	0	5.094350	4.029624	-3.436344
15	6	0	5.227992	5.054947	-1.120240
16	6	0	-0.447032	2.423191	-2.844988
17	6	0	4.084486	-0.896227	0.824721
18	6	0	-4.105605	0.774470	0.895603
19	6	0	-0.623755	-0.234231	-1.641851
20	6	0	-0.761184	-1.257477	-2.588799
21	6	0	-1.954563	-1.948589	-2.647368
22	6	0	-3.039187	-1.665479	-1.796463
23	6	0	-2.914025	-0.624323	-0.838107
24	6	0	-1.680014	0.060486	-0.789601
25	6	0	-4.479636	-3.501732	-2.965742
26	6	0	-5.822288	-3.326565	-3.690178
27	6	0	-4.263338	-2.465217	-1.875153
28	6	0	-5.194187	-2.316014	-0.902325
29	6	0	-5.126977	-1.268618	0.116837
30	6	0	-4.016428	-0.361021	0.087876
31	1	0	-3.366329	1.559940	0.850080
32	1	0	-2.029817	-2.753372	-3.364132
33	1	0	3.135293	-1.297770	1.153339
34	1	0	2.023666	3.435791	-2.590362
35	1	0	-6.789385	-2.709444	-0.055295
36	1	0	-4.447755	-5.662679	-3.195217
37	1	0	3.466215	4.493364	-2.129499
38	8	0	-1.522412	1.055948	0.136064
39	1	0	5.146235	5.031877	-3.869347
40	1	0	4.504956	3.394782	-4.102323
41	1	0	6.106801	3.625145	-3.379917
42	1	0	5.136675	6.068298	-1.519461
43	1	0	4.806171	5.047325	-0.112740
44	1	0	6.284521	4.802756	-1.053412
45	1	0	0.727673	-0.683424	-4.041597
46	1	0	0.054198	-2.305978	-4.280109
47	1	0	1.228687	-2.004200	-2.998837
48	8	0	6.711135	2.549981	-1.132186
49	1	0	7.281374	1.898900	-0.686272
50	8	0	6.518271	0.310505	0.100558
51	1	0	-0.184687	3.376025	-3.305001
52	1	0	-1.272088	2.590411	-2.146869
53	1	0	-0.819429	1.748507	-3.619994
54	8	0	1.582536	-1.225969	-0.305303
55	8	0	-6.094841	-1.204906	0.911312
56	1	0	-3.341339	-5.055148	-1.949220
57	1	0	-5.085188	-5.103550	-1.638107
58	8	0	-6.303569	-3.082564	-0.812443
59	1	0	-3.715996	-3.361817	-3.729310
60	1	0	-5.865360	-4.008658	-4.543449
61	1	0	-5.927868	-2.306334	-4.065624
62	1	0	-6.662349	-3.541357	-3.032261
63	1	0	1.961495	-1.893717	-0.887854
64	1	0	-0.596439	1.328417	0.130706
65	7	0	5.132395	-1.441770	1.421379
66	6	0	5.582919	-3.671761	1.978057
67	6	0	5.487339	-1.942803	3.685515
68	6	0	5.332594	-4.760024	3.015111

69	1	0	6.668321	-3.522317	1.842435
70	1	0	5.157031	-3.945124	1.011382
71	6	0	5.238663	-2.981778	4.772892
72	1	0	6.569668	-1.746531	3.591885
73	1	0	4.992120	-0.999807	3.921950
74	6	0	5.853471	-4.326182	4.384459
75	1	0	5.813801	-5.684513	2.688061
76	1	0	4.256157	-4.947453	3.071631
77	1	0	5.653664	-2.618503	5.715841
78	1	0	4.158626	-3.094618	4.907742
79	1	0	5.629365	-5.083380	5.138712
80	1	0	6.944399	-4.226150	4.341484
81	7	0	4.944809	-2.419112	2.405652
82	7	0	-5.084665	1.013319	1.754813
83	7	0	-5.130485	2.233185	2.439692
84	6	0	-6.302655	3.001978	1.998531
85	6	0	-5.160537	1.980992	3.885534
86	6	0	-6.327734	4.355374	2.698297
87	1	0	-7.230114	2.445548	2.219587
88	1	0	-6.230204	3.120030	0.916187
89	6	0	-5.153479	3.303910	4.642764
90	1	0	-6.059419	1.398782	4.154104
91	1	0	-4.283742	1.381182	4.133360
92	6	0	-6.334198	4.175659	4.216006
93	1	0	-7.205425	4.915425	2.367339
94	1	0	-5.440147	4.920542	2.397844
95	1	0	-5.182909	3.103435	5.716174
96	1	0	-4.214820	3.823604	4.427789
97	1	0	-6.296352	5.145079	4.717703
98	1	0	-7.270073	3.691570	4.519221
99	1	0	6.067330	-1.098431	1.176588
100	1	0	-5.836105	0.320020	1.841230

Structure 16bb χ = 326.2° (vacuum)

Energy (Hartrees): = -2224.3742355
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.534868	1.207679	-1.753780
2	6	0	4.440698	1.718827	-2.370884
3	6	0	3.132177	1.120165	-2.086198
4	6	0	2.998829	0.139267	-1.072125
5	6	0	4.154569	-0.197905	-0.237969
6	6	0	5.460294	0.237919	-0.657032
7	6	0	-4.646744	-5.331212	-0.637197
8	6	0	0.238917	-2.846406	-2.813947
9	6	0	4.607720	2.832001	-3.391105
10	6	0	1.764014	-0.529504	-0.954611
11	6	0	0.642109	-0.161963	-1.692266
12	6	0	0.760236	0.873171	-2.637699
13	6	0	1.995712	1.464712	-2.838070
14	6	0	5.297029	2.309892	-4.658984
15	6	0	5.339019	4.052120	-2.812382
16	6	0	-0.436825	1.285770	-3.454851
17	6	0	4.037623	-0.698514	1.054902
18	6	0	-4.012893	1.103538	0.584116
19	6	0	-0.651669	-0.881360	-1.507699
20	6	0	-0.859979	-2.155908	-2.051082
21	6	0	-2.088691	-2.757230	-1.869375
22	6	0	-3.140413	-2.144425	-1.162745
23	6	0	-2.941864	-0.851926	-0.607728
24	6	0	-1.673693	-0.260148	-0.798961
25	6	0	-4.700850	-4.180722	-1.651075
26	6	0	-6.030399	-4.170128	-2.419800
27	6	0	-4.408411	-2.852018	-0.973245
28	6	0	-5.317825	-2.329079	-0.116191
29	6	0	-5.174667	-1.009547	0.496949
30	6	0	-4.010945	-0.232388	0.178934
31	1	0	-3.222865	1.781352	0.299154
32	1	0	-2.218583	-3.750940	-2.272593
33	1	0	3.067426	-0.834679	1.521846
34	1	0	2.071167	2.201813	-3.624376
35	1	0	-6.921144	-2.320264	0.803210
36	1	0	-4.822788	-6.287735	-1.136602
37	1	0	3.619388	3.187891	-3.676698
38	8	0	-1.446750	0.980188	-0.263693
39	1	0	5.373166	3.106318	-5.403640
40	1	0	4.732321	1.482912	-5.095774
41	1	0	6.302878	1.957365	-4.425566
42	1	0	5.326593	4.863565	-3.544475
43	1	0	4.843391	4.405265	-1.905378

44	1	0	6.375171	3.819259	-2.572799
45	1	0	0.651447	-2.193555	-3.587750
46	1	0	-0.131057	-3.755760	-3.288397
47	1	0	1.060245	-3.117184	-2.145316
48	8	0	6.794829	1.607113	-2.031282
49	1	0	7.350717	1.134664	-1.387705
50	8	0	6.530276	-0.060789	-0.088293
51	1	0	-0.156828	2.025763	-4.204646
52	1	0	-1.213259	1.715707	-2.815838
53	1	0	-0.881371	0.423407	-3.957491
54	8	0	1.607576	-1.586986	-0.095875
55	8	0	-6.126890	-0.627336	1.218088
56	1	0	-3.670794	-5.372009	-0.147597
57	1	0	-5.412500	-5.194482	0.128401
58	8	0	-6.469660	-2.953414	0.216922
59	1	0	-3.932217	-4.361701	-2.400434
60	1	0	-6.126404	-5.097648	-2.990380
61	1	0	-6.062966	-3.333984	-3.121817
62	1	0	-6.880876	-4.088401	-1.745387
63	1	0	2.438082	-2.074946	-0.061585
64	1	0	-0.511591	1.189720	-0.377186
65	7	0	5.051078	-1.005035	1.854950
66	6	0	5.474212	-2.592969	3.522465
67	6	0	5.247583	-0.233150	4.065973
68	6	0	5.154128	-2.990295	4.958579
69	1	0	6.566103	-2.490430	3.394269
70	1	0	5.120806	-3.348088	2.818881
71	6	0	4.918411	-0.562134	5.517323
72	1	0	6.333111	-0.070962	3.950255
73	1	0	4.734134	0.673914	3.742561
74	6	0	5.565652	-1.884100	5.929565
75	1	0	5.665017	-3.926754	5.193118
76	1	0	4.077869	-3.170438	5.038554
77	1	0	5.258262	0.256191	6.156056
78	1	0	3.831491	-0.634873	5.620752
79	1	0	5.284200	-2.147087	6.951368
80	1	0	6.656292	-1.773964	5.913244
81	7	0	4.802258	-1.330052	3.193031
82	7	0	-4.959318	1.669336	1.318621
83	7	0	-4.905825	3.041928	1.586755
84	6	0	-6.024683	3.720731	0.918045
85	6	0	-4.931276	3.258909	3.038324
86	6	0	-5.935891	5.223707	1.157125
87	1	0	-6.987217	3.334095	1.295630
88	1	0	-5.962527	3.487162	-0.145994
89	6	0	-4.809989	4.747544	3.341387
90	1	0	-5.867793	2.862864	3.468854
91	1	0	-4.099138	2.700402	3.469215
92	6	0	-5.928616	5.530513	2.654325
93	1	0	-6.774384	5.717350	0.660450
94	1	0	-5.013643	5.595631	0.700365
95	1	0	-4.835656	4.897194	4.423185
96	1	0	-3.838574	5.098843	2.980288
97	1	0	-5.808953	6.602375	2.826571
98	1	0	-6.892599	5.238885	3.087493
99	1	0	6.004051	-0.851911	1.509568
100	1	0	-5.754869	1.093812	1.615633

Structure 16dd (vacuum)

Energy (Hartrees): = -2224.3777353
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.212938	2.397126	0.493632
2	6	0	-4.242844	2.687115	1.393040
3	6	0	-3.022026	1.877980	1.384804
4	6	0	-2.943368	0.688969	0.610163
5	6	0	-4.083047	0.295537	-0.220118
6	6	0	-5.191545	1.199388	-0.349365
7	6	0	4.211297	-5.192082	1.564047
8	6	0	-0.471667	-2.072885	2.943585
9	6	0	-4.406858	3.875019	2.326543
10	6	0	-1.719112	-0.014711	0.641953
11	6	0	-0.623708	0.409871	1.392330
12	6	0	-0.709432	1.597997	2.137580
13	6	0	-1.897577	2.300944	2.118864
14	6	0	-5.741378	3.861240	3.086552
15	6	0	-4.211415	5.192084	1.564469
16	6	0	0.471764	2.072594	2.943738
17	6	0	-4.195499	-0.939946	-0.856829
18	6	0	4.195518	0.940021	-0.856811

19	6	0	0.623775	-0.410015	1.392301
20	6	0	0.709517	-1.598196	2.137465
21	6	0	1.897686	-2.301100	2.118722
22	6	0	3.022142	-1.878050	1.384714
23	6	0	2.943464	-0.688984	0.610157
24	6	0	1.719191	0.014668	0.642003
25	6	0	4.406955	-3.875157	2.326304
26	6	0	5.741536	-3.861681	3.086198
27	6	0	4.242992	-2.687147	1.392937
28	6	0	5.213115	-2.397056	0.493604
29	6	0	5.191717	-1.199244	-0.349289
30	6	0	4.083157	-0.295456	-0.220064
31	1	0	3.430770	1.687857	-0.711617
32	1	0	1.939393	-3.223893	2.679163
33	1	0	-3.430821	-1.687849	-0.711605
34	1	0	-1.939261	3.223716	2.679345
35	1	0	6.840503	-2.666095	-0.340428
36	1	0	4.291690	-6.043418	2.244984
37	1	0	-3.636685	3.810241	3.094191
38	8	0	1.599570	1.161710	-0.093102
39	1	0	-5.724845	4.637630	3.855714
40	1	0	-5.896069	2.898311	3.578383
41	1	0	-6.583414	4.048557	2.423360
42	1	0	-4.291867	6.043292	2.245557
43	1	0	-3.230269	5.225532	1.084486
44	1	0	-4.976527	5.294544	0.792184
45	1	0	-0.808235	-1.295311	3.634203
46	1	0	-0.213853	-2.962381	3.518460
47	1	0	-1.320931	-2.313116	2.297420
48	8	0	-6.319655	3.149356	0.326489
49	1	0	-6.840299	2.666248	-0.340432
50	8	0	-6.186038	1.018145	-1.084575
51	1	0	0.213967	2.962040	3.518700
52	1	0	1.321031	2.312873	2.297590
53	1	0	0.808324	1.294948	3.634277
54	8	0	-1.599507	-1.161665	-0.093295
55	8	0	6.186222	-1.017946	-1.084472
56	1	0	3.230129	-5.225329	1.084093
57	1	0	4.976365	-5.294483	0.791705
58	8	0	6.319833	-3.149271	0.326424
59	1	0	3.636848	-3.810354	3.094019
60	1	0	5.724814	-4.637967	3.855461
61	1	0	5.896566	-2.898735	3.577888
62	1	0	6.583470	-4.049345	2.422977
63	1	0	-0.687490	-1.473264	-0.015558
64	1	0	0.687557	1.473306	-0.015296
65	7	0	-5.195707	-1.315279	-1.642084
66	6	0	-4.170219	-2.830337	-3.160067
67	6	0	-5.381829	-3.647048	-1.206538
68	6	0	-4.412321	-4.141861	-3.898797
69	1	0	-3.199513	-2.873919	-2.636001
70	1	0	-4.141177	-1.987604	-3.852407
71	6	0	-5.657417	-4.980395	-1.892336
72	1	0	-4.457691	-3.723745	-0.607894
73	1	0	-6.197657	-3.373939	-0.535408
74	6	0	-4.560718	-5.297942	-2.909065
75	1	0	-3.586366	-4.324010	-4.590256
76	1	0	-5.327383	-4.044534	-4.490718
77	1	0	-5.730287	-5.766326	-1.136957
78	1	0	-6.624229	-4.915943	-2.400568
79	1	0	-4.783907	-6.227695	-3.436693
80	1	0	-3.610692	-5.446276	-2.382168
81	7	0	-5.270759	-2.592475	-2.219877
82	7	0	5.195684	1.315436	-1.642080
83	7	0	5.270593	2.592627	-2.219903
84	6	0	4.169998	2.830397	-3.160042
85	6	0	5.381647	3.647214	-1.206581
86	6	0	4.411987	4.141921	-3.898809
87	1	0	3.199306	2.873942	-2.635947
88	1	0	4.140976	1.987643	-3.852358
89	6	0	5.657105	4.980574	-1.892403
90	1	0	4.457536	3.723847	-0.607884
91	1	0	6.197528	3.374164	-0.535491
92	6	0	4.560342	5.298023	-2.909093
93	1	0	3.585990	4.324010	-4.590234
94	1	0	5.327030	4.044646	-4.490767
95	1	0	5.729936	5.766523	-1.137039
96	1	0	6.623903	4.916197	-2.400671
97	1	0	4.783433	6.227793	-3.436733
98	1	0	3.610326	5.446285	-2.382157
99	1	0	-5.955421	-0.662493	-1.820023
100	1	0	5.955480	0.662736	-1.819988

Structure 16dd ($CHCl_3$)

Energy (Hartrees): = -2224.4232237

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.203903	2.410912	-0.473692
2	6	0	4.241661	2.693263	-1.385438
3	6	0	3.025398	1.877203	-1.385020
4	6	0	2.946534	0.693443	-0.602018
5	6	0	4.085636	0.305496	0.232163
6	6	0	5.181793	1.217112	0.373926
7	6	0	-4.191069	-5.199592	-1.573352
8	6	0	0.465495	-2.063086	-2.946777
9	6	0	4.405771	3.878915	-2.323313
10	6	0	1.718122	-0.008883	-0.623353
11	6	0	0.625335	0.408577	-1.380624
12	6	0	0.714081	1.589390	-2.139705
13	6	0	1.902950	2.291556	-2.129609
14	6	0	5.745867	3.874403	-3.072384
15	6	0	4.191078	5.199527	-1.573761
16	6	0	-0.465580	2.062948	-2.946876
17	6	0	4.209095	-0.943986	0.852826
18	6	0	-4.209085	0.944034	0.852902
19	6	0	-0.625385	-0.408631	-1.380587
20	6	0	-0.714148	-1.589485	-2.139603
21	6	0	-1.903017	-2.291650	-2.129443
22	6	0	-3.025447	-1.877260	-1.384848
23	6	0	-2.946565	-0.693458	-0.601910
24	6	0	-1.718155	0.008869	-0.623314
25	6	0	-4.405826	-3.879039	-2.322989
26	6	0	-5.745951	-3.874617	-3.072010
27	6	0	-4.241709	-2.693322	-1.385198
28	6	0	-5.203938	-2.410917	-0.473455
29	6	0	-5.181809	-1.217073	0.374099
30	6	0	-4.085650	-0.305470	0.232277
31	1	0	-3.463506	1.705368	0.679163
32	1	0	-1.943545	-3.208507	-2.700110
33	1	0	3.463522	-1.705335	0.679120
34	1	0	1.943465	3.208385	-2.700321
35	1	0	-6.828764	-2.704134	0.373624
36	1	0	-4.276845	-6.046052	-2.260270
37	1	0	3.643122	3.805003	-3.097144
38	8	0	-1.605357	1.139111	0.132521
39	1	0	5.725028	4.643582	-3.849245
40	1	0	5.917802	2.910225	-3.557741
41	1	0	6.584189	4.079924	-2.408715
42	1	0	4.276852	6.045935	-2.260743
43	1	0	3.201755	5.234764	-1.109990
44	1	0	4.941954	5.318006	-0.788970
45	1	0	0.797004	-1.291226	-3.646829
46	1	0	0.209629	-2.958159	-3.514780
47	1	0	1.317481	-2.298349	-2.301599
48	8	0	6.304652	3.174133	-0.301285
49	1	0	6.828745	2.704180	0.373342
50	8	0	6.172098	1.045475	1.122377
51	1	0	-0.209739	2.958013	-3.514904
52	1	0	-1.317563	2.298208	-2.301694
53	1	0	-0.797081	1.291065	-3.646907
54	8	0	1.605339	-1.139080	0.132552
55	8	0	-6.172102	-1.045394	1.122557
56	1	0	-3.201728	-5.234767	-1.109615
57	1	0	-4.941914	-5.318036	-0.788525
58	8	0	-6.304684	-3.174127	-0.300985
59	1	0	-3.643209	-3.805160	-3.096853
60	1	0	-5.725112	-4.643838	-3.848829
61	1	0	-5.917938	-2.910472	-3.557415
62	1	0	-6.584242	-4.080129	-2.408300
63	1	0	0.692717	-1.458564	0.088152
64	1	0	-0.692733	1.458587	0.088094
65	7	0	5.200113	-1.315655	1.642712
66	6	0	4.185715	-2.847075	3.148678
67	6	0	5.393967	-3.642723	1.178320
68	6	0	4.420998	-4.171001	3.865539
69	1	0	3.217477	-2.876028	2.621670
70	1	0	4.162970	-2.015699	3.855414
71	6	0	5.660804	-4.986533	1.846073
72	1	0	4.469338	-3.704133	0.581326
73	1	0	6.213113	-3.365478	0.512360
74	6	0	4.563054	-5.312671	2.858790
75	1	0	3.591795	-4.356643	4.552330
76	1	0	5.335238	-4.090184	4.462091
77	1	0	5.726317	-5.759684	1.076767
78	1	0	6.629332	-4.939257	2.353911
79	1	0	4.783459	-6.250559	3.373792
80	1	0	3.611893	-5.448194	2.330372
81	7	0	5.288809	-2.600147	2.208810

82	7	0	-5.200088	1.315741	1.642790
83	7	0	-5.288750	2.600250	2.208856
84	6	0	-4.185641	2.847175	3.148708
85	6	0	-5.393894	3.642801	1.178341
86	6	0	-4.420881	4.171127	3.865535
87	1	0	-3.217408	2.876086	2.621690
88	1	0	-4.162912	2.015817	3.855467
89	6	0	-5.660687	4.986637	1.846060
90	1	0	-4.469270	3.704173	0.581334
91	1	0	-6.213054	3.365560	0.512397
92	6	0	-4.562916	5.312772	2.858755
93	1	0	-3.591666	4.356766	4.552311
94	1	0	-5.335116	4.090352	4.462099
95	1	0	-5.726188	5.759768	1.076734
96	1	0	-6.629210	4.939401	2.353911
97	1	0	-4.783289	6.250681	3.373733
98	1	0	-3.611758	5.448253	2.330322
99	1	0	5.946054	-0.656140	1.850757
100	1	0	-5.946035	0.656243	1.850867

Structure 16dd (DMSO)

Energy (Hartrees): = -2224.4135198
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.182505	2.453272	-0.467283
2	6	0	4.216208	2.730348	-1.376666
3	6	0	3.007510	1.903397	-1.374634
4	6	0	2.939609	0.719097	-0.590483
5	6	0	4.083647	0.338087	0.240541
6	6	0	5.172835	1.256834	0.377513
7	6	0	-4.114316	-5.232686	-1.551572
8	6	0	0.481053	-2.056480	-2.942362
9	6	0	4.362604	3.922613	-2.308663
10	6	0	1.715769	0.007653	-0.609750
11	6	0	0.621448	0.414449	-1.370471
12	6	0	0.700625	1.593939	-2.132869
13	6	0	1.882238	2.308310	-2.120950
14	6	0	5.706783	3.952741	-3.048193
15	6	0	4.114279	5.232611	-1.552000
16	6	0	-0.481145	2.056349	-2.942455
17	6	0	4.220987	-0.916412	0.854103
18	6	0	-4.220984	0.916460	0.854175
19	6	0	-0.621505	-0.414501	-1.370436
20	6	0	-0.700699	-1.594030	-2.132771
21	6	0	-1.882310	-2.308404	-2.120786
22	6	0	-3.007563	-1.903457	-1.374462
23	6	0	-2.939648	-0.719114	-0.590375
24	6	0	-1.715810	-0.007669	-0.609710
25	6	0	-4.362649	-3.922746	-2.308334
26	6	0	-5.706822	-3.952940	-3.047871
27	6	0	-4.216258	-2.730413	-1.376423
28	6	0	-5.182541	-2.453284	-0.467042
29	6	0	-5.172861	-1.256796	0.377683
30	6	0	-4.083670	-0.338062	0.240652
31	1	0	-3.479290	1.683282	0.687303
32	1	0	-1.914458	-3.225149	-2.692375
33	1	0	3.479305	-1.683252	0.687263
34	1	0	1.914374	3.225028	-2.692584
35	1	0	-6.799104	-2.742010	0.381214
36	1	0	-4.188224	-6.085628	-2.231793
37	1	0	3.606771	3.838256	-3.087933
38	8	0	-1.608008	1.115871	0.153524
39	1	0	5.672043	4.725221	-3.821179
40	1	0	5.904457	2.995819	-3.538612
41	1	0	6.536433	4.173784	-2.378578
42	1	0	4.188204	6.085501	-2.232285
43	1	0	3.119415	5.243313	-1.098811
44	1	0	4.855566	5.360745	-0.759045
45	1	0	0.809915	-1.276746	-3.635168
46	1	0	0.227640	-2.947052	-3.518321
47	1	0	1.332777	-2.297667	-2.298960
48	8	0	6.278658	3.221746	-0.290073
49	1	0	6.799089	2.742041	0.380919
50	8	0	6.169414	1.096060	1.121626
51	1	0	-0.227751	2.946906	-3.518446
52	1	0	-1.332863	2.297545	-2.299049
53	1	0	-0.810006	1.276588	-3.635232
54	8	0	1.607983	-1.115844	0.153548
55	8	0	-6.169430	-1.095981	1.121801
56	1	0	-3.119457	-5.243340	-1.098372

57	1	0	-4.855610	-5.360770	-0.758615
58	8	0	-6.278685	-3.221755	-0.289758
59	1	0	-3.606813	-3.838442	-3.087607
60	1	0	-5.672062	-4.725465	-3.820812
61	1	0	-5.904509	-2.996051	-3.538348
62	1	0	-6.536474	-4.173959	-2.378251
63	1	0	0.703960	-1.455447	0.083071
64	1	0	-0.703986	1.455469	0.083013
65	7	0	5.224371	-1.282572	1.627876
66	6	0	4.267965	-2.839433	3.147808
67	6	0	5.432919	-3.605333	1.139308
68	6	0	4.546254	-4.162263	3.850810
69	1	0	3.289164	-2.885165	2.643143
70	1	0	4.249689	-2.011981	3.859490
71	6	0	5.742227	-4.946701	1.793081
72	1	0	4.491019	-3.679805	0.572987
73	1	0	6.227183	-3.311381	0.450477
74	6	0	4.679224	-5.296040	2.834385
75	1	0	3.738895	-4.364463	4.558666
76	1	0	5.475064	-4.069227	4.423095
77	1	0	5.798488	-5.714534	1.017798
78	1	0	6.724234	-4.885838	2.273528
79	1	0	4.929820	-6.232581	3.337939
80	1	0	3.716176	-5.443086	2.331694
81	7	0	5.343177	-2.570599	2.180575
82	7	0	-5.224351	1.282664	1.627948
83	7	0	-5.343117	2.570707	2.180616
84	6	0	-4.267889	2.839531	3.147834
85	6	0	-5.432835	3.605418	1.139324
86	6	0	-4.546124	4.162391	3.850802
87	1	0	-3.289091	2.885213	2.643160
88	1	0	-4.249637	2.012099	3.859539
89	6	0	-5.742091	4.946813	1.793064
90	1	0	-4.490939	3.679845	0.572991
91	1	0	-6.227117	3.311475	0.450509
92	6	0	-4.679064	5.296144	2.834347
93	1	0	-3.738752	4.364582	4.558645
94	1	0	-5.474933	4.069404	4.423099
95	1	0	-5.798334	5.714627	1.017761
96	1	0	-6.724095	4.885998	2.273524
97	1	0	-4.929619	6.232709	3.337877
98	1	0	-3.716016	5.443141	2.331641
99	1	0	5.966374	-0.617476	1.831131
100	1	0	-5.966363	0.617586	1.831235

Structure 17bb (vacuum)

Energy (Hartrees): = -2381.6179097
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.748430	3.122367	-0.536761
2	6	0	3.777371	3.305747	-1.464476
3	6	0	2.708742	2.309940	-1.556850
4	6	0	2.800273	1.085307	-0.843792
5	6	0	3.961867	0.828284	0.003790
6	6	0	4.891915	1.891153	0.243467
7	6	0	-3.391459	-5.788660	-1.483147
8	6	0	0.726037	-2.011998	-3.226999
9	6	0	3.779391	4.562213	-2.319630
10	6	0	1.697648	0.207023	-0.922041
11	6	0	0.564691	0.488201	-1.683716
12	6	0	0.491449	1.698857	-2.395824
13	6	0	1.553034	2.578341	-2.316173
14	6	0	5.112818	4.778953	-3.049764
15	6	0	3.392037	5.788833	-1.482850
16	6	0	-0.725907	2.012501	-3.226846
17	6	0	4.290779	-0.430533	0.513330
18	6	0	-4.290928	0.430508	0.513261
19	6	0	-0.564639	-0.487875	-1.683772
20	6	0	-0.491346	-1.698468	-2.395973
21	6	0	-1.552885	-2.578007	-2.316385
22	6	0	-2.708591	-2.309722	-1.557025
23	6	0	-2.800208	-1.085141	-0.843889
24	6	0	-1.697595	-0.206814	-0.922050
25	6	0	-3.778952	-4.562062	-2.319895
26	6	0	-5.112318	-4.778958	-3.050096
27	6	0	-3.777120	-3.305626	-1.464699
28	6	0	-4.748170	-3.122407	-0.536947
29	6	0	-4.891765	-1.891260	0.243355
30	6	0	-3.961833	-0.828274	0.003722
31	1	0	-3.741332	1.316106	0.230658

32	1	0	-1.462429	-3.516649	-2.843735
33	1	0	3.741039	-1.316052	0.230749
34	1	0	1.462628	3.517011	-2.843478
35	1	0	-6.277055	-3.604636	0.384095
36	1	0	-3.358913	-6.683591	-2.110083
37	1	0	3.033466	4.441655	-3.104108
38	8	0	-1.744062	0.956923	-0.209240
39	1	0	5.011123	5.612390	-3.749617
40	1	0	5.389871	3.889267	-3.619663
41	1	0	5.917534	5.007527	-2.353501
42	1	0	3.359670	6.683794	-2.109753
43	1	0	2.410069	5.653319	-1.022988
44	1	0	4.125566	5.948311	-0.690495
45	1	0	0.908745	-1.220757	-3.958680
46	1	0	0.597833	-2.955298	-3.757913
47	1	0	1.622997	-2.084517	-2.605481
48	8	0	5.710625	4.033669	-0.281543
49	1	0	6.277353	3.604394	0.384290
50	8	0	5.879207	1.831258	1.013991
51	1	0	-0.597633	2.955806	-3.757735
52	1	0	-1.622856	2.085075	-2.605319
53	1	0	-0.908685	1.221294	-3.958547
54	8	0	1.744151	-0.956819	-0.209406
55	8	0	-5.879108	-1.831531	1.013825
56	1	0	-2.409542	-5.653015	-1.023214
57	1	0	-4.125014	-5.948287	-0.690845
58	8	0	-5.710275	-4.033816	-0.281755
59	1	0	-3.033006	-4.441359	-3.104332
60	1	0	-5.010459	-5.612338	-3.749994
61	1	0	-5.389483	-3.889282	-3.619957
62	1	0	-5.917032	-5.007699	-2.353888
63	1	0	0.885842	-1.394570	-0.290304
64	1	0	-0.885740	1.394662	-0.290073
65	7	0	5.290563	-0.666786	1.344206
66	6	0	7.027161	-2.242240	1.354427
67	6	0	5.311426	-2.202816	3.135410
68	6	0	7.361253	-3.692839	1.690658
69	1	0	7.670924	-1.584682	1.967041
70	6	0	5.634458	-3.654245	3.483771
71	1	0	5.953550	-1.541147	3.744024
72	6	0	7.080724	-4.005036	3.155986
73	1	0	8.410982	-3.874453	1.446311
74	1	0	6.754899	-4.340436	1.047533
75	1	0	5.424083	-3.813160	4.544419
76	1	0	4.956990	-4.298840	2.912505
77	1	0	7.280324	-5.057158	3.371293
78	1	0	7.751574	-3.413081	3.789232
79	7	0	5.610139	-1.983607	1.700146
80	7	0	-5.290695	0.666640	1.344184
81	7	0	-5.610463	1.983437	1.700058
82	6	0	-7.027558	2.241836	1.354455
83	6	0	-5.311631	2.202781	3.135280
84	6	0	-7.361865	3.692387	1.690677
85	1	0	-7.671164	1.584190	1.967138
86	6	0	-5.634877	3.654172	3.483592
87	1	0	-5.953569	1.541036	3.744006
88	6	0	-7.081251	4.004679	3.155969
89	1	0	-8.411644	3.873817	1.446420
90	1	0	-6.755675	4.340072	1.047485
91	1	0	-5.424396	3.813192	4.544202
92	1	0	-4.957606	4.298858	2.912196
93	1	0	-7.281031	5.056767	3.371268
94	1	0	-7.751911	3.412610	3.789311
95	1	0	5.866919	0.125091	1.648438
96	1	0	-5.866924	-0.125311	1.648479
97	6	0	-7.271817	1.948221	-0.120217
98	1	0	-6.569121	2.520233	-0.731874
99	1	0	-7.152596	0.889319	-0.351919
100	1	0	-8.287684	2.242692	-0.389932
101	6	0	-3.848576	1.891842	3.423088
102	1	0	-3.611991	0.838813	3.271193
103	1	0	-3.207048	2.487368	2.767953
104	1	0	-3.617289	2.145751	4.459367
105	6	0	7.271315	-1.948682	-0.120267
106	1	0	6.568490	-2.520605	-0.731859
107	1	0	7.152207	-0.889765	-0.351970
108	1	0	8.287119	-2.243288	-0.390070
109	6	0	3.848453	-1.891601	3.423369
110	1	0	3.612044	-0.838531	3.271477
111	1	0	3.206745	-2.487023	2.768315
112	1	0	3.617236	-2.145448	4.459676

Structure 17bb ($CHCl_3$)

Energy (Hartrees): = -2381.6654628
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.693543	-3.204399	-0.484548
2	6	0	-3.701913	-3.393188	-1.390553
3	6	0	-2.663106	-2.368341	-1.503518
4	6	0	-2.795900	-1.129682	-0.821066
5	6	0	-3.982246	-0.876091	-0.006939
6	6	0	-4.888625	-1.951397	0.248127
7	6	0	3.224500	5.861563	-1.316006
8	6	0	-0.779401	2.031470	-3.141712
9	6	0	-3.647648	-4.680629	-2.198329
10	6	0	-1.702907	-0.234339	-0.886249
11	6	0	-0.555206	-0.500068	-1.631690
12	6	0	-0.448691	-1.720758	-2.326496
13	6	0	-1.490458	-2.623897	-2.242769
14	6	0	-4.959086	-4.979352	-2.938315
15	6	0	-3.224503	-5.861613	-1.315655
16	6	0	0.779332	-2.031588	-3.141625
17	6	0	-4.353484	0.398399	0.448318
18	6	0	4.353479	-0.398371	0.448224
19	6	0	0.555161	0.500022	-1.631726
20	6	0	0.448637	1.720678	-2.326591
21	6	0	1.490412	2.623814	-2.242937
22	6	0	2.663075	2.368289	-1.503700
23	6	0	2.795879	1.129664	-0.821190
24	6	0	1.702880	0.234324	-0.886299
25	6	0	3.647605	4.680539	-2.198646
26	6	0	4.959013	4.979228	-2.938701
27	6	0	3.701893	3.393135	-1.390813
28	6	0	4.693546	3.204382	-0.484826
29	6	0	4.888642	1.951412	0.247901
30	6	0	3.982242	0.876103	-0.007080
31	1	0	3.819510	-1.283951	0.135834
32	1	0	1.369476	3.569056	-2.752843
33	1	0	-3.819532	1.283972	0.135880
34	1	0	-1.369527	-3.569166	-2.752628
35	1	0	6.230200	3.707983	0.424341
36	1	0	3.149057	6.775095	-1.912656
37	1	0	-2.895117	-4.562598	-2.976301
38	8	0	1.783990	-0.923824	-0.171976
39	1	0	-4.808945	-5.829463	-3.609347
40	1	0	-5.268218	-4.123876	-3.544290
41	1	0	-5.766901	-5.223163	-2.249790
42	1	0	-3.149077	-6.775169	-1.912271
43	1	0	-2.253206	-5.677007	-0.849118
44	1	0	-3.958829	-6.029144	-0.524608
45	1	0	-0.943673	1.270448	-3.909441
46	1	0	-0.676274	2.998905	-3.634348
47	1	0	-1.677702	2.059680	-2.518540
48	8	0	-5.631260	-4.138392	-0.212989
49	1	0	-6.230173	-3.707966	0.424680
50	8	0	-5.894956	-1.893578	0.997404
51	1	0	0.676190	-2.999040	-3.634226
52	1	0	1.677642	-2.059784	-2.518464
53	1	0	0.943599	-1.270594	-3.909382
54	8	0	-1.784001	0.923843	-0.171979
55	8	0	5.894983	1.893632	0.997169
56	1	0	2.253219	5.676981	-0.849424
57	1	0	3.958857	6.029121	-0.524993
58	8	0	5.631272	4.138385	-0.213329
59	1	0	2.895043	4.562476	-2.976582
60	1	0	4.808839	5.829301	-3.609774
61	1	0	5.268124	4.123720	-3.544642
62	1	0	5.766854	5.223081	-2.250224
63	1	0	-0.931841	1.380784	-0.215378
64	1	0	0.931829	-1.380766	-0.215331
65	7	0	-5.369491	0.646386	1.246329
66	6	0	-7.122021	2.203762	1.259542
67	6	0	-5.387366	2.191229	3.025826
68	6	0	-7.472965	3.649276	1.599764
69	1	0	-7.743079	1.534942	1.880827
70	6	0	-5.728378	3.637534	3.375950
71	1	0	-6.017963	1.519595	3.633167
72	6	0	-7.182591	3.966276	3.061852
73	1	0	-8.528035	3.813196	1.365968
74	1	0	-6.883719	4.306926	0.950413
75	1	0	-5.510856	3.797208	4.435078
76	1	0	-5.065361	4.293207	2.799758
77	1	0	-7.394361	5.016379	3.277039
78	1	0	-7.838266	3.364516	3.701816
79	7	0	-5.693774	1.967248	1.588514
80	7	0	5.369505	-0.646339	1.246216
81	7	0	5.693799	-1.967192	1.588423
82	6	0	7.122037	-2.203705	1.259415

83	6	0	5.387435	-2.191148	3.025749
84	6	0	7.472994	-3.649214	1.599645
85	1	0	7.743110	-1.534877	1.880676
86	6	0	5.728462	-3.637447	3.375886
87	1	0	6.018049	-1.519502	3.633059
88	6	0	7.182664	-3.966194	3.061746
89	1	0	8.528057	-3.813135	1.365820
90	1	0	6.883730	-4.306873	0.950320
91	1	0	5.510973	-3.797104	4.435023
92	1	0	5.065427	-4.293130	2.799725
93	1	0	7.394441	-5.016295	3.276941
94	1	0	7.838359	-3.364426	3.701683
95	1	0	-5.932125	-0.137061	1.591490
96	1	0	5.932162	0.137117	1.591323
97	6	0	7.380342	-1.908235	-0.211457
98	1	0	6.705365	-2.499231	-0.837205
99	1	0	7.241607	-0.852565	-0.450201
100	1	0	8.408832	-2.176693	-0.462330
101	6	0	3.919437	-1.901457	3.306973
102	1	0	3.664231	-0.851516	3.157120
103	1	0	3.284342	-2.509323	2.655836
104	1	0	3.691760	-2.155835	4.344499
105	6	0	-7.380368	1.908276	-0.211320
106	1	0	-6.705407	2.499265	-0.837092
107	1	0	-7.241642	0.852604	-0.450057
108	1	0	-8.408864	2.176734	-0.462167
109	6	0	-3.919359	1.901538	3.307009
110	1	0	-3.664161	0.851594	3.157167
111	1	0	-3.284284	2.509391	2.655840
112	1	0	-3.691648	2.155935	4.344522

Structure 17bb (DMSO)

Energy (Hartrees): = -2381.6540251
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.688732	-3.202720	-0.483906
2	6	0	-3.705218	-3.387740	-1.399768
3	6	0	-2.664144	-2.364654	-1.512108
4	6	0	-2.790194	-1.130236	-0.819819
5	6	0	-3.970062	-0.879352	0.004337
6	6	0	-4.871879	-1.955903	0.265032
7	6	0	3.215434	5.850241	-1.336984
8	6	0	-0.763714	2.015070	-3.177948
9	6	0	-3.654675	-4.671288	-2.213215
10	6	0	-1.696205	-0.235819	-0.886504
11	6	0	-0.556491	-0.498545	-1.644456
12	6	0	-0.457545	-1.713279	-2.350487
13	6	0	-1.499061	-2.616858	-2.265290
14	6	0	-4.972655	-4.974879	-2.938078
15	6	0	-3.215556	-5.850308	-1.336542
16	6	0	0.763612	-2.015202	-3.177880
17	6	0	-4.341827	0.397351	0.457165
18	6	0	4.341814	-0.397321	0.457052
19	6	0	0.556442	0.498487	-1.644498
20	6	0	0.457474	1.713187	-2.350584
21	6	0	1.498995	2.616768	-2.265470
22	6	0	2.664106	2.364599	-1.512318
23	6	0	2.790172	1.130216	-0.819968
24	6	0	1.696181	0.235797	-0.886571
25	6	0	3.654655	4.671193	-2.213570
26	6	0	4.972685	4.974789	-2.938338
27	6	0	3.705191	3.387685	-1.400059
28	6	0	4.688741	3.202697	-0.484229
29	6	0	4.871909	1.955913	0.264758
30	6	0	3.970064	0.879363	0.004160
31	1	0	3.811346	-1.281691	0.134987
32	1	0	1.383154	3.557677	-2.784814
33	1	0	-3.811405	1.281717	0.135015
34	1	0	-1.383236	-3.557795	-2.784589
35	1	0	6.212757	3.694258	0.439284
36	1	0	3.144578	6.763353	-1.934699
37	1	0	-2.910773	-4.549388	-2.998669
38	8	0	1.765895	-0.913776	-0.159055
39	1	0	-4.824718	-5.820042	-3.615675
40	1	0	-5.294935	-4.118498	-3.536414
41	1	0	-5.770716	-5.227642	-2.241289
42	1	0	-3.144686	-6.763452	-1.934209
43	1	0	-2.237764	-5.661810	-0.884998
44	1	0	-3.938240	-6.020332	-0.534943
45	1	0	-0.925126	1.241197	-3.933753

46	1	0	-0.654637	2.974517	-3.684469
47	1	0	-1.666028	2.056717	-2.560639
48	8	0	-5.630027	-4.131524	-0.208707
49	1	0	-6.212681	-3.694263	0.439730
50	8	0	-5.866723	-1.906363	1.028759
51	1	0	0.654527	-2.974686	-3.684331
52	1	0	1.665953	-2.056794	-2.560607
53	1	0	0.924982	-1.241381	-3.933748
54	8	0	-1.765883	0.913786	-0.159035
55	8	0	5.866763	1.906413	1.028477
56	1	0	2.237614	5.661733	-0.885503
57	1	0	3.938053	6.020328	-0.535339
58	8	0	5.630070	4.131498	-0.209137
59	1	0	2.910817	4.549237	-2.999074
60	1	0	4.824793	5.819943	-3.615956
61	1	0	5.295020	4.118404	-3.536640
62	1	0	5.770689	5.227565	-2.241488
63	1	0	-0.921189	1.381072	-0.232519
64	1	0	0.921201	-1.381070	-0.232485
65	7	0	-5.352925	0.650372	1.256806
66	6	0	-7.101091	2.212323	1.260377
67	6	0	-5.373618	2.193983	3.034579
68	6	0	-7.453514	3.656080	1.605208
69	1	0	-7.722245	1.539534	1.875819
70	6	0	-5.716676	3.638553	3.388130
71	1	0	-6.006823	1.519382	3.634510
72	6	0	-7.169502	3.967534	3.069405
73	1	0	-8.507866	3.818453	1.367540
74	1	0	-6.862853	4.317872	0.960897
75	1	0	-5.503833	3.792243	4.449018
76	1	0	-5.051659	4.298007	2.818052
77	1	0	-7.382073	5.017024	3.287010
78	1	0	-7.826958	3.362450	3.704081
79	7	0	-5.672822	1.974413	1.593813
80	7	0	5.352957	-0.650323	1.256643
81	7	0	5.672832	-1.974353	1.593717
82	6	0	7.101053	-2.212348	1.260141
83	6	0	5.373780	-2.193800	3.034534
84	6	0	7.453451	-3.656096	1.605041
85	1	0	7.722306	-1.539540	1.875462
86	6	0	5.716816	-3.638358	3.388158
87	1	0	6.007084	-1.519180	3.634342
88	6	0	7.169591	-3.967426	3.069292
89	1	0	8.507769	-3.818533	1.367266
90	1	0	6.862686	-4.317910	0.960847
91	1	0	5.504088	-3.791957	4.449082
92	1	0	5.051705	-4.297827	2.818206
93	1	0	7.382140	-5.016909	3.286953
94	1	0	7.827146	-3.362323	3.703848
95	1	0	-5.916908	-0.125245	1.616288
96	1	0	5.917001	0.125298	1.616020
97	6	0	7.351718	-1.926129	-0.213633
98	1	0	6.677450	-2.524018	-0.834001
99	1	0	7.208377	-0.872577	-0.459530
100	1	0	8.380493	-2.192286	-0.465908
101	6	0	3.906989	-1.904645	3.320955
102	1	0	3.650209	-0.855352	3.167278
103	1	0	3.268743	-2.517780	2.677493
104	1	0	3.685958	-2.153312	4.361289
105	6	0	-7.351911	1.925981	-0.213347
106	1	0	-6.677738	2.523849	-0.833838
107	1	0	-7.208557	0.872415	-0.459180
108	1	0	-8.380726	2.192077	-0.465526
109	6	0	-3.906781	1.904915	3.320852
110	1	0	-3.649973	0.855622	3.167229
111	1	0	-3.268638	2.518027	2.677264
112	1	0	-3.685637	2.153677	4.361140

Structure 17dd (vacuum)

Energy (Hartrees): = -2381.6090643
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.920902	-2.924574	-0.627049
2	6	0	-3.925733	-3.134406	-1.521663
3	6	0	-2.804458	-2.192238	-1.548237
4	6	0	-2.850305	-0.984958	-0.798420
5	6	0	-4.023528	-0.694071	0.027571
6	6	0	-5.031921	-1.705351	0.177446
7	6	0	3.624665	5.625341	-1.592950
8	6	0	-0.669026	2.023226	-3.155574

9	6	0	-3.957455	-4.368568	-2.408514
10	6	0	-1.708527	-0.155192	-0.850441
11	6	0	-0.579561	-0.470111	-1.605765
12	6	0	-0.545783	-1.669544	-2.336979
13	6	0	-1.648369	-2.499389	-2.291073
14	6	0	-5.282574	-4.527309	-3.168104
15	6	0	-3.624601	-5.625259	-1.593282
16	6	0	0.669094	-2.023050	-3.155676
17	6	0	-4.262075	0.533244	0.648674
18	6	0	4.262086	-0.533276	0.648681
19	6	0	0.579618	0.470206	-1.605735
20	6	0	0.545844	1.669678	-2.336886
21	6	0	1.648431	2.499519	-2.290932
22	6	0	2.804518	2.192327	-1.548110
23	6	0	2.850358	0.985009	-0.798355
24	6	0	1.708580	0.155247	-0.850422
25	6	0	3.957520	4.368703	-2.408262
26	6	0	5.282637	4.527497	-3.167843
27	6	0	3.925799	3.134487	-1.521486
28	6	0	4.920971	2.924596	-0.626889
29	6	0	5.031986	1.705327	0.177537
30	6	0	4.023577	0.694068	0.027622
31	1	0	3.569000	-1.349024	0.508795
32	1	0	1.594116	3.428777	-2.838996
33	1	0	-3.569026	1.349026	0.508808
34	1	0	-1.594050	-3.428619	-2.839184
35	1	0	6.508053	3.347191	0.222108
36	1	0	3.611714	6.507876	-2.237804
37	1	0	-3.195339	-4.254362	-3.178140
38	8	0	1.706603	-1.005523	-0.128478
39	1	0	-5.183433	-5.333575	-3.899431
40	1	0	-5.532184	-3.610214	-3.706232
41	1	0	-6.104577	-4.767654	-2.496905
42	1	0	-3.611653	-6.507753	-2.238192
43	1	0	-2.646546	-5.532054	-1.114824
44	1	0	-4.376239	-5.776295	-0.816003
45	1	0	-0.911759	1.219235	-3.855032
46	1	0	-0.498736	2.939210	-3.721307
47	1	0	-1.547510	2.168533	-2.520188
48	8	0	-5.935996	-3.790103	-0.430531
49	1	0	-6.507977	-3.347229	0.221931
50	8	0	-6.043194	-1.612495	0.906990
51	1	0	0.498795	-2.938985	-3.721485
52	1	0	1.547564	-2.168428	-2.520285
53	1	0	0.911857	-1.219009	-3.855064
54	8	0	-1.706549	1.005539	-0.128436
55	8	0	6.043254	1.612433	0.907085
56	1	0	2.646610	5.532105	-1.114494
57	1	0	4.376304	5.776331	-0.815663
58	8	0	5.936070	3.790109	-0.430322
59	1	0	3.195404	4.254542	-3.177893
60	1	0	5.183488	5.333803	-3.899126
61	1	0	5.532255	3.610435	-3.706023
62	1	0	6.104639	4.767813	-2.496632
63	1	0	-0.833194	1.411755	-0.215693
64	1	0	0.833249	-1.411734	-0.215756
65	7	0	-5.308757	0.815674	1.409547
66	6	0	-4.467518	2.370441	3.001834
67	6	0	-5.659417	3.132652	0.962053
68	6	0	-4.813360	3.684598	3.697936
69	1	0	-3.487595	2.487784	2.504204
70	6	0	-6.013074	4.446611	1.655111
71	1	0	-4.703093	3.276540	0.428004
72	6	0	-4.972662	4.827269	2.702141
73	1	0	-4.030977	3.907110	4.428275
74	1	0	-5.749295	3.540540	4.249265
75	1	0	-6.108328	5.226308	0.894823
76	1	0	-6.993002	4.326874	2.130611
77	1	0	-5.260779	5.747454	3.215398
78	1	0	-4.012178	5.019928	2.210231
79	7	0	-5.509187	2.081053	1.991028
80	7	0	5.308762	-0.815780	1.409534
81	7	0	5.509127	-2.081182	1.990989
82	6	0	4.467464	-2.370515	3.001818
83	6	0	5.659260	-3.132776	0.961996
84	6	0	4.813235	-3.684705	3.697893
85	1	0	3.487520	-2.487784	2.504212
86	6	0	6.012844	-4.446769	1.655026
87	1	0	4.702913	-3.276592	0.427968
88	6	0	4.972432	-4.827371	2.702077
89	1	0	4.030855	-3.907173	4.428249
90	1	0	5.749195	-3.540719	4.249199
91	1	0	6.108026	-5.226462	0.894725
92	1	0	6.992792	-4.327107	2.130503
93	1	0	5.260500	-5.747585	3.215313
94	1	0	4.011922	-5.019957	2.210189
95	1	0	-6.001130	0.090252	1.580825
96	1	0	6.001172	-0.090396	1.580828

97	6	0	4.384841	-1.234084	4.013065
98	1	0	5.368561	-1.068585	4.459568
99	1	0	4.048918	-0.301098	3.560407
100	1	0	3.683027	-1.499942	4.805757
101	6	0	6.741425	-2.742707	-0.036863
102	1	0	6.473402	-1.858445	-0.615589
103	1	0	7.674064	-2.537409	0.494314
104	1	0	6.911067	-3.565865	-0.733463
105	6	0	-4.384792	1.234002	4.013063
106	1	0	-5.368490	1.068433	4.459591
107	1	0	-4.048821	0.301044	3.560385
108	1	0	-3.682974	1.499895	4.805739
109	6	0	-6.741580	2.742523	-0.036785
110	1	0	-6.473509	1.858290	-0.615533
111	1	0	-7.674190	2.537148	0.494414
112	1	0	-6.911299	3.565681	-0.733366

Structure 17dd ($CHCl_3$)

Energy (Hartrees): = -2381.6554421
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.892304	-3.009294	-0.622074
2	6	0	-3.862904	-3.218083	-1.478652
3	6	0	-2.759203	-2.255022	-1.483424
4	6	0	-2.850969	-1.039138	-0.751037
5	6	0	-4.058963	-0.755993	0.027628
6	6	0	-5.054343	-1.778934	0.155046
7	6	0	3.474540	5.697538	-1.476290
8	6	0	-0.737720	2.032698	-3.022596
9	6	0	-3.831083	-4.475984	-2.333351
10	6	0	-1.716923	-0.192754	-0.770391
11	6	0	-0.567578	-0.485788	-1.503402
12	6	0	-0.493202	-1.692052	-2.224154
13	6	0	-1.578120	-2.545816	-2.194650
14	6	0	-5.125329	-4.708560	-3.125467
15	6	0	-3.474472	-5.697463	-1.476637
16	6	0	0.737790	-2.032560	-3.022673
17	6	0	-4.339330	0.483176	0.620837
18	6	0	4.339341	-0.483205	0.620855
19	6	0	0.567628	0.485861	-1.503374
20	6	0	0.493261	1.692157	-2.224075
21	6	0	1.578179	2.545920	-2.194521
22	6	0	2.759253	2.255094	-1.483295
23	6	0	2.851012	1.039178	-0.750963
24	6	0	1.716966	0.192796	-0.770362
25	6	0	3.831111	4.476109	-2.333090
26	6	0	5.125319	4.708735	-3.125255
27	6	0	3.862952	3.218157	-1.478465
28	6	0	4.892340	3.009329	-0.621882
29	6	0	5.054377	1.778928	0.155175
30	6	0	4.058995	0.755995	0.027702
31	1	0	3.655665	-1.308582	0.491589
32	1	0	1.489281	3.478654	-2.732708
33	1	0	-3.655669	1.308572	0.491614
34	1	0	-1.489215	-3.478527	-2.732875
35	1	0	6.507009	3.456626	0.175230
36	1	0	3.412363	6.595973	-2.096850
37	1	0	-3.052029	-4.357195	-3.084414
38	8	0	1.757198	-0.958836	-0.040556
39	1	0	-4.968883	-5.524146	-3.836737
40	1	0	-5.401732	-3.817109	-3.694253
41	1	0	-5.958784	-4.973972	-2.477328
42	1	0	-3.412318	-6.595861	-2.097254
43	1	0	-2.511995	-5.559781	-0.976739
44	1	0	-4.237479	-5.861342	-0.711849
45	1	0	-0.940091	1.265631	-3.775246
46	1	0	-0.611039	2.988643	-3.531722
47	1	0	-1.623869	2.099671	-2.385178
48	8	0	-5.895949	-3.894842	-0.445605
49	1	0	-6.506998	-3.456618	0.174970
50	8	0	-6.096674	-1.693122	0.846354
51	1	0	0.611107	-2.988474	-3.531857
52	1	0	1.623925	-2.099581	-2.385241
53	1	0	0.940184	-1.265450	-3.775272
54	8	0	-1.757160	0.958849	-0.040539
55	8	0	6.096702	1.693087	0.846488
56	1	0	2.512086	5.559831	-0.976354
57	1	0	4.237584	5.861367	-0.711527
58	8	0	5.895968	3.894880	-0.445332
59	1	0	3.052025	4.357362	-3.084128

60	1	0	4.968824	5.524344	-3.836487
61	1	0	5.401710	3.817310	-3.694089
62	1	0	5.958800	4.974135	-2.477147
63	1	0	-0.889690	1.386924	-0.080124
64	1	0	0.889728	-1.386910	-0.080165
65	7	0	-5.413033	0.760691	1.336091
66	6	0	-4.636707	2.338633	2.938448
67	6	0	-5.789199	3.069187	0.857752
68	6	0	-5.009500	3.658181	3.609319
69	1	0	-3.648606	2.456288	2.460468
70	6	0	-6.168527	4.386633	1.530029
71	1	0	-4.823329	3.212701	0.344136
72	6	0	-5.154751	4.786564	2.595576
73	1	0	-4.243616	3.894819	4.352529
74	1	0	-5.956017	3.515553	4.143341
75	1	0	-6.251114	5.155944	0.757794
76	1	0	-7.158663	4.266771	1.984822
77	1	0	-5.463040	5.709954	3.091458
78	1	0	-4.184764	4.980298	2.123107
79	7	0	-5.652825	2.028257	1.903701
80	7	0	5.413031	-0.760776	1.336109
81	7	0	5.652780	-2.028367	1.903680
82	6	0	4.636637	-2.338744	2.938403
83	6	0	5.789141	-3.069272	0.857704
84	6	0	5.009384	-3.658320	3.609244
85	1	0	3.648542	-2.456360	2.460401
86	6	0	6.168421	-4.386747	1.529951
87	1	0	4.823274	-3.212747	0.344070
88	6	0	5.154619	-4.786678	2.595473
89	1	0	4.243481	-3.894957	4.352436
90	1	0	5.955896	-3.515732	4.143286
91	1	0	6.250998	-5.156040	0.757698
92	1	0	7.158554	-4.266925	1.984763
93	1	0	5.462877	-5.710091	3.091334
94	1	0	4.184633	-4.980373	2.122985
95	1	0	-6.102733	0.030748	1.496930
96	1	0	6.102739	-0.030852	1.496997
97	6	0	4.572156	-1.215045	3.964004
98	1	0	5.565511	-1.039345	4.386289
99	1	0	4.208769	-0.279816	3.535725
100	1	0	3.897268	-1.498331	4.774516
101	6	0	6.847044	-2.657855	-0.156949
102	1	0	6.559108	-1.771751	-0.724948
103	1	0	7.790793	-2.448274	0.353941
104	1	0	7.010656	-3.472885	-0.865174
105	6	0	-4.572215	1.214909	3.964022
106	1	0	-5.565572	1.039177	4.386288
107	1	0	-4.208801	0.279700	3.535724
108	1	0	-3.897344	1.498189	4.774551
109	6	0	-6.847075	2.657766	-0.156928
110	1	0	-6.559104	1.771687	-0.724947
111	1	0	-7.790825	2.448140	0.353944
112	1	0	-7.010704	3.472811	-0.865131

Structure 17dd (DMSO)

Energy (Hartrees): = -2381.6441442
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.892971	-2.983694	-0.617048
2	6	0	-3.883394	-3.189898	-1.497983
3	6	0	-2.776452	-2.230995	-1.518013
4	6	0	-2.848109	-1.022050	-0.771293
5	6	0	-4.039369	-0.738817	0.032497
6	6	0	-5.032536	-1.759680	0.175383
7	6	0	3.495699	5.666793	-1.523595
8	6	0	-0.701597	2.017008	-3.101899
9	6	0	-3.872106	-4.440084	-2.363595
10	6	0	-1.708627	-0.182560	-0.800921
11	6	0	-0.573188	-0.479284	-1.553001
12	6	0	-0.519167	-1.677410	-2.288907
13	6	0	-1.609457	-2.524031	-2.252755
14	6	0	-5.185375	-4.665957	-3.124376
15	6	0	-3.495912	-5.666792	-1.524106
16	6	0	0.701568	-2.017047	-3.101922
17	6	0	-4.308338	0.503666	0.629353
18	6	0	4.308301	-0.503723	0.629536
19	6	0	0.573088	0.479210	-1.552955
20	6	0	0.519092	1.677362	-2.288818
21	6	0	1.609361	2.524000	-2.252559
22	6	0	2.776311	2.230957	-1.517751

23	6	0	2.847962	1.021976	-0.771085
24	6	0	1.708485	0.182469	-0.800817
25	6	0	3.871859	4.440134	-2.363173
26	6	0	5.185050	4.666085	-3.124068
27	6	0	3.883210	3.189903	-1.497623
28	6	0	4.892735	2.983717	-0.616621
29	6	0	5.032298	1.759675	0.175765
30	6	0	4.039205	0.738765	0.032752
31	1	0	3.630501	-1.331271	0.482802
32	1	0	1.535451	3.451316	-2.802586
33	1	0	-3.630413	1.331129	0.482692
34	1	0	-1.535525	-3.451322	-2.802818
35	1	0	6.481716	3.419429	0.221700
36	1	0	3.446092	6.560466	-2.151991
37	1	0	-3.110498	-4.317026	-3.131547
38	8	0	1.727557	-0.958790	-0.057273
39	1	0	-5.047172	-5.475475	-3.846200
40	1	0	-5.475992	-3.769787	-3.679091
41	1	0	-6.002505	-4.936370	-2.457459
42	1	0	-3.446383	-6.560436	-2.152548
43	1	0	-2.521890	-5.531928	-1.045936
44	1	0	-4.241837	-5.836848	-0.743546
45	1	0	-0.920282	1.226567	-3.825461
46	1	0	-0.553243	2.951573	-3.643531
47	1	0	-1.586038	2.128302	-2.467377
48	8	0	-5.897905	-3.863748	-0.420962
49	1	0	-6.482074	-3.419351	0.221074
50	8	0	-6.058663	-1.680963	0.892638
51	1	0	0.553214	-2.951564	-3.643635
52	1	0	1.585955	-2.128431	-2.467338
53	1	0	0.920346	-1.226559	-3.825405
54	8	0	-1.727774	0.958677	-0.057344
55	8	0	6.058411	1.680924	0.893035
56	1	0	2.521723	5.531882	-1.045345
57	1	0	4.241690	5.836830	-0.743094
58	8	0	5.897588	3.863826	-0.420374
59	1	0	3.110191	4.317090	-3.131071
60	1	0	5.046724	5.475579	-3.845895
61	1	0	5.475679	3.769925	-3.678795
62	1	0	6.002220	4.936567	-2.457232
63	1	0	-0.866219	1.394515	-0.130781
64	1	0	0.866000	-1.394610	-0.130788
65	7	0	-5.366463	0.778951	1.365181
66	6	0	-4.571938	2.354456	2.961334
67	6	0	-5.748864	3.090209	0.895279
68	6	0	-4.940270	3.670283	3.640939
69	1	0	-3.591386	2.476080	2.470713
70	6	0	-6.123579	4.403754	1.576892
71	1	0	-4.788788	3.236229	0.373797
72	6	0	-5.098753	4.801422	2.632560
73	1	0	-4.165703	3.904977	4.375683
74	1	0	-5.880428	3.524814	4.185948
75	1	0	-6.215199	5.175031	0.807756
76	1	0	-7.108836	4.281589	2.042312
77	1	0	-5.403371	5.722572	3.135118
78	1	0	-4.134504	4.997147	2.149662
79	7	0	-5.601915	2.045755	1.937963
80	7	0	5.366455	-0.778888	1.365368
81	7	0	5.602109	-2.045688	1.938076
82	6	0	4.572183	-2.354629	2.961426
83	6	0	5.749242	-3.090058	0.895333
84	6	0	4.940759	-3.670422	3.640965
85	1	0	3.591658	-2.476414	2.470792
86	6	0	6.124200	-4.403569	1.576877
87	1	0	4.789192	-3.236226	0.373847
88	6	0	5.099450	-4.801480	2.632527
89	1	0	4.166236	-3.905296	4.375697
90	1	0	5.880890	-3.524806	4.185981
91	1	0	6.215959	-5.174789	0.807700
92	1	0	7.109436	-4.281246	2.042300
93	1	0	5.404240	-5.722600	3.135037
94	1	0	4.135236	-4.997358	2.149623
95	1	0	-6.049187	0.046738	1.544419
96	1	0	6.049059	-0.046578	1.544666
97	6	0	4.494319	-1.227750	3.981933
98	1	0	5.482196	-1.049043	4.416399
99	1	0	4.133803	-0.294744	3.545672
100	1	0	3.809781	-1.510137	4.784647
101	6	0	6.817417	-2.680326	-0.108756
102	1	0	6.529037	-1.803190	-0.690859
103	1	0	7.753477	-2.457458	0.411274
104	1	0	6.996689	-3.501852	-0.805646
105	6	0	-4.494292	1.227513	3.981786
106	1	0	-5.482203	1.048976	4.416242
107	1	0	-4.133956	0.294459	3.545480
108	1	0	-3.809699	1.509729	4.784514
109	6	0	-6.817119	2.680728	-0.108828
110	1	0	-6.528901	1.803577	-0.690988

111	1	0	-7.753214	2.457992	0.411197
112	1	0	-6.996253	3.502329	-0.805665

Structure 19a (vacuum)

Energy (Hartrees): = -1112.7767906
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.609811	-1.850183	-0.134112
2	6	0	-2.663656	-1.001065	0.078743
3	6	0	-2.400284	0.414327	0.062387
4	6	0	-1.060943	0.902035	-0.073549
5	6	0	0.034234	-0.031225	-0.179454
6	6	0	-0.275340	-1.377548	-0.248518
7	6	0	-4.053307	-1.585726	0.278209
8	6	0	-0.903089	2.318423	-0.159659
9	6	0	-1.966922	3.178821	-0.060964
10	6	0	-3.278432	2.699006	0.099979
11	6	0	-3.471787	1.344614	0.152711
12	6	0	-4.114349	-2.552715	1.470211
13	6	0	-4.571996	-2.240275	-1.009408
14	6	0	-4.422256	3.673130	0.190352
15	6	0	1.451476	0.357785	-0.127264
16	1	0	1.682204	1.379352	0.128233
17	1	0	-4.486197	0.986493	0.240693
18	1	0	-4.736388	-0.775312	0.522357
19	1	0	-5.151698	-2.848686	1.647301
20	1	0	-3.738652	-2.071855	2.376124
21	1	0	-3.526388	-3.450163	1.285147
22	1	0	-5.590974	-2.607419	-0.861164
23	1	0	-4.581865	-1.520937	-1.831510
24	1	0	-3.940655	-3.082761	-1.294171
25	8	0	-1.784334	-3.194472	-0.210922
26	1	0	-0.908877	-3.583482	-0.339238
27	8	0	0.634522	-2.358851	-0.392214
28	1	0	1.525148	-1.919014	-0.473104
29	1	0	-5.375765	3.152794	0.283177
30	1	0	-4.465100	4.307429	-0.698973
31	1	0	-4.307744	4.329560	1.057068
32	8	0	0.351429	2.829383	-0.371070
33	1	0	0.271437	3.778606	-0.495489
34	7	0	2.370299	-0.511689	-0.357030
35	6	0	4.088873	1.084706	0.238009
36	6	0	4.465417	-1.339607	0.164115
37	6	0	5.587143	1.324377	0.069592
38	1	0	3.803458	1.121773	1.304958
39	1	0	3.545156	1.877550	-0.279379
40	6	0	5.959831	-1.135875	-0.037455
41	1	0	4.249105	-1.488971	1.235561
42	1	0	4.113403	-2.221411	-0.373225
43	6	0	6.409296	0.164529	0.624564
44	1	0	5.848496	2.263233	0.563448
45	1	0	5.800807	1.443028	-0.997079
46	1	0	6.495529	-1.993594	0.375963
47	1	0	6.172095	-1.095937	-1.110376
48	1	0	7.474925	0.337477	0.458956
49	1	0	6.256755	0.092456	1.707923
50	7	0	3.704573	-0.195928	-0.342865
51	1	0	-1.789839	4.249441	-0.131221

Structure 19a ($CHCl_3$)

Energy (Hartrees): = -1112.8034809
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.595607	-1.850791	-0.128090
2	6	0	-2.657935	-1.007566	0.074984
3	6	0	-2.403783	0.410759	0.060341
4	6	0	-1.068659	0.905691	-0.097788
5	6	0	0.034078	-0.019520	-0.200233
6	6	0	-0.264360	-1.369967	-0.248385
7	6	0	-4.046786	-1.601134	0.260860
8	6	0	-0.917522	2.323360	-0.209563
9	6	0	-1.982391	3.181043	-0.088088
10	6	0	-3.285922	2.694851	0.122918

11	6	0	-3.475977	1.338699	0.184523
12	6	0	-4.125572	-2.539883	1.473296
13	6	0	-4.537257	-2.289993	-1.019797
14	6	0	-4.427000	3.666733	0.256522
15	6	0	1.449782	0.380957	-0.140059
16	1	0	1.678058	1.399984	0.129141
17	1	0	-4.486247	0.980947	0.314757
18	1	0	-4.744331	-0.792929	0.466087
19	1	0	-5.163786	-2.843544	1.634638
20	1	0	-3.778469	-2.036280	2.379151
21	1	0	-3.525784	-3.437671	1.326729
22	1	0	-5.559763	-2.652834	-0.883052
23	1	0	-4.534271	-1.592085	-1.860914
24	1	0	-3.904334	-3.140710	-1.276254
25	8	0	-1.762957	-3.196968	-0.187867
26	1	0	-0.889374	-3.593248	-0.317623
27	8	0	0.655865	-2.343926	-0.376524
28	1	0	1.543913	-1.892773	-0.468105
29	1	0	-5.375426	3.146417	0.395913
30	1	0	-4.509805	4.295297	-0.634509
31	1	0	-4.272754	4.331449	1.111031
32	8	0	0.325470	2.825115	-0.468485
33	1	0	0.256320	3.779561	-0.589523
34	7	0	2.370335	-0.485682	-0.375256
35	6	0	4.088731	1.090341	0.266646
36	6	0	4.457002	-1.339433	0.138924
37	6	0	5.589807	1.324718	0.122789
38	1	0	3.789243	1.100748	1.329160
39	1	0	3.556379	1.897707	-0.239506
40	6	0	5.953686	-1.134523	-0.038910
41	1	0	4.226159	-1.511461	1.202881
42	1	0	4.110115	-2.206830	-0.425225
43	6	0	6.399696	0.147924	0.659112
44	1	0	5.845961	2.249466	0.645176
45	1	0	5.819420	1.471268	-0.937514
46	1	0	6.478310	-2.004842	0.362464
47	1	0	6.181934	-1.071486	-1.108051
48	1	0	7.467775	0.320155	0.507747
49	1	0	6.234169	0.050397	1.738585
50	7	0	3.703506	-0.177873	-0.347835
51	1	0	-1.811391	4.250818	-0.178549

Structure 19a (DMSO)

Energy (Hartrees): = -1112.7985009
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.578073	-1.851104	-0.135858
2	6	0	-2.646959	-1.019998	0.082665
3	6	0	-2.408075	0.401344	0.061652
4	6	0	-1.076956	0.911012	-0.086218
5	6	0	0.035915	-0.002737	-0.191966
6	6	0	-0.251129	-1.355786	-0.256532
7	6	0	-4.028268	-1.623349	0.290231
8	6	0	-0.939311	2.331108	-0.186745
9	6	0	-2.015306	3.177254	-0.077453
10	6	0	-3.317245	2.675219	0.106145
11	6	0	-3.493967	1.316235	0.165023
12	6	0	-4.073622	-2.594442	1.477895
13	6	0	-4.549525	-2.279502	-0.994260
14	6	0	-4.472022	3.633308	0.211952
15	6	0	1.450204	0.406916	-0.128228
16	1	0	1.677576	1.422579	0.155487
17	1	0	-4.503804	0.947783	0.269152
18	1	0	-4.720436	-0.823309	0.540384
19	1	0	-5.108381	-2.897210	1.660819
20	1	0	-3.699641	-2.116181	2.387005
21	1	0	-3.482104	-3.490246	1.291237
22	1	0	-5.563909	-2.657218	-0.838889
23	1	0	-4.578915	-1.557803	-1.814907
24	1	0	-3.915514	-3.116523	-1.292343
25	8	0	-1.730442	-3.197962	-0.210704
26	1	0	-0.849899	-3.579326	-0.336281
27	8	0	0.676660	-2.318562	-0.399330
28	1	0	1.561793	-1.853362	-0.480015
29	1	0	-5.416540	3.101835	0.334837
30	1	0	-4.542172	4.257479	-0.683195
31	1	0	-4.341588	4.304969	1.064921
32	8	0	0.300530	2.845155	-0.423409
33	1	0	0.229170	3.805340	-0.496779
34	7	0	2.371076	-0.455894	-0.378793

35	6	0	4.097637	1.099052	0.289174
36	6	0	4.454917	-1.332239	0.106736
37	6	0	5.599425	1.327389	0.145515
38	1	0	3.801552	1.086149	1.351943
39	1	0	3.569186	1.920010	-0.198402
40	6	0	5.951094	-1.128999	-0.073130
41	1	0	4.228340	-1.523538	1.167766
42	1	0	4.101609	-2.185871	-0.474539
43	6	0	6.404551	0.134856	0.652535
44	1	0	5.861481	2.238797	0.687828
45	1	0	5.827421	1.497438	-0.911802
46	1	0	6.472827	-2.010918	0.305892
47	1	0	6.175992	-1.042679	-1.141516
48	1	0	7.473062	0.305547	0.502189
49	1	0	6.239848	0.013021	1.729542
50	7	0	3.703811	-0.155329	-0.350775
51	1	0	-1.854860	4.249524	-0.160605

Structure 19b (vacuum)

Energy (Hartrees): = -1112.7743696
Imaginary frequency -20.42

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.554545	-1.837717	-0.164170
2	6	0	-2.644354	-1.033968	0.035411
3	6	0	-2.438497	0.393655	0.064292
4	6	0	-1.117621	0.935046	0.000222
5	6	0	0.016448	0.045967	-0.088404
6	6	0	-0.232710	-1.311988	-0.214481
7	6	0	-4.016850	-1.673010	0.174736
8	6	0	-1.005714	2.355244	-0.035025
9	6	0	-2.105228	3.173867	0.036286
10	6	0	-3.402890	2.641404	0.118956
11	6	0	-3.547926	1.278581	0.126610
12	6	0	-4.075201	-2.691013	1.323628
13	6	0	-4.477734	-2.289170	-1.153221
14	6	0	-4.586514	3.569415	0.178376
15	6	0	1.415011	0.461993	0.036928
16	1	0	1.661813	1.479433	0.313669
17	1	0	-4.551336	0.881644	0.154062
18	1	0	-4.732113	-0.896058	0.435402
19	1	0	-5.107835	-3.020380	1.464530
20	1	0	-3.732089	-2.239186	2.257022
21	1	0	-3.459908	-3.564578	1.114970
22	1	0	-5.483158	-2.704462	-1.045834
23	1	0	-4.499873	-1.534764	-1.943135
24	1	0	-3.804589	-3.091123	-1.458761
25	8	0	-1.674931	-3.183539	-0.288883
26	1	0	-0.780521	-3.537929	-0.383291
27	8	0	0.715231	-2.246350	-0.350392
28	1	0	1.607044	-1.773003	-0.341479
29	1	0	-5.522598	3.011204	0.201753
30	1	0	-4.606289	4.231854	-0.690831
31	1	0	-4.543970	4.198811	1.071187
32	8	0	0.239734	2.903122	-0.168411
33	1	0	0.149689	3.857501	-0.231754
34	7	0	2.368848	-0.377582	-0.138769
35	6	0	4.317172	-0.634354	1.121415
36	6	0	4.411567	0.069245	-1.183083
37	6	0	5.720500	-0.102900	1.389805
38	1	0	4.363405	-1.692799	0.811430
39	1	0	3.699575	-0.575552	2.019536
40	6	0	5.819183	0.625559	-1.001994
41	1	0	4.455049	-0.981967	-1.516010
42	1	0	3.862892	0.636355	-1.937168
43	6	0	6.554956	-0.122913	0.109356
44	1	0	6.190448	-0.704466	2.171651
45	1	0	5.640996	0.922705	1.762924
46	1	0	6.360398	0.549783	-1.948193
47	1	0	5.745727	1.686883	-0.745666
48	1	0	7.540010	0.316386	0.283238
49	1	0	6.714592	-1.162373	-0.200437
50	7	0	3.668764	0.170565	0.079339
51	1	0	-1.965245	4.251672	0.004831

Structure 19b ($CHCl_3$)

Energy (Hartrees): = -1112.8001689
Imaginary frequency -21.90

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.542100	-1.837834	-0.183517
2	6	0	-2.636219	-1.042839	0.033260
3	6	0	-2.441781	0.387588	0.065602
4	6	0	-1.124517	0.937951	-0.003916
5	6	0	0.015015	0.056088	-0.098199
6	6	0	-0.223817	-1.302557	-0.237660
7	6	0	-4.004588	-1.688890	0.188413
8	6	0	-1.017911	2.360006	-0.047925
9	6	0	-2.122067	3.173089	0.033390
10	6	0	-3.416219	2.631446	0.131337
11	6	0	-3.556983	1.266330	0.138733
12	6	0	-4.045291	-2.719961	1.325526
13	6	0	-4.488639	-2.289462	-1.137612
14	6	0	-4.602800	3.553077	0.215185
15	6	0	1.410556	0.480247	0.048391
16	1	0	1.644374	1.488379	0.368717
17	1	0	-4.559662	0.866713	0.175032
18	1	0	-4.715557	-0.916108	0.470576
19	1	0	-5.077750	-3.042642	1.485706
20	1	0	-3.681088	-2.283996	2.259302
21	1	0	-3.442997	-3.598649	1.097724
22	1	0	-5.494822	-2.701224	-1.019993
23	1	0	-4.521777	-1.527562	-1.920703
24	1	0	-3.826544	-3.092775	-1.465945
25	8	0	-1.659310	-3.182851	-0.318432
26	1	0	-0.767310	-3.546417	-0.414626
27	8	0	0.733532	-2.225791	-0.385079
28	1	0	1.621471	-1.739703	-0.376741
29	1	0	-5.537961	2.991760	0.216856
30	1	0	-4.620648	4.247104	-0.629272
31	1	0	-4.563976	4.152494	1.129125
32	8	0	0.221480	2.905936	-0.201057
33	1	0	0.137693	3.864497	-0.268130
34	7	0	2.369195	-0.346037	-0.154565
35	6	0	4.306711	-0.658471	1.109768
36	6	0	4.419122	0.121319	-1.172412
37	6	0	5.715104	-0.153532	1.399748
38	1	0	4.342429	-1.704732	0.761915
39	1	0	3.687417	-0.623248	2.008170
40	6	0	5.831977	0.654271	-0.966980
41	1	0	4.452881	-0.919561	-1.535322
42	1	0	3.881170	0.718801	-1.910970
43	6	0	6.554089	-0.138309	0.122378
44	1	0	6.172492	-0.790980	2.160458
45	1	0	5.648694	0.858665	1.811168
46	1	0	6.374355	0.599384	-1.914149
47	1	0	5.773269	1.709133	-0.679597
48	1	0	7.542054	0.286529	0.315598
49	1	0	6.704795	-1.168157	-0.221986
50	7	0	3.669406	0.189711	0.091329
51	1	0	-1.986668	4.250879	-0.004780

Structure 19b (DMSO)

Energy (Hartrees): = -1112.7945042
Imaginary frequency -27.36

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.541826	-1.838000	-0.187278
2	6	0	-2.638256	-1.042809	0.021412
3	6	0	-2.443499	0.388043	0.062225
4	6	0	-1.126303	0.938282	-0.014617
5	6	0	0.013728	0.057274	-0.105075
6	6	0	-0.223103	-1.302335	-0.237775
7	6	0	-4.007305	-1.689466	0.165316
8	6	0	-1.018161	2.360196	-0.067223
9	6	0	-2.119448	3.175922	0.027458
10	6	0	-3.412365	2.634381	0.147930
11	6	0	-3.556352	1.268753	0.154408
12	6	0	-4.060107	-2.684490	1.332584
13	6	0	-4.466598	-2.332647	-1.149203
14	6	0	-4.596273	3.556649	0.251605
15	6	0	1.408203	0.482287	0.051350
16	1	0	1.639590	1.488968	0.378421
17	1	0	-4.559704	0.872972	0.211228
18	1	0	-4.729744	-0.914008	0.405744
19	1	0	-5.087584	-3.033124	1.467550

20	1	0	-3.741589	-2.208579	2.263686
21	1	0	-3.425017	-3.551734	1.153267
22	1	0	-5.478842	-2.730358	-1.036321
23	1	0	-4.480152	-1.596851	-1.957587
24	1	0	-3.807324	-3.152514	-1.438802
25	8	0	-1.653904	-3.183901	-0.316002
26	1	0	-0.759479	-3.540515	-0.413264
27	8	0	0.735941	-2.224026	-0.376310
28	1	0	1.622476	-1.732500	-0.365079
29	1	0	-5.531204	2.995179	0.269625
30	1	0	-4.625441	4.250463	-0.592657
31	1	0	-4.539777	4.157628	1.163586
32	8	0	0.219088	2.901001	-0.244102
33	1	0	0.135905	3.861771	-0.294233
34	7	0	2.366893	-0.344335	-0.147438
35	6	0	4.309562	-0.692161	1.097599
36	6	0	4.411471	0.158669	-1.161059
37	6	0	5.718047	-0.193618	1.397066
38	1	0	4.346202	-1.725901	0.715276
39	1	0	3.693706	-0.685680	1.999186
40	6	0	5.823622	0.687682	-0.943048
41	1	0	4.447072	-0.870865	-1.553782
42	1	0	3.870122	0.778159	-1.878918
43	6	0	6.551002	-0.138046	0.117352
44	1	0	6.178306	-0.853964	2.136068
45	1	0	5.652865	0.805624	1.839915
46	1	0	6.362108	0.664343	-1.893567
47	1	0	5.764611	1.732719	-0.621220
48	1	0	7.539343	0.282081	0.318985
49	1	0	6.699760	-1.156493	-0.259933
50	7	0	3.666385	0.186800	0.108115
51	1	0	-1.984384	4.253926	-0.016751

Structure 19c (vacuum)

Energy (Hartrees): = -1112.7769209
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.671973	-1.850779	-0.010927
2	6	0	-2.711779	-0.960516	0.052331
3	6	0	-2.398405	0.444951	0.023225
4	6	0	-1.035581	0.883223	-0.005854
5	6	0	0.031392	-0.087948	0.017095
6	6	0	-0.316691	-1.425852	-0.028772
7	6	0	-4.133624	-1.496177	0.119928
8	6	0	-0.819892	2.290874	-0.112523
9	6	0	-1.856029	3.189664	-0.124710
10	6	0	-3.192590	2.759469	-0.060645
11	6	0	-3.438708	1.414123	0.003604
12	6	0	-4.364999	-2.367064	1.363497
13	6	0	-4.518739	-2.233316	-1.170672
14	6	0	-4.304842	3.773087	-0.083071
15	6	0	1.452445	0.259500	0.167316
16	1	0	1.695663	1.279611	0.416353
17	1	0	-4.469670	1.095169	0.023263
18	1	0	-4.816864	-0.655748	0.215052
19	1	0	-5.419866	-2.647812	1.423742
20	1	0	-4.106327	-1.817262	2.271169
21	1	0	-3.767948	-3.277137	1.327957
22	1	0	-5.563313	-2.552161	-1.121564
23	1	0	-4.400775	-1.579083	-2.037541
24	1	0	-3.895649	-3.115828	-1.315057
25	8	0	-1.884694	-3.191606	-0.036814
26	1	0	-1.015001	-3.612496	-0.057629
27	8	0	0.567310	-2.439840	-0.055239
28	1	0	1.477490	-2.032427	-0.054806
29	1	0	-5.279107	3.288461	-0.014748
30	1	0	-4.280516	4.359957	-1.005145
31	1	0	-4.213304	4.471083	0.753194
32	8	0	0.465389	2.753340	-0.228227
33	1	0	0.431005	3.702250	-0.373861
34	7	0	2.357897	-0.644725	0.043217
35	6	0	4.495218	-1.171690	-0.663659
36	6	0	4.094870	1.003181	0.394612
37	6	0	5.969516	-1.123252	-0.290631
38	1	0	4.356399	-0.782417	-1.686347
39	1	0	4.114412	-2.193398	-0.642162
40	6	0	5.575101	1.101287	0.754999
41	1	0	3.881499	1.544766	-0.544703
42	1	0	3.509606	1.471932	1.187981
43	6	0	6.447447	0.325504	-0.228136

44	1	0	6.542377	-1.695784	-1.023800
45	1	0	6.106294	-1.599320	0.685411
46	1	0	5.858746	2.156064	0.785741
47	1	0	5.713714	0.693750	1.761225
48	1	0	7.497539	0.377686	0.067873
49	1	0	6.367250	0.777427	-1.224006
50	7	0	3.687057	-0.391493	0.277713
51	1	0	-1.635198	4.251474	-0.203894

Structure 19c ($CHCl_3$)

Energy (Hartrees): = -1112.8035285
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.665743	-1.850882	-0.008874
2	6	0	-2.710488	-0.964038	0.044948
3	6	0	-2.401754	0.443709	0.021098
4	6	0	-1.039834	0.885218	-0.021607
5	6	0	0.031537	-0.081546	0.009689
6	6	0	-0.311667	-1.421768	-0.024954
7	6	0	-4.132832	-1.503707	0.099315
8	6	0	-0.824448	2.293619	-0.148139
9	6	0	-1.861946	3.192354	-0.142436
10	6	0	-3.196903	2.759570	-0.041355
11	6	0	-3.444120	1.412887	0.026826
12	6	0	-4.382754	-2.341930	1.360979
13	6	0	-4.498338	-2.277806	-1.175090
14	6	0	-4.307659	3.774158	-0.036270
15	6	0	1.451909	0.273031	0.168364
16	1	0	1.693210	1.290210	0.432189
17	1	0	-4.474793	1.095530	0.076870
18	1	0	-4.821136	-0.664183	0.153731
19	1	0	-5.434876	-2.637131	1.405517
20	1	0	-4.155094	-1.765285	2.261121
21	1	0	-3.773698	-3.246324	1.367514
22	1	0	-5.550925	-2.573140	-1.141219
23	1	0	-4.349217	-1.657290	-2.062475
24	1	0	-3.893221	-3.179012	-1.278400
25	8	0	-1.877483	-3.192068	-0.025157
26	1	0	-1.011099	-3.623153	-0.041645
27	8	0	0.578528	-2.430752	-0.040016
28	1	0	1.488268	-2.014369	-0.049805
29	1	0	-5.280688	3.293637	0.073894
30	1	0	-4.314483	4.349245	-0.966514
31	1	0	-4.183090	4.485573	0.784595
32	8	0	0.454830	2.743983	-0.303131
33	1	0	0.434185	3.697805	-0.444185
34	7	0	2.357237	-0.631157	0.039944
35	6	0	4.494700	-1.172250	-0.658226
36	6	0	4.098540	1.007370	0.405298
37	6	0	5.967966	-1.126133	-0.283190
38	1	0	4.357533	-0.779140	-1.678516
39	1	0	4.113317	-2.194019	-0.638051
40	6	0	5.578341	1.098166	0.767222
41	1	0	3.889308	1.547392	-0.534762
42	1	0	3.514271	1.477390	1.198417
43	6	0	6.449411	0.321055	-0.215673
44	1	0	6.537498	-1.697011	-1.020434
45	1	0	6.105879	-1.607495	0.690613
46	1	0	5.862633	2.152815	0.797659
47	1	0	5.716114	0.691292	1.774176
48	1	0	7.498807	0.367694	0.084713
49	1	0	6.372867	0.775523	-1.210708
50	7	0	3.684288	-0.388173	0.283147
51	1	0	-1.642741	4.252985	-0.237052

Structure 19c (DMSO)

Energy (Hartrees): = -1112.7985147
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.654945	-1.851533	0.001587
2	6	0	-2.705890	-0.970785	0.038044
3	6	0	-2.404703	0.439070	0.012704
4	6	0	-1.044736	0.889393	-0.024731

5	6	0	0.032799	-0.071045	0.012907
6	6	0	-0.302879	-1.414069	-0.013461
7	6	0	-4.126009	-1.516990	0.079531
8	6	0	-0.837998	2.299762	-0.150885
9	6	0	-1.881440	3.192522	-0.143233
10	6	0	-3.213684	2.750431	-0.045771
11	6	0	-3.453671	1.401308	0.015566
12	6	0	-4.387930	-2.338382	1.349156
13	6	0	-4.467840	-2.313386	-1.187192
14	6	0	-4.330670	3.756997	-0.017823
15	6	0	1.452477	0.290800	0.169540
16	1	0	1.694645	1.309809	0.425970
17	1	0	-4.482998	1.078573	0.061797
18	1	0	-4.820702	-0.681781	0.109971
19	1	0	-5.439236	-2.637430	1.384404
20	1	0	-4.174849	-1.748650	2.244631
21	1	0	-3.774714	-3.240027	1.374970
22	1	0	-5.519266	-2.613365	-1.162785
23	1	0	-4.311078	-1.706366	-2.082757
24	1	0	-3.857067	-3.213311	-1.267551
25	8	0	-1.855785	-3.194260	-0.001812
26	1	0	-0.984391	-3.614375	-0.014257
27	8	0	0.593282	-2.416832	-0.020612
28	1	0	1.500614	-1.989695	-0.034270
29	1	0	-5.303511	3.266578	-0.071890
30	1	0	-4.249209	4.456778	-0.853556
31	1	0	-4.296081	4.347224	0.902552
32	8	0	0.436574	2.757225	-0.307665
33	1	0	0.410449	3.716311	-0.415925
34	7	0	2.357299	-0.615388	0.046857
35	6	0	4.490141	-1.176071	-0.648746
36	6	0	4.105026	1.019372	0.392900
37	6	0	5.963569	-1.131570	-0.275870
38	1	0	4.354139	-0.791164	-1.671952
39	1	0	4.104095	-2.196073	-0.616474
40	6	0	5.585775	1.106218	0.750481
41	1	0	3.898176	1.547914	-0.553559
42	1	0	3.524099	1.500915	1.181493
43	6	0	6.451074	0.313971	-0.224936
44	1	0	6.528498	-1.713052	-1.008293
45	1	0	6.102011	-1.603370	0.702749
46	1	0	5.873779	2.160032	0.766774
47	1	0	5.725077	0.711663	1.762320
48	1	0	7.501032	0.358767	0.073775
49	1	0	6.374291	0.757738	-1.224614
50	7	0	3.683876	-0.376567	0.285159
51	1	0	-1.669382	4.254893	-0.235521

Structure 19d (vacuum)

Energy (Hartrees): = -1112.7654254
Imaginary frequency -47.00

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.797148	-1.829768	-0.110680
2	6	0	-2.741389	-0.851423	0.043965
3	6	0	-2.304393	0.524855	0.040792
4	6	0	-0.911867	0.842300	-0.022550
5	6	0	0.059652	-0.224379	-0.095196
6	6	0	-0.406430	-1.529429	-0.176247
7	6	0	-4.200940	-1.254402	0.181157
8	6	0	-0.571122	2.225493	-0.057058
9	6	0	-1.523389	3.212851	-0.007664
10	6	0	-2.890977	2.900559	0.059812
11	6	0	-3.254614	1.579340	0.080607
12	6	0	-4.437291	-2.181772	1.382699
13	6	0	-4.733927	-1.865321	-1.122054
14	6	0	-3.909136	4.008593	0.092270
15	6	0	1.508683	-0.045166	-0.034687
16	1	0	1.904174	0.944150	0.154553
17	1	0	-4.309454	1.351900	0.106812
18	1	0	-4.788018	-0.361125	0.380914
19	1	0	-5.510610	-2.343134	1.512181
20	1	0	-4.048136	-1.732305	2.298991
21	1	0	-3.958221	-3.148940	1.240729
22	1	0	-5.795896	-2.102109	-1.017924
23	1	0	-4.618160	-1.165110	-1.952513
24	1	0	-4.197319	-2.783143	-1.364590
25	8	0	-2.132243	-3.141991	-0.182954
26	1	0	-1.305239	-3.636520	-0.265527
27	8	0	0.377176	-2.602637	-0.284742

28	1	0	1.343040	-2.266741	-0.294210
29	1	0	-4.919733	3.610326	0.184585
30	1	0	-3.862238	4.608895	-0.820219
31	1	0	-3.728860	4.678580	0.936747
32	8	0	0.750927	2.571637	-0.158292
33	1	0	0.811551	3.528774	-0.215594
34	7	0	2.297459	-1.049764	-0.179232
35	6	0	4.183068	0.046274	-1.159811
36	6	0	4.085568	-0.309495	1.243242
37	6	0	5.707481	0.089223	-1.130586
38	1	0	3.781519	1.072439	-1.072962
39	1	0	3.819749	-0.374544	-2.099605
40	6	0	5.607129	-0.283003	1.347210
41	1	0	3.689675	0.705163	1.427941
42	1	0	3.652556	-0.979194	1.989257
43	6	0	6.204173	0.575370	0.231565
44	1	0	6.068383	0.739072	-1.931624
45	1	0	6.086222	-0.919252	-1.321172
46	1	0	5.898170	0.097443	2.329414
47	1	0	5.978911	-1.308262	1.261906
48	1	0	7.295609	0.553721	0.272495
49	1	0	5.897068	1.618312	0.375983
50	7	0	3.705112	-0.813380	-0.076761
51	1	0	-1.208414	4.253343	-0.037439

Structure 19d ($CHCl_3$)

Energy (Hartrees): = -1112.7917333
Imaginary frequency -77.63

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.795357	-1.829501	-0.129783
2	6	0	-2.740086	-0.852135	0.038743
3	6	0	-2.305440	0.526015	0.037515
4	6	0	-0.914343	0.844776	-0.054796
5	6	0	0.058002	-0.220401	-0.139541
6	6	0	-0.406313	-1.526509	-0.215072
7	6	0	-4.198294	-1.257438	0.193616
8	6	0	-0.571251	2.228430	-0.114281
9	6	0	-1.521188	3.217006	-0.032066
10	6	0	-2.886320	2.903486	0.086861
11	6	0	-3.254099	1.581734	0.113726
12	6	0	-4.421858	-2.154862	1.419434
13	6	0	-4.743188	-1.902557	-1.087630
14	6	0	-3.900340	4.012887	0.161774
15	6	0	1.507565	-0.038561	-0.057720
16	1	0	1.899312	0.945063	0.167972
17	1	0	-4.308630	1.358021	0.176020
18	1	0	-4.788521	-0.362223	0.370761
19	1	0	-5.492834	-2.328902	1.555325
20	1	0	-4.041210	-1.677553	2.325926
21	1	0	-3.930459	-3.120877	1.306214
22	1	0	-5.807239	-2.125194	-0.969737
23	1	0	-4.630400	-1.228476	-1.940500
24	1	0	-4.220455	-2.833226	-1.312211
25	8	0	-2.133229	-3.141995	-0.191820
26	1	0	-1.313418	-3.650000	-0.281388
27	8	0	0.382737	-2.595653	-0.329849
28	1	0	1.348157	-2.249260	-0.340138
29	1	0	-4.910270	3.615993	0.271402
30	1	0	-3.871814	4.629226	-0.741128
31	1	0	-3.696241	4.669228	1.012023
32	8	0	0.742208	2.563356	-0.276856
33	1	0	0.815387	3.522665	-0.349173
34	7	0	2.296745	-1.040084	-0.217190
35	6	0	4.204736	0.060936	-1.141328
36	6	0	4.061311	-0.332489	1.256417
37	6	0	5.727454	0.109545	-1.080838
38	1	0	3.795387	1.080984	-1.039436
39	1	0	3.862214	-0.343339	-2.096548
40	6	0	5.580035	-0.305243	1.389219
41	1	0	3.661078	0.678153	1.443017
42	1	0	3.615935	-1.012251	1.986275
43	6	0	6.197380	0.571056	0.299104
44	1	0	6.097535	0.778298	-1.862112
45	1	0	6.117671	-0.892070	-1.286783
46	1	0	5.847595	0.062606	2.382969
47	1	0	5.959218	-1.327964	1.299781
48	1	0	7.288094	0.546831	0.359860
49	1	0	5.887356	1.611231	0.455779
50	7	0	3.705703	-0.820696	-0.080714
51	1	0	-1.204745	4.255785	-0.080769

Structure 19d (DMSO)

Energy (Hartrees): = -1112.7866405
Imaginary frequency -28.66

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.789015	-1.832636	-0.104161
2	6	0	2.740505	-0.857457	0.034681
3	6	0	2.309325	0.522305	0.038014
4	6	0	0.917078	0.846644	-0.029401
5	6	0	-0.060719	-0.216565	-0.098911
6	6	0	0.399158	-1.525803	-0.162509
7	6	0	4.201498	-1.264862	0.152940
8	6	0	0.580516	2.233522	-0.067388
9	6	0	1.537785	3.217362	-0.008940
10	6	0	2.903767	2.897013	0.074736
11	6	0	3.265436	1.572837	0.094128
12	6	0	4.712595	-1.906074	-1.143521
13	6	0	4.454576	-2.166090	1.369438
14	6	0	3.924775	4.000522	0.124413
15	6	0	-1.511947	-0.029398	-0.047125
16	1	0	-1.909452	0.962731	0.121423
17	1	0	4.320014	1.344343	0.136858
18	1	0	4.798258	-0.371879	0.317156
19	1	0	5.778289	-2.132666	-1.051330
20	1	0	4.584197	-1.226087	-1.989775
21	1	0	4.181535	-2.833844	-1.362215
22	1	0	5.528395	-2.342866	1.475109
23	1	0	4.101329	-1.688906	2.287310
24	1	0	3.956990	-3.130431	1.268008
25	8	0	2.118527	-3.146918	-0.168671
26	1	0	1.291655	-3.644922	-0.242099
27	8	0	-0.394554	-2.592999	-0.253989
28	1	0	-1.360827	-2.234698	-0.262739
29	1	0	4.933153	3.598355	0.229648
30	1	0	3.730601	4.670512	0.966158
31	1	0	3.888834	4.604439	-0.786605
32	8	0	-0.733199	2.579486	-0.180608
33	1	0	-0.801361	3.542116	-0.214310
34	7	0	-2.297542	-1.038754	-0.175857
35	6	0	-4.097663	-0.340823	1.243275
36	6	0	-4.182772	0.075120	-1.155180
37	6	0	-5.618713	-0.305398	1.339746
38	1	0	-3.691776	0.664677	1.441750
39	1	0	-3.674511	-1.029188	1.978542
40	6	0	-5.706609	0.118042	-1.130615
41	1	0	-3.785821	1.096154	-1.032096
42	1	0	-3.815743	-0.318885	-2.105754
43	6	0	-6.207000	0.577037	0.239039
44	1	0	-5.906134	0.060864	2.328430
45	1	0	-6.002908	-1.325670	1.239082
46	1	0	-6.058777	0.787763	-1.919104
47	1	0	-6.091903	-0.883577	-1.347497
48	1	0	-7.298937	0.556494	0.274598
49	1	0	-5.895559	1.615031	0.405717
50	7	0	-3.710201	-0.819276	-0.090271
51	1	0	1.224825	4.258002	-0.043182

Structure 20a (vacuum)

Energy (Hartrees): = -1112.7681389
Imaginary frequency -59.64

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.555313	-1.864895	-0.117521
2	6	0	-2.623203	-1.056511	0.103442
3	6	0	-2.422164	0.387600	0.051395
4	6	0	-1.111704	0.932653	-0.077157
5	6	0	0.031274	0.035482	-0.193174
6	6	0	-0.195721	-1.367384	-0.260883
7	6	0	-3.989582	-1.680605	0.340513
8	6	0	-1.016117	2.344492	-0.135445
9	6	0	-2.123412	3.163277	-0.072310
10	6	0	-3.409425	2.626737	0.034797
11	6	0	-3.534466	1.256738	0.095291
12	6	0	-3.983368	-2.685985	1.501619

13	6	0	-4.528898	-2.313349	-0.949155
14	6	0	-4.607410	3.538035	0.079024
15	6	0	1.381484	0.460381	-0.201149
16	1	0	1.621843	1.505445	-0.106896
17	1	0	-4.532490	0.848259	0.152690
18	1	0	-4.682349	-0.895781	0.638383
19	1	0	-5.007474	-3.007380	1.709105
20	1	0	-3.581371	-2.226217	2.407239
21	1	0	-3.385206	-3.564388	1.265487
22	1	0	-5.525098	-2.731278	-0.780957
23	1	0	-4.597045	-1.569781	-1.746872
24	1	0	-3.868599	-3.116686	-1.280436
25	8	0	-1.648745	-3.211434	-0.184692
26	1	0	-0.730099	-3.507519	-0.314291
27	8	0	0.706826	-2.246811	-0.403119
28	1	0	-5.534651	2.964858	0.101173
29	1	0	-4.633890	4.192921	-0.795620
30	1	0	-4.582474	4.174856	0.967351
31	8	0	0.226142	2.917114	-0.269601
32	1	0	0.111277	3.866246	-0.361518
33	7	0	2.375423	-0.386376	-0.309946
34	6	0	4.116072	1.042377	0.482189
35	6	0	4.491528	-1.289672	-0.091732
36	6	0	5.604931	1.338211	0.331019
37	1	0	3.867934	0.793340	1.528077
38	1	0	3.550134	1.930479	0.201567
39	6	0	5.982593	-1.051175	-0.275906
40	1	0	4.280257	-1.614069	0.940886
41	1	0	4.140552	-2.070485	-0.770280
42	6	0	6.448428	0.097867	0.615625
43	1	0	5.869119	2.156496	1.004449
44	1	0	5.788307	1.679795	-0.692164
45	1	0	6.521039	-1.972506	-0.043667
46	1	0	6.174623	-0.808587	-1.325298
47	1	0	7.507366	0.308856	0.452831
48	1	0	6.332140	-0.188765	1.667177
49	7	0	3.738860	-0.065937	-0.400463
50	1	0	2.076542	-1.379780	-0.426857
51	1	0	-1.987312	4.241248	-0.122295

Structure 20a ($CHCl_3$)

Energy (Hartrees): = -1112.7975316
Imaginary frequency -70.00

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.557730	-1.864536	-0.142917
2	6	0	-2.619645	-1.057130	0.113893
3	6	0	-2.420083	0.387825	0.054296
4	6	0	-1.113770	0.927972	-0.133320
5	6	0	0.026844	0.029731	-0.268207
6	6	0	-0.201387	-1.370693	-0.333726
7	6	0	-3.979036	-1.682512	0.390907
8	6	0	-1.017833	2.339801	-0.243424
9	6	0	-2.118520	3.163511	-0.130426
10	6	0	-3.397540	2.632408	0.069272
11	6	0	-3.526838	1.262538	0.151550
12	6	0	-3.943658	-2.667651	1.567965
13	6	0	-4.548350	-2.337319	-0.874194
14	6	0	-4.584391	3.550592	0.190874
15	6	0	1.379763	0.460408	-0.242258
16	1	0	1.616214	1.501931	-0.099483
17	1	0	-4.522832	0.861733	0.272231
18	1	0	-4.669898	-0.896644	0.688050
19	1	0	-4.960443	-2.997030	1.799394
20	1	0	-3.533632	-2.190660	2.461873
21	1	0	-3.340877	-3.546273	1.340354
22	1	0	-5.541104	-2.750711	-0.674909
23	1	0	-4.639620	-1.607662	-1.683157
24	1	0	-3.901061	-3.148489	-1.213378
25	8	0	-1.654259	-3.212997	-0.201730
26	1	0	-0.739682	-3.513332	-0.358138
27	8	0	0.695161	-2.252372	-0.500834
28	1	0	-5.517400	2.985779	0.215542
29	1	0	-4.629511	4.249044	-0.648688
30	1	0	-4.524672	4.144378	1.107658
31	8	0	0.210754	2.892149	-0.483513
32	1	0	0.106872	3.841831	-0.614704
33	7	0	2.383674	-0.368196	-0.360321
34	6	0	4.084124	0.989878	0.625673
35	6	0	4.510381	-1.265515	-0.187963
36	6	0	5.570290	1.320096	0.540407

37	1	0	3.820485	0.618116	1.629162
38	1	0	3.509431	1.894609	0.430899
39	6	0	6.000152	-0.986688	-0.312149
40	1	0	4.283364	-1.694225	0.801518
41	1	0	4.186774	-1.975967	-0.951976
42	6	0	6.428953	0.068844	0.704408
43	1	0	5.802784	2.060306	1.309316
44	1	0	5.770118	1.780390	-0.432451
45	1	0	6.544691	-1.921638	-0.162538
46	1	0	6.212314	-0.635646	-1.326900
47	1	0	7.486618	0.312806	0.582925
48	1	0	6.300254	-0.331183	1.716695
49	7	0	3.744142	-0.023822	-0.384451
50	1	0	2.124456	-1.359442	-0.512925
51	1	0	-1.981941	4.238482	-0.218326

Structure 20a (DMSO)

Energy (Hartrees): = -1112.7936294
Imaginary frequency -64.85

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.567933	-1.865754	-0.132117
2	6	0	-2.629664	-1.053680	0.111224
3	6	0	-2.422265	0.390226	0.049039
4	6	0	-1.110519	0.924753	-0.121928
5	6	0	0.027925	0.021297	-0.249480
6	6	0	-0.207132	-1.377505	-0.315741
7	6	0	-3.994867	-1.669535	0.380219
8	6	0	-1.008051	2.337983	-0.223011
9	6	0	-2.107332	3.166282	-0.125413
10	6	0	-3.391759	2.638887	0.051611
11	6	0	-3.528076	1.268959	0.130328
12	6	0	-3.973965	-2.652146	1.558990
13	6	0	-4.560115	-2.324482	-0.885902
14	6	0	-4.577418	3.560197	0.153235
15	6	0	1.385230	0.446759	-0.224367
16	1	0	1.626827	1.487003	-0.081489
17	1	0	-4.527872	0.872888	0.236045
18	1	0	-4.683262	-0.879119	0.670269
19	1	0	-4.994333	-2.977353	1.780025
20	1	0	-3.573219	-2.174706	2.457126
21	1	0	-3.371327	-3.533204	1.339666
22	1	0	-5.557261	-2.729137	-0.691024
23	1	0	-4.642606	-1.596810	-1.697829
24	1	0	-3.917490	-3.142384	-1.218624
25	8	0	-1.663814	-3.213904	-0.186833
26	1	0	-0.745190	-3.507012	-0.334830
27	8	0	0.683243	-2.264980	-0.478678
28	1	0	-5.511151	2.996415	0.175449
29	1	0	-4.611872	4.250944	-0.693129
30	1	0	-4.523674	4.164309	1.063535
31	8	0	0.224309	2.885414	-0.438385
32	1	0	0.131584	3.843162	-0.516072
33	7	0	2.387470	-0.381397	-0.347472
34	6	0	4.092241	0.984935	0.624137
35	6	0	4.520638	-1.272422	-0.190879
36	6	0	5.575832	1.320287	0.520849
37	1	0	3.842563	0.611561	1.630059
38	1	0	3.512559	1.887179	0.433973
39	6	0	6.006626	-0.984553	-0.334803
40	1	0	4.309447	-1.697313	0.803152
41	1	0	4.190381	-1.985966	-0.949357
42	6	0	6.442111	0.073519	0.675813
43	1	0	5.812598	2.062121	1.286777
44	1	0	5.762695	1.781609	-0.454285
45	1	0	6.557759	-1.916673	-0.192438
46	1	0	6.203953	-0.632471	-1.352407
47	1	0	7.497049	0.322663	0.541043
48	1	0	6.326105	-0.326698	1.689489
49	7	0	3.746103	-0.033676	-0.380801
50	1	0	2.137026	-1.373212	-0.498809
51	1	0	-1.965257	4.241429	-0.208060

Structure 20b χ=175.4 º (vacuum)

Energy (Hartrees): = -1112.7767894
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.594063	-1.854347	-0.199884
2	6	0	-2.648032	-1.047360	0.070305
3	6	0	-2.434365	0.401298	0.074094
4	6	0	-1.121626	0.939441	-0.018772
5	6	0	0.023181	0.035786	-0.141080
6	6	0	-0.219679	-1.367442	-0.315083
7	6	0	-4.021739	-1.660968	0.288895
8	6	0	-1.011415	2.347744	-0.056212
9	6	0	-2.115135	3.175263	0.012428
10	6	0	-3.403471	2.646376	0.097714
11	6	0	-3.540308	1.273865	0.125065
12	6	0	-4.021094	-2.737101	1.384429
13	6	0	-4.588066	-2.201853	-1.030905
14	6	0	-4.596589	3.563797	0.150351
15	6	0	1.355731	0.437949	-0.026719
16	1	0	1.621604	1.458690	0.203627
17	1	0	-4.542178	0.871705	0.157625
18	1	0	-4.694138	-0.882986	0.646453
19	1	0	-5.049351	-3.049069	1.585560
20	1	0	-3.598783	-2.342776	2.311462
21	1	0	-3.445411	-3.611635	1.086899
22	1	0	-5.589071	-2.613214	-0.876397
23	1	0	-4.651894	-1.409222	-1.780257
24	1	0	-3.944858	-2.993552	-1.418888
25	8	0	-1.701465	-3.193596	-0.339566
26	1	0	-0.785710	-3.492764	-0.482708
27	8	0	0.662938	-2.237713	-0.503084
28	1	0	-5.527264	2.995958	0.159659
29	1	0	-4.615034	4.231983	-0.714262
30	1	0	-4.571728	4.186651	1.048378
31	8	0	0.235432	2.904124	-0.178516
32	1	0	0.137543	3.855953	-0.261998
33	7	0	2.398927	-0.366098	-0.161645
34	6	0	4.304973	-0.540681	1.193541
35	6	0	4.484325	-0.067295	-1.184110
36	6	0	5.693380	0.034242	1.449059
37	1	0	4.373927	-1.627695	1.013827
38	1	0	3.648791	-0.381625	2.050615
39	6	0	5.877747	0.521041	-0.999049
40	1	0	4.558129	-1.142507	-1.424072
41	1	0	3.955160	0.424946	-2.001286
42	6	0	6.572781	-0.109511	0.207300
43	1	0	6.140920	-0.474206	2.306099
44	1	0	5.590630	1.092567	1.707576
45	1	0	6.457351	0.363367	-1.911486
46	1	0	5.782859	1.600640	-0.847663
47	1	0	7.549208	0.351134	0.372402
48	1	0	6.747274	-1.173402	0.008694
49	7	0	3.692861	0.128986	0.037490
50	1	0	2.225753	-1.355848	-0.370668
51	1	0	-1.970694	4.252697	-0.018975

Structure 20b ($CHCl_3$)

Energy (Hartrees): = -1112.8050791
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.599002	-1.852983	-0.202751
2	6	0	-2.653746	-1.044337	0.066078
3	6	0	-2.436845	0.404289	0.073199
4	6	0	-1.121953	0.936694	-0.042159
5	6	0	0.019479	0.029083	-0.166313
6	6	0	-0.224203	-1.371125	-0.328807
7	6	0	-4.029156	-1.658891	0.279783
8	6	0	-1.006112	2.346978	-0.103695
9	6	0	-2.104902	3.179570	-0.011300
10	6	0	-3.393368	2.655847	0.119786
11	6	0	-3.538416	1.283241	0.153407
12	6	0	-4.039210	-2.712723	1.395989
13	6	0	-4.579154	-2.227708	-1.034564
14	6	0	-4.577398	3.580064	0.222252
15	6	0	1.356087	0.435311	-0.036969
16	1	0	1.611415	1.456165	0.206103
17	1	0	-4.542185	0.889353	0.219076
18	1	0	-4.711789	-0.878297	0.608657
19	1	0	-5.068374	-3.028827	1.588049
20	1	0	-3.636315	-2.300122	2.324522
21	1	0	-3.454171	-3.591689	1.127758

22	1	0	-5.585111	-2.629650	-0.884802
23	1	0	-4.631931	-1.452332	-1.803335
24	1	0	-3.939305	-3.032815	-1.401417
25	8	0	-1.711203	-3.194380	-0.334798
26	1	0	-0.796982	-3.501525	-0.478419
27	8	0	0.657006	-2.246464	-0.516749
28	1	0	-5.514536	3.022067	0.203746
29	1	0	-4.589700	4.297107	-0.602555
30	1	0	-4.543460	4.153256	1.153140
31	8	0	0.235721	2.890049	-0.274101
32	1	0	0.150592	3.845666	-0.371269
33	7	0	2.401775	-0.356439	-0.162618
34	6	0	4.293324	-0.532539	1.209670
35	6	0	4.491971	-0.066176	-1.170989
36	6	0	5.686238	0.027621	1.470411
37	1	0	4.348904	-1.618459	1.026163
38	1	0	3.636171	-0.363972	2.064357
39	6	0	5.890269	0.506581	-0.979040
40	1	0	4.552896	-1.143313	-1.401065
41	1	0	3.974615	0.429412	-1.993992
42	6	0	6.571692	-0.125140	0.234238
43	1	0	6.121426	-0.488271	2.329559
44	1	0	5.595471	1.087039	1.731117
45	1	0	6.470711	0.333597	-1.888355
46	1	0	5.810179	1.588996	-0.836696
47	1	0	7.549092	0.331890	0.404895
48	1	0	6.741131	-1.190498	0.039677
49	7	0	3.693663	0.145085	0.047615
50	1	0	2.252449	-1.346120	-0.383874
51	1	0	-1.955008	4.255222	-0.060185

Structure 20b (DMSO)

Energy (Hartrees): = -1112.8004855
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.604942	-1.856206	-0.191121
2	6	0	-2.659336	-1.043554	0.067788
3	6	0	-2.436834	0.404434	0.071092
4	6	0	-1.118590	0.932870	-0.033526
5	6	0	0.021006	0.020942	-0.149411
6	6	0	-0.226468	-1.378653	-0.305674
7	6	0	-4.040071	-1.648418	0.273203
8	6	0	-0.999328	2.344221	-0.089001
9	6	0	-2.096876	3.180038	-0.006572
10	6	0	-3.388360	2.658867	0.108203
11	6	0	-3.537825	1.286174	0.139480
12	6	0	-4.063945	-2.714685	1.376707
13	6	0	-4.592642	-2.196719	-1.048028
14	6	0	-4.571396	3.585131	0.194404
15	6	0	1.361197	0.425334	-0.026678
16	1	0	1.618376	1.449073	0.200816
17	1	0	-4.543931	0.896056	0.194797
18	1	0	-4.716419	-0.865561	0.609249
19	1	0	-5.098062	-3.014980	1.567025
20	1	0	-3.653787	-2.319192	2.309836
21	1	0	-3.493885	-3.600294	1.098070
22	1	0	-5.602454	-2.590939	-0.904429
23	1	0	-4.638617	-1.411691	-1.807621
24	1	0	-3.959785	-3.003434	-1.424369
25	8	0	-1.715691	-3.197354	-0.321620
26	1	0	-0.797512	-3.497954	-0.454719
27	8	0	0.651412	-2.259100	-0.482066
28	1	0	-5.508547	3.027152	0.174435
29	1	0	-4.575045	4.295696	-0.636031
30	1	0	-4.542121	4.167573	1.119659
31	8	0	0.243617	2.885429	-0.244093
32	1	0	0.161110	3.845409	-0.304086
33	7	0	2.405430	-0.366215	-0.142060
34	6	0	4.310552	-0.515274	1.214027
35	6	0	4.483323	-0.088226	-1.177197
36	6	0	5.704963	0.051322	1.449308
37	1	0	4.366227	-1.602895	1.044540
38	1	0	3.663023	-0.332709	2.073384
39	6	0	5.882756	0.488307	-1.008780
40	1	0	4.541447	-1.168956	-1.387037
41	1	0	3.957669	0.394581	-2.002800
42	6	0	6.576834	-0.123434	0.206947
43	1	0	6.149099	-0.449174	2.312871
44	1	0	5.616900	1.115438	1.692026
45	1	0	6.452862	0.300427	-1.921631

46	1	0	5.804978	1.573286	-0.883665
47	1	0	7.556597	0.335275	0.359369
48	1	0	6.741127	-1.192289	0.028141
49	7	0	3.697502	0.144377	0.047205
50	1	0	2.265259	-1.359453	-0.350874
51	1	0	-1.943846	4.255811	-0.051754

Structure 20b χ = 38.6 º (vacuum)

Energy (Hartrees): = -1112.77402
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.575016	-1.841148	-0.361239
2	6	0	-2.586087	-1.059152	0.091224
3	6	0	-2.401061	0.396725	0.095569
4	6	0	-1.131822	0.955228	-0.201460
5	6	0	0.012519	0.069772	-0.427789
6	6	0	-0.227614	-1.334231	-0.632114
7	6	0	-3.906935	-1.693655	0.491184
8	6	0	-1.046818	2.355159	-0.338378
9	6	0	-2.122316	3.180546	-0.077869
10	6	0	-3.355145	2.640499	0.286438
11	6	0	-3.482338	1.262833	0.339501
12	6	0	-3.743269	-2.814105	1.528095
13	6	0	-4.667868	-2.182263	-0.748548
14	6	0	-4.520678	3.546235	0.586438
15	6	0	1.330027	0.466438	-0.229193
16	1	0	1.571047	1.458525	0.137410
17	1	0	-4.461604	0.858184	0.552089
18	1	0	-4.515262	-0.932142	0.976512
19	1	0	-4.729543	-3.128273	1.879003
20	1	0	-3.171898	-2.463113	2.390330
21	1	0	-3.235438	-3.678870	1.105769
22	1	0	-5.638890	-2.593569	-0.460566
23	1	0	-4.834992	-1.362843	-1.451572
24	1	0	-4.098751	-2.963188	-1.256389
25	8	0	-1.689542	-3.177889	-0.526926
26	1	0	-0.796804	-3.470813	-0.778729
27	8	0	0.649271	-2.175409	-0.921484
28	1	0	-5.455330	2.985701	0.626615
29	1	0	-4.620495	4.323935	-0.173846
30	1	0	-4.384662	4.043513	1.550647
31	8	0	0.112422	2.973434	-0.747019
32	1	0	0.519088	2.428278	-1.429760
33	7	0	2.398258	-0.303184	-0.404259
34	6	0	4.062911	-0.542355	1.239939
35	6	0	4.627520	-0.038008	-1.070366
36	6	0	5.397746	0.008954	1.725325
37	1	0	4.145530	-1.627088	1.053944
38	1	0	3.279642	-0.386067	1.983477
39	6	0	5.981371	0.524963	-0.652995
40	1	0	4.725513	-1.111204	-1.311322
41	1	0	4.244964	0.472894	-1.955091
42	6	0	6.463907	-0.132567	0.639603
43	1	0	5.693198	-0.517898	2.635415
44	1	0	5.267159	1.065111	1.979694
45	1	0	6.699125	0.370203	-1.461700
46	1	0	5.878805	1.603888	-0.502161
47	1	0	7.406832	0.310491	0.967012
48	1	0	6.653718	-1.196502	0.455557
49	7	0	3.653503	0.154345	0.010346
50	1	0	2.250331	-1.276437	-0.690786
51	1	0	-1.985016	4.248877	-0.200906

Structure 20b χ = 91.0 º (vacuum)

Energy (Hartrees): = -1112.772129
Imaginary frequency -314.45

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.573670	-1.847215	-0.284548
2	6	0	-2.614796	-1.055239	0.070452
3	6	0	-2.420434	0.397200	0.070529
4	6	0	-1.127843	0.952686	-0.140810
5	6	0	0.016894	0.062079	-0.331966
6	6	0	-0.217739	-1.342829	-0.505438

7	6	0	-3.956912	-1.691676	0.392657
8	6	0	-1.035674	2.357910	-0.217595
9	6	0	-2.127505	3.180158	-0.036197
10	6	0	-3.393279	2.642135	0.199718
11	6	0	-3.516545	1.265721	0.233611
12	6	0	-3.855123	-2.726436	1.522858
13	6	0	-4.592586	-2.293746	-0.867717
14	6	0	-4.580037	3.546360	0.405909
15	6	0	1.342281	0.473744	-0.193003
16	1	0	1.586669	1.484884	0.102906
17	1	0	-4.507603	0.858159	0.373846
18	1	0	-4.628100	-0.918788	0.762303
19	1	0	-4.857098	-3.068192	1.794913
20	1	0	-3.394494	-2.284743	2.409249
21	1	0	-3.265591	-3.590009	1.219953
22	1	0	-5.574358	-2.713801	-0.633835
23	1	0	-4.719431	-1.531375	-1.640059
24	1	0	-3.961137	-3.089198	-1.266069
25	8	0	-1.673611	-3.189034	-0.412521
26	1	0	-0.767890	-3.478783	-0.621343
27	8	0	0.664326	-2.196359	-0.754949
28	1	0	-5.509848	2.976898	0.426427
29	1	0	-4.652614	4.288942	-0.392044
30	1	0	-4.495270	4.087386	1.352115
31	8	0	0.185222	2.972514	-0.470680
32	1	0	0.274818	3.081200	-1.422642
33	7	0	2.397631	-0.308313	-0.364601
34	6	0	4.115096	-0.498811	1.222721
35	6	0	4.603411	-0.085539	-1.120983
36	6	0	5.471001	0.053951	1.643236
37	1	0	4.181336	-1.590275	1.072139
38	1	0	3.358841	-0.309141	1.986151
39	6	0	5.977959	0.474840	-0.771279
40	1	0	4.680611	-1.167959	-1.325886
41	1	0	4.195705	0.397323	-2.010199
42	6	0	6.497779	-0.140111	0.527895
43	1	0	5.792072	-0.442379	2.561804
44	1	0	5.360158	1.120252	1.862265
45	1	0	6.665119	0.280593	-1.597939
46	1	0	5.893370	1.559934	-0.657598
47	1	0	7.456051	0.304052	0.805523
48	1	0	6.670230	-1.212230	0.377241
49	7	0	3.670186	0.158392	-0.015429
50	1	0	2.234475	-1.293576	-0.602300
51	1	0	-1.971892	4.252202	-0.091817

Structure 20b χ = 269.0 º (vacuum)

Energy (Hartrees): = -1112.772129
Imaginary frequency -314.41

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.573659	-1.847200	-0.284579
2	6	0	2.614804	-1.055252	0.070425
3	6	0	2.420461	0.397188	0.070558
4	6	0	1.127867	0.952696	-0.140697
5	6	0	-0.016888	0.062110	-0.331839
6	6	0	0.217726	-1.342790	-0.505406
7	6	0	3.956919	-1.691718	0.392577
8	6	0	1.035710	2.357924	-0.217439
9	6	0	2.127562	3.180152	-0.036089
10	6	0	3.393344	2.642106	0.199739
11	6	0	3.516594	1.265691	0.233603
12	6	0	4.592560	-2.293760	-0.867826
13	6	0	3.855135	-2.726515	1.522746
14	6	0	4.580130	3.546316	0.405835
15	6	0	-1.342266	0.473780	-0.192796
16	1	0	-1.586637	1.484896	0.103206
17	1	0	4.507653	0.858112	0.373774
18	1	0	4.628124	-0.918852	0.762237
19	1	0	5.574333	-2.713828	-0.633977
20	1	0	4.719394	-1.531372	-1.640154
21	1	0	3.961095	-3.089199	-1.266181
22	1	0	4.857109	-3.068306	1.794761
23	1	0	3.394539	-2.284842	2.409164
24	1	0	3.265572	-3.590062	1.219824
25	8	0	1.673581	-3.189015	-0.412616
26	1	0	0.767851	-3.478744	-0.621428
27	8	0	-0.664353	-2.196298	-0.754939
28	1	0	5.509905	2.976804	0.426602
29	1	0	4.495291	4.087597	1.351887
30	1	0	4.652841	4.288683	-0.392308

31	8	0	-0.185195	2.972541	-0.470439
32	1	0	-0.274817	3.081306	-1.422388
33	7	0	-2.397623	-0.308256	-0.364440
34	6	0	-4.603292	-0.085099	-1.121023
35	6	0	-4.115279	-0.499168	1.222603
36	6	0	-5.977858	0.475222	-0.771304
37	1	0	-4.680511	-1.167447	-1.326297
38	1	0	-4.195454	0.398044	-2.010025
39	6	0	-5.471226	0.053480	1.643133
40	1	0	-4.181527	-1.590581	1.071649
41	1	0	-3.359116	-0.309772	1.986193
42	6	0	-6.497867	-0.140158	0.527590
43	1	0	-6.664922	0.281290	-1.598119
44	1	0	-5.893237	1.560273	-0.657236
45	1	0	-5.792428	-0.443175	2.561480
46	1	0	-5.360389	1.119699	1.862562
47	1	0	-7.456160	0.303941	0.805251
48	1	0	-6.670338	-1.212218	0.376541
49	7	0	-3.670189	0.158425	-0.015273
50	1	0	-2.234478	-1.293488	-0.602276
51	1	0	1.971963	4.252200	-0.091676

Structure 20b χ = 321.4 º (vacuum)

Energy (Hartrees): = -1112.77402
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.575026	-1.841128	-0.361640
2	6	0	2.585912	-1.059247	0.091369
3	6	0	2.400948	0.396646	0.095665
4	6	0	1.131760	0.955241	-0.201462
5	6	0	-0.012602	0.069798	-0.427954
6	6	0	0.227623	-1.334170	-0.632632
7	6	0	3.906686	-1.693611	0.491807
8	6	0	1.046842	2.355182	-0.338250
9	6	0	2.122518	3.180449	-0.077974
10	6	0	3.355265	2.640327	0.286345
11	6	0	3.482291	1.262619	0.339541
12	6	0	4.668520	-2.181237	-0.747754
13	6	0	3.742876	-2.814710	1.527990
14	6	0	4.520934	3.545832	0.586524
15	6	0	-1.330115	0.466405	-0.229278
16	1	0	-1.571160	1.458406	0.137500
17	1	0	4.461525	0.857873	0.552145
18	1	0	4.514380	-0.932120	0.977982
19	1	0	5.639495	-2.592433	-0.459452
20	1	0	4.835799	-1.361369	-1.450219
21	1	0	4.099917	-2.962046	-1.256369
22	1	0	4.729068	-3.128365	1.879588
23	1	0	3.170519	-2.464575	2.389920
24	1	0	3.236014	-3.679613	1.104801
25	8	0	1.689631	-3.177810	-0.527777
26	1	0	0.796963	-3.470691	-0.779864
27	8	0	-0.649158	-2.175326	-0.922230
28	1	0	5.455950	2.985658	0.623132
29	1	0	4.386667	4.040161	1.552509
30	1	0	4.618750	4.325821	-0.171651
31	8	0	-0.112408	2.973586	-0.746702
32	1	0	-0.519121	2.428485	-1.429474
33	7	0	-2.398400	-0.303156	-0.404472
34	6	0	-4.627717	-0.037589	-1.070276
35	6	0	-4.062907	-0.542719	1.239800
36	6	0	-5.981469	0.525375	-0.652586
37	1	0	-4.725843	-1.110702	-1.311563
38	1	0	-4.245200	0.473550	-1.954881
39	6	0	-5.397656	0.008518	1.725511
40	1	0	-4.145620	-1.627394	1.053484
41	1	0	-3.279556	-0.386719	1.983313
42	6	0	-6.463937	-0.132538	0.639848
43	1	0	-6.699323	0.370948	-1.461266
44	1	0	-5.878783	1.604240	-0.501405
45	1	0	-5.693055	-0.518631	2.635447
46	1	0	-5.266966	1.064575	1.980237
47	1	0	-7.406790	0.310495	0.967501
48	1	0	-6.653866	-1.196394	0.455467
49	7	0	-3.653572	0.154323	0.010391
50	1	0	-2.250584	-1.276369	-0.691116
51	1	0	1.985315	4.248787	-0.201079

Structure 20c (vacuum)

Energy (Hartrees): = -1112.7680766
Imaginary frequency -59.34

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.597878	-1.863306	0.090947
2	6	0	2.662250	-1.033593	-0.055513
3	6	0	2.425133	0.406419	-0.050774
4	6	0	1.096964	0.921052	-0.049819
5	6	0	-0.030539	-0.001755	-0.029902
6	6	0	0.219433	-1.396247	0.104347
7	6	0	4.058421	-1.626451	-0.160935
8	6	0	0.962105	2.330013	-0.011390
9	6	0	2.050989	3.175399	0.011165
10	6	0	3.353573	2.669136	0.020218
11	6	0	3.516134	1.301792	-0.009123
12	6	0	4.177688	-2.656515	-1.293847
13	6	0	4.502217	-2.216934	1.184108
14	6	0	4.529354	3.608749	0.067749
15	6	0	-1.380247	0.390218	-0.184836
16	1	0	-1.624975	1.418921	-0.388259
17	1	0	4.524646	0.917556	0.029308
18	1	0	4.753908	-0.829418	-0.417091
19	1	0	5.225467	-2.944269	-1.414053
20	1	0	3.830121	-2.232763	-2.238722
21	1	0	3.595174	-3.551148	-1.081645
22	1	0	5.521241	-2.606110	1.110967
23	1	0	4.478324	-1.457055	1.968954
24	1	0	3.840125	-3.034545	1.474395
25	8	0	1.715336	-3.205401	0.197254
26	1	0	0.795769	-3.521460	0.251123
27	8	0	-0.672717	-2.292070	0.192026
28	1	0	5.470069	3.057876	0.084462
29	1	0	4.491247	4.241520	0.958294
30	1	0	4.538646	4.267295	-0.804703
31	8	0	-0.301662	2.871176	0.016802
32	1	0	-0.217895	3.823512	0.109657
33	7	0	-2.367953	-0.468195	-0.107982
34	6	0	-4.500697	-1.305395	0.195418
35	6	0	-4.154833	1.097414	0.113514
36	6	0	-5.970817	-1.153453	-0.164058
37	1	0	-4.373720	-1.318587	1.290749
38	1	0	-4.102962	-2.241652	-0.202964
39	6	0	-5.626043	1.316740	-0.226697
40	1	0	-3.987874	1.155744	1.202582
41	1	0	-3.563340	1.879768	-0.361874
42	6	0	-6.498267	0.192796	0.328078
43	1	0	-6.531507	-1.980494	0.276997
44	1	0	-6.077079	-1.220441	-1.250920
45	1	0	-5.936403	2.286345	0.169008
46	1	0	-5.727527	1.356464	-1.315433
47	1	0	-7.539413	0.333337	0.030344
48	1	0	-6.467954	0.214970	1.423530
49	7	0	-3.719204	-0.208295	-0.390905
50	1	0	-2.062215	-1.456160	0.028506
51	1	0	1.886405	4.250121	0.038437

Structure 20c ($CHCl_3$)

Energy (Hartrees): = -1112.797514
Imaginary frequency -68.10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.613540	-1.861778	-0.107387
2	6	0	-2.673292	-1.027677	0.053434
3	6	0	-2.425857	0.410968	0.055875
4	6	0	-1.092454	0.914211	0.051314
5	6	0	0.029457	-0.017150	0.024681
6	6	0	-0.230430	-1.406165	-0.124073
7	6	0	-4.074102	-1.610244	0.172153
8	6	0	-0.944896	2.325225	0.006856
9	6	0	-2.028545	3.178901	-0.009596
10	6	0	-3.336390	2.681998	-0.007969
11	6	0	-3.512220	1.315258	0.023272
12	6	0	-4.189440	-2.646112	1.299420
13	6	0	-4.545966	-2.187814	-1.168459
14	6	0	-4.503108	3.631808	-0.062915
15	6	0	1.384115	0.369732	0.200696
16	1	0	1.629006	1.392419	0.435009

17	1	0	-4.525214	0.941118	-0.007450
18	1	0	-4.758832	-0.808801	0.442084
19	1	0	-5.239979	-2.915394	1.440372
20	1	0	-3.817436	-2.237628	2.242567
21	1	0	-3.629664	-3.552541	1.073030
22	1	0	-5.569670	-2.563165	-1.082496
23	1	0	-4.527307	-1.425385	-1.951623
24	1	0	-3.903474	-3.014867	-1.478387
25	8	0	-1.741778	-3.203710	-0.221825
26	1	0	-0.824396	-3.529390	-0.279952
27	8	0	0.653211	-2.310547	-0.223218
28	1	0	-5.450739	3.095292	0.001267
29	1	0	-4.498817	4.202494	-0.995834
30	1	0	-4.463350	4.351669	0.758983
31	8	0	0.319295	2.847746	-0.036190
32	1	0	0.257680	3.806614	-0.118117
33	7	0	2.375253	-0.478756	0.116778
34	6	0	4.512288	-1.317326	-0.165131
35	6	0	4.157721	1.091154	-0.128095
36	6	0	5.981891	-1.150653	0.187451
37	1	0	4.383086	-1.347058	-1.258801
38	1	0	4.119986	-2.247545	0.252451
39	6	0	5.628169	1.318783	0.206411
40	1	0	3.991454	1.121619	-1.217047
41	1	0	3.566104	1.881879	0.332330
42	6	0	6.502887	0.188325	-0.329669
43	1	0	6.541510	-1.984059	-0.243145
44	1	0	6.094630	-1.199832	1.275003
45	1	0	5.931651	2.282364	-0.209161
46	1	0	5.733140	1.380661	1.294213
47	1	0	7.543641	0.337469	-0.034026
48	1	0	6.470490	0.190796	-1.425326
49	7	0	3.724049	-0.210256	0.401890
50	1	0	2.101068	-1.463562	-0.052340
51	1	0	-1.853231	4.251329	-0.044025

Structure 20c (DMSO)

Energy (Hartrees): = -1112.7934899
Imaginary frequency -68.49

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.620222	-1.865449	-0.090339
2	6	0	-2.678275	-1.027945	0.065921
3	6	0	-2.424734	0.410091	0.066181
4	6	0	-1.088702	0.909060	0.061654
5	6	0	0.031196	-0.026060	0.037779
6	6	0	-0.234050	-1.414140	-0.104800
7	6	0	-4.085145	-1.598753	0.164105
8	6	0	-0.937972	2.320873	0.014302
9	6	0	-2.019447	3.177774	-0.003465
10	6	0	-3.328907	2.684207	-0.001457
11	6	0	-3.509429	1.317571	0.031514
12	6	0	-4.223830	-2.673343	1.251135
13	6	0	-4.555151	-2.121924	-1.198701
14	6	0	-4.492328	3.637179	-0.056355
15	6	0	1.390039	0.359840	0.205424
16	1	0	1.638602	1.383192	0.432967
17	1	0	-4.524305	0.947763	0.001707
18	1	0	-4.761278	-0.798995	0.458929
19	1	0	-5.281091	-2.919201	1.383089
20	1	0	-3.842487	-2.310768	2.209599
21	1	0	-3.688073	-3.584949	0.990744
22	1	0	-5.582435	-2.491167	-1.131905
23	1	0	-4.526106	-1.331531	-1.953609
24	1	0	-3.917610	-2.943250	-1.534839
25	8	0	-1.746748	-3.206763	-0.209024
26	1	0	-0.825908	-3.522864	-0.271450
27	8	0	0.643456	-2.323302	-0.203848
28	1	0	-5.441247	3.102575	0.005095
29	1	0	-4.483090	4.210715	-0.987497
30	1	0	-4.449532	4.355965	0.766240
31	8	0	0.325107	2.839265	-0.031636
32	1	0	0.265440	3.800291	-0.100605
33	7	0	2.381173	-0.487208	0.124108
34	6	0	4.522496	-1.322542	-0.159778
35	6	0	4.157994	1.086891	-0.146594
36	6	0	5.990826	-1.144837	0.192512
37	1	0	4.395077	-1.360674	-1.252894
38	1	0	4.134422	-2.250337	0.266682
39	6	0	5.627654	1.322930	0.183713
40	1	0	3.991256	1.102410	-1.235348

41	1	0	3.564814	1.880086	0.306603
42	6	0	6.506079	0.190046	-0.339618
43	1	0	6.553625	-1.980852	-0.228652
44	1	0	6.103753	-1.181628	1.280780
45	1	0	5.925044	2.282486	-0.245080
46	1	0	5.734430	1.399737	1.270605
47	1	0	7.546325	0.346932	-0.045724
48	1	0	6.471993	0.179541	-1.435063
49	7	0	3.730178	-0.212081	0.397532
50	1	0	2.117267	-1.472712	-0.043811
51	1	0	-1.841423	4.249842	-0.040774

Structure 20d (vacuum)

Energy (Hartrees): = -1112.7730666
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.854432	-1.844257	-0.175836
2	6	0	-2.751164	-0.865340	0.090751
3	6	0	-2.292616	0.526306	0.070777
4	6	0	-0.907060	0.832503	-0.019935
5	6	0	0.065051	-0.256876	-0.134374
6	6	0	-0.415635	-1.601070	-0.295419
7	6	0	-4.209384	-1.222512	0.325701
8	6	0	-0.560292	2.201642	-0.058991
9	6	0	-1.508710	3.204802	-0.008934
10	6	0	-2.868575	2.902900	0.060496
11	6	0	-3.235043	1.573124	0.099744
12	6	0	-4.397705	-2.302705	1.401012
13	6	0	-4.886380	-1.620332	-0.992292
14	6	0	-3.891007	4.008238	0.078970
15	6	0	1.445558	-0.086087	-0.053402
16	1	0	1.853975	0.893505	0.144245
17	1	0	-4.290897	1.345657	0.123774
18	1	0	-4.716856	-0.339799	0.711720
19	1	0	-5.461767	-2.397899	1.632589
20	1	0	-3.872514	-2.029855	2.318996
21	1	0	-4.028403	-3.270190	1.067225
22	1	0	-5.946327	-1.831802	-0.828554
23	1	0	-4.803250	-0.819736	-1.731295
24	1	0	-4.414349	-2.516190	-1.400486
25	8	0	-2.190060	-3.145413	-0.303679
26	1	0	-1.339598	-3.599202	-0.443637
27	8	0	0.305148	-2.607164	-0.476042
28	1	0	-4.899327	3.607047	0.183869
29	1	0	-3.853157	4.592171	-0.844372
30	1	0	-3.710845	4.694019	0.910528
31	8	0	0.765758	2.544819	-0.161510
32	1	0	0.826177	3.500074	-0.242529
33	7	0	2.349506	-1.049227	-0.185064
34	6	0	4.213942	0.078582	-1.132953
35	6	0	4.107513	-0.360803	1.263716
36	6	0	5.736921	0.135457	-1.088560
37	1	0	3.799920	1.095176	-1.013499
38	1	0	3.862192	-0.316810	-2.087152
39	6	0	5.627553	-0.315958	1.373414
40	1	0	3.693186	0.640042	1.475843
41	1	0	3.681298	-1.062002	1.982897
42	6	0	6.218292	0.586961	0.290478
43	1	0	6.096045	0.811479	-1.868098
44	1	0	6.128452	-0.862785	-1.306105
45	1	0	5.907170	0.034973	2.369503
46	1	0	6.015602	-1.332267	1.257280
47	1	0	7.309396	0.578927	0.337558
48	1	0	5.895466	1.620235	0.465570
49	7	0	3.729180	-0.817035	-0.077557
50	1	0	2.033019	-1.998423	-0.371988
51	1	0	-1.183147	4.242097	-0.041868

Structure 20d ($CHCl_3$)

Energy (Hartrees): = -1112.8008856
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.858876	-1.843320	-0.174044

2	6	0	-2.754204	-0.862227	0.095542
3	6	0	-2.291513	0.528029	0.074998
4	6	0	-0.904507	0.827851	-0.032862
5	6	0	0.063324	-0.265475	-0.149941
6	6	0	-0.420491	-1.605646	-0.301447
7	6	0	-4.215294	-1.213499	0.328367
8	6	0	-0.551118	2.198138	-0.089744
9	6	0	-1.495215	3.205012	-0.023955
10	6	0	-2.856102	2.908547	0.076124
11	6	0	-3.230233	1.580240	0.122768
12	6	0	-4.417862	-2.302933	1.391430
13	6	0	-4.895908	-1.591544	-0.993034
14	6	0	-3.870764	4.020070	0.115670
15	6	0	1.450031	-0.094534	-0.058600
16	1	0	1.856661	0.884700	0.144976
17	1	0	-4.287273	1.360423	0.167488
18	1	0	-4.717165	-0.331407	0.721992
19	1	0	-5.480950	-2.370065	1.638707
20	1	0	-3.874102	-2.060521	2.308095
21	1	0	-4.084770	-3.279262	1.043642
22	1	0	-5.957308	-1.798750	-0.830440
23	1	0	-4.812888	-0.783698	-1.724772
24	1	0	-4.433518	-2.486298	-1.416458
25	8	0	-2.202765	-3.144548	-0.299119
26	1	0	-1.357467	-3.609408	-0.440384
27	8	0	0.297017	-2.618297	-0.481731
28	1	0	-4.881464	3.625122	0.226487
29	1	0	-3.836506	4.613691	-0.802045
30	1	0	-3.675821	4.697163	0.951475
31	8	0	0.768962	2.529608	-0.226794
32	1	0	0.845247	3.487583	-0.310306
33	7	0	2.351018	-1.053732	-0.182299
34	6	0	4.222064	0.062401	-1.129773
35	6	0	4.102036	-0.355354	1.273531
36	6	0	5.743716	0.126920	-1.075330
37	1	0	3.801387	1.075449	-1.015802
38	1	0	3.879036	-0.341980	-2.083818
39	6	0	5.620750	-0.303895	1.390834
40	1	0	3.683615	0.646012	1.467024
41	1	0	3.674689	-1.050378	1.998362
42	6	0	6.215431	0.590102	0.302976
43	1	0	6.100643	0.801387	-1.857460
44	1	0	6.144277	-0.869609	-1.286396
45	1	0	5.889187	0.059981	2.385506
46	1	0	6.016112	-1.319607	1.290884
47	1	0	7.306557	0.582730	0.355991
48	1	0	5.889302	1.623995	0.467299
49	7	0	3.734241	-0.829144	-0.068008
50	1	0	2.041460	-2.003496	-0.375562
51	1	0	-1.163064	4.238971	-0.072227

Structure 20d (DMSO)

Energy (Hartrees): = -1112.7964679
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.859961	-1.845342	-0.169423
2	6	0	-2.754913	-0.863417	0.099165
3	6	0	-2.290263	0.525947	0.074522
4	6	0	-0.901958	0.823969	-0.026265
5	6	0	0.064890	-0.270635	-0.143481
6	6	0	-0.420942	-1.608146	-0.300183
7	6	0	-4.216923	-1.207076	0.335097
8	6	0	-0.547421	2.195241	-0.077670
9	6	0	-1.491972	3.202826	-0.022621
10	6	0	-2.854428	2.906555	0.064202
11	6	0	-3.230303	1.578266	0.111413
12	6	0	-4.424539	-2.306888	1.385290
13	6	0	-4.906661	-1.563298	-0.986932
14	6	0	-3.868710	4.018148	0.090135
15	6	0	1.454259	-0.100476	-0.051615
16	1	0	1.862974	0.876560	0.158560
17	1	0	-4.287911	1.358418	0.148320
18	1	0	-4.710194	-0.325734	0.740907
19	1	0	-5.486960	-2.364350	1.637333
20	1	0	-3.874174	-2.081194	2.302606
21	1	0	-4.103850	-3.282837	1.024620
22	1	0	-5.968558	-1.764645	-0.820550
23	1	0	-4.823301	-0.746073	-1.708408
24	1	0	-4.453212	-2.456289	-1.424679
25	8	0	-2.199515	-3.147514	-0.293204

26	1	0	-1.348787	-3.600857	-0.439641
27	8	0	0.292900	-2.622748	-0.487992
28	1	0	-4.880022	3.623513	0.196926
29	1	0	-3.826077	4.606505	-0.830610
30	1	0	-3.676915	4.700995	0.921927
31	8	0	0.772046	2.524758	-0.200729
32	1	0	0.851124	3.485221	-0.258557
33	7	0	2.352792	-1.058677	-0.179673
34	6	0	4.226141	0.040795	-1.138950
35	6	0	4.099756	-0.338317	1.271906
36	6	0	5.747039	0.112005	-1.080161
37	1	0	3.801716	1.052915	-1.038609
38	1	0	3.887951	-0.380265	-2.087688
39	6	0	5.617894	-0.279792	1.391050
40	1	0	3.679253	0.664954	1.445572
41	1	0	3.673474	-1.023059	2.007368
42	6	0	6.210497	0.600854	0.291664
43	1	0	6.102043	0.775224	-1.872551
44	1	0	6.155139	-0.885526	-1.273188
45	1	0	5.880850	0.100810	2.380861
46	1	0	6.019526	-1.294938	1.307948
47	1	0	7.301503	0.601881	0.348815
48	1	0	5.874672	1.634086	0.438075
49	7	0	3.737353	-0.836741	-0.063750
50	1	0	2.045554	-2.007571	-0.379905
51	1	0	-1.159178	4.236900	-0.068944

Structure 21a (vacuum)

Energy (Hartrees): = -1191.3849117
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.874940	-2.118858	1.167330
2	6	0	4.652778	3.693679	-0.521000
3	6	0	-1.168259	0.327499	0.084208
4	6	0	2.207470	3.187182	-0.202814
5	6	0	3.524095	2.714246	-0.340755
6	6	0	3.737245	1.362321	-0.289034
7	6	0	2.680448	0.427025	-0.118021
8	6	0	1.335568	0.905796	-0.016932
9	6	0	1.157547	2.321226	-0.032827
10	6	0	4.360257	-1.563219	-0.167998
11	6	0	4.437949	-2.612995	-1.286696
12	6	0	2.962271	-0.982901	-0.020993
13	6	0	1.919892	-1.828441	0.254749
14	6	0	0.577610	-1.367732	0.320866
15	6	0	0.253919	-0.032868	0.153350
16	1	0	-1.417972	1.331954	-0.215031
17	1	0	4.756043	1.012977	-0.360508
18	1	0	1.239840	-3.547883	0.597159
19	1	0	5.899802	-2.481482	1.053357
20	8	0	-0.104528	2.826173	0.152715
21	1	0	4.519320	4.276589	-1.436165
22	1	0	5.612311	3.179992	-0.583776
23	1	0	4.696782	4.397207	0.314382
24	8	0	-0.324850	-2.338536	0.536140
25	1	0	4.867972	-1.343307	1.936715
26	1	0	4.251311	-2.947536	1.504350
27	8	0	2.110877	-3.159706	0.438051
28	1	0	5.036980	-0.764984	-0.463916
29	1	0	5.477797	-2.917953	-1.430306
30	1	0	4.071154	-2.199854	-2.229012
31	1	0	3.849793	-3.496697	-1.043718
32	1	0	-1.223900	-1.884027	0.595153
33	1	0	-0.046885	3.784967	0.178536
34	7	0	-2.068783	-0.550336	0.347503
35	7	0	-3.430184	-0.262187	0.307151
36	6	0	-3.810302	1.159143	0.227803
37	6	0	-4.049731	-1.161779	-0.694877
38	6	0	-5.336858	1.283030	0.197545
39	1	0	-3.416465	1.614948	-0.698477
40	6	0	-5.566914	-1.012494	-0.681903
41	1	0	-3.682954	-0.867946	-1.695199
42	6	0	-5.978954	0.436464	-0.889656
43	1	0	-5.584019	2.340400	0.072305
44	1	0	-5.722645	0.970950	1.174805
45	1	0	-5.980221	-1.656571	-1.462243
46	1	0	-5.945943	-1.374909	0.280713
47	1	0	-7.066136	0.541842	-0.865653
48	1	0	-5.641487	0.777008	-1.875582
49	6	0	-3.660482	-2.614346	-0.431382

50	1	0	-2.620616	-2.821532	-0.678323
51	1	0	-3.826904	-2.852113	0.622427
52	1	0	-4.287481	-3.270148	-1.038729
53	6	0	-3.306612	1.921227	1.459426
54	1	0	-3.602766	1.369402	2.354218
55	1	0	-2.229748	2.071895	1.491971
56	1	0	-3.781793	2.904194	1.488826
57	1	0	2.016336	4.257614	-0.208429

Structure 21a ($CHCl_3$)

Energy (Hartrees): = -1191.4115246
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.872535	-2.127744	1.169557
2	6	0	4.644687	3.697770	-0.547846
3	6	0	-1.168739	0.330583	0.089174
4	6	0	2.205280	3.191772	-0.192085
5	6	0	3.519745	2.717091	-0.353724
6	6	0	3.736627	1.363837	-0.308056
7	6	0	2.681373	0.427663	-0.121864
8	6	0	1.336910	0.907294	-0.008598
9	6	0	1.156701	2.324724	-0.011009
10	6	0	4.362858	-1.563104	-0.163441
11	6	0	4.450666	-2.603308	-1.289355
12	6	0	2.962745	-0.983775	-0.020988
13	6	0	1.919040	-1.829293	0.255060
14	6	0	0.576768	-1.368097	0.324514
15	6	0	0.254464	-0.031911	0.161304
16	1	0	-1.418275	1.334994	-0.210930
17	1	0	4.755067	1.017053	-0.399215
18	1	0	1.246623	-3.562251	0.593790
19	1	0	5.901143	-2.482074	1.059039
20	8	0	-0.098969	2.820237	0.201025
21	1	0	4.499679	4.279806	-1.462336
22	1	0	5.605361	3.186307	-0.619464
23	1	0	4.693778	4.404964	0.284584
24	8	0	-0.329261	-2.335371	0.539262
25	1	0	4.859548	-1.359191	1.946673
26	1	0	4.256173	-2.964823	1.501024
27	8	0	2.113185	-3.160622	0.435268
28	1	0	5.042011	-0.762576	-0.445719
29	1	0	5.493064	-2.901217	-1.432968
30	1	0	4.086625	-2.186838	-2.232097
31	1	0	3.868176	-3.495115	-1.059240
32	1	0	-1.229997	-1.874312	0.590949
33	1	0	-0.054357	3.783406	0.231625
34	7	0	-2.068007	-0.549027	0.351009
35	7	0	-3.431030	-0.265989	0.314182
36	6	0	-3.810725	1.158151	0.224634
37	6	0	-4.047507	-1.168982	-0.692393
38	6	0	-5.336387	1.286267	0.175726
39	1	0	-3.402894	1.605935	-0.697766
40	6	0	-5.564031	-1.015040	-0.690229
41	1	0	-3.672986	-0.874569	-1.688418
42	6	0	-5.969483	0.433677	-0.911804
43	1	0	-5.575564	2.344112	0.039011
44	1	0	-5.736491	0.983843	1.150482
45	1	0	-5.971283	-1.663330	-1.470183
46	1	0	-5.952940	-1.370218	0.271510
47	1	0	-7.056728	0.541213	-0.896087
48	1	0	-5.622829	0.766121	-1.897319
49	6	0	-3.662514	-2.621387	-0.425842
50	1	0	-2.622828	-2.833611	-0.672847
51	1	0	-3.833166	-2.866198	0.626341
52	1	0	-4.287893	-3.275321	-1.037628
53	6	0	-3.321379	1.924097	1.457723
54	1	0	-3.683028	1.417400	2.355828
55	1	0	-2.240053	2.022502	1.535503
56	1	0	-3.743213	2.931808	1.439832
57	1	0	2.013081	4.261631	-0.187509

Structure 21a (DMSO)

Energy (Hartrees): = -1191.4053048
No imaginary frequencies

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	4.866976	-2.130201	1.184641
2	6	0	4.658691	3.689332	-0.533707
3	6	0	-1.170720	0.334262	0.082122
4	6	0	2.214720	3.190792	-0.205460
5	6	0	3.529779	2.712189	-0.349257
6	6	0	3.743653	1.357993	-0.297129
7	6	0	2.683618	0.425482	-0.118394
8	6	0	1.338539	0.908440	-0.018272
9	6	0	1.161560	2.326992	-0.032929
10	6	0	4.363435	-1.565775	-0.150070
11	6	0	4.456576	-2.606254	-1.274628
12	6	0	2.962650	-0.986807	-0.014958
13	6	0	1.915605	-1.830499	0.254365
14	6	0	0.573158	-1.366394	0.313561
15	6	0	0.253218	-0.029041	0.149298
16	1	0	-1.424735	1.340773	-0.205839
17	1	0	4.762633	1.009759	-0.377364
18	1	0	1.232165	-3.555613	0.590712
19	1	0	5.897414	-2.480304	1.078478
20	8	0	-0.094020	2.827402	0.155681
21	1	0	4.516441	4.277929	-1.444312
22	1	0	5.617347	3.174040	-0.605119
23	1	0	4.705176	4.391992	0.302659
24	8	0	-0.335094	-2.331318	0.522329
25	1	0	4.848658	-1.362484	1.962765
26	1	0	4.252351	-2.970234	1.512550
27	8	0	2.103094	-3.162291	0.437189
28	1	0	5.044582	-0.766259	-0.429222
29	1	0	5.499701	-2.904418	-1.411278
30	1	0	4.099959	-2.189716	-2.220421
31	1	0	3.872273	-3.497983	-1.048275
32	1	0	-1.237793	-1.865917	0.559710
33	1	0	-0.048644	3.792072	0.155567
34	7	0	-2.067831	-0.550249	0.336531
35	7	0	-3.431263	-0.269392	0.313585
36	6	0	-3.812953	1.157017	0.244298
37	6	0	-4.054216	-1.158968	-0.702997
38	6	0	-5.338761	1.282974	0.209194
39	1	0	-3.412435	1.615244	-0.675152
40	6	0	-5.570425	-1.006518	-0.687351
41	1	0	-3.686517	-0.848171	-1.695821
42	6	0	-5.978488	0.444620	-0.885082
43	1	0	-5.578724	2.342339	0.088258
44	1	0	-5.732391	0.967515	1.182717
45	1	0	-5.981366	-1.644017	-1.474165
46	1	0	-5.953126	-1.376150	0.271713
47	1	0	-7.065770	0.550405	-0.859613
48	1	0	-5.638532	0.790909	-1.868005
49	6	0	-3.666613	-2.614392	-0.460378
50	1	0	-2.628630	-2.822917	-0.717996
51	1	0	-3.830866	-2.876896	0.588844
52	1	0	-4.296106	-3.258433	-1.078330
53	6	0	-3.315722	1.907683	1.483101
54	1	0	-3.668270	1.389934	2.378996
55	1	0	-2.233977	2.010574	1.552512
56	1	0	-3.740188	2.914268	1.480960
57	1	0	2.025511	4.261346	-0.207744

Structure 21b (vacuum)

Energy (Hartrees): = -1191.3905497
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.394952	-2.765370	1.060887
2	6	0	4.789380	3.589555	0.538685
3	6	0	-1.128888	0.389252	0.162112
4	6	0	2.317980	3.158679	0.342676
5	6	0	3.626998	2.645636	0.383636
6	6	0	3.804763	1.292186	0.259710
7	6	0	2.715388	0.392711	0.107369
8	6	0	1.385994	0.912161	0.101808
9	6	0	1.238191	2.325987	0.190839
10	6	0	4.324564	-1.648355	0.008568
11	6	0	4.795345	-2.134740	-1.368741
12	6	0	2.942871	-1.020130	-0.071535
13	6	0	1.864897	-1.815197	-0.360096
14	6	0	0.535889	-1.307165	-0.358425
15	6	0	0.269068	0.020577	-0.072274
16	1	0	-1.369326	1.301015	0.696846

17	1	0	4.817274	0.917252	0.252371
18	1	0	1.120388	-3.495274	-0.767136
19	1	0	5.430163	-3.099031	1.169008
20	8	0	-0.023191	2.845001	0.087390
21	1	0	4.806824	4.323230	-0.271409
22	1	0	5.737001	3.050830	0.529839
23	1	0	4.720115	4.140186	1.480424
24	8	0	-0.404621	-2.233812	-0.595455
25	1	0	4.051628	-2.401647	2.031927
26	1	0	3.785069	-3.621273	0.776299
27	8	0	2.007169	-3.139378	-0.621920
28	1	0	5.027485	-0.887441	0.340759
29	1	0	5.808054	-2.539919	-1.298201
30	1	0	4.803483	-1.311631	-2.086972
31	1	0	4.135440	-2.917182	-1.745162
32	1	0	-1.292127	-1.760895	-0.595288
33	1	0	0.038291	3.803819	0.080681
34	7	0	-2.078226	-0.387287	-0.206507
35	7	0	-3.381727	0.062644	0.160862
36	6	0	-4.052766	0.578095	-1.055808
37	6	0	-4.092657	-1.103808	0.727196
38	6	0	-5.467662	1.020757	-0.684244
39	1	0	-4.114806	-0.233292	-1.802266
40	6	0	-5.504813	-0.684951	1.126477
41	1	0	-4.160201	-1.891301	-0.045030
42	6	0	-6.272059	-0.112868	-0.059286
43	1	0	-5.961311	1.399540	-1.583171
44	1	0	-5.387434	1.853007	0.024175
45	1	0	-6.021578	-1.552364	1.545778
46	1	0	-5.426868	0.067509	1.919403
47	1	0	-7.258656	0.239574	0.251019
48	1	0	-6.430812	-0.900393	-0.804977
49	6	0	-3.331859	-1.647822	1.930589
50	1	0	-2.364613	-2.062819	1.646657
51	1	0	-3.165106	-0.845860	2.654800
52	1	0	-3.913694	-2.436788	2.411735
53	6	0	-3.275329	1.745924	-1.652324
54	1	0	-3.114440	2.513376	-0.889921
55	1	0	-2.304569	1.442648	-2.043066
56	1	0	-3.849381	2.184348	-2.471442
57	1	0	2.157038	4.232112	0.404795

Structure 21b ($CHCl_3$)

Energy (Hartrees): = -1191.4169303
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.396794	-2.761096	1.063277
2	6	0	4.798083	3.584434	0.546655
3	6	0	-1.127311	0.399202	0.166144
4	6	0	2.326435	3.161767	0.340885
5	6	0	3.634318	2.643599	0.385455
6	6	0	3.811299	1.288521	0.259544
7	6	0	2.719051	0.391522	0.102477
8	6	0	1.390373	0.915180	0.097272
9	6	0	1.244115	2.331368	0.184594
10	6	0	4.323333	-1.654636	0.000509
11	6	0	4.791766	-2.156729	-1.371403
12	6	0	2.941910	-1.023168	-0.078077
13	6	0	1.860066	-1.816004	-0.362546
14	6	0	0.532089	-1.304470	-0.356383
15	6	0	0.270410	0.025092	-0.071989
16	1	0	-1.361114	1.313643	0.699310
17	1	0	4.824083	0.913433	0.258513
18	1	0	1.119171	-3.510763	-0.761493
19	1	0	5.432798	-3.092989	1.173607
20	8	0	-0.012631	2.848125	0.074215
21	1	0	4.808470	4.331580	-0.251652
22	1	0	5.746212	3.045837	0.523569
23	1	0	4.733524	4.122540	1.496434
24	8	0	-0.414067	-2.225868	-0.589001
25	1	0	4.056241	-2.390618	2.033557
26	1	0	3.788246	-3.623136	0.791269
27	8	0	2.002635	-3.140738	-0.621659
28	1	0	5.030219	-0.892633	0.319823
29	1	0	5.806911	-2.556462	-1.297441
30	1	0	4.798932	-1.343948	-2.102161
31	1	0	4.137596	-2.947662	-1.741619
32	1	0	-1.301496	-1.747634	-0.576071
33	1	0	0.039305	3.811156	0.090380
34	7	0	-2.078642	-0.377337	-0.195641

35	7	0	-3.383492	0.073111	0.167514
36	6	0	-4.055702	0.566589	-1.061529
37	6	0	-4.091871	-1.093226	0.744731
38	6	0	-5.473808	1.006599	-0.699928
39	1	0	-4.111007	-0.259507	-1.790973
40	6	0	-5.508412	-0.678318	1.132806
41	1	0	-4.150060	-1.887271	-0.020384
42	6	0	-6.274356	-0.121902	-0.061264
43	1	0	-5.965847	1.367952	-1.606865
44	1	0	-5.402388	1.850662	-0.004377
45	1	0	-6.020802	-1.546565	1.555994
46	1	0	-5.440774	0.080999	1.920737
47	1	0	-7.261786	0.232557	0.244977
48	1	0	-6.430442	-0.918698	-0.797510
49	6	0	-3.334639	-1.619600	1.957221
50	1	0	-2.362773	-2.033626	1.685187
51	1	0	-3.176095	-0.813129	2.679160
52	1	0	-3.914355	-2.408765	2.441735
53	6	0	-3.283920	1.726343	-1.679089
54	1	0	-3.129705	2.515610	-0.937161
55	1	0	-2.311127	1.421689	-2.065913
56	1	0	-3.860074	2.141720	-2.509294
57	1	0	2.165456	4.235057	0.400935

Structure 21b (DMSO)

Energy (Hartrees): = -1191.4103605
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.380010	-2.790574	1.050213
2	6	0	4.835070	3.555419	0.528421
3	6	0	-1.127003	0.421740	0.168420
4	6	0	2.358072	3.156982	0.340889
5	6	0	3.661170	2.626276	0.377960
6	6	0	3.824899	1.268702	0.252975
7	6	0	2.722415	0.382917	0.103114
8	6	0	1.397862	0.918662	0.102321
9	6	0	1.266667	2.336683	0.190667
10	6	0	4.311092	-1.673520	-0.000853
11	6	0	4.777209	-2.161964	-1.377768
12	6	0	2.933406	-1.034415	-0.075922
13	6	0	1.844615	-1.817897	-0.358963
14	6	0	0.520183	-1.295365	-0.348371
15	6	0	0.269297	0.037266	-0.064604
16	1	0	-1.357860	1.346431	0.684754
17	1	0	4.834603	0.884941	0.244934
18	1	0	1.082525	-3.498475	-0.757744
19	1	0	5.414573	-3.128821	1.153681
20	8	0	0.016526	2.867591	0.087478
21	1	0	4.850345	4.294744	-0.276980
22	1	0	5.776565	3.005146	0.509801
23	1	0	4.775775	4.104990	1.471880
24	8	0	-0.432157	-2.209121	-0.577708
25	1	0	4.046082	-2.427241	2.025733
26	1	0	3.765816	-3.647063	0.773352
27	8	0	1.972256	-3.142825	-0.622164
28	1	0	5.021359	-0.918637	0.326855
29	1	0	5.791315	-2.564903	-1.308108
30	1	0	4.787719	-1.340328	-2.098849
31	1	0	4.120833	-2.946729	-1.758055
32	1	0	-1.317844	-1.721767	-0.548931
33	1	0	0.082266	3.830731	0.111861
34	7	0	-2.079472	-0.359161	-0.181144
35	7	0	-3.386897	0.095437	0.166525
36	6	0	-4.062389	0.531154	-1.084518
37	6	0	-4.085363	-1.055441	0.788911
38	6	0	-5.487517	0.965605	-0.746899
39	1	0	-4.103728	-0.324721	-1.778931
40	6	0	-5.508992	-0.643527	1.151991
41	1	0	-4.128243	-1.880502	0.057283
42	6	0	-6.275299	-0.147821	-0.068102
43	1	0	-5.978371	1.282320	-1.670873
44	1	0	-5.433283	1.839054	-0.086489
45	1	0	-6.010520	-1.500983	1.608543
46	1	0	-5.457481	0.148414	1.908762
47	1	0	-7.269626	0.204129	0.217893
48	1	0	-6.413855	-0.976088	-0.772330
49	6	0	-3.328806	-1.519612	2.026638
50	1	0	-2.348980	-1.930301	1.778067
51	1	0	-3.187425	-0.682772	2.717338
52	1	0	-3.900031	-2.297348	2.538802

53	6	0	-3.304076	1.675546	-1.744329
54	1	0	-3.169186	2.498689	-1.036190
55	1	0	-2.323921	1.370266	-2.112394
56	1	0	-3.880881	2.044710	-2.595562
57	1	0	2.207908	4.232144	0.400241

Structure 21c (vacuum)

Energy (Hartrees): = -1191.3849118
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.438425	-2.612021	-1.286772
2	6	0	-4.651979	3.694202	-0.521607
3	6	0	1.168290	0.327163	0.084466
4	6	0	-2.206850	3.187269	-0.202851
5	6	0	-3.523525	2.714557	-0.341096
6	6	0	-3.736931	1.362679	-0.289273
7	6	0	-2.680348	0.427193	-0.117913
8	6	0	-1.335392	0.905739	-0.016710
9	6	0	-1.157119	2.321140	-0.032566
10	6	0	-4.360475	-1.562853	-0.167528
11	6	0	-4.874846	-2.119213	1.167619
12	6	0	-2.962403	-0.982686	-0.020757
13	6	0	-1.920097	-1.828441	0.254637
14	6	0	-0.577749	-1.367949	0.320791
15	6	0	-0.253900	-0.033094	0.153539
16	1	0	1.418038	1.331652	-0.214622
17	1	0	-4.755768	1.013533	-0.361089
18	1	0	-1.240275	-3.548074	0.596612
19	1	0	-5.478234	-2.917257	-1.430065
20	8	0	0.105004	2.825883	0.153268
21	1	0	-4.696894	4.396847	0.314476
22	1	0	-5.611468	3.180630	-0.585996
23	1	0	-4.517457	4.278093	-1.435988
24	8	0	0.324595	-2.338919	0.535868
25	1	0	-4.072163	-2.198279	-2.229029
26	1	0	-3.849876	-3.495663	-1.044488
27	8	0	-2.111248	-3.159752	0.437511
28	1	0	-5.037313	-0.764450	-0.462696
29	1	0	-5.899925	-2.481258	1.053749
30	1	0	-4.867257	-1.344203	1.937542
31	1	0	-4.251518	-2.948417	1.503872
32	1	0	1.223735	-1.884615	0.595047
33	1	0	0.047469	3.784674	0.179308
34	7	0	2.068770	-0.550739	0.347689
35	7	0	3.430089	-0.262555	0.307236
36	6	0	4.049570	-1.161763	-0.695126
37	6	0	3.810014	1.158836	0.228268
38	6	0	5.566724	-1.012167	-0.682475
39	1	0	3.682517	-0.867784	-1.695302
40	6	0	5.336507	1.283010	0.197738
41	1	0	3.416023	1.614949	-0.697808
42	6	0	5.978415	0.436922	-0.889937
43	1	0	5.979970	-1.655941	-1.463098
44	1	0	5.946075	-1.374769	0.279945
45	1	0	5.583434	2.340469	0.072792
46	1	0	5.722624	0.970668	1.174789
47	1	0	7.065586	0.542489	-0.866247
48	1	0	5.640572	0.777696	-1.875657
49	6	0	3.306384	1.920571	1.460131
50	1	0	3.781404	2.903611	1.489708
51	1	0	2.229499	2.071083	1.492735
52	1	0	3.602659	1.368580	2.354782
53	6	0	3.660694	-2.614478	-0.431908
54	1	0	3.827429	-2.852455	0.621798
55	1	0	2.620805	-2.821793	-0.678641
56	1	0	4.287656	-3.270023	-1.039583
57	1	0	-2.015519	4.257665	-0.208517

Structure 21c ($CHCl_3$)

Energy (Hartrees): = -1191.4115246
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.450665	-2.603337	-1.289342

2	6	0	-4.644679	3.697774	-0.547848
3	6	0	1.168738	0.330578	0.089165
4	6	0	-2.205280	3.191768	-0.192083
5	6	0	-3.519742	2.717087	-0.353743
6	6	0	-3.736624	1.363833	-0.308077
7	6	0	-2.681371	0.427660	-0.121872
8	6	0	-1.336910	0.907292	-0.008595
9	6	0	-1.156702	2.324722	-0.010996
10	6	0	-4.362855	-1.563104	-0.163455
11	6	0	-4.872540	-2.127709	1.169556
12	6	0	-2.962742	-0.983777	-0.021000
13	6	0	-1.919040	-1.829294	0.255061
14	6	0	-0.576768	-1.368099	0.324517
15	6	0	-0.254464	-0.031913	0.161306
16	1	0	1.418275	1.334990	-0.210935
17	1	0	-4.755063	1.017048	-0.399254
18	1	0	-1.246624	-3.562250	0.593791
19	1	0	-5.493068	-2.901225	-1.432965
20	8	0	0.098964	2.820238	0.201057
21	1	0	-4.693998	4.404717	0.284783
22	1	0	-5.605318	3.186300	-0.619845
23	1	0	-4.499469	4.280090	-1.462126
24	8	0	0.329261	-2.335372	0.539271
25	1	0	-4.086598	-2.186902	-2.232089
26	1	0	-3.868200	-3.495152	-1.059192
27	8	0	-2.113187	-3.160621	0.435279
28	1	0	-5.042001	-0.762579	-0.445759
29	1	0	-5.901142	-2.482055	1.059039
30	1	0	-4.859567	-1.359134	1.946649
31	1	0	-4.256169	-2.964771	1.501049
32	1	0	1.229995	-1.874314	0.590958
33	1	0	0.054348	3.783405	0.231657
34	7	0	2.068007	-0.549030	0.351004
35	7	0	3.431029	-0.265988	0.314181
36	6	0	4.047510	-1.168985	-0.692389
37	6	0	3.810720	1.158152	0.224624
38	6	0	5.564033	-1.015038	-0.690224
39	1	0	3.672989	-0.874580	-1.688416
40	6	0	5.336381	1.286272	0.175718
41	1	0	3.402890	1.605929	-0.697781
42	6	0	5.969481	0.433680	-0.911807
43	1	0	5.971288	-1.663331	-1.470175
44	1	0	5.952944	-1.370209	0.271517
45	1	0	5.575557	2.344118	0.039000
46	1	0	5.736485	0.983853	1.150475
47	1	0	7.056726	0.541219	-0.896090
48	1	0	5.622827	0.766117	-1.897324
49	6	0	3.321369	1.924105	1.457706
50	1	0	3.743180	2.931826	1.439796
51	1	0	2.240042	2.022483	1.535498
52	1	0	3.683041	1.417429	2.355814
53	6	0	3.662522	-2.621389	-0.425828
54	1	0	3.833170	-2.866190	0.626358
55	1	0	2.622838	-2.833620	-0.672836
56	1	0	4.287907	-3.275326	-1.037605
57	1	0	-2.013083	4.261628	-0.187504

Structure 21c (DMSO)

Energy (Hartrees): = -1191.4053048
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.456589	-2.606257	-1.274611
2	6	0	-4.658676	3.689344	-0.533705
3	6	0	1.170722	0.334254	0.082120
4	6	0	-2.214709	3.190792	-0.205476
5	6	0	-3.529770	2.712193	-0.349270
6	6	0	-3.743649	1.357998	-0.297135
7	6	0	-2.683616	0.425484	-0.118396
8	6	0	-1.338536	0.908438	-0.018276
9	6	0	-1.161552	2.326990	-0.032941
10	6	0	-4.363438	-1.565769	-0.150062
11	6	0	-4.866974	-2.130184	1.184656
12	6	0	-2.962652	-0.986804	-0.014957
13	6	0	-1.915608	-1.830499	0.254364
14	6	0	-0.573159	-1.366398	0.313557
15	6	0	-0.253217	-0.029045	0.149294
16	1	0	1.424742	1.340765	-0.205836
17	1	0	-4.762629	1.009767	-0.377372
18	1	0	-1.232173	-3.555617	0.590707

19	1	0	-5.499719	-2.904404	-1.411265
20	8	0	0.094030	2.827398	0.155663
21	1	0	-4.705291	4.391852	0.302784
22	1	0	-5.617316	3.174052	-0.605336
23	1	0	-4.516309	4.278109	-1.444182
24	8	0	0.335091	-2.331324	0.522323
25	1	0	-4.099960	-2.189733	-2.220406
26	1	0	-3.872302	-3.497994	-1.048247
27	8	0	-2.103101	-3.162290	0.437191
28	1	0	-5.044584	-0.766254	-0.429217
29	1	0	-5.897411	-2.480294	1.078499
30	1	0	-4.848658	-1.362460	1.962773
31	1	0	-4.252345	-2.970212	1.512571
32	1	0	1.237792	-1.865924	0.559702
33	1	0	0.048656	3.792068	0.155544
34	7	0	2.067829	-0.550261	0.336528
35	7	0	3.431262	-0.269402	0.313586
36	6	0	4.054215	-1.158958	-0.703012
37	6	0	3.812948	1.157010	0.244320
38	6	0	5.570424	-1.006508	-0.687361
39	1	0	3.686516	-0.848143	-1.695830
40	6	0	5.338756	1.282968	0.209224
41	1	0	3.412433	1.615248	-0.675126
42	6	0	5.978486	0.444634	-0.885066
43	1	0	5.981366	-1.643992	-1.474188
44	1	0	5.953124	-1.376157	0.271696
45	1	0	5.578719	2.342336	0.088307
46	1	0	5.732382	0.967493	1.182742
47	1	0	7.065768	0.550420	-0.859593
48	1	0	5.638532	0.790939	-1.867983
49	6	0	3.315711	1.907658	1.483131
50	1	0	3.740196	2.914235	1.481020
51	1	0	2.233967	2.010569	1.552525
52	1	0	3.668232	1.389882	2.379021
53	6	0	3.666611	-2.614387	-0.460421
54	1	0	3.830868	-2.876913	0.588796
55	1	0	2.628627	-2.822905	-0.718037
56	1	0	4.296102	-3.258416	-1.078387
57	1	0	-2.025497	4.261345	-0.207768

Structure 21d (vacuum)

Energy (Hartrees): = -1191.3797528
Imaginary frequency -24.26

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.664015	-2.246219	1.360856
2	6	0	4.302073	3.969148	0.106024
3	6	0	-1.217608	0.065244	-0.001997
4	6	0	1.896413	3.237269	-0.005496
5	6	0	3.255092	2.888518	0.067609
6	6	0	3.584894	1.558063	0.085249
7	6	0	2.607621	0.528652	0.039908
8	6	0	1.225027	0.883892	-0.020477
9	6	0	0.919446	2.274745	-0.059238
10	6	0	4.452660	-1.304132	0.166175
11	6	0	4.969006	-1.919985	-1.141366
12	6	0	3.005057	-0.859754	0.032242
13	6	0	2.033637	-1.809847	-0.132915
14	6	0	0.651867	-1.470189	-0.198655
15	6	0	0.223948	-0.153787	-0.097025
16	1	0	-1.578325	1.054443	0.248263
17	1	0	4.633630	1.303448	0.112349
18	1	0	1.491428	-3.601028	-0.301742
19	1	0	5.732883	-2.433641	1.491753
20	8	0	-0.392957	2.650979	-0.173615
21	1	0	4.273546	4.573144	-0.804791
22	1	0	5.301621	3.544094	0.200001
23	1	0	4.137354	4.641389	0.951893
24	8	0	-0.164659	-2.517127	-0.319819
25	1	0	4.282979	-1.795282	2.279835
26	1	0	4.163179	-3.200843	1.209902
27	8	0	2.331996	-3.130335	-0.216410
28	1	0	5.063751	-0.428386	0.372011
29	1	0	6.024394	-2.185461	-1.039489
30	1	0	4.871399	-1.211467	-1.967106
31	1	0	4.408441	-2.821794	-1.390016
32	1	0	-1.120427	-2.146679	-0.321884
33	1	0	-0.430431	3.607999	-0.249974
34	7	0	-2.035152	-0.910662	-0.175785
35	7	0	-3.437781	-0.650602	-0.021077
36	6	0	-3.761511	-0.058164	1.290807

37	6	0	-3.926765	0.125302	-1.176635
38	6	0	-5.279233	0.076280	1.402775
39	1	0	-3.332445	0.955223	1.388970
40	6	0	-5.441087	0.291612	-1.067759
41	1	0	-3.462577	1.130435	-1.174232
42	6	0	-5.850519	0.910368	0.262941
43	1	0	-5.517671	0.520848	2.372933
44	1	0	-5.714404	-0.929112	1.381588
45	1	0	-5.783547	0.902368	-1.907663
46	1	0	-5.899240	-0.698448	-1.171357
47	1	0	-6.938554	0.976679	0.339188
48	1	0	-5.460008	1.933039	0.327957
49	6	0	-3.567613	-0.586473	-2.477157
50	1	0	-4.035187	-0.071420	-3.318967
51	1	0	-2.491835	-0.617246	-2.645960
52	1	0	-3.939811	-1.613045	-2.442486
53	6	0	-3.224777	-0.944498	2.410044
54	1	0	-3.603479	-1.960790	2.278805
55	1	0	-2.135667	-0.985067	2.424029
56	1	0	-3.564755	-0.564698	3.375715
57	1	0	1.609400	4.285726	-0.038202

Structure 21d ($CHCl_3$)

Energy (Hartrees): = -1191.4067223
Imaginary frequency -36.16

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.647484	-2.213622	1.399303
2	6	0	4.287989	3.976178	0.178044
3	6	0	-1.214738	0.071844	-0.029086
4	6	0	1.891847	3.241440	-0.042696
5	6	0	3.247502	2.892513	0.090128
6	6	0	3.582874	1.561848	0.116696
7	6	0	2.608691	0.530032	0.030522
8	6	0	1.227728	0.885559	-0.062788
9	6	0	0.918884	2.276383	-0.131849
10	6	0	4.450199	-1.306363	0.176259
11	6	0	4.979011	-1.961460	-1.106619
12	6	0	3.004144	-0.859928	0.021799
13	6	0	2.032394	-1.809367	-0.156738
14	6	0	0.652082	-1.467937	-0.242330
15	6	0	0.226345	-0.150483	-0.149584
16	1	0	-1.568598	1.053549	0.259004
17	1	0	4.631117	1.311919	0.186602
18	1	0	1.500056	-3.614429	-0.318145
19	1	0	5.713215	-2.415434	1.537733
20	8	0	-0.384495	2.637876	-0.315307
21	1	0	4.281191	4.597724	-0.721736
22	1	0	5.287161	3.554304	0.293242
23	1	0	4.093463	4.633137	1.030099
24	8	0	-0.170258	-2.511163	-0.365221
25	1	0	4.276554	-1.730135	2.306570
26	1	0	4.132103	-3.166401	1.281306
27	8	0	2.333981	-3.130256	-0.227851
28	1	0	5.064982	-0.428211	0.356403
29	1	0	6.036444	-2.213421	-0.988408
30	1	0	4.885773	-1.280957	-1.956756
31	1	0	4.431684	-2.876585	-1.336206
32	1	0	-1.124712	-2.130456	-0.366923
33	1	0	-0.435552	3.597052	-0.405141
34	7	0	-2.034956	-0.899190	-0.212069
35	7	0	-3.435355	-0.655280	-0.011928
36	6	0	-3.724690	-0.060056	1.310984
37	6	0	-3.960587	0.123256	-1.153951
38	6	0	-5.239149	0.066834	1.464885
39	1	0	-3.298245	0.953823	1.393283
40	6	0	-5.471121	0.289363	-1.001553
41	1	0	-3.493736	1.125833	-1.158494
42	6	0	-5.844878	0.900935	0.342888
43	1	0	-5.449249	0.511063	2.441766
44	1	0	-5.672978	-0.939827	1.457209
45	1	0	-5.833402	0.907143	-1.827933
46	1	0	-5.936381	-0.698330	-1.100206
47	1	0	-6.930972	0.959953	0.449201
48	1	0	-5.457814	1.925250	0.400690
49	6	0	-3.637502	-0.583822	-2.465909
50	1	0	-4.133337	-0.068050	-3.291594
51	1	0	-2.566985	-0.606041	-2.671502
52	1	0	-4.002845	-1.613749	-2.429045
53	6	0	-3.151252	-0.941416	2.414775
54	1	0	-3.521945	-1.963502	2.299138

55	1	0	-2.060734	-0.969948	2.405772
56	1	0	-3.470711	-0.564142	3.388902
57	1	0	1.603266	4.288102	-0.098892

Structure 21d (DMSO)

Energy (Hartrees): = -1191.4009163
Imaginary frequency -37.02

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.651709	-2.230064	1.385657
2	6	0	4.299705	3.968278	0.157731
3	6	0	-1.216015	0.075888	-0.007167
4	6	0	1.899578	3.240444	-0.034576
5	6	0	3.255704	2.887704	0.084868
6	6	0	3.589045	1.555794	0.111557
7	6	0	2.610731	0.526677	0.036801
8	6	0	1.229546	0.885471	-0.045986
9	6	0	0.922948	2.277507	-0.111434
10	6	0	4.450098	-1.310919	0.173053
11	6	0	4.976727	-1.952079	-1.116994
12	6	0	3.003637	-0.864415	0.025804
13	6	0	2.028954	-1.811170	-0.151771
14	6	0	0.648700	-1.466499	-0.229209
15	6	0	0.225487	-0.148622	-0.128481
16	1	0	-1.571892	1.052952	0.293885
17	1	0	4.637698	1.304382	0.171396
18	1	0	1.487046	-3.608453	-0.323172
19	1	0	5.718708	-2.427402	1.520272
20	8	0	-0.379627	2.641607	-0.281648
21	1	0	4.289058	4.581698	-0.747543
22	1	0	5.297822	3.543631	0.272681
23	1	0	4.108878	4.634536	1.003291
24	8	0	-0.176824	-2.506664	-0.355165
25	1	0	4.280811	-1.757245	2.298785
26	1	0	4.140860	-3.184314	1.259038
27	8	0	2.325092	-3.132680	-0.231823
28	1	0	5.064759	-0.434642	0.361383
29	1	0	6.034514	-2.203889	-1.002398
30	1	0	4.883185	-1.261687	-1.959415
31	1	0	4.429682	-2.865258	-1.356605
32	1	0	-1.129436	-2.115189	-0.359862
33	1	0	-0.430092	3.603990	-0.343111
34	7	0	-2.034733	-0.892787	-0.208183
35	7	0	-3.437226	-0.656050	-0.015853
36	6	0	-3.737526	-0.056662	1.304821
37	6	0	-3.954951	0.128822	-1.159714
38	6	0	-5.253705	0.058727	1.448152
39	1	0	-3.318840	0.959590	1.382391
40	6	0	-5.467496	0.284625	-1.020811
41	1	0	-3.493163	1.132641	-1.148520
42	6	0	-5.857369	0.888565	0.322205
43	1	0	-5.472781	0.502471	2.423137
44	1	0	-5.681281	-0.950939	1.439258
45	1	0	-5.824599	0.904179	-1.847968
46	1	0	-5.926569	-0.705301	-1.129275
47	1	0	-6.944841	0.937337	0.419458
48	1	0	-5.478851	1.915543	0.385153
49	6	0	-3.615038	-0.566081	-2.473546
50	1	0	-4.109356	-0.047983	-3.298589
51	1	0	-2.542682	-0.576664	-2.671989
52	1	0	-3.972568	-1.599585	-2.449244
53	6	0	-3.164202	-0.929468	2.414638
54	1	0	-3.527598	-1.955156	2.303245
55	1	0	-2.073191	-0.948949	2.412826
56	1	0	-3.492160	-0.549694	3.384913
57	1	0	1.613861	4.288009	-0.089680

Structure 21e (vacuum)

Energy (Hartrees): = -1191.3788168
Imaginary frequency -151.98

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.606563	-2.634654	-0.952929
2	6	0	-4.970558	3.475301	-0.047544
3	6	0	1.114201	0.516214	-0.211778

4	6	0	-2.480616	3.130600	-0.183398
5	6	0	-3.765321	2.574034	-0.068351
6	6	0	-3.873206	1.212734	0.024644
7	6	0	-2.743075	0.350074	0.011822
8	6	0	-1.430751	0.914934	-0.107928
9	6	0	-1.360754	2.338618	-0.203912
10	6	0	-4.282699	-1.740616	0.252565
11	6	0	-4.409618	-2.503537	1.579253
12	6	0	-2.921566	-1.076156	0.110629
13	6	0	-1.803870	-1.867078	0.074211
14	6	0	-0.499819	-1.319636	-0.051799
15	6	0	-0.277070	0.044776	-0.130083
16	1	0	1.281200	1.573577	-0.260877
17	1	0	-4.864994	0.796180	0.108250
18	1	0	-0.980520	-3.556694	0.113039
19	1	0	-5.616189	-3.041482	-0.852036
20	8	0	-0.133263	2.938473	-0.327555
21	1	0	-4.947334	4.136642	0.822749
22	1	0	-5.893422	2.896151	-0.008560
23	1	0	-5.001396	4.106096	-0.939680
24	8	0	0.476714	-2.243470	-0.062669
25	1	0	-4.560583	-2.060650	-1.881179
26	1	0	-3.905759	-3.465995	-1.024251
27	8	0	-1.885440	-3.219685	0.156098
28	1	0	-5.047669	-0.968548	0.275403
29	1	0	-5.425413	-2.893077	1.685743
30	1	0	-4.207386	-1.841166	2.423978
31	1	0	-3.713808	-3.340619	1.621490
32	1	0	1.343806	-1.732197	-0.111594
33	1	0	-0.269012	3.883079	-0.438425
34	7	0	2.079379	-0.330059	-0.247900
35	7	0	3.417265	0.018832	-0.323432
36	6	0	3.823036	1.156997	0.545143
37	6	0	4.160805	-1.263602	-0.183485
38	6	0	5.345919	1.233665	0.706024
39	1	0	3.371024	0.995465	1.537379
40	6	0	5.664934	-1.062862	-0.070376
41	1	0	3.816221	-1.760040	0.738633
42	6	0	6.001071	-0.091476	1.046654
43	1	0	5.545283	1.988827	1.470819
44	1	0	5.771099	1.610119	-0.232159
45	1	0	6.120478	-2.042750	0.093185
46	1	0	6.051256	-0.678672	-1.021746
47	1	0	7.081407	0.032721	1.152078
48	1	0	5.620110	-0.472014	2.001332
49	6	0	3.854204	-2.155172	-1.384528
50	1	0	2.794636	-2.388327	-1.475630
51	1	0	4.170545	-1.648499	-2.299388
52	1	0	4.404466	-3.094655	-1.296005
53	6	0	3.370579	2.520685	-0.017738
54	1	0	3.297051	2.462434	-1.105901
55	1	0	2.419218	2.866777	0.383197
56	1	0	4.114963	3.280857	0.228597
57	1	0	-2.365456	4.209440	-0.258679

Structure 21e ($CHCl_3$)

Energy (Hartrees): = -1191.4054445
Imaginary frequency -152.46

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.594856	-2.687534	-0.889330
2	6	0	-4.983101	3.457762	0.026734
3	6	0	1.109788	0.543564	-0.222792
4	6	0	-2.505736	3.120319	-0.258931
5	6	0	-3.778017	2.560059	-0.046921
6	6	0	-3.877719	1.198526	0.075132
7	6	0	-2.744226	0.340095	0.013272
8	6	0	-1.441201	0.911957	-0.160137
9	6	0	-1.383325	2.332453	-0.321452
10	6	0	-4.262540	-1.760989	0.288908
11	6	0	-4.373725	-2.491069	1.634356
12	6	0	-2.907285	-1.088735	0.121142
13	6	0	-1.782726	-1.870654	0.064263
14	6	0	-0.485227	-1.313037	-0.089412
15	6	0	-0.278256	0.053744	-0.181380
16	1	0	1.270004	1.603682	-0.203624
17	1	0	-4.862122	0.781874	0.226172
18	1	0	-0.951788	-3.566786	0.108785
19	1	0	-5.609116	-3.080412	-0.775642
20	8	0	-0.171776	2.916655	-0.559725
21	1	0	-4.869869	4.198752	0.822797

22	1	0	-5.890584	2.884706	0.220974
23	1	0	-5.119170	4.005036	-0.910263
24	8	0	0.502971	-2.223539	-0.104071
25	1	0	-4.548346	-2.143062	-1.835895
26	1	0	-3.905661	-3.530281	-0.942918
27	8	0	-1.855182	-3.223062	0.160874
28	1	0	-5.032624	-0.994214	0.293310
29	1	0	-5.381583	-2.898147	1.754454
30	1	0	-4.184656	-1.805415	2.464246
31	1	0	-3.662232	-3.314748	1.699741
32	1	0	1.365084	-1.697705	-0.172758
33	1	0	-0.301291	3.861791	-0.701738
34	7	0	2.080127	-0.294569	-0.287234
35	7	0	3.418044	0.058735	-0.311693
36	6	0	3.809413	1.124732	0.657033
37	6	0	4.161045	-1.234085	-0.251853
38	6	0	5.330810	1.192256	0.833518
39	1	0	3.350556	0.873834	1.626420
40	6	0	5.663503	-1.041047	-0.110224
41	1	0	3.806229	-1.790555	0.630736
42	6	0	5.988047	-0.153202	1.077392
43	1	0	5.520986	1.886737	1.655729
44	1	0	5.761496	1.640301	-0.070163
45	1	0	6.116468	-2.030854	-0.011480
46	1	0	6.059594	-0.589359	-1.027597
47	1	0	7.067656	-0.032667	1.195950
48	1	0	5.603758	-0.604363	1.999337
49	6	0	3.865511	-2.041634	-1.512576
50	1	0	2.808209	-2.280933	-1.623427
51	1	0	4.178874	-1.474589	-2.393327
52	1	0	4.424406	-2.980225	-1.486745
53	6	0	3.354304	2.528623	0.212614
54	1	0	3.321317	2.585106	-0.878292
55	1	0	2.386083	2.826350	0.612985
56	1	0	4.076968	3.268692	0.564002
57	1	0	-2.400845	4.195235	-0.382034

Structure 21e (DMSO)

Energy (Hartrees): = -1191.3992282
Imaginary frequency -152.93

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.599500	-2.680366	-0.877799
2	6	0	-5.002475	3.442793	-0.046958
3	6	0	1.108979	0.554869	-0.186612
4	6	0	-2.517846	3.118471	-0.269299
5	6	0	-3.791643	2.551601	-0.083309
6	6	0	-3.887785	1.189863	0.048102
7	6	0	-2.748139	0.337182	0.015264
8	6	0	-1.445022	0.914616	-0.142306
9	6	0	-1.390595	2.335458	-0.305120
10	6	0	-4.258374	-1.766666	0.306914
11	6	0	-4.357720	-2.510776	1.645112
12	6	0	-2.905590	-1.092028	0.132249
13	6	0	-1.778038	-1.870151	0.073859
14	6	0	-0.481830	-1.307726	-0.077422
15	6	0	-0.278595	0.060503	-0.157472
16	1	0	1.267814	1.614237	-0.135325
17	1	0	-4.874549	0.770633	0.176887
18	1	0	-0.936417	-3.556979	0.111685
19	1	0	-5.607029	-3.086741	-0.753117
20	8	0	-0.178706	2.924051	-0.519061
21	1	0	-5.103666	3.998109	-0.983543
22	1	0	-4.920360	4.178863	0.757452
23	1	0	-5.913874	2.864157	0.108740
24	8	0	0.508361	-2.215000	-0.098325
25	1	0	-4.576194	-2.121728	-1.817226
26	1	0	-3.900894	-3.513994	-0.954604
27	8	0	-1.842879	-3.222741	0.167281
28	1	0	-5.028972	-1.001161	0.330231
29	1	0	-5.367019	-2.912519	1.770244
30	1	0	-4.158452	-1.834598	2.480645
31	1	0	-3.651025	-3.339495	1.696609
32	1	0	1.368459	-1.684876	-0.172555
33	1	0	-0.310066	3.873247	-0.637749
34	7	0	2.079279	-0.280915	-0.279673
35	7	0	3.417166	0.070038	-0.305764
36	6	0	3.825186	1.105045	0.691871
37	6	0	4.160321	-1.225333	-0.287739
38	6	0	5.350045	1.177532	0.824981
39	1	0	3.398533	0.811458	1.663765

40	6	0	5.665349	-1.033549	-0.176203
41	1	0	3.824627	-1.797779	0.591550
42	6	0	6.017719	-0.170025	1.020684
43	1	0	5.560586	1.853335	1.657475
44	1	0	5.752732	1.647825	-0.080400
45	1	0	6.119982	-2.025074	-0.107471
46	1	0	6.039184	-0.562613	-1.093374
47	1	0	7.099757	-0.048032	1.112388
48	1	0	5.658792	-0.642206	1.942361
49	6	0	3.841852	-2.007473	-1.558419
50	1	0	2.783874	-2.249972	-1.655718
51	1	0	4.138313	-1.422442	-2.433711
52	1	0	4.405183	-2.943603	-1.561445
53	6	0	3.346251	2.519537	0.314081
54	1	0	3.282724	2.621273	-0.772422
55	1	0	2.387731	2.791411	0.753770
56	1	0	4.071907	3.251442	0.675838
57	1	0	-2.416310	4.193238	-0.398835

Structure 21f (vacuum)

Energy (Hartrees): = -1191.3788168
Imaginary frequency -151.93

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.409594	-2.503837	1.579126
2	6	0	4.970590	3.475288	-0.048216
3	6	0	-1.114197	0.516219	-0.211654
4	6	0	2.480594	3.130626	-0.183160
5	6	0	3.765332	2.574038	-0.068607
6	6	0	3.873233	1.212735	0.024315
7	6	0	2.743088	0.350090	0.011837
8	6	0	1.430745	0.914956	-0.107677
9	6	0	1.360721	2.338653	-0.203427
10	6	0	4.282716	-1.740598	0.252613
11	6	0	4.606619	-2.634364	-0.953070
12	6	0	2.921580	-1.076135	0.110714
13	6	0	1.803886	-1.867059	0.074329
14	6	0	0.499827	-1.319623	-0.051619
15	6	0	0.277069	0.044792	-0.129827
16	1	0	-1.281193	1.573577	-0.260917
17	1	0	4.865046	0.796161	0.107514
18	1	0	0.980551	-3.556684	0.113122
19	1	0	5.425453	-2.893206	1.685629
20	8	0	0.133189	2.938529	-0.326568
21	1	0	5.001114	4.106105	-0.940346
22	1	0	5.893457	2.896119	-0.009583
23	1	0	4.947693	4.136606	0.822103
24	8	0	-0.476697	-2.243462	-0.062530
25	1	0	4.207142	-1.841723	2.424000
26	1	0	3.713947	-3.341064	1.621074
27	8	0	1.885471	-3.219670	0.156143
28	1	0	5.047666	-0.968518	0.275738
29	1	0	5.616180	-3.041353	-0.852182
30	1	0	4.560792	-2.060129	-1.881185
31	1	0	3.905696	-3.465590	-1.024637
32	1	0	-1.343796	-1.732186	-0.111418
33	1	0	0.268907	3.883166	-0.437219
34	7	0	-2.079369	-0.330063	-0.247770
35	7	0	-3.417253	0.018820	-0.323514
36	6	0	-4.160783	-1.263623	-0.183575
37	6	0	-3.823115	1.156990	0.545004
38	6	0	-5.664925	-1.062913	-0.070594
39	1	0	-3.816254	-1.760025	0.738583
40	6	0	-5.346008	1.233631	0.705762
41	1	0	-3.371170	0.995515	1.537278
42	6	0	-6.001149	-0.091513	1.046399
43	1	0	-6.120463	-2.042807	0.092950
44	1	0	-6.051181	-0.678747	-1.022003
45	1	0	-5.545442	1.988829	1.470504
46	1	0	-5.771122	1.610037	-0.232472
47	1	0	-7.081493	0.032662	1.151775
48	1	0	-5.620218	-0.472026	2.001098
49	6	0	-3.370634	2.520674	-0.017896
50	1	0	-2.419463	2.866919	0.383364
51	1	0	-3.296684	2.462319	-1.106023
52	1	0	-4.115203	3.280789	0.228055
53	6	0	-3.854055	-2.155211	-1.384574
54	1	0	-4.170217	-1.648501	-2.299475
55	1	0	-2.794489	-2.388443	-1.475510
56	1	0	-4.404398	-3.094656	-1.296148
57	1	0	2.365420	4.209477	-0.258266

Structure 21f ($CHCl_3$)

Energy (Hartrees): = -1191.405452
Imaginary frequency -161.58

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.401622	-2.481612	1.607330
2	6	0	4.980304	3.463921	0.008550
3	6	0	-1.112553	0.533408	-0.231333
4	6	0	2.497781	3.125897	-0.226418
5	6	0	3.774959	2.565375	-0.048371
6	6	0	3.877840	1.203031	0.059972
7	6	0	2.744515	0.343640	0.009801
8	6	0	1.437757	0.913861	-0.144264
9	6	0	1.375070	2.337454	-0.275897
10	6	0	4.271277	-1.754918	0.261727
11	6	0	4.589187	-2.684017	-0.918509
12	6	0	2.912624	-1.085045	0.111575
13	6	0	1.789082	-1.869235	0.071369
14	6	0	0.489135	-1.314821	-0.071663
15	6	0	0.277341	0.051321	-0.165516
16	1	0	-1.277717	1.592285	-0.255547
17	1	0	4.864995	0.786409	0.191567
18	1	0	0.962252	-3.566930	0.124549
19	1	0	5.411007	-2.888586	1.714117
20	8	0	0.157909	2.927615	-0.466956
21	1	0	5.097419	4.017827	-0.927134
22	1	0	5.892200	2.890850	0.180727
23	1	0	4.881766	4.199369	0.811660
24	8	0	-0.495909	-2.228705	-0.080428
25	1	0	4.224533	-1.793738	2.438006
26	1	0	3.690863	-3.304917	1.684890
27	8	0	1.865363	-3.221306	0.168792
28	1	0	5.040374	-0.987265	0.253385
29	1	0	5.605866	-3.074105	-0.817449
30	1	0	4.528551	-2.142533	-1.866002
31	1	0	3.901510	-3.528614	-0.960305
32	1	0	-1.360869	-1.706047	-0.143535
33	1	0	0.284244	3.876418	-0.585350
34	7	0	-2.080018	-0.309810	-0.272854
35	7	0	-3.417532	0.040458	-0.319560
36	6	0	-4.160254	-1.250110	-0.220743
37	6	0	-3.813350	1.145234	0.602702
38	6	0	-5.662216	-1.054933	-0.078473
39	1	0	-3.801776	-1.781827	0.675311
40	6	0	-5.333927	1.209208	0.788080
41	1	0	-3.344883	0.942513	1.578600
42	6	0	-5.981875	-0.130570	1.082253
43	1	0	-6.113298	-2.041874	0.052306
44	1	0	-6.063596	-0.631884	-1.007104
45	1	0	-5.521707	1.930576	1.587394
46	1	0	-5.774045	1.623854	-0.126955
47	1	0	-7.061101	-0.011284	1.205441
48	1	0	-5.588226	-0.549600	2.015401
49	6	0	-3.374633	2.531509	0.091941
50	1	0	-2.400220	2.851773	0.458414
51	1	0	-3.364668	2.541707	-1.000808
52	1	0	-4.094669	3.281722	0.426955
53	6	0	-3.867268	-2.091002	-1.460073
54	1	0	-4.194189	-1.553236	-2.354106
55	1	0	-2.808203	-2.321903	-1.573134
56	1	0	-4.415180	-3.034674	-1.402536
57	1	0	2.388213	4.202774	-0.327346

Structure 21f (DMSO)

Energy (Hartrees): = -1191.3992282
Imaginary frequency -152.94

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.357867	-2.510655	1.645034
2	6	0	5.002519	3.442761	-0.047152
3	6	0	-1.108992	0.554842	-0.186538
4	6	0	2.517845	3.118488	-0.269210
5	6	0	3.791657	2.551605	-0.083387
6	6	0	3.887803	1.189858	0.047943

7	6	0	2.748149	0.337187	0.015197
8	6	0	1.445016	0.914626	-0.142264
9	6	0	1.390586	2.335481	-0.304983
10	6	0	4.258406	-1.766657	0.306783
11	6	0	4.599411	-2.680455	-0.877890
12	6	0	2.905611	-1.092020	0.132196
13	6	0	1.778052	-1.870143	0.073962
14	6	0	0.481838	-1.307724	-0.077287
15	6	0	0.278590	0.060503	-0.157368
16	1	0	-1.267849	1.614201	-0.135259
17	1	0	4.874574	0.770616	0.176637
18	1	0	0.936432	-3.556967	0.111924
19	1	0	5.367217	-2.912262	1.770183
20	8	0	0.178687	2.924119	-0.518738
21	1	0	4.920187	4.179341	0.756769
22	1	0	5.104054	3.997464	-0.984063
23	1	0	5.913831	2.864160	0.109218
24	8	0	-0.508348	-2.215007	-0.098141
25	1	0	4.158523	-1.834442	2.480521
26	1	0	3.651275	-3.339459	1.696602
27	8	0	1.842895	-3.222725	0.167480
28	1	0	5.029016	-1.001160	0.329950
29	1	0	5.606865	-3.087001	-0.753158
30	1	0	4.576238	-2.121835	-1.817331
31	1	0	3.900666	-3.513965	-0.954703
32	1	0	-1.368450	-1.684896	-0.172429
33	1	0	0.310049	3.873328	-0.637324
34	7	0	-2.079281	-0.280951	-0.279627
35	7	0	-3.417165	0.070006	-0.305782
36	6	0	-4.160336	-1.225355	-0.287763
37	6	0	-3.825225	1.105051	0.691801
38	6	0	-5.665365	-1.033535	-0.176323
39	1	0	-3.824709	-1.797778	0.591566
40	6	0	-5.350088	1.177538	0.824887
41	1	0	-3.398591	0.811507	1.663716
42	6	0	-6.017785	-0.170013	1.020551
43	1	0	-6.120036	-2.025046	-0.107633
44	1	0	-6.039126	-0.562573	-1.093510
45	1	0	-5.560632	1.853317	1.657401
46	1	0	-5.752767	1.647862	-0.080481
47	1	0	-7.099826	-0.048003	1.112195
48	1	0	-5.658917	-0.642202	1.942245
49	6	0	-3.346299	2.519538	0.313971
50	1	0	-2.387782	2.791436	0.753652
51	1	0	-3.282777	2.621248	-0.772536
52	1	0	-4.071961	3.251444	0.675714
53	6	0	-3.841813	-2.007553	-1.558393
54	1	0	-4.138433	-1.422657	-2.433722
55	1	0	-2.783798	-2.249872	-1.655739
56	1	0	-4.404985	-2.943778	-1.561293
57	1	0	2.416294	4.193265	-0.398651

Structure 22a (vacuum)

Energy (Hartrees): = -1191.3733217
Imaginary frequency -115.52

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.784083	-1.880032	-0.045187
2	6	0	-2.881431	-1.104897	0.158186
3	6	0	-2.734917	0.342095	0.062759
4	6	0	-1.445259	0.929233	-0.093011
5	6	0	-0.273703	0.070739	-0.191364
6	6	0	-0.448734	-1.336165	-0.219516
7	6	0	-4.221770	-1.771800	0.424647
8	6	0	-1.400009	2.342697	-0.189936
9	6	0	-2.534675	3.122655	-0.141359
10	6	0	-3.800974	2.544105	-0.010099
11	6	0	-3.877531	1.173446	0.089208
12	6	0	-4.171972	-2.739266	1.616576
13	6	0	-4.746294	-2.462497	-0.840957
14	6	0	-5.029515	3.414438	0.020493
15	6	0	1.062260	0.553563	-0.217160
16	1	0	1.249163	1.605940	-0.148924
17	1	0	-4.860226	0.731905	0.166109
18	1	0	-4.940863	-1.003678	0.703188
19	1	0	-5.181902	-3.093933	1.838724
20	1	0	-3.785357	-2.235557	2.505385
21	1	0	-3.540511	-3.600573	1.405594
22	1	0	-5.726479	-2.909119	-0.653450
23	1	0	-4.844997	-1.746028	-1.659972
24	1	0	-4.060701	-3.252106	-1.153177

25	8	0	-1.828827	-3.230883	-0.068781
26	1	0	-0.901617	-3.498367	-0.197466
27	8	0	0.490757	-2.186471	-0.345431
28	1	0	-5.936902	2.810270	0.044969
29	1	0	-5.074658	4.059893	-0.860358
30	1	0	-5.029274	4.060023	0.902895
31	8	0	-0.179487	2.956927	-0.351099
32	1	0	-0.330912	3.894583	-0.494502
33	7	0	2.080053	-0.261211	-0.317733
34	6	0	3.811851	1.194346	0.488680
35	6	0	4.133113	-1.260641	-0.078343
36	6	0	5.328117	1.274720	0.685907
37	1	0	3.331733	1.057414	1.471313
38	6	0	5.635792	-1.080933	0.082738
39	1	0	3.731205	-1.660610	0.867476
40	6	0	5.955311	-0.032409	1.134146
41	1	0	5.512939	2.076949	1.404699
42	1	0	5.780798	1.583765	-0.263476
43	1	0	6.059321	-2.053869	0.342864
44	1	0	6.065670	-0.783993	-0.880859
45	1	0	7.034381	0.083839	1.257570
46	1	0	5.546318	-0.338458	2.103770
47	7	0	3.452677	0.034452	-0.367338
48	1	0	1.779332	-1.263402	-0.374343
49	6	0	3.361310	2.528538	-0.147691
50	1	0	3.185282	2.388298	-1.216094
51	1	0	2.462142	2.945580	0.304990
52	1	0	4.149601	3.274991	-0.035676
53	6	0	3.856175	-2.248698	-1.212500
54	1	0	2.808372	-2.535748	-1.304784
55	1	0	4.180699	-1.807778	-2.157652
56	1	0	4.427975	-3.162093	-1.037252
57	1	0	-2.437554	4.203174	-0.220887

Structure 22a ($CHCl_3$)

Energy (Hartrees): = -1191.402163
Imaginary frequency -110.90

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.792426	-1.881703	-0.041002
2	6	0	-2.887813	-1.103192	0.165386
3	6	0	-2.735759	0.343698	0.065516
4	6	0	-1.444889	0.922012	-0.121580
5	6	0	-0.275460	0.058677	-0.217575
6	6	0	-0.454837	-1.346108	-0.228810
7	6	0	-4.232029	-1.765165	0.430806
8	6	0	-1.394287	2.335994	-0.251632
9	6	0	-2.523708	3.123100	-0.178544
10	6	0	-3.789015	2.553566	0.006887
11	6	0	-3.873648	1.183260	0.120098
12	6	0	-4.194489	-2.728750	1.625737
13	6	0	-4.756531	-2.457271	-0.833733
14	6	0	-5.008277	3.433512	0.079911
15	6	0	1.065663	0.543396	-0.234756
16	1	0	1.252738	1.596066	-0.161761
17	1	0	-4.857298	0.751790	0.236585
18	1	0	-4.950346	-0.994168	0.700647
19	1	0	-5.208503	-3.072936	1.847666
20	1	0	-3.807166	-2.228554	2.517111
21	1	0	-3.572398	-3.599844	1.423184
22	1	0	-5.739645	-2.898745	-0.647092
23	1	0	-4.854351	-1.743683	-1.656139
24	1	0	-4.077653	-3.252833	-1.147664
25	8	0	-1.843346	-3.233958	-0.056544
26	1	0	-0.917375	-3.509626	-0.187311
27	8	0	0.479652	-2.203718	-0.350815
28	1	0	-5.921671	2.837797	0.113610
29	1	0	-5.066196	4.097932	-0.786241
30	1	0	-4.982380	4.063609	0.973688
31	8	0	-0.180068	2.929542	-0.471309
32	1	0	-0.312757	3.873670	-0.615937
33	7	0	2.086883	-0.263523	-0.326455
34	6	0	3.803528	1.187650	0.528119
35	6	0	4.145938	-1.259481	-0.102220
36	6	0	5.316609	1.263731	0.747027
37	1	0	3.309639	1.024699	1.498486
38	6	0	5.644145	-1.074519	0.088069
39	1	0	3.732189	-1.689624	0.823869
40	6	0	5.939726	-0.052717	1.171795
41	1	0	5.486848	2.047522	1.489223
42	1	0	5.782384	1.598184	-0.187450

43	1	0	6.067137	-2.052597	0.329296
44	1	0	6.089307	-0.748345	-0.859080
45	1	0	7.016576	0.064476	1.313798
46	1	0	5.516198	-0.385425	2.126442
47	7	0	3.456645	0.041962	-0.359985
48	1	0	1.809262	-1.265881	-0.382048
49	6	0	3.359305	2.534162	-0.082506
50	1	0	3.212183	2.430448	-1.160241
51	1	0	2.447067	2.934945	0.359934
52	1	0	4.137780	3.283580	0.073030
53	6	0	3.893410	-2.210004	-1.271946
54	1	0	2.845400	-2.482282	-1.407353
55	1	0	4.250744	-1.751405	-2.197240
56	1	0	4.447226	-3.136356	-1.105177
57	1	0	-2.420487	4.200486	-0.281691

Structure 22a (DMSO)

Energy (Hartrees): = -1191.3967557
Imaginary frequency -104.11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.791433	-1.884119	-0.042262
2	6	0	-2.886388	-1.107018	0.173054
3	6	0	-2.736691	0.339701	0.064797
4	6	0	-1.446329	0.919484	-0.123458
5	6	0	-0.275087	0.057752	-0.220449
6	6	0	-0.454101	-1.346838	-0.238768
7	6	0	-4.228889	-1.764516	0.455752
8	6	0	-1.398750	2.333498	-0.262317
9	6	0	-2.530079	3.119043	-0.194544
10	6	0	-3.794676	2.546984	-0.008228
11	6	0	-3.877595	1.176573	0.112805
12	6	0	-4.177570	-2.736711	1.642320
13	6	0	-4.778673	-2.444242	-0.803946
14	6	0	-5.015574	3.424274	0.057413
15	6	0	1.066949	0.545604	-0.227540
16	1	0	1.252796	1.597364	-0.136014
17	1	0	-4.861341	0.743942	0.227808
18	1	0	-4.938190	-0.991713	0.743371
19	1	0	-5.189994	-3.077369	1.876002
20	1	0	-3.776861	-2.244221	2.532362
21	1	0	-3.561905	-3.609176	1.426061
22	1	0	-5.761178	-2.880676	-0.603224
23	1	0	-4.888039	-1.724189	-1.619501
24	1	0	-4.110669	-3.242223	-1.135726
25	8	0	-1.836127	-3.236042	-0.057634
26	1	0	-0.907775	-3.500410	-0.195761
27	8	0	0.477136	-2.205419	-0.370824
28	1	0	-5.927644	2.826184	0.087118
29	1	0	-5.068036	4.088878	-0.808830
30	1	0	-4.994151	4.055948	0.950166
31	8	0	-0.187612	2.925999	-0.487103
32	1	0	-0.320265	3.874799	-0.605866
33	7	0	2.089903	-0.256569	-0.329562
34	6	0	3.804322	1.178301	0.560948
35	6	0	4.153159	-1.252269	-0.129354
36	6	0	5.317469	1.253145	0.776154
37	1	0	3.314035	0.986991	1.527224
38	6	0	5.650900	-1.066847	0.061054
39	1	0	3.743380	-1.703076	0.788210
40	6	0	5.945529	-0.070722	1.168126
41	1	0	5.486583	2.020534	1.535403
42	1	0	5.779216	1.610718	-0.151917
43	1	0	6.075788	-2.050104	0.276395
44	1	0	6.092754	-0.716049	-0.878958
45	1	0	7.022442	0.046984	1.309257
46	1	0	5.525109	-0.427700	2.115217
47	7	0	3.458623	0.053348	-0.356414
48	1	0	1.821018	-1.258477	-0.394773
49	6	0	3.352608	2.537827	-0.012860
50	1	0	3.183272	2.461001	-1.089735
51	1	0	2.451279	2.929056	0.459374
52	1	0	4.135323	3.282223	0.144428
53	6	0	3.902903	-2.175770	-1.320427
54	1	0	2.853802	-2.435852	-1.472373
55	1	0	4.272948	-1.702151	-2.233274
56	1	0	4.447766	-3.109734	-1.167682
57	1	0	-2.430351	4.195929	-0.308054

Structure 22b (vacuum)

Energy (Hartrees): = -1191.3928566
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.883273	-1.840099	-0.318848
2	6	0	2.937768	-1.044977	-0.015821
3	6	0	2.716669	0.398788	0.086924
4	6	0	1.399966	0.933748	0.041981
5	6	0	0.259342	0.033758	-0.128757
6	6	0	0.506305	-1.354100	-0.390383
7	6	0	4.315563	-1.667119	0.146350
8	6	0	1.280495	2.341030	0.095846
9	6	0	2.379548	3.169164	0.211371
10	6	0	3.671631	2.643826	0.253843
11	6	0	3.817381	1.273721	0.188770
12	6	0	4.852452	-2.159809	-1.204247
13	6	0	4.333907	-2.782481	1.201949
14	6	0	4.859600	3.563604	0.357179
15	6	0	-1.075180	0.421082	0.022200
16	1	0	-1.345162	1.417656	0.337035
17	1	0	4.822124	0.877810	0.188725
18	1	0	4.999209	-0.905262	0.516270
19	1	0	5.856919	-2.574464	-1.085555
20	1	0	4.900087	-1.340075	-1.925022
21	1	0	4.201943	-2.937583	-1.607241
22	1	0	5.363438	-3.113088	1.362690
23	1	0	3.941607	-2.417700	2.153938
24	1	0	3.740523	-3.639571	0.888684
25	8	0	1.994729	-3.168833	-0.535866
26	1	0	1.078787	-3.463849	-0.686214
27	8	0	-0.375519	-2.217144	-0.619857
28	1	0	5.792770	2.999845	0.355907
29	1	0	4.820723	4.151150	1.278073
30	1	0	4.885683	4.264788	-0.480773
31	8	0	0.029127	2.896107	0.016053
32	1	0	0.121103	3.851980	-0.004501
33	7	0	-2.113152	-0.373487	-0.177145
34	6	0	-4.177042	0.095617	-1.200196
35	6	0	-4.033854	-0.755975	1.115917
36	6	0	-5.582966	0.624491	-0.926201
37	1	0	-4.257567	-0.939946	-1.577205
38	6	0	-5.438225	-0.232558	1.406909
39	1	0	-4.116423	-1.791365	0.737741
40	6	0	-6.293877	-0.192634	0.146305
41	1	0	-6.146974	0.615549	-1.862423
42	1	0	-5.497218	1.668208	-0.603130
43	1	0	-5.895108	-0.867938	2.169984
44	1	0	-5.345930	0.775029	1.827716
45	1	0	-7.278655	0.228552	0.361271
46	1	0	-6.452951	-1.213774	-0.218987
47	7	0	-3.412756	0.088798	0.068930
48	1	0	-1.932212	-1.341785	-0.466803
49	6	0	-3.467591	0.956330	-2.237411
50	1	0	-3.299483	1.958151	-1.832914
51	1	0	-2.505377	0.537815	-2.531849
52	1	0	-4.089525	1.040869	-3.130652
53	6	0	-3.176479	-0.749320	2.374902
54	1	0	-2.211749	-1.231670	2.216505
55	1	0	-3.001724	0.280712	2.696970
56	1	0	-3.695320	-1.280305	3.175197
57	1	0	2.228994	4.245517	0.249937

Structure 22b ($CHCl_3$)

Energy (Hartrees): = -1191.4216749
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.898838	-1.835027	-0.339662
2	6	0	2.949540	-1.036239	-0.027658
3	6	0	2.718048	0.405107	0.090291
4	6	0	1.395669	0.928271	0.039962
5	6	0	0.263330	0.019416	-0.137087
6	6	0	0.518229	-1.359917	-0.413519
7	6	0	4.331331	-1.652181	0.133936
8	6	0	1.261323	2.337545	0.087572
9	6	0	2.351880	3.174950	0.221648
10	6	0	3.648922	2.659320	0.285151

11	6	0	3.810917	1.290236	0.213450
12	6	0	4.869835	-2.154862	-1.211693
13	6	0	4.356672	-2.758017	1.198678
14	6	0	4.824417	3.590231	0.422287
15	6	0	-1.076177	0.399517	0.040937
16	1	0	-1.338602	1.386149	0.392560
17	1	0	4.820746	0.906611	0.227656
18	1	0	5.015145	-0.885634	0.491813
19	1	0	5.878917	-2.558444	-1.090165
20	1	0	4.912481	-1.343273	-1.942661
21	1	0	4.230106	-2.944042	-1.611014
22	1	0	5.387175	-3.088000	1.357203
23	1	0	3.971563	-2.387507	2.152225
24	1	0	3.762543	-3.620801	0.899405
25	8	0	2.021951	-3.163206	-0.564168
26	1	0	1.108846	-3.469000	-0.717523
27	8	0	-0.357669	-2.228975	-0.655320
28	1	0	5.766704	3.041883	0.386455
29	1	0	4.783023	4.132230	1.371209
30	1	0	4.831211	4.334066	-0.378849
31	8	0	0.009618	2.874869	-0.020576
32	1	0	0.081206	3.836304	-0.037996
33	7	0	-2.114183	-0.383153	-0.165901
34	6	0	-4.165458	0.141345	-1.189445
35	6	0	-4.050098	-0.807014	1.093084
36	6	0	-5.568353	0.672649	-0.905624
37	1	0	-4.249678	-0.879286	-1.600464
38	6	0	-5.452480	-0.283489	1.392569
39	1	0	-4.135469	-1.821200	0.665223
40	6	0	-6.295508	-0.180532	0.127184
41	1	0	-6.122943	0.703805	-1.846947
42	1	0	-5.477471	1.702723	-0.541741
43	1	0	-5.920707	-0.949761	2.121682
44	1	0	-5.357264	0.703844	1.859147
45	1	0	-7.276928	0.243602	0.352617
46	1	0	-6.462016	-1.183677	-0.282272
47	7	0	-3.412580	0.081837	0.089230
48	1	0	-1.954172	-1.340763	-0.494590
49	6	0	-3.440903	1.031950	-2.189255
50	1	0	-3.261982	2.019082	-1.752773
51	1	0	-2.483389	0.613768	-2.502451
52	1	0	-4.059852	1.156235	-3.080549
53	6	0	-3.205912	-0.863519	2.358790
54	1	0	-2.245548	-1.354040	2.193221
55	1	0	-3.020931	0.147842	2.732330
56	1	0	-3.740254	-1.422797	3.129745
57	1	0	2.189295	4.249351	0.255137

Structure 22b (DMSO)

Energy (Hartrees): = -1191.4163264
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.905282	-1.838451	-0.328467
2	6	0	2.954975	-1.035523	-0.022316
3	6	0	2.717849	0.405302	0.095273
4	6	0	1.393044	0.924257	0.042358
5	6	0	0.262878	0.011139	-0.129092
6	6	0	0.521079	-1.369025	-0.393909
7	6	0	4.341837	-1.642965	0.126456
8	6	0	1.255500	2.334503	0.082554
9	6	0	2.343362	3.175818	0.216807
10	6	0	3.641730	2.663274	0.287676
11	6	0	3.808516	1.293927	0.220155
12	6	0	4.873431	-2.130632	-1.226822
13	6	0	4.383641	-2.755971	1.182407
14	6	0	4.814597	3.596957	0.424155
15	6	0	-1.079337	0.390916	0.045245
16	1	0	-1.342033	1.381301	0.385337
17	1	0	4.819985	0.914513	0.240205
18	1	0	5.024076	-0.874943	0.483395
19	1	0	5.887429	-2.524781	-1.116501
20	1	0	4.903679	-1.312236	-1.951140
21	1	0	4.238413	-2.922843	-1.628413
22	1	0	5.417570	-3.080801	1.328085
23	1	0	4.007275	-2.394416	2.143133
24	1	0	3.791085	-3.620339	0.884000
25	8	0	2.027745	-3.165895	-0.555242
26	1	0	1.111288	-3.465414	-0.702256
27	8	0	-0.351111	-2.244517	-0.622333

28	1	0	5.757167	3.048436	0.400774
29	1	0	4.764173	4.149443	1.366531
30	1	0	4.824003	4.333341	-0.383710
31	8	0	0.004758	2.868495	-0.034308
32	1	0	0.075820	3.831242	-0.039984
33	7	0	-2.116828	-0.391226	-0.151977
34	6	0	-4.158695	0.131426	-1.194147
35	6	0	-4.061685	-0.799435	1.096392
36	6	0	-5.561844	0.667939	-0.924361
37	1	0	-4.239929	-0.893050	-1.594186
38	6	0	-5.465124	-0.271885	1.381510
39	1	0	-4.143651	-1.814768	0.672591
40	6	0	-6.298190	-0.175868	0.109183
41	1	0	-6.108616	0.692322	-1.870409
42	1	0	-5.472196	1.701061	-0.568144
43	1	0	-5.938535	-0.934147	2.110827
44	1	0	-5.373190	0.718095	1.843685
45	1	0	-7.279957	0.252978	0.324237
46	1	0	-6.463199	-1.181385	-0.294616
47	7	0	-3.414709	0.083320	0.091695
48	1	0	-1.966718	-1.353332	-0.470478
49	6	0	-3.426269	1.012252	-2.196083
50	1	0	-3.256138	2.006369	-1.771430
51	1	0	-2.464232	0.592448	-2.493830
52	1	0	-4.036209	1.121505	-3.095485
53	6	0	-3.227597	-0.847224	2.368628
54	1	0	-2.267775	-1.343034	2.214458
55	1	0	-3.041560	0.166662	2.735378
56	1	0	-3.770255	-1.398241	3.139747
57	1	0	2.177993	4.250295	0.243614

Structure 22c (vacuum)

Energy (Hartrees): = -1191.3733218
Imaginary frequency -115.43

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.784041	-1.880059	-0.045199
2	6	0	2.881345	-1.104943	0.158443
3	6	0	2.734878	0.342051	0.062920
4	6	0	1.445250	0.929219	-0.092926
5	6	0	0.273685	0.070748	-0.191357
6	6	0	0.448700	-1.336158	-0.219588
7	6	0	4.221699	-1.771742	0.425051
8	6	0	1.400051	2.342667	-0.190000
9	6	0	2.534746	3.122591	-0.141441
10	6	0	3.801019	2.544007	-0.010100
11	6	0	3.877525	1.173349	0.089326
12	6	0	4.746873	-2.461431	-0.840841
13	6	0	4.171763	-2.740116	1.616236
14	6	0	5.029601	3.414286	0.020479
15	6	0	-1.062262	0.553603	-0.217026
16	1	0	-1.249141	1.605967	-0.148524
17	1	0	4.860201	0.731762	0.166275
18	1	0	4.940440	-1.003594	0.704449
19	1	0	5.726948	-2.908242	-0.653206
20	1	0	4.845969	-1.744362	-1.659283
21	1	0	4.061387	-3.250782	-1.153966
22	1	0	5.181850	-3.093927	1.839030
23	1	0	3.783830	-2.237462	2.505069
24	1	0	3.541362	-3.601900	1.404066
25	8	0	1.828785	-3.230901	-0.068966
26	1	0	0.901575	-3.498369	-0.197685
27	8	0	-0.490793	-2.186436	-0.345595
28	1	0	5.936968	2.810080	0.044835
29	1	0	5.029455	4.059777	0.902949
30	1	0	5.074711	4.059827	-0.860309
31	8	0	0.179550	2.956910	-0.351278
32	1	0	0.331012	3.894527	-0.494895
33	7	0	-2.080083	-0.261113	-0.317813
34	6	0	-4.133118	-1.260602	-0.078525
35	6	0	-3.811920	1.194303	0.488880
36	6	0	-5.635803	-1.080947	0.082553
37	1	0	-3.731214	-1.660701	0.867242
38	6	0	-5.328194	1.274611	0.686092
39	1	0	-3.331828	1.057236	1.471510
40	6	0	-5.955373	-0.032601	1.134118
41	1	0	-6.059337	-2.053934	0.342483
42	1	0	-6.065645	-0.783832	-0.881006
43	1	0	-5.513049	2.076723	1.405004
44	1	0	-5.780867	1.583791	-0.263250
45	1	0	-7.034451	0.083609	1.257513

46	1	0	-5.546411	-0.338776	2.103714
47	7	0	-3.452708	0.034551	-0.367321
48	1	0	-1.779426	-1.263293	-0.374602
49	6	0	-3.856152	-2.248496	-1.212820
50	1	0	-4.180751	-1.807486	-2.157905
51	1	0	-2.808333	-2.535465	-1.305184
52	1	0	-4.427882	-3.161952	-1.037663
53	6	0	-3.361423	2.528624	-0.147233
54	1	0	-2.462155	2.945514	0.305384
55	1	0	-3.185610	2.388650	-1.215708
56	1	0	-4.149663	3.275078	-0.034855
57	1	0	2.437668	4.203106	-0.221072

Structure 22c ($CHCl_3$)

Energy (Hartrees): = -1191.402163
Imaginary frequency -110.94

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.792426	-1.881705	-0.040967
2	6	0	2.887816	-1.103192	0.165401
3	6	0	2.735761	0.343696	0.065517
4	6	0	1.444888	0.922012	-0.121552
5	6	0	0.275457	0.058676	-0.217532
6	6	0	0.454835	-1.346110	-0.228751
7	6	0	4.232038	-1.765157	0.430804
8	6	0	1.394288	2.335999	-0.251569
9	6	0	2.523715	3.123099	-0.178507
10	6	0	3.789027	2.553557	0.006867
11	6	0	3.873657	1.183252	0.120065
12	6	0	4.756576	-2.457146	-0.833783
13	6	0	4.194509	-2.728842	1.625655
14	6	0	5.008299	3.433496	0.079828
15	6	0	-1.065667	0.543394	-0.234756
16	1	0	-1.252745	1.596067	-0.161824
17	1	0	4.857307	0.751773	0.236526
18	1	0	4.950326	-0.994162	0.700728
19	1	0	5.739667	-2.898676	-0.647147
20	1	0	4.854457	-1.743475	-1.656111
21	1	0	4.077682	-3.252650	-1.147828
22	1	0	5.208553	-3.072873	1.847683
23	1	0	3.806993	-2.228781	2.517021
24	1	0	3.572585	-3.600024	1.422964
25	8	0	1.843350	-3.233959	-0.056514
26	1	0	0.917378	-3.509630	-0.187265
27	8	0	-0.479655	-2.203723	-0.350731
28	1	0	5.921673	2.837764	0.113780
29	1	0	4.982309	4.063813	0.973446
30	1	0	5.066345	4.097702	-0.786481
31	8	0	0.180062	2.929561	-0.471176
32	1	0	0.312747	3.873697	-0.615748
33	7	0	-2.086887	-0.263530	-0.326420
34	6	0	-4.145949	-1.259481	-0.102244
35	6	0	-3.803552	1.187648	0.528107
36	6	0	-5.644161	-1.074520	0.088008
37	1	0	-3.732224	-1.689619	0.823858
38	6	0	-5.316639	1.263728	0.746981
39	1	0	-3.309683	1.024692	1.498483
40	6	0	-5.939769	-0.052720	1.171729
41	1	0	-6.067157	-2.052599	0.329223
42	1	0	-6.089300	-0.748346	-0.859152
43	1	0	-5.486893	2.047517	1.489176
44	1	0	-5.782392	1.598186	-0.187506
45	1	0	-7.016623	0.064475	1.313700
46	1	0	-5.516270	-0.385433	2.126387
47	7	0	-3.456648	0.041961	-0.359995
48	1	0	-1.809266	-1.265892	-0.381958
49	6	0	-3.893389	-2.210008	-1.271959
50	1	0	-4.250687	-1.751409	-2.197266
51	1	0	-2.845376	-2.482294	-1.407329
52	1	0	-4.447218	-3.136355	-1.105206
53	6	0	-3.359319	2.534161	-0.082506
54	1	0	-2.447085	2.934942	0.359945
55	1	0	-3.212183	2.430450	-1.160240
56	1	0	-4.137795	3.283580	0.073021
57	1	0	2.420491	4.200488	-0.281622

Structure 22c (DMSO)

Energy (Hartrees): = -1191.3967557
Imaginary frequency -104.11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.791437	-1.884118	-0.042263
2	6	0	2.886392	-1.107015	0.173049
3	6	0	2.736692	0.339703	0.064797
4	6	0	1.446329	0.919485	-0.123453
5	6	0	0.275088	0.057752	-0.220441
6	6	0	0.454103	-1.346839	-0.238762
7	6	0	4.228895	-1.764513	0.455737
8	6	0	1.398747	2.333499	-0.262310
9	6	0	2.530074	3.119046	-0.194536
10	6	0	3.794673	2.546988	-0.008223
11	6	0	3.877595	1.176577	0.112806
12	6	0	4.778670	-2.444244	-0.803962
13	6	0	4.177584	-2.736704	1.642311
14	6	0	5.015570	3.424280	0.057420
15	6	0	-1.066949	0.545603	-0.227529
16	1	0	-1.252796	1.597362	-0.135997
17	1	0	4.861342	0.743949	0.227807
18	1	0	4.938200	-0.991710	0.743347
19	1	0	5.761178	-2.880675	-0.603246
20	1	0	4.888026	-1.724196	-1.619522
21	1	0	4.110666	-3.242229	-1.135732
22	1	0	5.190009	-3.077366	1.875982
23	1	0	3.776887	-2.244209	2.532354
24	1	0	3.561913	-3.609167	1.426060
25	8	0	1.836132	-3.236041	-0.057635
26	1	0	0.907779	-3.500409	-0.195759
27	8	0	-0.477134	-2.205420	-0.370815
28	1	0	5.927640	2.826193	0.087127
29	1	0	4.994143	4.055957	0.950170
30	1	0	5.068032	4.088883	-0.808825
31	8	0	0.187608	2.925998	-0.487093
32	1	0	0.320260	3.874798	-0.605859
33	7	0	-2.089902	-0.256571	-0.329554
34	6	0	-4.153155	-1.252276	-0.129332
35	6	0	-3.804329	1.178306	0.560933
36	6	0	-5.650899	-1.066856	0.061061
37	1	0	-3.743379	-1.703067	0.788241
38	6	0	-5.317479	1.253151	0.776120
39	1	0	-3.314053	0.987011	1.527217
40	6	0	-5.945542	-0.070708	1.168109
41	1	0	-6.075784	-2.050110	0.276419
42	1	0	-6.092745	-0.716080	-0.878963
43	1	0	-5.486604	2.020554	1.535352
44	1	0	-5.779214	1.610706	-0.151965
45	1	0	-7.022457	0.046999	1.309223
46	1	0	-5.525135	-0.427667	2.115213
47	7	0	-3.458623	0.053340	-0.356410
48	1	0	-1.821014	-1.258477	-0.394773
49	6	0	-3.902890	-2.175794	-1.320390
50	1	0	-4.272917	-1.702183	-2.233248
51	1	0	-2.853792	-2.435893	-1.472316
52	1	0	-4.447768	-3.109750	-1.167641
53	6	0	-3.352614	2.537825	-0.012890
54	1	0	-2.451281	2.929057	0.459333
55	1	0	-3.183287	2.460988	-1.089766
56	1	0	-4.135326	3.282224	0.144398
57	1	0	2.430345	4.195931	-0.308044

Structure 22d (vacuum)

Energy (Hartrees): = -1191.3888113
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.050417	-1.794709	0.406005
2	6	0	2.978439	-0.906663	-0.026543
3	6	0	2.596768	0.503456	-0.141560
4	6	0	1.238098	0.892258	-0.005668
5	6	0	0.222328	-0.118979	0.276048
6	6	0	0.638394	-1.454240	0.593844
7	6	0	4.395544	-1.378624	-0.307068
8	6	0	0.955564	2.274823	-0.061134
9	6	0	1.942740	3.217825	-0.269194
10	6	0	3.278481	2.836673	-0.405314
11	6	0	3.582473	1.491969	-0.335623
12	6	0	4.442665	-2.550454	-1.298472

13	6	0	5.123655	-1.718806	1.000039
14	6	0	4.346076	3.880466	-0.603606
15	6	0	-1.147618	0.107681	0.156814
16	1	0	-1.502368	1.036205	-0.265520
17	1	0	4.622928	1.208415	-0.402347
18	1	0	4.936286	-0.566277	-0.790667
19	1	0	5.483022	-2.762597	-1.558685
20	1	0	3.906112	-2.300836	-2.216498
21	1	0	4.001869	-3.450721	-0.874527
22	1	0	6.155198	-2.017019	0.795001
23	1	0	5.140180	-0.857164	1.671719
24	1	0	4.619418	-2.542949	1.508037
25	8	0	2.326035	-3.092202	0.658843
26	1	0	1.466088	-3.476276	0.906956
27	8	0	-0.123862	-2.384681	0.940065
28	1	0	5.328094	3.420461	-0.717136
29	1	0	4.387735	4.563696	0.248580
30	1	0	4.146368	4.478160	-1.496563
31	8	0	-0.343127	2.686527	0.117200
32	1	0	-0.354031	3.646280	0.157061
33	7	0	-2.096330	-0.740481	0.523738
34	6	0	-3.917777	0.801115	0.736048
35	6	0	-3.778786	-0.801608	-1.146760
36	6	0	-5.436627	0.862508	0.582658
37	1	0	-3.490957	1.597337	0.099758
38	6	0	-5.292109	-0.724881	-1.334638
39	1	0	-3.300754	-0.030884	-1.779449
40	6	0	-5.857703	0.608522	-0.860453
41	1	0	-5.781884	1.842836	0.921439
42	1	0	-5.878244	0.107817	1.242688
43	1	0	-5.522077	-0.893582	-2.389976
44	1	0	-5.745205	-1.543092	-0.763749
45	1	0	-6.946250	0.618041	-0.952208
46	1	0	-5.474804	1.414590	-1.497308
47	7	0	-3.463440	-0.526777	0.273792
48	1	0	-1.818466	-1.636898	0.917196
49	6	0	-3.499013	1.038827	2.181391
50	1	0	-3.805596	0.190641	2.798168
51	1	0	-2.421412	1.171053	2.283174
52	1	0	-3.987560	1.939517	2.557814
53	6	0	-3.257821	-2.176545	-1.546918
54	1	0	-2.170189	-2.238238	-1.501689
55	1	0	-3.673475	-2.934966	-0.878327
56	1	0	-3.570924	-2.404103	-2.567501
57	1	0	1.671781	4.270515	-0.306410

Structure 22d ($CHCl_3$)

Energy (Hartrees): = -1191.41722
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.050667	-1.798128	0.393042
2	6	0	2.987596	-0.910002	-0.023443
3	6	0	2.606898	0.499544	-0.145999
4	6	0	1.245163	0.887545	-0.019307
5	6	0	0.226836	-0.124243	0.254817
6	6	0	0.638516	-1.457295	0.569442
7	6	0	4.409472	-1.383645	-0.283862
8	6	0	0.962642	2.273770	-0.080025
9	6	0	1.953114	3.215934	-0.278855
10	6	0	3.290807	2.833444	-0.409103
11	6	0	3.595953	1.488487	-0.336887
12	6	0	4.473279	-2.546906	-1.283793
13	6	0	5.120465	-1.734824	1.029061
14	6	0	4.358273	3.877393	-0.603696
15	6	0	-1.150149	0.110246	0.136439
16	1	0	-1.501087	1.039198	-0.287033
17	1	0	4.637373	1.206693	-0.400345
18	1	0	4.961719	-0.569630	-0.750431
19	1	0	5.518138	-2.754933	-1.530701
20	1	0	3.951672	-2.293306	-2.210207
21	1	0	4.030348	-3.455270	-0.877507
22	1	0	6.154279	-2.032446	0.832458
23	1	0	5.135019	-0.878430	1.708219
24	1	0	4.614367	-2.562256	1.531092
25	8	0	2.326126	-3.097914	0.644226
26	1	0	1.466200	-3.490085	0.883221
27	8	0	-0.127069	-2.391578	0.912101
28	1	0	5.342776	3.418878	-0.705578
29	1	0	4.389558	4.568270	0.243230
30	1	0	4.165452	4.470591	-1.501746

31	8	0	-0.332883	2.681705	0.085301
32	1	0	-0.359254	3.645598	0.102644
33	7	0	-2.096718	-0.732005	0.501196
34	6	0	-3.898640	0.842433	0.702385
35	6	0	-3.828301	-0.843896	-1.114670
36	6	0	-5.420432	0.913787	0.584929
37	1	0	-3.480270	1.601581	0.019858
38	6	0	-5.345283	-0.758845	-1.263340
39	1	0	-3.357746	-0.104384	-1.786274
40	6	0	-5.883861	0.600020	-0.833121
41	1	0	-5.742306	1.914146	0.886054
42	1	0	-5.855299	0.197120	1.290955
43	1	0	-5.603844	-0.969899	-2.304402
44	1	0	-5.792281	-1.546390	-0.645854
45	1	0	-6.974820	0.615227	-0.892404
46	1	0	-5.512195	1.372892	-1.516173
47	7	0	-3.471237	-0.512990	0.287158
48	1	0	-1.824275	-1.628560	0.898654
49	6	0	-3.445728	1.135950	2.126592
50	1	0	-3.747288	0.320876	2.789919
51	1	0	-2.365165	1.264423	2.206164
52	1	0	-3.917565	2.057751	2.473434
53	6	0	-3.332701	-2.239478	-1.471163
54	1	0	-2.243942	-2.308864	-1.469229
55	1	0	-3.726416	-2.968889	-0.757324
56	1	0	-3.685407	-2.508556	-2.468915
57	1	0	1.681034	4.268163	-0.309934

Structure 22d (DMSO)

Energy (Hartrees): = -1191.411896
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.100769	-1.822192	-0.219559
2	6	0	-3.021793	-0.868915	0.065417
3	6	0	-2.592787	0.532252	0.073821
4	6	0	-1.212423	0.866755	-0.021164
5	6	0	-0.217572	-0.200235	-0.154267
6	6	0	-0.667399	-1.546881	-0.335452
7	6	0	-4.474413	-1.257869	0.289697
8	6	0	-0.891396	2.247085	-0.046012
9	6	0	-1.859789	3.229947	0.034999
10	6	0	-3.213906	2.898527	0.122924
11	6	0	-3.557586	1.560695	0.139380
12	6	0	-4.650876	-2.366031	1.336862
13	6	0	-5.145869	-1.631598	-1.036923
14	6	0	-4.254754	3.983861	0.182904
15	6	0	1.166276	0.004498	-0.048555
16	1	0	1.547896	0.989524	0.174025
17	1	0	-4.609656	1.315839	0.176218
18	1	0	-4.998465	-0.393918	0.693550
19	1	0	-5.713989	-2.475044	1.568115
20	1	0	-4.129478	-2.114270	2.264187
21	1	0	-4.277445	-3.325671	0.982739
22	1	0	-6.203031	-1.860788	-0.876678
23	1	0	-5.080738	-0.810688	-1.756115
24	1	0	-4.666619	-2.510775	-1.474542
25	8	0	-2.406720	-3.129851	-0.371018
26	1	0	-1.543709	-3.559068	-0.518272
27	8	0	0.073742	-2.539855	-0.534453
28	1	0	-5.254476	3.562624	0.297507
29	1	0	-4.241029	4.589581	-0.727440
30	1	0	-4.067205	4.656602	1.023863
31	8	0	0.418787	2.611552	-0.169065
32	1	0	0.473841	3.574626	-0.207032
33	7	0	2.089038	-0.929247	-0.173018
34	6	0	3.940934	0.209211	-1.138169
35	6	0	3.787496	-0.159456	1.316819
36	6	0	5.454772	0.366069	-1.021124
37	1	0	3.477420	1.204864	-1.034926
38	6	0	5.301759	-0.007133	1.435544
39	1	0	3.331486	0.834629	1.457111
40	6	0	5.862398	0.899444	0.346639
41	1	0	5.793540	1.031909	-1.819122
42	1	0	5.916148	-0.614247	-1.189801
43	1	0	5.528688	0.387545	2.429377
44	1	0	5.756685	-1.002145	1.362467
45	1	0	6.950474	0.964650	0.424175
46	1	0	5.464944	1.912729	0.476163
47	7	0	3.468571	-0.669437	-0.039256
48	1	0	1.806952	-1.883200	-0.381329

49	6	0	3.565043	-0.389138	-2.486776
50	1	0	3.953340	-1.408748	-2.565636
51	1	0	2.485521	-0.416551	-2.643420
52	1	0	4.005754	0.210584	-3.286018
53	6	0	3.257853	-1.116398	2.375651
54	1	0	2.167877	-1.169189	2.381558
55	1	0	3.653474	-2.121367	2.202826
56	1	0	3.583577	-0.781832	3.362917
57	1	0	-1.552699	4.272816	0.009795

Structure 23 (vacuum)

Energy (Hartrees): = -1245.0083025
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.825275	-1.860108	-0.121103
2	6	0	-2.867445	-0.989817	0.054152
3	6	0	-2.581788	0.425996	0.053858
4	6	0	-1.233166	0.891025	-0.022652
5	6	0	-0.152888	-0.064917	-0.090045
6	6	0	-0.476801	-1.410157	-0.185583
7	6	0	-4.275069	-1.546381	0.194998
8	6	0	-1.042576	2.301078	-0.097055
9	6	0	-2.094059	3.181488	-0.043265
10	6	0	-3.418480	2.725128	0.059379
11	6	0	-3.639050	1.372677	0.099557
12	6	0	-4.404899	-2.522103	1.374271
13	6	0	-4.754449	-2.177451	-1.119518
14	6	0	-4.548690	3.718004	0.103055
15	6	0	1.263809	0.274481	0.020468
16	1	0	1.510924	1.298347	0.276634
17	1	0	-4.662873	1.033591	0.141770
18	1	0	-4.948952	-0.723182	0.420369
19	1	0	-5.457228	-2.780899	1.516054
20	1	0	-4.040639	-2.064485	2.296699
21	1	0	-3.845830	-3.439160	1.197934
22	1	0	-5.785909	-2.523369	-1.014990
23	1	0	-4.716511	-1.450988	-1.934513
24	1	0	-4.130673	-3.031205	-1.387008
25	8	0	-2.020664	-3.199354	-0.210893
26	1	0	-1.148724	-3.607394	-0.298747
27	8	0	0.423709	-2.389977	-0.302371
28	1	0	1.333165	-1.946148	-0.308892
29	1	0	-5.512735	3.213235	0.168130
30	1	0	-4.552012	4.345045	-0.792251
31	1	0	-4.452805	4.379511	0.967921
32	8	0	0.231951	2.781187	-0.249886
33	1	0	0.186995	3.733911	-0.366893
34	7	0	2.182916	-0.608988	-0.143322
35	1	0	-1.895073	4.248746	-0.102397
36	6	0	3.586603	-0.223230	-0.000392
37	6	0	3.926694	0.841404	-1.063688
38	1	0	3.351103	1.755249	-0.866419
39	1	0	3.624033	0.462841	-2.042689
40	6	0	3.850672	0.302969	1.424633
41	1	0	3.607666	-0.489760	2.143551
42	1	0	3.198850	1.153858	1.633684
43	6	0	4.386926	-1.512652	-0.251698
44	1	0	4.179535	-1.860833	-1.271465
45	1	0	4.033235	-2.278744	0.442509
46	8	0	5.312142	1.127060	-1.142562
47	1	0	5.563285	1.468324	-0.274174
48	8	0	5.177790	0.768641	1.604624
49	1	0	5.749781	0.003194	1.458470
50	8	0	5.780234	-1.371987	-0.031030
51	1	0	6.089254	-0.725946	-0.679317

Structure 23 ($CHCl_3$)

Energy (Hartrees): = -1245.0351186
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.811140	-1.859106	-0.133947
2	6	0	-2.860989	-0.996608	0.042751
3	6	0	-2.585946	0.422410	0.048557

4	6	0	-1.241728	0.896141	-0.056589
5	6	0	-0.153609	-0.050309	-0.127690
6	6	0	-0.465871	-1.399469	-0.208464
7	6	0	-4.264940	-1.564868	0.186189
8	6	0	-1.058360	2.307578	-0.156626
9	6	0	-2.111804	3.184431	-0.070538
10	6	0	-3.429115	2.719969	0.090677
11	6	0	-3.645684	1.365511	0.137927
12	6	0	-4.393044	-2.505987	1.392439
13	6	0	-4.731762	-2.239146	-1.111015
14	6	0	-4.558305	3.709818	0.186220
15	6	0	1.262086	0.300907	-0.002889
16	1	0	1.505730	1.322452	0.266348
17	1	0	-4.666270	1.025321	0.227349
18	1	0	-4.952487	-0.744666	0.376192
19	1	0	-5.442022	-2.782701	1.529104
20	1	0	-4.053559	-2.014645	2.307761
21	1	0	-3.814397	-3.418890	1.255695
22	1	0	-5.763699	-2.583938	-1.002484
23	1	0	-4.694701	-1.537399	-1.948086
24	1	0	-4.107608	-3.099874	-1.355048
25	8	0	-1.998535	-3.200569	-0.211566
26	1	0	-1.126998	-3.613676	-0.296409
27	8	0	0.445167	-2.370432	-0.317249
28	1	0	1.353083	-1.909554	-0.323970
29	1	0	-5.517668	3.204623	0.304409
30	1	0	-4.608100	4.332163	-0.711596
31	1	0	-4.416842	4.379040	1.039210
32	8	0	0.204950	2.779738	-0.367506
33	1	0	0.166648	3.735895	-0.489777
34	7	0	2.181067	-0.581907	-0.162630
35	1	0	-1.919711	4.251566	-0.149936
36	6	0	3.586702	-0.210564	0.005567
37	6	0	3.945974	0.866927	-1.036249
38	1	0	3.391563	1.788999	-0.820655
39	1	0	3.639265	0.512788	-2.023190
40	6	0	3.828368	0.291467	1.442083
41	1	0	3.577765	-0.511862	2.145889
42	1	0	3.174200	1.140046	1.653200
43	6	0	4.372545	-1.505695	-0.256247
44	1	0	4.186601	-1.828115	-1.288406
45	1	0	3.993380	-2.280820	0.414291
46	8	0	5.339755	1.128037	-1.108971
47	1	0	5.595497	1.468924	-0.241265
48	8	0	5.155756	0.754721	1.650038
49	1	0	5.732016	-0.010577	1.518648
50	8	0	5.765002	-1.392436	-0.000832
51	1	0	6.103832	-0.744671	-0.633118

Structure 23 (DMSO)

Energy (Hartrees): = -1245.0334552
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.789567	-1.858663	-0.148919
2	6	0	-2.847059	-1.012081	0.055095
3	6	0	-2.590974	0.410926	0.054078
4	6	0	-1.252412	0.903417	-0.041227
5	6	0	-0.152399	-0.029050	-0.123930
6	6	0	-0.449629	-1.380763	-0.229112
7	6	0	-4.242026	-1.593213	0.228186
8	6	0	-1.087039	2.318259	-0.124058
9	6	0	-2.154736	3.180086	-0.052284
10	6	0	-3.468690	2.695490	0.075449
11	6	0	-3.667247	1.337257	0.119661
12	6	0	-4.325782	-2.581932	1.398978
13	6	0	-4.748735	-2.218986	-1.077092
14	6	0	-4.614492	3.667876	0.135748
15	6	0	1.261531	0.332642	0.003327
16	1	0	1.502760	1.348575	0.294840
17	1	0	-4.685607	0.982526	0.178426
18	1	0	-4.923268	-0.784447	0.480430
19	1	0	-5.370999	-2.855474	1.567006
20	1	0	-3.946670	-2.129759	2.319215
21	1	0	-3.760319	-3.492283	1.203470
22	1	0	-5.772714	-2.579771	-0.947806
23	1	0	-4.747424	-1.484165	-1.886491
24	1	0	-4.123948	-3.063234	-1.374854
25	8	0	-1.958330	-3.201093	-0.248443
26	1	0	-1.079379	-3.594379	-0.347687
27	8	0	0.471483	-2.336242	-0.364205

28	1	0	1.376425	-1.855420	-0.361306
29	1	0	-5.567769	3.148256	0.240464
30	1	0	-4.653488	4.278871	-0.770362
31	1	0	-4.500106	4.351003	0.981668
32	8	0	0.171744	2.808592	-0.305567
33	1	0	0.124696	3.770469	-0.378758
34	7	0	2.180743	-0.545473	-0.179412
35	1	0	-1.976672	4.250497	-0.120867
36	6	0	3.588765	-0.190773	-0.002037
37	6	0	3.963009	0.898097	-1.025633
38	1	0	3.409806	1.818702	-0.803762
39	1	0	3.670276	0.557292	-2.021422
40	6	0	3.829273	0.284528	1.443031
41	1	0	3.548241	-0.522660	2.130839
42	1	0	3.200214	1.150187	1.659682
43	6	0	4.359168	-1.491641	-0.282921
44	1	0	4.158484	-1.801303	-1.316112
45	1	0	3.980963	-2.269225	0.385178
46	8	0	5.361007	1.156505	-1.073589
47	1	0	5.603419	1.464023	-0.189828
48	8	0	5.171059	0.700675	1.668777
49	1	0	5.720458	-0.075170	1.491893
50	8	0	5.758074	-1.392130	-0.044840
51	1	0	6.081366	-0.714110	-0.653082

Structure 24 (vacuum)

Energy (Hartrees): = -1245.011005
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.862295	-1.875238	-0.180198
2	6	0	-2.868409	-1.007718	0.085502
3	6	0	-2.577934	0.428247	0.065646
4	6	0	-1.238441	0.894145	-0.026685
5	6	0	-0.145063	-0.073580	-0.130477
6	6	0	-0.464200	-1.464753	-0.297336
7	6	0	-4.273534	-1.538041	0.319360
8	6	0	-1.052352	2.293367	-0.088574
9	6	0	-2.110958	3.179447	-0.043321
10	6	0	-3.425968	2.721325	0.039734
11	6	0	-3.636072	1.358266	0.090671
12	6	0	-4.328969	-2.613944	1.413991
13	6	0	-4.886378	-2.040991	-0.994689
14	6	0	-4.569193	3.700978	0.067676
15	6	0	1.202385	0.258587	-0.009416
16	1	0	1.476114	1.277015	0.220255
17	1	0	-4.658041	1.009523	0.119305
18	1	0	-4.890670	-0.719493	0.685948
19	1	0	-5.373096	-2.849241	1.635240
20	1	0	-3.859659	-2.254912	2.332552
21	1	0	-3.826382	-3.527770	1.103691
22	1	0	-5.910337	-2.385980	-0.829940
23	1	0	-4.905674	-1.247082	-1.745065
24	1	0	-4.300118	-2.873605	-1.387628
25	8	0	-2.045425	-3.207095	-0.306360
26	1	0	-1.150209	-3.563707	-0.443796
27	8	0	0.373413	-2.379864	-0.474360
28	1	0	-4.539988	4.362401	-0.801593
29	1	0	-4.522882	4.328271	0.961567
30	1	0	-5.528805	3.183671	0.068240
31	8	0	0.224202	2.785044	-0.210500
32	1	0	0.173387	3.738237	-0.319583
33	7	0	2.211491	-0.598419	-0.134824
34	1	0	-1.910039	4.247049	-0.092780
35	6	0	3.615570	-0.229624	0.008101
36	6	0	3.957250	0.862407	-1.027491
37	1	0	3.384061	1.772685	-0.810206
38	1	0	3.656132	0.507198	-2.015259
39	6	0	3.866592	0.256802	1.449613
40	1	0	3.652202	-0.566840	2.141430
41	1	0	3.181172	1.074824	1.682517
42	6	0	4.417726	-1.511183	-0.277355
43	1	0	4.236220	-1.822882	-1.314097
44	1	0	4.057637	-2.305355	0.382086
45	8	0	5.342722	1.145659	-1.094333
46	1	0	5.587565	1.494588	-0.227278
47	8	0	5.173466	0.767025	1.641835
48	1	0	5.773002	0.020316	1.514668
49	8	0	5.799730	-1.365124	-0.020291
50	1	0	6.121000	-0.703978	-0.647484
51	1	0	1.933563	-1.562163	-0.345455

Structure 24 ($CHCl_3$)

Energy (Hartrees): = -1245.0405081
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.869977	-1.869455	-0.203950
2	6	0	-2.873746	-0.998715	0.068454
3	6	0	-2.577522	0.436704	0.052497
4	6	0	-1.237106	0.892404	-0.085488
5	6	0	-0.150002	-0.079583	-0.206695
6	6	0	-0.473010	-1.466357	-0.358300
7	6	0	-4.274882	-1.534948	0.322192
8	6	0	-1.041790	2.291648	-0.178502
9	6	0	-2.089969	3.187307	-0.085556
10	6	0	-3.403011	2.739560	0.074643
11	6	0	-3.625572	1.377596	0.133502
12	6	0	-4.312424	-2.532476	1.488428
13	6	0	-4.874529	-2.138302	-0.954593
14	6	0	-4.531376	3.730213	0.182996
15	6	0	1.202549	0.253464	-0.066061
16	1	0	1.473637	1.265883	0.193943
17	1	0	-4.649106	1.042634	0.216160
18	1	0	-4.915925	-0.708386	0.620729
19	1	0	-5.349494	-2.806801	1.701145
20	1	0	-3.890434	-2.088757	2.393775
21	1	0	-3.756459	-3.440853	1.258585
22	1	0	-5.901387	-2.466428	-0.770910
23	1	0	-4.890984	-1.402081	-1.762381
24	1	0	-4.292173	-3.000489	-1.284731
25	8	0	-2.059590	-3.204601	-0.307413
26	1	0	-1.169340	-3.569496	-0.462693
27	8	0	0.358504	-2.388266	-0.547583
28	1	0	-4.482507	4.471976	-0.618085
29	1	0	-4.482591	4.270829	1.132661
30	1	0	-5.499841	3.231214	0.128270
31	8	0	0.226601	2.761370	-0.381297
32	1	0	0.190080	3.715725	-0.515419
33	7	0	2.211501	-0.592988	-0.193365
34	1	0	-1.882014	4.251994	-0.159341
35	6	0	3.613793	-0.229248	0.009677
36	6	0	3.972480	0.930670	-0.940729
37	1	0	3.413262	1.831802	-0.659875
38	1	0	3.678359	0.650343	-1.954607
39	6	0	3.813105	0.162427	1.486422
40	1	0	3.600302	-0.708817	2.117698
41	1	0	3.102847	0.950677	1.747384
42	6	0	4.424252	-1.488237	-0.339988
43	1	0	4.295834	-1.713389	-1.406320
44	1	0	4.031285	-2.330454	0.236170
45	8	0	5.364697	1.200483	-0.975958
46	1	0	5.602483	1.521392	-0.095931
47	8	0	5.104143	0.686864	1.750682
48	1	0	5.724810	-0.041301	1.614811
49	8	0	5.794483	-1.371800	-0.002953
50	1	0	6.155737	-0.679806	-0.573083
51	1	0	1.954821	-1.556923	-0.421932

Structure 24 (DMSO)

Energy (Hartrees): = -1245.0399931
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.856151	-1.875576	-0.210692
2	6	0	-2.858602	-1.017689	0.102240
3	6	0	-2.575166	0.419826	0.077596
4	6	0	-1.239671	0.888691	-0.059459
5	6	0	-0.144960	-0.074089	-0.189635
6	6	0	-0.461269	-1.458436	-0.366773
7	6	0	-4.257887	-1.544566	0.377262
8	6	0	-1.059673	2.291088	-0.149513
9	6	0	-2.120240	3.174241	-0.069676
10	6	0	-3.430670	2.710760	0.074539
11	6	0	-3.637987	1.346308	0.140671
12	6	0	-4.291102	-2.682902	1.405949

13	6	0	-4.944442	-1.953631	-0.931103
14	6	0	-4.572673	3.687570	0.154973
15	6	0	1.207877	0.266980	-0.039756
16	1	0	1.471172	1.276652	0.239951
17	1	0	-4.658409	0.996218	0.210832
18	1	0	-4.840278	-0.738941	0.821566
19	1	0	-5.330852	-2.896767	1.668383
20	1	0	-3.765472	-2.398287	2.321406
21	1	0	-3.839207	-3.595977	1.021422
22	1	0	-5.966004	-2.291909	-0.736978
23	1	0	-4.989255	-1.114030	-1.629879
24	1	0	-4.397717	-2.769841	-1.410262
25	8	0	-2.033916	-3.208086	-0.351187
26	1	0	-1.136445	-3.552087	-0.514072
27	8	0	0.371855	-2.374410	-0.577331
28	1	0	-4.525841	4.415049	-0.659164
29	1	0	-4.537791	4.248219	1.093539
30	1	0	-5.533266	3.173195	0.103081
31	8	0	0.203445	2.773046	-0.340063
32	1	0	0.161028	3.733058	-0.433334
33	7	0	2.218150	-0.572423	-0.179374
34	1	0	-1.925041	4.241318	-0.144623
35	6	0	3.624421	-0.214148	0.012658
36	6	0	4.006257	0.861188	-1.023939
37	1	0	3.449233	1.784477	-0.822718
38	1	0	3.725239	0.501287	-2.015967
39	6	0	3.819030	0.286088	1.456333
40	1	0	3.574026	-0.528925	2.147910
41	1	0	3.137196	1.115934	1.652031
42	6	0	4.414161	-1.511710	-0.228128
43	1	0	4.269587	-1.829870	-1.268236
44	1	0	4.016095	-2.290409	0.427596
45	8	0	5.403062	1.119854	-1.058024
46	1	0	5.627762	1.477164	-0.188795
47	8	0	5.128944	0.783019	1.692580
48	1	0	5.721294	0.027257	1.585115
49	8	0	5.792559	-1.383160	0.079443
50	1	0	6.142580	-0.727740	-0.538938
51	1	0	1.968225	-1.530135	-0.438872

Structure 25ab (vacuum)

Energy (Hartrees): = -2224.3850487
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.155216	2.550230	-0.614868
2	6	0	4.101679	2.900000	-1.417650
3	6	0	2.952637	2.032771	-1.432609
4	6	0	2.936958	0.827371	-0.658704
5	6	0	4.091025	0.468677	0.133141
6	6	0	5.155893	1.352398	0.148804
7	6	0	-3.962851	-5.374249	-1.569098
8	6	0	0.603469	-2.099011	-2.975774
9	6	0	4.196639	4.180364	-2.233752
10	6	0	1.732219	0.061016	-0.693763
11	6	0	0.639476	0.417416	-1.464803
12	6	0	0.681419	1.596927	-2.247450
13	6	0	1.812907	2.367224	-2.212626
14	6	0	5.338605	4.115026	-3.258521
15	6	0	4.305908	5.422641	-1.337724
16	6	0	-0.506185	1.974470	-3.093473
17	6	0	4.231964	-0.800353	0.865744
18	6	0	-4.216091	0.798770	0.726841
19	6	0	-0.573249	-0.453243	-1.465672
20	6	0	-0.604999	-1.655700	-2.192452
21	6	0	-1.764942	-2.403630	-2.174406
22	6	0	-2.913090	-2.013117	-1.457870
23	6	0	-2.889778	-0.808407	-0.704317
24	6	0	-1.692972	-0.057691	-0.736165
25	6	0	-4.205462	-4.086087	-2.366274
26	6	0	-5.531241	-4.146822	-3.138907
27	6	0	-4.099576	-2.870200	-1.460640
28	6	0	-5.090643	-2.598878	-0.577928
29	6	0	-5.125811	-1.384476	0.238667
30	6	0	-4.051261	-0.443421	0.107888
31	1	0	-3.494617	1.591539	0.602432
32	1	0	-1.764876	-3.336038	-2.720133
33	1	0	3.469185	-1.548210	0.732018
34	1	0	1.818309	3.265487	-2.810594
35	1	0	-6.714892	-2.914633	0.244521
36	1	0	-3.997530	-6.245400	-2.228545

37	1	0	3.280675	4.297397	-2.807776
38	8	0	-1.629689	1.104309	-0.022657
39	1	0	5.334668	5.017600	-3.875295
40	1	0	5.216619	3.251799	-3.916640
41	1	0	6.306799	4.039817	-2.764658
42	1	0	4.296444	6.325559	-1.953856
43	1	0	3.462554	5.472807	-0.645261
44	1	0	5.228777	5.409911	-0.758783
45	1	0	0.923439	-1.319019	-3.671498
46	1	0	0.384513	-3.004229	-3.542231
47	1	0	1.450764	-2.301984	-2.314418
48	8	0	6.267753	3.321718	-0.526502
49	1	0	6.871420	2.872927	0.080650
50	8	0	6.286098	1.165942	0.852934
51	1	0	6.170475	0.316504	1.367579
52	1	0	-0.285909	2.856839	-3.694418
53	1	0	-1.379950	2.188228	-2.470793
54	1	0	-0.784165	1.154462	-3.760543
55	8	0	1.648422	-1.071321	0.063999
56	8	0	-6.139785	-1.230550	0.958604
57	1	0	-2.987209	-5.351523	-1.077448
58	1	0	-4.732155	-5.490196	-0.802893
59	8	0	-6.168860	-3.391597	-0.406145
60	1	0	-3.430647	-4.008384	-3.127964
61	1	0	-5.473918	-4.940451	-3.888344
62	1	0	-5.720564	-3.203661	-3.656191
63	1	0	-6.371862	-4.352812	-2.479441
64	1	0	0.752846	-1.424415	-0.028609
65	1	0	-0.728189	1.447886	-0.084164
66	7	0	5.248502	-0.996376	1.629277
67	6	0	4.558849	-3.280112	2.042157
68	6	0	6.832663	-2.457242	2.472781
69	6	0	4.780955	-4.414170	3.039883
70	1	0	4.755523	-3.621460	1.009831
71	1	0	3.515017	-2.965092	2.095040
72	6	0	7.072309	-3.552694	3.501299
73	1	0	7.220484	-2.775319	1.490308
74	1	0	7.345856	-1.535973	2.751987
75	6	0	6.255752	-4.793200	3.146505
76	1	0	4.175610	-5.271306	2.735906
77	1	0	4.419097	-4.087778	4.019701
78	1	0	8.139971	-3.781007	3.538451
79	1	0	6.774510	-3.184882	4.488058
80	1	0	6.395304	-5.577756	3.893449
81	1	0	6.602962	-5.193414	2.186596
82	7	0	5.407138	-2.139321	2.366665
83	7	0	-5.243897	1.133575	1.489460
84	7	0	-5.327838	2.429001	2.013080
85	6	0	-6.508855	3.109744	1.464957
86	6	0	-5.372788	2.361776	3.479468
87	6	0	-6.569127	4.540655	1.987667
88	1	0	-7.427958	2.565887	1.744365
89	1	0	-6.423844	3.091737	0.377339
90	6	0	-5.400415	3.769736	4.061995
91	1	0	-6.264518	1.800491	3.809441
92	1	0	-4.488132	1.815973	3.810651
93	6	0	-6.591978	4.555926	3.515805
94	1	0	-7.452766	5.034872	1.577652
95	1	0	-5.688593	5.080747	1.626576
96	1	0	-5.440511	3.705738	5.151787
97	1	0	-4.468970	4.277243	3.793584
98	1	0	-6.579173	5.581796	3.889837
99	1	0	-7.522154	4.094943	3.868106
100	1	0	-5.978922	0.437992	1.654436

Structure 25ab ($CHCl_3$)

Energy (Hartrees): = -2224.4301114
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.149459	-2.571438	-0.628640
2	6	0	-4.082266	-2.924396	-1.413458
3	6	0	-2.935261	-2.052865	-1.417502
4	6	0	-2.933866	-0.841657	-0.652221
5	6	0	-4.099951	-0.481632	0.123452
6	6	0	-5.163863	-1.368713	0.128008
7	6	0	3.909759	5.405714	-1.560759
8	6	0	-0.600127	2.077791	-2.969370
9	6	0	-4.150267	-4.219151	-2.211259
10	6	0	-1.729680	-0.070390	-0.673493
11	6	0	-0.626348	-0.425383	-1.430085

12	6	0	-0.652923	-1.614195	-2.201223
13	6	0	-1.781970	-2.390019	-2.177706
14	6	0	-5.278777	-4.195882	-3.251642
15	6	0	-4.249802	-5.447235	-1.295502
16	6	0	0.546536	-2.003211	-3.023396
17	6	0	-4.262490	0.796102	0.840630
18	6	0	4.252048	-0.774805	0.726076
19	6	0	0.581042	0.454730	-1.433426
20	6	0	0.607012	1.648319	-2.177975
21	6	0	1.760972	2.406269	-2.168596
22	6	0	2.911247	2.034021	-1.443188
23	6	0	2.897419	0.835108	-0.679514
24	6	0	1.700753	0.078910	-0.694319
25	6	0	4.180463	4.120585	-2.352686
26	6	0	5.507668	4.205629	-3.118941
27	6	0	4.088754	2.903554	-1.445525
28	6	0	5.078569	2.644456	-0.556112
29	6	0	5.123738	1.434511	0.266594
30	6	0	4.064891	0.481624	0.129412
31	1	0	3.548509	-1.578655	0.571635
32	1	0	1.751924	3.331630	-2.726714
33	1	0	-3.521939	1.563709	0.692698
34	1	0	-1.773081	-3.293449	-2.768345
35	1	0	6.703307	2.991026	0.269278
36	1	0	3.931725	6.275804	-2.222760
37	1	0	-3.225856	-4.332033	-2.771620
38	8	0	1.648971	-1.061989	0.048601
39	1	0	-5.251814	-5.113466	-3.845989
40	1	0	-5.162824	-3.349256	-3.933038
41	1	0	-6.257688	-4.124724	-2.777419
42	1	0	-4.213536	-6.361304	-1.894844
43	1	0	-3.416151	-5.472727	-0.589036
44	1	0	-5.181384	-5.446659	-0.728896
45	1	0	-0.904138	1.298854	-3.673917
46	1	0	-0.387607	2.988412	-3.530477
47	1	0	-1.455226	2.271093	-2.314609
48	8	0	-6.257197	-3.350894	-0.551615
49	1	0	-6.881876	-2.913720	0.044938
50	8	0	-6.301946	-1.179918	0.818067
51	1	0	-6.187045	-0.329126	1.338485
52	1	0	0.341498	-2.907035	-3.597979
53	1	0	1.416120	-2.191423	-2.386274
54	1	0	0.822480	-1.204206	-3.716857
55	8	0	-1.670053	1.058912	0.084604
56	8	0	6.137379	1.294209	0.993561
57	1	0	2.931029	5.369605	-1.075060
58	1	0	4.670380	5.543015	-0.788362
59	8	0	6.147632	3.452539	-0.385539
60	1	0	3.411123	4.029954	-3.118008
61	1	0	5.436182	4.990923	-3.876590
62	1	0	5.723564	3.264182	-3.630489
63	1	0	6.343500	4.438832	-2.461433
64	1	0	-0.775431	1.424836	0.029532
65	1	0	0.748636	-1.416138	0.021505
66	7	0	-5.279224	0.972059	1.609385
67	6	0	-4.677441	3.286237	1.987083
68	6	0	-6.913732	2.374083	2.458162
69	6	0	-4.935141	4.420701	2.975107
70	1	0	-4.906254	3.603042	0.954784
71	1	0	-3.620329	3.018438	2.030042
72	6	0	-7.184536	3.472224	3.475226
73	1	0	-7.321542	2.664298	1.476193
74	1	0	-7.386753	1.436976	2.756490
75	6	0	-6.422544	4.740149	3.098178
76	1	0	-4.369386	5.297324	2.650862
77	1	0	-4.545879	4.122830	3.953986
78	1	0	-8.260516	3.656731	3.517716
79	1	0	-6.864904	3.129360	4.464714
80	1	0	-6.582455	5.524050	3.842161
81	1	0	-6.797539	5.117576	2.139469
82	7	0	-5.474452	2.112550	2.336546
83	7	0	5.275089	-1.110518	1.484594
84	7	0	5.379220	-2.416954	1.981657
85	6	0	6.576386	-3.060344	1.415129
86	6	0	5.438705	-2.364769	3.451204
87	6	0	6.677911	-4.494061	1.921797
88	1	0	7.479796	-2.493649	1.696205
89	1	0	6.482299	-3.034345	0.328189
90	6	0	5.510799	-3.777456	4.017200
91	1	0	6.319294	-1.784117	3.772927
92	1	0	4.543096	-1.847565	3.798990
93	6	0	6.715784	-4.526616	3.449154
94	1	0	7.571943	-4.956733	1.497363
95	1	0	5.810148	-5.056112	1.561893
96	1	0	5.563986	-3.719665	5.107013
97	1	0	4.589260	-4.308715	3.758218
98	1	0	6.730332	-5.557426	3.809964
99	1	0	7.637574	-4.046532	3.797893

100	1	0	6.000671	-0.415552	1.683638

Structure 25ab (DMSO)

Energy (Hartrees): = -2224.419749
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.148521	-2.543926	-0.612047
2	6	0	-4.117722	-2.870205	-1.455228
3	6	0	-2.958938	-2.013683	-1.458871
4	6	0	-2.929284	-0.821139	-0.665508
5	6	0	-4.075771	-0.465495	0.140435
6	6	0	-5.137452	-1.355098	0.167636
7	6	0	3.949603	5.365832	-1.621100
8	6	0	-0.561818	2.062884	-3.037828
9	6	0	-4.227070	-4.123911	-2.310824
10	6	0	-1.715776	-0.065186	-0.686971
11	6	0	-0.630267	-0.417506	-1.470036
12	6	0	-0.682495	-1.589557	-2.264764
13	6	0	-1.820555	-2.352960	-2.240618
14	6	0	-5.443671	-4.087797	-3.246328
15	6	0	-4.215799	-5.392728	-1.448583
16	6	0	0.500805	-1.976736	-3.109600
17	6	0	-4.223032	0.810480	0.865029
18	6	0	4.221143	-0.788470	0.751499
19	6	0	0.587856	0.447865	-1.471086
20	6	0	0.633469	1.631012	-2.231110
21	6	0	1.793499	2.379429	-2.216309
22	6	0	2.930471	2.005010	-1.470497
23	6	0	2.896699	0.816407	-0.690162
24	6	0	1.692792	0.070664	-0.710823
25	6	0	4.226308	4.069335	-2.391127
26	6	0	5.565401	4.138505	-3.136809
27	6	0	4.114741	2.865650	-1.468848
28	6	0	5.090404	2.609555	-0.562857
29	6	0	5.114978	1.409548	0.276194
30	6	0	4.050434	0.464597	0.139045
31	1	0	3.514338	-1.588862	0.594389
32	1	0	1.799010	3.298514	-2.785055
33	1	0	-3.491554	1.583873	0.699137
34	1	0	-1.825455	-3.251882	-2.838907
35	1	0	6.698716	2.937831	0.285328
36	1	0	3.992795	6.226566	-2.294113
37	1	0	-3.357640	-4.178021	-2.960999
38	8	0	1.616025	-1.055943	0.050602
39	1	0	-5.412395	-4.948982	-3.919521
40	1	0	-5.437514	-3.182879	-3.859751
41	1	0	-6.380835	-4.121731	-2.691540
42	1	0	-4.229163	-6.280268	-2.087310
43	1	0	-3.314719	-5.435102	-0.830834
44	1	0	-5.086883	-5.429981	-0.792384
45	1	0	-0.872175	1.275542	-3.730497
46	1	0	-0.332613	2.960383	-3.613194
47	1	0	-1.417995	2.281422	-2.392183
48	8	0	-6.250733	-3.326986	-0.502579
49	1	0	-6.848309	-2.893455	0.123317
50	8	0	-6.252856	-1.176687	0.894832
51	1	0	-6.125212	-0.322310	1.410206
52	1	0	0.274291	-2.862317	-3.704128
53	1	0	1.375037	-2.196107	-2.488907
54	1	0	0.780692	-1.164345	-3.786040
55	8	0	-1.627756	1.039290	0.101857
56	8	0	6.118059	1.273763	1.018200
57	1	0	2.959295	5.343955	-1.158382
58	1	0	4.694493	5.507634	-0.833912
59	8	0	6.165668	3.406848	-0.383456
60	1	0	3.468514	3.973807	-3.167106
61	1	0	5.510216	4.918798	-3.900797
62	1	0	5.782236	3.192139	-3.639405
63	1	0	6.393293	4.370038	-2.468493
64	1	0	-0.741169	1.417387	0.006082
65	1	0	0.719934	-1.416564	-0.016830
66	7	0	-5.222473	0.976948	1.658756
67	6	0	-4.629090	3.293203	2.028618
68	6	0	-6.857030	2.367235	2.523583
69	6	0	-4.888409	4.430548	3.012352
70	1	0	-4.869697	3.602371	0.997310
71	1	0	-3.569748	3.033227	2.065042
72	6	0	-7.126839	3.470702	3.534519
73	1	0	-7.272718	2.649286	1.543077
74	1	0	-7.321987	1.429258	2.832317

75	6	0	-6.376763	4.740605	3.142623
76	1	0	-4.330615	5.308271	2.677790
77	1	0	-4.490576	4.142792	3.991054
78	1	0	-8.203925	3.647021	3.582347
79	1	0	-6.799036	3.137928	4.525007
80	1	0	-6.537186	5.529073	3.881698
81	1	0	-6.759922	5.107375	2.183093
82	7	0	-5.415393	2.114508	2.389766
83	7	0	5.228427	-1.125766	1.526446
84	7	0	5.319269	-2.432025	2.027900
85	6	0	6.508988	-3.086889	1.454704
86	6	0	5.396349	-2.369400	3.497440
87	6	0	6.606508	-4.517081	1.970750
88	1	0	7.415537	-2.522053	1.726354
89	1	0	6.404401	-3.068172	0.368465
90	6	0	5.464362	-3.778562	4.071765
91	1	0	6.286003	-1.794274	3.801870
92	1	0	4.508591	-1.843279	3.852458
93	6	0	6.658748	-4.539069	3.497591
94	1	0	7.494489	-4.986884	1.541563
95	1	0	5.733056	-5.078257	1.622721
96	1	0	5.528948	-3.711987	5.160416
97	1	0	4.536859	-4.306553	3.827056
98	1	0	6.670599	-5.567669	3.865058
99	1	0	7.586041	-4.060653	3.833349
100	1	0	5.962063	-0.441850	1.732946

Structure 25cd (vacuum)

Energy (Hartrees): = -2224.3812215
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.149458	2.299965	-0.749329
2	6	0	4.078210	2.733673	-1.485154
3	6	0	2.888633	1.922559	-1.480299
4	6	0	2.857730	0.677377	-0.774356
5	6	0	4.034664	0.221882	-0.071375
6	6	0	5.132030	1.064249	-0.047948
7	6	0	-4.374253	-5.167121	-1.620522
8	6	0	0.279891	-2.008576	-3.089812
9	6	0	4.193797	4.043698	-2.249264
10	6	0	1.617433	-0.029588	-0.776737
11	6	0	0.500118	0.419273	-1.459149
12	6	0	0.554880	1.638662	-2.177430
13	6	0	1.723120	2.353554	-2.169272
14	6	0	5.302382	3.989082	-3.310786
15	6	0	4.369572	5.240691	-1.304160
16	6	0	-0.658202	2.117137	-2.931093
17	6	0	4.162352	-1.105018	0.550857
18	6	0	-4.224321	0.878768	0.992988
19	6	0	-0.748409	-0.399391	-1.439100
20	6	0	-0.867401	-1.559909	-2.222146
21	6	0	-2.055842	-2.261476	-2.180916
22	6	0	-3.150276	-1.861875	-1.390527
23	6	0	-3.037783	-0.700456	-0.578728
24	6	0	-1.812114	-0.000526	-0.631269
25	6	0	-4.574877	-3.827638	-2.341265
26	6	0	-5.928824	-3.777993	-3.064312
27	6	0	-4.373735	-2.667260	-1.380475
28	6	0	-5.312422	-2.400871	-0.441342
29	6	0	-5.254490	-1.233007	0.440927
30	6	0	-4.144702	-0.331769	0.305794
31	1	0	-3.458361	1.625681	0.849571
32	1	0	-2.120809	-3.164759	-2.770055
33	1	0	3.379146	-1.822027	0.371097
34	1	0	1.736778	3.285291	-2.713374
35	1	0	-6.911113	-2.689996	0.440244
36	1	0	-4.482867	-5.997998	-2.322463
37	1	0	3.267094	4.212906	-2.792290
38	8	0	-1.657507	1.117945	0.140898
39	1	0	5.301241	4.914243	-3.892998
40	1	0	5.137769	3.155134	-3.996649
41	1	0	6.283410	3.872088	-2.852139
42	1	0	4.374284	6.170237	-1.879287
43	1	0	3.548738	5.287669	-0.584862
44	1	0	5.308025	5.170707	-0.755004
45	1	0	0.593232	-1.207352	-3.764012
46	1	0	-0.003278	-2.875846	-3.686376
47	1	0	1.152168	-2.274836	-2.485812
48	8	0	6.295196	3.021843	-0.670477
49	1	0	6.909442	2.514984	-0.122489

50	8	0	6.281972	0.793903	0.593412
51	1	0	6.169224	-0.095934	1.032916
52	1	0	-0.433024	3.028339	-3.485240
53	1	0	-1.489526	2.322327	-2.250472
54	1	0	-1.004635	1.355179	-3.634245
55	8	0	1.525468	-1.195801	-0.074137
56	8	0	-6.221154	-1.072644	1.216991
57	1	0	-3.380787	-5.224152	-1.169020
58	1	0	-5.119319	-5.282760	-0.830886
59	8	0	-6.417886	-3.152335	-0.261414
60	1	0	-3.824725	-3.751304	-3.127168
61	1	0	-5.946438	-4.538663	-3.849043
62	1	0	-6.081145	-2.802961	-3.532589
63	1	0	-6.755281	-3.965663	-2.381998
64	1	0	0.611781	-1.507160	-0.131414
65	1	0	-0.744066	1.420925	0.047936
66	7	0	5.200412	-1.396352	1.252219
67	6	0	6.062977	-2.547208	3.066356
68	6	0	4.296702	-3.591315	1.720924
69	6	0	6.548431	-3.906820	3.547093
70	1	0	5.356745	-2.123254	3.799550
71	1	0	6.890660	-1.845463	2.956757
72	6	0	4.734033	-4.968590	2.212696
73	1	0	3.454403	-3.207840	2.324383
74	1	0	3.951152	-3.681636	0.689494
75	6	0	5.384001	-4.894022	3.591334
76	1	0	7.007027	-3.794031	4.532266
77	1	0	7.317589	-4.274115	2.860628
78	1	0	3.863098	-5.628054	2.222523
79	1	0	5.450964	-5.380803	1.495963
80	1	0	5.722604	-5.882324	3.909555
81	1	0	4.645831	-4.551266	4.326081
82	7	0	5.413072	-2.653860	1.757064
83	7	0	-5.192803	1.231245	1.827180
84	7	0	-5.230870	2.483262	2.461185
85	6	0	-4.094270	2.666316	3.370329
86	6	0	-5.363013	3.581343	1.497561
87	6	0	-4.287534	3.949555	4.170695
88	1	0	-3.142198	2.715635	2.813774
89	1	0	-4.055341	1.795422	4.026474
90	6	0	-5.592684	4.887967	2.248312
91	1	0	-4.459721	3.671426	0.869656
92	1	0	-6.206136	3.347287	0.845707
93	6	0	-4.454493	5.147342	3.235314
94	1	0	-3.433644	4.090627	4.837377
95	1	0	-5.181477	3.840906	4.792199
96	1	0	-5.680076	5.705882	1.529324
97	1	0	-6.541223	4.816641	2.788940
98	1	0	-4.644945	6.057517	3.808138
99	1	0	-3.522396	5.305451	2.679904
100	1	0	-5.951867	0.578359	2.007243

Structure 25cd ($CHCl_3$)

Energy (Hartrees): = -2224.4256613
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.117529	2.385682	-0.715164
2	6	0	4.038263	2.800296	-1.452128
3	6	0	2.860758	1.969946	-1.443496
4	6	0	2.854903	0.721650	-0.743193
5	6	0	4.045846	0.278790	-0.054628
6	6	0	5.127310	1.142678	-0.025790
7	6	0	-4.265226	-5.255991	-1.566582
8	6	0	0.329960	-2.021451	-3.014777
9	6	0	4.123444	4.115128	-2.213443
10	6	0	1.621913	-0.000727	-0.724696
11	6	0	0.494218	0.426499	-1.403843
12	6	0	0.526453	1.647254	-2.123414
13	6	0	1.682856	2.383207	-2.123666
14	6	0	5.242184	4.104143	-3.264981
15	6	0	4.250356	5.314412	-1.264505
16	6	0	-0.695580	2.113544	-2.868795
17	6	0	4.210300	-1.062267	0.531266
18	6	0	-4.284523	0.840240	0.968170
19	6	0	-0.740973	-0.413922	-1.383611
20	6	0	-0.832122	-1.581027	-2.163954
21	6	0	-2.008418	-2.303742	-2.133633
22	6	0	-3.118502	-1.920245	-1.354843
23	6	0	-3.036663	-0.751440	-0.549557
24	6	0	-1.818183	-0.032450	-0.585673

25	6	0	-4.492230	-3.926274	-2.296340
26	6	0	-5.839937	-3.916268	-3.031499
27	6	0	-4.323826	-2.752236	-1.344481
28	6	0	-5.273598	-2.495128	-0.412359
29	6	0	-5.248033	-1.317480	0.457243
30	6	0	-4.162824	-0.392760	0.315031
31	1	0	-3.546962	1.610835	0.801930
32	1	0	-2.049174	-3.210317	-2.720372
33	1	0	3.456026	-1.802827	0.323025
34	1	0	1.672664	3.318226	-2.663257
35	1	0	-6.879992	-2.821126	0.458021
36	1	0	-4.353649	-6.093143	-2.264498
37	1	0	3.198187	4.255443	-2.766217
38	8	0	-1.698568	1.079897	0.195518
39	1	0	5.212390	5.032454	-3.842201
40	1	0	5.113991	3.270925	-3.960533
41	1	0	6.226109	4.019540	-2.804137
42	1	0	4.231758	6.245967	-1.837016
43	1	0	3.420167	5.336603	-0.553791
44	1	0	5.184165	5.276851	-0.702389
45	1	0	0.636675	-1.227544	-3.701088
46	1	0	0.065562	-2.902135	-3.601161
47	1	0	1.200252	-2.269005	-2.399459
48	8	0	6.244977	3.135473	-0.632588
49	1	0	6.885174	2.645290	-0.096876
50	8	0	6.283136	0.884367	0.609594
51	1	0	6.185543	-0.017310	1.036929
52	1	0	-0.485712	3.035086	-3.412688
53	1	0	-1.528877	2.301501	-2.185128
54	1	0	-1.031504	1.357001	-3.583239
55	8	0	1.560874	-1.152569	-0.001622
56	8	0	-6.226510	-1.170689	1.226395
57	1	0	-3.271234	-5.292812	-1.113086
58	1	0	-5.008074	-5.388752	-0.776648
59	8	0	-6.363746	-3.272501	-0.235085
60	1	0	-3.737535	-3.840678	-3.076446
61	1	0	-5.827379	-4.679511	-3.814377
62	1	0	-6.016807	-2.948444	-3.507753
63	1	0	-6.671029	-4.127220	-2.360450
64	1	0	0.651279	-1.483541	-0.017060
65	1	0	-0.787603	1.403091	0.145113
66	7	0	5.257033	-1.336328	1.227258
67	6	0	6.181076	-2.496915	3.005152
68	6	0	4.436142	-3.572268	1.646325
69	6	0	6.711785	-3.850425	3.452618
70	1	0	5.465726	-2.112258	3.749746
71	1	0	6.986979	-1.768229	2.905447
72	6	0	4.923186	-4.942997	2.106859
73	1	0	3.589453	-3.228391	2.265556
74	1	0	4.085848	-3.653193	0.615865
75	6	0	5.581031	-4.875947	3.481773
76	1	0	7.170691	-3.740787	4.438162
77	1	0	7.490592	-4.178794	2.756598
78	1	0	4.072057	-5.628018	2.109689
79	1	0	5.645988	-5.320460	1.376379
80	1	0	5.955612	-5.859484	3.774556
81	1	0	4.837548	-4.573919	4.228857
82	7	0	5.521660	-2.595516	1.696312
83	7	0	-5.264966	1.184221	1.783397
84	7	0	-5.356109	2.453032	2.382908
85	6	0	-4.245331	2.684888	3.317274
86	6	0	-5.480200	3.521448	1.381533
87	6	0	-4.486729	3.985932	4.073181
88	1	0	-3.283339	2.738510	2.780733
89	1	0	-4.206687	1.834666	4.000394
90	6	0	-5.755575	4.843234	2.088476
91	1	0	-4.560616	3.609091	0.779978
92	1	0	-6.301500	3.253575	0.714485
93	6	0	-4.652242	5.153509	3.100220
94	1	0	-3.652329	4.161783	4.756222
95	1	0	-5.393572	3.877919	4.676689
96	1	0	-5.836173	5.636776	1.341749
97	1	0	-6.719032	4.771044	2.602938
98	1	0	-4.879238	6.073809	3.643439
99	1	0	-3.707888	5.315775	2.567148
100	1	0	-6.001908	0.513330	1.986978

Structure 26cd (DMSO)

Energy (Hartrees): = -2224.4153511
No imaginary frequencies

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	5.118095	2.369045	-0.716479
2	6	0	4.045247	2.784752	-1.462859
3	6	0	2.866189	1.955736	-1.462689
4	6	0	2.850479	0.711953	-0.754176
5	6	0	4.035619	0.266182	-0.057871
6	6	0	5.119759	1.127069	-0.024114
7	6	0	-4.265409	-5.236058	-1.578195
8	6	0	0.296086	-1.997406	-3.078868
9	6	0	4.133719	4.101080	-2.220566
10	6	0	1.613954	-0.004637	-0.735708
11	6	0	0.494820	0.421395	-1.429345
12	6	0	0.537976	1.634271	-2.161332
13	6	0	1.696261	2.367692	-2.158012
14	6	0	5.259594	4.095288	-3.263624
15	6	0	4.251352	5.296830	-1.266700
16	6	0	-0.677902	2.098284	-2.916829
17	6	0	4.193783	-1.075347	0.529758
18	6	0	-4.260433	0.844796	0.984105
19	6	0	-0.745258	-0.411797	-1.409062
20	6	0	-0.851712	-1.566537	-2.205331
21	6	0	-2.029402	-2.286659	-2.167457
22	6	0	-3.127235	-1.907725	-1.368448
23	6	0	-3.032527	-0.746523	-0.552856
24	6	0	-1.810164	-0.033574	-0.593949
25	6	0	-4.510897	-3.908137	-2.304163
26	6	0	-5.867920	-3.906664	-3.020504
27	6	0	-4.334760	-2.736396	-1.351298
28	6	0	-5.273632	-2.481223	-0.407337
29	6	0	-5.232055	-1.312279	0.474424
30	6	0	-4.146920	-0.390283	0.327981
31	1	0	-3.525410	1.616872	0.811782
32	1	0	-2.080143	-3.185711	-2.765046
33	1	0	3.443820	-1.819014	0.315495
34	1	0	1.693137	3.297238	-2.707115
35	1	0	-6.861845	-2.793010	0.485544
36	1	0	-4.361249	-6.073429	-2.274835
37	1	0	3.212228	4.243383	-2.778513
38	8	0	-1.673006	1.064350	0.201344
39	1	0	5.234654	5.027371	-3.834842
40	1	0	5.134671	3.267590	-3.966692
41	1	0	6.240687	4.005640	-2.797334
42	1	0	4.232831	6.229492	-1.837237
43	1	0	3.415706	5.315043	-0.562140
44	1	0	5.181548	5.261635	-0.698195
45	1	0	0.601404	-1.189606	-3.749703
46	1	0	0.016619	-2.861586	-3.682496
47	1	0	1.171096	-2.269959	-2.480844
48	8	0	6.248345	3.113579	-0.623822
49	1	0	6.872850	2.620487	-0.072995
50	8	0	6.270214	0.865344	0.618087
51	1	0	6.159757	-0.035347	1.049978
52	1	0	-0.461409	3.013307	-3.468840
53	1	0	-1.512675	2.298270	-2.237951
54	1	0	-1.013764	1.335059	-3.624592
55	8	0	1.540624	-1.142849	0.005207
56	8	0	-6.200550	-1.175397	1.259065
57	1	0	-3.262672	-5.267447	-1.143686
58	1	0	-4.993863	-5.372586	-0.775106
59	8	0	-6.366872	-3.251369	-0.218837
60	1	0	-3.767455	-3.819279	-3.094283
61	1	0	-5.859874	-4.670117	-3.803111
62	1	0	-6.057489	-2.940587	-3.495965
63	1	0	-6.689273	-4.122336	-2.338962
64	1	0	0.637499	-1.488510	-0.046713
65	1	0	-0.768369	1.399018	0.116754
66	7	0	5.236312	-1.343892	1.234688
67	6	0	6.154779	-2.487717	3.025182
68	6	0	4.426014	-3.582380	1.656098
69	6	0	6.688213	-3.835539	3.484826
70	1	0	5.429835	-2.104356	3.760493
71	1	0	6.957576	-1.755038	2.927519
72	6	0	4.919049	-4.946528	2.128576
73	1	0	3.574336	-3.240365	2.268769
74	1	0	4.083744	-3.670135	0.623461
75	6	0	5.562845	-4.866612	3.509247
76	1	0	7.136570	-3.716390	4.474044
77	1	0	7.476197	-4.164474	2.799180
78	1	0	4.071937	-5.636355	2.127537
79	1	0	5.650952	-5.324498	1.407187
80	1	0	5.940389	-5.845864	3.812535
81	1	0	4.810026	-4.562659	4.246118
82	7	0	5.505700	-2.597860	1.710651
83	7	0	-5.233210	1.186073	1.806806
84	7	0	-5.330422	2.455946	2.404373
85	6	0	-4.214878	2.697325	3.332421
86	6	0	-5.463915	3.521915	1.399949

87	6	0	-4.463549	3.997548	4.086994
88	1	0	-3.258587	2.759921	2.788243
89	1	0	-4.165869	1.848719	4.017128
90	6	0	-5.748290	4.841458	2.106852
91	1	0	-4.545449	3.615375	0.799004
92	1	0	-6.285093	3.247355	0.735176
93	6	0	-4.643734	5.162225	3.113495
94	1	0	-3.626109	4.181020	4.764299
95	1	0	-5.365822	3.884079	4.696819
96	1	0	-5.838264	5.632533	1.358625
97	1	0	-6.709673	4.762936	2.624916
98	1	0	-4.876758	6.080694	3.657361
99	1	0	-3.703568	5.330891	2.575466
100	1	0	-5.967527	0.514649	2.016981

Structure 26ad (vacuum)

Energy (Hartrees): = -2381.6047972
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.829864	2.807812	-0.789681
2	6	0	3.777193	3.074510	-1.625350
3	6	0	2.683816	2.136554	-1.649930
4	6	0	2.741564	0.930879	-0.881260
5	6	0	3.918536	0.636607	-0.099820
6	6	0	4.913422	1.596836	-0.049120
7	6	0	-4.458053	-5.635036	-1.017658
8	6	0	0.494149	-2.134612	-3.136706
9	6	0	3.797152	4.351670	-2.450875
10	6	0	1.579363	0.105038	-0.891677
11	6	0	0.460532	0.396397	-1.652458
12	6	0	0.436527	1.567800	-2.449234
13	6	0	1.523229	2.402682	-2.424535
14	6	0	5.007510	4.409019	-3.394711
15	6	0	3.711095	5.598287	-1.559101
16	6	0	-0.772401	1.870226	-3.296200
17	6	0	4.163436	-0.642235	0.582508
18	6	0	-4.317656	0.558285	0.733507
19	6	0	-0.709035	-0.529909	-1.604490
20	6	0	-0.699207	-1.749612	-2.301062
21	6	0	-1.807572	-2.566988	-2.209248
22	6	0	-2.945779	-2.228646	-1.451891
23	6	0	-2.985214	-0.980557	-0.770172
24	6	0	-1.834314	-0.165842	-0.866196
25	6	0	-4.023816	-4.542116	-2.005623
26	6	0	-4.836048	-4.604369	-3.305985
27	6	0	-4.084237	-3.148501	-1.400864
28	6	0	-5.238547	-2.715145	-0.840438
29	6	0	-5.358319	-1.436656	-0.136883
30	6	0	-4.201181	-0.590516	-0.051765
31	1	0	-3.468181	1.211521	0.857475
32	1	0	-1.795018	-3.486374	-2.776014
33	1	0	3.468543	-1.446392	0.411178
34	1	0	1.472469	3.300686	-3.021227
35	1	0	-7.006956	-2.891196	-0.331254
36	1	0	-4.273370	-6.616851	-1.461302
37	1	0	2.919561	4.363232	-3.093202
38	8	0	-1.824369	1.041309	-0.224257
39	1	0	4.931266	5.290383	-4.036746
40	1	0	5.038240	3.524028	-4.034235
41	1	0	5.942187	4.467902	-2.839276
42	1	0	3.673533	6.498550	-2.177981
43	1	0	2.811146	5.569580	-0.940377
44	1	0	4.579687	5.666633	-0.904111
45	1	0	0.730783	-1.351870	-3.861931
46	1	0	0.304348	-3.063661	-3.674262
47	1	0	1.384161	-2.272477	-2.515549
48	8	0	5.869467	3.668208	-0.656571
49	1	0	6.494764	3.259229	-0.042673
50	8	0	6.037848	1.476199	0.672508
51	1	0	5.962376	0.600041	1.172450
52	1	0	-0.600682	2.754657	-3.909641
53	1	0	-1.657562	2.045037	-2.677448
54	1	0	-1.006044	1.027983	-3.952554
55	8	0	1.566099	-1.014218	-0.109497
56	8	0	-6.469579	-1.191994	0.382134
57	1	0	-3.884830	-5.567799	-0.090239
58	1	0	-5.516330	-5.558728	-0.775376
59	8	0	-6.376535	-3.438750	-0.833131
60	1	0	-2.986647	-4.767228	-2.249060
61	1	0	-4.758728	-5.597661	-3.755788

62	1	0	-4.471667	-3.869513	-4.027929
63	1	0	-5.888214	-4.397096	-3.103057
64	1	0	0.692657	-1.422782	-0.186760
65	1	0	-0.954497	1.443596	-0.353407
66	7	0	5.197242	-0.780701	1.333173
67	6	0	4.423671	-2.983936	2.044887
68	6	0	6.826224	-2.411076	1.575589
69	6	0	4.915048	-4.219577	2.806736
70	1	0	4.162124	-3.301161	1.019648
71	6	0	7.272298	-3.624329	2.383035
72	1	0	6.761360	-2.710880	0.514109
73	6	0	6.247426	-4.744373	2.298218
74	1	0	4.136508	-4.983526	2.736911
75	1	0	5.013690	-3.950984	3.864629
76	1	0	8.244149	-3.949436	2.003139
77	1	0	7.410185	-3.319854	3.427038
78	1	0	6.564173	-5.611380	2.882664
79	1	0	6.148065	-5.073771	1.257399
80	7	0	5.482687	-1.959452	2.011409
81	7	0	-5.407451	0.940528	1.381524
82	7	0	-5.456474	2.117927	2.151648
83	6	0	-4.498031	2.065253	3.276703
84	6	0	-5.318303	3.314225	1.290455
85	6	0	-4.682612	3.312234	4.138548
86	1	0	-3.462451	2.068881	2.891616
87	6	0	-5.498807	4.563487	2.150015
88	1	0	-4.304795	3.340346	0.849873
89	6	0	-4.525109	4.588707	3.321200
90	1	0	-3.958562	3.278266	4.956777
91	1	0	-5.684311	3.275356	4.581377
92	1	0	-5.370030	5.443299	1.513965
93	1	0	-6.528973	4.574295	2.523414
94	1	0	-4.697137	5.468919	3.944931
95	1	0	-3.498589	4.657565	2.942949
96	6	0	3.185160	-2.454369	2.777282
97	1	0	3.498936	-2.058245	3.745507
98	1	0	2.640803	-1.674110	2.249547
99	1	0	2.493367	-3.281218	2.951685
100	6	0	7.845494	-1.281857	1.710078
101	1	0	7.719425	-0.509999	0.952609
102	1	0	7.756575	-0.824696	2.698907
103	1	0	8.851980	-1.691696	1.605864
104	6	0	-6.352469	3.278351	0.172510
105	1	0	-6.189731	2.448601	-0.515553
106	1	0	-7.352710	3.180750	0.601801
107	1	0	-6.307642	4.207878	-0.398032
108	6	0	-4.725124	0.804172	4.100846
109	1	0	-5.766863	0.764283	4.428628
110	1	0	-4.505647	-0.103662	3.538687
111	1	0	-4.082411	0.821584	4.983110
112	1	0	-6.249202	0.374390	1.308237

Structure 26ad ($CHCl_3$)

Energy (Hartrees): = -2381.6494566
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.903475	2.754495	-0.846058
2	6	0	3.847490	3.032912	-1.674551
3	6	0	2.724126	2.129446	-1.659335
4	6	0	2.761832	0.932193	-0.875714
5	6	0	3.941476	0.621587	-0.101636
6	6	0	4.961335	1.558067	-0.079189
7	6	0	-4.516929	-5.583910	-1.192038
8	6	0	0.506674	-2.081014	-3.131301
9	6	0	3.887763	4.290478	-2.530498
10	6	0	1.582225	0.127774	-0.869392
11	6	0	0.463178	0.435528	-1.623923
12	6	0	0.449536	1.611642	-2.415623
13	6	0	1.554352	2.424042	-2.410725
14	6	0	5.100121	4.320264	-3.472462
15	6	0	3.811956	5.556057	-1.666141
16	6	0	-0.764444	1.948443	-3.240264
17	6	0	4.164974	-0.650695	0.604346
18	6	0	-4.336062	0.552633	0.752978
19	6	0	-0.711193	-0.487647	-1.592823
20	6	0	-0.696145	-1.696902	-2.310774
21	6	0	-1.810339	-2.509586	-2.254385
22	6	0	-2.959346	-2.178790	-1.507650
23	6	0	-3.002448	-0.945429	-0.799223
24	6	0	-1.843792	-0.133360	-0.862009

25	6	0	-4.041733	-4.469645	-2.135940
26	6	0	-4.809063	-4.495744	-3.463747
27	6	0	-4.106280	-3.089096	-1.500279
28	6	0	-5.266620	-2.656683	-0.950020
29	6	0	-5.385882	-1.398210	-0.212790
30	6	0	-4.224970	-0.568089	-0.083522
31	1	0	-3.479804	1.188475	0.917077
32	1	0	-1.791551	-3.418347	-2.838686
33	1	0	3.456849	-1.446615	0.450816
34	1	0	1.508659	3.326215	-3.002414
35	1	0	-7.051984	-2.839333	-0.478373
36	1	0	-4.305383	-6.556202	-1.645517
37	1	0	3.013850	4.295543	-3.177567
38	8	0	-1.846751	1.057307	-0.196687
39	1	0	5.015351	5.174418	-4.149930
40	1	0	5.142409	3.413018	-4.080665
41	1	0	6.036939	4.410803	-2.923986
42	1	0	3.789458	6.445338	-2.302235
43	1	0	2.907353	5.554999	-1.052386
44	1	0	4.676831	5.630024	-1.005150
45	1	0	0.760775	-1.295523	-3.848038
46	1	0	0.317749	-3.003884	-3.680611
47	1	0	1.385402	-2.235773	-2.497656
48	8	0	5.964642	3.592856	-0.746291
49	1	0	6.600518	3.190904	-0.136530
50	8	0	6.086537	1.420712	0.637153
51	1	0	5.989772	0.550848	1.152655
52	1	0	-0.594119	2.855985	-3.820092
53	1	0	-1.644189	2.105016	-2.608820
54	1	0	-1.005620	1.135052	-3.930087
55	8	0	1.563984	-0.983643	-0.081486
56	8	0	-6.506478	-1.159600	0.296735
57	1	0	-3.988758	-5.536522	-0.236263
58	1	0	-5.586484	-5.523067	-0.996525
59	8	0	-6.411179	-3.372263	-0.984329
60	1	0	-2.999874	-4.699007	-2.351936
61	1	0	-4.721394	-5.478923	-3.934757
62	1	0	-4.417654	-3.748664	-4.159255
63	1	0	-5.868261	-4.287761	-3.297413
64	1	0	0.683250	-1.383881	-0.123869
65	1	0	-0.970858	1.462556	-0.272714
66	7	0	5.199587	-0.791072	1.354131
67	6	0	4.401481	-2.970998	2.112876
68	6	0	6.815363	-2.429646	1.640396
69	6	0	4.880322	-4.198985	2.895292
70	1	0	4.139723	-3.298813	1.092471
71	6	0	7.244792	-3.632432	2.471548
72	1	0	6.747237	-2.748225	0.585841
73	6	0	6.209454	-4.743418	2.399698
74	1	0	4.094262	-4.956028	2.833528
75	1	0	4.978728	-3.916449	3.949827
76	1	0	8.214801	-3.972298	2.099734
77	1	0	7.382024	-3.313533	3.511726
78	1	0	6.515856	-5.602913	3.000793
79	1	0	6.111664	-5.088052	1.363721
80	7	0	5.471602	-1.954200	2.063152
81	7	0	-5.424601	0.916553	1.403802
82	7	0	-5.483768	2.064573	2.219263
83	6	0	-4.515198	1.985490	3.337715
84	6	0	-5.364382	3.292557	1.395981
85	6	0	-4.713822	3.199400	4.242348
86	1	0	-3.484009	2.019052	2.946691
87	6	0	-5.557486	4.508241	2.299096
88	1	0	-4.354220	3.341593	0.953054
89	6	0	-4.580816	4.505494	3.468344
90	1	0	-3.980025	3.146641	5.050996
91	1	0	-5.710203	3.132692	4.694448
92	1	0	-5.439538	5.410382	1.692878
93	1	0	-6.587048	4.495796	2.674989
94	1	0	-4.765822	5.359926	4.123635
95	1	0	-3.556809	4.603051	3.089609
96	6	0	3.168635	-2.419699	2.836286
97	1	0	3.472560	-2.048953	3.818242
98	1	0	2.651166	-1.615284	2.316226
99	1	0	2.451152	-3.230176	2.984329
100	6	0	7.846330	-1.309912	1.755258
101	1	0	7.739851	-0.556758	0.975200
102	1	0	7.762181	-0.823132	2.730986
103	1	0	8.848342	-1.735296	1.666912
104	6	0	-6.403470	3.280051	0.283258
105	1	0	-6.233904	2.477363	-0.436027
106	1	0	-7.403472	3.157074	0.708443
107	1	0	-6.371094	4.228697	-0.256773
108	6	0	-4.721465	0.693954	4.117404
109	1	0	-5.762896	0.620040	4.442350
110	1	0	-4.480036	-0.192623	3.529152
111	1	0	-4.081969	0.694538	5.002742
112	1	0	-6.273562	0.366932	1.297142

Structure 26ad (DMSO)

Energy (Hartrees): = -2381.6373954
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.904883	2.713083	-0.867935
2	6	0	3.860097	2.980488	-1.714636
3	6	0	2.737781	2.074773	-1.704750
4	6	0	2.759997	0.895350	-0.893503
5	6	0	3.930318	0.592876	-0.102296
6	6	0	4.953329	1.526106	-0.085221
7	6	0	-4.650103	-5.509158	-1.198867
8	6	0	0.477434	-2.151157	-3.123216
9	6	0	3.911136	4.225755	-2.587422
10	6	0	1.574393	0.100024	-0.878166
11	6	0	0.471079	0.390961	-1.661054
12	6	0	0.479617	1.537941	-2.493890
13	6	0	1.585581	2.349173	-2.490508
14	6	0	5.126086	4.229129	-3.525287
15	6	0	3.844230	5.504680	-1.743051
16	6	0	-0.715706	1.849246	-3.353831
17	6	0	4.143807	-0.671607	0.621302
18	6	0	-4.304622	0.599314	0.753011
19	6	0	-0.715912	-0.514537	-1.612598
20	6	0	-0.721464	-1.733238	-2.314554
21	6	0	-1.853389	-2.521229	-2.257333
22	6	0	-2.998570	-2.156079	-1.520149
23	6	0	-3.014090	-0.920257	-0.815097
24	6	0	-1.842229	-0.127982	-0.888763
25	6	0	-4.138170	-4.417370	-2.148084
26	6	0	-4.893864	-4.434086	-3.482039
27	6	0	-4.172257	-3.031599	-1.522782
28	6	0	-5.327774	-2.555426	-0.998264
29	6	0	-5.421256	-1.283510	-0.278063
30	6	0	-4.231926	-0.503462	-0.114411
31	1	0	-3.414551	1.165330	0.983996
32	1	0	-1.850374	-3.435343	-2.833778
33	1	0	3.432250	-1.466677	0.478125
34	1	0	1.554380	3.231351	-3.112694
35	1	0	-7.119004	-2.658128	-0.554517
36	1	0	-4.480102	-6.490085	-1.651212
37	1	0	3.038092	4.232139	-3.235124
38	8	0	-1.830360	1.072906	-0.245227
39	1	0	5.058217	5.080155	-4.208499
40	1	0	5.154870	3.317640	-4.128255
41	1	0	6.062577	4.307097	-2.973780
42	1	0	3.821315	6.382441	-2.394735
43	1	0	2.940876	5.517717	-1.127379
44	1	0	4.711455	5.588442	-1.086299
45	1	0	0.751007	-1.378506	-3.847104
46	1	0	0.272572	-3.076231	-3.662887
47	1	0	1.348870	-2.318198	-2.482507
48	8	0	5.968630	3.547823	-0.764827
49	1	0	6.587600	3.147440	-0.137333
50	8	0	6.072519	1.394762	0.640905
51	1	0	5.973697	0.522528	1.155159
52	1	0	-0.521866	2.723491	-3.975806
53	1	0	-1.601825	2.052830	-2.744529
54	1	0	-0.959260	1.004661	-4.004539
55	8	0	1.532761	-0.979079	-0.049186
56	8	0	-6.547335	-1.001376	0.197265
57	1	0	-4.112632	-5.480831	-0.247341
58	1	0	-5.715188	-5.404849	-0.996727
59	8	0	-6.497383	-3.229123	-1.043217
60	1	0	-3.101596	-4.675828	-2.355169
61	1	0	-4.815933	-5.419637	-3.949505
62	1	0	-4.482405	-3.696018	-4.175857
63	1	0	-5.951636	-4.209543	-3.327365
64	1	0	0.657614	-1.388925	-0.116635
65	1	0	-0.961246	1.483327	-0.363255
66	7	0	5.177639	-0.807046	1.373287
67	6	0	4.365195	-2.971660	2.160620
68	6	0	6.782037	-2.455435	1.678861
69	6	0	4.834907	-4.191060	2.960972
70	1	0	4.105051	-3.310732	1.144292
71	6	0	7.203216	-3.647888	2.528203
72	1	0	6.704966	-2.790849	0.630781
73	6	0	6.159900	-4.752107	2.474228
74	1	0	4.042655	-4.942086	2.908303
75	1	0	4.934637	-3.895273	4.011944

76	1	0	8.170109	-3.999889	2.159914
77	1	0	7.343936	-3.313933	3.563387
78	1	0	6.460595	-5.603994	3.088986
79	1	0	6.059282	-5.111982	1.443792
80	7	0	5.442762	-1.961358	2.099847
81	7	0	-5.397974	1.021927	1.355286
82	7	0	-5.423384	2.135889	2.218990
83	6	0	-4.609581	1.887873	3.434617
84	6	0	-5.057588	3.376505	1.492163
85	6	0	-4.781368	3.072355	4.381899
86	1	0	-3.544219	1.816357	3.158925
87	6	0	-5.230352	4.562105	2.437312
88	1	0	-3.999074	3.329655	1.186593
89	6	0	-4.412001	4.389817	3.711170
90	1	0	-4.162910	2.895909	5.265884
91	1	0	-5.827136	3.102397	4.710133
92	1	0	-4.938649	5.470231	1.903440
93	1	0	-6.294340	4.652035	2.686515
94	1	0	-4.581664	5.226712	4.392830
95	1	0	-3.345002	4.384699	3.460237
96	6	0	3.135285	-2.403522	2.874904
97	1	0	3.437428	-2.028702	3.856319
98	1	0	2.625822	-1.598898	2.347045
99	1	0	2.410609	-3.206958	3.025828
100	6	0	7.823097	-1.343605	1.771742
101	1	0	7.721241	-0.602730	0.979293
102	1	0	7.749051	-0.839564	2.739820
103	1	0	8.820508	-1.780114	1.685941
104	6	0	-5.937170	3.541297	0.260438
105	1	0	-5.758532	2.767840	-0.488415
106	1	0	-6.991739	3.507185	0.549368
107	1	0	-5.738244	4.510163	-0.202818
108	6	0	-5.050850	0.593451	4.103321
109	1	0	-6.125603	0.624318	4.304173
110	1	0	-4.839011	-0.283562	3.489245
111	1	0	-4.524354	0.475288	5.052771
112	1	0	-6.276134	0.537532	1.189483

Structure 26bb (vacuum)

Energy (Hartrees): = -2381.6145661
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.766893	3.099738	-0.577672
2	6	0	3.696221	3.358255	-1.392640
3	6	0	2.666492	2.353419	-1.499029
4	6	0	2.800122	1.108763	-0.813838
5	6	0	3.990756	0.834527	-0.050218
6	6	0	4.922554	1.849726	0.086103
7	6	0	-3.308816	-5.834775	-1.338194
8	6	0	0.775725	-2.065226	-3.105545
9	6	0	3.624332	4.695444	-2.112615
10	6	0	1.695390	0.212241	-0.864860
11	6	0	0.563157	0.468512	-1.619127
12	6	0	0.470866	1.677873	-2.352568
13	6	0	1.496351	2.585102	-2.269067
14	6	0	4.810205	4.901833	-3.066074
15	6	0	3.481527	5.858948	-1.120947
16	6	0	-0.744873	1.943285	-3.201435
17	6	0	4.356092	-0.484396	0.472519
18	6	0	-4.336474	0.416742	0.474715
19	6	0	-0.553466	-0.521984	-1.611271
20	6	0	-0.456437	-1.745592	-2.298537
21	6	0	-1.511295	-2.633240	-2.219604
22	6	0	-2.685007	-2.359138	-1.490800
23	6	0	-2.802395	-1.119442	-0.807859
24	6	0	-1.703017	-0.236753	-0.876436
25	6	0	-3.711420	-4.642925	-2.216892
26	6	0	-5.028389	-4.913126	-2.959054
27	6	0	-3.746546	-3.362643	-1.398819
28	6	0	-4.741683	-3.164926	-0.499842
29	6	0	-4.916588	-1.914502	0.242915
30	6	0	-3.987468	-0.851146	0.002502
31	1	0	-3.782259	1.298674	0.189747
32	1	0	-1.401793	-3.582199	-2.724444
33	1	0	3.821504	-1.369416	0.147685
34	1	0	1.387223	3.508978	-2.816290
35	1	0	-6.289316	-3.637196	0.394640
36	1	0	-3.251227	-6.747870	-1.936476
37	1	0	2.732955	4.705359	-2.735567
38	8	0	-1.771202	0.938678	-0.183676

39	1	0	4.669566	5.827361	-3.630129
40	1	0	4.881310	4.076386	-3.777695
41	1	0	5.749935	4.971036	-2.520243
42	1	0	3.364139	6.799960	-1.664322
43	1	0	2.603872	5.718774	-0.485751
44	1	0	4.362026	5.936380	-0.483438
45	1	0	0.967404	-1.282828	-3.844421
46	1	0	0.658364	-3.015254	-3.626786
47	1	0	1.663552	-2.128842	-2.470166
48	8	0	5.752459	4.011625	-0.386189
49	1	0	6.407620	3.601655	0.194550
50	8	0	6.055140	1.745591	0.793318
51	1	0	6.052586	0.833276	1.224833
52	1	0	-0.638606	2.882754	-3.743707
53	1	0	-1.650355	1.996271	-2.590658
54	1	0	-0.894812	1.136551	-3.923540
55	8	0	1.763914	-0.926720	-0.121269
56	8	0	-5.925086	-1.842462	0.983968
57	1	0	-2.335440	-5.665607	-0.871325
58	1	0	-4.048515	-5.985066	-0.549552
59	8	0	-5.700004	-4.079179	-0.242693
60	1	0	-2.957572	-4.528430	-2.994810
61	1	0	-4.892743	-5.757765	-3.639381
62	1	0	-5.322940	-4.044011	-3.551555
63	1	0	-5.835876	-5.150196	-2.269092
64	1	0	0.915934	-1.386041	-0.192254
65	1	0	-0.910758	1.374841	-0.242000
66	7	0	5.350347	-0.617199	1.269393
67	6	0	7.085824	-2.181840	1.332270
68	6	0	5.327530	-2.170161	3.041293
69	6	0	7.452168	-3.620738	1.684665
70	1	0	7.677402	-1.498222	1.967487
71	6	0	5.672531	-3.608508	3.424250
72	1	0	5.942836	-1.480775	3.645870
73	6	0	7.134574	-3.933665	3.141793
74	1	0	8.514022	-3.773887	1.474543
75	1	0	6.884843	-4.288728	1.026912
76	1	0	5.438378	-3.753557	4.482190
77	1	0	5.024157	-4.277784	2.847646
78	1	0	7.348170	-4.980840	3.369135
79	1	0	7.774351	-3.325103	3.791301
80	7	0	5.647336	-1.971699	1.608538
81	7	0	-5.359339	0.666323	1.272487
82	7	0	-5.676167	1.987583	1.614043
83	6	0	-7.091690	2.246670	1.263735
84	6	0	-5.377868	2.219079	3.047977
85	6	0	-7.424291	3.700166	1.589616
86	1	0	-7.738191	1.594312	1.879015
87	6	0	-5.699302	3.673568	3.384154
88	1	0	-6.021096	1.563241	3.661549
89	6	0	-7.145044	4.022718	3.052893
90	1	0	-8.473506	3.881149	1.342590
91	1	0	-6.816554	4.342634	0.942636
92	1	0	-5.489222	3.840914	4.443541
93	1	0	-5.021059	4.312949	2.807944
94	1	0	-7.344437	5.076443	3.260321
95	1	0	-7.816687	3.435610	3.689767
96	6	0	7.389164	-1.889627	-0.132316
97	1	0	6.731146	-2.484918	-0.771378
98	1	0	7.247017	-0.836114	-0.374290
99	1	0	8.424812	-2.153873	-0.355825
100	6	0	3.853188	-1.887623	3.304604
101	1	0	3.601935	-0.838172	3.153475
102	1	0	3.233794	-2.489712	2.633855
103	1	0	3.607432	-2.151589	4.335387
104	6	0	-3.915339	1.908969	3.339873
105	1	0	-3.679253	0.854197	3.199719
106	1	0	-3.272553	2.496934	2.679104
107	1	0	-3.684557	2.173460	4.373575
108	6	0	-7.332500	1.944152	-0.209679
109	1	0	-6.628919	2.513348	-0.822897
110	1	0	-7.211282	0.884095	-0.434819
111	1	0	-8.348074	2.235875	-0.483498
112	1	0	-5.938209	-0.121270	1.582765

Structure 26bb ($CHCl_3$)

Energy (Hartrees): = -2381.660049
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.742013	3.135784	-0.559260

2	6	0	3.661152	3.394448	-1.362062
3	6	0	2.644561	2.376245	-1.481421
4	6	0	2.797688	1.123684	-0.814995
5	6	0	4.000786	0.850222	-0.069694
6	6	0	4.921229	1.874789	0.078036
7	6	0	-3.235271	-5.877551	-1.259279
8	6	0	0.793318	-2.081110	-3.066167
9	6	0	3.559359	4.745148	-2.054167
10	6	0	1.695942	0.220840	-0.854716
11	6	0	0.554006	0.472094	-1.596706
12	6	0	0.444202	1.689778	-2.316628
13	6	0	1.462549	2.606764	-2.234403
14	6	0	4.738176	5.002211	-3.003058
15	6	0	3.387134	5.882671	-1.038465
16	6	0	-0.781429	1.966376	-3.146154
17	6	0	4.386617	-0.475005	0.425682
18	6	0	-4.373636	0.400833	0.438212
19	6	0	-0.554530	-0.529686	-1.587331
20	6	0	-0.442931	-1.757783	-2.268251
21	6	0	-1.488537	-2.656750	-2.187835
22	6	0	-2.669076	-2.390044	-1.465439
23	6	0	-2.805644	-1.144650	-0.795824
24	6	0	-1.708863	-0.253989	-0.856101
25	6	0	-3.653971	-4.703676	-2.153364
26	6	0	-4.960872	-5.008755	-2.898790
27	6	0	-3.712906	-3.410139	-1.355921
28	6	0	-4.713115	-3.210778	-0.461689
29	6	0	-4.913913	-1.949435	0.255224
30	6	0	-4.001188	-0.879386	0.000570
31	1	0	-3.831640	1.281181	0.124775
32	1	0	-1.364470	-3.607899	-2.686045
33	1	0	3.862330	-1.359695	0.082667
34	1	0	1.335167	3.536327	-2.769010
35	1	0	-6.262148	-3.701094	0.433749
36	1	0	-3.158152	-6.796177	-1.847806
37	1	0	2.668096	4.747247	-2.676806
38	8	0	-1.793724	0.911776	-0.154058
39	1	0	4.570506	5.933000	-3.551760
40	1	0	4.833195	4.193674	-3.732147
41	1	0	5.679083	5.090083	-2.460720
42	1	0	3.242318	6.831927	-1.561377
43	1	0	2.513258	5.707138	-0.405812
44	1	0	4.264755	5.975023	-0.397592
45	1	0	0.974479	-1.323546	-3.833484
46	1	0	0.688209	-3.048879	-3.557636
47	1	0	1.683247	-2.116669	-2.431261
48	8	0	5.710301	4.063423	-0.356788
49	1	0	6.386459	3.667430	0.211667
50	8	0	6.059052	1.768987	0.775802
51	1	0	6.068513	0.845889	1.188484
52	1	0	-0.688378	2.924632	-3.658029
53	1	0	-1.683335	1.994142	-2.528191
54	1	0	-0.929952	1.185886	-3.897349
55	8	0	1.785713	-0.912265	-0.108306
56	8	0	-5.929709	-1.880634	0.990393
57	1	0	-2.265768	-5.689908	-0.790261
58	1	0	-3.972939	-6.038032	-0.469794
59	8	0	-5.655787	-4.139787	-0.191162
60	1	0	-2.897192	-4.590670	-2.928036
61	1	0	-4.804997	-5.861765	-3.564812
62	1	0	-5.268537	-4.156828	-3.510502
63	1	0	-5.771978	-5.251026	-2.213657
64	1	0	0.940634	-1.383042	-0.146837
65	1	0	-0.935836	1.358698	-0.179115
66	7	0	5.383879	-0.607106	1.217797
67	6	0	7.141816	-2.149681	1.278346
68	6	0	5.384452	-2.154860	2.990549
69	6	0	7.529919	-3.580586	1.639697
70	1	0	7.718332	-1.452750	1.911396
71	6	0	5.751252	-3.585077	3.381806
72	1	0	5.994431	-1.452860	3.584470
73	6	0	7.217102	-3.891153	3.098333
74	1	0	8.594501	-3.716042	1.430997
75	1	0	6.975479	-4.262691	0.984832
76	1	0	5.522135	-3.724251	4.441696
77	1	0	5.110714	-4.269085	2.813112
78	1	0	7.443781	-4.935371	3.328366
79	1	0	7.849514	-3.271468	3.744740
80	7	0	5.697059	-1.959297	1.552190
81	7	0	-5.399103	0.660882	1.220020
82	7	0	-5.717695	1.986001	1.551278
83	6	0	-7.144198	2.226238	1.217831
84	6	0	-5.412198	2.218891	2.987594
85	6	0	-7.491201	3.674783	1.549629
86	1	0	-7.769150	1.562771	1.840956
87	6	0	-5.749354	3.668382	3.327916
88	1	0	-6.045155	1.553000	3.598713
89	6	0	-7.202267	3.998974	3.010357

90	1	0	-8.545378	3.840492	1.313041
91	1	0	-6.898949	4.327214	0.897728
92	1	0	-5.532237	3.834344	4.386145
93	1	0	-5.084161	4.318567	2.748003
94	1	0	-7.411859	5.050688	3.219568
95	1	0	-7.860219	3.402181	3.652590
96	6	0	7.443151	-1.861044	-0.186573
97	1	0	6.802694	-2.472987	-0.828871
98	1	0	7.282889	-0.811435	-0.437359
99	1	0	8.485733	-2.104435	-0.403920
100	6	0	3.908861	-1.890840	3.262395
101	1	0	3.636677	-0.847421	3.100083
102	1	0	3.287535	-2.514747	2.612664
103	1	0	3.679643	-2.140161	4.301173
104	6	0	-3.945204	1.927581	3.272359
105	1	0	-3.691920	0.876180	3.129843
106	1	0	-3.308092	2.530104	2.618222
107	1	0	-3.718323	2.188107	4.308519
108	6	0	-7.399801	1.924289	-0.252214
109	1	0	-6.721569	2.510417	-0.878995
110	1	0	-7.263438	0.867122	-0.485567
111	1	0	-8.426879	2.194484	-0.506989
112	1	0	-5.968475	-0.116677	1.567312

Structure 26bb (DMSO)

Energy (Hartrees): = -2381.6474668
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.736218	3.123812	-0.553652
2	6	0	3.670310	3.378686	-1.377828
3	6	0	2.648631	2.365275	-1.499456
4	6	0	2.789407	1.116149	-0.823714
5	6	0	3.983223	0.841848	-0.064022
6	6	0	4.903082	1.865514	0.093475
7	6	0	-3.237155	-5.862274	-1.283285
8	6	0	0.763636	-2.059872	-3.127816
9	6	0	3.580860	4.722166	-2.084536
10	6	0	1.685253	0.217065	-0.869997
11	6	0	0.552555	0.470622	-1.624608
12	6	0	0.454764	1.683849	-2.352786
13	6	0	1.476268	2.597479	-2.267400
14	6	0	4.781640	4.982795	-3.003753
15	6	0	3.374650	5.864564	-1.081680
16	6	0	-0.762522	1.956645	-3.194481
17	6	0	4.362831	-0.483538	0.435454
18	6	0	-4.357430	0.404185	0.450600
19	6	0	-0.561502	-0.524656	-1.616213
20	6	0	-0.461520	-1.745902	-2.310685
21	6	0	-1.506819	-2.644971	-2.224334
22	6	0	-2.676451	-2.381571	-1.482155
23	6	0	-2.802774	-1.140704	-0.801340
24	6	0	-1.704755	-0.251455	-0.867613
25	6	0	-3.670646	-4.689856	-2.171438
26	6	0	-4.985732	-4.997685	-2.899757
27	6	0	-3.722318	-3.399588	-1.368858
28	6	0	-4.711283	-3.203187	-0.461260
29	6	0	-4.895554	-1.948776	0.274790
30	6	0	-3.987813	-0.877879	0.011335
31	1	0	-3.820295	1.283635	0.125927
32	1	0	-1.390679	-3.591154	-2.734012
33	1	0	3.841855	-1.367966	0.086394
34	1	0	1.356609	3.525082	-2.807549
35	1	0	-6.244060	-3.680632	0.454964
36	1	0	-3.165744	-6.780459	-1.873107
37	1	0	2.707036	4.714607	-2.730860
38	8	0	-1.774963	0.905046	-0.150924
39	1	0	4.615800	5.906349	-3.564919
40	1	0	4.905103	4.169710	-3.723741
41	1	0	5.707821	5.087077	-2.439393
42	1	0	3.252069	6.811378	-1.614502
43	1	0	2.476924	5.695405	-0.481253
44	1	0	4.228328	5.957812	-0.408933
45	1	0	0.937444	-1.288789	-3.883684
46	1	0	0.649957	-3.019308	-3.633304
47	1	0	1.661184	-2.109058	-2.503967
48	8	0	5.704646	4.048000	-0.338600
49	1	0	6.367772	3.645150	0.239823
50	8	0	6.029090	1.760614	0.808839
51	1	0	6.034939	0.831349	1.212011
52	1	0	-0.663283	2.910607	-3.712921

53	1	0	-1.669901	1.991768	-2.584258
54	1	0	-0.905550	1.168813	-3.939502
55	8	0	1.759827	-0.910754	-0.115237
56	8	0	-5.895796	-1.888880	1.030590
57	1	0	-2.260737	-5.671980	-0.829538
58	1	0	-3.963184	-6.024553	-0.483050
59	8	0	-5.657609	-4.126157	-0.184364
60	1	0	-2.923259	-4.575222	-2.954698
61	1	0	-4.835070	-5.847752	-3.570596
62	1	0	-5.304811	-4.145410	-3.505618
63	1	0	-5.787046	-5.245111	-2.204809
64	1	0	0.921723	-1.390592	-0.187461
65	1	0	-0.924335	1.363023	-0.210947
66	7	0	5.353937	-0.614601	1.235260
67	6	0	7.116118	-2.152684	1.288715
68	6	0	5.370478	-2.154906	3.013778
69	6	0	7.510604	-3.580447	1.654807
70	1	0	7.693161	-1.450635	1.914665
71	6	0	5.743272	-3.582197	3.408198
72	1	0	5.983874	-1.449253	3.599024
73	6	0	7.207742	-3.885172	3.116605
74	1	0	8.574441	-3.711898	1.440393
75	1	0	6.955330	-4.268461	1.006387
76	1	0	5.521069	-3.716040	4.470118
77	1	0	5.100821	-4.271159	2.847164
78	1	0	7.438537	-4.927846	3.349347
79	1	0	7.842097	-3.260580	3.756074
80	7	0	5.671258	-1.965260	1.571094
81	7	0	-5.373699	0.668266	1.239949
82	7	0	-5.687847	1.996036	1.567663
83	6	0	-7.114821	2.237403	1.231298
84	6	0	-5.388761	2.223116	3.007472
85	6	0	-7.463402	3.683841	1.569041
86	1	0	-7.738996	1.569399	1.848885
87	6	0	-5.728357	3.670380	3.353204
88	1	0	-6.023754	1.553292	3.610793
89	6	0	-7.180148	4.001256	3.032056
90	1	0	-8.516995	3.848034	1.329245
91	1	0	-6.870123	4.341063	0.922459
92	1	0	-5.515507	3.829069	4.413347
93	1	0	-5.061578	4.325298	2.779964
94	1	0	-7.390562	5.052173	3.244712
95	1	0	-7.839495	3.400431	3.668801
96	6	0	7.406754	-1.871200	-0.179462
97	1	0	6.764916	-2.488260	-0.815912
98	1	0	7.242598	-0.823212	-0.435587
99	1	0	8.448811	-2.112931	-0.400976
100	6	0	3.896663	-1.894321	3.295948
101	1	0	3.617903	-0.853592	3.125918
102	1	0	3.271415	-2.528819	2.660012
103	1	0	3.678980	-2.133877	4.339415
104	6	0	-3.922677	1.932620	3.296125
105	1	0	-3.667351	0.882250	3.147545
106	1	0	-3.283084	2.542079	2.650538
107	1	0	-3.702062	2.185537	4.335525
108	6	0	-7.364379	1.945233	-0.241494
109	1	0	-6.688154	2.539127	-0.863537
110	1	0	-7.222928	0.890329	-0.482626
111	1	0	-8.392303	2.212432	-0.496156
112	1	0	-5.943595	-0.101727	1.602096

Structure 27 (vacuum)

Energy (Hartrees): = -1112.7639881
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.608918	-1.879587	-0.147416
2	6	0	-2.634923	-1.016060	0.133481
3	6	0	-2.367092	0.399188	0.099719
4	6	0	-1.028725	0.868601	-0.056088
5	6	0	0.051939	-0.080677	-0.174406
6	6	0	-0.260107	-1.429002	-0.274671
7	6	0	-4.046405	-1.524042	0.400179
8	6	0	-0.860027	2.282480	-0.160269
9	6	0	-1.917872	3.152701	-0.062133
10	6	0	-3.232183	2.686603	0.107863
11	6	0	-3.434927	1.333167	0.178581
12	6	0	-4.147786	-2.769609	1.305784
13	6	0	-4.820378	-1.724156	-0.910405
14	6	0	-4.369217	3.669847	0.184927
15	6	0	1.466661	0.312305	-0.099345

16	1	0	1.684794	1.316452	0.227800
17	1	0	-4.453933	0.981931	0.259667
18	1	0	-4.549145	-0.741496	0.965809
19	1	0	-5.107792	-2.755012	1.825290
20	1	0	-3.354041	-2.791272	2.053891
21	1	0	-4.126198	-3.716756	0.757154
22	1	0	-5.848071	-2.040669	-0.712881
23	1	0	-4.843849	-0.801742	-1.494066
24	1	0	-4.344352	-2.490527	-1.530606
25	8	0	-1.743538	-3.223155	-0.281569
26	1	0	-2.673937	-3.450486	-0.292932
27	8	0	0.642693	-2.392440	-0.451754
28	1	0	1.522373	-1.951033	-0.540210
29	1	0	-5.326725	3.157672	0.283710
30	1	0	-4.407314	4.294032	-0.711700
31	1	0	-4.250838	4.335759	1.043832
32	8	0	0.394394	2.782027	-0.393485
33	1	0	0.317731	3.727882	-0.543078
34	7	0	2.397057	-0.526038	-0.386960
35	6	0	4.090180	1.056285	0.316778
36	6	0	4.505308	-1.351780	0.083796
37	6	0	5.584347	1.330240	0.163180
38	1	0	3.806219	1.021604	1.384387
39	1	0	3.533204	1.871934	-0.148884
40	6	0	5.995669	-1.110815	-0.107339
41	1	0	4.294975	-1.574465	1.143658
42	1	0	4.163973	-2.201464	-0.508852
43	6	0	6.425817	0.149457	0.639869
44	1	0	5.832936	2.239002	0.716638
45	1	0	5.794068	1.520935	-0.893865
46	1	0	6.547696	-1.985541	0.244412
47	1	0	6.202375	-0.993855	-1.175766
48	1	0	7.488489	0.350198	0.486471
49	1	0	6.274643	0.002883	1.715936
50	7	0	3.725648	-0.189557	-0.345422
51	1	0	-1.732788	4.220868	-0.147198

Structure 27 ($CHCl_3$)

Energy (Hartrees): = -1112.794847
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.592687	-1.878856	-0.155708
2	6	0	-2.628012	-1.026085	0.130098
3	6	0	-2.370947	0.392435	0.092204
4	6	0	-1.037725	0.875089	-0.075237
5	6	0	0.052631	-0.063371	-0.195389
6	6	0	-0.250040	-1.414234	-0.287998
7	6	0	-4.032688	-1.545557	0.414330
8	6	0	-0.878965	2.291286	-0.190264
9	6	0	-1.942330	3.153937	-0.077163
10	6	0	-3.250563	2.675153	0.117790
11	6	0	-3.445362	1.319140	0.189769
12	6	0	-4.110690	-2.793030	1.316867
13	6	0	-4.826181	-1.750835	-0.883319
14	6	0	-4.390965	3.651395	0.221743
15	6	0	1.465825	0.340343	-0.111589
16	1	0	1.680777	1.340015	0.232310
17	1	0	-4.460196	0.959944	0.287755
18	1	0	-4.533942	-0.767594	0.987340
19	1	0	-5.073180	-2.794805	1.832975
20	1	0	-3.322893	-2.797986	2.072897
21	1	0	-4.068028	-3.738815	0.768168
22	1	0	-5.850518	-2.063327	-0.662038
23	1	0	-4.864233	-0.832243	-1.473360
24	1	0	-4.365669	-2.525467	-1.505765
25	8	0	-1.709724	-3.226048	-0.283029
26	1	0	-2.636811	-3.470645	-0.342783
27	8	0	0.668524	-2.370390	-0.461519
28	1	0	1.544373	-1.912778	-0.551435
29	1	0	-5.343373	3.134922	0.348410
30	1	0	-4.456052	4.273670	-0.675097
31	1	0	-4.250901	4.322201	1.073967
32	8	0	0.366284	2.787785	-0.447541
33	1	0	0.299520	3.740889	-0.579984
34	7	0	2.398004	-0.493147	-0.409495
35	6	0	4.091721	1.062247	0.345924
36	6	0	4.498053	-1.346159	0.048532
37	6	0	5.589418	1.328974	0.222335
38	1	0	3.791216	0.995881	1.406287
39	1	0	3.548290	1.894999	-0.104741

40	6	0	5.991391	-1.106012	-0.113474
41	1	0	4.270154	-1.595575	1.097738
42	1	0	4.163245	-2.176902	-0.574736
43	6	0	6.416547	0.129573	0.676303
44	1	0	5.832092	2.219152	0.807683
45	1	0	5.818118	1.551992	-0.824875
46	1	0	6.531285	-1.994581	0.222349
47	1	0	6.217004	-0.960496	-1.175079
48	1	0	7.482329	0.328517	0.542118
49	1	0	6.248877	-0.047728	1.745175
50	7	0	3.726796	-0.165321	-0.356481
51	1	0	-1.766330	4.222661	-0.171284

Structure 27 (DMSO)

Energy (Hartrees): = -1112.7913118
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.583037	-1.878779	-0.154745
2	6	0	-2.621987	-1.031174	0.136148
3	6	0	-2.372877	0.388834	0.098190
4	6	0	-1.042576	0.879063	-0.072001
5	6	0	0.053156	-0.053591	-0.191777
6	6	0	-0.242128	-1.406883	-0.286537
7	6	0	-4.024453	-1.558036	0.416259
8	6	0	-0.891138	2.295923	-0.192633
9	6	0	-1.959262	3.153315	-0.080405
10	6	0	-3.264691	2.666680	0.117429
11	6	0	-3.453211	1.309347	0.194292
12	6	0	-4.100227	-2.806528	1.316870
13	6	0	-4.808824	-1.767806	-0.885406
14	6	0	-4.410723	3.636195	0.214586
15	6	0	1.465062	0.356971	-0.102678
16	1	0	1.678313	1.352016	0.257119
17	1	0	-4.466300	0.945628	0.295097
18	1	0	-4.534084	-0.783465	0.986028
19	1	0	-5.066831	-2.812948	1.824821
20	1	0	-3.319784	-2.806469	2.080861
21	1	0	-4.051365	-3.753476	0.769762
22	1	0	-5.830530	-2.090458	-0.667592
23	1	0	-4.855241	-0.846343	-1.470896
24	1	0	-4.340107	-2.537154	-1.508208
25	8	0	-1.698878	-3.223796	-0.290783
26	1	0	-2.628638	-3.468838	-0.303592
27	8	0	0.683616	-2.355169	-0.462079
28	1	0	1.555350	-1.886336	-0.548875
29	1	0	-5.359757	3.114269	0.343926
30	1	0	-4.476739	4.252684	-0.686133
31	1	0	-4.273635	4.314534	1.061244
32	8	0	0.349299	2.795385	-0.458191
33	1	0	0.282401	3.753689	-0.555923
34	7	0	2.397663	-0.471444	-0.414805
35	6	0	4.097722	1.065000	0.365247
36	6	0	4.493711	-1.341649	0.028209
37	6	0	5.596285	1.325973	0.242834
38	1	0	3.799439	0.979081	1.424223
39	1	0	3.557863	1.908242	-0.069336
40	6	0	5.987316	-1.104644	-0.131927
41	1	0	4.266604	-1.602792	1.074363
42	1	0	4.154281	-2.162034	-0.606582
43	6	0	6.418096	0.116063	0.677030
44	1	0	5.843236	2.205960	0.841388
45	1	0	5.825341	1.564408	-0.801087
46	1	0	6.523157	-2.000990	0.189181
47	1	0	6.213135	-0.942853	-1.191298
48	1	0	7.484581	0.312277	0.544097
49	1	0	6.249619	-0.077599	1.742850
50	7	0	3.726719	-0.150112	-0.358052
51	1	0	-1.790567	4.222850	-0.180939

Structure 28 (vacuum)

Energy (Hartrees): = -1112.7465402
Imaginary frequency -392.77

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.657084	-1.872382	-0.125742
2	6	0	2.695091	-0.969747	-0.120228
3	6	0	2.370177	0.428089	-0.081365
4	6	0	1.007205	0.846466	-0.154770
5	6	0	-0.038772	-0.130794	-0.239141
6	6	0	0.301362	-1.460881	-0.236150
7	6	0	4.148330	-1.427287	-0.096983
8	6	0	0.748525	2.250533	-0.087867
9	6	0	1.761305	3.165764	0.041283
10	6	0	3.104350	2.751885	0.130808
11	6	0	3.387785	1.413578	0.068369
12	6	0	4.492748	-2.605941	-1.032032
13	6	0	4.620019	-1.700093	1.337855
14	6	0	4.186130	3.785731	0.294252
15	6	0	-1.476229	0.221650	-0.348613
16	1	0	-1.751735	0.948708	-1.103144
17	1	0	4.421506	1.114292	0.168623
18	1	0	4.736108	-0.598239	-0.486442
19	1	0	5.544496	-2.540401	-1.317234
20	1	0	3.890577	-2.591633	-1.941786
21	1	0	4.382056	-3.589302	-0.561934
22	1	0	5.676250	-1.982125	1.355564
23	1	0	4.481767	-0.817931	1.966111
24	1	0	4.045061	-2.516051	1.787968
25	8	0	1.809810	-3.221233	-0.040735
26	1	0	2.732721	-3.430724	0.108563
27	8	0	-0.635132	-2.440342	-0.421624
28	1	0	-0.823705	-2.859192	0.422984
29	1	0	5.166065	3.319059	0.398096
30	1	0	4.004709	4.401778	1.178726
31	1	0	4.216624	4.453553	-0.570775
32	8	0	-0.548187	2.667664	-0.151078
33	1	0	-0.570537	3.617348	-0.006216
34	7	0	-2.303490	-0.343468	0.438702
35	6	0	-4.140450	0.765230	-0.705389
36	6	0	-4.421924	-1.228733	0.694796
37	6	0	-5.605902	1.131688	-0.482800
38	1	0	-4.013904	0.222340	-1.659783
39	1	0	-3.552207	1.683259	-0.764436
40	6	0	-5.878641	-0.878592	0.964480
41	1	0	-4.359325	-1.931944	-0.153416
42	1	0	-3.955968	-1.706320	1.556954
43	6	0	-6.460599	-0.104405	-0.216867
44	1	0	-5.969407	1.680206	-1.355460
45	1	0	-5.666442	1.805139	0.378032
46	1	0	-6.441996	-1.796619	1.148906
47	1	0	-5.934297	-0.265350	1.869693
48	1	0	-7.497627	0.180458	-0.023844
49	1	0	-6.460409	-0.746205	-1.105996
50	7	0	-3.636211	-0.030547	0.405039
51	1	0	1.520050	4.224735	0.088179

Structure 28 ($CHCl_3$)

Energy (Hartrees): = -1112.7794426
Imaginary frequency -366.08

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.660246	-1.883873	-0.102741
2	6	0	2.697588	-0.979376	-0.125262
3	6	0	2.368290	0.419710	-0.082419
4	6	0	1.004164	0.837901	-0.130438
5	6	0	-0.041483	-0.141620	-0.205398
6	6	0	0.301133	-1.471399	-0.194358
7	6	0	4.157974	-1.418324	-0.146977
8	6	0	0.741591	2.242254	-0.053165
9	6	0	1.755972	3.159913	0.052807
10	6	0	3.102338	2.746435	0.105482
11	6	0	3.388856	1.406976	0.038384
12	6	0	4.480625	-2.644598	-1.022529
13	6	0	4.708157	-1.597365	1.273826
14	6	0	4.185203	3.781206	0.249706
15	6	0	-1.478374	0.213434	-0.329593
16	1	0	-1.746154	0.914606	-1.111432
17	1	0	4.425434	1.107926	0.109640
18	1	0	4.707365	-0.603462	-0.616357
19	1	0	5.526857	-2.589818	-1.331253
20	1	0	3.865962	-2.678332	-1.924434
21	1	0	4.382570	-3.600910	-0.498316
22	1	0	5.771826	-1.850321	1.247406
23	1	0	4.583756	-0.685226	1.861994

24	1	0	4.182406	-2.403735	1.795492
25	8	0	1.811936	-3.231883	-0.019722
26	1	0	2.728237	-3.447718	0.173445
27	8	0	-0.638068	-2.455073	-0.358581
28	1	0	-0.851540	-2.836953	0.500875
29	1	0	4.125077	4.521466	-0.552756
30	1	0	5.175200	3.324531	0.219826
31	1	0	4.084085	4.319122	1.196570
32	8	0	-0.555673	2.649055	-0.079902
33	1	0	-0.588144	3.604934	0.045478
34	7	0	-2.315472	-0.318352	0.471440
35	6	0	-4.138222	0.739565	-0.744020
36	6	0	-4.438817	-1.193328	0.736895
37	6	0	-5.609938	1.104671	-0.570001
38	1	0	-3.988039	0.149303	-1.665342
39	1	0	-3.558204	1.659544	-0.838350
40	6	0	-5.903251	-0.842718	0.956998
41	1	0	-4.350577	-1.927630	-0.081330
42	1	0	-3.996245	-1.634755	1.630814
43	6	0	-6.463881	-0.123061	-0.268039
44	1	0	-5.953644	1.609239	-1.476404
45	1	0	-5.696109	1.818482	0.255754
46	1	0	-6.461662	-1.758557	1.166071
47	1	0	-5.986144	-0.194315	1.835812
48	1	0	-7.505420	0.165493	-0.106354
49	1	0	-6.443014	-0.802784	-1.128146
50	7	0	-3.650154	-0.000584	0.415857
51	1	0	1.510916	4.217203	0.110916

Structure 28 (DMSO)

Energy (Hartrees): = -1112.7751443
Imaginary frequency -405.23

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.667993	-1.886002	-0.107041
2	6	0	2.701793	-0.976656	-0.125662
3	6	0	2.366791	0.421393	-0.081534
4	6	0	1.000578	0.834952	-0.128971
5	6	0	-0.040854	-0.149240	-0.207848
6	6	0	0.306946	-1.478150	-0.201216
7	6	0	4.164297	-1.408473	-0.139733
8	6	0	0.732180	2.238509	-0.047710
9	6	0	1.743823	3.160165	0.051481
10	6	0	3.092002	2.750939	0.102196
11	6	0	3.384523	1.411961	0.038699
12	6	0	4.498660	-2.638964	-1.004242
13	6	0	4.706922	-1.575858	1.284984
14	6	0	4.170781	3.790867	0.231407
15	6	0	-1.478535	0.202734	-0.334982
16	1	0	-1.747799	0.903037	-1.117289
17	1	0	4.422472	1.117714	0.110908
18	1	0	4.712200	-0.594057	-0.611251
19	1	0	5.547214	-2.579103	-1.303538
20	1	0	3.893947	-2.680493	-1.912832
21	1	0	4.404118	-3.593207	-0.474890
22	1	0	5.773240	-1.816890	1.263400
23	1	0	4.571898	-0.661521	1.867726
24	1	0	4.189012	-2.387516	1.806496
25	8	0	1.825656	-3.231063	-0.023735
26	1	0	2.746675	-3.440966	0.156961
27	8	0	-0.627614	-2.464108	-0.374177
28	1	0	-0.848201	-2.844285	0.484385
29	1	0	5.154070	3.329845	0.333127
30	1	0	3.993559	4.425893	1.103503
31	1	0	4.185732	4.443439	-0.646187
32	8	0	-0.566544	2.639743	-0.059478
33	1	0	-0.596348	3.601028	0.028303
34	7	0	-2.315027	-0.329428	0.467305
35	6	0	-4.138114	0.741119	-0.739840
36	6	0	-4.442476	-1.204049	0.724778
37	6	0	-5.606880	1.111722	-0.555574
38	1	0	-3.996005	0.154877	-1.664518
39	1	0	-3.553834	1.658642	-0.831513
40	6	0	-5.904915	-0.850202	0.951629
41	1	0	-4.360698	-1.927956	-0.103061
42	1	0	-4.001332	-1.659124	1.612793
43	6	0	-6.465680	-0.114659	-0.263346
44	1	0	-5.950426	1.627542	-1.455525
45	1	0	-5.685847	1.817812	0.277749
46	1	0	-6.464943	-1.766976	1.151602
47	1	0	-5.985017	-0.212226	1.838520

48	1	0	-7.504848	0.177576	-0.093563
49	1	0	-6.451389	-0.785159	-1.130726
50	7	0	-3.650019	-0.009744	0.414466
51	1	0	1.496874	4.217043	0.111316

Structure $TS_{19b/20b}$ (vacuum)

Energy (Hartrees): = -1112.7703062
Imaginary frequency -1072.92

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.452938	-1.841367	0.062009
2	6	0	-2.585210	-1.087355	-0.034226
3	6	0	-2.457157	0.359378	-0.015579
4	6	0	-1.169147	0.969651	0.040366
5	6	0	0.015101	0.136717	0.092187
6	6	0	-0.140909	-1.258832	0.124785
7	6	0	-3.927420	-1.794836	-0.139294
8	6	0	-1.129831	2.388276	0.063709
9	6	0	-2.272469	3.152995	0.031099
10	6	0	-3.538763	2.555111	-0.018012
11	6	0	-3.609583	1.183149	-0.039964
12	6	0	-4.247102	-2.579607	1.140886
13	6	0	-4.005897	-2.688864	-1.386080
14	6	0	-4.773927	3.415920	-0.043755
15	6	0	1.375326	0.600604	0.083289
16	1	0	1.632902	1.648491	0.014699
17	1	0	-4.591439	0.735891	-0.065578
18	1	0	-4.708732	-1.047751	-0.256490
19	1	0	-5.237916	-3.034638	1.061695
20	1	0	-4.241216	-1.919386	2.011142
21	1	0	-3.514621	-3.371104	1.300328
22	1	0	-5.014826	-3.098291	-1.482002
23	1	0	-3.783923	-2.113067	-2.287341
24	1	0	-3.301712	-3.517093	-1.322097
25	8	0	-1.477443	-3.195610	0.089923
26	1	0	-0.547966	-3.468246	0.146290
27	8	0	0.848790	-2.100121	0.189992
28	1	0	-4.813857	4.067891	0.832657
29	1	0	-5.677423	2.805699	-0.054086
30	1	0	-4.785678	4.054865	-0.930706
31	8	0	0.093358	3.001287	0.126077
32	1	0	-0.042356	3.951723	0.157123
33	7	0	2.344546	-0.259730	0.143286
34	6	0	4.439235	-0.363650	1.169430
35	6	0	4.235795	-0.128096	-1.232453
36	6	0	5.868237	0.166023	1.141247
37	1	0	4.440668	-1.463520	1.080028
38	1	0	3.942434	-0.102811	2.105134
39	6	0	5.656649	0.411127	-1.340763
40	1	0	4.232588	-1.223956	-1.359567
41	1	0	3.594309	0.302026	-2.003605
42	6	0	6.525140	-0.131694	-0.206258
43	1	0	6.434063	-0.285280	1.959675
44	1	0	5.844545	1.246862	1.309997
45	1	0	6.070703	0.138638	-2.314403
46	1	0	5.620993	1.503619	-1.288660
47	1	0	7.527946	0.299033	-0.249759
48	1	0	6.634159	-1.216359	-0.323058
49	7	0	3.665147	0.234133	0.074108
50	1	0	1.855526	-1.383223	0.181366
51	1	0	-2.185464	4.236810	0.051794

Structure $TS_{19b/20b}$ ($CHCl_3$)

Energy (Hartrees): = -1112.7970938
Imaginary frequency -1087.92

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.446888	-1.841616	0.001475
2	6	0	2.586651	-1.090055	0.005544
3	6	0	2.460538	0.356330	0.023149
4	6	0	1.171325	0.968736	0.067667
5	6	0	-0.015529	0.137393	0.081175
6	6	0	0.137450	-1.256170	0.048663
7	6	0	3.933164	-1.798118	-0.031072

8	6	0	1.133404	2.390901	0.091990
9	6	0	2.277807	3.153834	0.053458
10	6	0	3.543971	2.552345	-0.003412
11	6	0	3.615647	1.179546	-0.013764
12	6	0	4.135323	-2.540282	-1.358925
13	6	0	4.136479	-2.727830	1.173560
14	6	0	4.778788	3.411053	-0.059205
15	6	0	-1.381469	0.607581	0.103250
16	1	0	-1.634184	1.659043	0.108962
17	1	0	4.597468	0.733508	-0.063345
18	1	0	4.721621	-1.052706	0.033606
19	1	0	5.129542	-2.994891	-1.385526
20	1	0	4.054493	-1.851942	-2.204000
21	1	0	3.393280	-3.329990	-1.485000
22	1	0	5.154569	-3.126633	1.159226
23	1	0	4.001173	-2.184106	2.112055
24	1	0	3.440291	-3.565664	1.157808
25	8	0	1.472495	-3.196392	-0.044512
26	1	0	0.544883	-3.482930	-0.029067
27	8	0	-0.859930	-2.098916	0.053875
28	1	0	4.783884	4.028867	-0.961616
29	1	0	5.682712	2.800380	-0.060973
30	1	0	4.825278	4.086945	0.798933
31	8	0	-0.085488	3.000663	0.153955
32	1	0	0.040831	3.956696	0.162918
33	7	0	-2.347548	-0.252175	0.106117
34	6	0	-4.254285	-0.043713	-1.234902
35	6	0	-4.426407	-0.433006	1.152561
36	6	0	-5.682662	0.482621	-1.291364
37	1	0	-4.240008	-1.129194	-1.426396
38	1	0	-3.629006	0.442336	-1.986122
39	6	0	-5.860949	0.080809	1.172899
40	1	0	-4.416472	-1.523473	0.989649
41	1	0	-3.922835	-0.226386	2.098609
42	6	0	-6.530761	-0.139747	-0.182799
43	1	0	-6.103637	0.264292	-2.275703
44	1	0	-5.661838	1.570824	-1.173560
45	1	0	-6.409376	-0.429457	1.968383
46	1	0	-5.849670	1.149461	1.410431
47	1	0	-7.538127	0.283267	-0.186854
48	1	0	-6.628954	-1.216157	-0.365619
49	7	0	-3.670593	0.244275	0.087199
50	1	0	-1.847046	-1.390784	0.077542
51	1	0	2.189257	4.237471	0.066231

Structure $TS_{19b/20b}$ (DMSO)

Energy (Hartrees): = -1112.7917492
Imaginary frequency -1086.84

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.439481	-1.843330	0.057962
2	6	0	2.574940	-1.093585	-0.061480
3	6	0	2.453566	0.352834	-0.019106
4	6	0	1.167989	0.966981	0.086112
5	6	0	-0.017789	0.137656	0.151782
6	6	0	0.134823	-1.255227	0.167010
7	6	0	3.913853	-1.802231	-0.204652
8	6	0	1.134093	2.388852	0.149973
9	6	0	2.278919	3.149892	0.092529
10	6	0	3.541359	2.546654	-0.019498
11	6	0	3.610284	1.173957	-0.070203
12	6	0	3.964463	-2.695475	-1.452176
13	6	0	4.266089	-2.587531	1.065323
14	6	0	4.775345	3.404775	-0.084281
15	6	0	-1.384447	0.610470	0.161567
16	1	0	-1.634734	1.659995	0.083589
17	1	0	4.591029	0.727811	-0.144536
18	1	0	4.693468	-1.056941	-0.338421
19	1	0	4.972639	-3.101488	-1.571529
20	1	0	3.724279	-2.121644	-2.351163
21	1	0	3.265630	-3.528321	-1.377745
22	1	0	5.255433	-3.041480	0.960476
23	1	0	4.287241	-1.929085	1.937797
24	1	0	3.540963	-3.381912	1.248945
25	8	0	1.459658	-3.198695	0.070500
26	1	0	0.531892	-3.473753	0.147634
27	8	0	-0.860515	-2.096652	0.253056
28	1	0	4.765404	4.033449	-0.979158
29	1	0	5.678642	2.793432	-0.106641
30	1	0	4.832829	4.072031	0.779823
31	8	0	-0.078772	2.997318	0.280445

32	1	0	0.053594	3.952711	0.322662
33	7	0	-2.347709	-0.247211	0.239276
34	6	0	-4.145055	0.138609	-1.223576
35	6	0	-4.498464	-0.594154	1.062443
36	6	0	-5.572805	0.661229	-1.315937
37	1	0	-4.097897	-0.908022	-1.565026
38	1	0	-3.473122	0.734040	-1.844573
39	6	0	-5.936819	-0.092950	1.043330
40	1	0	-4.459655	-1.648168	0.742220
41	1	0	-4.074419	-0.525664	2.065911
42	6	0	-6.495784	-0.115859	-0.378310
43	1	0	-5.911211	0.582578	-2.351828
44	1	0	-5.578354	1.722364	-1.045538
45	1	0	-6.538704	-0.715690	1.709396
46	1	0	-5.959662	0.929473	1.434534
47	1	0	-7.505132	0.301613	-0.401150
48	1	0	-6.563893	-1.154795	-0.721273
49	7	0	-3.671563	0.233772	0.171353
50	1	0	-1.845118	-1.386462	0.262115
51	1	0	2.196538	4.232826	0.144195

Structure $TS_{19a/20a}$ (vacuum)

Energy (Hartrees): = -1112.7687782
Imaginary frequency -846.49

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.573584	-1.854502	-0.018673
2	6	0	-2.651000	-1.020121	-0.036454
3	6	0	-2.415011	0.412405	0.003169
4	6	0	-1.083263	0.926721	0.005077
5	6	0	0.036859	0.008560	-0.022901
6	6	0	-0.215779	-1.374678	-0.001828
7	6	0	-4.045252	-1.626254	-0.083751
8	6	0	-0.944031	2.338435	0.062365
9	6	0	-2.028047	3.183840	0.101335
10	6	0	-3.335258	2.679412	0.098696
11	6	0	-3.503956	1.316689	0.052595
12	6	0	-4.350272	-2.428078	1.189323
13	6	0	-4.258140	-2.470228	-1.348840
14	6	0	-4.505697	3.625323	0.147705
15	6	0	1.420635	0.390111	-0.116749
16	1	0	1.700877	1.426930	-0.203173
17	1	0	-4.515360	0.940079	0.066223
18	1	0	-4.776358	-0.822749	-0.133130
19	1	0	-5.374636	-2.808461	1.155251
20	1	0	-4.247925	-1.798129	2.075977
21	1	0	-3.669881	-3.274578	1.284381
22	1	0	-5.296529	-2.809092	-1.395397
23	1	0	-4.050700	-1.880312	-2.244469
24	1	0	-3.609077	-3.345012	-1.352828
25	8	0	-1.691358	-3.203379	-0.024573
26	1	0	-0.777445	-3.533020	-0.022702
27	8	0	0.706876	-2.283069	0.001607
28	1	0	-5.449772	3.080061	0.155320
29	1	0	-4.506274	4.291086	-0.719392
30	1	0	-4.468117	4.250818	1.043455
31	8	0	0.322448	2.870832	0.086497
32	1	0	0.245820	3.825071	0.165222
33	7	0	2.332392	-0.537176	-0.125761
34	6	0	4.115325	1.038570	-0.401192
35	6	0	4.425554	-1.126146	0.685037
36	6	0	5.605312	1.105760	-0.722973
37	1	0	3.902805	1.564149	0.547379
38	1	0	3.546764	1.529674	-1.194104
39	6	0	5.915801	-1.114559	0.376429
40	1	0	4.239073	-0.703209	1.686263
41	1	0	4.029076	-2.142938	0.671478
42	6	0	6.428016	0.322491	0.298107
43	1	0	5.911974	2.153838	-0.752461
44	1	0	5.763161	0.685965	-1.720911
45	1	0	6.444292	-1.677983	1.148604
46	1	0	6.082821	-1.620391	-0.579259
47	1	0	7.487043	0.342377	0.032246
48	1	0	6.331766	0.795390	1.282619
49	7	0	3.691438	-0.353310	-0.326294
50	1	0	1.818714	-1.571579	-0.081563
51	1	0	-1.861918	4.257836	0.142252

Structure $TS_{19a/20a}$ ($CHCl_3$)

Energy (Hartrees): = -1112.7972018
Imaginary frequency -899.52

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.558181	-1.852925	-0.019774
2	6	0	2.642670	-1.028646	0.064204
3	6	0	2.418827	0.404253	0.022451
4	6	0	1.089742	0.927542	0.006391
5	6	0	-0.036848	0.018532	0.013830
6	6	0	0.207621	-1.360659	-0.049141
7	6	0	4.033477	-1.638565	0.162216
8	6	0	0.957172	2.342975	-0.067273
9	6	0	2.048130	3.180299	-0.100546
10	6	0	3.353788	2.665213	-0.085510
11	6	0	3.516881	1.301601	-0.027133
12	6	0	4.426849	-2.339670	-1.144664
13	6	0	4.179658	-2.576378	1.369091
14	6	0	4.528054	3.604756	-0.151383
15	6	0	-1.425537	0.409971	0.139783
16	1	0	-1.697516	1.441261	0.294154
17	1	0	4.526622	0.918881	-0.043559
18	1	0	4.752867	-0.839263	0.325266
19	1	0	5.446074	-2.729851	-1.072220
20	1	0	4.387963	-1.643933	-1.986848
21	1	0	3.754551	-3.173181	-1.355574
22	1	0	5.225730	-2.878169	1.471983
23	1	0	3.882485	-2.071690	2.291878
24	1	0	3.574417	-3.475193	1.257814
25	8	0	1.671581	-3.203000	-0.057943
26	1	0	0.759588	-3.538252	-0.086673
27	8	0	-0.728438	-2.265488	-0.092361
28	1	0	5.471673	3.060482	-0.094534
29	1	0	4.500345	4.325300	0.670613
30	1	0	4.520047	4.175350	-1.084306
31	8	0	-0.302787	2.871456	-0.120169
32	1	0	-0.235900	3.829287	-0.210594
33	7	0	-2.334820	-0.513175	0.103775
34	6	0	-4.123368	1.049358	0.414726
35	6	0	-4.430249	-1.123587	-0.676587
36	6	0	-5.612217	1.104285	0.741188
37	1	0	-3.913636	1.578242	-0.531149
38	1	0	-3.558786	1.539326	1.210804
39	6	0	-5.917129	-1.116601	-0.356291
40	1	0	-4.254400	-0.700465	-1.678253
41	1	0	-4.030272	-2.139110	-0.662476
42	6	0	-6.435237	0.317836	-0.276339
43	1	0	-5.921674	2.151471	0.771970
44	1	0	-5.765896	0.684424	1.740163
45	1	0	-6.445089	-1.683052	-1.126881
46	1	0	-6.078403	-1.623489	0.600422
47	1	0	-7.492959	0.331497	-0.003679
48	1	0	-6.344818	0.790955	-1.261339
49	7	0	-3.686902	-0.341608	0.325617
50	1	0	-1.804026	-1.562681	0.002234
51	1	0	1.887435	4.254049	-0.156619

Structure $TS_{19a/20a}$ (DMSO)

Energy (Hartrees): = -1112.792892
Imaginary frequency -938.04

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.558854	-1.852382	0.017081
2	6	0	2.647539	-1.027911	0.035163
3	6	0	2.422317	0.405018	0.003711
4	6	0	1.091369	0.927249	-0.023056
5	6	0	-0.035970	0.019573	0.001730
6	6	0	0.209089	-1.359925	-0.009348
7	6	0	4.038819	-1.643589	0.069872
8	6	0	0.958137	2.343495	-0.108700
9	6	0	2.047716	3.183040	-0.119055
10	6	0	3.353759	2.670120	-0.061499
11	6	0	3.519719	1.306429	-0.007361
12	6	0	4.323839	-2.468985	-1.191855
13	6	0	4.268386	-2.465804	1.344778
14	6	0	4.525716	3.613372	-0.076028
15	6	0	-1.428775	0.415340	0.108957

16	1	0	-1.705592	1.450514	0.222550
17	1	0	4.531462	0.929936	0.022401
18	1	0	4.776085	-0.845261	0.086743
19	1	0	5.353650	-2.836349	-1.170411
20	1	0	4.202123	-1.859258	-2.091148
21	1	0	3.654551	-3.327477	-1.263306
22	1	0	5.302132	-2.821286	1.374381
23	1	0	4.095501	-1.857026	2.236192
24	1	0	3.606934	-3.332093	1.384787
25	8	0	1.667166	-3.203549	0.029962
26	1	0	0.751960	-3.530737	0.023849
27	8	0	-0.727157	-2.267628	-0.014564
28	1	0	5.468968	3.070582	-0.000979
29	1	0	4.469225	4.320675	0.755836
30	1	0	4.541522	4.200790	-0.998428
31	8	0	-0.299024	2.867325	-0.195526
32	1	0	-0.232326	3.827657	-0.268923
33	7	0	-2.334019	-0.511165	0.107092
34	6	0	-4.121127	1.061314	0.386534
35	6	0	-4.434193	-1.140026	-0.651008
36	6	0	-5.607285	1.121108	0.723000
37	1	0	-3.920529	1.565958	-0.573619
38	1	0	-3.550287	1.570403	1.166045
39	6	0	-5.918215	-1.125404	-0.319140
40	1	0	-4.266938	-0.738520	-1.662550
41	1	0	-4.034410	-2.155149	-0.614848
42	6	0	-6.436718	0.309851	-0.269044
43	1	0	-5.916548	2.168694	0.730102
44	1	0	-5.754270	0.726048	1.733294
45	1	0	-6.450766	-1.710271	-1.072536
46	1	0	-6.072281	-1.610214	0.650408
47	1	0	-7.492336	0.328666	0.011491
48	1	0	-6.353205	0.759689	-1.265296
49	7	0	-3.683692	-0.332355	0.326421
50	1	0	-1.793660	-1.568388	0.045155
51	1	0	1.887268	4.256579	-0.183153

Structure $TS_{21b/22b}$ (vacuum)

Energy (Hartrees): = -1191.3861697
Imaginary frequency -1092.67

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.246481	-2.840974	1.162346
2	6	0	5.024770	3.421278	0.297195
3	6	0	-1.099330	0.568047	0.043326
4	6	0	2.525039	3.144813	0.215365
5	6	0	3.796319	2.554061	0.219837
6	6	0	3.878895	1.184844	0.141147
7	6	0	2.732273	0.356546	0.059172
8	6	0	1.440693	0.959470	0.052733
9	6	0	1.388638	2.375803	0.124830
10	6	0	4.214334	-1.788727	0.043942
11	6	0	4.615232	-2.387750	-1.310932
12	6	0	2.869494	-1.085184	-0.043004
13	6	0	1.746703	-1.831288	-0.252112
14	6	0	0.431476	-1.253882	-0.268142
15	6	0	0.264009	0.126192	-0.075706
16	1	0	-1.361795	1.582395	0.312200
17	1	0	4.864456	0.744716	0.118615
18	1	0	0.860718	-3.449769	-0.521218
19	1	0	5.260570	-3.236501	1.262085
20	8	0	0.159525	2.978718	0.088515
21	1	0	5.932363	2.817109	0.295644
22	1	0	5.020260	4.024788	1.208542
23	1	0	5.072040	4.107748	-0.552183
24	8	0	-0.554487	-2.090688	-0.426497
25	1	0	3.959412	-2.395457	2.117473
26	1	0	3.571972	-3.668966	0.950174
27	8	0	1.785891	-3.174080	-0.426884
28	1	0	4.972377	-1.054753	0.308496
29	1	0	5.602436	-2.851705	-1.238622
30	1	0	4.655352	-1.612639	-2.079820
31	1	0	3.898284	-3.148191	-1.622522
32	1	0	-1.556783	-1.387070	-0.349036
33	1	0	0.285828	3.930972	0.095400
34	7	0	-2.061690	-0.279627	-0.144137
35	7	0	-3.385356	0.170922	0.064256
36	6	0	-4.119505	0.095620	-1.220584
37	6	0	-3.999151	-0.683475	1.107907
38	6	0	-5.546390	0.591050	-0.995364

39	1	0	-4.154942	-0.956497	-1.553754
40	6	0	-5.422455	-0.195207	1.365775
41	1	0	-4.041941	-1.723951	0.739475
42	6	0	-6.257549	-0.208567	0.090424
43	1	0	-6.089300	0.531299	-1.942337
44	1	0	-5.498090	1.647785	-0.709059
45	1	0	-5.874650	-0.827278	2.134561
46	1	0	-5.366074	0.823327	1.766004
47	1	0	-7.254493	0.197679	0.276925
48	1	0	-6.389169	-1.243027	-0.246941
49	6	0	-3.167698	-0.639023	2.383634
50	1	0	-2.193522	-1.110586	2.251614
51	1	0	-3.013291	0.399620	2.688521
52	1	0	-3.693411	-1.162451	3.184550
53	6	0	-3.419163	0.934793	-2.281396
54	1	0	-3.285067	1.956680	-1.915855
55	1	0	-2.441840	0.530301	-2.543830
56	1	0	-4.029029	0.966146	-3.186492
57	1	0	2.430541	4.226978	0.267131

Structure $TS_{21b/22b}$ ($CHCl_3$)

Energy (Hartrees): = -1191.4134583
Imaginary frequency -1071.44

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.285662	-2.740907	1.242834
2	6	0	5.038193	3.417513	0.249052
3	6	0	-1.102132	0.586855	0.015637
4	6	0	2.538660	3.150661	0.135438
5	6	0	3.808602	2.553922	0.161256
6	6	0	3.889069	1.182881	0.100868
7	6	0	2.738599	0.355856	0.025750
8	6	0	1.446876	0.963395	0.008157
9	6	0	1.399218	2.384558	0.050432
10	6	0	4.215604	-1.796378	0.033992
11	6	0	4.553831	-2.525265	-1.273543
12	6	0	2.871142	-1.087922	-0.047109
13	6	0	1.739193	-1.837110	-0.198631
14	6	0	0.428226	-1.254757	-0.219355
15	6	0	0.266229	0.130333	-0.083123
16	1	0	-1.355009	1.617564	0.225626
17	1	0	4.874382	0.741604	0.100608
18	1	0	0.850073	-3.476930	-0.377817
19	1	0	5.292050	-3.160370	1.326508
20	8	0	0.176380	2.986894	-0.007326
21	1	0	5.945870	2.812496	0.237975
22	1	0	5.034547	4.007873	1.169534
23	1	0	5.084894	4.119220	-0.588177
24	8	0	-0.566189	-2.095938	-0.334118
25	1	0	4.066932	-2.202069	2.168269
26	1	0	3.577489	-3.563840	1.147062
27	8	0	1.774436	-3.187965	-0.311146
28	1	0	4.994142	-1.053251	0.187444
29	1	0	5.553365	-2.963896	-1.206893
30	1	0	4.543398	-1.832585	-2.118905
31	1	0	3.840328	-3.325321	-1.473611
32	1	0	-1.548766	-1.396628	-0.274392
33	1	0	0.295735	3.943784	0.004700
34	7	0	-2.062979	-0.266549	-0.119053
35	7	0	-3.389437	0.196713	0.048013
36	6	0	-4.123699	-0.035190	-1.221781
37	6	0	-3.992923	-0.553684	1.178749
38	6	0	-5.557972	0.460431	-1.052698
39	1	0	-4.141685	-1.118766	-1.429323
40	6	0	-5.423312	-0.061746	1.382422
41	1	0	-4.018453	-1.625810	0.918998
42	6	0	-6.257832	-0.223075	0.116727
43	1	0	-6.096599	0.281956	-1.987224
44	1	0	-5.529462	1.543971	-0.889420
45	1	0	-5.865939	-0.617057	2.213641
46	1	0	-5.385763	0.994288	1.674017
47	1	0	-7.258507	0.191716	0.260408
48	1	0	-6.378393	-1.289593	-0.104925
49	6	0	-3.166007	-0.365299	2.443379
50	1	0	-2.181608	-0.828989	2.362522
51	1	0	-3.032123	0.700409	2.651227
52	1	0	-3.683787	-0.820930	3.290313
53	6	0	-3.433238	0.685001	-2.372012
54	1	0	-3.301440	1.743419	-2.129012
55	1	0	-2.455031	0.257253	-2.595720
56	1	0	-4.047221	0.611697	-3.272469

57	1	0	2.444543	4.233273	0.168390

Structure $TS_{21b/22b}$ (DMSO)

Energy (Hartrees): = -1191.407273
Imaginary frequency -1108.93

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.532015	-2.515886	-1.298017
2	6	0	-5.034578	3.421252	0.225307
3	6	0	1.105409	0.582257	0.030441
4	6	0	-2.536293	3.151467	0.110483
5	6	0	-3.807085	2.555322	0.142571
6	6	0	-3.889697	1.183535	0.095803
7	6	0	-2.738737	0.355072	0.030155
8	6	0	-1.445061	0.960838	0.014869
9	6	0	-1.396831	2.383989	0.038410
10	6	0	-4.222693	-1.791525	0.018665
11	6	0	-4.328387	-2.736881	1.223261
12	6	0	-2.873873	-1.088996	-0.032923
13	6	0	-1.740754	-1.841954	-0.156520
14	6	0	-0.428692	-1.262342	-0.165263
15	6	0	-0.265176	0.124443	-0.055207
16	1	0	1.360407	1.619605	0.198426
17	1	0	-4.875818	0.743553	0.101893
18	1	0	-0.846786	-3.476564	-0.311464
19	1	0	-5.537138	-2.944408	-1.258323
20	8	0	-0.175488	2.986149	-0.023550
21	1	0	-5.062800	4.138700	-0.599030
22	1	0	-5.041614	3.996325	1.155408
23	1	0	-5.943806	2.819700	0.189391
24	8	0	0.564658	-2.108931	-0.255544
25	1	0	-4.494580	-1.821161	-2.141182
26	1	0	-3.821387	-3.322469	-1.482834
27	8	0	-1.773651	-3.193474	-0.257794
28	1	0	-5.002627	-1.046717	0.153111
29	1	0	-5.337535	-3.154621	1.274483
30	1	0	-4.139860	-2.199099	2.156141
31	1	0	-3.618146	-3.560513	1.149977
32	1	0	1.542934	-1.414893	-0.203226
33	1	0	-0.298184	3.943839	-0.019371
34	7	0	2.063068	-0.276487	-0.074519
35	7	0	3.391188	0.196966	0.048972
36	6	0	4.023118	-0.514253	1.190181
37	6	0	4.095719	-0.076889	-1.230568
38	6	0	5.457700	-0.014832	1.341089
39	1	0	4.043096	-1.594074	0.967041
40	6	0	5.531719	0.427565	-1.112083
41	1	0	4.112282	-1.166440	-1.399447
42	6	0	6.260234	-0.217736	0.061157
43	1	0	5.920127	-0.542618	2.179168
44	1	0	5.426655	1.050413	1.598365
45	1	0	6.048209	0.220803	-2.052971
46	1	0	5.504752	1.515873	-0.982569
47	1	0	7.264064	0.200752	0.166810
48	1	0	6.374005	-1.290978	-0.128859
49	6	0	3.377369	0.602832	-2.388247
50	1	0	2.396162	0.165447	-2.578379
51	1	0	3.247672	1.668961	-2.178706
52	1	0	3.973745	0.500429	-3.297481
53	6	0	3.227989	-0.278293	2.466971
54	1	0	3.101226	0.794603	2.640482
55	1	0	2.241122	-0.742236	2.428162
56	1	0	3.767376	-0.703971	3.315889
57	1	0	-2.443781	4.234545	0.129829

Structure $TS_{21a/22d}$ (vacuum)

Energy (Hartrees): = -1191.3807627
Imaginary frequency -984.98

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.864551	-1.822324	0.279122
2	6	0	2.927190	-1.006543	0.017711
3	6	0	2.683283	0.415927	-0.126463
4	6	0	1.351374	0.927407	-0.093368

5	6	0	0.243561	0.015046	0.079158
6	6	0	0.512611	-1.341902	0.295757
7	6	0	4.318422	-1.614473	-0.063954
8	6	0	1.201396	2.337057	-0.178568
9	6	0	2.276376	3.180417	-0.325532
10	6	0	3.585193	2.677908	-0.373861
11	6	0	3.765003	1.320365	-0.270725
12	6	0	4.410767	-2.716842	-1.129707
13	6	0	4.779320	-2.116798	1.311192
14	6	0	4.745743	3.625513	-0.522941
15	6	0	-1.153386	0.373266	0.021071
16	1	0	-1.448325	1.377921	-0.236499
17	1	0	4.778670	0.948738	-0.280083
18	1	0	5.017425	-0.842200	-0.377554
19	1	0	5.450239	-3.039399	-1.231592
20	1	0	4.073017	-2.344125	-2.099316
21	1	0	3.805574	-3.581432	-0.861544
22	1	0	5.796713	-2.511496	1.247304
23	1	0	4.770312	-1.304583	2.041827
24	1	0	4.121691	-2.910895	1.667274
25	8	0	2.002887	-3.150480	0.506025
26	1	0	1.101447	-3.484099	0.638489
27	8	0	-0.411466	-2.240674	0.502374
28	1	0	4.763794	4.353413	0.292320
29	1	0	4.677124	4.182595	-1.461010
30	1	0	5.694010	3.087684	-0.517954
31	8	0	-0.064807	2.862981	-0.091895
32	1	0	0.003221	3.821134	-0.109237
33	7	0	-2.043081	-0.531036	0.286026
34	6	0	-3.832676	1.089865	0.476025
35	6	0	-4.012676	-0.985107	-0.890890
36	6	0	-5.360343	1.144281	0.554244
37	1	0	-3.520932	1.702899	-0.388787
38	6	0	-5.534282	-0.920659	-0.811187
39	1	0	-3.679865	-0.446046	-1.796821
40	6	0	-6.025082	0.512677	-0.660849
41	1	0	-5.657763	2.190483	0.661622
42	1	0	-5.672491	0.617624	1.462973
43	1	0	-5.947470	-1.385291	-1.710092
44	1	0	-5.857695	-1.517932	0.048777
45	1	0	-7.112598	0.542019	-0.561357
46	1	0	-5.767625	1.085225	-1.559605
47	7	0	-3.425285	-0.314445	0.293228
48	1	0	-1.452259	-1.582593	0.494506
49	6	0	-3.247956	1.661271	1.769550
50	1	0	-3.414104	0.947542	2.579441
51	1	0	-2.182243	1.879715	1.717599
52	1	0	-3.765539	2.590411	2.015505
53	6	0	-3.546068	-2.435361	-0.972471
54	1	0	-2.480645	-2.524197	-1.181688
55	1	0	-3.755437	-2.942526	-0.026850
56	1	0	-4.092460	-2.945503	-1.767934
57	1	0	2.105949	4.252712	-0.386410

Structure $TS_{21a/22d}$ ($CHCl_3$)

Energy (Hartrees): = -1191.4083433
Imaginary frequency -987.23

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.863000	-1.823280	0.270905
2	6	0	2.931481	-1.006996	0.027744
3	6	0	2.688836	0.415224	-0.117866
4	6	0	1.354789	0.927071	-0.097854
5	6	0	0.244967	0.014242	0.064538
6	6	0	0.513584	-1.341566	0.274505
7	6	0	4.324341	-1.615327	-0.042487
8	6	0	1.204493	2.339950	-0.193248
9	6	0	2.282436	3.182063	-0.331250
10	6	0	3.592762	2.678036	-0.363875
11	6	0	3.773751	1.320279	-0.256222
12	6	0	4.432350	-2.701495	-1.122862
13	6	0	4.773177	-2.138618	1.328143
14	6	0	4.753227	3.626271	-0.506563
15	6	0	-1.158605	0.378712	0.012537
16	1	0	-1.452501	1.387469	-0.228653
17	1	0	4.788552	0.950906	-0.260729
18	1	0	5.027798	-0.839001	-0.333232
19	1	0	5.475155	-3.015121	-1.223078
20	1	0	4.099655	-2.320357	-2.091747
21	1	0	3.833486	-3.577140	-0.873864
22	1	0	5.794566	-2.524838	1.267495

23	1	0	4.755228	-1.340507	2.074855
24	1	0	4.121205	-2.944810	1.668908
25	8	0	2.003224	-3.153662	0.490976
26	1	0	1.104325	-3.501506	0.608566
27	8	0	-0.416532	-2.244587	0.470320
28	1	0	4.745558	4.375729	0.289606
29	1	0	4.704258	4.161482	-1.458991
30	1	0	5.704152	3.093654	-0.464132
31	8	0	-0.057998	2.861044	-0.127046
32	1	0	-0.002662	3.823018	-0.168683
33	7	0	-2.044687	-0.529526	0.261521
34	6	0	-3.833917	1.093751	0.483424
35	6	0	-4.030061	-0.984933	-0.887033
36	6	0	-5.361152	1.146662	0.572700
37	1	0	-3.525771	1.707228	-0.380159
38	6	0	-5.550158	-0.918820	-0.789559
39	1	0	-3.707609	-0.443875	-1.793898
40	6	0	-6.036459	0.515468	-0.636238
41	1	0	-5.655308	2.193476	0.681811
42	1	0	-5.668409	0.621022	1.484094
43	1	0	-5.971331	-1.382910	-1.685026
44	1	0	-5.867619	-1.514940	0.073811
45	1	0	-7.123036	0.545238	-0.525250
46	1	0	-5.786248	1.086713	-1.537892
47	7	0	-3.425492	-0.312911	0.292201
48	1	0	-1.438517	-1.597120	0.455701
49	6	0	-3.245087	1.659088	1.776776
50	1	0	-3.425393	0.955922	2.593905
51	1	0	-2.175797	1.864072	1.732025
52	1	0	-3.748394	2.598366	2.015459
53	6	0	-3.563596	-2.433848	-0.977333
54	1	0	-2.504970	-2.520930	-1.222662
55	1	0	-3.742923	-2.945423	-0.027165
56	1	0	-4.130930	-2.946193	-1.757167
57	1	0	2.110231	4.253469	-0.397259

Structure $TS_{21a/22d}$ (DMSO)

Energy (Hartrees): = -1191.4026218
Imaginary frequency -992.33

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.860471	-1.822776	0.275544
2	6	0	2.930569	-1.010283	0.024138
3	6	0	2.690336	0.412286	-0.121287
4	6	0	1.357083	0.927799	-0.094366
5	6	0	0.244774	0.018211	0.071321
6	6	0	0.512364	-1.337391	0.279586
7	6	0	4.322434	-1.619749	-0.050842
8	6	0	1.210599	2.342356	-0.184429
9	6	0	2.290240	3.181657	-0.328466
10	6	0	3.599120	2.673008	-0.370207
11	6	0	3.778045	1.314194	-0.264907
12	6	0	4.423650	-2.714558	-1.122430
13	6	0	4.778671	-2.130634	1.321439
14	6	0	4.761549	3.617757	-0.515534
15	6	0	-1.160789	0.386012	0.019064
16	1	0	-1.454114	1.395492	-0.219965
17	1	0	4.792403	0.943086	-0.274305
18	1	0	5.024873	-0.846892	-0.352207
19	1	0	5.464238	-3.036615	-1.217642
20	1	0	4.097706	-2.337334	-2.095399
21	1	0	3.817195	-3.584190	-0.870062
22	1	0	5.800104	-2.516055	1.258418
23	1	0	4.765355	-1.325335	2.060784
24	1	0	4.129518	-2.934277	1.674309
25	8	0	1.995161	-3.152745	0.501363
26	1	0	1.093527	-3.491307	0.622658
27	8	0	-0.418779	-2.241145	0.475060
28	1	0	5.710012	3.079721	-0.490121
29	1	0	4.763522	4.358715	0.288479
30	1	0	4.702145	4.164971	-1.460451
31	8	0	-0.047791	2.865478	-0.105151
32	1	0	0.010472	3.828406	-0.147044
33	7	0	-2.045569	-0.523750	0.263222
34	6	0	-3.838312	1.098802	0.474100
35	6	0	-4.028390	-0.991670	-0.881938
36	6	0	-5.365744	1.151823	0.553335
37	1	0	-3.523537	1.705046	-0.390960
38	6	0	-5.548378	-0.924489	-0.791321
39	1	0	-3.701637	-0.456189	-1.789620
40	6	0	-6.034034	0.511151	-0.653865

41	1	0	-5.658489	2.199978	0.651752
42	1	0	-5.680246	0.634106	1.467142
43	1	0	-5.963589	-1.396685	-1.685246
44	1	0	-5.871293	-1.513068	0.075580
45	1	0	-7.121214	0.542881	-0.548986
46	1	0	-5.776898	1.073893	-1.558665
47	7	0	-3.426512	-0.310109	0.295471
48	1	0	-1.433098	-1.597433	0.453485
49	6	0	-3.261330	1.672291	1.768588
50	1	0	-3.469710	0.987156	2.594689
51	1	0	-2.187847	1.857634	1.740623
52	1	0	-3.750464	2.625008	1.982167
53	6	0	-3.563524	-2.441380	-0.959700
54	1	0	-2.504807	-2.531878	-1.203608
55	1	0	-3.745683	-2.947433	-0.006785
56	1	0	-4.130085	-2.957623	-1.737424
57	1	0	2.121062	4.254031	-0.389570

Structure $TS_{23/24}$ (vacuum)

Energy (Hartrees): = -1245.0052286
Imaginary frequency -984.11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.729191	-1.861996	0.014315
2	6	0	-2.819954	-1.043639	-0.006268
3	6	0	-2.609360	0.394377	-0.004851
4	6	0	-1.288449	0.933495	0.000919
5	6	0	-0.151791	0.033519	0.010184
6	6	0	-0.387423	-1.352140	0.024686
7	6	0	-4.203674	-1.674075	-0.025836
8	6	0	-1.172554	2.347712	0.004762
9	6	0	-2.272513	3.173375	0.002369
10	6	0	-3.570004	2.645480	-0.001390
11	6	0	-3.715039	1.278967	-0.004857
12	6	0	-4.471953	-2.483852	1.250803
13	6	0	-4.425225	-2.516255	-1.290555
14	6	0	-4.756866	3.571699	-0.000462
15	6	0	1.230782	0.419037	0.003984
16	1	0	1.496727	1.467494	-0.022429
17	1	0	-4.720097	0.886365	-0.003665
18	1	0	-4.949032	-0.883283	-0.053197
19	1	0	-5.496159	-2.865254	1.238379
20	1	0	-4.351342	-1.857632	2.137673
21	1	0	-3.789266	-3.329839	1.327195
22	1	0	-5.455898	-2.879247	-1.315143
23	1	0	-4.252602	-1.917788	-2.187877
24	1	0	-3.756419	-3.375905	-1.313185
25	8	0	-1.831184	-3.212456	0.023768
26	1	0	-0.920346	-3.544567	0.036779
27	8	0	0.559053	-2.244685	0.041727
28	1	0	1.573674	-1.578511	0.039778
29	1	0	-4.748336	4.217980	-0.881912
30	1	0	-4.748015	4.216868	0.881787
31	1	0	-5.691820	3.011141	-0.000726
32	8	0	0.083311	2.900011	0.012838
33	1	0	-0.004873	3.856725	0.020481
34	7	0	2.162060	-0.490193	0.027367
35	1	0	-2.126420	4.250877	0.005847
36	6	0	3.583661	-0.166070	0.006086
37	6	0	3.916960	0.557687	-1.314506
38	1	0	3.394272	1.522710	-1.344975
39	1	0	3.549470	-0.048736	-2.145331
40	6	0	3.933813	0.705576	1.228778
41	1	0	3.695454	0.144699	2.140986
42	1	0	3.321753	1.610261	1.224070
43	6	0	4.313317	-1.519069	0.082140
44	1	0	4.052765	-2.112003	-0.803934
45	1	0	3.956303	-2.058325	0.963012
46	8	0	5.307590	0.731874	-1.516171
47	1	0	5.617096	1.288354	-0.789447
48	8	0	5.282532	1.139102	1.227056
49	1	0	5.819880	0.337076	1.281408
50	8	0	5.716624	-1.392296	0.220511
51	1	0	6.028188	-0.963468	-0.586796

Structure $TS_{23/24}$ ($CHCl_3$)

Energy (Hartrees): = -1245.0332153
Imaginary frequency -1074.62

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.724232	-1.860115	-0.018854
2	6	0	2.819394	-1.044991	-0.000132
3	6	0	2.611562	0.392373	-0.000508
4	6	0	1.289243	0.932579	-0.011086
5	6	0	0.150620	0.035214	-0.020300
6	6	0	0.385868	-1.347042	-0.032380
7	6	0	4.203198	-1.678379	0.021385
8	6	0	1.173783	2.351027	-0.021483
9	6	0	2.275461	3.174876	-0.010988
10	6	0	3.573932	2.644217	0.005146
11	6	0	3.720406	1.277318	0.008148
12	6	0	4.470580	-2.506540	-1.243345
13	6	0	4.430123	-2.499545	1.298525
14	6	0	4.760488	3.569606	0.028765
15	6	0	-1.240404	0.425999	-0.006922
16	1	0	-1.507701	1.473733	0.028968
17	1	0	4.726191	0.885550	0.016791
18	1	0	4.950272	-0.889495	0.030878
19	1	0	5.499639	-2.875886	-1.232105
20	1	0	4.339970	-1.896339	-2.140653
21	1	0	3.799763	-3.363380	-1.308191
22	1	0	5.455861	-2.877722	1.317299
23	1	0	4.281009	-1.881792	2.187657
24	1	0	3.750208	-3.350086	1.351260
25	8	0	1.827413	-3.211832	-0.022111
26	1	0	0.918972	-3.553538	-0.032150
27	8	0	-0.565660	-2.243656	-0.047933
28	1	0	4.780077	4.152929	0.953634
29	1	0	4.723054	4.278521	-0.802453
30	1	0	5.695545	3.012232	-0.039772
31	8	0	-0.077247	2.898457	-0.044715
32	1	0	0.001199	3.859811	-0.056460
33	7	0	-2.164481	-0.483086	-0.031687
34	1	0	-1.559711	-1.590365	-0.046697
35	1	0	2.127703	4.251870	-0.018396
36	6	0	-3.589190	-0.162947	-0.004193
37	6	0	-4.307463	-1.521828	-0.038934
38	1	0	-4.054958	-2.082109	0.870040
39	1	0	-3.938948	-2.086014	-0.899119
40	6	0	-3.944543	0.676228	-1.246188
41	1	0	-3.314860	1.567891	-1.275403
42	1	0	-3.738313	0.084608	-2.146205
43	6	0	-3.908311	0.595298	1.299072
44	1	0	-3.507647	0.025594	2.140317
45	1	0	-3.414551	1.574454	1.283210
46	8	0	-5.712924	-1.411031	-0.195834
47	1	0	-6.040402	-0.975032	0.602226
48	8	0	-5.301083	0.740693	1.528202
49	1	0	-5.637695	1.288838	0.806556
50	8	0	-5.287238	1.137296	-1.232627
51	1	0	-5.843274	0.347828	-1.283649

Structure $TS_{23/24}$ (DMSO)

Energy (Hartrees): = -1245.0319493
Imaginary frequency -1011.75

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.716417	-1.858446	-0.073797
2	6	0	2.814030	-1.049782	0.012598
3	6	0	2.612741	0.388192	0.016156
4	6	0	1.293745	0.933882	-0.042889
5	6	0	0.152313	0.043121	-0.086778
6	6	0	0.381959	-1.337534	-0.130769
7	6	0	4.193283	-1.687433	0.089093
8	6	0	1.183557	2.352246	-0.094637
9	6	0	2.286165	3.173557	-0.042441
10	6	0	3.580421	2.637481	0.048853
11	6	0	3.723816	1.269778	0.070097
12	6	0	4.518192	-2.494170	-1.175181
13	6	0	4.357859	-2.532762	1.359242
14	6	0	4.767108	3.559628	0.119121
15	6	0	-1.239206	0.440875	-0.026174
16	1	0	-1.500133	1.481956	0.114142
17	1	0	4.727935	0.876437	0.125213
18	1	0	4.940688	-0.901141	0.149922

19	1	0	5.543373	-2.870387	-1.119172
20	1	0	4.437575	-1.867908	-2.067658
21	1	0	3.845659	-3.345140	-1.287989
22	1	0	5.383511	-2.906175	1.423528
23	1	0	4.160529	-1.933784	2.252180
24	1	0	3.681494	-3.388072	1.361096
25	8	0	1.811019	-3.210507	-0.098814
26	1	0	0.900326	-3.541193	-0.150022
27	8	0	-0.572989	-2.230224	-0.198181
28	1	0	-1.554914	-1.576962	-0.186528
29	1	0	4.732129	4.169280	1.026400
30	1	0	4.780437	4.245592	-0.731927
31	1	0	5.701523	2.996869	0.122163
32	8	0	-0.061538	2.895813	-0.210956
33	1	0	0.019065	3.857148	-0.252225
34	7	0	-2.163657	-0.461172	-0.111729
35	1	0	2.144612	4.250953	-0.082958
36	6	0	-3.586594	-0.149565	-0.006214
37	6	0	-3.865886	0.427847	1.394711
38	1	0	-3.369867	1.400740	1.496115
39	1	0	-3.446457	-0.250999	2.140622
40	6	0	-3.977819	0.843540	-1.116102
41	1	0	-3.782857	0.381131	-2.091329
42	1	0	-3.366521	1.744718	-1.036888
43	6	0	-4.304619	-1.496003	-0.199222
44	1	0	-4.018114	-2.171159	0.617016
45	1	0	-3.967091	-1.935904	-1.140773
46	8	0	-5.254506	0.542847	1.676419
47	1	0	-5.603633	1.168037	1.027233
48	8	0	-5.331212	1.268540	-1.014682
49	1	0	-5.866295	0.471806	-1.131092
50	8	0	-5.717706	-1.376415	-0.286178
51	1	0	-6.006804	-1.034780	0.570170

Structure $TS_{14bb/26bb}$ (vacuum)

Energy (Hartrees): =-2381.6073421
Imaginary frequency -1107.65

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.040477	-2.838360	-0.692492
2	6	0	-4.010310	-3.151770	-1.539703
3	6	0	-2.901168	-2.233791	-1.626681
4	6	0	-2.928000	-0.998457	-0.911159
5	6	0	-4.077716	-0.660119	-0.109546
6	6	0	-5.082444	-1.604792	0.016322
7	6	0	3.960733	5.492626	-1.828028
8	6	0	-0.724486	1.943963	-3.337321
9	6	0	-4.063282	-4.461515	-2.310356
10	6	0	-1.761336	-0.183375	-0.976170
11	6	0	-0.660466	-0.519890	-1.744307
12	6	0	-0.659942	-1.729927	-2.480334
13	6	0	-1.755166	-2.551491	-2.402889
14	6	0	-5.299925	-4.551538	-3.216876
15	6	0	-3.960894	-5.667746	-1.366105
16	6	0	0.536535	-2.089317	-3.322123
17	6	0	-4.306884	0.648498	0.507927
18	6	0	4.193118	-0.631874	0.538497
19	6	0	0.516655	0.397383	-1.771668
20	6	0	0.500134	1.585198	-2.536154
21	6	0	1.615908	2.387833	-2.531655
22	6	0	2.782816	2.077147	-1.792281
23	6	0	2.808554	0.882727	-1.014362
24	6	0	1.643792	0.072627	-1.031395
25	6	0	3.984303	4.215783	-2.679560
26	6	0	5.185818	4.192745	-3.636133
27	6	0	3.926445	2.970493	-1.808631
28	6	0	4.980229	2.687688	-0.989386
29	6	0	5.032048	1.498452	-0.184402
30	6	0	3.976476	0.575423	-0.216545
31	1	0	3.505388	-1.465822	0.514124
32	1	0	1.574769	3.296427	-3.113191
33	1	0	-3.695520	1.498563	0.232689
34	1	0	-1.719540	-3.479215	-2.953323
35	1	0	6.662860	3.047845	-0.271881
36	1	0	3.950210	6.374299	-2.473924
37	1	0	-3.204205	-4.505837	-2.975804
38	8	0	1.642463	-1.070543	-0.287056
39	1	0	-5.243678	-5.459462	-3.822767
40	1	0	-5.345143	-3.694300	-3.892173
41	1	0	-6.219157	-4.582808	-2.634208

42	1	0	-3.943456	-6.594749	-1.944883
43	1	0	-3.045683	-5.617473	-0.771706
44	1	0	-4.813771	-5.700864	-0.687950
45	1	0	-1.003948	1.127105	-4.007601
46	1	0	-0.546551	2.839683	-3.932366
47	1	0	-1.582868	2.128591	-2.684686
48	8	0	-6.088967	-3.677857	-0.504961
49	1	0	-6.695241	-3.239332	0.107146
50	8	0	-6.183178	-1.441828	0.762096
51	1	0	-6.088035	-0.561300	1.245097
52	1	0	0.357450	-3.012990	-3.872293
53	1	0	1.428840	-2.222201	-2.703483
54	1	0	0.760476	-1.292746	-4.036409
55	8	0	-1.732706	0.962705	-0.240246
56	8	0	6.114729	1.340867	0.522937
57	1	0	3.069970	5.519245	-1.196047
58	1	0	4.841764	5.543969	-1.187755
59	8	0	6.065251	3.491210	-0.894361
60	1	0	3.100977	4.237728	-3.313940
61	1	0	5.131425	5.049799	-4.312355
62	1	0	5.180690	3.282463	-4.239795
63	1	0	6.127523	4.242544	-3.091856
64	1	0	5.942266	0.274425	1.096405
65	1	0	-0.855206	1.358544	-0.332508
66	1	0	0.763865	-1.469227	-0.346725
67	7	0	-5.254792	0.815332	1.353552
68	6	0	-6.793948	2.522356	1.794706
69	6	0	-4.839774	2.170086	3.234522
70	6	0	-6.955752	3.944877	2.325129
71	1	0	-7.369305	1.833616	2.439340
72	6	0	-4.974068	3.587932	3.786629
73	1	0	-5.444434	1.486280	3.855726
74	6	0	-6.416963	4.075551	3.744438
75	1	0	-8.013934	4.216603	2.282193
76	1	0	-6.413107	4.622639	1.656522
77	1	0	-4.588320	3.601642	4.809339
78	1	0	-4.339211	4.248127	3.185161
79	1	0	-6.486054	5.109225	4.091636
80	1	0	-7.026462	3.466028	4.421486
81	7	0	-5.364095	2.149143	1.846859
82	7	0	5.257820	-0.741681	1.267124
83	7	0	5.447345	-1.947879	1.978167
84	6	0	6.816046	-2.435840	1.692240
85	6	0	5.237902	-1.687490	3.423813
86	6	0	7.030378	-3.754564	2.429732
87	1	0	7.546229	-1.697020	2.067875
88	6	0	5.433471	-2.997282	4.185089
89	1	0	5.989890	-0.957002	3.770066
90	6	0	6.810940	-3.598051	3.930030
91	1	0	8.041406	-4.112540	2.218388
92	1	0	6.327461	-4.490612	2.023842
93	1	0	5.282262	-2.806751	5.250763
94	1	0	4.655229	-3.697494	3.861251
95	1	0	6.912135	-4.560269	4.437367
96	1	0	7.578871	-2.933635	4.342550
97	6	0	-7.309413	2.416153	0.364754
98	1	0	-6.682102	3.018233	-0.298163
99	1	0	-7.301511	1.386242	0.006982
100	1	0	-8.334012	2.789551	0.310351
101	6	0	-3.382556	1.723880	3.274438
102	1	0	-3.262876	0.672651	3.014317
103	1	0	-2.789336	2.320752	2.576109
104	1	0	-2.984821	1.871086	4.280670
105	6	0	3.843267	-1.126926	3.672292
106	1	0	3.716936	-0.130138	3.249756
107	1	0	3.092555	-1.788927	3.231546
108	1	0	3.661174	-1.064083	4.746837
109	6	0	7.008454	-2.611288	0.191421
110	1	0	6.222324	-3.256910	-0.208994
111	1	0	6.977445	-1.657685	-0.336252
112	1	0	7.976094	-3.077461	-0.003994

Structure $TS_{26bb/17bb}$ (vacuum)

Energy (Hartrees): = -1245.0052286
Imaginary frequency -1074.53

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.793115	2.989165	-0.659799
2	6	0	3.739467	3.249722	-1.487820
3	6	0	2.670064	2.271775	-1.570796

4	6	0	2.770729	1.033914	-0.873595
5	6	0	3.950722	0.749080	-0.089252
6	6	0	4.925899	1.746479	0.049967
7	6	0	-3.440215	-5.818777	-1.357038
8	6	0	0.666318	-2.073578	-3.194126
9	6	0	3.713057	4.561470	-2.255984
10	6	0	1.656640	0.158735	-0.930413
11	6	0	0.519737	0.442871	-1.672856
12	6	0	0.445000	1.656622	-2.393439
13	6	0	1.500238	2.535826	-2.323609
14	6	0	4.928709	4.709856	-3.182632
15	6	0	3.572530	5.759459	-1.306558
16	6	0	-0.776610	1.960186	-3.221594
17	6	0	4.290339	-0.525870	0.485679
18	6	0	-4.339169	0.435356	0.514390
19	6	0	-0.613048	-0.528843	-1.659573
20	6	0	-0.545285	-1.747217	-2.359125
21	6	0	-1.608030	-2.623956	-2.264430
22	6	0	-2.761450	-2.344011	-1.505841
23	6	0	-2.850071	-1.108433	-0.811280
24	6	0	-1.743660	-0.236028	-0.898844
25	6	0	-3.829746	-4.612706	-2.222235
26	6	0	-5.161501	-4.850003	-2.949023
27	6	0	-3.830743	-3.337291	-1.395556
28	6	0	-4.804007	-3.134748	-0.473991
29	6	0	-4.948096	-1.888531	0.282014
30	6	0	-4.013198	-0.833429	0.028261
31	1	0	-3.783210	1.313471	0.220843
32	1	0	-1.520508	-3.568808	-2.780935
33	1	0	3.717431	-1.422788	0.289874
34	1	0	1.406946	3.465593	-2.864345
35	1	0	-6.335930	-3.596521	0.452253
36	1	0	-3.404411	-6.727563	-1.963525
37	1	0	2.840667	4.566979	-2.905842
38	8	0	-1.784372	0.934926	-0.197027
39	1	0	4.826002	5.620257	-3.778700
40	1	0	4.996890	3.860878	-3.866388
41	1	0	5.855314	4.772516	-2.614140
42	1	0	3.507784	6.687104	-1.881122
43	1	0	2.668586	5.668230	-0.699831
44	1	0	4.432440	5.825765	-0.639839
45	1	0	0.852400	-1.286420	-3.929313
46	1	0	0.527214	-3.017250	-3.721593
47	1	0	1.565965	-2.153025	-2.577353
48	8	0	5.807082	3.866633	-0.472891
49	1	0	6.428962	3.422044	0.124300
50	8	0	6.008706	1.608225	0.761903
51	1	0	5.923988	0.470245	1.208114
52	1	0	-0.655714	2.902515	-3.755885
53	1	0	-1.672047	2.028751	-2.597574
54	1	0	-0.956382	1.165247	-3.950051
55	8	0	1.717174	-0.998356	-0.210790
56	8	0	-5.938668	-1.811444	1.046659
57	1	0	-2.459338	-5.670325	-0.898896
58	1	0	-4.174402	-5.962789	-0.562258
59	8	0	-5.767440	-4.039884	-0.202784
60	1	0	-3.083227	-4.508685	-3.008402
61	1	0	-5.055525	-5.697301	-3.631361
62	1	0	-5.441791	-3.973398	-3.537345
63	1	0	-5.965993	-5.067695	-2.249132
64	1	0	0.861325	-1.442852	-0.280821
65	1	0	-0.922084	1.364797	-0.275615
66	7	0	5.346483	-0.624388	1.228046
67	6	0	7.143554	-2.115418	1.355421
68	6	0	5.454190	-2.012571	3.137401
69	6	0	7.547248	-3.522136	1.785866
70	1	0	7.747313	-1.384036	1.922151
71	6	0	5.835267	-3.419630	3.594875
72	1	0	6.086216	-1.279140	3.668131
73	6	0	7.288758	-3.746655	3.271494
74	1	0	8.603401	-3.671987	1.547319
75	1	0	6.968993	-4.238948	1.192279
76	1	0	5.648129	-3.500105	4.668834
77	1	0	5.171664	-4.130538	3.089968
78	1	0	7.523466	-4.775908	3.552991
79	1	0	7.946682	-3.094681	3.857586
80	7	0	5.713009	-1.912247	1.680684
81	7	0	-5.342453	0.690575	1.335187
82	7	0	-5.651878	2.014277	1.674630
83	6	0	-7.067646	2.278023	1.327695
84	6	0	-5.348273	2.248070	3.106773
85	6	0	-7.394269	3.733244	1.651574
86	1	0	-7.714627	1.629129	1.946086
87	6	0	-5.664677	3.704127	3.441394
88	1	0	-5.990962	1.595172	3.724078
89	6	0	-7.110287	4.057105	3.113590
90	1	0	-8.443457	3.917504	1.406865
91	1	0	-6.785857	4.372552	1.002104

92	1	0	-5.451045	3.872626	4.499902
93	1	0	-4.986275	4.340656	2.862224
94	1	0	-7.305874	5.111723	3.320093
95	1	0	-7.782009	3.472908	3.753057
96	6	0	7.381300	-1.910082	-0.135534
97	1	0	6.705156	-2.548572	-0.710396
98	1	0	7.219516	-0.873884	-0.434248
99	1	0	8.409810	-2.178419	-0.384659
100	6	0	3.989495	-1.726621	3.443676
101	1	0	3.720404	-0.690133	3.240291
102	1	0	3.348476	-2.375119	2.839979
103	1	0	3.790613	-1.927749	4.498108
104	6	0	-3.885489	1.934656	3.393585
105	1	0	-3.652818	0.879290	3.252317
106	1	0	-3.243930	2.521092	2.730308
107	1	0	-3.650177	2.198667	4.426417
108	6	0	-7.313694	1.973251	-0.144391
109	1	0	-6.608003	2.536522	-0.760660
110	1	0	-7.199792	0.911859	-0.367136
111	1	0	-8.328023	2.270630	-0.416658
112	1	0	-5.923581	-0.093147	1.651230