Supporting Information

Synthesis, Resolution, and Absolute Stereochemistry of (–)-Blestriarene C

Tetsutaro Hattori,[*,†] *Yuhi Shimazumi,*[†] *Hitoshi Goto,*[‡] *Osamu Yamabe,*[†] *Naoya Morohashi,*[†] *Wataru Kawai,*[‡] *and Sotaro Miyano*[*,†]

[†]Department of Biomolecular Engineering, Graduate School of Engineering, Tohoku University, Aramaki-Aoba 07, Aoba-ku, Sendai 980-8579, Japan

[‡]Department of Knowledge-based Information Engineering, Toyohashi University of Technology, 1-1 Hibarigaoka, Tempaku-cho, Toyohashi 441-8066, Japan

Contents:

1. ORTEP Drawing of Compound (R_a,R_a)-21

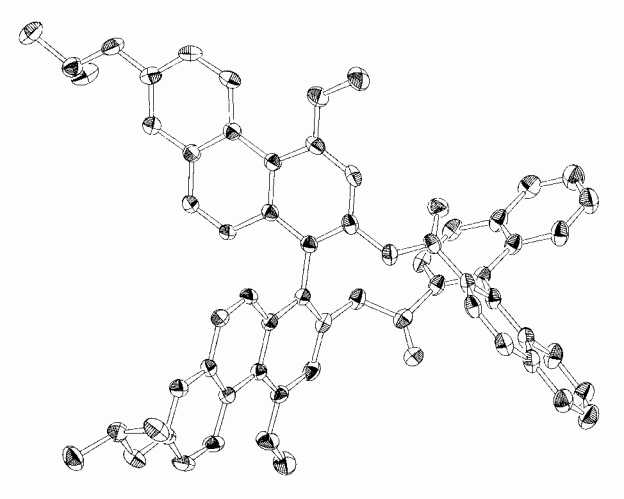


Figure S1. ORTEP drawing of compound (R_a,R_a)-**21**. Hydrogen atoms are omitted for clarity.

2. Conformational Analyses of Compounds 22–24 by MOPAC

Table S1. Dihedral Angles for Optimized 22–24

Compound	Conformation Index	Hamiltonian	(R_a,R_a)-Isomer			(S_a,R_a)-Isomer		
			θ^a (°)	ϕ^b (°)	η^c (°)	θ^a (°)	ϕ^b (°)	η^c (°)
22	sym	AM1	–74.9	–77.7	–64.4	107.5	–104.1	–75.6
		PM3	–82.2	–82.6	–65.9	93.5	–93.4	–71.8
	asym	AM1	–63.3	–83.6	–56.3			
					–125.1			
		PM3	–76.2	–87.1	–59.2			
					–93.0			
23	sym	AM1	–74.0	–76.8	–63.1	109.4	–104.0	–74.9
		PM3	–81.1	–81.4	–64.2	94.1	–93.4	–71.6
	asym	AM1	–62.3	–83.3	–55.5			
					–127.6			
		PM3	–75.4	–87.0	–59.0			
					–92.9			
24	sym	AM1	–61.7	–71.8	–62.5	124.7	–122.0	–80.3
		PM3	–70.4	–76.1	–61.9	99.2	–99.2	–72.5
	asym	AM1	–52.8	–80.6	–57.2			
					–128.2			
		PM3	–66.0	–89.2	–59.6			
					–118.2			

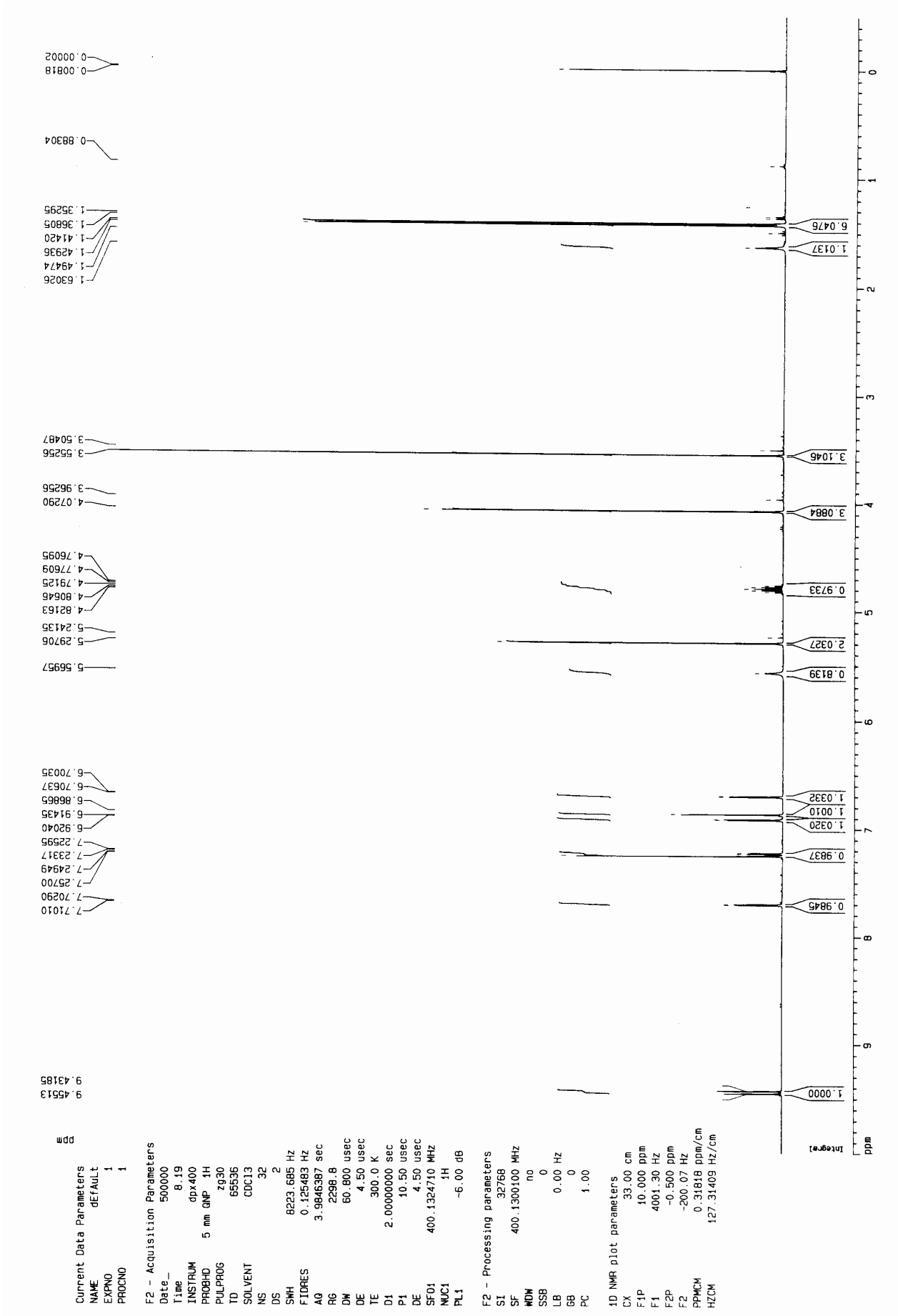
[a] Dihedral angle between C_2–C_3 and C_4–C_5 bonds. [b] Dihedral angle between C_8–C_9 and C_{10}–C_{11} bonds. [c] Dihedral angle between C_7=O (C_{12}=O) and C_8–C_9 (C_{10}–C_{11}) bonds.

Table S2. Heats of Formation and Relative Energies for Optimized 22–24[a]

Compound	Hamiltonian	Conformation Index	$E(R_a,R_a)$	$E(S_a,R_a)$	ΔE^b
22	AM1	sym	102.84	109.37	6.53
		asym	102.85		6.52
	PM3	sym	80.00	74.15	–5.85
		asym	79.71		–5.56
23	AM1	sym	68.66	74.81	6.15
		asym	68.66		6.15
	PM3	sym	50.99	44.99	–6.00
		asym	50.75		–5.76
24	AM1	sym	–15.08	–11.49	3.59
		asym	–14.84		3.35
	PM3	sym	–26.43	-32.19	–5.76
		asym	–25.57		–6.62

[a] kcal mol^{-1}. [b] Relative energy given by $E(S_a,R_a)$–$E(R_a,R_a)$.

3. ^{1}H NMR Spectrum of Compound 15 (Figure S2)



Current Data Parameters
NAME dEfAult
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 500000
Time 8.19
INSTRUM dpx400
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 2298.8
DW 60.800 usec
DE 4.50 usec
TE 300.0 K
D1 2.00000000 sec
P1 10.50 usec
DE 4.50 usec
SFO1 400.1324710 MHz
NUC1 1H
PL1 -6.00 dB

F2 - Processing parameters
SI 32768
SF 400.1300100 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 33.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.31818 ppm/cm
HZCM 127.31409 Hz/cm

4. Cartesian Coordinates for Calculated Structures

4.1. Compound (R_a,R_a)-22

4.1.1. AM1 Structure

(a) symmetric

Heat of formation: 102.84 kcal/mol

82 rr22-sym-AM1

C	1	-1.426000	-2.181000	-0.347000	63	2	12	13
C	2	-2.792000	-2.177000	0.218000	63	1	3	15
C	3	-3.759000	-1.308000	-0.263000	63	2	4	18
C	4	-3.441000	-0.319000	-1.308000	63	3	5	19
C	5	-2.760000	0.849000	-1.005000	63	4	6	22
C	6	-2.384000	1.169000	0.388000	63	5	7	14
O	7	-1.013000	1.266000	0.545000	82	6	8	
C	8	-0.469000	1.153000	1.824000	63	7	9	23
C	9	0.659000	0.342000	1.969000	63	8	10	26
C	10	1.320000	-0.302000	0.826000	63	9	11	27
C	11	0.781000	-1.416000	0.177000	63	10	12	30
O	12	-0.473000	-1.856000	0.602000	82	1	11	
O	13	-1.077000	-2.474000	-1.486000	81	1		
O	14	-3.124000	1.392000	1.342000	81	6		
C	15	-3.086000	-3.100000	1.253000	63	2	16	55
C	16	-4.350000	-3.164000	1.781000	63	15	17	56
C	17	-5.374000	-2.302000	1.305000	63	16	18	31
C	18	-5.081000	-1.364000	0.281000	63	3	17	34
C	19	-3.826000	-0.573000	-2.662000	63	4	20	35
C	20	-3.496000	0.372000	-3.668000	63	19	21	38
C	21	-2.782000	1.550000	-3.318000	63	20	22	57
C	22	-2.418000	1.781000	-2.017000	63	5	21	58
C	23	-0.987000	1.885000	2.912000	63	8	24	59
C	24	-0.422000	1.745000	4.162000	63	23	25	60
C	25	0.668000	0.874000	4.379000	63	24	26	39
C	26	1.210000	0.176000	3.272000	63	9	25	46
C	27	2.581000	0.193000	0.383000	63	10	28	47
C	28	3.299000	-0.473000	-0.640000	63	27	29	54
C	29	2.744000	-1.643000	-1.205000	63	28	30	61
C	30	1.509000	-2.110000	-0.811000	63	11	29	62
C	31	-6.688000	-2.357000	1.845000	63	17	32	63
C	32	-7.667000	-1.508000	1.390000	63	31	33	64

C	33	-7.376000	-0.567000	0.374000	63	32	34	65
C	34	-6.116000	-0.495000	-0.167000	63	18	33	66
C	35	-4.522000	-1.756000	-3.038000	63	19	36	67
C	36	-4.876000	-1.978000	-4.346000	63	35	37	68
C	37	-4.551000	-1.030000	-5.346000	63	36	38	69
C	38	-3.877000	0.119000	-5.015000	63	20	37	70
C	39	1.238000	0.683000	5.695000	63	25	40	44
C	40	0.745000	1.354000	6.839000	63	39	41	71
C	41	1.311000	1.150000	8.083000	63	40	42	72
C	42	2.393000	0.266000	8.236000	63	41	43	73
C	43	2.893000	-0.403000	7.138000	63	42	44	74
C	44	2.326000	-0.206000	5.858000	63	39	43	45
C	45	2.845000	-0.904000	4.719000	63	44	46	75
C	46	2.314000	-0.720000	3.485000	63	26	45	76
C	47	3.132000	1.390000	0.958000	63	27	48	77
C	48	4.323000	1.888000	0.542000	63	47	49	78
C	49	5.080000	1.232000	-0.485000	63	48	50	54
C	50	6.323000	1.758000	-0.904000	63	49	51	79
C	51	7.051000	1.131000	-1.893000	63	50	52	80
C	52	6.553000	-0.040000	-2.491000	63	51	53	81
C	53	5.340000	-0.568000	-2.093000	63	52	54	82
C	54	4.573000	0.053000	-1.080000	63	28	49	53
H	55	-2.278000	-3.750000	1.626000	11	15		
H	56	-4.588000	-3.878000	2.585000	11	16		
H	57	-2.521000	2.267000	-4.111000	11	21		
H	58	-1.848000	2.681000	-1.735000	11	22		
H	59	-1.850000	2.552000	2.761000	11	23		
H	60	-0.844000	2.325000	4.996000	11	24		
H	61	3.294000	-2.199000	-1.979000	11	29		
H	62	1.079000	-3.012000	-1.274000	11	30		
H	63	-6.900000	-3.090000	2.638000	11	31		
H	64	-8.683000	-1.547000	1.809000	11	32		
H	65	-8.172000	0.109000	0.027000	11	33		
H	66	-5.884000	0.239000	-0.955000	11	34		
H	67	-4.769000	-2.493000	-2.257000	11	35		
H	68	-5.411000	-2.895000	-4.632000	11	36		
H	69	-4.844000	-1.229000	-6.387000	11	37		
H	70	-3.614000	0.861000	-5.784000	11	38		

H	71	-0.103000	2.049000	6.750000	11	40	
H	72	0.916000	1.679000	8.963000	11	41	
H	73	2.834000	0.114000	9.232000	11	42	
H	74	3.739000	-1.098000	7.243000	11	43	
H	75	3.688000	-1.595000	4.876000	11	45	
H	76	2.718000	-1.260000	2.613000	11	46	
H	77	2.556000	1.898000	1.748000	11	47	
H	78	4.738000	2.807000	0.983000	11	48	
H	79	6.699000	2.676000	-0.428000	11	50	
H	80	8.019000	1.539000	-2.220000	11	51	
H	81	7.138000	-0.535000	-3.281000	11	52	
H	82	4.975000	-1.483000	-2.580000	11	53	

(b) asymmetric

Heat of formation: 102.85 kcal/mol

82 rr22-asym-AM1

C	1	4.385000	-2.799000	1.882000	63	2	6	47
C	2	5.438000	-2.539000	0.972000	63	1	3	48
C	3	5.322000	-1.447000	0.051000	63	2	4	55
C	4	4.218000	-0.659000	0.037000	63	3	5	56
C	5	3.121000	-0.893000	0.936000	63	4	6	10
C	6	3.199000	-1.971000	1.852000	63	1	5	7
C	7	2.103000	-2.218000	2.709000	63	6	8	57
C	8	0.958000	-1.453000	2.642000	63	7	9	58
C	9	0.884000	-0.395000	1.715000	63	8	10	11
C	10	1.960000	-0.071000	0.884000	63	5	9	18
O	11	-0.252000	0.411000	1.643000	82	9	34	
C	12	3.665000	2.242000	1.281000	63	13	17	59
C	13	4.489000	3.301000	1.481000	63	12	14	60
C	14	4.489000	4.417000	0.581000	63	13	15	49
C	15	3.607000	4.421000	-0.525000	63	14	16	50
C	16	2.712000	3.302000	-0.724000	63	15	17	21
C	17	2.756000	2.202000	0.168000	63	12	16	18
C	18	1.896000	1.084000	-0.020000	63	10	17	19
C	19	0.959000	1.136000	-1.058000	63	18	20	22
C	20	0.906000	2.227000	-1.948000	63	19	21	61
C	21	1.779000	3.280000	-1.785000	63	16	20	62
O	22	0.011000	0.118000	-1.070000	82	19	45	

C	23	-4.887000	3.524000	-1.287000	63	24	28	63
C	24	-5.476000	3.212000	-2.487000	63	23	25	64
C	25	-5.253000	1.946000	-3.080000	63	24	26	65
C	26	-4.450000	1.020000	-2.461000	63	25	27	66
C	27	-3.826000	1.313000	-1.215000	63	26	28	32
C	28	-4.048000	2.585000	-0.626000	63	23	27	29
C	29	-3.421000	2.905000	0.609000	63	28	30	67
C	30	-2.601000	1.997000	1.225000	63	29	31	68
C	31	-2.383000	0.718000	0.648000	63	30	32	34
C	32	-2.981000	0.366000	-0.551000	63	27	31	41
O	33	-0.163000	0.062000	-3.320000	81	45		
C	34	-1.463000	-0.201000	1.350000	63	11	31	46
C	35	-4.939000	-1.716000	-0.148000	63	36	40	69
C	36	-5.886000	-2.692000	0.043000	63	35	37	70
C	37	-5.742000	-3.959000	-0.571000	63	36	38	71
C	38	-4.651000	-4.223000	-1.361000	63	37	39	72
C	39	-3.655000	-3.231000	-1.573000	63	38	40	44
C	40	-3.796000	-1.958000	-0.963000	63	35	39	41
C	41	-2.788000	-0.959000	-1.167000	63	32	40	42
C	42	-1.692000	-1.259000	-1.956000	63	41	43	45
C	43	-1.562000	-2.533000	-2.574000	63	42	44	73
C	44	-2.519000	-3.495000	-2.386000	63	39	43	74
C	45	-0.594000	-0.307000	-2.231000	63	22	33	42
O	46	-1.654000	-1.351000	1.733000	81	34		
C	47	4.536000	-3.875000	2.787000	63	1	54	75
C	48	6.596000	-3.349000	0.980000	63	2	53	76
C	49	5.363000	5.507000	0.793000	63	14	52	77
C	50	3.636000	5.534000	-1.399000	63	15	51	78
C	51	4.499000	6.590000	-1.177000	63	50	52	79
C	52	5.369000	6.580000	-0.073000	63	49	51	80
C	53	6.715000	-4.394000	1.873000	63	48	54	81
C	54	5.676000	-4.656000	2.783000	63	47	53	82
H	55	6.156000	-1.267000	-0.646000	11	3		
H	56	4.135000	0.182000	-0.672000	11	4		
H	57	2.144000	-3.041000	3.438000	11	7		
H	58	0.090000	-1.670000	3.283000	11	8		
H	59	3.672000	1.384000	1.973000	11	12		
H	60	5.178000	3.328000	2.340000	11	13		

H	61	0.173000	2.229000	-2.770000	11	20
H	62	1.727000	4.119000	-2.495000	11	21
H	63	-5.050000	4.505000	-0.816000	11	23
H	64	-6.124000	3.937000	-3.001000	11	24
H	65	-5.730000	1.715000	-4.044000	11	25
H	66	-4.276000	0.034000	-2.920000	11	26
H	67	-3.598000	3.896000	1.052000	11	29
H	68	-2.085000	2.241000	2.168000	11	30
H	69	-5.046000	-0.731000	0.333000	11	35
H	70	-6.764000	-2.501000	0.677000	11	36
H	71	-6.513000	-4.726000	-0.403000	11	37
H	72	-4.524000	-5.205000	-1.841000	11	38
H	73	-0.680000	-2.724000	-3.205000	11	43
H	74	-2.423000	-4.485000	-2.858000	11	44
H	75	3.741000	-4.104000	3.511000	11	47
H	76	7.402000	-3.131000	0.263000	11	48
H	77	6.040000	5.484000	1.661000	11	49
H	78	2.969000	5.568000	-2.272000	11	50
H	79	4.510000	7.447000	-1.867000	11	51
H	80	6.049000	7.428000	0.091000	11	52
H	81	7.616000	-5.025000	1.879000	11	53
H	82	5.778000	-5.489000	3.494000	11	54

4.1.2. PM3 Structure

(a) symmetric

Heat of formation: 80.00 kcal/mol

82 rr22-sym-PM3

C	1	-1.497000	-1.448000	0.091000	63	2	12	13
C	2	-2.725000	-0.756000	-0.399000	63	1	3	15
C	3	-2.847000	-0.361000	-1.716000	63	2	4	18
C	4	-1.752000	-0.574000	-2.689000	63	3	5	19
C	5	-0.691000	0.303000	-2.781000	63	4	6	22
C	6	-0.621000	1.525000	-1.926000	63	5	7	14
O	7	0.467000	1.502000	-1.074000	82	6	8	
C	8	0.432000	2.250000	0.101000	63	7	9	23
C	9	0.800000	1.594000	1.275000	63	8	10	26
C	10	1.338000	0.218000	1.296000	63	9	11	27
C	11	0.530000	-0.917000	1.252000	63	10	12	30

O	12	-0.833000	-0.710000	1.052000	82	1	11	
O	13	-1.109000	-2.546000	-0.239000	81	1		
O	14	-1.368000	2.476000	-1.967000	81	6		
C	15	-3.778000	-0.545000	0.527000	63	2	16	55
C	16	-4.939000	0.053000	0.124000	63	15	17	56
C	17	-5.101000	0.471000	-1.223000	63	16	18	31
C	18	-4.057000	0.268000	-2.150000	63	3	17	34
C	19	-1.796000	-1.714000	-3.553000	63	4	20	35
C	20	-0.753000	-1.917000	-4.482000	63	19	21	38
C	21	0.324000	-0.994000	-4.546000	63	20	22	57
C	22	0.355000	0.090000	-3.714000	63	5	21	58
C	23	0.141000	3.633000	0.102000	63	8	24	59
C	24	0.108000	4.319000	1.290000	63	23	25	60
C	25	0.362000	3.665000	2.513000	63	24	26	39
C	26	0.719000	2.304000	2.506000	63	9	25	46
C	27	2.745000	0.048000	1.438000	63	10	28	47
C	28	3.285000	-1.238000	1.622000	63	27	29	54
C	29	2.418000	-2.349000	1.685000	63	28	30	61
C	30	1.066000	-2.201000	1.505000	63	11	29	62
C	31	-6.305000	1.097000	-1.648000	63	17	32	63
C	32	-6.452000	1.505000	-2.945000	63	31	33	64
C	33	-5.406000	1.308000	-3.876000	63	32	34	65
C	34	-4.239000	0.706000	-3.492000	63	18	33	66
C	35	-2.858000	-2.659000	-3.500000	63	19	36	67
C	36	-2.870000	-3.742000	-4.337000	63	35	37	68
C	37	-1.826000	-3.939000	-5.269000	63	36	38	69
C	38	-0.790000	-3.048000	-5.342000	63	20	37	70
C	39	0.272000	4.380000	3.767000	63	25	40	44
C	40	-0.079000	5.747000	3.815000	63	39	41	71
C	41	-0.161000	6.408000	5.019000	63	40	42	72
C	42	0.103000	5.727000	6.220000	63	41	43	73
C	43	0.447000	4.395000	6.197000	63	42	44	74
C	44	0.537000	3.703000	4.970000	63	39	43	45
C	45	0.896000	2.314000	4.935000	63	44	46	75
C	46	0.986000	1.649000	3.760000	63	26	45	76
C	47	3.638000	1.176000	1.385000	63	27	48	77
C	48	4.977000	1.020000	1.503000	63	47	49	78
C	49	5.553000	-0.280000	1.694000	63	48	50	54

C	50	6.950000	-0.439000	1.821000	63	49	51	79
C	51	7.493000	-1.690000	2.005000	63	50	52	80
C	52	6.658000	-2.819000	2.068000	63	51	53	81
C	53	5.295000	-2.680000	1.946000	63	52	54	82
C	54	4.715000	-1.406000	1.756000	63	28	49	53
H	55	-3.645000	-0.862000	1.567000	11	15		
H	56	-5.757000	0.221000	0.835000	11	16		
H	57	1.129000	-1.166000	-5.270000	11	21		
H	58	1.187000	0.801000	-3.754000	11	22		
H	59	-0.066000	4.162000	-0.836000	11	23		
H	60	-0.128000	5.395000	1.309000	11	24		
H	61	2.852000	-3.343000	1.872000	11	29		
H	62	0.413000	-3.080000	1.553000	11	30		
H	63	-7.107000	1.248000	-0.917000	11	31		
H	64	-7.376000	1.990000	-3.276000	11	32		
H	65	-5.541000	1.646000	-4.909000	11	33		
H	66	-3.423000	0.556000	-4.210000	11	34		
H	67	-3.664000	-2.506000	-2.772000	11	35		
H	68	-3.687000	-4.469000	-4.290000	11	36		
H	69	-1.856000	-4.814000	-5.927000	11	37		
H	70	0.027000	-3.194000	-6.058000	11	38		
H	71	-0.283000	6.270000	2.869000	11	40		
H	72	-0.434000	7.468000	5.049000	11	41		
H	73	0.033000	6.265000	7.171000	11	42		
H	74	0.655000	3.857000	7.130000	11	43		
H	75	1.096000	1.806000	5.886000	11	45		
H	76	1.265000	0.588000	3.740000	11	46		
H	77	3.203000	2.173000	1.243000	11	47		
H	78	5.650000	1.884000	1.456000	11	48		
H	79	7.595000	0.446000	1.771000	11	50		
H	80	8.576000	-1.815000	2.103000	11	51		
H	81	7.101000	-3.809000	2.215000	11	52		
H	82	4.631000	-3.557000	1.994000	11	53		

(b) asymmetric

Heat of formation: 79.71 kcal/mol

82 rr22-asym-PM3

C	1	1.224000	-3.688000	-3.116000	63	2	6	47

C	2	2.264000	-3.099000	-3.855000	63	1	3	48
C	3	2.645000	-1.742000	-3.584000	63	2	4	55
C	4	2.012000	-1.020000	-2.630000	63	3	5	56
C	5	0.928000	-1.580000	-1.867000	63	4	6	10
C	6	0.534000	-2.908000	-2.112000	63	1	5	7
C	7	-0.535000	-3.462000	-1.377000	63	6	8	57
C	8	-1.232000	-2.708000	-0.465000	63	7	9	58
C	9	-0.866000	-1.360000	-0.254000	63	8	10	11
C	10	0.244000	-0.805000	-0.890000	63	5	9	18
O	11	-1.530000	-0.564000	0.676000	82	9	34	
C	12	2.576000	-0.502000	0.783000	63	13	17	59
C	13	3.680000	-0.395000	1.558000	63	12	14	60
C	14	4.230000	0.890000	1.883000	63	13	15	49
C	15	3.611000	2.052000	1.392000	63	14	16	50
C	16	2.426000	1.935000	0.570000	63	15	17	21
C	17	1.912000	0.662000	0.260000	63	12	16	18
C	18	0.745000	0.541000	-0.545000	63	10	17	19
C	19	0.110000	1.705000	-0.974000	63	18	20	22
C	20	0.633000	2.982000	-0.674000	63	19	21	61
C	21	1.774000	3.087000	0.080000	63	16	20	62
O	22	-1.057000	1.513000	-1.704000	82	19	45	
C	23	-4.306000	4.711000	2.821000	63	24	28	63
C	24	-4.904000	5.690000	2.074000	63	23	25	64
C	25	-5.186000	5.468000	0.706000	63	24	26	65
C	26	-4.868000	4.275000	0.117000	63	25	27	66
C	27	-4.246000	3.238000	0.867000	63	26	28	32
C	28	-3.964000	3.465000	2.230000	63	23	27	29
C	29	-3.338000	2.447000	2.998000	63	28	30	67
C	30	-3.001000	1.256000	2.420000	63	29	31	68
C	31	-3.279000	1.018000	1.049000	63	30	32	34
C	32	-3.899000	1.980000	0.277000	63	27	31	41
O	33	-1.621000	3.694000	-1.877000	81	45		
C	34	-2.878000	-0.307000	0.487000	63	11	31	46
C	35	-6.521000	0.995000	-0.483000	63	36	40	69
C	36	-7.761000	0.533000	-0.832000	63	35	37	70
C	37	-8.092000	0.322000	-2.190000	63	36	38	71
C	38	-7.173000	0.577000	-3.170000	63	37	39	72
C	39	-5.877000	1.056000	-2.833000	63	38	40	44

C	40	-5.543000	1.270000	-1.479000	63	35	39	41
C	41	-4.236000	1.748000	-1.146000	63	32	40	42
C	42	-3.332000	1.998000	-2.157000	63	41	43	45
C	43	-3.675000	1.781000	-3.516000	63	42	44	73
C	44	-4.918000	1.320000	-3.847000	63	39	43	74
C	45	-1.964000	2.531000	-1.884000	63	22	33	42
O	46	-3.596000	-1.136000	-0.023000	81	34		
C	47	0.870000	-5.029000	-3.383000	63	1	54	75
C	48	2.930000	-3.850000	-4.848000	63	2	53	76
C	49	5.385000	0.998000	2.688000	63	14	52	77
C	50	4.163000	3.310000	1.720000	63	15	51	78
C	51	5.288000	3.399000	2.505000	63	50	52	79
C	52	5.905000	2.234000	2.994000	63	49	51	80
C	53	2.567000	-5.155000	-5.092000	63	48	54	81
C	54	1.530000	-5.748000	-4.352000	63	47	53	82
H	55	3.464000	-1.306000	-4.169000	11	3		
H	56	2.310000	0.015000	-2.419000	11	4		
H	57	-0.809000	-4.513000	-1.559000	11	7		
H	58	-2.074000	-3.146000	0.084000	11	8		
H	59	2.162000	-1.488000	0.534000	11	12		
H	60	4.178000	-1.288000	1.954000	11	13		
H	61	0.085000	3.868000	-1.048000	11	20		
H	62	2.194000	4.075000	0.323000	11	21		
H	63	-4.080000	4.873000	3.881000	11	23		
H	64	-5.167000	6.652000	2.524000	11	24		
H	65	-5.661000	6.264000	0.124000	11	25		
H	66	-5.083000	4.103000	-0.946000	11	26		
H	67	-3.126000	2.635000	4.057000	11	29		
H	68	-2.507000	0.474000	3.008000	11	30		
H	69	-6.261000	1.153000	0.571000	11	35		
H	70	-8.510000	0.319000	-0.061000	11	36		
H	71	-9.090000	-0.050000	-2.445000	11	37		
H	72	-7.417000	0.414000	-4.226000	11	38		
H	73	-2.930000	1.987000	-4.293000	11	43		
H	74	-5.189000	1.146000	-4.894000	11	44		
H	75	0.054000	-5.482000	-2.800000	11	47		
H	76	3.739000	-3.381000	-5.420000	11	48		
H	77	5.860000	0.085000	3.065000	11	49		

H	78	3.671000	4.215000	1.332000	11	50
H	79	5.711000	4.377000	2.755000	11	51
H	80	6.800000	2.320000	3.618000	11	52
H	81	3.083000	-5.738000	-5.861000	11	53
H	82	1.251000	-6.787000	-4.555000	11	54

4.1.3. HF/6-31G* Structure

(a) symmetric

Total energy: -1386347.11 kcal/mol

82 rr22-sym-631

C	1	-0.521000	1.479000	-1.809000	63	2	12	13
C	2	-1.309000	0.557000	-2.686000	63	1	3	15
C	3	-2.606000	0.261000	-2.368000	63	2	4	18
C	4	-3.205000	0.778000	-1.086000	63	3	5	19
C	5	-2.796000	0.268000	0.115000	63	4	6	22
C	6	-1.830000	-0.873000	0.147000	63	5	7	14
O	7	-0.766000	-0.599000	0.924000	82	6	8	
C	8	0.356000	-1.401000	0.840000	63	7	9	23
C	9	1.567000	-0.800000	0.626000	63	8	10	26
C	10	1.745000	0.694000	0.644000	63	9	11	27
C	11	1.360000	1.496000	-0.396000	63	10	12	30
O	12	0.645000	0.925000	-1.431000	82	1	11	
O	13	-0.878000	2.557000	-1.482000	81	1		
O	14	-1.976000	-1.889000	-0.441000	81	6		
C	15	-0.689000	0.015000	-3.840000	63	2	16	55
C	16	-1.393000	-0.777000	-4.680000	63	15	17	56
C	17	-2.744000	-1.109000	-4.397000	63	16	18	31
C	18	-3.352000	-0.608000	-3.228000	63	3	17	34
C	19	-4.145000	1.860000	-1.099000	63	4	20	35
C	20	-4.651000	2.347000	0.122000	63	19	21	38
C	21	-4.191000	1.788000	1.343000	63	20	22	57
C	22	-3.275000	0.793000	1.342000	63	5	21	58
C	23	0.245000	-2.786000	1.018000	63	8	24	59
C	24	1.350000	-3.572000	0.909000	63	23	25	60
C	25	2.612000	-3.028000	0.597000	63	24	26	39
C	26	2.714000	-1.634000	0.458000	63	9	25	46
C	27	2.412000	1.301000	1.752000	63	10	28	47
C	28	2.740000	2.666000	1.730000	63	27	29	54

C	29	2.395000	3.412000	0.586000	63	28	30	61
C	30	1.713000	2.850000	-0.449000	63	11	29	62
C	31	-3.486000	-1.958000	-5.259000	63	17	32	63
C	32	-4.766000	-2.300000	-4.965000	63	31	33	64
C	33	-5.373000	-1.816000	-3.783000	63	32	34	65
C	34	-4.688000	-1.000000	-2.940000	63	18	33	66
C	35	-4.581000	2.474000	-2.305000	63	19	36	67
C	36	-5.483000	3.489000	-2.284000	63	35	37	68
C	37	-6.003000	3.963000	-1.057000	63	36	38	69
C	38	-5.594000	3.408000	0.112000	63	20	37	70
C	39	3.796000	-3.866000	0.426000	63	25	40	44
C	40	3.770000	-5.271000	0.561000	63	39	41	71
C	41	4.901000	-6.022000	0.394000	63	40	42	72
C	42	6.123000	-5.409000	0.081000	63	41	43	73
C	43	6.176000	-4.052000	-0.057000	63	42	44	74
C	44	5.021000	-3.261000	0.112000	63	39	43	45
C	45	5.082000	-1.834000	-0.041000	63	44	46	75
C	46	3.998000	-1.064000	0.125000	63	26	45	76
C	47	2.748000	0.527000	2.924000	63	27	48	77
C	48	3.369000	1.084000	3.973000	63	47	49	78
C	49	3.738000	2.472000	3.980000	63	48	50	54
C	50	4.400000	3.034000	5.089000	63	49	51	79
C	51	4.748000	4.354000	5.103000	63	50	52	80
C	52	4.439000	5.160000	3.997000	63	51	53	81
C	53	3.796000	4.632000	2.913000	63	52	54	82
C	54	3.427000	3.269000	2.869000	63	28	49	53
H	55	0.340000	0.249000	-4.041000	11	15		
H	56	-0.933000	-1.176000	-5.566000	11	16		
H	57	-4.570000	2.177000	2.271000	11	21		
H	58	-2.909000	0.384000	2.265000	11	22		
H	59	-0.711000	-3.218000	1.226000	11	23		
H	60	1.233000	-4.627000	1.052000	11	24		
H	61	2.651000	4.450000	0.515000	11	29		
H	62	1.431000	3.438000	-1.298000	11	30		
H	63	-3.012000	-2.331000	-6.150000	11	31		
H	64	-5.321000	-2.945000	-5.622000	11	32		
H	65	-6.383000	-2.102000	-3.550000	11	33		
H	66	-5.157000	-0.648000	-2.042000	11	34		

H	67	-4.187000	2.131000	-3.242000	11	35
H	68	-5.802000	3.942000	-3.206000	11	36
H	69	-6.717000	4.767000	-1.057000	11	37
H	70	-5.975000	3.769000	1.051000	11	38
H	71	2.854000	-5.776000	0.796000	11	40
H	72	4.851000	-7.091000	0.503000	11	41
H	73	7.007000	-6.005000	-0.049000	11	42
H	74	7.105000	-3.566000	-0.299000	11	43
H	75	6.026000	-1.387000	-0.298000	11	45
H	76	4.079000	-0.004000	-0.005000	11	46
H	77	2.481000	-0.509000	2.957000	11	47
H	78	3.601000	0.489000	4.839000	11	48
H	79	4.628000	2.403000	5.930000	11	50
H	80	5.253000	4.776000	5.953000	11	51
H	81	4.708000	6.201000	4.002000	11	52
H	82	3.573000	5.280000	2.088000	11	53

(b) asymmetric

Total energy: -1386349.51 kcal/mol

82 rr22-asym-631

C	1	4.586000	0.518000	0.626000	63	2	6	47
C	2	4.782000	-0.579000	1.477000	63	1	3	48
C	3	3.729000	-1.544000	1.637000	63	2	4	55
C	4	2.569000	-1.432000	0.976000	63	3	5	56
C	5	2.321000	-0.329000	0.079000	63	4	6	10
C	6	3.315000	0.652000	-0.082000	63	1	5	7
C	7	3.042000	1.746000	-0.927000	63	6	8	57
C	8	1.838000	1.880000	-1.550000	63	7	9	58
C	9	0.858000	0.901000	-1.371000	63	8	10	11
C	10	1.081000	-0.220000	-0.615000	63	5	9	18
O	11	-0.372000	1.038000	-1.979000	82	9	34	
C	12	1.513000	-2.811000	-1.920000	63	13	17	59
C	13	1.759000	-3.994000	-2.498000	63	12	14	60
C	14	0.843000	-5.095000	-2.381000	63	13	15	49
C	15	-0.350000	-4.921000	-1.665000	63	14	16	50
C	16	-0.631000	-3.624000	-1.055000	63	15	17	21
C	17	0.307000	-2.583000	-1.159000	63	12	16	18
C	18	0.056000	-1.318000	-0.549000	63	10	17	19

C	19	-1.150000	-1.127000	0.071000	63	18	20	22
C	20	-2.105000	-2.145000	0.164000	63	19	21	61
C	21	-1.837000	-3.366000	-0.373000	63	16	20	62
O	22	-1.453000	0.150000	0.486000	82	19	45	
C	23	-6.589000	0.328000	-2.246000	63	24	28	63
C	24	-7.500000	0.478000	-1.252000	63	23	25	64
C	25	-7.119000	1.083000	-0.031000	63	24	26	65
C	26	-5.848000	1.523000	0.155000	63	25	27	66
C	27	-4.867000	1.388000	-0.869000	63	26	28	32
C	28	-5.251000	0.774000	-2.080000	63	23	27	29
C	29	-4.290000	0.595000	-3.107000	63	28	30	67
C	30	-3.010000	0.993000	-2.925000	63	29	31	68
C	31	-2.623000	1.637000	-1.723000	63	30	32	34
C	32	-3.515000	1.845000	-0.708000	63	27	31	41
O	33	-2.290000	-0.334000	2.490000	81	45		
C	34	-1.190000	2.014000	-1.538000	63	11	31	46
C	35	-4.062000	4.675000	-0.307000	63	36	40	69
C	36	-4.382000	5.983000	-0.131000	63	35	37	70
C	37	-4.159000	6.615000	1.114000	63	36	38	71
C	38	-3.617000	5.914000	2.142000	63	37	39	72
C	39	-3.270000	4.547000	1.986000	63	38	40	44
C	40	-3.495000	3.909000	0.750000	63	35	39	41
C	41	-3.139000	2.528000	0.586000	63	32	40	42
C	42	-2.569000	1.864000	1.641000	63	41	43	45
C	43	-2.374000	2.510000	2.892000	63	42	44	73
C	44	-2.706000	3.809000	3.058000	63	39	43	74
C	45	-2.124000	0.435000	1.605000	63	22	33	42
O	46	-0.805000	3.023000	-1.058000	81	34		
C	47	5.641000	1.448000	0.496000	63	1	54	75
C	48	6.000000	-0.725000	2.170000	63	2	53	76
C	49	1.132000	-6.336000	-2.981000	63	14	52	77
C	50	-1.225000	-6.024000	-1.566000	63	15	51	78
C	51	-0.927000	-7.223000	-2.153000	63	50	52	79
C	52	0.266000	-7.386000	-2.872000	63	49	51	80
C	53	7.004000	0.189000	2.026000	63	48	54	81
C	54	6.817000	1.288000	1.175000	63	47	53	82
H	55	3.889000	-2.368000	2.310000	11	3		
H	56	1.800000	-2.163000	1.125000	11	4		

H	57	3.777000	2.510000	-1.080000	11	7	
H	58	1.624000	2.731000	-2.165000	11	8	
H	59	2.215000	-2.011000	-2.032000	11	12	
H	60	2.660000	-4.137000	-3.068000	11	13	
H	61	-3.036000	-1.961000	0.661000	11	20	
H	62	-2.583000	-4.130000	-0.283000	11	21	
H	63	-6.866000	-0.135000	-3.176000	11	23	
H	64	-8.511000	0.137000	-1.384000	11	24	
H	65	-7.844000	1.194000	0.755000	11	25	
H	66	-5.578000	1.978000	1.087000	11	26	
H	67	-4.588000	0.120000	-4.025000	11	29	
H	68	-2.272000	0.825000	-3.687000	11	30	
H	69	-4.228000	4.214000	-1.260000	11	35	
H	70	-4.803000	6.546000	-0.944000	11	36	
H	71	-4.418000	7.651000	1.240000	11	37	
H	72	-3.440000	6.386000	3.093000	11	38	
H	73	-1.953000	1.940000	3.699000	11	43	
H	74	-2.546000	4.296000	4.004000	11	44	
H	75	5.535000	2.301000	-0.144000	11	47	
H	76	6.127000	-1.574000	2.819000	11	48	
H	77	2.052000	-6.446000	-3.528000	11	49	
H	78	-2.144000	-5.940000	-1.020000	11	50	
H	79	-1.612000	-8.047000	-2.059000	11	51	
H	80	0.494000	-8.331000	-3.331000	11	52	
H	81	7.930000	0.070000	2.558000	11	53	
H	82	7.603000	2.012000	1.056000	11	54	

4.2. Compound (S_a,R_a)-22

4.2.1. AM1 Structure

Heat of formation: 109.37 kcal/mol

82 sr22-AM1

C	1	-1.858000	0.627000	1.790000	63	2	12	13
C	2	-2.986000	0.772000	0.847000	63	1	3	15
C	3	-3.560000	-0.298000	0.183000	63	2	4	18
C	4	-3.109000	-1.688000	0.375000	63	3	5	19
C	5	-2.333000	-2.357000	-0.556000	63	4	6	22
C	6	-1.868000	-1.738000	-1.814000	63	5	7	14
O	7	-0.546000	-1.384000	-2.026000	82	6	8	

C	8	0.404000	-1.576000	-1.028000	63	7	9	23
C	9	0.950000	-0.470000	-0.379000	63	8	10	26
C	10	0.487000	0.894000	-0.668000	63	9	11	27
C	11	-0.291000	1.606000	0.244000	63	10	12	30
O	12	-0.574000	1.047000	1.486000	82	1	11	
O	13	-1.909000	0.197000	2.941000	81	1		
O	14	-2.539000	-1.522000	-2.822000	81	6		
C	15	-3.541000	2.076000	0.730000	63	2	16	55
C	16	-4.629000	2.305000	-0.068000	63	15	17	56
C	17	-5.226000	1.238000	-0.792000	63	16	18	31
C	18	-4.693000	-0.071000	-0.669000	63	3	17	34
C	19	-3.566000	-2.388000	1.541000	63	4	20	35
C	20	-3.245000	-3.760000	1.706000	63	19	21	38
C	21	-2.475000	-4.421000	0.712000	63	20	22	57
C	22	-2.034000	-3.737000	-0.389000	63	5	21	58
C	23	0.928000	-2.871000	-0.832000	63	8	24	59
C	24	1.968000	-3.063000	0.050000	63	23	25	60
C	25	2.530000	-1.979000	0.764000	63	24	26	39
C	26	2.018000	-0.678000	0.541000	63	9	25	46
C	27	0.881000	1.536000	-1.877000	63	10	28	47
C	28	0.513000	2.881000	-2.128000	63	27	29	54
C	29	-0.243000	3.572000	-1.154000	63	28	30	61
C	30	-0.637000	2.954000	0.012000	63	11	29	62
C	31	-6.356000	1.461000	-1.625000	63	17	32	63
C	32	-6.936000	0.421000	-2.308000	63	31	33	64
C	33	-6.407000	-0.886000	-2.190000	63	32	34	65
C	34	-5.315000	-1.126000	-1.394000	63	18	33	66
C	35	-4.349000	-1.751000	2.545000	63	19	36	67
C	36	-4.788000	-2.446000	3.645000	63	35	37	68
C	37	-4.467000	-3.815000	3.803000	63	36	38	69
C	38	-3.709000	-4.458000	2.855000	63	20	37	70
C	39	3.619000	-2.170000	1.697000	63	25	40	44
C	40	4.168000	-3.445000	1.973000	63	39	41	71
C	41	5.211000	-3.592000	2.866000	63	40	42	72
C	42	5.748000	-2.472000	3.525000	63	41	43	73
C	43	5.229000	-1.218000	3.278000	63	42	44	74
C	44	4.162000	-1.049000	2.367000	63	39	43	45
C	45	3.619000	0.255000	2.121000	63	44	46	75

C	46	2.594000	0.432000	1.250000	63	26	45	76
C	47	1.663000	0.831000	-2.854000	63	27	48	77
C	48	2.056000	1.429000	-4.007000	63	47	49	78
C	49	1.703000	2.789000	-4.290000	63	48	50	54
C	50	2.120000	3.400000	-5.495000	63	49	51	79
C	51	1.774000	4.706000	-5.775000	63	50	52	80
C	52	0.999000	5.435000	-4.857000	63	51	53	81
C	53	0.584000	4.854000	-3.674000	63	52	54	82
C	54	0.927000	3.518000	-3.359000	63	28	49	53
H	55	-3.093000	2.895000	1.313000	11	15		
H	56	-5.061000	3.314000	-0.157000	11	16		
H	57	-2.246000	-5.490000	0.841000	11	21		
H	58	-1.460000	-4.252000	-1.174000	11	22		
H	59	0.514000	-3.712000	-1.406000	11	23		
H	60	2.365000	-4.080000	0.187000	11	24		
H	61	-0.521000	4.624000	-1.314000	11	29		
H	62	-1.200000	3.505000	0.780000	11	30		
H	63	-6.751000	2.485000	-1.712000	11	31		
H	64	-7.810000	0.591000	-2.955000	11	32		
H	65	-6.877000	-1.707000	-2.753000	11	33		
H	66	-4.887000	-2.139000	-1.326000	11	34		
H	67	-4.576000	-0.678000	2.438000	11	35		
H	68	-5.387000	-1.944000	4.419000	11	36		
H	69	-4.826000	-4.351000	4.693000	11	37		
H	70	-3.445000	-5.520000	2.967000	11	38		
H	71	3.766000	-4.339000	1.476000	11	40		
H	72	5.627000	-4.590000	3.070000	11	41		
H	73	6.579000	-2.605000	4.234000	11	42		
H	74	5.637000	-0.332000	3.789000	11	43		
H	75	4.054000	1.108000	2.665000	11	45		
H	76	2.163000	1.432000	1.081000	11	46		
H	77	1.917000	-0.222000	-2.650000	11	47		
H	78	2.651000	0.882000	-4.755000	11	48		
H	79	2.723000	2.815000	-6.206000	11	50		
H	80	2.097000	5.181000	-6.713000	11	51		
H	81	0.724000	6.475000	-5.088000	11	52		
H	82	-0.024000	5.448000	-2.977000	11	53		

4.2.2. PM3 Structure

Heat of formation: 74.15 kcal/mol

82 sr22-PM3

C	1	-1.303000	1.303000	1.987000	63	2	12	13
C	2	-2.143000	1.691000	0.820000	63	1	3	15
C	3	-2.824000	0.768000	0.053000	63	2	4	18
C	4	-2.732000	-0.687000	0.308000	63	3	5	19
C	5	-1.819000	-1.488000	-0.345000	63	4	6	22
C	6	-0.890000	-0.967000	-1.386000	63	5	7	14
O	7	0.467000	-0.814000	-1.256000	82	6	8	
C	8	1.147000	-1.260000	-0.130000	63	7	9	23
C	9	1.842000	-0.335000	0.644000	63	8	10	26
C	10	1.752000	1.112000	0.369000	63	9	11	27
C	11	0.824000	1.913000	1.028000	63	10	12	30
O	12	0.066000	1.357000	2.051000	82	1	11	
O	13	-1.692000	0.903000	3.062000	81	1		
O	14	-1.180000	-0.619000	-2.510000	81	6		
C	15	-2.305000	3.081000	0.586000	63	2	16	55
C	16	-3.130000	3.532000	-0.405000	63	15	17	56
C	17	-3.840000	2.608000	-1.218000	63	16	18	31
C	18	-3.691000	1.223000	-0.993000	63	3	17	34
C	19	-3.659000	-1.278000	1.227000	63	4	20	35
C	20	-3.628000	-2.671000	1.443000	63	19	21	38
C	21	-2.680000	-3.469000	0.749000	63	20	22	57
C	22	-1.801000	-2.890000	-0.120000	63	5	21	58
C	23	1.273000	-2.647000	0.104000	63	8	24	59
C	24	2.077000	-3.095000	1.122000	63	23	25	60
C	25	2.787000	-2.187000	1.936000	63	24	26	39
C	26	2.671000	-0.805000	1.698000	63	9	25	46
C	27	2.641000	1.713000	-0.564000	63	10	28	47
C	28	2.579000	3.099000	-0.798000	63	27	29	54
C	29	1.633000	3.881000	-0.101000	63	28	30	61
C	30	0.771000	3.306000	0.799000	63	11	29	62
C	31	-4.700000	3.067000	-2.251000	63	17	32	63
C	32	-5.385000	2.172000	-3.027000	63	31	33	64
C	33	-5.242000	0.783000	-2.805000	63	32	34	65
C	34	-4.418000	0.319000	-1.816000	63	18	33	66
C	35	-4.624000	-0.502000	1.928000	63	19	36	67

C	36	-5.500000	-1.095000	2.796000	63	35	37	68
C	37	-5.463000	-2.492000	3.011000	63	36	38	69
C	38	-4.548000	-3.265000	2.350000	63	20	37	70
C	39	3.634000	-2.662000	3.009000	63	25	40	44
C	40	3.778000	-4.040000	3.283000	63	39	41	71
C	41	4.587000	-4.470000	4.308000	63	40	42	72
C	42	5.283000	-3.539000	5.098000	63	41	43	73
C	43	5.158000	-2.192000	4.850000	63	42	44	74
C	44	4.331000	-1.734000	3.801000	63	39	43	45
C	45	4.194000	-0.331000	3.536000	63	44	46	75
C	46	3.403000	0.112000	2.531000	63	26	45	76
C	47	3.611000	0.925000	-1.275000	63	27	48	77
C	48	4.461000	1.492000	-2.163000	63	47	49	78
C	49	4.421000	2.904000	-2.422000	63	48	50	54
C	50	5.309000	3.491000	-3.349000	63	49	51	79
C	51	5.263000	4.845000	-3.592000	63	50	52	80
C	52	4.331000	5.652000	-2.917000	63	51	53	81
C	53	3.459000	5.094000	-2.011000	63	52	54	82
C	54	3.487000	3.707000	-1.746000	63	28	49	53
H	55	-1.738000	3.791000	1.209000	11	15		
H	56	-3.253000	4.606000	-0.586000	11	16		
H	57	-2.665000	-4.551000	0.923000	11	21		
H	58	-1.052000	-3.499000	-0.649000	11	22		
H	59	0.713000	-3.357000	-0.524000	11	23		
H	60	2.184000	-4.173000	1.321000	11	24		
H	61	1.603000	4.964000	-0.294000	11	29		
H	62	0.027000	3.916000	1.334000	11	30		
H	63	-4.801000	4.145000	-2.415000	11	31		
H	64	-6.047000	2.520000	-3.827000	11	32		
H	65	-5.795000	0.082000	-3.440000	11	33		
H	66	-4.299000	-0.759000	-1.652000	11	34		
H	67	-4.645000	0.584000	1.771000	11	35		
H	68	-6.235000	-0.492000	3.338000	11	36		
H	69	-6.171000	-2.943000	3.713000	11	37		
H	70	-4.507000	-4.348000	2.510000	11	38		
H	71	3.227000	-4.760000	2.658000	11	40		
H	72	4.694000	-5.540000	4.516000	11	41		
H	73	5.923000	-3.895000	5.912000	11	42		

H	74	5.697000	-1.460000	5.463000	11	43
H	75	4.745000	0.374000	4.169000	11	45
H	76	3.295000	1.186000	2.333000	11	46
H	77	3.640000	-0.155000	-1.083000	11	47
H	78	5.195000	0.886000	-2.705000	11	48
H	79	6.032000	2.856000	-3.872000	11	50
H	80	5.950000	5.302000	-4.311000	11	51
H	81	4.303000	6.728000	-3.119000	11	52
H	82	2.724000	5.716000	-1.478000	11	53

4.2.3. HF/6-31G* Structure

Total energy: -1386333.13 kcal/mol

82 sr22-631

C	1	1.451000	0.422000	-1.599000	63	2	14	28
C	2	1.236000	1.478000	-0.751000	63	1	3	26
C	3	1.350000	2.799000	-1.195000	63	2	4	55
C	4	1.617000	3.058000	-2.505000	63	3	5	56
C	5	1.808000	2.017000	-3.434000	63	4	6	14
C	6	2.099000	2.282000	-4.841000	63	5	7	11
C	7	2.135000	3.582000	-5.388000	63	6	8	57
C	8	2.416000	3.789000	-6.710000	63	7	9	58
C	9	2.678000	2.704000	-7.560000	63	8	10	59
C	10	2.644000	1.435000	-7.057000	63	9	11	60
C	11	2.354000	1.203000	-5.699000	63	6	10	12
C	12	2.314000	-0.135000	-5.176000	63	11	13	61
C	13	2.023000	-0.380000	-3.892000	63	12	14	62
C	14	1.745000	0.693000	-2.968000	63	1	5	13
C	15	-2.495000	1.053000	0.361000	63	16	24	42
C	16	-1.331000	1.680000	0.703000	63	15	17	25
C	17	-1.254000	3.100000	0.734000	63	16	18	63
C	18	-2.321000	3.858000	0.401000	63	17	19	64
C	19	-3.531000	3.250000	-0.023000	63	18	20	24
C	20	-4.648000	4.033000	-0.411000	63	19	21	65
C	21	-5.802000	3.442000	-0.814000	63	20	22	66
C	22	-5.897000	2.033000	-0.852000	63	21	23	67
C	23	-4.843000	1.259000	-0.482000	63	22	24	68
C	24	-3.622000	1.844000	-0.049000	63	15	19	23
C	25	-0.122000	0.922000	1.171000	63	16	26	27

O	26	1.061000	1.257000	0.600000	82	2	25	
O	27	-0.134000	0.142000	2.055000	81	25		
C	28	1.469000	-0.988000	-1.083000	63	1	29	41
C	29	0.466000	-1.866000	-1.403000	63	28	30	53
C	30	0.539000	-3.214000	-1.040000	63	29	31	69
C	31	1.590000	-3.665000	-0.301000	63	30	32	70
C	32	2.632000	-2.805000	0.095000	63	31	33	41
C	33	3.766000	-3.278000	0.884000	63	32	34	38
C	34	3.867000	-4.598000	1.372000	63	33	35	71
C	35	4.949000	-5.004000	2.104000	63	34	36	72
C	36	5.991000	-4.110000	2.389000	63	35	37	73
C	37	5.915000	-2.825000	1.933000	63	36	38	74
C	38	4.808000	-2.388000	1.180000	63	33	37	39
C	39	4.731000	-1.033000	0.708000	63	38	40	75
C	40	3.680000	-0.593000	0.006000	63	39	41	76
C	41	2.577000	-1.464000	-0.321000	63	28	32	40
C	42	-2.671000	-0.438000	0.458000	63	15	43	51
C	43	-2.305000	-1.287000	-0.546000	63	42	44	52
C	44	-2.620000	-2.672000	-0.473000	63	43	45	77
C	45	-3.264000	-3.181000	0.600000	63	44	46	78
C	46	-3.604000	-2.346000	1.696000	63	45	47	51
C	47	-4.247000	-2.872000	2.846000	63	46	48	79
C	48	-4.570000	-2.066000	3.889000	63	47	49	80
C	49	-4.264000	-0.687000	3.836000	63	48	50	81
C	50	-3.653000	-0.156000	2.744000	63	49	51	82
C	51	-3.306000	-0.971000	1.632000	63	42	46	50
C	52	-1.666000	-0.800000	-1.814000	63	43	53	54
O	53	-0.564000	-1.469000	-2.232000	82	29	52	
O	54	-2.119000	0.048000	-2.496000	81	52		
H	55	1.242000	3.602000	-0.494000	11	3		
H	56	1.698000	4.081000	-2.812000	11	4		
H	57	1.931000	4.436000	-4.772000	11	7		
H	58	2.434000	4.791000	-7.101000	11	8		
H	59	2.899000	2.874000	-8.598000	11	9		
H	60	2.838000	0.592000	-7.697000	11	10		
H	61	2.521000	-0.951000	-5.846000	11	12		
H	62	1.999000	-1.390000	-3.538000	11	13		
H	63	-0.347000	3.563000	1.070000	11	17		

H	64	-2.264000	4.931000	0.453000	11	18
H	65	-4.562000	5.105000	-0.383000	11	20
H	66	-6.645000	4.041000	-1.110000	11	21
H	67	-6.810000	1.571000	-1.182000	11	22
H	68	-4.928000	0.191000	-0.528000	11	23
H	69	-0.228000	-3.889000	-1.362000	11	30
H	70	1.615000	-4.704000	-0.039000	11	31
H	71	3.086000	-5.308000	1.183000	11	34
H	72	4.999000	-6.016000	2.465000	11	35
H	73	6.838000	-4.435000	2.964000	11	36
H	74	6.704000	-2.125000	2.147000	11	37
H	75	5.544000	-0.366000	0.937000	11	39
H	76	3.654000	0.425000	-0.327000	11	40
H	77	-2.380000	-3.304000	-1.307000	11	44
H	78	-3.522000	-4.224000	0.636000	11	45
H	79	-4.470000	-3.924000	2.877000	11	47
H	80	-5.055000	-2.471000	4.759000	11	48
H	81	-4.514000	-0.056000	4.669000	11	49
H	82	-3.417000	0.889000	2.726000	11	50

4.3. Compound (R_a,R_a)-23

4.3.1. AM1 Structure

(a) symmetric

Heat of formation: 68.66 kcal/mol

70 rr23-sym-AM1

C	1	-0.298000	1.627000	-1.336000	63	2	12	13
C	2	-1.275000	0.779000	-2.051000	63	1	3	15
C	3	-2.434000	0.347000	-1.426000	63	2	4	22
C	4	-2.702000	0.668000	-0.014000	63	3	5	30
C	5	-2.061000	-0.012000	1.010000	63	4	6	23
C	6	-1.132000	-1.124000	0.716000	63	5	7	14
O	7	0.145000	-0.867000	1.183000	82	6	8	
C	8	1.212000	-1.605000	0.668000	63	7	9	39
C	9	2.351000	-0.906000	0.290000	63	8	10	46
C	10	2.509000	0.541000	0.482000	63	9	11	38
C	11	1.852000	1.488000	-0.293000	63	10	12	31
O	12	0.943000	1.022000	-1.246000	82	1	11	
O	13	-0.459000	2.758000	-0.888000	81	1		

O	14	-1.380000	-2.199000	0.178000	81	6		
C	15	-0.997000	0.436000	-3.399000	63	2	16	47
C	16	-1.891000	-0.314000	-4.117000	63	15	17	48
C	17	-3.098000	-0.765000	-3.518000	63	16	18	22
C	18	-4.033000	-1.548000	-4.251000	63	17	19	49
C	19	-5.188000	-1.993000	-3.658000	63	18	20	50
C	20	-5.462000	-1.677000	-2.306000	63	19	21	51
C	21	-4.578000	-0.920000	-1.577000	63	20	22	52
C	22	-3.374000	-0.439000	-2.165000	63	3	17	21
C	23	-2.288000	0.324000	2.368000	63	5	24	53
C	24	-3.173000	1.320000	2.693000	63	23	25	54
C	25	-3.861000	2.032000	1.675000	63	24	26	30
C	26	-4.778000	3.071000	1.998000	63	25	27	55
C	27	-5.425000	3.765000	1.006000	63	26	28	56
C	28	-5.186000	3.453000	-0.354000	63	27	29	57
C	29	-4.308000	2.453000	-0.693000	63	28	30	58
C	30	-3.625000	1.712000	0.312000	63	4	25	29
C	31	2.145000	2.875000	-0.190000	63	11	32	59
C	32	3.044000	3.311000	0.747000	63	31	33	60
C	33	3.683000	2.391000	1.621000	63	32	34	38
C	34	4.579000	2.842000	2.628000	63	33	35	61
C	35	5.183000	1.950000	3.478000	63	34	36	62
C	36	4.918000	0.565000	3.356000	63	35	37	63
C	37	4.062000	0.104000	2.387000	63	36	38	64
C	38	3.420000	1.004000	1.488000	63	10	33	37
C	39	1.152000	-3.024000	0.616000	63	8	40	65
C	40	2.212000	-3.731000	0.113000	63	39	41	66
C	41	3.369000	-3.059000	-0.363000	63	40	42	46
C	42	4.452000	-3.783000	-0.933000	63	41	43	67
C	43	5.562000	-3.128000	-1.404000	63	42	44	68
C	44	5.638000	-1.717000	-1.324000	63	43	45	69
C	45	4.609000	-0.995000	-0.772000	63	44	46	70
C	46	3.444000	-1.646000	-0.273000	63	9	41	45
H	47	-0.048000	0.775000	-3.844000	11	15		
H	48	-1.685000	-0.585000	-5.164000	11	16		
H	49	-3.806000	-1.791000	-5.300000	11	18		
H	50	-5.910000	-2.602000	-4.223000	11	19		
H	51	-6.390000	-2.048000	-1.847000	11	20		

H	52	-4.785000	-0.674000	-0.523000	11	21
H	53	-1.733000	-0.223000	3.146000	11	23
H	54	-3.356000	1.588000	3.745000	11	24
H	55	-4.951000	3.307000	3.058000	11	26
H	56	-6.132000	4.571000	1.254000	11	27
H	57	-5.709000	4.025000	-1.134000	11	28
H	58	-4.116000	2.209000	-1.750000	11	29
H	59	1.632000	3.583000	-0.858000	11	31
H	60	3.278000	4.383000	0.840000	11	32
H	61	4.773000	3.922000	2.712000	11	34
H	62	5.875000	2.297000	4.260000	11	35
H	63	5.406000	-0.136000	4.049000	11	36
H	64	3.856000	-0.974000	2.290000	11	37
H	65	0.244000	-3.536000	0.970000	11	39
H	66	2.178000	-4.830000	0.064000	11	40
H	67	4.377000	-4.880000	-0.991000	11	42
H	68	6.400000	-3.686000	-1.847000	11	43
H	69	6.532000	-1.206000	-1.711000	11	44
H	70	4.668000	0.103000	-0.708000	11	45

(b) asymmetric

Heat of formation: 68.66 kcal/mol

70 rr23-asym-AM1

C	1	6.030000	0.998000	-0.677000	63	2	6	47
C	2	6.291000	2.336000	-0.830000	63	1	3	48
C	3	5.294000	3.292000	-0.520000	63	2	4	49
C	4	4.066000	2.891000	-0.058000	63	3	5	50
C	5	3.764000	1.510000	0.116000	63	4	6	10
C	6	4.761000	0.554000	-0.211000	63	1	5	7
C	7	4.478000	-0.833000	-0.082000	63	6	8	51
C	8	3.241000	-1.257000	0.325000	63	7	9	52
C	9	2.241000	-0.299000	0.636000	63	8	10	11
C	10	2.482000	1.070000	0.578000	63	5	9	18
O	11	0.988000	-0.718000	1.085000	82	9	34	
C	12	2.868000	2.803000	2.900000	63	13	17	53
C	13	3.062000	3.627000	3.981000	63	12	14	54
C	14	2.090000	4.594000	4.328000	63	13	15	55
C	15	0.939000	4.707000	3.589000	63	14	16	56

C	16	0.708000	3.859000	2.471000	63	15	17	21
C	17	1.689000	2.900000	2.107000	63	12	16	18
C	18	1.464000	2.047000	0.979000	63	10	17	19
C	19	0.245000	2.144000	0.315000	63	18	20	22
C	20	-0.736000	3.104000	0.675000	63	19	21	57
C	21	-0.497000	3.951000	1.725000	63	16	20	58
O	22	-0.015000	1.159000	-0.635000	82	19	45	
C	23	-5.311000	-0.691000	1.313000	63	24	28	59
C	24	-6.185000	-0.380000	0.302000	63	23	25	60
C	25	-5.722000	-0.279000	-1.032000	63	24	26	61
C	26	-4.398000	-0.492000	-1.326000	63	25	27	62
C	27	-3.467000	-0.819000	-0.299000	63	26	28	32
C	28	-3.934000	-0.914000	1.037000	63	23	27	29
C	29	-3.018000	-1.221000	2.079000	63	28	30	63
C	30	-1.690000	-1.415000	1.801000	63	29	31	64
C	31	-1.217000	-1.331000	0.464000	63	30	32	34
C	32	-2.080000	-1.042000	-0.580000	63	27	31	41
O	33	-1.123000	2.553000	-2.022000	81	45		
C	34	0.231000	-1.517000	0.238000	63	11	31	46
C	35	-2.394000	-3.320000	-2.321000	63	36	40	65
C	36	-2.564000	-4.408000	-3.141000	63	35	37	66
C	37	-2.173000	-4.350000	-4.500000	63	36	38	67
C	38	-1.618000	-3.202000	-5.008000	63	37	39	68
C	39	-1.429000	-2.062000	-4.181000	63	38	40	44
C	40	-1.822000	-2.115000	-2.819000	63	35	39	41
C	41	-1.624000	-0.969000	-1.980000	63	32	40	42
C	42	-1.046000	0.168000	-2.516000	63	41	43	45
C	43	-0.665000	0.217000	-3.886000	63	42	44	69
C	44	-0.851000	-0.870000	-4.697000	63	39	43	70
C	45	-0.788000	1.404000	-1.745000	63	22	33	42
O	46	0.808000	-2.289000	-0.520000	81	34		
H	47	6.793000	0.242000	-0.918000	11	1		
H	48	7.270000	2.681000	-1.194000	11	2		
H	49	5.517000	4.361000	-0.656000	11	3		
H	50	3.289000	3.633000	0.187000	11	4		
H	51	5.267000	-1.560000	-0.327000	11	7		
H	52	2.991000	-2.327000	0.397000	11	8		
H	53	3.625000	2.051000	2.627000	11	12		

H	54	3.974000	3.543000	4.589000	11	13
H	55	2.268000	5.247000	5.195000	11	14
H	56	0.171000	5.452000	3.849000	11	15
H	57	-1.673000	3.161000	0.100000	11	20
H	58	-1.243000	4.708000	2.013000	11	21
H	59	-5.657000	-0.771000	2.355000	11	23
H	60	-7.251000	-0.205000	0.514000	11	24
H	61	-6.437000	-0.025000	-1.829000	11	25
H	62	-4.036000	-0.415000	-2.363000	11	26
H	63	-3.392000	-1.289000	3.112000	11	29
H	64	-0.963000	-1.623000	2.601000	11	30
H	65	-2.693000	-3.365000	-1.262000	11	35
H	66	-3.002000	-5.339000	-2.749000	11	36
H	67	-2.317000	-5.235000	-5.137000	11	37
H	68	-1.305000	-3.144000	-6.062000	11	38
H	69	-0.223000	1.149000	-4.274000	11	43
H	70	-0.554000	-0.840000	-5.756000	11	44

4.3.2. PM3 Structure

(a) symmetric

Heat of formation: 50.99 kcal/mol

70 rr23-sym-PM3

C	1	-0.090000	-1.436000	1.162000	63	2	12	13
C	2	-1.344000	-0.878000	1.749000	63	1	3	15
C	3	-2.465000	-0.667000	0.972000	63	2	4	22
C	4	-2.463000	-0.958000	-0.479000	63	3	5	30
C	5	-1.939000	-0.064000	-1.392000	63	4	6	23
C	6	-1.376000	1.247000	-0.954000	63	5	7	14
O	7	-0.034000	1.363000	-1.258000	82	6	8	
C	8	0.748000	2.270000	-0.544000	63	7	9	39
C	9	1.936000	1.800000	-0.008000	63	8	10	46
C	10	2.476000	0.449000	-0.264000	63	9	11	38
C	11	2.053000	-0.689000	0.403000	63	10	12	31
O	12	0.970000	-0.556000	1.270000	82	1	11	
O	13	0.052000	-2.537000	0.679000	81	1		
O	14	-1.985000	2.155000	-0.432000	81	6		
C	15	-1.356000	-0.598000	3.139000	63	2	16	47
C	16	-2.487000	-0.115000	3.734000	63	15	17	48

C	17	-3.659000	0.118000	2.966000	63	16	18	22
C	18	-4.836000	0.628000	3.577000	63	17	19	49
C	19	-5.958000	0.860000	2.830000	63	18	20	50
C	20	-5.956000	0.593000	1.441000	63	19	21	51
C	21	-4.836000	0.099000	0.831000	63	20	22	52
C	22	-3.654000	-0.155000	1.581000	63	3	17	21
C	23	-1.945000	-0.351000	-2.780000	63	5	24	53
C	24	-2.475000	-1.524000	-3.239000	63	23	25	54
C	25	-3.021000	-2.468000	-2.330000	63	24	26	30
C	26	-3.567000	-3.694000	-2.799000	63	25	27	55
C	27	-4.081000	-4.605000	-1.918000	63	26	28	56
C	28	-4.074000	-4.334000	-0.530000	63	27	29	57
C	29	-3.556000	-3.161000	-0.054000	63	28	30	58
C	30	-3.016000	-2.192000	-0.946000	63	4	25	29
C	31	2.766000	-1.917000	0.294000	63	11	32	59
C	32	3.819000	-2.018000	-0.569000	63	31	33	60
C	33	4.208000	-0.908000	-1.365000	63	32	34	38
C	34	5.260000	-1.033000	-2.312000	63	33	35	61
C	35	5.633000	0.038000	-3.077000	63	34	36	62
C	36	4.974000	1.279000	-2.928000	63	35	37	63
C	37	3.961000	1.423000	-2.019000	63	36	38	64
C	38	3.548000	0.328000	-1.210000	63	10	33	37
C	39	0.396000	3.647000	-0.466000	63	8	40	65
C	40	1.178000	4.510000	0.247000	63	39	41	66
C	41	2.340000	4.044000	0.917000	63	40	42	46
C	42	3.117000	4.927000	1.714000	63	41	43	67
C	43	4.237000	4.475000	2.358000	63	42	44	68
C	44	4.630000	3.124000	2.232000	63	43	45	69
C	45	3.900000	2.257000	1.465000	63	44	46	70
C	46	2.729000	2.695000	0.785000	63	9	41	45
H	47	-0.446000	-0.770000	3.725000	11	15		
H	48	-2.504000	0.105000	4.808000	11	16		
H	49	-4.825000	0.835000	4.653000	11	18		
H	50	-6.867000	1.256000	3.296000	11	19		
H	51	-6.863000	0.791000	0.859000	11	20		
H	52	-4.830000	-0.104000	-0.247000	11	21		
H	53	-1.514000	0.377000	-3.476000	11	23		
H	54	-2.482000	-1.752000	-4.311000	11	24		

H	55	-3.563000	-3.895000	-3.877000	11	26
H	56	-4.500000	-5.552000	-2.275000	11	27
H	57	-4.485000	-5.079000	0.160000	11	28
H	58	-3.545000	-2.950000	1.022000	11	29
H	59	2.469000	-2.781000	0.901000	11	31
H	60	4.372000	-2.960000	-0.664000	11	32
H	61	5.763000	-2.001000	-2.418000	11	34
H	62	6.442000	-0.053000	-3.810000	11	35
H	63	5.283000	2.125000	-3.551000	11	36
H	64	3.453000	2.388000	-1.902000	11	37
H	65	-0.502000	4.015000	-0.975000	11	39
H	66	0.915000	5.572000	0.318000	11	40
H	67	2.801000	5.972000	1.805000	11	42
H	68	4.837000	5.151000	2.976000	11	43
H	69	5.527000	2.779000	2.756000	11	44
H	70	4.208000	1.209000	1.365000	11	45

(b) asymmetric

Heat of formation: 50.75 kcal/mol

70 rr23-asym-PM3

C	1	0.000000	0.000000	0.000000	63	2	6	47
C	2	1.368000	0.000000	0.000000	63	1	3	48
C	3	2.078000	1.222000	0.000000	63	2	4	49
C	4	1.407000	2.415000	0.004000	63	3	5	50
C	5	-0.016000	2.448000	0.004000	63	4	6	10
C	6	-0.720000	1.226000	-0.003000	63	1	5	7
C	7	-2.140000	1.228000	-0.011000	63	6	8	51
C	8	-2.832000	2.405000	-0.065000	63	7	9	52
C	9	-2.124000	3.638000	-0.106000	63	8	10	11
C	10	-0.741000	3.683000	-0.010000	63	5	9	18
O	11	-2.803000	4.854000	-0.131000	82	9	34	
C	12	0.318000	4.518000	2.553000	63	13	17	53
C	13	0.830000	4.890000	3.766000	63	12	14	54
C	14	1.589000	6.076000	3.892000	63	13	15	55
C	15	1.811000	6.867000	2.798000	63	14	16	56
C	16	1.282000	6.505000	1.529000	63	15	17	21
C	17	0.534000	5.317000	1.395000	63	12	16	18
C	18	-0.001000	4.953000	0.117000	63	10	17	19

C	19	0.197000	5.816000	-0.950000	63	18	20	22
C	20	0.961000	7.007000	-0.814000	63	19	21	57
C	21	1.495000	7.337000	0.397000	63	16	20	58
O	22	-0.394000	5.431000	-2.148000	82	19	45	
C	23	-3.958000	10.779000	-2.051000	63	24	28	59
C	24	-3.641000	11.329000	-3.263000	63	23	25	60
C	25	-3.232000	10.501000	-4.334000	63	24	26	61
C	26	-3.151000	9.145000	-4.172000	63	25	27	62
C	27	-3.475000	8.543000	-2.924000	63	26	28	32
C	28	-3.880000	9.373000	-1.858000	63	23	27	29
C	29	-4.202000	8.796000	-0.601000	63	28	30	63
C	30	-4.112000	7.445000	-0.419000	63	29	31	64
C	31	-3.704000	6.601000	-1.485000	63	30	32	34
C	32	-3.397000	7.128000	-2.724000	63	27	31	41
O	33	0.123000	7.297000	-3.315000	81	45		
C	34	-3.624000	5.135000	-1.210000	63	11	31	46
C	35	-5.382000	6.206000	-4.630000	63	36	40	65
C	36	-6.325000	5.778000	-5.525000	63	35	37	66
C	37	-5.955000	4.967000	-6.623000	63	36	38	67
C	38	-4.649000	4.601000	-6.800000	63	37	39	68
C	39	-3.652000	5.032000	-5.883000	63	38	40	44
C	40	-4.016000	5.843000	-4.787000	63	35	39	41
C	41	-3.007000	6.270000	-3.865000	63	32	40	42
C	42	-1.699000	5.888000	-4.073000	63	41	43	45
C	43	-1.341000	5.072000	-5.177000	63	42	44	69
C	44	-2.294000	4.653000	-6.061000	63	39	43	70
C	45	-0.590000	6.327000	-3.173000	63	22	33	42
O	46	-4.225000	4.249000	-1.772000	81	34		
H	47	-0.561000	-0.941000	-0.002000	11	1		
H	48	1.926000	-0.942000	-0.001000	11	2		
H	49	3.173000	1.203000	-0.003000	11	3		
H	50	1.955000	3.365000	0.009000	11	4		
H	51	-2.672000	0.271000	0.018000	11	7		
H	52	-3.928000	2.404000	-0.084000	11	8		
H	53	-0.267000	3.595000	2.455000	11	12		
H	54	0.658000	4.271000	4.653000	11	13		
H	55	1.992000	6.351000	4.871000	11	14		
H	56	2.395000	7.790000	2.882000	11	15		

H	57	1.082000	7.643000	-1.713000	11	20		
H	58	2.087000	8.253000	0.512000	11	21		
H	59	-4.274000	11.410000	-1.213000	11	23		
H	60	-3.698000	12.411000	-3.416000	11	24		
H	61	-2.978000	10.961000	-5.295000	11	25		
H	62	-2.830000	8.502000	-5.002000	11	26		
H	63	-4.518000	9.451000	0.220000	11	29		
H	64	-4.348000	6.998000	0.554000	11	30		
H	65	-5.668000	6.830000	-3.774000	11	35		
H	66	-7.376000	6.057000	-5.398000	11	36		
H	67	-6.727000	4.635000	-7.325000	11	37		
H	68	-4.352000	3.970000	-7.645000	11	38		
H	69	-0.292000	4.783000	-5.308000	11	43		
H	70	-2.026000	4.020000	-6.914000	11	44		

4.3.3. HF/6-31G* Structure

(a) symmetric

Total energy: -1194763.49 kcal/mol

70 rr23-sym-631

C	1	-1.040000	1.601000	-0.164000	63	2	12	13
C	2	-1.941000	0.621000	-0.844000	63	1	3	15
C	3	-2.688000	-0.248000	-0.096000	63	2	4	22
C	4	-2.535000	-0.281000	1.402000	63	3	5	30
C	5	-1.390000	-0.776000	1.965000	63	4	6	23
C	6	-0.329000	-1.368000	1.094000	63	5	7	14
O	7	0.875000	-0.822000	1.342000	82	6	8	
C	8	1.907000	-1.045000	0.449000	63	7	9	39
C	9	2.558000	0.030000	-0.071000	63	8	10	46
C	10	2.324000	1.441000	0.390000	63	9	11	38
C	11	1.230000	2.171000	0.040000	63	10	12	31
O	12	0.212000	1.541000	-0.652000	82	1	11	
O	13	-1.376000	2.334000	0.700000	81	1		
O	14	-0.519000	-2.205000	0.281000	81	6		
C	15	-2.003000	0.617000	-2.260000	63	2	16	47
C	16	-2.845000	-0.225000	-2.901000	63	15	17	48
C	17	-3.642000	-1.144000	-2.170000	63	16	18	22
C	18	-4.510000	-2.050000	-2.833000	63	17	19	49
C	19	-5.243000	-2.951000	-2.130000	63	18	20	50

C	20	-5.141000	-2.999000	-0.721000	63	19	21	51
C	21	-4.320000	-2.142000	-0.059000	63	20	22	52
C	22	-3.553000	-1.175000	-0.763000	63	3	17	21
C	23	-1.183000	-0.744000	3.368000	63	5	24	53
C	24	-2.146000	-0.258000	4.185000	63	23	25	54
C	25	-3.352000	0.264000	3.650000	63	24	26	30
C	26	-4.357000	0.800000	4.496000	63	25	27	55
C	27	-5.493000	1.331000	3.976000	63	26	28	56
C	28	-5.681000	1.362000	2.575000	63	27	29	57
C	29	-4.737000	0.855000	1.740000	63	28	30	58
C	30	-3.544000	0.275000	2.253000	63	4	25	29
C	31	1.122000	3.556000	0.314000	63	11	32	59
C	32	2.100000	4.180000	1.007000	63	31	33	60
C	33	3.226000	3.459000	1.483000	63	32	34	38
C	34	4.229000	4.096000	2.258000	63	33	35	61
C	35	5.297000	3.399000	2.723000	63	34	36	62
C	36	5.413000	2.021000	2.433000	63	35	37	63
C	37	4.472000	1.388000	1.682000	63	36	38	64
C	38	3.343000	2.089000	1.176000	63	10	33	37
C	39	2.281000	-2.378000	0.149000	63	8	40	65
C	40	3.275000	-2.611000	-0.736000	63	39	41	66
C	41	3.935000	-1.537000	-1.386000	63	40	42	46
C	42	4.941000	-1.775000	-2.358000	63	41	43	67
C	43	5.560000	-0.744000	-2.988000	63	42	44	68
C	44	5.198000	0.585000	-2.674000	63	43	45	69
C	45	4.246000	0.843000	-1.738000	63	44	46	70
C	46	3.581000	-0.214000	-1.057000	63	9	41	45
H	47	-1.381000	1.296000	-2.813000	11	15		
H	48	-2.908000	-0.219000	-3.975000	11	16		
H	49	-4.572000	-2.014000	-3.906000	11	18		
H	50	-5.897000	-3.636000	-2.640000	11	19		
H	51	-5.714000	-3.725000	-0.172000	11	20		
H	52	-4.245000	-2.197000	1.009000	11	21		
H	53	-0.260000	-1.117000	3.769000	11	23		
H	54	-2.000000	-0.248000	5.251000	11	24		
H	55	-4.200000	0.782000	5.560000	11	26		
H	56	-6.249000	1.737000	4.624000	11	27		
H	57	-6.577000	1.797000	2.170000	11	28		

H	58	-4.888000	0.894000	0.679000	11	29
H	59	0.258000	4.089000	-0.024000	11	31
H	60	2.024000	5.232000	1.218000	11	32
H	61	4.123000	5.144000	2.476000	11	34
H	62	6.052000	3.886000	3.314000	11	35
H	63	6.254000	1.468000	2.811000	11	36
H	64	4.577000	0.341000	1.478000	11	37
H	65	1.762000	-3.185000	0.622000	11	39
H	66	3.564000	-3.621000	-0.968000	11	40
H	67	5.200000	-2.793000	-2.591000	11	42
H	68	6.318000	-0.932000	-3.727000	11	43
H	69	5.682000	1.401000	-3.181000	11	44
H	70	3.984000	1.859000	-1.519000	11	45

(b) asymmetric

Total energy: -1194765.79 kcal/mol

70 rr23-asym-631

C	1	4.908000	-1.678000	-2.310000	63	2	6	47
C	2	5.370000	-0.553000	-2.912000	63	1	3	48
C	3	4.853000	0.707000	-2.535000	63	2	4	49
C	4	3.908000	0.806000	-1.563000	63	3	5	50
C	5	3.410000	-0.352000	-0.904000	63	4	6	10
C	6	3.912000	-1.609000	-1.300000	63	1	5	7
C	7	3.405000	-2.785000	-0.690000	63	6	8	51
C	8	2.421000	-2.714000	0.236000	63	7	9	52
C	9	1.914000	-1.452000	0.615000	63	8	10	11
C	10	2.403000	-0.281000	0.119000	63	5	9	18
O	11	0.896000	-1.388000	1.546000	82	9	34	
C	12	4.142000	1.465000	1.757000	63	13	17	53
C	13	4.960000	2.272000	2.484000	63	12	14	54
C	14	4.522000	3.544000	2.916000	63	13	15	55
C	15	3.266000	3.960000	2.613000	63	14	16	56
C	16	2.387000	3.136000	1.864000	63	15	17	21
C	17	2.826000	1.876000	1.409000	63	12	16	18
C	18	1.934000	1.045000	0.644000	63	10	17	19
C	19	0.663000	1.488000	0.444000	63	18	20	22
C	20	0.207000	2.744000	0.910000	63	19	21	57
C	21	1.058000	3.549000	1.586000	63	16	20	58

O	22	-0.235000	0.609000	-0.120000	82	19	45	
C	23	-4.261000	1.145000	4.034000	63	24	28	59
C	24	-5.342000	1.661000	3.397000	63	23	25	60
C	25	-5.516000	1.440000	2.011000	63	24	26	61
C	26	-4.611000	0.709000	1.309000	63	25	27	62
C	27	-3.468000	0.147000	1.946000	63	26	28	32
C	28	-3.295000	0.381000	3.327000	63	23	27	29
C	29	-2.151000	-0.137000	3.985000	63	28	30	63
C	30	-1.220000	-0.835000	3.294000	63	29	31	64
C	31	-1.400000	-1.098000	1.913000	63	30	32	34
C	32	-2.494000	-0.633000	1.236000	63	27	31	41
O	33	-1.169000	1.989000	-1.594000	81	45		
C	34	-0.324000	-1.821000	1.172000	63	11	31	46
C	35	-4.237000	-2.794000	0.374000	63	36	40	65
C	36	-5.101000	-3.776000	0.007000	63	35	37	66
C	37	-5.437000	-3.964000	-1.354000	63	36	38	67
C	38	-4.890000	-3.165000	-2.304000	63	37	39	68
C	39	-3.980000	-2.133000	-1.950000	63	38	40	44
C	40	-3.646000	-1.936000	-0.595000	63	35	39	41
C	41	-2.722000	-0.898000	-0.234000	63	32	40	42
C	42	-2.170000	-0.131000	-1.227000	63	41	43	45
C	43	-2.536000	-0.322000	-2.587000	63	42	44	69
C	44	-3.407000	-1.293000	-2.939000	63	39	43	70
C	45	-1.169000	0.960000	-1.006000	63	22	33	42
O	46	-0.500000	-2.654000	0.352000	81	34		
H	47	5.285000	-2.645000	-2.595000	11	1		
H	48	6.120000	-0.614000	-3.680000	11	2		
H	49	5.210000	1.595000	-3.025000	11	3		
H	50	3.521000	1.770000	-1.295000	11	4		
H	51	3.800000	-3.740000	-0.987000	11	7		
H	52	2.005000	-3.595000	0.682000	11	8		
H	53	4.493000	0.502000	1.445000	11	12		
H	54	5.950000	1.938000	2.738000	11	13		
H	55	5.182000	4.172000	3.487000	11	14		
H	56	2.914000	4.921000	2.944000	11	15		
H	57	-0.802000	3.045000	0.715000	11	20		
H	58	0.724000	4.508000	1.938000	11	21		
H	59	-4.116000	1.311000	5.087000	11	23		

H	60	-6.068000	2.240000	3.939000	11	24
H	61	-6.371000	1.856000	1.510000	11	25
H	62	-4.759000	0.554000	0.259000	11	26
H	63	-2.023000	0.049000	5.036000	11	29
H	64	-0.335000	-1.196000	3.782000	11	30
H	65	-3.986000	-2.672000	1.409000	11	35
H	66	-5.531000	-4.418000	0.754000	11	36
H	67	-6.124000	-4.745000	-1.630000	11	37
H	68	-5.135000	-3.301000	-3.342000	11	38
H	69	-2.101000	0.323000	-3.326000	11	43
H	70	-3.673000	-1.440000	-3.970000	11	44

4.4. Compound (S_a,R_a)-23

4.4.1. AM1 Structure

Heat of formation: 74.81 kcal/mol

70 sr23-AM1

C	1	2.732000	4.250000	-2.488000	63	2	22	47
C	2	3.610000	3.660000	-3.363000	63	1	7	48
C	3	-1.607000	-1.323000	0.122000	63	29	30	31
C	4	-3.165000	2.666000	-0.226000	63	5	39	49
C	5	-2.203000	2.390000	0.708000	63	4	40	50
C	6	2.069000	-1.027000	-0.724000	63	13	15	17
C	7	3.971000	2.302000	-3.198000	63	2	16	51
C	8	3.788000	0.783000	2.062000	63	9	14	52
C	9	4.677000	0.512000	3.073000	63	8	10	53
C	10	5.200000	-0.793000	3.236000	63	9	11	54
C	11	4.817000	-1.799000	2.384000	63	10	12	55
C	12	3.898000	-1.544000	1.330000	63	11	14	18
O	13	1.277000	-0.779000	-1.842000	82	6	37	
C	14	3.374000	-0.237000	1.160000	63	8	12	15
C	15	2.453000	0.026000	0.094000	63	6	14	19
C	16	3.452000	1.566000	-2.162000	63	7	21	56
C	17	2.614000	-2.331000	-0.570000	63	6	18	57
C	18	3.507000	-2.580000	0.438000	63	12	17	58
C	19	1.995000	1.401000	-0.142000	63	15	21	25
C	20	-0.358000	-3.275000	-0.628000	63	27	30	59
C	21	2.543000	2.149000	-1.235000	63	16	19	22
C	22	2.180000	3.509000	-1.407000	63	1	21	23

C	23	1.279000	4.119000	-0.492000	63	22	24	60
C	24	0.744000	3.398000	0.542000	63	23	25	61
C	25	1.087000	2.028000	0.699000	63	19	24	26
O	26	0.635000	1.369000	1.840000	82	25	45	
C	27	-0.936000	-4.059000	0.335000	63	20	28	62
C	28	-1.871000	-3.502000	1.247000	63	27	29	35
C	29	-2.212000	-2.129000	1.145000	63	3	28	32
C	30	-0.678000	-1.893000	-0.731000	63	3	20	37
C	31	-2.069000	0.070000	-0.023000	63	3	38	40
C	32	-3.160000	-1.596000	2.063000	63	29	33	63
C	33	-3.736000	-2.391000	3.022000	63	32	34	64
C	34	-3.395000	-3.761000	3.118000	63	33	35	65
C	35	-2.480000	-4.304000	2.251000	63	28	34	66
O	36	-0.874000	0.352000	2.986000	81	45		
C	37	-0.053000	-1.163000	-1.852000	63	13	30	46
C	38	-3.068000	0.347000	-1.015000	63	31	39	44
C	39	-3.615000	1.652000	-1.114000	63	4	38	41
C	40	-1.635000	1.090000	0.806000	63	5	31	45
C	41	-4.614000	1.924000	-2.088000	63	39	42	67
C	42	-5.054000	0.934000	-2.931000	63	41	43	68
C	43	-4.510000	-0.369000	-2.839000	63	42	44	69
C	44	-3.542000	-0.655000	-1.908000	63	38	43	70
C	45	-0.661000	0.887000	1.899000	63	26	36	40
O	46	-0.578000	-0.871000	-2.926000	81	37		
H	47	2.438000	5.303000	-2.608000	11	1		
H	48	4.037000	4.231000	-4.201000	11	2		
H	49	-3.607000	3.671000	-0.301000	11	4		
H	50	-1.870000	3.166000	1.414000	11	5		
H	51	4.669000	1.843000	-3.914000	11	7		
H	52	3.361000	1.793000	1.947000	11	8		
H	53	4.988000	1.304000	3.770000	11	9		
H	54	5.910000	-0.988000	4.053000	11	10		
H	55	5.211000	-2.819000	2.502000	11	11		
H	56	3.714000	0.502000	-2.043000	11	16		
H	57	2.325000	-3.114000	-1.285000	11	17		
H	58	3.940000	-3.583000	0.570000	11	18		
H	59	0.349000	-3.708000	-1.352000	11	20		
H	60	1.026000	5.181000	-0.627000	11	23		

H	61	0.069000	3.863000	1.274000	11	24
H	62	-0.690000	-5.129000	0.413000	11	27
H	63	-3.405000	-0.523000	2.008000	11	32
H	64	-4.463000	-1.970000	3.732000	11	33
H	65	-3.867000	-4.379000	3.896000	11	34
H	66	-2.199000	-5.366000	2.317000	11	35
H	67	-5.022000	2.943000	-2.152000	11	41
H	68	-5.826000	1.141000	-3.687000	11	42
H	69	-4.866000	-1.148000	-3.530000	11	43
H	70	-3.099000	-1.662000	-1.857000	11	44

4.4.2. PM3 Structure

Heat of formation: 44.99 kcal/mol

70 sr23-PM3

C	1	4.352000	-3.097000	2.014000	63	2	22	47
C	2	5.241000	-2.232000	2.592000	63	1	7	48
C	3	-2.271000	0.709000	0.159000	63	29	30	31
C	4	-2.298000	-3.480000	1.114000	63	5	39	49
C	5	-1.572000	-3.027000	0.050000	63	4	40	50
C	6	1.571000	1.588000	0.327000	63	13	15	17
C	7	5.185000	-0.852000	2.296000	63	2	16	51
C	8	3.744000	0.264000	-2.412000	63	9	14	52
C	9	4.437000	0.739000	-3.492000	63	8	10	53
C	10	4.433000	2.120000	-3.795000	63	9	11	54
C	11	3.734000	2.995000	-3.008000	63	10	12	55
C	12	3.007000	2.525000	-1.882000	63	11	14	18
O	13	0.994000	1.165000	1.518000	82	6	37	
C	14	3.007000	1.148000	-1.576000	63	8	12	15
C	15	2.275000	0.677000	-0.440000	63	6	14	19
C	16	4.243000	-0.366000	1.430000	63	7	21	56
C	17	1.582000	2.978000	0.019000	63	6	18	57
C	18	2.283000	3.431000	-1.061000	63	12	17	58
C	19	2.311000	-0.757000	-0.097000	63	15	21	25
C	20	-1.486000	2.995000	0.412000	63	27	30	59
C	21	3.305000	-1.239000	0.813000	63	16	19	22
C	22	3.366000	-2.616000	1.112000	63	1	21	23
C	23	2.443000	-3.512000	0.507000	63	22	24	60
C	24	1.494000	-3.049000	-0.357000	63	23	25	61

C	25	1.422000	-1.659000	-0.655000	63	19	24	26
O	26	0.564000	-1.227000	-1.658000	82	25	45	
C	27	-2.455000	3.459000	-0.430000	63	20	28	62
C	28	-3.380000	2.556000	-1.020000	63	27	29	35
C	29	-3.292000	1.179000	-0.730000	63	3	28	32
C	30	-1.385000	1.611000	0.711000	63	3	20	37
C	31	-2.236000	-0.732000	0.493000	63	3	38	40
C	32	-4.235000	0.296000	-1.328000	63	29	33	63
C	33	-5.203000	0.775000	-2.169000	63	32	34	64
C	34	-5.284000	2.156000	-2.458000	63	33	35	65
C	35	-4.393000	3.029000	-1.897000	63	28	34	66
O	36	-1.284000	-0.954000	-2.572000	81	45		
C	37	-0.361000	1.219000	1.720000	63	13	30	46
C	38	-3.001000	-1.190000	1.615000	63	31	39	44
C	39	-3.029000	-2.567000	1.920000	63	4	38	41
C	40	-1.534000	-1.644000	-0.267000	63	5	31	45
C	41	-3.788000	-3.028000	3.029000	63	39	42	67
C	42	-4.494000	-2.144000	3.798000	63	41	43	68
C	43	-4.473000	-0.764000	3.496000	63	42	44	69
C	44	-3.747000	-0.297000	2.433000	63	38	43	70
C	45	-0.798000	-1.264000	-1.505000	63	26	36	40
O	46	-0.560000	0.913000	2.875000	81	37		
H	47	4.386000	-4.169000	2.239000	11	1		
H	48	6.002000	-2.598000	3.290000	11	2		
H	49	-2.327000	-4.548000	1.359000	11	4		
H	50	-0.989000	-3.726000	-0.570000	11	5		
H	51	5.902000	-0.175000	2.771000	11	7		
H	52	3.740000	-0.808000	-2.178000	11	8		
H	53	4.999000	0.054000	-4.135000	11	9		
H	54	4.993000	2.477000	-4.665000	11	10		
H	55	3.723000	4.067000	-3.235000	11	11		
H	56	4.193000	0.707000	1.202000	11	16		
H	57	1.008000	3.671000	0.654000	11	17		
H	58	2.297000	4.499000	-1.309000	11	18		
H	59	-0.755000	3.686000	0.860000	11	20		
H	60	2.507000	-4.580000	0.745000	11	23		
H	61	0.768000	-3.734000	-0.822000	11	24		
H	62	-2.532000	4.527000	-0.661000	11	27		

H	63	-4.165000	-0.777000	-1.113000	11	32
H	64	-5.921000	0.090000	-2.632000	11	33
H	65	-6.064000	2.515000	-3.138000	11	34
H	66	-4.444000	4.102000	-2.116000	11	35
H	67	-3.795000	-4.101000	3.255000	11	41
H	68	-5.079000	-2.494000	4.656000	11	42
H	69	-5.040000	-0.071000	4.126000	11	43
H	70	-3.722000	0.776000	2.206000	11	44

4.4.3. HF/6-31G* Structure

Total energy: -1194749.57 kcal/mol

70 sr23-631

C	1	5.131000	-2.579000	2.609000	63	2	22	47
C	2	5.435000	-1.766000	3.652000	63	1	7	48
C	3	-1.512000	-0.093000	-0.141000	63	29	30	31
C	4	-0.395000	-4.068000	-1.379000	63	5	39	49
C	5	0.351000	-3.008000	-1.762000	63	4	40	50
C	6	1.746000	1.653000	1.160000	63	13	15	17
C	7	4.985000	-0.426000	3.649000	63	2	16	51
C	8	4.456000	1.632000	-1.396000	63	9	14	52
C	9	5.110000	2.517000	-2.193000	63	8	10	53
C	10	4.774000	3.889000	-2.177000	63	9	11	54
C	11	3.794000	4.331000	-1.348000	63	10	12	55
C	12	3.099000	3.431000	-0.501000	63	11	14	18
O	13	1.122000	0.837000	2.083000	82	6	37	
C	14	3.416000	2.058000	-0.525000	63	8	12	15
C	15	2.711000	1.150000	0.340000	63	6	14	19
C	16	4.241000	0.055000	2.619000	63	7	21	56
C	17	1.458000	3.036000	1.217000	63	6	18	57
C	18	2.108000	3.896000	0.401000	63	12	17	58
C	19	3.118000	-0.293000	0.404000	63	15	21	25
C	20	-1.564000	1.829000	1.329000	63	27	30	59
C	21	3.894000	-0.773000	1.516000	63	16	19	22
C	22	4.361000	-2.102000	1.517000	63	1	21	23
C	23	4.083000	-2.934000	0.403000	63	22	24	60
C	24	3.361000	-2.471000	-0.642000	63	23	25	61
C	25	2.854000	-1.151000	-0.621000	63	19	24	26
O	26	2.209000	-0.702000	-1.757000	82	25	45	

C	27	-2.596000	2.375000	0.650000	63	20	28	62
C	28	-3.116000	1.734000	-0.504000	63	27	29	35
C	29	-2.574000	0.498000	-0.907000	63	3	28	32
C	30	-1.001000	0.587000	0.926000	63	3	20	37
C	31	-1.050000	-1.475000	-0.516000	63	3	38	40
C	32	-3.109000	-0.123000	-2.069000	63	29	33	63
C	33	-4.123000	0.454000	-2.766000	63	32	34	64
C	34	-4.669000	1.690000	-2.350000	63	33	35	65
C	35	-4.176000	2.312000	-1.248000	63	28	34	66
O	36	0.422000	0.346000	-2.460000	81	45		
C	37	0.083000	0.016000	1.795000	63	13	30	46
C	38	-1.821000	-2.597000	-0.056000	63	31	39	44
C	39	-1.491000	-3.894000	-0.495000	63	4	38	41
C	40	0.033000	-1.695000	-1.318000	63	5	31	45
C	41	-2.261000	-5.001000	-0.057000	63	39	42	67
C	42	-3.310000	-4.825000	0.788000	63	41	43	68
C	43	-3.641000	-3.527000	1.240000	63	42	44	69
C	44	-2.921000	-2.449000	0.833000	63	38	43	70
C	45	0.864000	-0.571000	-1.866000	63	26	36	40
O	46	0.028000	-1.044000	2.305000	81	37		
H	47	5.472000	-3.599000	2.593000	11	1		
H	48	6.019000	-2.132000	4.478000	11	2		
H	49	-0.164000	-5.054000	-1.740000	11	4		
H	50	1.167000	-3.142000	-2.445000	11	5		
H	51	5.234000	0.218000	4.473000	11	7		
H	52	4.727000	0.595000	-1.425000	11	8		
H	53	5.891000	2.170000	-2.845000	11	9		
H	54	5.298000	4.576000	-2.817000	11	10		
H	55	3.531000	5.374000	-1.319000	11	11		
H	56	3.910000	1.073000	2.638000	11	16		
H	57	0.734000	3.387000	1.925000	11	17		
H	58	1.889000	4.948000	0.440000	11	18		
H	59	-1.186000	2.309000	2.211000	11	20		
H	60	4.466000	-3.939000	0.392000	11	23		
H	61	3.178000	-3.084000	-1.501000	11	24		
H	62	-3.033000	3.302000	0.976000	11	27		
H	63	-2.699000	-1.054000	-2.405000	11	32		
H	64	-4.511000	-0.028000	-3.645000	11	33		

H	65	-5.471000	2.134000	-2.911000	11	34
H	66	-4.580000	3.255000	-0.925000	11	35
H	67	-1.997000	-5.984000	-0.403000	11	41
H	68	-3.888000	-5.668000	1.119000	11	42
H	69	-4.465000	-3.396000	1.917000	11	43
H	70	-3.178000	-1.474000	1.195000	11	44

4.5. Compound (R_a,R_a)-24

4.5.1. AM1 Structure

(a) symmetric

Heat of formation: -15.08 kcal/mol

46 rr24-sym-AM1

C	1	-1.411000	-0.754000	1.238000	63	2	12	13
C	2	-2.496000	0.166000	1.637000	63	1	3	15
C	3	-3.287000	0.798000	0.660000	63	2	4	18
C	4	-3.027000	0.624000	-0.774000	63	3	5	19
C	5	-1.912000	1.208000	-1.400000	63	4	6	22
C	6	-0.997000	2.080000	-0.633000	63	5	7	14
O	7	0.289000	1.578000	-0.606000	82	6	8	
C	8	1.240000	2.171000	0.223000	63	7	9	23
C	9	2.093000	1.313000	0.944000	63	8	10	26
C	10	2.070000	-0.150000	0.872000	63	9	11	27
C	11	0.977000	-0.960000	1.234000	63	10	12	30
O	12	-0.178000	-0.315000	1.676000	82	1	11	
O	13	-1.503000	-1.814000	0.624000	81	1		
O	14	-1.251000	3.148000	-0.084000	81	6		
C	15	-2.746000	0.378000	2.996000	63	2	16	31
C	16	-3.803000	1.196000	3.391000	63	15	17	32
C	17	-4.606000	1.808000	2.429000	63	16	18	33
C	18	-4.349000	1.612000	1.073000	63	3	17	34
C	19	-3.911000	-0.143000	-1.545000	63	4	20	35
C	20	-3.677000	-0.338000	-2.905000	63	19	21	36
C	21	-2.557000	0.227000	-3.513000	63	20	22	37
C	22	-1.672000	0.997000	-2.761000	63	5	21	38
C	23	1.407000	3.563000	0.265000	63	8	24	39
C	24	2.408000	4.114000	1.060000	63	23	25	40
C	25	3.247000	3.283000	1.802000	63	24	26	41
C	26	3.095000	1.902000	1.734000	63	9	25	42
C	27	3.258000	-0.794000	0.484000	63	10	28	43
C	28	3.358000	-2.181000	0.463000	63	27	29	44
C	29	2.271000	-2.964000	0.852000	63	28	30	45
C	30	1.081000	-2.358000	1.244000	63	11	29	46
H	31	-2.100000	-0.101000	3.748000	11	15		

H	32	-3.998000	1.360000	4.461000	11	16
H	33	-5.440000	2.455000	2.739000	11	17
H	34	-4.974000	2.110000	0.315000	11	18
H	35	-4.787000	-0.604000	-1.063000	11	19
H	36	-4.377000	-0.948000	-3.497000	11	20
H	37	-2.366000	0.062000	-4.584000	11	21
H	38	-0.778000	1.438000	-3.229000	11	22
H	39	0.737000	4.215000	-0.316000	11	23
H	40	2.532000	5.206000	1.101000	11	24
H	41	4.031000	3.718000	2.438000	11	25
H	42	3.768000	1.248000	2.311000	11	26
H	43	4.123000	-0.178000	0.190000	11	27
H	44	4.295000	-2.659000	0.144000	11	28
H	45	2.350000	-4.061000	0.849000	11	29
H	46	0.218000	-2.973000	1.543000	11	30

(b) asymmetric

Heat of formation: -14.84 kcal/mol

46 rr24-asym-AM1

C	1	-0.282000	1.910000	0.175000	63	2	12	13
C	2	-0.941000	1.445000	-1.062000	63	1	3	15
C	3	-2.017000	0.544000	-1.002000	63	2	4	18
C	4	-2.579000	0.068000	0.270000	63	3	5	19
C	5	-2.007000	-0.962000	1.032000	63	4	6	22
C	6	-0.768000	-1.674000	0.654000	63	5	7	14
O	7	0.290000	-0.820000	0.438000	82	6	8	
C	8	1.539000	-1.312000	0.060000	63	7	9	23
C	9	2.663000	-0.640000	0.582000	63	8	10	26
C	10	2.579000	0.458000	1.544000	63	9	11	27
C	11	1.782000	1.604000	1.341000	63	10	12	30
O	12	1.082000	1.681000	0.139000	82	1	11	
O	13	-0.770000	2.481000	1.146000	81	1		
O	14	-0.600000	-2.889000	0.573000	81	6		
C	15	-0.459000	1.890000	-2.298000	63	2	16	31
C	16	-1.058000	1.457000	-3.479000	63	15	17	32
C	17	-2.131000	0.568000	-3.428000	63	16	18	33
C	18	-2.607000	0.114000	-2.199000	63	3	17	34
C	19	-3.774000	0.656000	0.716000	63	4	20	35
C	20	-4.378000	0.235000	1.897000	63	19	21	36
C	21	-3.806000	-0.792000	2.648000	63	20	22	37
C	22	-2.627000	-1.391000	2.215000	63	5	21	38
C	23	1.678000	-2.347000	-0.873000	63	8	24	39
C	24	2.951000	-2.733000	-1.284000	63	23	25	40
C	25	4.077000	-2.086000	-0.776000	63	24	26	41
C	26	3.932000	-1.052000	0.145000	63	9	25	42

C	27	3.366000	0.407000	2.705000	63	10	28	43
C	28	3.351000	1.449000	3.629000	63	27	29	44
C	29	2.556000	2.574000	3.408000	63	28	30	45
C	30	1.770000	2.659000	2.261000	63	11	29	46
H	31	0.403000	2.575000	-2.327000	11	15		
H	32	-0.680000	1.813000	-4.449000	11	16		
H	33	-2.604000	0.220000	-4.359000	11	17		
H	34	-3.452000	-0.590000	-2.162000	11	18		
H	35	-4.226000	1.467000	0.125000	11	19		
H	36	-5.307000	0.716000	2.238000	11	20		
H	37	-4.283000	-1.129000	3.580000	11	21		
H	38	-2.173000	-2.211000	2.794000	11	22		
H	39	0.786000	-2.861000	-1.263000	11	23		
H	40	3.064000	-3.549000	-2.013000	11	24		
H	41	5.082000	-2.391000	-1.102000	11	25		
H	42	4.822000	-0.538000	0.538000	11	26		
H	43	3.996000	-0.477000	2.885000	11	27		
H	44	3.969000	1.382000	4.537000	11	28		
H	45	2.547000	3.396000	4.138000	11	29		
H	46	1.126000	3.532000	2.082000	11	30		

4.5.2. PM3 Structure

(a) symmetric

Heat of formation: -26.43 kcal/mol

46 rr24-sym-PM3

C	1	-1.393000	-2.321000	-1.653000	63	2	12	13
C	2	-2.018000	-2.899000	-0.429000	63	1	3	15
C	3	-2.783000	-2.096000	0.426000	63	2	4	18
C	4	-2.990000	-0.656000	0.179000	63	3	5	19
C	5	-1.995000	0.297000	0.435000	63	4	6	22
C	6	-0.677000	-0.116000	0.998000	63	5	7	14
O	7	0.364000	0.194000	0.149000	82	6	8	
C	8	1.629000	-0.336000	0.394000	63	7	9	23
C	9	2.300000	-0.937000	-0.685000	63	8	10	26
C	10	1.828000	-0.975000	-2.081000	63	9	11	27
C	11	0.740000	-1.726000	-2.561000	63	10	12	30
O	12	-0.019000	-2.426000	-1.628000	82	1	11	
O	13	-1.972000	-1.824000	-2.594000	81	1		
O	14	-0.483000	-0.646000	2.070000	81	6		
C	15	-1.859000	-4.259000	-0.158000	63	2	16	31
C	16	-2.463000	-4.820000	0.960000	63	15	17	32
C	17	-3.226000	-4.028000	1.811000	63	16	18	33
C	18	-3.387000	-2.673000	1.546000	63	3	17	34
C	19	-4.228000	-0.235000	-0.313000	63	4	20	35
C	20	-4.467000	1.113000	-0.551000	63	19	21	36

C	21	-3.475000	2.055000	-0.298000	63	20	22	37
C	22	-2.240000	1.649000	0.193000	63	5	21	38
C	23	2.265000	-0.182000	1.634000	63	8	24	39
C	24	3.535000	-0.708000	1.828000	63	23	25	40
C	25	4.182000	-1.371000	0.791000	63	24	26	41
C	26	3.576000	-1.469000	-0.454000	63	9	25	42
C	27	2.603000	-0.270000	-3.012000	63	10	28	43
C	28	2.336000	-0.338000	-4.371000	63	27	29	44
C	29	1.302000	-1.144000	-4.836000	63	28	30	45
C	30	0.508000	-1.845000	-3.939000	63	11	29	46
H	31	-1.254000	-4.883000	-0.826000	11	15		
H	32	-2.334000	-5.887000	1.172000	11	16		
H	33	-3.698000	-4.470000	2.695000	11	17		
H	34	-3.982000	-2.048000	2.222000	11	18		
H	35	-5.007000	-0.977000	-0.520000	11	19		
H	36	-5.439000	1.433000	-0.944000	11	20		
H	37	-3.664000	3.116000	-0.489000	11	21		
H	38	-1.457000	2.391000	0.388000	11	22		
H	39	1.766000	0.336000	2.461000	11	23		
H	40	4.024000	-0.601000	2.802000	11	24		
H	41	5.174000	-1.805000	0.951000	11	25		
H	42	4.105000	-1.961000	-1.278000	11	26		
H	43	3.442000	0.338000	-2.653000	11	27		
H	44	2.948000	0.232000	-5.078000	11	28		
H	45	1.110000	-1.226000	-5.911000	11	29		
H	46	-0.305000	-2.474000	-4.319000	11	30		

(b) asymmetric

Heat of formation: -25.57 kcal/mol

46 rr24-asym-PM3

C	1	-0.796000	2.069000	-0.425000	63	2	12	13
C	2	-2.015000	1.267000	-0.739000	63	1	3	15
C	3	-2.701000	0.568000	0.263000	63	2	4	18
C	4	-2.330000	0.641000	1.690000	63	3	5	19
C	5	-1.404000	-0.219000	2.290000	63	4	6	22
C	6	-0.673000	-1.279000	1.532000	63	5	7	14
O	7	0.176000	-0.715000	0.617000	82	6	8	
C	8	0.797000	-1.407000	-0.410000	63	7	9	23
C	9	1.865000	-0.705000	-1.007000	63	8	10	26
C	10	2.340000	0.614000	-0.555000	63	9	11	27
C	11	1.571000	1.790000	-0.645000	63	10	12	30
O	12	0.292000	1.671000	-1.183000	82	1	11	
O	13	-0.705000	3.004000	0.338000	81	1		
O	14	-0.725000	-2.475000	1.715000	81	6		
C	15	-2.461000	1.207000	-2.061000	63	2	16	31

C	16	-3.580000	0.450000	-2.388000	63	15	17	32
C	17	-4.253000	-0.259000	-1.399000	63	16	18	33
C	18	-3.818000	-0.199000	-0.081000	63	3	17	34
C	19	-2.978000	1.601000	2.475000	63	4	20	35
C	20	-2.703000	1.704000	3.833000	63	19	21	36
C	21	-1.783000	0.845000	4.425000	63	20	22	37
C	22	-1.137000	-0.116000	3.657000	63	5	21	38
C	23	0.381000	-2.640000	-0.923000	63	8	24	39
C	24	1.050000	-3.191000	-2.009000	63	23	25	40
C	25	2.118000	-2.521000	-2.593000	63	24	26	41
C	26	2.517000	-1.286000	-2.097000	63	9	25	42
C	27	3.650000	0.712000	-0.079000	63	10	28	43
C	28	4.187000	1.942000	0.282000	63	27	29	44
C	29	3.428000	3.100000	0.153000	63	28	30	45
C	30	2.122000	3.034000	-0.316000	63	11	29	46
H	31	-1.924000	1.754000	-2.845000	11	15		
H	32	-3.926000	0.408000	-3.426000	11	16		
H	33	-5.129000	-0.863000	-1.657000	11	17		
H	34	-4.354000	-0.753000	0.699000	11	18		
H	35	-3.699000	2.282000	2.009000	11	19		
H	36	-3.209000	2.466000	4.435000	11	20		
H	37	-1.567000	0.925000	5.496000	11	21		
H	38	-0.416000	-0.796000	4.125000	11	22		
H	39	-0.463000	-3.188000	-0.488000	11	23		
H	40	0.729000	-4.160000	-2.405000	11	24		
H	41	2.643000	-2.961000	-3.447000	11	25		
H	42	3.354000	-0.754000	-2.564000	11	26		
H	43	4.259000	-0.196000	0.002000	11	27		
H	44	5.212000	1.998000	0.662000	11	28		
H	45	3.859000	4.070000	0.423000	11	29		
H	46	1.529000	3.951000	-0.411000	11	30		

4.5.3. HF/6-31G* Structure

(a) symmetric

Total energy: -811610.37 kcal/mol

46 rr24-sym-631

C	1	-0.306000	2.067000	-0.151000	63	2	12	13
C	2	-1.221000	1.834000	-1.312000	63	1	3	15
C	3	-2.491000	1.288000	-1.103000	63	2	4	18
C	4	-2.907000	0.765000	0.237000	63	3	5	19
C	5	-2.192000	-0.250000	0.879000	63	4	6	22
C	6	-1.090000	-0.961000	0.158000	63	5	7	14
O	7	0.032000	-1.026000	0.892000	82	6	8	

C	8	1.170000	-1.593000	0.348000	63	7	9	23
C	9	2.352000	-0.862000	0.371000	63	8	10	26
C	10	2.531000	0.483000	1.007000	63	9	11	27
C	11	1.875000	1.648000	0.628000	63	10	12	30
O	12	0.924000	1.576000	-0.371000	82	1	11	
O	13	-0.627000	2.625000	0.842000	81	1		
O	14	-1.197000	-1.417000	-0.928000	81	6		
C	15	-0.824000	2.229000	-2.580000	63	2	16	31
C	16	-1.700000	2.133000	-3.647000	63	15	17	32
C	17	-2.968000	1.618000	-3.444000	63	16	18	33
C	18	-3.354000	1.190000	-2.185000	63	3	17	34
C	19	-3.993000	1.325000	0.893000	63	4	20	35
C	20	-4.362000	0.893000	2.157000	63	19	21	36
C	21	-3.633000	-0.094000	2.795000	63	20	22	37
C	22	-2.541000	-0.657000	2.157000	63	5	21	38
C	23	1.129000	-2.889000	-0.137000	63	8	24	39
C	24	2.270000	-3.472000	-0.650000	63	23	25	40
C	25	3.456000	-2.758000	-0.672000	63	24	26	41
C	26	3.488000	-1.477000	-0.160000	63	9	25	42
C	27	3.507000	0.597000	1.999000	63	10	28	43
C	28	3.828000	1.810000	2.574000	63	27	29	44
C	29	3.180000	2.959000	2.151000	63	28	30	45
C	30	2.206000	2.876000	1.177000	63	11	29	46
H	31	0.164000	2.624000	-2.727000	11	15		
H	32	-1.392000	2.453000	-4.625000	11	16		
H	33	-3.653000	1.531000	-4.269000	11	17		
H	34	-4.324000	0.751000	-2.043000	11	18		
H	35	-4.537000	2.123000	0.421000	11	19		
H	36	-5.206000	1.342000	2.647000	11	20		
H	37	-3.907000	-0.422000	3.781000	11	21		
H	38	-1.965000	-1.421000	2.646000	11	22		
H	39	0.203000	-3.428000	-0.123000	11	23		
H	40	2.228000	-4.476000	-1.032000	11	24		
H	41	4.349000	-3.196000	-1.079000	11	25		
H	42	4.410000	-0.925000	-0.170000	11	26		
H	43	4.016000	-0.293000	2.321000	11	27		
H	44	4.581000	1.859000	3.341000	11	28		
H	45	3.425000	3.914000	2.579000	11	29		

H	46	1.690000	3.755000	0.848000	11	30		

(b) asymmetric

Total energy: -811613.31 kcal/mol

46 rr24-asym-631

C	1	-0.603000	-1.305000	1.271000	63	2	12	13
C	2	-1.468000	-0.260000	1.893000	63	1	3	15
C	3	-2.390000	0.429000	1.101000	63	2	4	18
C	4	-2.630000	0.152000	-0.360000	63	3	5	19
C	5	-1.776000	0.505000	-1.415000	63	4	6	22
C	6	-0.433000	1.151000	-1.279000	63	5	7	14
O	7	0.206000	0.803000	-0.157000	82	6	8	
C	8	1.381000	1.417000	0.231000	63	7	9	23
C	9	2.493000	0.628000	0.493000	63	8	10	26
C	10	2.547000	-0.854000	0.296000	63	9	11	27
C	11	1.668000	-1.739000	0.911000	63	10	12	30
O	12	0.668000	-1.208000	1.697000	82	1	11	
O	13	-0.974000	-2.115000	0.494000	81	1		
O	14	0.035000	1.871000	-2.095000	81	6		
C	15	-1.327000	0.043000	3.238000	63	2	16	31
C	16	-2.123000	1.010000	3.828000	63	15	17	32
C	17	-3.041000	1.697000	3.057000	63	16	18	33
C	18	-3.166000	1.410000	1.706000	63	3	17	34
C	19	-3.858000	-0.419000	-0.679000	63	4	20	35
C	20	-4.233000	-0.655000	-1.989000	63	19	21	36
C	21	-3.390000	-0.299000	-3.025000	63	20	22	37
C	22	-2.175000	0.288000	-2.730000	63	5	21	38
C	23	1.396000	2.786000	0.425000	63	8	24	39
C	24	2.546000	3.404000	0.877000	63	23	25	40
C	25	3.674000	2.646000	1.145000	63	24	26	41
C	26	3.638000	1.278000	0.956000	63	9	25	42
C	27	3.571000	-1.402000	-0.474000	63	10	28	43
C	28	3.716000	-2.769000	-0.617000	63	27	29	44
C	29	2.834000	-3.625000	0.022000	63	28	30	45
C	30	1.807000	-3.108000	0.790000	63	11	29	46
H	31	-0.593000	-0.480000	3.821000	11	15		
H	32	-2.016000	1.229000	4.875000	11	16		
H	33	-3.657000	2.460000	3.498000	11	17		
H	34	-3.872000	1.958000	1.110000	11	18		
H	35	-4.523000	-0.693000	0.120000	11	19		
H	36	-5.185000	-1.112000	-2.195000	11	20		
H	37	-3.672000	-0.471000	-4.047000	11	21		
H	38	-1.514000	0.588000	-3.520000	11	22		
H	39	0.515000	3.359000	0.212000	11	23		

H	40	2.556000	4.468000	1.023000	11	24
H	41	4.572000	3.114000	1.505000	11	25
H	42	4.507000	0.688000	1.183000	11	26
H	43	4.255000	-0.739000	-0.972000	11	27
H	44	4.512000	-3.163000	-1.223000	11	28
H	45	2.940000	-4.690000	-0.079000	11	29
H	46	1.108000	-3.753000	1.285000	11	30

4.6. Compound (S_a,R_a)-24

4.6.1. AM1 Structure

Heat of formation: -11.49 kcal/mol

46 sr24-AM1

C	1	1.099000	1.879000	0.955000	63	2	12	13
C	2	-0.304000	2.171000	0.600000	63	1	3	15
C	3	-1.344000	1.278000	0.904000	63	2	4	18
C	4	-1.141000	0.077000	1.722000	63	3	5	19
C	5	-1.433000	-1.215000	1.256000	63	4	6	22
C	6	-1.818000	-1.465000	-0.147000	63	5	7	14
O	7	-0.895000	-1.970000	-1.052000	82	6	8	
C	8	0.405000	-2.196000	-0.598000	63	7	9	23
C	9	1.424000	-1.275000	-0.901000	63	8	10	26
C	10	1.200000	-0.092000	-1.731000	63	9	11	27
C	11	1.501000	1.211000	-1.296000	63	10	12	30
O	12	1.988000	1.418000	-0.005000	82	1	11	
O	13	1.649000	2.019000	2.046000	81	1		
O	14	-2.920000	-1.311000	-0.669000	81	6		
C	15	-0.586000	3.380000	-0.048000	63	2	16	31
C	16	-1.889000	3.686000	-0.431000	63	15	17	32
C	17	-2.917000	2.776000	-0.184000	63	16	18	33
C	18	-2.647000	1.582000	0.478000	63	3	17	34
C	19	-0.715000	0.239000	3.050000	63	4	20	35
C	20	-0.636000	-0.853000	3.910000	63	19	21	36
C	21	-0.984000	-2.125000	3.456000	63	20	22	37
C	22	-1.373000	-2.306000	2.132000	63	5	21	38
C	23	0.688000	-3.399000	0.063000	63	8	24	39
C	24	1.992000	-3.669000	0.468000	63	23	25	40
C	25	3.004000	-2.739000	0.227000	63	24	26	41
C	26	2.724000	-1.557000	-0.452000	63	9	25	42
C	27	0.743000	-0.259000	-3.048000	63	10	28	43
C	28	0.643000	0.827000	-3.913000	63	27	29	44
C	29	1.003000	2.104000	-3.482000	63	28	30	45
C	30	1.427000	2.304000	-2.171000	63	11	29	46
H	31	0.231000	4.090000	-0.254000	11	15		
H	32	-2.103000	4.641000	-0.935000	11	16		
H	33	-3.944000	3.001000	-0.510000	11	17		

H	34	-3.455000	0.856000	0.664000	11	18
H	35	-0.429000	1.245000	3.403000	11	19
H	36	-0.302000	-0.708000	4.948000	11	20
H	37	-0.944000	-2.987000	4.139000	11	21
H	38	-1.633000	-3.312000	1.766000	11	22
H	39	-0.122000	-4.119000	0.251000	11	23
H	40	2.221000	-4.613000	0.983000	11	24
H	41	4.029000	-2.941000	0.571000	11	25
H	42	3.521000	-0.820000	-0.641000	11	26
H	43	0.458000	-1.268000	-3.386000	11	27
H	44	0.283000	0.675000	-4.941000	11	28
H	45	0.946000	2.957000	-4.174000	11	29
H	46	1.707000	3.305000	-1.814000	11	30

4.6.2. PM3 Structure

Heat of formation: -32.19 kcal/mol

46 sr24-PM3

C	1	-0.626000	1.572000	1.381000	63	2	12	13
C	2	-1.406000	1.758000	0.128000	63	1	3	15
C	3	-2.165000	0.723000	-0.430000	63	2	4	18
C	4	-2.237000	-0.622000	0.171000	63	3	5	19
C	5	-1.472000	-1.697000	-0.293000	63	4	6	22
C	6	-0.536000	-1.555000	-1.442000	63	5	7	14
O	7	0.833000	-1.553000	-1.349000	82	6	8	
C	8	1.458000	-1.771000	-0.126000	63	7	9	23
C	9	2.221000	-0.739000	0.441000	63	8	10	26
C	10	2.293000	0.605000	-0.153000	63	9	11	27
C	11	1.521000	1.678000	0.320000	63	10	12	30
O	12	0.741000	1.497000	1.456000	82	1	11	
O	13	-1.060000	1.474000	2.509000	81	1		
O	14	-0.823000	-1.438000	-2.613000	81	6		
C	15	-1.422000	3.026000	-0.458000	63	2	16	31
C	16	-2.189000	3.267000	-1.590000	63	15	17	32
C	17	-2.940000	2.238000	-2.151000	63	16	18	33
C	18	-2.927000	0.973000	-1.576000	63	3	17	34
C	19	-3.144000	-0.828000	1.216000	63	4	20	35
C	20	-3.294000	-2.089000	1.780000	63	19	21	36
C	21	-2.536000	-3.157000	1.311000	63	20	22	37
C	22	-1.625000	-2.961000	0.282000	63	5	21	38
C	23	1.445000	-3.049000	0.447000	63	8	24	39
C	24	2.194000	-3.295000	1.590000	63	23	25	40
C	25	2.952000	-2.277000	2.162000	63	24	26	41
C	26	2.964000	-1.009000	1.594000	63	9	25	42
C	27	3.184000	0.832000	-1.206000	63	10	28	43
C	28	3.307000	2.097000	-1.767000	63	27	29	44

C	29	2.541000	3.155000	-1.289000	63	28	30	45
C	30	1.646000	2.952000	-0.247000	63	11	29	46
H	31	-0.796000	3.826000	-0.030000	11	15		
H	32	-2.198000	4.264000	-2.042000	11	16		
H	33	-3.539000	2.422000	-3.048000	11	17		
H	34	-3.509000	0.160000	-2.025000	11	18		
H	35	-3.733000	0.016000	1.594000	11	19		
H	36	-4.007000	-2.239000	2.598000	11	20		
H	37	-2.652000	-4.151000	1.756000	11	21		
H	38	-0.995000	-3.793000	-0.069000	11	22		
H	39	0.821000	-3.841000	0.006000	11	23		
H	40	2.187000	-4.292000	2.041000	11	24		
H	41	3.538000	-2.474000	3.065000	11	25		
H	42	3.556000	-0.208000	2.052000	11	26		
H	43	3.785000	-0.001000	-1.590000	11	27		
H	44	4.009000	2.259000	-2.592000	11	28		
H	45	2.641000	4.150000	-1.734000	11	29		
H	46	1.015000	3.778000	0.117000	11	30		

4.6.3. HF/6-31G* Structure

Total energy: -811596.64 kcal/mol

46 sr24-631

C	1	0.499000	-1.298000	1.780000	63	2	12	13
C	2	-0.379000	-2.007000	0.786000	63	1	3	15
C	3	-0.233000	-1.842000	-0.589000	63	2	4	18
C	4	0.829000	-0.988000	-1.221000	63	3	5	19
C	5	0.618000	0.321000	-1.648000	63	4	6	22
C	6	-0.700000	1.023000	-1.473000	63	5	7	14
O	7	-0.677000	2.222000	-0.845000	82	6	8	
C	8	0.205000	2.507000	0.178000	63	7	9	23
C	9	-0.032000	2.022000	1.458000	63	8	10	26
C	10	-1.294000	1.313000	1.839000	63	9	11	27
C	11	-1.304000	0.100000	2.516000	63	10	12	30
O	12	-0.122000	-0.576000	2.742000	82	1	11	
O	13	1.673000	-1.406000	1.813000	81	1		
O	14	-1.717000	0.630000	-1.921000	81	6		
C	15	-1.310000	-2.915000	1.282000	63	2	16	31
C	16	-2.108000	-3.649000	0.428000	63	15	17	32
C	17	-1.997000	-3.458000	-0.939000	63	16	18	33
C	18	-1.070000	-2.564000	-1.437000	63	3	17	34
C	19	2.072000	-1.571000	-1.454000	63	4	20	35

C	20	3.067000	-0.893000	-2.130000	63	19	21	36
C	21	2.837000	0.393000	-2.590000	63	20	22	37
C	22	1.622000	0.996000	-2.337000	63	5	21	38
C	23	1.271000	3.348000	-0.088000	63	8	24	39
C	24	2.165000	3.666000	0.915000	63	23	25	40
C	25	1.989000	3.141000	2.185000	63	24	26	41
C	26	0.898000	2.338000	2.450000	63	9	25	42
C	27	-2.520000	1.948000	1.635000	63	10	28	43
C	28	-3.697000	1.418000	2.126000	63	27	29	44
C	29	-3.669000	0.240000	2.855000	63	28	30	45
C	30	-2.471000	-0.418000	3.049000	63	11	29	46
H	31	-1.393000	-3.061000	2.343000	11	15		
H	32	-2.813000	-4.356000	0.826000	11	16		
H	33	-2.626000	-4.008000	-1.616000	11	17		
H	34	-0.983000	-2.417000	-2.497000	11	18		
H	35	2.250000	-2.568000	-1.098000	11	19		
H	36	4.015000	-1.369000	-2.303000	11	20		
H	37	3.597000	0.922000	-3.135000	11	21		
H	38	1.439000	1.993000	-2.693000	11	22		
H	39	1.389000	3.745000	-1.078000	11	23		
H	40	2.996000	4.314000	0.704000	11	24		
H	41	2.686000	3.372000	2.970000	11	25		
H	42	0.743000	1.959000	3.442000	11	26		
H	43	-2.537000	2.877000	1.098000	11	27		
H	44	-4.626000	1.932000	1.957000	11	28		
H	45	-4.575000	-0.168000	3.265000	11	29		
H	46	-2.427000	-1.330000	3.612000	11	30		

5. CIF for Compound (R_a,R_a)-21

```
d;----------------------------------------------------------------------
data_cyclic_diester_(Ra,Ra)-21
#----------------------------------------------------------------------
# CHEMICAL DATA
_chemical_formula_sum                   'C58 H44 O8 '
_chemical_formula_moiety                'C58 H44 O8 '
_chemical_formula_weight                868.98
_chemical_melting_point                 ?
#----------------------------------------------------------------------
```

```
# CRYSTAL DATA
_symmetry_cell_setting                orthorhombic
_symmetry_space_group_name_H-M         'C 2 2 21        '
_symmetry_Int_Tables_number            20
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
x,-y,-z
-x,-y,1/2+z
-x,y,1/2-z
1/2+x,1/2+y,z
1/2+x,1/2-y,-z
1/2-x,1/2-y,1/2+z
1/2-x,1/2+y,1/2-z
_cell_length_a                        14.090(2)
_cell_length_b                        28.820(4)
_cell_length_c                        11.160(2)
_cell_angle_alpha                     90
_cell_angle_beta                      90
_cell_angle_gamma                      90
_cell_volume                           4531(1)
_cell_formula_units_Z                 4
_cell_measurement_reflns_used         8786
_cell_measurement_theta_min           3.2
_cell_measurement_theta_max           27.5
_cell_measurement_temperature         173.2
#------------------------------------------------------------------------------
_exptl_crystal_description            'Prism'
_exptl_crystal_colour                  'Colorless'
_exptl_crystal_size_max                0.300
_exptl_crystal_size_mid                0.300
_exptl_crystal_size_min                0.250
_exptl_crystal_size_rad                ?
_exptl_crystal_density_diffrn         1.274
_exptl_crystal_density_meas            ?
_exptl_crystal_density_method          'not measured'
_exptl_absorpt_coefficient_mu          0.084
_exptl_absorpt_correction_type         multi-scan
```

```
_exptl_absorpt_process_details          '(Jacobson, 1998)'
_exptl_absorpt_correction_T_min          0.880
_exptl_absorpt_correction_T_max          0.979
#------------------------------------------------------------------------
# EXPERIMENTAL DATA
_diffrn_radiation_type                   'Mo K¥a'
_diffrn_radiation_wavelength             0.7107
_diffrn_measurement_device_type          'Rigaku/MSC Mercury CCD'
_diffrn_measurement_method                ¥w
_diffrn_detector_area_resol_mean         14.62
_diffrn_reflns_number                     21216
_diffrn_reflns_av_R_equivalents          0.028
_diffrn_reflns_theta_max                  27.48
_diffrn_measured_fraction_theta_max      0.9910
_diffrn_reflns_theta_full                27.48
_diffrn_measured_fraction_theta_full     0.9910
_diffrn_reflns_limit_h_min               -18
_diffrn_reflns_limit_h_max                17
_diffrn_reflns_limit_k_min               -27
_diffrn_reflns_limit_k_max                37
_diffrn_reflns_limit_l_min               -14
_diffrn_reflns_limit_l_max                14
#------------------------------------------------------------------------
# REFINEMENT DATA
_refine_special_details
;
Refinement using reflections with F^2^ > 3.0 sigma(F^2^). The weighted R-factor
(wR), goodness of fit (S) and R-factor (gt) are based on F, with F set to zero
for negative F. The threshold expression of F^2^ > 3.0 sigma(F^2^) is used only
for calculating R-factor (gt).
;
_reflns_number_total                      2876
_reflns_number_gt                         2184
_reflns_threshold_expression             F^2^>3.0¥s(F^2^)
_refine_ls_structure_factor_coef         F
_refine_ls_R_factor_gt                    0.0469
_refine_ls_wR_factor_ref                  0.0483
_refine_ls_hydrogen_treatment             noref
```

```
_refine_ls_number_reflns                 2184
_refine_ls_number_parameters             299
_refine_ls_goodness_of_fit_ref           1.418
_refine_ls_weighting_scheme              unit
_refine_ls_shift/su_max                  0.0075
_refine_diff_density_max                 0.19
_refine_diff_density_min                 -0.16
_refine_ls_extinction_method             none
_refine_ls_extinction_coef               ?
_refine_ls_abs_structure_details         ?
_refine_ls_abs_structure_Flack           1(1)
loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
  'C' 'C'    0.003 0.002
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
  'H' 'H'    0.000 0.000
;International Tables for Crystallography
(1992, Vol. C, Table 6.1.1.2)
;
  'O' 'O'    0.011 0.006
;International Tables for Crystallography
(1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1)
;
#---------------------------------------------------------------------------
# ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
```

_atom_site_adp_type
_atom_site_occupancy
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group

O(1)	O	-0.1474(2)	0.33756(7)	0.6922(2)	0.0363(6)	Uani 1.00 d . . .
O(2)	O	-0.0423(1)	0.39020(6)	0.6186(2)	0.0292(5)	Uani 1.00 d . . .
O(3)	O	-0.3404(2)	0.47131(8)	0.6487(2)	0.0395(6)	Uani 1.00 d . . .
O(4)	O	-0.4132(1)	0.64099(8)	1.0046(2)	0.0366(6)	Uani 1.00 d . . .
C(1)	C	0.0004(2)	0.31124(9)	0.6093(3)	0.0270(6)	Uani 1.00 d . . .
C(2)	C	0.0487(2)	0.31592(10)	0.4985(3)	0.0306(7)	Uani 1.00 d . . .
C(3)	C	0.1182(2)	0.2850(1)	0.4675(3)	0.0318(7)	Uani 1.00 d . . .
C(4)	C	0.1432(2)	0.2479(1)	0.5453(3)	0.0332(7)	Uani 1.00 d . . .
C(5)	C	0.2164(2)	0.2164(1)	0.5147(3)	0.0392(9)	Uani 1.00 d . . .
C(6)	C	0.2408(3)	0.1814(1)	0.5909(4)	0.0457(9)	Uani 1.00 d . . .
C(7)	C	0.1938(3)	0.1763(1)	0.7019(3)	0.0433(9)	Uani 1.00 d . . .
C(8)	C	0.1226(3)	0.2062(1)	0.7344(3)	0.0371(8)	Uani 1.00 d . . .
C(9)	C	0.0951(2)	0.24314(10)	0.6570(3)	0.0296(7)	Uani 1.00 d . . .
C(10)	C	0.0224(2)	0.27586(9)	0.6894(3)	0.0271(7)	Uani 1.00 d . . .
C(11)	C	-0.0732(2)	0.34594(10)	0.6445(3)	0.0276(6)	Uani 1.00 d . . .
C(12)	C	-0.0974(2)	0.42700(9)	0.6653(3)	0.0272(7)	Uani 1.00 d . . .
C(13)	C	-0.0526(2)	0.45816(9)	0.7392(3)	0.0243(7)	Uani 1.00 d . . .
C(14)	C	-0.1099(2)	0.49410(9)	0.7901(3)	0.0239(6)	Uani 1.00 d . . .
C(15)	C	-0.0661(2)	0.52608(9)	0.8720(3)	0.0268(7)	Uani 1.00 d . . .
C(16)	C	-0.1165(2)	0.55920(10)	0.9291(3)	0.0281(7)	Uani 1.00 d . . .
C(17)	C	-0.2163(2)	0.56409(10)	0.9083(3)	0.0266(7)	Uani 1.00 d . . .
C(18)	C	-0.2647(2)	0.5993(1)	0.9721(3)	0.0298(7)	Uani 1.00 d . . .
C(19)	C	-0.3606(2)	0.6062(1)	0.9538(3)	0.0308(7)	Uani 1.00 d . . .
C(20)	C	-0.4092(2)	0.5775(1)	0.8729(3)	0.0335(8)	Uani 1.00 d . . .
C(21)	C	-0.3631(2)	0.5427(1)	0.8122(3)	0.0314(7)	Uani 1.00 d . . .
C(22)	C	-0.2638(2)	0.53454(10)	0.8263(3)	0.0260(7)	Uani 1.00 d . . .
C(23)	C	-0.2090(2)	0.49835(10)	0.7648(3)	0.0246(6)	Uani 1.00 d . . .
C(24)	C	-0.2470(2)	0.4665(1)	0.6798(3)	0.0283(7)	Uani 1.00 d . . .
C(25)	C	-0.1922(2)	0.43142(10)	0.6318(3)	0.0291(7)	Uani 1.00 d . . .
C(26)	C	-0.3790(3)	0.4424(1)	0.5561(3)	0.0451(10)	Uani 1.00 d . . .
C(27)	C	-0.3680(2)	0.6699(1)	1.0940(3)	0.0358(8)	Uani 1.00 d . . .
C(28)	C	-0.3603(3)	0.6442(1)	1.2118(3)	0.047(1)	Uani 1.00 d . . .

C(29)	C	-0.4287(3)	0.7129(1)	1.1030(3)	0.047(1)	Uani 1.00 d . . .
H(1)	H	0.0331	0.3427	0.4443	0.0412	Uiso 1.00 calc . . .
H(2)	H	0.1474	0.2897	0.3871	0.0412	Uiso 1.00 calc . . .
H(3)	H	0.2470	0.2207	0.4346	0.0412	Uiso 1.00 calc . . .
H(4)	H	0.2920	0.1581	0.5628	0.0412	Uiso 1.00 calc . . .
H(5)	H	0.2254	0.1519	0.7618	0.0412	Uiso 1.00 calc . . .
H(6)	H	0.0852	0.2010	0.8154	0.0412	Uiso 1.00 calc . . .
H(7)	H	0.0039	0.5223	0.8903	0.0412	Uiso 1.00 calc . . .
H(8)	H	-0.0842	0.5811	0.9924	0.0412	Uiso 1.00 calc . . .
H(9)	H	-0.2318	0.6138	1.0445	0.0412	Uiso 1.00 calc . . .
H(10)	H	-0.4755	0.5845	0.8579	0.0412	Uiso 1.00 calc . . .
H(11)	H	-0.3930	0.5226	0.7547	0.0412	Uiso 1.00 calc . . .
H(12)	H	-0.2214	0.4068	0.5770	0.0412	Uiso 1.00 calc . . .
H(13)	H	-0.3716	0.4071	0.5827	0.0412	Uiso 1.00 calc . . .
H(14)	H	-0.3413	0.4476	0.4711	0.0412	Uiso 1.00 calc . . .
H(15)	H	-0.4372	0.4539	0.5234	0.0412	Uiso 1.00 calc . . .
H(16)	H	-0.3001	0.6785	1.0737	0.0412	Uiso 1.00 calc . . .
H(17)	H	-0.3301	0.6140	1.1925	0.0412	Uiso 1.00 calc . . .
H(18)	H	-0.4267	0.6359	1.2258	0.0412	Uiso 1.00 calc . . .
H(19)	H	-0.3465	0.6592	1.2990	0.0412	Uiso 1.00 calc . . .
H(20)	H	-0.3881	0.7353	1.1590	0.0412	Uiso 1.00 calc . . .
H(21)	H	-0.4919	0.7086	1.1254	0.0412	Uiso 1.00 calc . . .
H(22)	H	-0.4519	0.7305	1.0280	0.0412	Uiso 1.00 calc . . .

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23

O(1)	0.030(1)	0.033(1)	0.047(1)	-0.0038(9)	0.0019(10)	0.007(1)
O(2)	0.037(1)	0.0203(8)	0.030(1)	-0.0037(8)	0.0045(10)	-0.0020(8)
O(3)	0.032(1)	0.040(1)	0.047(1)	-0.0004(10)	-0.018(1)	-0.007(1)
O(4)	0.027(1)	0.041(1)	0.041(1)	0.0127(9)	-0.002(1)	-0.0022(10)
C(1)	0.035(1)	0.020(1)	0.026(1)	-0.006(1)	0.002(1)	-0.004(1)
C(2)	0.042(2)	0.024(1)	0.026(1)	-0.010(1)	0.001(1)	0.002(1)

C(3)	0.042(2)	0.031(1)	0.022(1)	-0.010(1)	0.007(1)	-0.003(1)
C(4)	0.043(2)	0.025(1)	0.032(1)	-0.006(1)	0.008(1)	-0.004(1)
C(5)	0.045(2)	0.036(2)	0.036(2)	-0.004(1)	0.014(2)	-0.010(1)
C(6)	0.052(2)	0.034(2)	0.051(2)	0.007(2)	0.016(2)	-0.005(1)
C(7)	0.053(2)	0.031(2)	0.046(2)	0.009(1)	0.007(2)	0.003(1)
C(8)	0.054(2)	0.027(1)	0.031(2)	0.002(1)	0.010(2)	0.002(1)
C(9)	0.037(2)	0.023(1)	0.029(1)	-0.004(1)	0.006(1)	-0.003(1)
C(10)	0.036(2)	0.022(1)	0.022(1)	-0.004(1)	0.005(1)	-0.004(1)
C(11)	0.033(1)	0.028(1)	0.022(1)	-0.007(1)	-0.003(1)	-0.002(1)
C(12)	0.033(1)	0.021(1)	0.027(1)	-0.006(1)	0.002(1)	0.002(1)
C(13)	0.024(1)	0.021(1)	0.028(1)	-0.0023(10)	-0.001(1)	0.004(1)
C(14)	0.024(1)	0.022(1)	0.026(1)	-0.0037(10)	0.001(1)	0.003(1)
C(15)	0.020(1)	0.024(1)	0.036(2)	0.000(1)	-0.007(1)	-0.002(1)
C(16)	0.025(1)	0.023(1)	0.036(2)	-0.003(1)	-0.005(1)	-0.002(1)
C(17)	0.025(1)	0.023(1)	0.032(2)	0.000(1)	-0.004(1)	0.004(1)
C(18)	0.026(1)	0.027(1)	0.036(2)	0.000(1)	-0.003(1)	-0.002(1)
C(19)	0.025(1)	0.036(2)	0.031(1)	0.005(1)	0.003(1)	0.005(1)
C(20)	0.019(1)	0.046(2)	0.036(2)	0.003(1)	-0.001(1)	0.003(1)
C(21)	0.024(1)	0.039(2)	0.031(2)	-0.006(1)	-0.006(1)	0.001(1)
C(22)	0.024(1)	0.025(1)	0.029(1)	-0.001(1)	-0.003(1)	0.004(1)
C(23)	0.024(1)	0.022(1)	0.027(1)	-0.001(1)	-0.003(1)	0.004(1)
C(24)	0.027(1)	0.029(1)	0.029(1)	-0.006(1)	-0.006(1)	0.005(1)
C(25)	0.036(1)	0.023(1)	0.028(1)	-0.009(1)	-0.007(1)	0.000(1)
C(26)	0.046(2)	0.041(2)	0.049(2)	-0.002(2)	-0.025(2)	-0.003(2)
C(27)	0.033(2)	0.033(1)	0.042(2)	0.002(1)	0.007(1)	0.001(1)
C(28)	0.043(2)	0.059(2)	0.040(2)	0.018(2)	0.002(2)	0.005(2)
C(29)	0.046(2)	0.039(2)	0.055(2)	0.018(1)	0.009(2)	0.004(2)

#---

_computing_data_collection '.'
_computing_cell_refinement '.'
_computing_data_reduction 'teXsan Ver. 1.11'
_computing_structure_solution SIR92
_computing_structure_refinement 'teXsan Ver. 1.10'
_computing_publication_material 'teXsan Ver. 1.11'
_computing_molecular_graphics ?

#---

_geom_special_details
;

?
;
loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
O(1) C(11) 1.198(4) . . yes
O(2) C(11) 1.379(4) . . yes
O(2) C(12) 1.414(4) . . yes
O(3) C(24) 1.368(4) . . yes
O(3) C(26) 1.434(5) . . yes
O(4) C(19) 1.370(4) . . yes
O(4) C(27) 1.448(5) . . yes
C(1) C(2) 1.418(5) . . yes
C(1) C(10) 1.391(4) . . yes
C(1) C(11) 1.493(5) . . yes
C(2) C(3) 1.367(5) . . yes
C(3) C(4) 1.421(5) . . yes
C(4) C(5) 1.418(5) . . yes
C(4) C(9) 1.426(5) . . yes
C(5) C(6) 1.362(6) . . yes
C(6) C(7) 1.412(6) . . yes
C(7) C(8) 1.371(5) . . yes
C(8) C(9) 1.426(5) . . yes
C(9) C(10) 1.438(5) . . yes
C(10) C(10) 1.493(7) . 4_556 yes
C(12) C(13) 1.373(5) . . yes
C(12) C(25) 1.393(5) . . yes
C(13) C(13) 1.501(7) . 4_556 yes
C(13) C(14) 1.431(4) . . yes
C(14) C(15) 1.437(4) . . yes
C(14) C(23) 1.429(4) . . yes
C(15) C(16) 1.349(5) . . yes
C(16) C(17) 1.432(5) . . yes
C(17) C(18) 1.415(5) . . yes

```
  C(17)        C(22)        1.418(5)     . . yes
  C(18)        C(19)        1.381(5)     . . yes
  C(19)        C(20)        1.403(5)     . . yes
  C(20)        C(21)        1.375(5)     . . yes
  C(21)        C(22)        1.428(5)     . . yes
  C(22)        C(23)        1.468(5)     . . yes
  C(23)        C(24)        1.425(5)     . . yes
  C(24)        C(25)        1.380(5)     . . yes
  C(27)        C(28)        1.513(6)     . . yes
  C(27)        C(29)        1.509(5)     . . yes
#------------------------------------------------------------------------------
loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
     C(11)        O(2)         C(12)        116.3(3)     . . . yes
     C(24)        O(3)         C(26)        119.2(3)     . . . yes
     C(19)        O(4)         C(27)        117.9(3)     . . . yes
     C(2)         C(1)         C(10)        121.5(3)     . . . yes
     C(2)         C(1)         C(11)        119.9(3)     . . . yes
     C(10)        C(1)         C(11)        118.5(3)     . . . yes
     C(1)         C(2)         C(3)         120.2(3)     . . . yes
     C(2)         C(3)         C(4)         120.8(3)     . . . yes
     C(3)         C(4)         C(5)         121.0(3)     . . . yes
     C(3)         C(4)         C(9)         119.3(3)     . . . yes
     C(5)         C(4)         C(9)         119.6(3)     . . . yes
     C(4)         C(5)         C(6)         120.5(4)     . . . yes
     C(5)         C(6)         C(7)         120.4(4)     . . . yes
     C(6)         C(7)         C(8)         120.7(4)     . . . yes
     C(7)         C(8)         C(9)         120.5(4)     . . . yes
     C(4)         C(9)         C(8)         118.2(3)     . . . yes
     C(4)         C(9)         C(10)        119.6(3)     . . . yes
     C(8)         C(9)         C(10)        122.2(3)     . . . yes
```

C(1)	C(10)	C(9)	118.6(3)	. . . yes
C(1)	C(10)	C(10)	119.2(3)	. . 4_556 yes
C(9)	C(10)	C(10)	121.9(3)	. . 4_556 yes
O(1)	C(11)	O(2)	123.7(3)	. . . yes
O(1)	C(11)	C(1)	126.0(3)	. . . yes
O(2)	C(11)	C(1)	110.2(3)	. . . yes
O(2)	C(12)	C(13)	117.3(3)	. . . yes
O(2)	C(12)	C(25)	119.8(3)	. . . yes
C(13)	C(12)	C(25)	122.9(3)	. . . yes
C(12)	C(13)	C(13)	123.4(3)	. . 4_556 yes
C(12)	C(13)	C(14)	116.9(3)	. . . yes
C(13)	C(13)	C(14)	119.5(3)	4_556 . . yes
C(13)	C(14)	C(15)	118.3(3)	. . . yes
C(13)	C(14)	C(23)	122.3(3)	. . . yes
C(15)	C(14)	C(23)	119.4(3)	. . . yes
C(14)	C(15)	C(16)	121.9(3)	. . . yes
C(15)	C(16)	C(17)	120.6(3)	. . . yes
C(16)	C(17)	C(18)	117.6(3)	. . . yes
C(16)	C(17)	C(22)	120.6(3)	. . . yes
C(18)	C(17)	C(22)	121.8(3)	. . . yes
C(17)	C(18)	C(19)	120.1(3)	. . . yes
O(4)	C(19)	C(18)	125.1(3)	. . . yes
O(4)	C(19)	C(20)	115.7(3)	. . . yes
C(18)	C(19)	C(20)	119.2(3)	. . . yes
C(19)	C(20)	C(21)	121.1(3)	. . . yes
C(20)	C(21)	C(22)	121.9(3)	. . . yes
C(17)	C(22)	C(21)	115.8(3)	. . . yes
C(17)	C(22)	C(23)	118.7(3)	. . . yes
C(21)	C(22)	C(23)	125.5(3)	. . . yes
C(14)	C(23)	C(22)	118.8(3)	. . . yes
C(14)	C(23)	C(24)	116.4(3)	. . . yes
C(22)	C(23)	C(24)	124.8(3)	. . . yes
O(3)	C(24)	C(23)	117.7(3)	. . . yes
O(3)	C(24)	C(25)	120.9(3)	. . . yes
C(23)	C(24)	C(25)	121.3(3)	. . . yes
C(12)	C(25)	C(24)	119.9(3)	. . . yes
O(4)	C(27)	C(28)	110.4(3)	. . . yes
O(4)	C(27)	C(29)	105.6(3)	. . . yes

```
     C(28)         C(27)         C(29)         112.6(3)      . . . yes
#-------------------------------------------------------------------------------
l
#-------------------------------------------------------------------------------
*==END
→
```