STUDY OF SYNTHETIC ROUTES FOR THE SPIROKETAL FRAGMENT IN CALYCULIN A BASED ON CONFORMATIONAL ANALYSIS

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Supproting Information

1. Coordinate of the global minimum of **5**

No	Atom	X	Y	Z	No.	Atom	X	Y	Z
1	O	0.1639	0.1769	0.5885	34	H	-2.2053	-0.0382	1.7536
2	C	-0.5880	-0.0108	-0.6070	35	H	-4.1499	1.3081	1.0723
3	C	-2.0477	0.4058	-0.3641	36	H	-4.5362	-0.3144	2.9705
4	C	-2.7224	-0.3079	0.8242	37	H	-5.2266	-1.4627	1.7915
5	C	-4.1612	0.2266	0.8883	38	H	-6.6195	0.2398	1.1350
6	C	-5.0154	-0.4082	1.9919	39	H	-3.1450	-2.3270	1.5421
7	O	-6.2791	0.2580	2.0503	40	H	-3.1755	-2.1821	-0.2232
8	O	-2.7873	0.1704	-1.5628	41	H	-1.6402	-2.1990	0.6603
9	C	-2.6724	-1.8367	0.6856	42	H	-4.7291	-1.1544	-2.6979
10	O	-4.8330	-0.0039	-0.3571	43	H	-5.9047	0.1587	-2.7404
11	C	-4.1598	0.5555	-1.4867	44	H	-4.3707	0.2886	-3.6451
12	C	-4.8322	-0.0627	-2.7158	45	H	-5.3908	2.3531	-1.5500
13	C	-4.3307	2.0771	-1.5571	46	H	-3.8695	2.5884	-0.7076
14	Si	1.8156	-0.0653	0.5878	47	H	-3.8593	2.4831	-2.4588
15	C	2.4994	-0.3041	2.4433	48	H	2.8928	0.9520	4.2007

16	C	2.5829	1.0711	3.1556	49	H	1.6143	1.5848	3.1564
17	C	1.5287	-1.1865	3.2656	50	H	3.3138	1.7339	2.6791
18	C	3.9032	-0.9451	2.4619	51	H	1.4440	-2.1985	2.8614
19	C	2.2287	-1.5141	-0.5373	52	H	0.5205	-0.7566	3.2953
20	C	2.5888	-1.3113	-1.8857	53	H	1.8732	-1.2837	4.3021
21	C	2.8737	-2.3857	-2.7341	54	H	4.2707	-1.0469	3.4899
22	C	2.7927	-3.6899	-2.2601	55	H	3.9030	-1.9467	2.0204
23	C	2.4186	-3.9198	-0.9409	56	H	4.6338	-0.3401	1.9150
24	C	2.1334	-2.8452	-0.0918	57	H	2.6457	-0.3085	-2.3085
25	C	2.6478	1.4812	-0.1080	58	H	3.1526	-2.1992	-3.7681
26	C	4.0100	1.4860	-0.4644	59	H	3.0114	-4.5251	-2.9196
27	C	4.6179	2.6396	-0.9663	60	H	2.3415	-4.9384	-0.5691
28	C	3.8800	3.8102	-1.1161	61	H	1.8281	-3.0793	0.9242
29	C	2.5340	3.8304	-0.7625	62	H	4.6185	0.5881	-0.3626
30	C	1.9227	2.6784	-0.2608	63	H	5.6699	2.6223	-1.2394
31	H	-0.5464	-1.0541	-0.9431	64	H	4.3545	4.7070	-1.5052
32	H	-0.1827	0.6026	-1.4234	65	H	1.9574	4.7451	-0.8736
33	H	-2.0322	1.4836	-0.1569	66	H	0.8705	2.7323	0.0151

2. Coordinate of the 29th minimum of **5**

No	Atom	X	Y	Z	No.	Atom	X	Y	Z
1	O	-0.1922	-0.2777	0.2848	34	H	1.9420	-1.6431	-0.4748
2	C	0.7669	0.6223	0.8263	35	H	3.8276	-0.6266	-1.6882
3	C	2.1115	0.4408	0.1038	36	H	4.0423	-3.0907	-1.1739
4	C	2.6380	-1.0076	0.0871	37	H	5.0387	-2.6647	0.2441
5	C	3.9812	-0.9697	-0.6576	38	H	6.3445	-1.4424	-1.1973
6	C	4.6909	-2.3264	-0.7364	39	H	3.1308	-2.6240	1.4708
7	O	5.8518	-2.2030	-1.5617	40	H	3.4601	-1.0097	2.1216
8	O	3.0684	1.3037	0.7200	41	H	1.8020	-1.6223	2.0096
9	C	2.7705	-1.5912	1.5015	42	H	5.3049	1.4775	2.0543
10	O	4.8794	-0.0550	-0.0151	43	H	6.3274	2.0003	0.7167
11	C	4.3593	1.2701	0.1107	44	H	4.9692	3.0196	1.2688
12	C	5.2958	1.9903	1.0850	45	H	5.3897	2.0320	-1.6523

13	C	4.3812	2.0222	-1.2248	46	H	3.7298	1.5626	-1.9734
14	Si	-1.8265	0.0012	0.4952	47	H	4.0334	3.0533	-1.0996
15	C	-2.3941	-0.0172	2.3710	48	H	-2.0416	-1.2587	4.1510
16	C	-1.7420	-1.2259	3.0967	49	H	-0.6476	-1.1730	3.0709
17	C	-1.9569	1.2624	3.1226	50	H	-2.0389	-2.1794	2.6447
18	C	-3.9272	-0.1712	2.5163	51	H	-2.4093	2.1654	2.7033
19	C	-2.2639	1.5440	-0.4818	52	H	-0.8711	1.3991	3.1021
20	C	-3.2089	2.4920	-0.0566	53	H	-2.2546	1.2161	4.1771
21	C	-3.4977	3.6228	-0.8284	54	H	-4.2224	-0.1580	3.5724
22	C	-2.8527	3.8275	-2.0440	55	H	-4.4759	0.6328	2.0180
23	C	-1.9197	2.8999	-2.4930	56	H	-4.2812	-1.1205	2.0984
24	C	-1.6299	1.7708	-1.7226	57	H	-3.7481	2.3772	0.8788
25	C	-2.7100	-1.4185	-0.3919	58	H	-4.2323	4.3437	-0.4778
26	C	-2.0984	-2.6833	-0.4872	59	H	-3.0809	4.7053	-2.6422
27	C	-2.7401	-3.7443	-1.1307	60	H	-1.4183	3.0492	-3.4456
28	C	-4.0011	-3.5615	-1.6912	61	H	-0.9012	1.0585	-2.1106
29	C	-4.6217	-2.3177	-1.6109	62	H	-1.1104	-2.8561	-0.0620
30	C	-3.9835	-1.2540	-0.9675	63	H	-2.2523	-4.7134	-1.1953
31	H	0.8864	0.4459	1.9015	64	H	-4.4987	-4.3866	-2.1933
32	H	0.4550	1.6697	0.7137	65	H	-5.6042	-2.1718	-2.0520
33	H	1.9512	0.7627	-0.9332	66	H	-4.4977	-0.2948	-0.9281

3. Coordinate of the global minimum of **6**

No	Atom	X	Y	Z	No.	Atom	X	Y	Z
1	O	0.7615	-0.1367	-0.0146	37	H	-1.1613	0.8713	1.5419
2	C	0.4646	1.2364	0.2205	38	H	-1.8177	-0.3186	-0.4917
3	C	-1.0225	1.3849	0.5819	39	H	-3.5244	0.5385	1.0523
4	C	-1.9883	0.7638	-0.4462	40	H	-5.5061	0.6279	-0.3361
5	C	-3.4111	1.0298	0.0798	41	H	-4.5969	1.0951	-1.7424
6	C	-4.5328	0.4980	-0.8258	42	H	-5.1042	-3.3419	-2.0580
7	O	-4.3414	-0.8582	-1.2030	43	H	-4.6570	-4.3202	-0.6285
8	S	-4.7348	-2.0188	-0.1313	44	H	-3.3946	-3.4035	-1.5040
9	C	-4.4412	-3.4111	-1.1936	45	H	-1.9194	2.4178	-1.8868

10	O	-1.3083	2.7745	0.7483	46	H	-2.4675	0.8810	-2.5748
11	C	-1.7763	1.3330	-1.8570	47	H	-0.7690	1.1144	-2.2248
12	O	-3.6131	2.4333	0.2572	48	H	-2.6601	4.8344	-0.1140
13	O	-6.1520	-1.9339	0.1466	49	H	-3.8615	4.8731	1.1756
14	O	-3.7448	-2.0232	0.9245	50	H	-2.1328	5.1293	1.5422
15	C	-2.6582	3.0500	1.1235	51	H	-2.2185	3.2448	3.2494
16	C	-2.8410	4.5584	0.9319	52	H	-2.8014	1.6498	2.8102
17	C	-2.9209	2.7156	2.5963	53	H	-3.9453	2.9788	2.8812
18	Si	2.3364	-0.6289	-0.2575	54	H	1.1143	-3.3530	0.4112
19	C	2.3910	-2.4214	-1.1259	55	H	2.8481	-3.5747	0.6999
20	C	2.0799	-3.5234	-0.0796	56	H	2.0381	-4.5115	-0.5532
21	C	3.7722	-2.7189	-1.7466	57	H	4.5699	-2.6880	-0.9970
22	C	1.3075	-2.5188	-2.2276	58	H	3.7889	-3.7183	-2.1974
23	C	3.2549	0.6887	-1.2350	59	H	4.0295	-2.0062	-2.5364
24	C	4.0057	1.6889	-0.5830	60	H	1.2995	-3.5180	-2.6793
25	C	4.6719	2.6861	-1.3020	61	H	1.4734	-1.8037	-3.0375
26	C	4.5936	2.7167	-2.6894	62	H	0.3048	-2.3346	-1.8241
27	C	3.8423	1.7558	-3.3568	63	H	4.0794	1.7183	0.5039
28	C	3.1754	0.7581	-2.6379	64	H	5.2463	3.4421	-0.7727
29	C	3.1744	-0.8101	1.4252	65	H	5.1087	3.4930	-3.2483
30	C	4.5691	-0.9649	1.5403	66	H	3.7673	1.7835	-4.4410
31	C	5.1754	-1.1106	2.7908	67	H	2.5871	0.0426	-3.2053
32	C	4.4013	-1.1106	3.9476	68	H	5.2067	-0.9682	0.6570
33	C	3.0198	-0.9672	3.8564	69	H	6.2541	-1.2251	2.8595
34	C	2.4102	-0.8206	2.6078	70	H	4.8738	-1.2255	4.9192
35	H	0.7003	1.8472	-0.6597	71	H	2.4125	-0.9728	4.7579
36	H	1.0647	1.6309	1.0519	72	H	1.3259	-0.7211	2.5724

4. Coordinate of the 4th minimum of **6**

No	Atom	X	Y	Z	No.	Atom	X	Y	Z
1	O	1.1070	-0.2742	-0.1933	37	H	-0.9836	-0.0283	1.4409
2	C	0.6948	0.8917	0.5138	38	H	-1.4279	-0.3519	-0.9449
3	C	-0.8193	0.8261	0.7717	39	H	-3.2868	-0.2308	0.6613

4	C	-1.6703	0.6203	-0.4976	40	H	-4.2169	1.3588	-1.7684
5	C	-3.1380	0.5980	-0.0375	41	H	-3.8317	-0.3703	-1.8720
6	C	-4.1384	0.4319	-1.1913	42	H	-7.3289	-0.5383	1.1688
7	O	-5.4468	0.1776	-0.6816	43	H	-7.9865	-2.0125	0.3975
8	S	-5.9245	-1.3706	-0.5437	44	H	-8.0995	-0.4427	-0.4530
9	C	-7.4956	-1.0533	0.2208	45	H	-1.6207	2.7073	-1.1745
10	O	-1.2128	2.0254	1.4399	46	H	-2.0172	1.5419	-2.4478
11	C	-1.4063	1.7034	-1.5544	47	H	-0.3648	1.6835	-1.8899
12	O	-3.4461	1.8167	0.6479	48	H	-2.6443	4.2052	1.3247
13	O	-5.0655	-2.0388	0.4110	49	H	-3.9315	3.6890	2.4132
14	O	-6.1476	-1.9016	-1.8713	50	H	-2.2547	3.8471	3.0063
15	C	-2.6012	2.0800	1.7686	51	H	-3.9996	1.2724	3.2326
16	C	-2.8768	3.5345	2.1606	52	H	-2.3279	1.4458	3.8359
17	C	-2.9407	1.1852	2.9661	53	H	-2.7559	0.1268	2.7624
18	Si	2.7274	-0.5538	-0.4793	54	H	1.6995	-3.3975	-0.9438
19	C	2.9726	-1.8933	-1.9323	55	H	3.4285	-3.6101	-0.6218
20	C	2.6996	-3.3193	-1.3864	56	H	2.7633	-4.0640	-2.1887
21	C	4.4036	-1.8620	-2.5096	57	H	5.1566	-2.0647	-1.7409
22	C	1.9593	-1.6401	-3.0752	58	H	4.5245	-2.6219	-3.2908
23	C	3.5838	1.0820	-0.8367	59	H	4.6423	-0.8948	-2.9629
24	C	3.5685	1.6589	-2.1198	60	H	2.0558	-2.4022	-3.8578
25	C	4.1868	2.8880	-2.3732	61	H	2.1084	-0.6694	-3.5550
26	C	4.8236	3.5766	-1.3467	62	H	0.9254	-1.6740	-2.7117
27	C	4.8354	3.0411	-0.0641	63	H	3.0694	1.1704	-2.9518
28	C	4.2176	1.8127	0.1897	64	H	4.1639	3.3087	-3.3753
29	C	3.4930	-1.2931	1.0816	65	H	5.3012	4.5323	-1.5439
30	C	2.6752	-1.7825	2.1180	66	H	5.3198	3.5803	0.7460
31	C	3.2327	-2.3429	3.2701	67	H	4.2350	1.4434	1.2149
32	C	4.6152	-2.4294	3.4070	68	H	1.5896	-1.7401	2.0393
33	C	5.4425	-1.9587	2.3915	69	H	2.5847	-2.7154	4.0592
34	C	4.8884	-1.3983	1.2377	70	H	5.0474	-2.8666	4.3030
35	H	0.9411	1.8023	-0.0461	71	H	6.5223	-2.0280	2.4950
36	H	1.2091	0.9647	1.4819	72	H	5.5668	-1.0395	0.4645

5. Coordinate of the global minimum of **19**

No	Atom	X	Y	Z	No.	Atom	X	Y	Z
1	C	-0.1740	0.1761	0.1146	17	H	0.0211	1.1723	0.5218
2	C	-1.6071	-0.2687	0.4478	18	H	-1.7375	-1.3273	0.1877
3	C	-2.6645	0.5581	-0.3230	19	H	-2.4054	0.5292	-1.3901
4	C	-4.0291	-0.0614	-0.1450	20	H	-4.4122	-0.0058	0.8665
5	C	-4.5088	-1.1751	-1.0401	21	H	-5.2338	-1.8743	-0.6425
6	O	-4.9354	0.1815	-1.2296	22	H	-3.8312	-1.5931	-1.7732
7	O	-1.8379	-0.1458	1.8566	23	H	-1.1172	-0.6347	2.2979
8	C	-2.7128	2.0286	0.1055	24	H	-1.7567	2.5291	-0.0730
9	S	1.0286	-0.9842	0.8717	25	H	-3.4779	2.5688	-0.4632
10	C	2.5431	-0.3347	0.1898	26	H	-2.9638	2.1331	1.1664
11	C	3.3538	-1.1688	-0.5861	27	H	3.0624	-2.1989	-0.7777
12	C	4.5484	-0.6878	-1.1266	28	H	5.1720	-1.3412	-1.7315
13	C	4.9430	0.6272	-0.8865	29	H	5.8744	1.0006	-1.3047
14	C	4.1471	1.4598	-0.1017	30	H	4.4599	2.4820	0.0959
15	C	2.9520	0.9792	0.4387	31	H	2.3551	1.6380	1.0640
16	H	-0.0184	0.1888	-0.9688					

6. Coordinate of the 2nd minimum of **19**

No	Atom	X	Y	Z	No.	Atom	X	Y	Z
1	C	0.1783	-0.0742	0.0262	17	H	-0.1140	-0.1557	1.0778
2	C	1.6013	0.4938	-0.0980	18	H	1.8158	0.7301	-1.1484
3	C	2.6701	-0.5057	0.4065	19	H	2.5059	-1.4641	-0.1047
4	C	4.0489	-0.0046	0.0522	20	H	4.3412	0.8961	0.5778
5	C	4.6672	-0.2903	-1.2923	21	H	5.3961	0.4110	-1.6791
6	O	5.0273	-1.0384	-0.1224	22	H	4.0796	-0.7956	-2.0478
7	O	1.7037	1.7168	0.6414	23	H	0.9715	2.2857	0.3360
8	C	2.5935	-0.7629	1.9151	24	H	1.6281	-1.1915	2.1996
9	S	-1.0155	1.0551	-0.7892	25	H	3.3712	-1.4706	2.2235
10	C	-2.5403	0.2458	-0.3425	26	H	2.7455	0.1564	2.4908
11	C	-2.8280	-1.0528	-0.7742	27	H	-2.1268	-1.5977	-1.4004

12	C	-4.0325	-1.6632	-0.4169	28	H	-4.2512	-2.6727	-0.7556
13	C	-4.9577	-0.9759	0.3669	29	H	-5.8961	-1.4502	0.6431
14	C	-4.6826	0.3235	0.7893	30	H	-5.4060	0.8636	1.3947
15	C	-3.4786	0.9345	0.4320	31	H	-3.2804	1.9503	0.7656
16	H	0.1190	-1.0600	-0.4447					

7. Coordinate of the 3rd minimum of **19**

No	Atom	X	Y	Z	No.	Atom	X	Y	Z
1	C	0.3105	-1.5329	-0.7378	17	H	0.8415	-2.4703	-0.9310
2	C	1.1283	-0.6478	0.2180	18	H	0.5258	0.2052	0.5520
3	C	2.4084	-0.0983	-0.4561	19	H	2.1159	0.3742	-1.4037
4	C	3.0408	0.9508	0.4253	20	H	3.4509	0.5642	1.3500
5	C	2.5892	2.3881	0.3801	21	H	2.7070	2.9891	1.2731
6	O	3.7836	1.9513	-0.2842	22	H	1.7418	2.6560	-0.2377
7	O	1.4842	-1.3952	1.3874	23	H	0.6617	-1.8053	1.7158
8	C	3.4394	-1.1856	-0.7757	24	H	3.0342	-1.9305	-1.4667
9	S	-1.2961	-2.0241	0.0059	25	H	4.3257	-0.7467	-1.2474
10	C	-2.1650	-0.4670	-0.0448	26	H	3.7767	-1.7024	0.1292
11	C	-2.6139	0.1032	1.1504	27	H	-2.4390	-0.3953	2.1009
12	C	-3.2923	1.3238	1.1380	28	H	-3.6362	1.7629	2.0711
13	C	-3.5341	1.9752	-0.0702	29	H	-4.0663	2.9232	-0.0799
14	C	-3.1045	1.4039	-1.2667	30	H	-3.3057	1.9044	-2.2106
15	C	-2.4255	0.1834	-1.2549	31	H	-2.1170	-0.2565	-2.1997
16	H	0.1403	-1.0366	-1.6976					

8. Coordinate of the 4th minimum of **19**

No	Atom	X	Y	Z	No.	Atom	X	Y	Z
1	C	0.3399	-0.3167	0.1239	17	H	0.3907	0.5639	-0.5231
2	C	1.6710	-1.0848	0.0867	18	H	1.5616	-2.0422	0.6127
3	C	2.8649	-0.3326	0.7229	19	H	3.7574	-0.9541	0.5630
4	C	3.1092	1.0094	0.0763	20	H	2.3266	1.7384	0.2354
5	C	3.9905	1.1374	-1.1386	21	H	3.8010	1.9509	-1.8269
6	O	4.4640	1.4729	0.1735	22	H	4.3747	0.2356	-1.5998

7	O	2.0111	-1.3987	-1.2721	23	H	1.2403	-1.8669	-1.6463
8	C	2.6935	-0.1618	2.2342	24	H	2.4955	-1.1237	2.7179
9	S	-1.0149	-1.3879	-0.4980	25	H	3.6044	0.2555	2.6777
10	C	-2.4048	-0.3111	-0.2005	26	H	1.8753	0.5233	2.4780
11	C	-2.5121	0.9311	-0.8338	27	H	-1.7494	1.2662	-1.5318
12	C	-3.6139	1.7538	-0.5889	28	H	-3.6926	2.7180	-1.0847
13	C	-4.6171	1.3355	0.2838	29	H	-5.4761	1.9747	0.4721
14	C	-4.5229	0.0925	0.9074	30	H	-5.3084	-0.2388	1.5817
15	C	-3.4215	-0.7306	0.6625	31	H	-3.3650	-1.7001	1.1520
16	H	0.0921	-0.0051	1.1420					

9. Coordinate of the global minimum of **8**

No	Atom	X	Y	Z	No.	Atom	X	Y	Z
1	O	1.5069	-0.3014	-0.2529	34	H	-1.0203	-0.3525	-1.0278
2	C	1.0221	0.6241	0.7160	35	H	-2.8591	-0.7823	0.5324
3	C	-0.4813	0.3918	0.9371	36	H	-3.3739	-0.2606	-1.9698
4	C	-1.3276	0.4546	-0.3509	37	H	-3.9795	1.3120	-1.3913
5	C	-2.7888	0.2119	0.0747	38	H	-1.4236	2.6442	-0.4723
6	C	-3.7735	0.2757	-1.1025	39	H	-1.7646	1.8190	-2.0013
7	I	-5.6636	-0.6449	-0.5729	40	H	-0.1156	1.9220	-1.4233
8	O	-0.9498	1.3526	1.8836	41	H	-3.7710	2.5362	3.2060
9	C	-1.1510	1.7868	-1.0958	42	H	-2.5264	3.3924	2.2971
10	O	-3.1665	1.1998	1.0363	43	H	-2.1063	2.6530	3.8414
11	C	-2.3375	1.2315	2.1982	44	H	-3.6707	-0.0086	3.3961
12	C	-2.7094	2.5204	2.9366	45	H	-2.0123	0.1211	4.0451
13	C	-2.6095	0.0453	3.1299	46	H	-2.3531	-0.9135	2.6707
14	Si	3.1386	-0.3775	-0.5972	47	H	2.3174	-3.0899	-1.7504
15	C	3.4545	-1.2947	-2.3372	48	H	4.0636	-3.2409	-1.4925
16	C	3.2998	-2.8278	-2.1607	49	H	3.4029	-3.3445	-3.1224
17	C	2.4024	-0.8463	-3.3809	50	H	1.3814	-1.0483	-3.0361
18	C	4.8671	-1.0108	-2.8901	51	H	2.4694	0.2212	-3.6057
19	C	3.8660	1.3553	-0.5400	52	H	2.5396	-1.3821	-4.3278
20	C	3.7762	2.2302	-1.6382	53	H	5.0236	0.0540	-3.0895

21	C	4.2978	3.5270	-1.5809	54	H	5.0287	-1.5422	-3.8355
22	C	4.9097	3.9852	-0.4195	55	H	5.6486	-1.3383	-2.1966
23	C	4.9930	3.1502	0.6886	56	H	3.2920	1.9275	-2.5623
24	C	4.4719	1.8539	0.6318	57	H	4.2188	4.1808	-2.4459
25	C	3.9841	-1.4192	0.7325	58	H	5.3120	4.9934	-0.3750
26	C	3.2232	-2.2021	1.6216	59	H	5.4580	3.5065	1.6043
27	C	3.8413	-2.9854	2.5998	60	H	4.5422	1.2442	1.5323
28	C	5.2290	-3.0055	2.7056	61	H	2.1359	-2.2174	1.5610
29	C	6.0012	-2.2448	1.8324	62	H	3.2368	-3.5826	3.2775
30	C	5.3864	-1.4608	0.8528	63	H	5.7085	-3.6156	3.4662
31	H	1.1992	1.6594	0.3998	64	H	7.0852	-2.2608	1.9118
32	H	1.5395	0.4914	1.6761	65	H	6.0228	-0.8773	0.1886
33	H	-0.5806	-0.6131	1.3675					

10. Coordinate of the global minimum of **13**

No	Atom	X	Y	Z	No.	Atom	X	Y	Z
1	C	-2.5292	0.7586	-0.2127	21	H	-2.9774	1.6360	-0.6935
2	C	-1.0003	0.8543	-0.3527	22	H	-0.7753	0.8766	-1.4267
3	C	-0.1917	-0.2795	0.3148	23	H	-0.4174	-1.2338	-0.1757
4	C	1.2977	0.0441	0.0771	24	H	1.4815	0.0700	-1.0039
5	O	1.5934	1.3255	0.6358	25	H	-1.5722	-0.6929	1.9577
6	C	0.7916	2.3863	0.1185	26	H	0.0650	-1.2290	2.2663
7	O	-0.6074	2.1129	0.2094	27	H	-0.3241	0.4950	2.3651
8	C	-0.5216	-0.4266	1.8085	28	H	1.0499	1.9722	-2.0234
9	C	1.2071	2.7800	-1.3033	29	H	0.6209	3.6338	-1.6603
10	C	1.0408	3.5818	1.0423	30	H	2.2722	3.0326	-1.3443
11	C	2.2429	-0.9911	0.7058	31	H	0.7535	3.3349	2.0715
12	I	4.2309	-0.8309	-0.1442	32	H	2.1003	3.8595	1.0620
13	S	-3.2145	-0.7482	-0.9868	33	H	0.4463	4.4516	0.7423
14	C	-4.8985	-0.6591	-0.4054	34	H	1.8818	-2.0079	0.5184
15	C	-5.4395	-1.7569	0.2713	35	H	2.3323	-0.8411	1.7871
16	C	-6.7575	-1.7237	0.7324	36	H	-4.8391	-2.6463	0.4477
17	C	-7.5453	-0.5957	0.5114	37	H	-7.1688	-2.5797	1.2611

18	C	-7.0180	0.4966	-0.1751	38	H	-8.5718	-0.5704	0.8683
19	C	-5.6996	0.4637	-0.6361	39	H	-7.6348	1.3730	-0.3574
20	H	-2.8251	0.8104	0.8407	40	H	-5.3144	1.3184	-1.1855

11. Coordinate of the global minimum of **17**

No	Atom	X	Y	Z	No.	Atom	X	Y	Z
1	C	-1.6470	0.9861	0.1268	26	H	-1.9001	1.1691	1.1747
2	C	-0.1792	1.2718	-0.1781	27	H	-2.2724	1.6614	-0.4697
3	C	0.8533	0.4829	0.6516	28	H	-0.0164	1.0661	-1.2428
4	C	2.2459	0.9817	0.2140	29	H	0.7753	-0.5824	0.4095
5	O	2.3455	2.3917	0.4183	30	H	2.3705	0.7768	-0.8544
6	C	1.3325	3.1441	-0.2501	31	H	-0.3420	0.2671	2.4702
7	O	0.0139	2.6761	0.0446	32	H	1.3763	0.0789	2.7347
8	C	0.6364	0.6479	2.1637	33	H	0.7035	1.6951	2.4752
9	C	1.5844	3.2354	-1.7592	34	H	1.5412	2.2593	-2.2503
10	C	1.4103	4.5559	0.3380	35	H	0.8288	3.8623	-2.2451
11	C	3.4184	0.3060	0.9431	36	H	2.5789	3.6452	-1.9661
12	O	3.2952	-1.1085	0.9677	37	H	1.2336	4.5285	1.4201
13	S	-2.1210	-0.6700	-0.3010	38	H	2.3997	5.0004	0.1848
14	C	-3.8862	-0.6471	-0.0878	39	H	0.6492	5.2137	-0.0955
15	C	-4.7125	-0.3904	-1.1850	40	H	3.4751	0.6569	1.9797
16	C	-6.0962	-0.3797	-1.0108	41	H	4.3706	0.6066	0.4879
17	C	-6.6447	-0.6330	0.2478	42	H	-4.2937	-0.2054	-2.1718
18	C	-5.8137	-0.9046	1.3364	43	H	-6.7495	-0.1816	-1.8575
19	C	-4.4290	-0.9173	1.1716	44	H	-7.7246	-0.6287	0.3786
20	O	-1.5842	-1.5845	0.6894	45	H	-6.2481	-1.1142	2.3111
21	O	-1.8563	-0.8720	-1.7128	46	H	-3.7885	-1.1446	2.0210
22	S	3.8515	-1.9504	-0.3093	47	H	3.5944	-4.2812	-0.5365
23	O	5.2977	-1.9168	-0.2855	48	H	2.2154	-3.5366	0.3265
24	O	3.0950	-1.5627	-1.4805	49	H	3.7802	-3.7925	1.1745
25	C	3.3020	-3.5532	0.2229					