

**Adsorption and electron injection of the N3 metal-organic dye on the TiO₂
rutile (110) surface**

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Supporting Information

Table ST1 Interatomic distances in carboxylic and thiocyanate groups of the N3 molecule adsorbed on TiO₂

Number	Configuration	Structure		Distances, Ang												S...O _{2c} (TiO ₂)	S...Ti _{5c} (TiO ₂)	H(COOH _{ads}) -O(TiO ₂)
		starting	final	C-O (COOH1)		C-O (COOH2)		C-O (COOH1)		Ti-O (COOH1)		Ti-O (COOH2)		Ti-O (COOH3)				
				O1	O2	O1	O2	O1	O2	O1	O2	O1	O2	O1	O2			
1	1COOH-trans	1BB	1BB	1.23	1.33					1.98	2.01							
1	1COOH-cis	1BB	1BB	1.27	1.28					2.08	2.09							
2	2COOH-same-2rows	2BB	2BB	1.28	1.27	1.29	1.27			2.04	2.17	2.05	2.22					
3	2COOH-same-1row	2BB	2M+2Hbonds	1.31	1.24	1.31	1.23			1.92	3.35	1.92	3.38					
3	2COOH-same-1row	2BB	2M	1.32	1.23	1.32	1.23			1.91	3.27	1.92	3.29					
3	2COOH-same-1row	2MH	2MH	1.23	1.32	1.24	1.33			2.24		2.22					2.25, 2.41	
4	2COOH-same-2rows-S	2BB+S	2BB+S	1.28	1.26	1.27	1.27			2.03	2.26	2.08	2.12		4.32	4.37		
5	2COOH-same-1row-S	2BB+S	2M+S	1.33	1.24	1.32	1.24			2.02	3.14	1.95	3.27		3.08	2.73		
5	2COOH-same-1row-S	2MH+S	2MH+S	1.24	1.35	1.24	1.35			2.28		2.3			3.13	2.92	3.12, 3.22	
6	2COOH-diff(2trans)-2rows	2BB	1BB1M	1.34	1.23	1.30	1.26			1.99	3.49	1.97	2.46					
7	2COOH-diff(cis,trans)-2rows	2BB	2BB	1.30	1.25	1.29	1.26			2.00	2.45	1.98	2.33					
8	2COOH-diff(2trans)-1row	2BB	2BB	1.30	1.25	1.29	1.25			1.94	2.58	1.98	2.35					
8	2COOH-diff(2trans)-1row	1B1MH	1BB1M	1.28	1.26	1.24	1.33			2.03	2.17	2.21						
8	2COOH-diff(2trans)-1row	2MH	2MH	1.24	1.32	1.24	1.32			2.20		2.24						
9	2COOH-diff(cis,trans)-1row	2BB	1BB1M	1.28	1.25	1.31	1.23			2.01	2.33	1.91	3.03					
9	2COOH-diff(cis,trans)-1row	1B1MH	1BB1MH	1.28	1.26	1.23	1.34			2.05	2.16	2.22					2.90	
9	2COOH-diff(cis,trans)-1row	2MH	2MH	1.24	1.35	1.26	1.32			2.18		2.22					1.50, 3.07	
10	2COOH-diff(cis,trans)-2rows-S	2BB+S	1BB1M+S	1.28	1.27	1.31	1.22			2.05	2.20	1.92	3.38		3.36	2.87		
10	2COOH-diff(cis,trans)-2rows-S	1BB1MH+S	1BB1MH+S	1.27	1.27	1.23	1.33			2.08	2.14	2.25			3.43	3.05	2.66	
10	2COOH-diff(cis,trans)-2rows-S	2MH+S	2MH+S	1.24	1.35	1.24	1.35			2.26		2.29			3.56	2.73	2.57, 2.98	

	2rows-S																
11	2COOH-diff(cis,trans)- 1row-S	2BB+S	1BB1M+S	1.28	1.26	1.32	1.22			2.09	2.19	1.93	3.68		3.34	2.84	
11	2COOH-diff(cis,trans)- 1row-S	1BB1MH +S	1BB1MH+S	1.28	1.26	1.22	1.34			2.11	2.18	2.30			3.38	2.93	
11	2COOH-diff(cis,trans)- 1row-S	2MH+S	2MH+S	1.25	1.33	1.24	1.35			2.20		2.30			3.48	2.91	1.90, 2.88
12	3COOH	2BB1MH	2BB1MH	1.29	1.27	1.29	1.25	1.24	1.33	2.08	2.15	1.96	2.35	2.34			1.76
12	3COOH	3BB	3BB	1.29	1.27	1.30	1.25	1.30	1.25	2.13	2.11	1.96	2.40	1.97	2.47		

Table ST2 Coordinates of all adsorbed structures (see Table ST1 and Table 1 in the main text for labelling)

(1) 1COOH-trans

203

Ti	-0.423095	-7.663958	-0.073198
Ti	-3.678131	8.752204	-0.017130
Ti	-3.679126	-7.653240	-3.279279
Ti	-0.406474	8.748475	-3.279279
Ti	-0.404930	-4.667867	-0.056694
Ti	-3.672772	-6.161277	-0.009219
Ti	-3.679126	-4.671110	-3.279279
Ti	-0.406474	-6.162175	-3.279279
Ti	-0.404078	-1.686855	-0.032629
Ti	-3.671038	-3.187342	-0.010759
Ti	-3.679126	-1.688979	-3.279279
Ti	-0.406474	-3.180045	-3.279279
Ti	-0.404597	1.285658	-0.032017
Ti	-3.669225	-0.224121	-0.027263
Ti	-3.679126	1.293151	-3.279279
Ti	-0.406474	-0.197914	-3.279279
Ti	-0.404732	4.272920	-0.060599
Ti	-3.671091	2.814210	-0.019730
Ti	-3.679126	4.275281	-3.279279
Ti	-0.406474	2.784216	-3.279279
Ti	-0.402721	7.258042	-0.065637
Ti	-3.675239	5.774220	-0.009363
Ti	-3.679126	7.257412	-3.279279
Ti	-0.406474	5.766346	-3.279279
Ti	-6.949911	1.293229	-0.070364
Ti	2.871361	8.753624	-0.021896
Ti	2.866178	-7.653241	-3.279279
Ti	-6.951781	-0.197914	-3.279279
Ti	6.125460	-4.672717	-0.077609
Ti	2.867659	-6.164197	-0.009195
Ti	2.866178	-4.671111	-3.279279
Ti	-6.951781	2.784215	-3.279279
Ti	6.139478	-1.685044	-0.065354
Ti	2.867768	-3.179441	-0.008049
Ti	2.866178	-1.688981	-3.279279
Ti	6.138830	-3.180046	-3.279279
Ti	6.138259	1.293832	-0.066965
Ti	2.863836	-0.196099	-0.016643
Ti	2.866178	1.293150	-3.279279
Ti	6.138830	-0.197916	-3.279279
Ti	6.139380	4.273000	-0.066524
Ti	2.866935	2.786380	-0.011691
Ti	2.866178	4.275280	-3.279279
Ti	6.138830	2.784215	-3.279279
Ti	-6.951670	-1.692896	-0.069342
Ti	2.871462	5.767858	-0.012418
Ti	2.866178	7.257411	-3.279279
Ti	-6.951781	-3.180042	-3.279279

O	-3.681397	-7.658993	1.210231
O	-1.662114	8.744239	-0.014415
O	0.857289	8.756996	-0.032934
O	-3.675653	-7.650458	-1.316328
O	-0.406474	-7.653241	-2.009489
O	-4.948923	8.748473	-3.279279
O	-2.409337	8.748475	-3.279279
O	-0.406474	-7.653241	-4.549068
O	-3.680432	-4.670458	1.209306
O	-1.651857	-6.156625	-0.022838
O	0.845506	-6.168436	-0.006830
O	-3.679583	-4.672160	-1.314828
O	-0.406474	-4.671110	-2.009489
O	-4.948915	-6.162175	-3.279279
O	-2.409337	-6.162176	-3.279279
O	-0.406474	-4.671110	-4.549068
O	-3.678821	-1.678942	1.202982
O	-1.660882	-3.188185	-0.011653
O	0.853894	-3.189007	-0.008588
O	-3.678850	-1.693369	-1.316545
O	-0.406474	-1.688980	-2.009489
O	-4.948915	-3.180044	-3.279279
O	-2.409337	-3.180045	-3.279279
O	-0.406474	-1.688980	-4.549068
O	-3.678510	1.295014	1.255183
O	-1.683266	-0.205561	-0.042103
O	0.859730	-0.194716	-0.037344
O	-3.676203	1.297926	-1.298328
O	-0.406474	1.293150	-2.009489
O	-4.948915	-0.197913	-3.279279
O	-2.409337	-0.197914	-3.279279
O	-0.406474	1.293150	-4.549068
O	-3.677908	4.268565	1.210296
O	-1.669413	2.798790	-0.010198
O	0.850171	2.794431	-0.013469
O	-3.678870	4.279644	-1.311556
O	-0.406474	4.275281	-2.009489
O	-4.948915	2.784217	-3.279279
O	-2.409337	2.784216	-3.279279
O	-0.406474	4.275281	-4.549068
O	-3.681225	7.257671	1.208252
O	-1.656884	5.771624	-0.016346
O	0.852487	5.769384	-0.024582
O	-3.684322	7.254665	-1.313196
O	-0.406474	7.257412	-2.009489
O	-4.948915	5.766347	-3.279279
O	-2.409337	5.766347	-3.279279
O	-0.406474	7.257412	-4.549068
O	2.870029	-7.659887	1.207468
O	4.897552	8.751391	-0.029804
O	-5.689204	-0.202279	-0.021298
O	2.868170	-7.650141	-1.320707
O	-6.951781	1.293151	-2.009489
O	1.596389	8.748474	-3.279279
O	4.135976	8.748477	-3.279279

O	-6.951781	1.293151	-4.549068
O	2.869626	-4.676942	1.209417
O	4.892390	-6.166609	-0.030344
O	-5.685680	2.795423	-0.011180
O	2.864450	-4.672934	-1.316693
O	6.138830	-4.671112	-2.009489
O	1.596389	-6.162176	-3.279279
O	4.135967	-6.162177	-3.279279
O	6.138830	-4.671112	-4.549068
O	2.866965	-1.689664	1.205191
O	4.896311	-3.174912	-0.013636
O	7.393456	-3.181341	-0.022981
O	2.863918	-1.691029	-1.320130
O	6.138830	-1.688981	-2.009489
O	1.596389	-3.180046	-3.279279
O	4.135967	-3.180046	-3.279279
O	6.138830	-1.688981	-4.549068
O	2.866910	1.296964	1.203385
O	4.892149	-0.196950	-0.023982
O	7.395979	-0.196260	-0.026114
O	2.863519	1.296513	-1.321588
O	6.138830	1.293149	-2.009489
O	1.596389	-0.197915	-3.279279
O	4.135967	-0.197915	-3.279279
O	6.138830	1.293149	-4.549068
O	2.868659	4.281766	1.206675
O	4.891669	2.784956	-0.023964
O	7.396804	2.784244	-0.021709
O	2.864827	4.277925	-1.319392
O	6.138830	4.275279	-2.009489
O	1.596389	2.784216	-3.279279
O	4.135967	2.784215	-3.279279
O	6.138830	4.275279	-4.549068
O	2.872933	7.264922	1.201792
O	4.893528	5.767450	-0.024846
O	-5.693784	-3.181193	-0.021876
O	2.866817	7.256369	-1.319808
O	-6.951781	-1.688977	-2.009489
O	1.596389	5.766346	-3.279279
O	4.135967	5.766346	-3.279279
O	-6.951781	-1.688977	-4.549068
O	6.937569	-1.014427	9.444199
O	7.008386	1.223693	9.217192
O	3.417007	-6.077138	9.420596
O	1.343337	-6.936850	9.574885
O	-0.486982	1.007735	1.959654
O	-0.386978	-1.243039	1.898442
O	-0.466459	6.082461	5.498494
O	-0.749965	6.930468	7.567865
C	0.061221	0.467645	12.066345
C	-3.173866	-0.459847	8.868390
C	2.816353	1.305185	8.940517
C	4.189020	1.344351	9.046236
C	4.882508	0.148710	9.186556
C	4.166693	-1.037799	9.234494

C	2.779794	-1.005687	9.135090
C	6.367267	0.203248	9.283513
C	1.934295	-2.206786	9.235913
C	-0.236166	-3.029210	9.386299
C	0.218252	-4.329458	9.483892
C	1.586259	-4.569547	9.435832
C	2.452675	-3.493383	9.318671
C	2.069128	-5.977823	9.502732
C	-0.039211	-1.311899	6.090544
C	-0.152970	-1.353843	4.717393
C	-0.279319	-0.154003	4.018177
C	-0.328770	1.035260	4.736740
C	-0.218687	1.004398	6.124798
C	-0.393066	-0.186861	2.535789
C	-0.327560	2.204604	6.969764
C	-0.522362	3.020000	9.140909
C	-0.639719	4.319049	8.688438
C	-0.560884	4.565733	7.322457
C	-0.420647	3.492809	6.452581
C	-0.639008	5.973734	6.842669
H	2.246438	2.210061	8.854138
H	4.717808	2.280118	9.036415
H	4.689903	-1.965334	9.349780
H	-1.279701	-2.784908	9.414177
H	-0.471868	-5.144138	9.599150
H	3.509512	-3.666308	9.285336
H	0.041659	-2.219339	6.660175
H	-0.159425	-2.296075	4.188068
H	-0.468439	1.963544	4.207350
H	-0.565230	2.772030	10.181230
H	-0.794358	5.128193	9.377430
H	-0.382661	3.669947	5.391968
H	7.894839	-0.880766	9.436831
H	3.640801	-7.014434	9.369757
H	-3.660432	1.293317	2.256843
H	-0.509640	7.022048	5.272902
N	0.001657	0.386797	10.904216
N	-2.006760	-0.389393	8.906847
N	2.117076	0.164573	8.967034
N	0.595713	-1.990428	9.233569
N	-0.057384	-0.168481	6.792374
N	-0.341188	1.985636	8.309694
S	0.164670	0.595535	13.649319
S	-4.776257	-0.572864	8.791045
Ru	0.007050	-0.002426	8.894347

(1) 1COOH-cis

203

Ti	-3.298824	-7.460798	-0.196999
Ti	-0.003427	-5.998774	0.084667
Ti	0.000001	-7.455331	-3.279280
Ti	-3.272651	-5.964265	-3.279280
Ti	-3.263795	-4.484888	-0.196364

Ti	0.003361	-3.013580	0.084678
Ti	0.000001	-4.473201	-3.279280
Ti	-3.272651	-2.982134	-3.279280
Ti	-3.290860	-1.496116	-0.199625
Ti	0.005246	-0.035173	0.076931
Ti	0.000001	-1.491070	-3.279280
Ti	-3.272651	-0.000004	-3.279280
Ti	-3.262130	1.490987	-0.196012
Ti	0.009290	2.945603	0.046416
Ti	0.000001	1.491060	-3.279280
Ti	-3.272651	2.982126	-3.279280
Ti	-3.276337	4.472777	-0.196670
Ti	0.009937	5.929306	0.073289
Ti	0.000001	4.473190	-3.279280
Ti	-3.272651	5.964256	-3.279280
Ti	-3.257614	7.455280	-0.195717
Ti	0.004132	8.908689	0.086072
Ti	0.000001	7.455321	-3.279280
Ti	-3.272651	8.946387	-3.279280
Ti	3.256423	-7.456478	-0.196286
Ti	6.538872	-5.897315	0.102572
Ti	6.545306	-7.455332	-3.279280
Ti	3.272653	-5.964266	-3.279280
Ti	3.277627	-4.468794	-0.197433
Ti	6.545607	-2.954399	0.089189
Ti	6.545306	-4.473203	-3.279280
Ti	3.272653	-2.982136	-3.279280
Ti	3.266268	-1.484433	-0.207664
Ti	6.521443	-0.019784	0.078768
Ti	6.545306	-1.491072	-3.279280
Ti	3.272653	-0.000005	-3.279280
Ti	3.261836	1.503982	-0.100948
Ti	6.506101	2.918064	0.058419
Ti	6.545306	1.491059	-3.279280
Ti	3.272653	2.982125	-3.279280
Ti	3.246938	4.458390	-0.100407
Ti	6.537200	5.852714	0.001886
Ti	6.545306	4.473189	-3.279280
Ti	3.272653	5.964255	-3.279280
Ti	3.294524	7.443639	-0.211592
Ti	6.536787	9.057496	0.006304
Ti	6.545306	7.455320	-3.279280
Ti	3.272653	8.946385	-3.279280
O	-0.001177	-7.466509	1.135476
O	2.056016	-5.969770	0.117574
O	-2.056735	-5.970505	0.109130
O	0.002634	-7.444050	-1.421657
O	-3.272651	-7.455331	-2.009489
O	-1.269787	-5.964266	-3.279280
O	1.269790	-5.964266	-3.279280
O	-3.272651	-7.455331	-4.549070
O	-0.008680	-4.489963	1.133707
O	2.050053	-3.003965	0.114423
O	-2.067714	-2.987901	0.115959
O	-0.004610	-4.467382	-1.421815

O	-3.272651	-4.473200	-2.009489
O	-1.269787	-2.982135	-3.279280
O	1.269790	-2.982135	-3.279280
O	-3.272651	-4.473200	-4.549070
O	-0.008537	-1.510208	1.133754
O	2.036108	-0.047176	0.072310
O	-2.070476	-0.010531	0.126287
O	-0.012173	-1.492865	-1.419186
O	-3.272651	-1.491070	-2.009489
O	-1.269787	-0.000005	-3.279280
O	1.269790	-0.000005	-3.279280
O	-3.272651	-1.491070	-4.549070
O	0.017707	1.480249	1.113530
O	1.999811	2.975380	-0.123275
O	-2.060556	2.975851	0.113283
O	-0.045507	1.480575	-1.426616
O	-3.272651	1.491061	-2.009489
O	-1.269787	2.982126	-3.279280
O	1.269790	2.982125	-3.279280
O	-3.272651	1.491061	-4.549070
O	0.026192	4.454731	1.112757
O	2.050959	6.002558	0.068970
O	-2.054538	5.958837	0.118933
O	-0.038097	4.495522	-1.428188
O	-3.272651	4.473191	-2.009489
O	-1.269787	5.964256	-3.279280
O	1.269790	5.964256	-3.279280
O	-3.272651	4.473191	-4.549070
O	-0.000742	7.443229	1.134079
O	2.064490	-8.939004	0.119982
O	-2.053052	-8.949009	0.110106
O	-0.006329	7.472480	-1.419065
O	-3.272651	7.455322	-2.009489
O	-1.269787	8.946386	-3.279280
O	1.269790	8.946386	-3.279280
O	-3.272651	7.455322	-4.549070
O	6.551062	-7.460586	1.137615
O	-4.508367	2.981434	0.109366
O	4.510532	-5.964666	0.119492
O	6.545818	-7.468680	-1.404643
O	3.272653	-7.455332	-2.009489
O	5.275517	-5.964267	-3.279280
O	-5.275517	2.982126	-3.279280
O	3.272653	-7.455332	-4.549070
O	6.551452	-4.459971	1.165051
O	-4.503222	5.960265	0.108836
O	4.509272	-2.999780	0.114975
O	6.545996	-4.491541	-1.404559
O	3.272653	-4.473202	-2.009489
O	5.275517	-2.982136	-3.279280
O	-5.275517	5.964256	-3.279280
O	3.272653	-4.473202	-4.549070
O	6.550591	-1.492503	1.156261
O	-4.501945	-8.954970	0.116961
O	4.519021	-0.047870	0.066977

O	6.553203	-1.503545	-1.405912
O	3.272653	-1.491071	-2.009489
O	5.275517	-0.000006	-3.279280
O	-5.275526	8.946384	-3.279280
O	3.272653	-1.491071	-4.549070
O	6.520628	1.478782	1.142318
O	-4.504122	-5.969250	0.116925
O	4.559869	2.971321	-0.111579
O	6.587494	1.484634	-1.411617
O	3.272653	1.491059	-2.009489
O	5.275517	2.982124	-3.279280
O	-5.275517	-5.964263	-3.279280
O	3.272653	1.491059	-4.549070
O	6.522599	4.471416	1.121974
O	-4.517830	-2.985164	0.118546
O	4.538086	6.001775	0.060093
O	6.584729	4.497466	-1.409231
O	3.272653	4.473190	-2.009489
O	5.275517	5.964255	-3.279280
O	-5.275517	-2.982133	-3.279280
O	3.272653	4.473190	-4.549070
O	6.551032	7.458407	1.210418
O	-4.520293	0.000291	0.103759
O	4.524525	8.961481	0.109339
O	6.555956	7.465502	-1.410429
O	3.272653	7.455321	-2.009489
O	5.275525	8.946388	-3.279280
O	-5.275517	-0.000003	-3.279280
O	3.272653	7.455321	-4.549070
O	11.077239	3.083835	10.010848
O	11.187971	3.430945	7.779847
O	7.382937	2.752912	15.028061
O	5.274261	2.617319	15.835626
O	3.151584	-3.231643	5.835013
O	3.360484	-3.962923	7.964847
O	3.274926	1.850598	1.961448
O	3.280386	4.109824	1.936666
C	4.214808	6.264552	9.130043
C	0.957735	2.886537	9.235274
C	6.972164	3.166763	7.580671
C	8.355738	3.227864	7.575955
C	9.036102	3.192204	8.797996
C	8.292778	3.100094	9.975491
C	6.896971	3.044943	9.910996
C	10.528654	3.254872	8.783084
C	6.026588	2.940495	11.098004
C	3.814120	2.784722	11.851478
C	4.224350	2.729867	13.177903
C	5.593664	2.782601	13.466310
C	6.501901	2.895734	12.412391
C	6.032125	2.708968	14.891983
C	4.106022	-0.004998	9.227629
C	3.907777	-1.327400	8.866601
C	3.618582	-1.625199	7.531037
C	3.547677	-0.580591	6.609787

C	3.758748	0.732778	7.039766
C	3.369822	-3.051422	7.164316
C	3.668066	1.908535	6.153458
C	3.634576	4.248670	6.079447
C	3.445735	4.242134	4.705611
C	3.407106	3.018278	4.030018
C	3.498573	1.838521	4.768546
C	3.306626	2.985027	2.539363
H	6.411184	3.196704	6.654106
H	8.909045	3.291106	6.644622
H	8.806740	3.077189	10.928866
H	2.769305	2.765759	11.560678
H	3.501894	2.641213	13.981704
H	7.561703	2.954677	12.623944
H	4.317405	0.267419	10.254329
H	3.975519	-2.123894	9.597595
H	3.310700	-0.792876	5.575102
H	3.684688	5.166017	6.655274
H	3.353693	5.173794	4.162867
H	3.461543	0.887710	4.251412
H	12.042911	3.123379	9.910540
H	7.584662	2.724073	15.976302
H	2.998072	-4.185043	5.702777
H	6.534634	7.464416	2.170447
N	4.197401	5.086172	9.025672
N	2.137218	2.981256	9.200265
N	6.244159	3.074600	8.712400
N	4.691978	2.870498	10.831014
N	4.032963	1.012534	8.346944
N	3.775913	3.110993	6.787425
S	4.260391	7.889021	9.228871
S	-0.659191	2.741117	9.313254
Ru	4.158462	3.039792	8.824843

(2) 2COOH-same-2rows

203

Ti	-4.539915	10.428263	-0.195765
Ti	-1.253023	-5.854629	0.027390
Ti	-1.269788	-7.455331	-3.279280
Ti	-4.542442	-5.964265	-3.279280
Ti	-4.534096	-4.474863	-0.200419
Ti	-1.251106	-2.925693	0.030108
Ti	-1.269788	-4.473200	-3.279280
Ti	-4.542442	-2.982135	-3.279280
Ti	-4.533354	-1.508295	-0.104486
Ti	-1.269753	0.048258	0.019166
Ti	-1.269788	-1.491070	-3.279280
Ti	-4.542442	-0.000005	-3.279280
Ti	-4.571549	1.443001	-0.098981
Ti	-1.272022	2.979953	0.082128
Ti	-1.269788	1.491060	-3.279280
Ti	-4.542442	2.982126	-3.279280
Ti	-4.525424	4.439684	-0.199530

Ti	-1.263483	5.909066	0.124476
Ti	-1.269788	4.473190	-3.279280
Ti	-4.542442	5.964256	-3.279280
Ti	-4.534529	7.432508	-0.189429
Ti	-1.257245	8.842715	-0.001552
Ti	-1.269788	7.455321	-3.279280
Ti	-4.542445	8.946388	-3.279280
Ti	1.985948	-7.446065	-0.201825
Ti	5.286106	-5.989251	0.079495
Ti	5.275522	10.437447	-3.279280
Ti	2.002865	-5.964265	-3.279280
Ti	2.043903	-4.452672	-0.091384
Ti	5.286511	-3.056749	0.074560
Ti	5.275518	-4.473201	-3.279280
Ti	2.002865	-2.982135	-3.279280
Ti	2.011719	-1.506323	-0.100195
Ti	5.288612	-0.111183	-0.006995
Ti	5.275518	-1.491071	-3.279280
Ti	2.002865	-0.000005	-3.279280
Ti	2.012536	1.475219	-0.207075
Ti	5.282434	3.087910	0.019589
Ti	5.275518	1.491060	-3.279280
Ti	2.002865	2.982125	-3.279280
Ti	2.004097	4.465385	-0.188801
Ti	5.282960	6.026794	0.096047
Ti	5.275518	4.473190	-3.279280
Ti	2.002865	5.964256	-3.279280
Ti	2.025903	7.455952	-0.190685
Ti	5.290175	8.968361	0.054712
Ti	5.275522	7.455320	-3.279280
Ti	2.002865	8.946387	-3.279280
O	-1.228615	-7.464824	1.233950
O	0.744095	-6.006964	0.078642
O	-3.302934	-5.991191	0.170011
O	-1.281548	-7.472130	-1.402854
O	-4.542445	10.437450	-2.009489
O	-2.539577	-5.964265	-3.279280
O	0.000001	-5.964265	-3.279280
O	-4.542445	10.437450	-4.549070
O	-1.240936	-4.457082	1.128692
O	0.738689	-2.975289	-0.073750
O	-3.293011	-3.027648	0.063266
O	-1.300761	-4.512382	-1.401103
O	-4.542442	-4.473200	-2.009489
O	-2.539577	-2.982135	-3.279280
O	0.000001	-2.982135	-3.279280
O	-4.542442	-4.473200	-4.549070
O	-1.268839	-1.473842	1.105158
O	0.778371	0.045716	0.070114
O	-3.270193	0.015381	-0.070300
O	-1.272253	-1.502238	-1.425593
O	-4.542442	-1.491070	-2.009489
O	-2.539577	-0.000005	-3.279280
O	0.000001	-0.000005	-3.279280
O	-4.542442	-1.491070	-4.549070

O	-1.282729	1.485810	1.134386
O	0.788792	3.001302	0.133867
O	-3.291284	3.016205	0.080098
O	-1.231960	1.513996	-1.410628
O	-4.542442	1.491060	-2.009489
O	-2.539577	2.982126	-3.279280
O	0.000001	2.982126	-3.279280
O	-4.542442	1.491060	-4.549070
O	-1.260896	4.459908	1.185320
O	0.782259	5.958593	0.133955
O	-3.299049	5.981198	0.141313
O	-1.263435	4.493530	-1.391500
O	-4.542442	4.473191	-2.009489
O	-2.539577	5.964256	-3.279280
O	0.000001	5.964255	-3.279280
O	-4.542442	4.473191	-4.549070
O	-1.254264	7.465496	1.147611
O	0.753103	8.927193	0.089039
O	-3.304734	8.947359	0.165465
O	-1.285011	7.467757	-1.395741
O	-4.542445	7.455322	-2.009489
O	-2.539577	8.946387	-3.279280
O	0.000001	8.946385	-3.279280
O	-4.542445	7.455322	-4.549070
O	5.309842	10.429780	1.142689
O	-5.780380	3.027714	0.085435
O	3.233524	-5.994603	0.092571
O	5.231026	10.448715	-1.407692
O	2.002865	-7.455331	-2.009489
O	4.005729	-5.964265	-3.279280
O	6.545309	-5.964265	-3.279280
O	2.002865	-7.455331	-4.549070
O	5.251366	-4.483834	1.160741
O	-5.760166	5.981158	0.134540
O	3.293265	-2.997381	-0.106852
O	5.315397	-4.467276	-1.406203
O	2.002865	-4.473200	-2.009489
O	4.005729	-2.982135	-3.279280
O	6.545308	-2.982135	-3.279280
O	2.002865	-4.473200	-4.549070
O	5.250946	-1.493075	1.118236
O	-5.770906	8.948135	0.120766
O	3.279507	0.062179	0.084543
O	5.317814	-1.462426	-1.410399
O	2.002865	-1.491070	-2.009489
O	4.005729	-0.000005	-3.279280
O	6.545308	-0.000005	-3.279280
O	2.002865	-1.491070	-4.549070
O	5.326690	1.484354	1.240377
O	-5.776933	-5.989336	0.107044
O	3.255745	2.988378	0.169016
O	5.294046	1.502018	-1.413836
O	2.002865	1.491060	-2.009489
O	4.005729	2.982125	-3.279280
O	6.545308	2.982125	-3.279280

O	2.002865	1.491060	-4.549070
O	5.291942	4.470919	1.143913
O	-5.780382	-3.036902	0.067195
O	3.236716	5.963621	0.149186
O	5.255367	4.447255	-1.396706
O	2.002865	4.473190	-2.009489
O	4.005729	5.964255	-3.279280
O	6.545309	5.964256	-3.279280
O	2.002865	4.473190	-4.549070
O	5.311022	7.473547	1.151660
O	-5.834553	0.002302	-0.141917
O	3.215230	8.936289	0.152245
O	5.229921	7.423689	-1.406550
O	2.002865	7.455320	-2.009489
O	4.005732	8.946385	-3.279280
O	6.545309	8.946387	-3.279280
O	2.002865	7.455320	-4.549070
O	2.201805	5.002091	8.968757
O	0.841372	5.775119	7.332441
O	4.423200	0.056623	11.904692
O	4.242035	-2.163324	12.322156
O	2.047397	-1.788480	1.932740
O	1.986308	-4.051334	2.086490
O	-4.587079	-1.165439	1.905383
O	-4.602900	1.097089	2.043411
C	-3.187837	-0.049599	10.179367
C	-2.201698	-4.059746	8.074304
C	-0.905201	1.923777	7.077987
C	-0.399116	3.209968	7.132652
C	0.674730	3.477464	7.989059
C	1.179163	2.440623	8.769784
C	0.621714	1.165767	8.670643
C	1.222614	4.860201	8.039897
C	1.074845	0.017166	9.462687
C	0.687217	-2.224423	10.006952
C	1.801711	-2.258067	10.827891
C	2.583330	-1.107644	10.957812
C	2.192670	0.050174	10.292858
C	3.816071	-1.158891	11.790032
C	1.240544	-2.335716	6.333676
C	1.904184	-2.807541	5.199976
C	1.292930	-2.644147	3.953100
C	0.021425	-2.072116	3.923263
C	-0.602357	-1.667017	5.098846
C	1.861303	-2.888756	2.570771
C	-1.949733	-1.085487	5.092083
C	-3.709893	-0.187135	6.320670
C	-4.436619	0.105027	5.165318
C	-3.889166	-0.242486	3.926529
C	-2.644459	-0.870736	3.907422
C	-4.458088	-0.059898	2.543146
H	-1.723740	1.679834	6.410919
H	-0.825395	4.004600	6.528200
H	1.973500	2.644906	9.476354
H	0.044726	-3.081798	9.857329

H	2.067015	-3.156371	11.368295
H	2.771171	0.956534	10.403461
H	1.710171	-2.396206	7.307848
H	2.884326	-3.263731	5.298787
H	-0.462937	-1.922914	2.965486
H	-4.087900	0.039929	7.309771
H	-5.412825	0.575132	5.241913
H	-2.225536	-1.178809	2.956021
H	2.527229	5.919617	8.914020
H	5.176763	-0.058555	12.517137
H	-1.703772	-7.485608	2.081568
H	4.715457	1.429625	1.996777
N	-2.512424	-0.376210	9.266973
N	-1.776546	-2.959862	8.145288
N	-0.409726	0.906784	7.814604
N	0.346427	-1.125884	9.303740
N	0.024073	-1.755554	6.302550
N	-2.480046	-0.741832	6.295361
S	-4.137652	0.418530	11.400822
S	-2.756373	-5.585638	7.989175
Ru	-1.166496	-1.025887	7.898403

(3) 3CG.2COOH-same-tmp 2M+2Hbond

203

Ti	-0.389834	-6.141567	-0.198758
Ti	-3.659107	-7.592158	0.094229
Ti	-3.679127	-6.163242	-3.279279
Ti	-0.406474	-7.654306	-3.279279
Ti	-0.415797	-3.166128	-0.022730
Ti	-3.663212	-4.651490	0.071561
Ti	-3.679127	-3.181111	-3.279279
Ti	-0.406474	-4.672175	-3.279279
Ti	-0.405561	-0.195392	-0.237953
Ti	-3.663832	-1.704315	0.072132
Ti	-3.679127	-0.198981	-3.279279
Ti	-0.406474	-1.690045	-3.279279
Ti	-0.406349	2.773774	-0.021369
Ti	-3.659427	1.232144	0.079958
Ti	-3.679127	2.783150	-3.279279
Ti	-0.406474	1.292086	-3.279279
Ti	-0.434011	5.742887	-0.202044
Ti	-3.672817	4.174518	-0.017338
Ti	-3.679127	5.765281	-3.279279
Ti	-0.406474	4.274216	-3.279279
Ti	-0.404274	8.746714	-0.194993
Ti	-3.671538	7.356914	0.028504
Ti	-3.679130	-9.145368	-3.279279
Ti	-0.406474	7.256347	-3.279279
Ti	-6.971139	2.779888	-0.195367
Ti	2.854495	-7.759345	0.027432
Ti	2.866178	-6.163241	-3.279279
Ti	-6.951782	1.292083	-3.279279
Ti	6.151783	-3.180313	-0.195194

Ti	2.845211	-4.570239	-0.022500
Ti	2.866178	-3.181110	-3.279279
Ti	6.138831	-4.672175	-3.279279
Ti	6.132934	-0.194475	-0.192913
Ti	2.840108	-1.630561	0.085179
Ti	2.866178	-0.198980	-3.279279
Ti	6.138831	-1.690044	-3.279279
Ti	6.146966	2.786562	-0.194989
Ti	2.850856	1.307884	0.072568
Ti	2.866178	2.783151	-3.279279
Ti	6.138831	1.292087	-3.279279
Ti	-6.961363	-3.182287	-0.194409
Ti	2.845647	4.254585	0.073036
Ti	2.866178	5.765282	-3.279279
Ti	6.138831	4.274217	-3.279279
Ti	-6.944380	-0.204614	-0.192505
Ti	2.842986	7.192672	0.092518
Ti	2.866178	8.747412	-3.279279
Ti	-6.951782	-1.690045	-3.279279
O	-3.678339	-6.147447	1.148667
O	-1.629891	-7.665692	0.108023
O	0.843313	-7.670265	0.111063
O	-3.692582	-6.187352	-1.409896
O	-0.406474	-6.163241	-2.009489
O	-4.948920	-7.654305	-3.279279
O	-2.409337	-7.654306	-3.279279
O	-0.406474	-6.163241	-4.549068
O	-3.659459	-3.183759	1.132008
O	-1.646723	-4.722400	0.025225
O	0.883139	-4.721417	-0.031604
O	-3.704176	-3.185684	-1.413272
O	-0.406474	-3.181111	-2.009489
O	-4.948916	-4.672176	-3.279279
O	-2.409337	-4.672175	-3.279279
O	-0.406474	-3.181111	-4.549068
O	-3.683613	-0.214272	1.146623
O	-1.657497	-1.657161	0.030474
O	0.860761	-1.642840	0.010500
O	-3.716018	-0.191906	-1.411332
O	-0.406474	-0.198980	-2.009489
O	-4.948916	-1.690046	-3.279279
O	-2.409337	-1.690045	-3.279279
O	-0.406474	-0.198980	-4.549068
O	-3.657312	2.789665	1.108447
O	-1.673974	1.244980	0.008380
O	0.844686	1.264599	0.036951
O	-3.722980	2.792518	-1.414362
O	-0.406474	2.783151	-2.009489
O	-4.948916	1.292085	-3.279279
O	-2.409337	1.292085	-3.279279
O	-0.406474	2.783151	-4.549068
O	-3.648119	5.752936	1.226038
O	-1.696872	4.320735	-0.045060
O	0.831193	4.326607	0.036433
O	-3.715870	5.777892	-1.418192

O	-0.406474	5.765281	-2.009489
O	-4.948916	4.274216	-3.279279
O	-2.409337	4.274216	-3.279279
O	-0.406474	5.765281	-4.549068
O	-3.681408	-9.145116	1.134884
O	-1.653738	7.272901	0.110137
O	0.818782	7.266051	0.108501
O	-3.677079	-9.166124	-1.402936
O	-0.406474	8.747411	-2.009489
O	8.141697	-1.690042	-3.279279
O	-2.409337	7.256347	-3.279279
O	-0.406474	8.747411	-4.549068
O	2.852185	-6.154842	1.216885
O	-8.198087	1.296651	0.104228
O	-5.742271	1.290984	0.121935
O	2.901552	-6.174792	-1.416870
O	-6.951782	2.783148	-2.009489
O	1.596389	-7.654306	-3.279279
O	4.135968	-7.654305	-3.279279
O	-6.951782	2.783148	-4.549068
O	2.845227	-3.185401	1.115205
O	4.908761	-4.675517	0.108387
O	-5.721278	4.279401	0.109705
O	2.908336	-3.188539	-1.412452
O	6.138831	-3.181109	-2.009489
O	1.596389	-4.672175	-3.279279
O	4.135968	-4.672175	-3.279279
O	6.138831	-3.181109	-4.549068
O	2.870110	-0.184293	1.153214
O	4.931080	-1.687308	0.126942
O	7.387046	-1.697291	0.109306
O	2.902438	-0.204420	-1.410235
O	6.138831	-0.198979	-2.009489
O	1.596389	-1.690045	-3.279279
O	4.135968	-1.690045	-3.279279
O	6.138831	-0.198979	-4.549068
O	2.849580	2.785611	1.135059
O	4.920401	1.292109	0.113023
O	7.371282	1.291198	0.111788
O	2.889016	2.787179	-1.411909
O	6.138831	2.783152	-2.009489
O	1.596389	1.292086	-3.279279
O	4.135968	1.292086	-3.279279
O	6.138831	2.783152	-4.549068
O	2.867529	5.749530	1.150369
O	4.911922	4.270952	0.107536
O	-5.725844	-4.671382	0.108088
O	2.878343	5.786805	-1.408995
O	-6.951782	-3.181110	-2.009489
O	1.596389	4.274216	-3.279279
O	4.135968	4.274217	-3.279279
O	-6.951782	-3.181110	-4.549068
O	2.868061	8.743848	1.133422
O	-8.184573	-1.690821	0.108231
O	-5.732951	-1.691762	0.109048

O	2.866361	8.766385	-1.404532
O	-6.951782	-0.198980	-2.009489
O	1.596389	7.256347	-3.279279
O	4.135968	7.256347	-3.279279
O	-6.951782	-0.198980	-4.549068
O	6.225107	-1.290004	9.950301
O	6.657148	0.172190	8.277955
O	1.952219	-4.347177	13.224560
O	-0.237553	-4.819985	13.548185
O	-0.330321	-3.182013	1.892351
O	0.162091	-5.111601	2.937728
O	-0.519663	2.792219	1.897441
O	-1.175828	4.686313	2.921528
C	-0.638324	2.257276	10.259170
C	-3.649615	-0.484732	7.794603
C	2.483404	0.589992	7.666009
C	3.857139	0.527364	7.837748
C	4.377680	-0.349886	8.795763
C	3.491766	-1.114244	9.555142
C	2.116285	-0.999617	9.336328
C	5.859588	-0.439613	8.959415
C	1.103056	-1.761056	10.091582
C	-1.185121	-2.191087	10.342570
C	-0.948213	-3.064401	11.396351
C	0.371220	-3.293914	11.802304
C	1.405750	-2.629181	11.142755
C	0.628960	-4.230906	12.938520
C	-0.144961	-2.858805	6.616034
C	-0.066301	-3.676780	5.495748
C	-0.162217	-3.093226	4.229070
C	-0.340284	-1.709960	4.158592
C	-0.401381	-0.939472	5.317680
C	-0.093619	-3.904171	2.960928
C	-0.567562	0.529217	5.310009
C	-0.771637	2.458118	6.614964
C	-0.881526	3.268584	5.487795
C	-0.812098	2.679490	4.222362
C	-0.664376	1.292398	4.147116
C	-0.860747	3.492421	2.952918
H	2.039882	1.262227	6.941879
H	4.520371	1.146563	7.244435
H	3.875745	-1.793706	10.304158
H	-2.184014	-1.960393	9.989608
H	-1.771869	-3.556360	11.900670
H	2.429245	-2.789564	11.455268
H	-0.096660	-3.280337	7.613065
H	0.060172	-4.747632	5.604721
H	-0.411277	-1.242108	3.188435
H	-0.811571	2.863967	7.619279
H	-1.012293	4.339397	5.595688
H	-0.634871	0.820395	3.176135
H	7.194822	-1.301219	9.997115
H	2.047778	-4.905763	14.016383
H	2.305258	-6.091842	2.017382
H	-3.059547	5.648080	1.995470

N	-0.599726	1.319743	9.538159
N	-2.501282	-0.412537	8.072287
N	1.620752	-0.161881	8.379586
N	-0.184681	-1.564029	9.691695
N	-0.303714	-1.520384	6.548405
N	-0.593872	1.123189	6.534760
S	-0.678895	3.561864	11.229714
S	-5.231128	-0.606475	7.430082
Ru	-0.452117	-0.189023	8.151893

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203

Ti	-0.400519	-6.154862	-0.187558
Ti	-3.666301	-7.674027	0.083606
Ti	-3.679127	-6.163242	-3.279279
Ti	-0.406474	-7.654306	-3.279279
Ti	-0.412674	-3.192544	-0.023712
Ti	-3.668789	-4.735101	0.088065
Ti	-3.679127	-3.181111	-3.279279
Ti	-0.406474	-4.672175	-3.279279
Ti	-0.406475	-0.198409	-0.243080
Ti	-3.651771	-1.794034	-0.007640
Ti	-3.679127	-0.198981	-3.279279
Ti	-0.406474	-1.690045	-3.279279
Ti	-0.405568	2.796089	-0.023809
Ti	-3.647105	1.396913	-0.009848
Ti	-3.679127	2.783150	-3.279279
Ti	-0.406474	1.292086	-3.279279
Ti	-0.406391	5.757359	-0.187082
Ti	-3.666587	4.338770	0.089063
Ti	-3.679127	5.765281	-3.279279
Ti	-0.406474	4.274216	-3.279279
Ti	-0.405919	8.747349	-0.196364
Ti	-3.669414	7.279945	0.087591
Ti	-3.679133	-9.145367	-3.279279
Ti	-0.406474	7.256347	-3.279279
Ti	-6.956748	2.782038	-0.193896
Ti	2.860380	-7.674387	0.084190
Ti	2.866178	-6.163241	-3.279279
Ti	-6.951782	1.292083	-3.279279
Ti	6.143740	-3.179764	-0.194470
Ti	2.853614	-4.735446	0.090337
Ti	2.866178	-3.181110	-3.279279
Ti	6.138831	-4.672175	-3.279279
Ti	6.109831	-0.199443	-0.196839
Ti	2.835617	-1.794427	-0.015728
Ti	2.866178	-0.198980	-3.279279
Ti	6.138831	-1.690044	-3.279279
Ti	6.146594	2.781960	-0.194369
Ti	2.839979	1.398556	-0.015482
Ti	2.866178	2.783151	-3.279279
Ti	6.138831	1.292087	-3.279279
Ti	-6.960640	-3.178647	-0.193913

Ti	2.854417	4.339647	0.088879
Ti	2.866178	5.765282	-3.279279
Ti	6.138831	4.274217	-3.279279
Ti	-6.919741	-0.198305	-0.196153
Ti	2.856552	7.280430	0.086306
Ti	2.866178	8.747412	-3.279279
Ti	-6.951782	-1.690045	-3.279279
O	-3.689867	-6.180100	1.150209
O	-1.643425	-7.669709	0.098565
O	0.832492	-7.670173	0.095276
O	-3.702366	-6.161345	-1.409456
O	-0.406474	-6.163241	-2.009489
O	-4.948923	-7.654304	-3.279279
O	-2.409337	-7.654306	-3.279279
O	-0.406474	-6.163241	-4.549068
O	-3.654014	-3.179732	1.115869
O	-1.664132	-4.719945	0.008229
O	0.855101	-4.717282	-0.000238
O	-3.706075	-3.167584	-1.410109
O	-0.406474	-3.181111	-2.009489
O	-4.948916	-4.672176	-3.279279
O	-2.409337	-4.672175	-3.279279
O	-0.406474	-3.181111	-4.549068
O	-3.707571	-0.198969	1.202803
O	-1.671741	-1.648158	0.022702
O	0.863813	-1.640083	0.025935
O	-3.716326	-0.199086	-1.413113
O	-0.406474	-0.198980	-2.009489
O	-4.948916	-1.690046	-3.279279
O	-2.409337	-1.690045	-3.279279
O	-0.406474	-0.198980	-4.549068
O	-3.655385	2.784585	1.117379
O	-1.672561	1.249134	0.022355
O	0.863618	1.245403	0.026820
O	-3.706785	2.770261	-1.410406
O	-0.406474	2.783151	-2.009489
O	-4.948916	1.292085	-3.279279
O	-2.409337	1.292085	-3.279279
O	-0.406474	2.783151	-4.549068
O	-3.688963	5.784263	1.155703
O	-1.666254	4.322396	0.002314
O	0.853698	4.320339	0.000654
O	-3.704820	5.763168	-1.410019
O	-0.406474	5.765281	-2.009489
O	-4.948916	4.274216	-3.279279
O	-2.409337	4.274216	-3.279279
O	-0.406474	5.765281	-4.549068
O	-3.693578	-9.145617	1.151083
O	-1.644053	7.272953	0.096964
O	0.831300	7.272812	0.098204
O	-3.689855	-9.144578	-1.409126
O	-0.406474	8.747411	-2.009489
O	8.141697	-1.690042	-3.279279
O	-2.409337	7.256347	-3.279279
O	-0.406474	8.747411	-4.549068

O	2.875528	-6.180415	1.151566
O	-8.162736	1.286846	0.113182
O	-5.709210	1.298307	0.100678
O	2.891363	-6.161252	-1.409883
O	-6.951782	2.783148	-2.009489
O	1.596389	-7.654306	-3.279279
O	4.135968	-7.654305	-3.279279
O	-6.951782	2.783148	-4.549068
O	2.839879	-3.178825	1.121921
O	4.912781	-4.674452	0.115428
O	-5.727563	4.278791	0.114758
O	2.893783	-3.167273	-1.409484
O	6.138831	-3.181109	-2.009489
O	1.596389	-4.672175	-3.279279
O	4.135968	-4.672175	-3.279279
O	6.138831	-3.181109	-4.549068
O	2.898899	-0.199374	1.212962
O	4.893760	-1.692921	0.103858
O	7.347298	-1.684633	0.117336
O	2.907178	-0.198791	-1.414305
O	6.138831	-0.198979	-2.009489
O	1.596389	-1.690045	-3.279279
O	4.135968	-1.690045	-3.279279
O	6.138831	-0.198979	-4.549068
O	2.839125	2.781650	1.116568
O	4.893915	1.297232	0.103599
O	7.348187	1.287356	0.116958
O	2.894460	2.769457	-1.410354
O	6.138831	2.783152	-2.009489
O	1.596389	1.292086	-3.279279
O	4.135968	1.292086	-3.279279
O	6.138831	2.783152	-4.549068
O	2.877347	5.782698	1.150844
O	4.913343	4.275971	0.115433
O	-5.726218	-4.675552	0.113400
O	2.889805	5.762153	-1.410293
O	-6.951782	-3.181110	-2.009489
O	1.596389	4.274216	-3.279279
O	4.135968	4.274217	-3.279279
O	-6.951782	-3.181110	-4.549068
O	2.880237	8.748649	1.148367
O	-8.162860	-1.684630	0.113968
O	-5.709434	-1.697437	0.100580
O	2.876193	8.746284	-1.409727
O	-6.951782	-0.198980	-2.009489
O	1.596389	7.256347	-3.279279
O	4.135968	7.256347	-3.279279
O	-6.951782	-0.198980	-4.549068
O	6.052976	-1.955920	10.518225
O	6.754998	-0.469403	8.963639
O	1.169979	-4.467451	13.474542
O	-1.076784	-4.684828	13.598711
O	-0.391307	-3.135889	1.891421
O	-0.307146	-5.129482	2.935314
O	-0.404647	2.747266	1.889309

O	-0.359705	4.746995	2.921581
C	-0.511994	2.245606	10.287189
C	-3.411652	-0.272965	7.303294
C	2.720117	0.325164	7.971331
C	4.059214	0.129985	8.270065
C	4.403202	-0.803771	9.254586
C	3.381755	-1.485735	9.915910
C	2.049007	-1.230349	9.578596
C	5.850951	-1.036147	9.542818
C	0.899676	-1.886187	10.230327
C	-1.433961	-2.093597	10.251026
C	-1.388834	-2.964706	11.331231
C	-0.144666	-3.304196	11.875196
C	1.010843	-2.757554	11.315846
C	-0.098304	-4.218351	13.056597
C	-0.154713	-2.867327	6.618628
C	-0.189771	-3.686656	5.495110
C	-0.250781	-3.092027	4.232283
C	-0.250489	-1.696779	4.167673
C	-0.211864	-0.926512	5.329329
C	-0.317991	-3.903758	2.959969
C	-0.230891	0.552416	5.325249
C	-0.217195	2.495058	6.624345
C	-0.258468	3.312212	5.496094
C	-0.292843	2.715917	4.233010
C	-0.277096	1.320354	4.163125
C	-0.355306	3.522217	2.955724
H	2.417232	1.043657	7.218334
H	4.833844	0.686420	7.754853
H	3.629465	-2.213917	10.678902
H	-2.363632	-1.763870	9.800467
H	-2.299000	-3.369618	11.760014
H	1.976500	-3.006710	11.734669
H	-0.129730	-3.296001	7.613703
H	-0.186635	-4.766367	5.595530
H	-0.288532	-1.223298	3.196389
H	-0.214238	2.905614	7.627714
H	-0.282385	4.391123	5.598407
H	-0.305968	0.849262	3.190530
H	7.013757	-2.052347	10.642206
H	1.115570	-5.012031	14.278614
H	2.469301	-0.200023	2.077138
H	-3.479564	-0.198936	2.138352
N	-0.462685	1.325287	9.545563
N	-2.349672	-0.228543	7.825014
N	1.726445	-0.345543	8.589418
N	-0.317304	-1.574631	9.701619
N	-0.170242	-1.519663	6.556363
N	-0.195353	1.148278	6.548054
S	-0.565087	3.521829	11.293676
S	-4.875866	-0.349191	6.589123
Ru	-0.302959	-0.181225	8.159456

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203

Ti	-0.427537	-6.170722	-0.219216
Ti	-3.685252	-7.658241	0.084079
Ti	-3.679128	-6.163241	-3.279279
Ti	-0.406474	-7.654306	-3.279279
Ti	-0.399691	-3.181560	-0.107426
Ti	-3.681266	-4.678355	0.077269
Ti	-3.679128	-3.181111	-3.279279
Ti	-0.406474	-4.672175	-3.279279
Ti	-0.406898	-0.198328	-0.222377
Ti	-3.674777	-1.699962	0.078907
Ti	-3.679128	-0.198980	-3.279279
Ti	-0.406474	-1.690045	-3.279279
Ti	-0.435844	2.789977	-0.115307
Ti	-3.680823	1.276129	0.074382
Ti	-3.679128	2.783150	-3.279279
Ti	-0.406474	1.292086	-3.279279
Ti	-0.384417	5.768524	-0.218804
Ti	-3.703639	4.265555	0.042506
Ti	-3.679128	5.765281	-3.279279
Ti	-0.406474	4.274216	-3.279279
Ti	-0.419164	8.741738	-0.192887
Ti	-3.676111	7.252135	0.092931
Ti	-3.679131	-9.145367	-3.279279
Ti	-0.406474	7.256347	-3.279279
Ti	-6.958424	2.775899	-0.197077
Ti	2.850219	-7.649788	0.086310
Ti	2.866179	-6.163241	-3.279279
Ti	-6.951784	1.292083	-3.279279
Ti	6.139189	-3.176073	-0.197319
Ti	2.882785	-4.662093	0.053630
Ti	2.866179	-3.181110	-3.279279
Ti	6.138833	-4.672175	-3.279279
Ti	6.133117	-0.195544	-0.196223
Ti	2.859886	-1.671037	0.070724
Ti	2.866179	-0.198980	-3.279279
Ti	6.138833	-1.690044	-3.279279
Ti	6.133005	2.783160	-0.196773
Ti	2.846124	1.306744	0.077785
Ti	2.866179	2.783151	-3.279279
Ti	6.138833	1.292086	-3.279279
Ti	-6.949417	-3.180900	-0.196318
Ti	2.863620	4.285484	0.076875
Ti	2.866179	5.765281	-3.279279
Ti	6.138833	4.274216	-3.279279
Ti	-6.953134	-0.201073	-0.195746
Ti	2.865185	7.266922	0.084338
Ti	2.866179	8.747411	-3.279279
Ti	-6.951784	-1.690044	-3.279279
O	-3.679582	-6.167838	1.135973
O	-1.640592	-7.662691	0.103480
O	0.808389	-7.659561	0.141094
O	-3.685941	-6.169191	-1.418449
O	-0.406474	-6.163241	-2.009489

O	-4.948920	-7.654305	-3.279279
O	-2.409338	-7.654306	-3.279279
O	-0.406474	-6.163241	-4.549068
O	-3.671926	-3.186402	1.131780
O	-1.638480	-4.695737	0.076345
O	0.835263	-4.732742	0.092865
O	-3.691838	-3.180522	-1.418089
O	-0.406474	-3.181111	-2.009489
O	-4.948917	-4.672176	-3.279279
O	-2.409338	-4.672176	-3.279279
O	-0.406474	-3.181111	-4.549068
O	-3.669300	-0.200772	1.136481
O	-1.633815	-1.685703	0.074687
O	0.837584	-1.669129	0.045606
O	-3.694048	-0.195522	-1.417741
O	-0.406474	-0.198980	-2.009489
O	-4.948917	-1.690045	-3.279279
O	-2.409338	-1.690045	-3.279279
O	-0.406474	-0.198980	-4.549068
O	-3.659400	2.790925	1.118950
O	-1.650269	1.273658	0.050572
O	0.818293	1.287539	0.078962
O	-3.696348	2.789704	-1.424086
O	-0.406474	2.783150	-2.009489
O	-4.948917	1.292085	-3.279279
O	-2.409338	1.292085	-3.279279
O	-0.406474	2.783150	-4.549068
O	-3.649644	5.744165	1.148814
O	-1.654254	4.336448	0.044382
O	0.824344	4.300508	0.075475
O	-3.697565	5.775261	-1.419236
O	-0.406474	5.765281	-2.009489
O	-4.948917	4.274216	-3.279279
O	-2.409338	4.274216	-3.279279
O	-0.406474	5.765281	-4.549068
O	-3.682472	-9.152461	1.142518
O	-1.623840	7.260375	0.140979
O	0.830143	7.276028	0.098946
O	-3.677770	-9.153505	-1.413843
O	-0.406474	8.747411	-2.009489
O	8.141700	-1.690043	-3.279279
O	-2.409338	7.256347	-3.279279
O	-0.406474	8.747411	-4.549068
O	2.858323	-6.150102	1.138187
O	-8.176250	1.294630	0.113895
O	-5.729726	1.294600	0.115955
O	2.877074	-6.169538	-1.419983
O	-6.951784	2.783149	-2.009489
O	1.596390	-7.654305	-3.279279
O	4.135969	-7.654306	-3.279279
O	-6.951784	2.783149	-4.549068
O	2.853411	-3.180245	1.122819
O	4.918589	-4.672137	0.115874
O	-5.730018	4.277133	0.112644
O	2.882350	-3.189350	-1.421801

O	6.138833	-3.181110	-2.009489
O	1.596390	-4.672175	-3.279279
O	4.135969	-4.672175	-3.279279
O	6.138833	-3.181110	-4.549068
O	2.855667	-0.194410	1.138242
O	4.918591	-1.688848	0.118293
O	7.365158	-1.695041	0.121827
O	2.882536	-0.201010	-1.417986
O	6.138833	-0.198980	-2.009489
O	1.596390	-1.690045	-3.279279
O	4.135969	-1.690045	-3.279279
O	6.138833	-0.198980	-4.549068
O	2.857867	2.790253	1.135204
O	4.914943	1.291141	0.116137
O	7.359675	1.289364	0.115683
O	2.878930	2.781383	-1.416954
O	6.138833	2.783151	-2.009489
O	1.596390	1.292086	-3.279279
O	4.135969	1.292086	-3.279279
O	6.138833	2.783151	-4.549068
O	2.863353	5.770751	1.136487
O	4.916781	4.275892	0.116602
O	-5.729309	-4.674755	0.111444
O	2.874341	5.767744	-1.418742
O	-6.951784	-3.181110	-2.009489
O	1.596390	4.274216	-3.279279
O	4.135969	4.274216	-3.279279
O	-6.951784	-3.181110	-4.549068
O	2.872492	8.754836	1.141978
O	-8.172703	-1.688283	0.111613
O	-5.727670	-1.689596	0.114356
O	2.866724	8.752513	-1.415184
O	-6.951784	-0.198979	-2.009489
O	1.596390	7.256347	-3.279279
O	4.135969	7.256347	-3.279279
O	-6.951784	-0.198979	-4.549068
O	7.028943	-0.338013	10.049958
O	7.284516	1.072431	8.300174
O	3.213474	-3.943884	13.305204
O	1.098559	-4.664442	13.670568
O	-0.244071	-3.152756	2.132889
O	0.854526	-4.833791	3.197792
O	-0.595329	2.863541	2.095085
O	-1.635992	4.530889	3.244617
C	-0.005031	2.447665	10.422205
C	-2.934605	-0.587576	8.221469
C	3.080446	1.012525	7.742858
C	4.455798	1.106470	7.890843
C	5.081247	0.324183	8.867483
C	4.299183	-0.514921	9.660073
C	2.918122	-0.566728	9.455072
C	6.565658	0.411846	9.019699
C	2.010646	-1.425761	10.239132
C	-0.212823	-2.089334	10.553642
C	0.143539	-2.936323	11.594844

C	1.490723	-3.032192	11.958563
C	2.431792	-2.262031	11.274832
C	1.878913	-3.963083	13.063686
C	0.690558	-2.662269	6.784193
C	0.685284	-3.471791	5.655588
C	0.292150	-2.910358	4.431823
C	-0.050354	-1.563849	4.399449
C	0.033778	-0.796804	5.555911
C	0.266585	-3.645593	3.144300
C	-0.208539	0.647868	5.553261
C	-0.396630	2.595431	6.823026
C	-0.701000	3.354586	5.696020
C	-0.699566	2.723654	4.445957
C	-0.448954	1.358455	4.384345
C	-0.971022	3.389903	3.145613
H	2.550156	1.611979	7.013272
H	5.044323	1.770115	7.267615
H	4.772121	-1.117164	10.423812
H	-1.239882	-1.959813	10.230669
H	-0.605185	-3.513986	12.124078
H	3.474758	-2.322432	11.554737
H	0.955860	-3.063251	7.754374
H	0.961811	-4.515852	5.734660
H	-0.379776	-1.136618	3.464139
H	-0.361722	3.034571	7.813678
H	-0.914992	4.411484	5.800941
H	-0.451744	0.870014	3.420808
H	7.993514	-0.230229	10.088395
H	3.414207	-4.578472	14.015594
H	0.966749	-5.223855	2.311974
H	-1.997932	4.860335	2.392352
N	0.054952	1.477972	9.747347
N	-1.779379	-0.411497	8.413056
N	2.318969	0.191838	8.492723
N	0.699302	-1.362952	9.877680
N	0.377384	-1.347388	6.755626
N	-0.139034	1.272177	6.759165
S	-0.076792	3.789212	11.334682
S	-4.517001	-0.853631	7.976713
Ru	0.238472	-0.018892	8.358250

(4) 2COOH-same-2rows-S

203

Ti	-2.375267	-5.537101	-0.193618
Ti	-5.666735	-6.985602	0.071613
Ti	-5.646657	-5.531121	-3.279279
Ti	-2.374004	-7.022186	-3.279279
Ti	-2.354827	-2.550821	-0.184179
Ti	-5.641262	-4.080791	0.100855
Ti	-5.646657	-2.548990	-3.279279
Ti	-2.374004	-4.040055	-3.279279
Ti	-2.377547	0.424531	-0.204545
Ti	-5.649454	-1.174503	0.016065

Ti	-5.646657	0.433140	-3.279279
Ti	-2.374004	-1.057925	-3.279279
Ti	-2.354073	3.401835	-0.106393
Ti	-5.641880	1.972395	0.017556
Ti	-5.646657	3.415271	-3.279279
Ti	-2.374004	1.924206	-3.279279
Ti	-2.380773	6.380086	-0.114879
Ti	-5.611135	4.862773	-0.035030
Ti	-5.646660	6.397402	-3.279279
Ti	-2.374004	4.906336	-3.279279
Ti	-2.374940	-8.519513	-0.200685
Ti	-5.653076	8.005390	0.001357
Ti	-5.646660	9.379533	-3.279279
Ti	-2.374004	7.888466	-3.279279
Ti	4.167739	-5.527360	-0.192689
Ti	0.898332	-7.025733	0.083448
Ti	0.898650	-5.531121	-3.279279
Ti	4.171303	-7.022186	-3.279279
Ti	4.202237	-2.542539	-0.206318
Ti	0.907591	-4.041408	0.082402
Ti	0.898650	-2.548990	-3.279279
Ti	4.171303	-4.040056	-3.279279
Ti	4.158543	0.447028	-0.103473
Ti	0.912752	-1.064773	0.077928
Ti	0.898650	0.433140	-3.279279
Ti	4.171303	-1.057925	-3.279279
Ti	4.186245	3.401862	-0.101032
Ti	0.912042	1.911061	0.023584
Ti	0.898650	3.415270	-3.279279
Ti	4.171303	1.924205	-3.279279
Ti	4.164012	6.380983	-0.204780
Ti	0.903661	4.910558	0.018420
Ti	0.898650	6.397401	-3.279279
Ti	4.171303	4.906336	-3.279279
Ti	4.183360	9.370010	-0.195724
Ti	0.892299	7.886657	0.081946
Ti	0.898650	-8.513249	-3.279279
Ti	4.171303	7.888467	-3.279279
O	-5.668076	-5.535977	1.171188
O	-3.608716	-7.011063	0.112762
O	-1.152080	-7.016784	0.112188
O	-5.606586	-5.509315	-1.398462
O	-2.374004	-5.531121	-2.009489
O	-6.916450	-7.022185	-3.279279
O	-4.376868	-7.022186	-3.279279
O	-2.374004	-5.531121	-4.549068
O	-5.643735	-2.545814	1.149303
O	-3.608249	-4.042915	0.120466
O	-1.150004	-4.044294	0.105941
O	-5.637188	-2.529378	-1.395973
O	-2.374004	-2.548990	-2.009489
O	-6.916450	-4.040054	-3.279279
O	-4.376868	-4.040055	-3.279279
O	-2.374004	-2.548990	-4.549068
O	-5.670635	0.424633	1.249797

O	-3.627618	-1.069501	0.100669
O	-1.152633	-1.073828	0.091758
O	-5.658429	0.447169	-1.398143
O	-2.374004	0.433140	-2.009489
O	-6.916447	-1.057925	-3.279279
O	-4.376868	-1.057925	-3.279279
O	-2.374004	0.433140	-4.549068
O	-5.601482	3.419858	1.106574
O	-3.648531	1.866508	0.059949
O	-1.156744	1.889072	0.061138
O	-5.683688	3.394672	-1.396046
O	-2.374004	3.415271	-2.009489
O	-6.916447	1.924206	-3.279279
O	-4.376868	1.924206	-3.279279
O	-2.374004	3.415271	-4.549068
O	-5.611162	6.397655	1.231399
O	-3.695661	4.930263	-0.132308
O	-1.132716	4.913352	-0.058420
O	-5.688879	6.388415	-1.405721
O	-2.374004	6.397402	-2.009489
O	-6.916450	4.906337	-3.279279
O	-4.376868	4.906336	-3.279279
O	-2.374004	6.397402	-4.549068
O	-5.664983	9.386145	1.135608
O	-3.637301	7.917321	0.088799
O	-1.156139	7.914652	0.088210
O	-5.612080	9.360848	-1.402646
O	-2.374004	-8.513249	-2.009489
O	-6.916450	7.888467	-3.279279
O	-4.376871	7.888467	-3.279279
O	-2.374004	-8.513249	-4.549068
O	0.910217	-5.535684	1.132969
O	2.977702	-7.021708	0.126406
O	5.438689	-7.025765	0.110526
O	0.907082	-5.534523	-1.419539
O	4.171303	-5.531122	-2.009489
O	-0.371140	-7.022186	-3.279279
O	2.168439	-7.022186	-3.279279
O	4.171303	-5.531122	-4.549068
O	0.916710	-2.554933	1.128693
O	2.976689	-4.054349	0.121708
O	5.438882	-4.052822	0.101768
O	0.900060	-2.559026	-1.418117
O	4.171303	-2.548990	-2.009489
O	-0.371140	-4.040056	-3.279279
O	2.168439	-4.040056	-3.279279
O	4.171303	-2.548990	-4.549068
O	0.933042	0.444232	1.109526
O	2.961790	-1.099324	0.071058
O	5.450917	-1.101399	0.068515
O	0.872152	0.415057	-1.424971
O	4.171303	0.433140	-2.009489
O	-0.371140	-1.057925	-3.279279
O	2.168439	-1.057925	-3.279279
O	4.171303	0.433140	-4.549068

O	0.903213	3.419012	1.089946
O	2.914149	1.910892	-0.106642
O	5.470938	1.931801	-0.114316
O	0.891713	3.421488	-1.436163
O	4.171303	3.415270	-2.009489
O	-0.371140	1.924206	-3.279279
O	2.168439	1.924205	-3.279279
O	4.171303	3.415270	-4.549068
O	0.880293	6.382609	1.118302
O	2.945306	4.949231	0.058392
O	5.428911	4.944661	0.071760
O	0.922276	6.420558	-1.422637
O	4.171303	6.397401	-2.009489
O	-0.371140	4.906336	-3.279279
O	2.168439	4.906336	-3.279279
O	4.171303	6.397401	-4.549068
O	0.903387	-8.514320	1.137230
O	2.971729	7.903144	0.135344
O	5.437483	7.906830	0.093284
O	0.907934	-8.509148	-1.415399
O	4.171306	9.379530	-2.009489
O	-0.371140	7.888467	-3.279279
O	2.168439	7.888466	-3.279279
O	4.171303	9.379531	-4.549068
O	2.975313	3.508529	13.237013
O	2.142683	5.524080	12.648177
O	3.395123	-2.596767	11.806528
O	2.693701	-4.261674	10.444741
O	4.089167	3.059993	1.954780
O	4.188984	0.800414	1.990832
O	-2.458055	5.968225	2.107745
O	-2.489541	3.719384	1.900757
C	-2.825469	1.367023	9.161751
C	-1.460675	-0.589855	5.138133
C	0.603195	3.805372	9.102584
C	1.109517	4.436534	10.227565
C	1.776442	3.665583	11.187258
C	1.903316	2.290577	10.978093
C	1.359502	1.716258	9.826777
C	2.298127	4.345380	12.406528
C	1.383255	0.269757	9.541159
C	0.605373	-1.415466	8.109983
C	1.245602	-2.397439	8.849878
C	1.994772	-2.022933	9.971293
C	2.052218	-0.674827	10.324957
C	2.710189	-3.084384	10.737613
C	2.548444	0.876045	5.894936
C	3.425563	0.931489	4.819181
C	3.228088	1.911193	3.842116
C	2.170967	2.800409	4.001119
C	1.262540	2.614694	5.044606
C	3.929333	1.928017	2.517123
C	-0.037334	3.308683	5.075524
C	-2.092183	3.536655	6.145344
C	-2.622942	4.261416	5.076916

C	-1.823678	4.474454	3.954632
C	-0.497551	4.044297	3.986312
C	-2.325228	4.798759	2.563798
H	0.071611	4.359542	8.338651
H	0.970944	5.497439	10.383082
H	2.412816	1.684709	11.712693
H	0.002871	-1.644575	7.239806
H	1.169950	-3.440810	8.570072
H	2.619867	-0.371094	11.194639
H	2.685605	0.142227	6.680505
H	4.224683	0.207246	4.721508
H	2.000116	3.557936	3.249027
H	-2.695598	3.266272	7.005882
H	-3.663399	4.563738	5.107255
H	0.116573	4.159737	3.106329
H	3.274902	4.044350	13.988171
H	3.828550	-3.354683	12.237971
H	-5.248654	0.418920	2.119063
H	-5.046908	6.423597	2.015023
N	-1.870167	1.372855	8.465070
N	-0.993946	0.168107	5.914170
N	0.723938	2.479528	8.889795
N	0.689650	-0.105784	8.428642
N	1.461600	1.667205	5.999536
N	-0.845328	3.031711	6.133138
S	-4.144072	1.381680	10.116556
S	-2.096457	-1.669323	4.088646
Ru	-0.154172	1.430202	7.334843

(5) 2COOH-same-1row-S 2M+S

203

Ti	-2.287783	-6.158716	-0.189206
Ti	7.511611	1.290503	0.122108
Ti	7.518478	2.783148	-3.279279
Ti	-2.299481	-7.654305	-3.279279
Ti	-2.340392	-3.175937	-0.199154
Ti	-5.599255	-4.753261	-0.010729
Ti	-5.572133	-3.181109	-3.279279
Ti	-2.299481	-4.672175	-3.279279
Ti	-2.264064	-0.203548	-0.090031
Ti	-5.592604	-1.604739	0.000367
Ti	-5.572133	-0.198978	-3.279279
Ti	-2.299481	-1.690044	-3.279279
Ti	-2.319806	2.773070	-0.194728
Ti	-5.575979	1.301216	0.123833
Ti	-5.572133	2.783153	-3.279279
Ti	-2.299481	1.292087	-3.279279
Ti	-2.297927	5.762568	-0.189275
Ti	-5.575225	4.200137	-0.008440
Ti	-5.572133	5.765283	-3.279279
Ti	-2.299481	4.274217	-3.279279
Ti	-2.309323	8.746799	-0.184381
Ti	7.515926	-1.613109	0.011282

Ti	7.518478	-0.198980	-3.279279
Ti	-2.299481	7.256347	-3.279279
Ti	4.249462	-6.139894	-0.175837
Ti	0.989839	-7.656104	0.089751
Ti	0.973171	-6.163241	-3.279279
Ti	4.245823	-7.654307	-3.279279
Ti	4.254843	-3.172859	-0.074286
Ti	0.966420	-4.672330	0.077020
Ti	0.973171	-3.181111	-3.279279
Ti	4.245823	-4.672177	-3.279279
Ti	4.249891	-0.196005	-0.226588
Ti	0.986864	-1.693147	0.071179
Ti	0.973171	-0.198980	-3.279279
Ti	4.245823	-1.690046	-3.279279
Ti	4.248403	2.774293	-0.039426
Ti	0.991533	1.292622	0.067967
Ti	0.973171	2.783150	-3.279279
Ti	4.245823	1.292084	-3.279279
Ti	4.230208	5.752633	-0.183217
Ti	0.963995	4.275830	0.075721
Ti	0.973171	5.765281	-3.279279
Ti	4.245823	4.274215	-3.279279
Ti	4.250223	8.758996	-0.190920
Ti	0.988198	7.258427	0.089374
Ti	0.973171	8.747411	-3.279279
Ti	4.245823	7.256345	-3.279279
O	7.483148	2.805109	1.166782
O	-3.547572	-7.651309	0.133289
O	-1.090010	-7.665598	0.128213
O	7.544153	2.781024	-1.390718
O	-2.299481	-6.163241	-2.009489
O	6.248689	1.292084	-3.279279
O	-4.302344	-7.654304	-3.279279
O	-2.299481	-6.163241	-4.549068
O	-5.556633	-3.184329	1.243787
O	-3.564010	-4.682459	0.104298
O	-1.094547	-4.680255	0.142978
O	-5.551823	-3.175974	-1.405956
O	-2.299481	-3.181110	-2.009489
O	6.248689	4.274214	-3.279279
O	-4.302344	-4.672174	-3.279279
O	-2.299481	-3.181110	-4.549068
O	-5.554968	-0.217189	1.167546
O	-3.588088	-1.718013	0.022876
O	-1.083518	-1.717431	0.091272
O	-5.606765	-0.205527	-1.390668
O	-2.299481	-0.198979	-2.009489
O	6.248698	7.256348	-3.279279
O	-4.302344	-1.690044	-3.279279
O	-2.299481	-0.198979	-4.549068
O	-5.577318	2.802933	1.164491
O	-3.573147	1.324714	0.036723
O	-1.081564	1.316863	0.098442
O	-5.555752	2.776518	-1.397900
O	-2.299481	2.783151	-2.009489

O	6.248698	-7.654301	-3.279279
O	-4.302344	1.292087	-3.279279
O	-2.299481	2.783151	-4.549068
O	-5.693817	5.752451	1.256108
O	-3.568456	4.299409	0.120039
O	-1.096189	4.283238	0.141773
O	-5.522269	5.772524	-1.404653
O	-2.299481	5.765282	-2.009489
O	6.248689	-4.672174	-3.279279
O	-4.302344	4.274218	-3.279279
O	-2.299481	5.765282	-4.549068
O	7.510364	-0.211634	1.179265
O	-3.563212	7.241599	0.146825
O	-1.091173	7.266390	0.121549
O	7.560797	-0.205249	-1.389894
O	-2.299481	8.747412	-2.009489
O	6.248689	-1.690044	-3.279279
O	-4.302344	7.256348	-3.279279
O	-2.299481	8.747412	-4.549068
O	0.961822	-6.160153	1.151282
O	3.014288	-7.670040	0.113759
O	5.490234	-7.666117	0.128608
O	0.954664	-6.169026	-1.413825
O	4.245823	-6.163242	-2.009489
O	-0.296618	-7.654306	-3.279279
O	2.242960	-7.654306	-3.279279
O	4.245823	-6.163242	-4.549068
O	0.985337	-3.182960	1.151575
O	3.011077	-4.683551	0.051624
O	5.546772	-4.730951	-0.055246
O	0.950604	-3.186368	-1.413524
O	4.245823	-3.181112	-2.009489
O	-0.296618	-4.672175	-3.279279
O	2.242960	-4.672176	-3.279279
O	4.245823	-3.181112	-4.549068
O	0.961765	-0.200840	1.142752
O	3.012375	-1.669255	0.068522
O	5.541370	-1.651636	0.005219
O	0.954835	-0.202067	-1.416794
O	4.245823	-0.198981	-2.009489
O	-0.296618	-1.690045	-3.279279
O	2.242960	-1.690046	-3.279279
O	4.245823	-0.198981	-4.549068
O	0.992980	2.783612	1.145641
O	3.000173	1.253683	0.041214
O	5.523323	1.246572	0.024637
O	0.946723	2.787933	-1.414719
O	4.245823	2.783149	-2.009489
O	-0.296618	1.292086	-3.279279
O	2.242960	1.292085	-3.279279
O	4.245823	2.783149	-4.549068
O	0.965216	5.764556	1.149548
O	3.003803	4.301017	0.034766
O	5.542462	4.346374	-0.013610
O	0.953743	5.773982	-1.414990

O	4.245823	5.765280	-2.009489
O	-0.296618	4.274216	-3.279279
O	2.242960	4.274215	-3.279279
O	4.245823	5.765280	-4.549068
O	0.959700	8.747825	1.159029
O	3.018511	7.277746	0.113689
O	5.497780	7.260307	0.142457
O	0.965337	8.749095	-1.414093
O	4.245831	8.747413	-2.009489
O	-0.296618	7.256346	-3.279279
O	2.242960	7.256346	-3.279279
O	4.245831	8.747413	-4.549068
O	1.875535	-1.896952	12.947899
O	3.697828	-0.587499	12.538659
O	-3.348567	-4.544531	10.630039
O	-4.668067	-4.819675	8.794354
O	4.567947	-3.181006	1.922591
O	3.924473	-5.185484	2.794822
O	4.371671	2.795774	1.904450
O	3.966324	4.780979	2.925354
C	-1.515371	2.082646	7.799459
C	-1.607061	-0.177866	3.692709
C	2.259899	0.055043	8.582957
C	2.785709	-0.126249	9.855626
C	2.092241	-0.934947	10.780002
C	0.892468	-1.535597	10.373721
C	0.408738	-1.319712	9.074999
C	2.654853	-1.100838	12.147748
C	-0.811262	-1.932080	8.540012
C	-2.164585	-2.165044	6.621655
C	-3.029111	-3.022388	7.291086
C	-2.770728	-3.352924	8.638991
C	-1.647766	-2.795040	9.262325
C	-3.695231	-4.295006	9.325118
C	1.389018	-2.911544	5.436533
C	2.202345	-3.729314	4.655790
C	3.151667	-3.131448	3.809573
C	3.268736	-1.734500	3.827808
C	2.423036	-0.959259	4.630548
C	3.932703	-3.947878	2.808914
C	2.440975	0.513773	4.667792
C	1.476398	2.438844	5.619137
C	2.260669	3.281172	4.828315
C	3.147082	2.710938	3.901604
C	3.253730	1.313305	3.857078
C	3.879837	3.544313	2.874096
H	2.762883	0.681083	7.842636
H	3.719764	0.353167	10.158383
H	0.334935	-2.166558	11.066656
H	-2.331059	-1.872785	5.582742
H	-3.912167	-3.434842	6.799438
H	-1.441222	-3.024382	10.311646
H	0.611502	-3.328092	6.079099
H	2.077808	-4.814634	4.657981
H	4.007709	-1.260022	3.182434

H	0.726422	2.813473	6.318311
H	2.149950	4.365733	4.892455
H	3.938752	0.868206	3.136524
H	2.326198	-1.916602	13.822644
H	-4.009957	-5.203492	10.936252
H	-6.554270	5.756800	1.758165
H	-6.067582	-3.186542	2.075272
N	-0.922223	1.232726	7.198077
N	-0.872298	-0.137243	4.626324
N	1.093616	-0.518908	8.181756
N	-1.067084	-1.626566	7.218183
N	1.468910	-1.556008	5.418992
N	1.542518	1.086646	5.530516
S	-2.300542	3.248408	8.603277
S	-2.818884	-0.299254	2.583003
Ru	0.189776	-0.244743	6.378996

(5) 2COOH-same-1row-S 2MH+S

203

Ti	-2.483360	-5.913353	-0.200376
Ti	7.335065	1.539387	0.079072
Ti	7.328688	3.027883	-3.279279
Ti	-2.489258	-7.409565	-3.279279
Ti	-2.507678	-2.924485	-0.205385
Ti	-5.761164	-4.422493	0.069922
Ti	-5.761904	-2.936365	-3.279279
Ti	-2.489258	-4.427434	-3.279279
Ti	-2.470580	0.047223	-0.129069
Ti	-5.768410	-1.443687	0.068538
Ti	-5.761904	0.045765	-3.279279
Ti	-2.489258	-1.445303	-3.279279
Ti	-2.507676	3.017843	-0.204319
Ti	-5.765626	1.543289	0.075023
Ti	-5.761904	3.027897	-3.279279
Ti	-2.489258	1.536828	-3.279279
Ti	-2.485578	6.005799	-0.199451
Ti	-5.762468	4.520817	0.066797
Ti	7.328697	-2.936370	-3.279279
Ti	-2.489258	4.518958	-3.279279
Ti	-2.490383	-8.899798	-0.199501
Ti	7.336153	-1.441061	0.073986
Ti	7.328688	0.045755	-3.279279
Ti	-2.489258	7.501089	-3.279279
Ti	4.036892	-5.919980	-0.219551
Ti	0.784299	-7.409948	0.086055
Ti	0.783390	-5.918503	-3.279279
Ti	4.056037	-7.409570	-3.279279
Ti	4.075807	-2.931532	-0.141071
Ti	0.771883	-4.427791	0.072322
Ti	0.783390	-2.936371	-3.279279
Ti	4.056037	-4.427439	-3.279279
Ti	4.061237	0.047960	-0.224858
Ti	0.790586	-1.445584	0.067111

Ti	0.783390	0.045759	-3.279279
Ti	4.056037	-1.445309	-3.279279
Ti	4.074001	3.030032	-0.141713
Ti	0.793006	1.541168	0.069262
Ti	0.783390	3.027890	-3.279279
Ti	4.056037	1.536822	-3.279279
Ti	4.033941	6.014152	-0.219367
Ti	0.768564	4.522775	0.071611
Ti	0.783390	6.010020	-3.279279
Ti	4.056037	4.518953	-3.279279
Ti	4.062264	-8.899272	-0.198710
Ti	0.781650	7.504866	0.085694
Ti	0.783390	-8.900629	-3.279279
Ti	4.056037	7.501083	-3.279279
O	7.313631	3.033302	1.132335
O	-3.711479	-7.409049	0.121645
O	-1.267137	-7.410252	0.119731
O	7.339685	3.028752	-1.419501
O	-2.489258	-5.918499	-2.009489
O	6.058901	1.536820	-3.279279
O	-4.492118	-7.409561	-3.279279
O	-2.489258	-5.918499	-4.549068
O	-5.776845	-2.937801	1.137372
O	-3.713956	-4.433398	0.117566
O	-1.265327	-4.433890	0.118716
O	-5.762742	-2.937440	-1.420908
O	-2.489258	-2.936368	-2.009489
O	6.058901	4.518950	-3.279279
O	-4.492118	-4.427431	-3.279279
O	-2.489258	-2.936368	-4.549068
O	-5.761385	0.045783	1.119799
O	-3.734356	-1.463986	0.040439
O	-1.258016	-1.462095	0.080072
O	-5.791034	0.043780	-1.421714
O	-2.489258	0.045763	-2.009489
O	-7.031693	-1.445297	-3.279279
O	-4.492118	-1.445301	-3.279279
O	-2.489258	0.045763	-4.549068
O	-5.778243	3.034094	1.138219
O	-3.735525	1.557052	0.035721
O	-1.260119	1.553887	0.085678
O	-5.762628	3.026342	-1.421316
O	-2.489258	3.027893	-2.009489
O	-7.031693	1.536834	-3.279279
O	-4.492118	1.536830	-3.279279
O	-2.489258	3.027893	-4.549068
O	7.311371	-2.937742	1.127078
O	-3.714976	4.526218	0.112889
O	-1.265659	4.527696	0.115337
O	7.342006	-2.936497	-1.420234
O	-2.489258	6.010024	-2.009489
O	6.058901	-4.427438	-3.279279
O	-4.492118	4.518961	-3.279279
O	-2.489258	6.010024	-4.549068
O	7.320069	0.047473	1.136414

O	-3.711018	7.503842	0.123222
O	-1.266647	7.503903	0.116645
O	7.348513	0.045689	-1.419636
O	-2.489258	-8.900626	-2.009489
O	6.058901	-1.445308	-3.279279
O	-4.492136	7.501083	-3.279279
O	-2.489258	-8.900626	-4.549068
O	0.787091	-5.914858	1.140822
O	2.823148	-7.421305	0.118086
O	5.269217	-7.410912	0.134895
O	0.779275	-5.921678	-1.416481
O	4.056037	-5.918506	-2.009489
O	-0.486397	-7.409566	-3.279279
O	2.053177	-7.409567	-3.279279
O	4.056037	-5.918506	-4.549068
O	0.800563	-2.936453	1.135474
O	2.827669	-4.447467	0.092384
O	5.292721	-4.473315	0.058628
O	0.779035	-2.941941	-1.417722
O	4.056037	-2.936375	-2.009489
O	-0.486397	-4.427435	-3.279279
O	2.053177	-4.427437	-3.279279
O	4.056037	-2.936375	-4.549068
O	0.797146	0.045706	1.130186
O	2.828784	-1.435400	0.071780
O	5.297154	-1.427729	0.052056
O	0.781897	0.045554	-1.419294
O	4.056037	0.045756	-2.009489
O	-0.486397	-1.445305	-3.279279
O	2.053177	-1.445307	-3.279279
O	4.056037	0.045756	-4.549068
O	0.799869	3.030350	1.134433
O	2.827496	1.527897	0.073423
O	5.294375	1.524478	0.058935
O	0.777527	3.031932	-1.417813
O	4.056037	3.027886	-2.009489
O	-0.486397	1.536826	-3.279279
O	2.053177	1.536824	-3.279279
O	4.056037	3.027886	-4.549068
O	0.787242	6.009079	1.138157
O	2.824427	4.540540	0.086632
O	5.289992	4.563018	0.065621
O	0.779085	6.013927	-1.417428
O	4.056037	6.010017	-2.009489
O	-0.486397	4.518957	-3.279279
O	2.053177	4.518954	-3.279279
O	4.056037	6.010017	-4.549068
O	0.776026	-8.899006	1.143465
O	2.823220	7.513446	0.118412
O	5.268644	7.502408	0.135550
O	0.779837	-8.900091	-1.415907
O	4.056064	-8.900620	-2.009489
O	-0.486397	7.501087	-3.279279
O	2.053177	7.501085	-3.279279
O	4.056064	-8.900620	-4.549068

O	1.445434	-1.719909	13.220291
O	3.225050	-0.374555	12.858857
O	-3.710785	-4.335400	10.852937
O	-5.041128	-4.579996	9.045352
O	4.176862	-2.946453	2.137460
O	4.181843	-4.738543	3.505751
O	4.119152	3.049445	2.157005
O	4.105226	4.817549	3.553543
C	-1.840263	2.329369	8.144112
C	-1.942383	0.099552	3.916058
C	1.854831	0.289618	8.906143
C	2.362411	0.106063	10.182728
C	1.662603	-0.714587	11.075701
C	0.479050	-1.315311	10.648747
C	0.025195	-1.096078	9.344789
C	2.208195	-0.898480	12.452185
C	-1.196021	-1.710320	8.792504
C	-2.554793	-1.908009	6.895206
C	-3.417522	-2.774918	7.551808
C	-3.147695	-3.122455	8.880254
C	-2.025853	-2.578894	9.506848
C	-4.070410	-4.073548	9.568261
C	1.103773	-2.688139	5.714585
C	1.973956	-3.479069	4.969645
C	2.829917	-2.843020	4.065682
C	2.810285	-1.455097	3.984366
C	1.954108	-0.723012	4.797062
C	3.776808	-3.520176	3.142439
C	1.966148	0.746062	4.820542
C	1.178815	2.681384	5.863401
C	2.010859	3.492640	5.092413
C	2.809427	2.885503	4.118194
C	2.770379	1.501715	3.976646
C	3.719792	3.594271	3.177858
H	2.360598	0.924455	8.188637
H	3.281338	0.587064	10.498152
H	-0.080256	-1.945627	11.327881
H	-2.722784	-1.599982	5.869898
H	-4.290526	-3.179026	7.051376
H	-1.812266	-2.832581	10.537263
H	0.381403	-3.138691	6.385784
H	1.954556	-4.557602	5.069331
H	3.476693	-0.966570	3.289415
H	0.482815	3.088856	6.587850
H	2.001755	4.567386	5.228659
H	3.362824	1.045212	3.198525
H	1.870060	-1.766056	14.094571
H	-4.358067	-4.972844	11.194135
H	4.796689	5.125853	2.939449
H	4.888519	-5.030219	2.898230
N	-1.280022	1.504353	7.506409
N	-1.243872	0.123534	4.864393
N	0.713849	-0.291939	8.482676
N	-1.461817	-1.392222	7.493981
N	1.090570	-1.340497	5.648939

N	1.168237	1.338513	5.746321
S	-2.589145	3.475501	9.022103
S	-3.079223	0.024812	2.734715
Ru	-0.182786	0.000424	6.634831

(6) 2COOH-diff(2trans)-2rows

203

Ti	-3.327267	-6.192065	-0.190073
Ti	6.450870	-7.668958	0.148009
Ti	6.477579	-6.173821	-3.279279
Ti	-3.340384	-7.664886	-3.279279
Ti	-3.350418	-3.204383	-0.194089
Ti	6.491265	-4.773048	-0.010270
Ti	6.477579	-3.191690	-3.279279
Ti	-3.340384	-4.682755	-3.279279
Ti	-3.340815	-0.227352	-0.204362
Ti	6.478121	-1.614932	0.005090
Ti	6.477579	-0.209560	-3.279279
Ti	-3.340384	-1.700625	-3.279279
Ti	-3.340127	2.723354	-0.104043
Ti	6.466687	1.283480	0.136611
Ti	6.477579	2.772570	-3.279279
Ti	-3.340384	1.281505	-3.279279
Ti	-3.292863	5.706948	-0.121100
Ti	6.528547	4.184503	-0.032583
Ti	6.477579	5.754701	-3.279279
Ti	-3.340384	4.263636	-3.279279
Ti	-3.374398	8.715487	-0.196387
Ti	6.473168	7.329541	0.017048
Ti	6.477579	8.736831	-3.279279
Ti	-3.340384	7.245766	-3.279279
Ti	3.204748	-6.160414	-0.190931
Ti	-0.085099	-7.674617	0.093104
Ti	-0.067730	-6.173821	-3.279279
Ti	3.204924	-7.664886	-3.279279
Ti	3.226080	-3.190697	-0.045295
Ti	-0.056373	-4.690089	0.075162
Ti	-0.067730	-3.191690	-3.279279
Ti	3.204924	-4.682755	-3.279279
Ti	3.195284	-0.216029	-0.208570
Ti	-0.068644	-1.703165	0.078329
Ti	-0.067730	-0.209560	-3.279279
Ti	3.204924	-1.700625	-3.279279
Ti	3.207784	2.776584	-0.192831
Ti	-0.059258	1.276264	0.081491
Ti	-0.067730	2.772570	-3.279279
Ti	3.204924	1.281505	-3.279279
Ti	3.242893	5.754533	-0.192905
Ti	-0.049719	4.260202	0.059409
Ti	-0.067730	5.754701	-3.279279
Ti	3.204924	4.263636	-3.279279
Ti	3.163980	8.744875	-0.192095
Ti	-0.085972	7.241643	0.095744

Ti	-0.067730	8.736831	-3.279279
Ti	3.204924	7.245766	-3.279279
O	6.469953	-6.158589	1.181483
O	-4.585607	-7.661100	0.161387
O	-2.122477	-7.665067	0.128864
O	6.509784	-6.193229	-1.382286
O	-3.340384	-6.173821	-2.009489
O	5.207789	-7.664886	-3.279279
O	-5.343249	-7.664886	-3.279279
O	-3.340384	-6.173821	-4.549068
O	6.373627	-3.201720	1.257710
O	-4.601292	-4.685104	0.131377
O	-2.130082	-4.690643	0.139036
O	6.521780	-3.195466	-1.396674
O	-3.340384	-3.191690	-2.009489
O	5.207789	-4.682755	-3.279279
O	-5.343249	-4.682755	-3.279279
O	-3.340384	-3.191690	-4.549068
O	6.469596	-0.225083	1.186672
O	-4.608584	-1.737105	0.136785
O	-2.127945	-1.729609	0.146842
O	6.482070	-0.210535	-1.381883
O	-3.340384	-0.209560	-2.009489
O	5.207789	-1.700625	-3.279279
O	-5.343249	-1.700625	-3.279279
O	-3.340384	-0.209560	-4.549068
O	6.526980	2.803298	1.165170
O	-4.609144	1.207548	0.049468
O	-2.105229	1.223088	0.060857
O	6.445650	2.757997	-1.385650
O	-3.340384	2.772570	-2.009489
O	5.207789	1.281505	-3.279279
O	-5.343249	1.281505	-3.279279
O	-3.340384	2.772570	-4.549068
O	6.481986	5.748222	1.253013
O	-4.649226	4.330382	-0.094902
O	-2.076076	4.241482	-0.076414
O	6.422725	5.777148	-1.395592
O	-3.340384	5.754701	-2.009489
O	5.207789	4.263636	-3.279279
O	-5.343249	4.263636	-3.279279
O	-3.340384	5.754701	-4.549068
O	6.483608	8.714296	1.197666
O	-4.603134	7.258962	0.110281
O	-2.116412	7.274328	0.123108
O	6.482834	8.734019	-1.370098
O	-3.340384	8.736831	-2.009489
O	5.207789	7.245766	-3.279279
O	-5.343249	7.245766	-3.279279
O	-3.340384	8.736831	-4.549068
O	-0.076612	-6.172836	1.144862
O	1.976778	-7.681231	0.129311
O	4.451129	-7.687956	0.130055
O	-0.076138	-6.179481	-1.413273
O	3.204924	-6.173821	-2.009489

O	-1.337520	-7.664886	-3.279279
O	1.202060	-7.664886	-3.279279
O	3.204924	-6.173821	-4.549068
O	-0.042311	-3.197005	1.148774
O	1.977100	-4.697290	0.045325
O	4.503960	-4.748242	-0.023185
O	-0.097086	-3.192208	-1.412919
O	3.204924	-3.191690	-2.009489
O	-1.337520	-4.682755	-3.279279
O	1.202060	-4.682755	-3.279279
O	3.204924	-3.191690	-4.549068
O	-0.066857	-0.213926	1.154948
O	1.971466	-1.657410	0.063381
O	4.493605	-1.638545	0.012051
O	-0.068321	-0.211253	-1.411048
O	3.204924	-0.209560	-2.009489
O	-1.337520	-1.700625	-3.279279
O	1.202060	-1.700625	-3.279279
O	3.204924	-0.209560	-4.549068
O	-0.097383	2.775512	1.145740
O	1.986684	1.300823	0.145858
O	4.452587	1.301499	0.149966
O	-0.025026	2.760468	-1.416572
O	3.204924	2.772570	-2.009489
O	-1.337520	1.281505	-3.279279
O	1.202060	1.281505	-3.279279
O	3.204924	2.772570	-4.549068
O	-0.078685	5.738598	1.149995
O	1.998457	4.269445	0.147968
O	4.466445	4.269882	0.111767
O	-0.038322	5.767874	-1.413383
O	3.204924	5.754701	-2.009489
O	-1.337520	4.263636	-3.279279
O	1.202060	4.263636	-3.279279
O	3.204924	5.754701	-4.549068
O	-0.063232	8.731400	1.161405
O	1.998592	7.239699	0.148558
O	4.465643	7.239176	0.143790
O	-0.060954	8.735037	-1.407044
O	3.204924	8.736831	-2.009489
O	-1.337520	7.245766	-3.279279
O	1.202060	7.245766	-3.279279
O	3.204924	8.736831	-4.549068
O	2.548335	-4.958932	3.014051
O	3.439454	-3.166644	1.930131
O	-3.797258	-5.260825	4.892239
O	-5.386869	-4.422827	6.301867
O	-3.112973	5.178367	2.278198
O	-3.487764	2.980365	1.842603
O	3.282834	6.099773	4.905179
O	5.021208	5.137503	6.032801
C	1.731868	-1.351587	8.867226
C	-1.821748	1.846187	9.183675
C	1.932507	-0.535726	4.801119
C	2.581708	-1.442526	3.967589

C	2.038939	-2.728924	3.788612
C	0.838312	-3.033341	4.441812
C	0.201025	-2.055652	5.222329
C	2.696728	-3.743261	2.885958
C	-1.096133	-2.247354	5.882161
C	-2.627980	-1.375976	7.443184
C	-3.541176	-2.393337	7.177485
C	-3.227049	-3.361634	6.203115
C	-1.974900	-3.296690	5.575980
C	-4.255975	-4.379595	5.835906
C	-2.507231	1.373127	5.245119
C	-3.176026	2.215253	4.372790
C	-2.513566	3.352983	3.859658
C	-1.231203	3.645652	4.334714
C	-0.603301	2.745958	5.222198
C	-3.083609	3.960257	2.600312
C	0.739881	2.925573	5.784629
C	2.341536	2.053122	7.283456
C	3.233407	3.081140	6.994697
C	2.863900	4.066643	6.056464
C	1.593891	3.990644	5.466267
C	3.844518	5.127974	5.691229
H	2.355496	0.448870	5.005476
H	3.516799	-1.155228	3.482665
H	0.412852	-4.033498	4.332276
H	-2.823498	-0.599437	8.189772
H	-4.502646	-2.427399	7.698559
H	-1.709307	-4.041791	4.823226
H	-2.974831	0.468880	5.641533
H	-4.185196	1.963947	4.042932
H	-0.708282	4.525083	3.950417
H	2.567305	1.267081	8.011075
H	4.207486	3.122380	7.490856
H	1.295533	4.748185	4.739034
H	5.529291	-3.250619	1.772161
H	-4.535026	-5.879640	4.696896
H	7.011513	5.748433	2.072115
H	3.995963	6.738096	4.682006
N	1.055796	-0.634643	8.182693
N	-1.165007	1.218354	8.396377
N	0.760446	-0.815668	5.417925
N	-1.442414	-1.266778	6.783097
N	-1.222428	1.587845	5.621300
N	1.127429	1.947054	6.676500
S	2.673277	-2.282726	9.797429
S	-2.721823	2.662134	10.249711
Ru	-0.148941	0.348159	6.903224

(7) 2COOH-diff(cis,trans)-2rows

203

Ti	-2.413563	-8.094822	-0.199757
Ti	0.844320	-6.625181	0.077746
Ti	0.847190	-8.110935	-3.279279

Ti	-2.425464	-6.619870	-3.279279
Ti	-2.415794	-5.085643	-0.113102
Ti	0.840847	-3.646414	0.050265
Ti	0.847190	-5.128805	-3.279279
Ti	-2.425464	-3.637739	-3.279279
Ti	-2.414477	-2.118221	-0.102803
Ti	0.849125	-0.664887	0.027091
Ti	0.847190	-2.146674	-3.279279
Ti	-2.425464	-0.655609	-3.279279
Ti	-2.420136	0.844182	-0.209841
Ti	0.840703	2.335613	0.036847
Ti	0.847190	0.835456	-3.279279
Ti	-2.425464	2.326522	-3.279279
Ti	-2.442658	3.829694	-0.196768
Ti	0.845266	5.311217	0.082360
Ti	0.847190	3.817587	-3.279279
Ti	-2.425464	5.308652	-3.279279
Ti	-2.427446	6.809756	-0.193774
Ti	0.859379	8.289720	0.081996
Ti	0.847190	6.799717	-3.279279
Ti	-2.425464	8.290782	-3.279279
Ti	4.145688	-8.121104	-0.197464
Ti	-5.665382	-3.562543	-0.044918
Ti	-5.698121	-5.128805	-3.279279
Ti	4.119843	-6.619870	-3.279279
Ti	4.120007	-5.140357	-0.196116
Ti	-5.693665	-0.664670	0.126272
Ti	-5.698121	-2.146674	-3.279279
Ti	4.119843	-3.637739	-3.279279
Ti	4.114644	-2.157015	-0.209318
Ti	-5.692765	2.230504	-0.006857
Ti	-5.698121	0.835456	-3.279279
Ti	4.119843	-0.655609	-3.279279
Ti	4.151485	0.816481	-0.100642
Ti	7.367801	2.412431	-0.045348
Ti	-5.698121	3.817586	-3.279279
Ti	4.119843	2.326521	-3.279279
Ti	4.099237	3.778072	-0.114564
Ti	7.386062	5.300533	0.132401
Ti	7.392496	3.817587	-3.279279
Ti	4.119843	5.308652	-3.279279
Ti	4.120820	6.777158	-0.200084
Ti	-5.681037	-6.714539	0.004791
Ti	-5.698121	-8.110933	-3.279279
Ti	4.119843	8.290782	-3.279279
O	0.853554	-8.110855	1.132578
O	2.921872	-6.626764	0.135326
O	-1.200887	-6.646860	0.086080
O	0.857731	-8.112128	-1.418639
O	-2.425464	-8.110935	-2.009489
O	-0.422599	-6.619870	-3.279279
O	2.116979	-6.619870	-3.279279
O	-2.425464	-8.110935	-4.549068
O	0.832641	-5.124184	1.122500
O	2.908355	-3.658054	0.111258

O	-1.168596	-3.638788	-0.087841
O	0.882723	-5.143022	-1.423578
O	-2.425464	-5.128805	-2.009489
O	-0.422599	-3.637739	-3.279279
O	2.116979	-3.637739	-3.279279
O	-2.425464	-5.128805	-4.549068
O	0.820852	-2.147015	1.104956
O	2.901730	-0.699500	0.072769
O	-1.198539	-0.609661	0.038983
O	0.876255	-2.142076	-1.430416
O	-2.425464	-2.146674	-2.009489
O	-0.422599	-0.655609	-3.279279
O	2.116979	-0.655609	-3.279279
O	-2.425464	-2.146674	-4.549068
O	0.837181	0.832488	1.075521
O	2.877724	2.313582	-0.044887
O	-1.223827	2.349040	0.109424
O	0.826020	0.833058	-1.439331
O	-2.425464	0.835456	-2.009489
O	-0.422599	2.326522	-3.279279
O	2.116979	2.326522	-3.279279
O	-2.425464	0.835456	-4.549068
O	0.862395	3.809900	1.109290
O	2.896985	5.330698	0.078791
O	-1.220645	5.316203	0.124693
O	0.818431	3.828607	-1.426043
O	-2.425464	3.817587	-2.009489
O	-0.422599	5.308652	-3.279279
O	2.116979	5.308652	-3.279279
O	-2.425464	3.817587	-4.549068
O	0.850435	6.803102	1.131469
O	2.920446	8.295634	0.122154
O	-1.207222	8.288137	0.105061
O	0.845091	6.804554	-1.419558
O	-2.425464	6.799716	-2.009489
O	-0.422599	8.290782	-3.279279
O	2.116979	8.290782	-3.279279
O	-2.425464	6.799716	-4.549068
O	-5.686376	-5.126415	1.216970
O	-3.735633	-3.677636	-0.108121
O	5.381555	-6.629391	0.090406
O	-5.739659	-5.146122	-1.409275
O	4.119843	-8.110935	-2.009489
O	-6.967910	-3.637740	-3.279279
O	-4.428331	-3.637740	-3.279279
O	4.119843	-8.110935	-4.549068
O	-5.655517	-2.182261	1.137216
O	-3.688391	-0.599009	0.045924
O	5.367224	-3.660574	0.129727
O	-5.732718	-2.135599	-1.398981
O	4.119843	-5.128805	-2.009489
O	-6.967910	-0.655609	-3.279279
O	-4.428331	-0.655609	-3.279279
O	4.119843	-5.128805	-4.549068
O	-5.699472	0.851122	1.156192

O	-3.689514	2.349512	0.097613
O	5.397311	-0.715830	0.030509
O	-5.697382	0.836129	-1.394134
O	4.119843	-2.146674	-2.009489
O	6.122707	-0.655609	-3.279279
O	-4.428331	2.326522	-3.279279
O	4.119843	-2.146674	-4.549068
O	-5.740909	3.824793	1.192365
O	-3.681902	5.312479	0.084947
O	5.431836	2.371513	-0.135429
O	-5.657189	3.806518	-1.411630
O	4.119843	0.835456	-2.009489
O	6.122707	2.326522	-3.279279
O	-4.428331	5.308652	-3.279279
O	4.119843	0.835456	-4.549068
O	7.372257	3.784643	1.139879
O	-3.667074	8.284751	0.129138
O	5.373047	5.332695	0.098933
O	7.437554	3.842684	-1.401442
O	4.119843	3.817587	-2.009489
O	6.122707	5.308652	-3.279279
O	-4.428331	8.290782	-3.279279
O	4.119843	3.817587	-4.549068
O	-5.691962	-8.093473	1.162465
O	-3.684015	-6.642544	0.098169
O	5.384061	8.297108	0.102534
O	-5.695541	-8.106689	-1.388078
O	4.119843	6.799717	-2.009489
O	-6.967910	-6.619867	-3.279279
O	-4.428331	-6.619868	-3.279279
O	4.119843	6.799717	-4.549068
O	2.375820	-7.251061	6.398418
O	3.988584	-6.793719	7.916912
O	-2.342953	-4.620794	2.169301
O	-2.514115	-2.395232	1.854872
O	4.007536	3.248495	2.274662
O	4.340592	1.060238	1.872948
O	6.075484	3.219505	9.470313
O	5.223862	2.845025	11.534060
C	-1.233082	-1.573712	9.850642
C	-1.246662	2.083787	6.862531
C	2.496558	-2.818475	8.160548
C	3.022216	-4.103331	8.150897
C	2.477923	-5.047177	7.272042
C	1.417825	-4.665073	6.449172
C	0.934329	-3.356848	6.511669
C	3.039744	-6.430547	7.255604
C	-0.227318	-2.887062	5.734613
C	-1.824043	-1.190032	5.556695
C	-2.429893	-1.825476	4.486863
C	-1.872819	-3.011164	3.974421
C	-0.795962	-3.582353	4.652844
C	-2.284192	-3.431484	2.586859
C	1.600008	-0.114271	4.551907
C	2.351892	0.466878	3.557550

C	3.243656	1.505179	3.858271
C	3.415646	1.842099	5.203545
C	2.692151	1.134459	6.185197
C	3.932190	2.049995	2.618159
C	2.874295	1.277748	7.644697
C	2.063150	0.649114	9.752564
C	3.051921	1.383046	10.397510
C	4.009377	2.051965	9.627041
C	3.906123	2.010530	8.235715
C	5.135824	2.742523	10.329299
H	2.871888	-2.062170	8.839155
H	3.824812	-4.377529	8.826112
H	0.959575	-5.389346	5.788657
H	-2.187055	-0.248966	5.951869
H	-3.301253	-1.377099	4.023756
H	-0.356865	-4.502656	4.286076
H	0.854055	-0.860808	4.311948
H	2.205531	0.152235	2.542684
H	4.116876	2.618703	5.491407
H	1.298145	0.098375	10.290985
H	3.098515	1.423550	11.479721
H	4.635352	2.534114	7.629469
H	2.801146	-8.125510	6.435211
H	-6.250025	3.825466	2.017185
H	-5.188149	-5.125807	2.045983
H	6.801420	3.586032	10.002771
N	-0.484178	-1.135863	9.043421
N	-0.583481	1.159351	7.181950
N	1.484984	-2.434242	7.357305
N	-0.692757	-1.664316	6.119018
N	1.753274	0.202549	5.845612
N	1.991719	0.566039	8.409010
S	-2.230761	-2.179024	10.977457
S	-2.164774	3.347568	6.396115
Ru	0.557323	-0.555611	7.371034

(8) 2COOH-diff(2trans)-1row 2BB

203

Ti	6.728149	2.992399	-0.197701
Ti	-3.035316	-7.484913	0.085172
Ti	-3.064949	8.945033	-3.279281
Ti	6.753019	4.471836	-3.279281
Ti	-6.301932	-5.962026	-0.197721
Ti	-3.041038	-4.544504	0.073118
Ti	-3.064949	-5.965622	-3.279281
Ti	-6.337604	-4.474557	-3.279281
Ti	-6.384870	-2.981512	-0.196903
Ti	-3.099814	-1.615435	0.008695
Ti	-3.064949	-2.983492	-3.279281
Ti	-6.337604	-1.492425	-3.279281
Ti	-6.361628	0.009362	-0.199879
Ti	-3.077756	1.614017	-0.006953
Ti	-3.064949	-0.001360	-3.279281

Ti	-6.337604	1.489706	-3.279281
Ti	-6.333761	3.005363	-0.196756
Ti	-3.016905	4.549802	0.066827
Ti	-3.064949	2.980772	-3.279281
Ti	6.753019	-1.492425	-3.279281
Ti	6.761196	0.008949	-0.197951
Ti	-3.068004	7.477342	0.081536
Ti	-3.064949	5.962903	-3.279281
Ti	6.753019	1.489707	-3.279281
Ti	0.187817	8.940640	-0.205005
Ti	3.406178	-7.361176	0.000088
Ti	3.480361	8.945032	-3.279281
Ti	0.207705	-7.456688	-3.279281
Ti	0.196996	-5.904566	-0.134920
Ti	3.455945	-4.416858	0.060248
Ti	3.480361	-5.965623	-3.279281
Ti	0.207705	-4.474557	-3.279281
Ti	0.211681	-2.922623	-0.114657
Ti	3.465101	-1.460353	0.084132
Ti	3.480361	-2.983492	-3.279281
Ti	0.207705	-1.492426	-3.279281
Ti	0.152720	0.008875	-0.223128
Ti	3.470490	1.465913	0.079572
Ti	3.480361	-0.001360	-3.279281
Ti	0.207705	1.489706	-3.279281
Ti	0.243781	2.945437	-0.127967
Ti	3.465562	4.410290	0.063057
Ti	3.480361	2.980771	-3.279281
Ti	0.207705	4.471837	-3.279281
Ti	0.206569	5.923302	-0.105952
Ti	3.453767	7.328978	0.031173
Ti	3.480361	5.962904	-3.279281
Ti	0.207705	7.453970	-3.279281
O	-3.074690	-8.945564	1.164672
O	-1.025850	-7.467621	0.089424
O	-5.120920	-7.457708	0.138739
O	-3.076129	-8.934102	-1.400778
O	6.753019	2.980769	-2.009491
O	-4.334739	-7.456688	-3.279281
O	-1.795159	-7.456688	-3.279281
O	6.753019	2.980769	-4.549073
O	-3.065153	-5.973209	1.159061
O	-1.076296	-4.498510	-0.067527
O	-5.114044	-4.464640	0.092116
O	-3.102974	-5.963715	-1.408559
O	-6.337604	-5.965623	-2.009491
O	-4.334739	-4.474556	-3.279281
O	-1.795159	-4.474557	-3.279281
O	-6.337604	-5.965623	-4.549073
O	-3.059945	-2.988712	1.144684
O	-1.077540	-1.454803	0.019813
O	-5.115790	-1.483977	0.157834
O	-3.106330	-2.949709	-1.402640
O	-6.337604	-2.983492	-2.009491
O	-4.334739	-1.492425	-3.279281

O	-1.795159	-1.492426	-3.279281
O	-6.337604	-2.983492	-4.549073
O	-3.024448	0.006853	1.211878
O	-1.064886	1.483271	0.034462
O	-5.109539	1.492857	0.157164
O	-3.099179	0.011248	-1.415339
O	-6.337604	-0.001360	-2.009491
O	-4.334739	1.489706	-3.279281
O	-1.795159	1.489706	-3.279281
O	-6.337604	-0.001360	-4.549073
O	-3.059116	2.997202	1.129573
O	-1.076016	4.494484	-0.092907
O	-5.106720	4.486391	0.090529
O	-3.111914	2.958218	-1.406496
O	-6.337604	2.980772	-2.009491
O	-4.334739	4.471837	-3.279281
O	-1.795159	4.471837	-3.279281
O	-6.337604	2.980772	-4.549073
O	-3.060213	5.982492	1.160248
O	-1.028606	7.482988	0.075490
O	7.979193	1.495070	0.104920
O	-3.096771	5.977668	-1.409811
O	6.753019	-0.001359	-2.009491
O	-4.334739	7.453970	-3.279281
O	-1.795159	7.453970	-3.279281
O	6.753019	-0.001359	-4.549073
O	3.540723	-8.941229	1.237629
O	-7.571077	-1.483981	0.089601
O	1.462891	-7.469476	0.128380
O	3.496413	-8.934087	-1.407659
O	0.207705	8.945032	-2.009491
O	2.210571	-7.456688	-3.279281
O	-8.340472	-1.492426	-3.279281
O	0.207705	8.945032	-4.549073
O	3.492592	-5.955647	1.114451
O	5.528511	-4.462354	0.085052
O	1.486373	-4.495234	-0.080836
O	3.505575	-5.996707	-1.408451
O	0.207705	-5.965623	-2.009491
O	2.210571	-4.474557	-3.279281
O	4.750150	-4.474557	-3.279281
O	0.207705	-5.965623	-4.549073
O	3.448066	-2.970606	1.144963
O	5.533044	-1.489538	0.145124
O	1.445838	-1.430982	0.042021
O	3.510821	-2.972518	-1.413836
O	0.207705	-2.983491	-2.009491
O	2.210571	-1.492426	-3.279281
O	4.750150	-1.492425	-3.279281
O	0.207705	-2.983491	-4.549073
O	3.482186	0.006802	1.169666
O	5.529616	1.496743	0.142723
O	1.451531	1.447526	0.045095
O	3.516142	0.001554	-1.398454
O	0.207705	-0.001360	-2.009491

O	2.210571	1.489706	-3.279281
O	4.750150	1.489707	-3.279281
O	0.207705	-0.001360	-4.549073
O	3.450490	2.976918	1.154890
O	5.518818	4.479083	0.082914
O	1.497571	4.503233	-0.099099
O	3.519605	2.973515	-1.409572
O	0.207705	2.980772	-2.009491
O	2.210571	4.471838	-3.279281
O	4.750150	4.471838	-3.279281
O	0.207705	2.980772	-4.549073
O	3.470015	5.946326	1.151804
O	-7.569180	-4.473352	0.137591
O	1.469199	7.486874	0.113583
O	3.513190	6.001213	-1.397435
O	0.207705	5.962903	-2.009491
O	2.210571	7.453970	-3.279281
O	4.750150	7.453970	-3.279281
O	0.207705	5.962903	-4.549073
O	0.462585	-5.295167	2.355218
O	0.182300	-3.119336	1.815318
O	-6.070396	-2.930150	5.328142
O	-7.006404	-1.263851	6.524766
O	0.244748	3.204691	1.833235
O	0.137494	5.427419	2.192709
O	6.148032	2.784442	5.686522
O	6.879163	1.434659	7.339388
C	0.458752	-2.402789	9.211760
C	-0.888734	2.483875	9.421960
C	1.316897	-1.811238	5.432835
C	1.412384	-2.823791	4.494029
C	0.238801	-3.436176	4.030403
C	-0.969917	-3.067026	4.613092
C	-0.991465	-2.049818	5.582452
C	0.281922	-4.100512	2.661966
C	-2.224051	-1.547875	6.217197
C	-3.138166	-0.009105	7.730999
C	-4.424991	-0.450725	7.474633
C	-4.616331	-1.466312	6.530156
C	-3.499996	-2.020954	5.904629
C	-6.005809	-1.844372	6.156219
C	-1.292844	2.312478	5.471419
C	-1.256106	3.303162	4.499338
C	-0.011449	3.705334	4.002786
C	1.137349	3.211429	4.623032
C	1.026674	2.257940	5.638470
C	0.106066	4.239053	2.586435
C	2.177860	1.703219	6.372756
C	2.862721	0.270494	8.093183
C	4.189294	0.645410	7.935385
C	4.522688	1.555678	6.926243
C	3.498340	2.090569	6.142402
C	5.953489	1.896512	6.707235
H	2.192314	-1.257268	5.734923
H	2.372728	-3.057827	4.048764

H	-1.892938	-3.517596	4.262514
H	-2.928911	0.813875	8.406178
H	-5.278124	-0.009979	7.977760
H	-3.638318	-2.793438	5.157301
H	-2.237203	1.924251	5.835267
H	-2.180000	3.689136	4.079280
H	2.111535	3.497269	4.245104
H	2.554403	-0.470995	8.820871
H	4.963287	0.232317	8.574951
H	3.735557	2.790802	5.350802
H	3.063869	-8.936027	2.082261
H	-7.020984	-3.161899	5.277735
H	-3.433508	0.014602	2.087404
H	7.118566	2.855593	5.567515
N	0.240887	-1.342227	8.734058
N	-0.625412	1.517898	8.792369
N	0.148412	-1.399069	5.957942
N	-2.053722	-0.528760	7.114345
N	-0.186624	1.747773	5.997237
N	1.869870	0.770394	7.324104
S	0.784438	-3.836149	9.887042
S	-1.288333	3.792941	10.282695
Ru	-0.109444	0.145093	7.378828

(8) 2COOH-diff(2trans)-1row 1BB1MH

203

Ti	6.752467	2.976481	-0.196777
Ti	-3.053548	-7.492311	0.094444
Ti	-3.064949	8.945033	-3.279281
Ti	6.753019	4.471836	-3.279281
Ti	-6.347539	-5.975193	-0.197906
Ti	-3.083849	-4.547105	0.064982
Ti	-3.064949	-5.965622	-3.279281
Ti	-6.337604	-4.474557	-3.279281
Ti	-6.350623	-2.986447	-0.195302
Ti	-3.046100	-1.600970	-0.011766
Ti	-3.064949	-2.983492	-3.279281
Ti	-6.337604	-1.492425	-3.279281
Ti	-6.324687	-0.001095	-0.201228
Ti	-3.037480	1.597542	0.000468
Ti	-3.064949	-0.001360	-3.279281
Ti	-6.337604	1.489706	-3.279281
Ti	-6.331410	2.987695	-0.195717
Ti	-3.034703	4.529947	0.056899
Ti	-3.064949	2.980772	-3.279281
Ti	6.753019	-1.492425	-3.279281
Ti	6.752187	-0.002336	-0.197131
Ti	-3.053910	7.463237	0.084658
Ti	-3.064949	5.962903	-3.279281
Ti	6.753019	1.489707	-3.279281
Ti	0.209422	8.926201	-0.204895
Ti	3.467151	-7.466435	0.084166
Ti	3.480361	8.945032	-3.279281

Ti	0.207705	-7.456688	-3.279281
Ti	0.209077	-5.977609	-0.211226
Ti	3.489187	-4.484009	0.073903
Ti	3.480361	-5.965623	-3.279281
Ti	0.207705	-4.474557	-3.279281
Ti	0.230087	-2.995688	-0.099105
Ti	3.466542	-1.496174	0.069999
Ti	3.480361	-2.983492	-3.279281
Ti	0.207705	-1.492426	-3.279281
Ti	0.186471	-0.006186	-0.224110
Ti	3.467538	1.481815	0.074068
Ti	3.480361	-0.001360	-3.279281
Ti	0.207705	1.489706	-3.279281
Ti	0.234689	2.978320	-0.112583
Ti	3.462014	4.465342	0.044656
Ti	3.480361	2.980771	-3.279281
Ti	0.207705	4.471837	-3.279281
Ti	0.201525	5.937292	-0.101945
Ti	3.460531	7.445334	0.077373
Ti	3.480361	5.962904	-3.279281
Ti	0.207705	7.453970	-3.279281
O	-3.073679	8.944364	1.159232
O	-1.030550	-7.456091	0.115130
O	-5.104428	-7.453797	0.116006
O	-3.073498	-8.933459	-1.401850
O	6.753019	2.980769	-2.009491
O	-4.334739	-7.456688	-3.279281
O	-1.795159	-7.456688	-3.279281
O	6.753019	2.980769	-4.549073
O	-3.054669	-5.965734	1.168978
O	-1.043030	-4.516395	0.091864
O	-5.104973	-4.479399	0.113179
O	-3.077890	-5.953252	-1.406826
O	-6.337604	-5.965623	-2.009491
O	-4.334739	-4.474556	-3.279281
O	-1.795159	-4.474557	-3.279281
O	-6.337604	-5.965623	-4.549073
O	-3.056079	-2.990096	1.119102
O	-1.066653	-1.481800	0.038446
O	-5.090880	-1.491108	0.135269
O	-3.088860	-2.974034	-1.409675
O	-6.337604	-2.983492	-2.009491
O	-4.334739	-1.492425	-3.279281
O	-1.795159	-1.492426	-3.279281
O	-6.337604	-2.983492	-4.549073
O	-3.037887	-0.009822	1.227628
O	-1.066038	1.452385	0.041339
O	-5.092034	1.479999	0.145118
O	-3.086820	-0.009198	-1.411699
O	-6.337604	-0.001360	-2.009491
O	-4.334739	1.489706	-3.279281
O	-1.795159	1.489706	-3.279281
O	-6.337604	-0.001360	-4.549073
O	-3.048754	2.983732	1.123797
O	-1.085737	4.483304	-0.114320

O	-5.107753	4.473194	0.112702
O	-3.111137	2.954526	-1.407817
O	-6.337604	2.980772	-2.009491
O	-4.334739	4.471837	-3.279281
O	-1.795159	4.471837	-3.279281
O	-6.337604	2.980772	-4.549073
O	-3.048146	5.967728	1.147230
O	-1.042445	7.487843	0.071721
O	7.982790	1.491005	0.116901
O	-3.107959	5.973244	-1.410328
O	6.753019	-0.001359	-2.009491
O	-4.334739	7.453970	-3.279281
O	-1.795159	7.453970	-3.279281
O	6.753019	-0.001359	-4.549073
O	3.491952	8.942397	1.133065
O	-7.540671	-1.490960	0.121200
O	1.431622	-7.455930	0.116623
O	3.491099	-8.938654	-1.417854
O	0.207705	8.945032	-2.009491
O	2.210571	-7.456688	-3.279281
O	-8.340472	-1.492426	-3.279281
O	0.207705	8.945032	-4.549073
O	3.489383	-5.965891	1.130946
O	5.549283	-4.477650	0.117798
O	1.441263	-4.500265	0.059141
O	3.494199	-5.967569	-1.420801
O	0.207705	-5.965623	-2.009491
O	2.210571	-4.474557	-3.279281
O	4.750150	-4.474557	-3.279281
O	0.207705	-5.965623	-4.549073
O	3.474974	-2.987011	1.122983
O	5.538363	-1.499205	0.115098
O	1.432994	-1.481167	0.045315
O	3.500121	-2.985774	-1.422875
O	0.207705	-2.983491	-2.009491
O	2.210571	-1.492426	-3.279281
O	4.750150	-1.492425	-3.279281
O	0.207705	-2.983491	-4.549073
O	3.477554	-0.009193	1.133126
O	5.536549	1.488234	0.123925
O	1.430443	1.448555	0.064620
O	3.500862	-0.003488	-1.418795
O	0.207705	-0.001360	-2.009491
O	2.210571	1.489706	-3.279281
O	4.750150	1.489707	-3.279281
O	0.207705	-0.001360	-4.549073
O	3.454965	2.982413	1.117791
O	5.539516	4.469371	0.116487
O	1.477520	4.480457	-0.113606
O	3.518649	2.966078	-1.424486
O	0.207705	2.980772	-2.009491
O	2.210571	4.471838	-3.279281
O	4.750150	4.471838	-3.279281
O	0.207705	2.980772	-4.549073
O	3.465441	5.950788	1.118264

O	-7.548640	-4.471641	0.123571
O	1.439646	7.483362	0.077469
O	3.523518	5.979976	-1.424799
O	0.207705	5.962903	-2.009491
O	2.210571	7.453970	-3.279281
O	4.750150	7.453970	-3.279281
O	0.207705	5.962903	-4.549073
O	-1.347994	-3.945454	3.379602
O	0.203784	-2.898761	2.106874
O	-5.977683	-2.178372	7.239943
O	-6.739958	-0.573087	8.640114
O	0.192444	3.307307	1.886724
O	0.186154	5.563641	2.031797
O	6.180924	4.337598	6.351387
O	7.002363	2.905035	7.894668
C	0.691718	-1.377855	9.639281
C	-0.306495	3.595198	9.982041
C	1.059402	-0.417811	5.441757
C	0.940672	-1.321400	4.402853
C	-0.245027	-2.068813	4.291531
C	-1.263931	-1.846495	5.224499
C	-1.106868	-0.868181	6.204475
C	-0.434527	-3.000075	3.166904
C	-2.186399	-0.458963	7.118285
C	-2.820892	1.061359	8.783277
C	-4.106179	0.537587	8.833664
C	-4.431996	-0.533634	7.994565
C	-3.456078	-1.042522	7.137489
C	-5.826677	-1.072214	8.021007
C	-1.150558	3.172052	5.811282
C	-1.134715	3.867184	4.609058
C	0.103138	4.137786	4.016126
C	1.269932	3.835417	4.714988
C	1.175832	3.160564	5.935397
C	0.169143	4.408672	2.536264
C	2.347051	2.749344	6.735219
C	3.082302	1.391344	8.493761
C	4.380256	1.876464	8.375852
C	4.660790	2.827939	7.390293
C	3.627101	3.279763	6.567906
C	6.060409	3.334396	7.265197
H	1.976651	0.139497	5.582456
H	1.755110	-1.471835	3.701490
H	-2.186037	-2.409399	5.157812
H	-2.499711	1.872541	9.426669
H	-4.845689	0.942431	9.513767
H	-3.696715	-1.874256	6.488769
H	-2.081966	2.870734	6.277200
H	-2.062978	4.120547	4.110300
H	2.238179	4.038171	4.272457
H	2.801433	0.655305	9.238971
H	5.162815	1.539248	9.046407
H	3.823899	4.042675	5.824189
H	-1.523378	-4.455668	2.570439
H	-6.907808	-2.449868	7.297408

H	-3.529847	-0.007187	2.057586
H	7.111346	4.612323	6.350486
N	0.516818	-0.302487	9.170203
N	-0.148216	2.610063	9.340873
N	0.066915	-0.168905	6.331897
N	-1.887193	0.590507	7.932555
N	-0.028723	2.755815	6.422942
N	2.090270	1.807292	7.684376
S	0.953173	-2.837291	10.290088
S	-0.547586	4.936734	10.855208
Ru	0.101926	1.216431	7.867326

(8) 2COOH-diff(2trans)-1row 2MH

203

Ti	6.768178	2.977174	-0.197836
Ti	-3.050851	-7.472374	0.094301
Ti	-3.064950	8.945036	-3.279283
Ti	6.753021	4.471838	-3.279283
Ti	-6.347255	-5.973210	-0.199400
Ti	-3.098494	-4.488514	0.028142
Ti	-3.064950	-5.965626	-3.279283
Ti	-6.337607	-4.474559	-3.279283
Ti	-6.346549	-2.981450	-0.199490
Ti	-3.053782	-1.502806	0.072291
Ti	-3.064950	-2.983493	-3.279283
Ti	-6.337607	-1.492426	-3.279283
Ti	-6.327309	-0.004147	-0.198884
Ti	-3.056364	1.466122	0.077630
Ti	-3.064950	-0.001360	-3.279283
Ti	-6.337607	1.489707	-3.279283
Ti	-6.352439	2.973907	-0.199745
Ti	-3.107127	4.449010	0.024250
Ti	-3.064950	2.980773	-3.279283
Ti	6.753021	-1.492426	-3.279283
Ti	6.739603	0.002195	-0.199002
Ti	-3.048564	7.438966	0.092059
Ti	-3.064950	5.962906	-3.279283
Ti	6.753021	1.489708	-3.279283
Ti	0.211495	-8.948565	-0.197580
Ti	3.476827	-7.467052	0.084122
Ti	3.480362	8.945036	-3.279283
Ti	0.207706	-7.456692	-3.279283
Ti	0.215210	-5.967604	-0.215402
Ti	3.474942	-4.486216	0.073991
Ti	3.480362	-5.965626	-3.279283
Ti	0.207706	-4.474559	-3.279283
Ti	0.202741	-2.987858	-0.107680
Ti	3.467023	-1.501046	0.073985
Ti	3.480362	-2.983493	-3.279283
Ti	0.207706	-1.492426	-3.279283
Ti	0.211455	-0.002517	-0.219348
Ti	3.468885	1.480907	0.075413
Ti	3.480362	-0.001360	-3.279283

Ti	0.207706	1.489707	-3.279283
Ti	0.201527	2.982939	-0.108392
Ti	3.477569	4.462062	0.073049
Ti	3.480362	2.980773	-3.279283
Ti	0.207706	4.471839	-3.279283
Ti	0.220718	5.963433	-0.217983
Ti	3.476972	7.444870	0.085233
Ti	3.480362	5.962906	-3.279283
Ti	0.207706	7.453973	-3.279283
O	-3.066102	8.937370	1.145033
O	-1.017533	-7.467138	0.121932
O	-5.105870	-7.455511	0.120956
O	-3.061086	-8.944575	-1.409376
O	6.753021	2.980771	-2.009491
O	-4.334740	-7.456691	-3.279283
O	-1.795160	-7.456692	-3.279283
O	6.753021	2.980771	-4.549075
O	-3.036301	-5.948996	1.139536
O	-1.038872	-4.524226	0.065476
O	-5.114696	-4.479797	0.109847
O	-3.081308	-5.971332	-1.420589
O	-6.337607	-5.965626	-2.009491
O	-4.334740	-4.474559	-3.279283
O	-1.795160	-4.474559	-3.279283
O	-6.337607	-5.965626	-4.549075
O	-3.047307	-3.002918	1.114880
O	-1.036292	-1.475692	0.050319
O	-5.112065	-1.498703	0.116723
O	-3.084491	-2.984622	-1.424576
O	-6.337607	-2.983493	-2.009491
O	-4.334740	-1.492426	-3.279283
O	-1.795160	-1.492426	-3.279283
O	-6.337607	-2.983493	-4.549075
O	-3.060414	-0.010459	1.139847
O	-1.034085	1.474931	0.060267
O	-5.113400	1.490076	0.117780
O	-3.084100	0.002285	-1.414966
O	-6.337607	-0.001360	-2.009491
O	-4.334740	1.489707	-3.279283
O	-1.795160	1.489707	-3.279283
O	-6.337607	-0.001360	-4.549075
O	-3.051131	2.987900	1.117362
O	-1.038459	4.521142	0.065899
O	-5.116789	4.470557	0.108501
O	-3.083678	2.986192	-1.424080
O	-6.337607	2.980773	-2.009491
O	-4.334740	4.471839	-3.279283
O	-1.795160	4.471839	-3.279283
O	-6.337607	2.980773	-4.549075
O	-3.031805	5.932020	1.136820
O	-1.015645	7.459430	0.122382
O	7.984003	1.481269	0.119983
O	-3.082554	5.974206	-1.421656
O	6.753021	-0.001359	-2.009491
O	-4.334740	7.453972	-3.279283

O	-1.795160	7.453973	-3.279283
O	6.753021	-0.001359	-4.549075
O	3.490093	8.939811	1.136762
O	-7.556248	-1.493733	0.113166
O	1.435707	-7.469658	0.113401
O	3.485217	-8.946592	-1.418628
O	0.207706	8.945036	-2.009491
O	2.210572	-7.456692	-3.279283
O	-8.340476	-1.492427	-3.279283
O	0.207706	8.945036	-4.549075
O	3.480665	-5.969575	1.131903
O	5.532642	-4.479906	0.113262
O	1.443042	-4.506033	0.057551
O	3.489230	-5.969550	-1.422176
O	0.207706	-5.965626	-2.009491
O	2.210572	-4.474559	-3.279283
O	4.750152	-4.474559	-3.279283
O	0.207706	-5.965626	-4.549075
O	3.470778	-2.989112	1.128171
O	5.531973	-1.494516	0.119946
O	1.440996	-1.481723	0.055461
O	3.498661	-2.982810	-1.420423
O	0.207706	-2.983493	-2.009491
O	2.210572	-1.492426	-3.279283
O	4.750152	-1.492426	-3.279283
O	0.207706	-2.983493	-4.549075
O	3.474434	-0.005090	1.132547
O	5.536142	1.491213	0.117162
O	1.440275	1.481303	0.062929
O	3.497623	0.001567	-1.419615
O	0.207706	-0.001360	-2.009491
O	2.210572	1.489707	-3.279283
O	4.750152	1.489707	-3.279283
O	0.207706	-0.001360	-4.549075
O	3.473619	2.978313	1.130550
O	5.538303	4.466023	0.115943
O	1.445904	4.501342	0.056481
O	3.497458	2.983881	-1.420040
O	0.207706	2.980773	-2.009491
O	2.210572	4.471839	-3.279283
O	4.750152	4.471840	-3.279283
O	0.207706	2.980773	-4.549075
O	3.483726	5.955319	1.133320
O	-7.555625	-4.478272	0.117872
O	1.437682	7.463000	0.112646
O	3.493000	5.970148	-1.420595
O	0.207706	5.962906	-2.009491
O	2.210572	7.453972	-3.279283
O	4.750152	7.453973	-3.279283
O	0.207706	5.962906	-4.549075
O	-1.315430	-4.348239	3.199172
O	0.151771	-3.002896	2.095375
O	-5.970234	-3.023091	7.323343
O	-6.695162	-1.587998	8.913742
O	0.167833	3.057298	2.125440

O	-1.197064	4.634698	3.052157
O	6.056178	3.343527	6.218734
O	6.996854	2.079395	7.837962
C	0.934469	-2.421691	9.956783
C	-0.283864	2.546761	10.429660
C	1.160020	-1.333651	5.842352
C	1.019738	-2.051874	4.668780
C	-0.214444	-2.662223	4.409742
C	-1.250463	-2.524995	5.336204
C	-1.063043	-1.725579	6.464556
C	-0.439715	-3.357025	3.125150
C	-2.136577	-1.401137	7.423686
C	-2.733048	-0.096318	9.273030
C	-4.033388	-0.587927	9.253065
C	-4.385462	-1.526637	8.277768
C	-3.419401	-1.949629	7.365533
C	-5.794458	-2.025923	8.233998
C	-1.273036	2.168998	6.433196
C	-1.383411	2.886218	5.253756
C	-0.233166	3.057506	4.471517
C	1.006547	2.654441	4.971961
C	1.055416	2.043100	6.225610
C	-0.387992	3.589070	3.094863
C	2.294708	1.698754	6.950605
C	3.165008	0.529680	8.787170
C	4.441459	1.019436	8.541013
C	4.639345	1.882801	7.458239
C	3.549740	2.230372	6.654152
C	6.012426	2.418805	7.218160
H	2.109060	-0.894359	6.118469
H	1.848746	-2.161076	3.978067
H	-2.204577	-2.997646	5.144649
H	-2.398717	0.622917	10.012243
H	-4.765274	-0.262386	9.982812
H	-3.674315	-2.692203	6.620530
H	-2.137346	1.935653	7.042667
H	-2.344292	3.253345	4.914171
H	1.906356	2.801137	4.385572
H	2.941705	-0.148856	9.603137
H	5.267756	0.753110	9.189650
H	3.685532	2.925668	5.835165
H	-1.598829	-4.689692	2.325367
H	-6.904607	-3.283861	7.353620
H	-1.506981	4.883035	2.154425
H	6.970351	3.667191	6.176223
N	0.695097	-1.333136	9.549695
N	-0.088547	1.548907	9.818008
N	0.142199	-1.127820	6.707987
N	-1.810620	-0.475037	8.367300
N	-0.094553	1.701562	6.883195
N	2.118165	0.851431	8.004375
S	1.282940	-3.897494	10.522724
S	-0.571835	3.901277	11.266988
Ru	0.170517	0.199496	8.303988

(9) 2COOH-diff(cis,trans)-1row 1BB1M

203

Ti	6.585017	-2.222961	-0.206784
Ti	-3.226493	-6.576135	0.026822
Ti	-3.272659	-8.205334	-3.279281
Ti	6.545309	-0.750005	-3.279281
Ti	6.553866	0.758440	-0.202980
Ti	-3.220532	-3.647805	0.046725
Ti	-3.272659	-5.223203	-3.279281
Ti	6.545309	2.232126	-3.279281
Ti	-6.505196	-2.231143	-0.203824
Ti	-3.236550	-0.715267	0.058394
Ti	-3.272659	-2.241071	-3.279281
Ti	-6.545314	-0.750005	-3.279281
Ti	-6.571049	0.739475	-0.200158
Ti	-3.310772	2.219673	0.073339
Ti	-3.272659	0.741060	-3.279281
Ti	-6.545314	2.232126	-3.279281
Ti	-6.579620	3.725243	-0.205228
Ti	-3.223835	5.163261	0.084634
Ti	-3.272659	3.723192	-3.279281
Ti	-6.545314	5.214258	-3.279281
Ti	6.606195	-5.217694	-0.203222
Ti	-3.206394	8.106021	-0.045784
Ti	-3.272659	6.705324	-3.279281
Ti	6.545309	-3.732135	-3.279281
Ti	0.007429	-8.183412	-0.217278
Ti	3.272927	-6.613212	-0.009084
Ti	3.272651	-8.205334	-3.279281
Ti	-0.000005	-6.714267	-3.279281
Ti	0.031893	-5.162073	-0.108902
Ti	3.324295	-3.686568	0.049771
Ti	3.272651	-5.223202	-3.279281
Ti	-0.000005	-3.732137	-3.279281
Ti	0.069350	-2.217896	-0.119750
Ti	3.287651	-0.730741	0.061183
Ti	3.272651	-2.241071	-3.279281
Ti	-0.000005	-0.750005	-3.279281
Ti	-0.030985	0.737556	-0.232148
Ti	3.285173	2.213252	0.059054
Ti	3.272651	0.741060	-3.279281
Ti	-0.000005	2.232127	-3.279281
Ti	0.052535	3.668230	-0.090351
Ti	3.261944	5.167912	0.047555
Ti	3.272651	3.723192	-3.279281
Ti	-0.000005	5.214258	-3.279281
Ti	0.002337	6.655498	-0.175822
Ti	3.212390	8.095747	-0.002636
Ti	3.272651	6.705324	-3.279281
Ti	-0.000005	8.196390	-3.279281
O	-3.313346	-8.203598	1.210246
O	-1.246128	-6.735021	0.102680
O	7.797257	-0.738734	0.096108

O	-3.289019	-8.220601	-1.406710
O	6.545309	-2.241071	-2.009491
O	-4.542449	-6.714267	-3.279281
O	-2.002869	-6.714268	-3.279281
O	6.545309	-2.241071	-4.549073
O	-3.251725	-5.195305	1.154106
O	-1.264339	-3.733011	-0.071357
O	-5.302803	-3.727751	0.100078
O	-3.296409	-5.253522	-1.397473
O	6.545309	0.741060	-2.009491
O	-4.542449	-3.732137	-3.279281
O	-2.002869	-3.732137	-3.279281
O	6.545309	0.741060	-4.549073
O	-3.248355	-2.223601	1.152520
O	-1.246656	-0.730934	0.046340
O	-5.318470	-0.736292	0.121096
O	-3.308709	-2.239636	-1.404454
O	-6.545314	-2.241071	-2.009491
O	-4.542449	-0.750005	-3.279281
O	-2.002869	-0.750005	-3.279281
O	-6.545314	-2.241071	-4.549073
O	-3.262287	0.743099	1.155784
O	-1.237235	2.224866	0.078497
O	-5.334819	2.238174	0.133926
O	-3.290889	0.745219	-1.399102
O	-6.545314	0.741060	-2.009491
O	-4.542449	2.232126	-3.279281
O	-2.002869	2.232126	-3.279281
O	-6.545314	0.741060	-4.549073
O	-3.253049	3.710692	1.162132
O	-1.257199	5.234541	-0.008995
O	-5.323117	5.201861	0.089677
O	-3.299477	3.717333	-1.404107
O	-6.545314	3.723192	-2.009491
O	-4.542449	5.214258	-3.279281
O	-2.002869	5.214258	-3.279281
O	-6.545314	3.723192	-4.549073
O	-3.296508	6.714201	1.113391
O	-1.249930	8.231595	0.089288
O	7.795078	-3.724083	0.080723
O	-3.276806	6.725583	-1.406573
O	6.545309	-5.223200	-2.009491
O	8.548174	-3.732135	-3.279281
O	-2.002869	8.196391	-3.279281
O	6.545309	-5.223200	-4.549073
O	3.271798	-8.198395	1.222307
O	5.315432	-6.704070	0.147368
O	1.250326	-6.728814	0.095296
O	3.274929	-8.196735	-1.391623
O	-0.000005	-8.205334	-2.009491
O	2.002860	-6.714268	-3.279281
O	4.542441	-6.714268	-3.279281
O	-0.000005	-8.205334	-4.549073
O	3.265695	-5.221885	1.128056
O	5.349215	-3.723228	0.140648

O	1.299375	-3.752610	-0.120927
O	3.324525	-5.244407	-1.398867
O	-0.000005	-5.223202	-2.009491
O	2.002860	-3.732137	-3.279281
O	4.542441	-3.732137	-3.279281
O	-0.000005	-5.223202	-4.549073
O	3.257807	-2.240698	1.133901
O	5.346939	-0.744205	0.144719
O	1.254760	-0.697222	0.051175
O	3.322327	-2.231029	-1.408845
O	-0.000005	-2.241071	-2.009491
O	2.002860	-0.750005	-3.279281
O	4.542441	-0.750005	-3.279281
O	-0.000005	-2.241071	-4.549073
O	3.292970	0.739516	1.142624
O	5.341977	2.242483	0.139247
O	1.267373	2.166552	0.012377
O	3.318131	0.739463	-1.407252
O	-0.000005	0.741060	-2.009491
O	2.002860	2.232126	-3.279281
O	4.542441	2.232126	-3.279281
O	-0.000005	0.741060	-4.549073
O	3.251020	3.722763	1.127252
O	5.324715	5.215533	0.103073
O	1.311820	5.323506	-0.143714
O	3.310127	3.720767	-1.410837
O	-0.000005	3.723192	-2.009491
O	2.002860	5.214258	-3.279281
O	4.542441	5.214259	-3.279281
O	-0.000005	3.723192	-4.549073
O	3.273108	6.715475	1.128944
O	-7.785827	2.237622	0.130502
O	1.230371	8.223696	0.131614
O	3.321538	6.751262	-1.406242
O	-0.000005	6.705325	-2.009491
O	2.002860	8.196390	-3.279281
O	-8.548182	2.232127	-3.279281
O	-0.000005	6.705325	-4.549073
O	5.573538	-2.370357	6.739541
O	6.055646	-0.943624	8.405841
O	0.077539	-2.476294	1.874402
O	0.037678	-4.712023	2.177953
O	-0.211429	5.914951	2.751396
O	0.293457	3.952730	1.786472
O	0.359136	6.881512	9.657905
O	-0.276293	6.047930	11.646977
C	-1.342887	-1.799686	9.914527
C	-4.063009	0.937182	6.879103
C	2.078442	0.494275	8.288059
C	3.394504	0.084130	8.366492
C	3.824353	-0.948357	7.546115
C	2.906336	-1.551028	6.686156
C	1.578438	-1.124707	6.694847
C	5.248432	-1.397529	7.628650
C	0.517812	-1.752294	5.878906

C	-1.763067	-1.854131	5.461145
C	-1.581565	-2.751337	4.414610
C	-0.273272	-3.090850	4.033504
C	0.780006	-2.636142	4.831365
C	-0.016713	-3.533873	2.596438
C	-0.731868	1.482129	4.608430
C	-0.621870	2.435154	3.623150
C	-0.376361	3.777442	3.970394
C	-0.228382	4.087078	5.320993
C	-0.387557	3.069911	6.274571
C	-0.115747	4.687310	2.786524
C	-0.413016	3.276502	7.738838
C	-0.897098	2.279060	9.794540
C	-0.689423	3.472043	10.465208
C	-0.321680	4.595573	9.743180
C	-0.208915	4.507859	8.355664
C	-0.092303	5.892667	10.458998
H	1.716820	1.290242	8.903620
H	4.069113	0.534361	9.068605
H	3.222893	-2.342743	6.024026
H	-2.738739	-1.483963	5.722359
H	-2.435348	-3.101530	3.844818
H	1.797655	-2.882976	4.561382
H	-0.906724	0.450017	4.356099
H	-0.668745	2.145946	2.582277
H	0.040059	5.093280	5.606879
H	-1.183713	1.379475	10.293105
H	-0.811850	3.532570	11.527030
H	0.004656	5.385357	7.770715
H	6.513128	-2.558480	6.855593
H	-2.922049	-8.220824	2.088410
H	3.611901	-8.206925	2.119822
H	0.512213	7.665888	10.180153
N	-1.189721	-0.773696	8.959849
N	-2.847168	0.626112	7.103351
N	1.180611	-0.098658	7.500221
N	-0.740077	-1.327549	6.142038
N	-0.612129	1.784556	5.906857
N	-0.734972	2.169325	8.478630
S	-1.490712	-2.821789	10.900007
S	-5.548843	1.303716	6.591843
Ru	-0.874233	0.368925	7.398772

(9) 2COOH-diff(cis,trans)-1row 1BB1MH

203

Ti	6.566209	-2.241185	-0.199852
Ti	-3.261520	-6.606615	0.000830
Ti	-3.272658	-8.205331	-3.279280
Ti	6.545306	-0.750005	-3.279280
Ti	6.541650	0.746965	-0.196560
Ti	-3.238710	-3.671024	0.053355
Ti	-3.272658	-5.223201	-3.279280
Ti	6.545306	2.232125	-3.279280

Ti	-6.527675	-2.240955	-0.196499
Ti	-3.251864	-0.732942	0.078002
Ti	-3.272658	-2.241070	-3.279280
Ti	-6.545311	-0.750005	-3.279280
Ti	-6.552302	0.738823	-0.195295
Ti	-3.277086	2.204846	0.078168
Ti	-3.272658	0.741060	-3.279280
Ti	-6.545311	2.232126	-3.279280
Ti	-6.550028	3.720690	-0.195656
Ti	-3.261432	5.148554	0.092324
Ti	-3.272658	3.723190	-3.279280
Ti	-6.545311	5.214256	-3.279280
Ti	6.539083	-5.229469	-0.196840
Ti	-3.263950	8.086765	0.009320
Ti	-3.272658	6.705321	-3.279280
Ti	6.545306	-3.732133	-3.279280
Ti	-0.010739	-8.190263	-0.209697
Ti	3.251993	-6.716191	0.075659
Ti	3.272649	-8.205331	-3.279280
Ti	-0.000005	-6.714265	-3.279280
Ti	0.003706	-5.190871	-0.103177
Ti	3.270681	-3.736621	0.048977
Ti	3.272649	-5.223200	-3.279280
Ti	-0.000005	-3.732135	-3.279280
Ti	0.025360	-2.236528	-0.110399
Ti	3.274080	-0.754648	0.074877
Ti	3.272649	-2.241070	-3.279280
Ti	-0.000005	-0.750005	-3.279280
Ti	-0.000945	0.737433	-0.225902
Ti	3.270615	2.223067	0.071955
Ti	3.272649	0.741060	-3.279280
Ti	-0.000005	2.232126	-3.279280
Ti	0.007650	3.709688	-0.114117
Ti	3.277998	5.211860	0.061078
Ti	3.272649	3.723190	-3.279280
Ti	-0.000005	5.214256	-3.279280
Ti	0.001000	6.703422	-0.211820
Ti	3.256377	8.197437	0.087466
Ti	3.272649	6.705320	-3.279280
Ti	-0.000005	8.196386	-3.279280
O	-3.314294	-8.206359	1.230208
O	-1.271454	-6.760347	0.081869
O	7.793605	-0.752253	0.104275
O	-3.287989	-8.215083	-1.410701
O	6.545306	-2.241071	-2.009489
O	-4.542447	-6.714265	-3.279280
O	-2.002868	-6.714265	-3.279280
O	6.545306	-2.241071	-4.549070
O	-3.253381	-5.218654	1.120184
O	-1.289035	-3.736771	-0.119109
O	-5.313714	-3.732862	0.110368
O	-3.309259	-5.252765	-1.411609
O	6.545306	0.741060	-2.009489
O	-4.542447	-3.732135	-3.279280
O	-2.002868	-3.732135	-3.279280

O	6.545306	0.741060	-4.549070
O	-3.245668	-2.237999	1.145197
O	-1.245078	-0.715772	0.059990
O	-5.314562	-0.747332	0.116344
O	-3.314820	-2.235254	-1.411868
O	-6.545311	-2.241070	-2.009489
O	-4.542447	-0.750005	-3.279280
O	-2.002868	-0.750005	-3.279280
O	-6.545311	-2.241070	-4.549070
O	-3.264761	0.741852	1.150527
O	-1.247498	2.220198	0.037539
O	-5.316154	2.231908	0.109774
O	-3.293559	0.744406	-1.408221
O	-6.545311	0.741060	-2.009489
O	-4.542447	2.232126	-3.279280
O	-2.002868	2.232126	-3.279280
O	-6.545311	0.741060	-4.549070
O	-3.263168	3.707614	1.155371
O	-1.245394	5.236610	0.075529
O	-5.313090	5.210475	0.114193
O	-3.288814	3.740329	-1.407140
O	-6.545311	3.723190	-2.009489
O	-4.542447	5.214255	-3.279280
O	-2.002868	5.214255	-3.279280
O	-6.545311	3.723190	-4.549070
O	-3.274772	6.704662	1.137098
O	-1.257068	8.199530	0.134463
O	7.795143	-3.734649	0.100007
O	-3.276536	6.724120	-1.403572
O	6.545306	-5.223197	-2.009489
O	8.548170	-3.732133	-3.279280
O	-2.002868	8.196386	-3.279280
O	6.545306	-5.223197	-4.549070
O	3.272139	-8.208387	1.134723
O	5.327969	-6.715762	0.116961
O	1.218237	-6.746663	0.085257
O	3.273214	-8.214021	-1.415212
O	-0.000005	-8.205331	-2.009489
O	2.002860	-6.714265	-3.279280
O	4.542439	-6.714265	-3.279280
O	-0.000005	-8.205331	-4.549070
O	3.257972	-5.219799	1.118176
O	5.345178	-3.732415	0.124857
O	1.271589	-3.753197	-0.099658
O	3.313666	-5.239757	-1.425707
O	-0.000005	-5.223201	-2.009489
O	2.002860	-3.732135	-3.279280
O	4.542439	-3.732135	-3.279280
O	-0.000005	-5.223201	-4.549070
O	3.258076	-2.251044	1.118624
O	5.343333	-0.752710	0.131903
O	1.241404	-0.719689	0.064305
O	3.314855	-2.228734	-1.424346
O	-0.000005	-2.241070	-2.009489
O	2.002860	-0.750005	-3.279280

O	4.542439	-0.750005	-3.279280
O	-0.000005	-2.241070	-4.549070
O	3.277727	0.742837	1.132323
O	5.330226	2.233726	0.114657
O	1.241905	2.217921	0.040509
O	3.297580	0.743497	-1.418076
O	-0.000005	0.741060	-2.009489
O	2.002860	2.232125	-3.279280
O	4.542439	2.232125	-3.279280
O	-0.000005	0.741060	-4.549070
O	3.253176	3.728809	1.125367
O	5.326300	5.213904	0.110926
O	1.232719	5.255624	0.064867
O	3.291098	3.728609	-1.424311
O	-0.000005	3.723190	-2.009489
O	2.002860	5.214256	-3.279280
O	4.542439	5.214256	-3.279280
O	-0.000005	3.723190	-4.549070
O	3.254503	6.695014	1.139127
O	-7.767241	2.229425	0.115301
O	1.206555	8.194140	0.128432
O	3.283548	6.710642	-1.421286
O	-0.000005	6.705321	-2.009489
O	2.002860	8.196386	-3.279280
O	-8.548178	2.232126	-3.279280
O	-0.000005	6.705321	-4.549070
O	5.293445	-3.533136	7.059377
O	5.917471	-2.098622	8.694685
O	-0.026715	-2.585320	1.909041
O	-0.101435	-4.842570	2.029146
O	1.069916	4.850491	3.711628
O	0.073633	3.628438	2.099529
O	0.015679	6.032743	9.963440
O	-0.637778	5.188632	11.960338
C	-1.293743	-2.555145	10.195146
C	-4.141740	-0.037267	7.229746
C	1.948723	-0.581596	8.747169
C	3.257088	-1.044670	8.799302
C	3.661122	-2.023896	7.888051
C	2.733068	-2.508590	6.967160
C	1.438823	-1.989986	6.966025
C	5.066468	-2.528851	7.946503
C	0.387169	-2.465078	6.047311
C	-1.908828	-2.611057	5.672844
C	-1.711059	-3.274040	4.465390
C	-0.401800	-3.449484	4.004646
C	0.659693	-3.107716	4.839674
C	-0.149381	-3.688798	2.538591
C	-0.766603	0.630554	4.896403
C	-0.497603	1.584847	3.935758
C	-0.047596	2.848980	4.337429
C	0.028569	3.125002	5.707624
C	-0.331017	2.138137	6.628324
C	0.355436	3.804905	3.285688
C	-0.456843	2.363042	8.079782

C	-1.082226	1.391399	10.119461
C	-0.948853	2.603071	10.784135
C	-0.541171	3.730171	10.062433
C	-0.292292	3.605234	8.694872
C	-0.404363	5.034495	10.781897
H	1.595678	0.161290	9.450887
H	3.954157	-0.675096	9.543155
H	3.011386	-3.287765	6.269405
H	-2.896710	-2.351441	6.034268
H	-2.560017	-3.550974	3.851071
H	1.681615	-3.242868	4.506934
H	-1.081045	-0.361241	4.608400
H	-0.627471	1.351428	2.887783
H	0.343424	4.102303	6.045799
H	-1.408603	0.483672	10.614576
H	-1.160910	2.685314	11.843909
H	0.012222	4.473101	8.125646
H	6.219149	-3.806583	7.148776
H	-2.851460	-8.198864	2.076399
H	1.458062	5.333152	2.958756
H	0.070534	6.852591	10.483882
N	-1.263948	-1.699939	9.376288
N	-3.007310	-0.248418	7.481547
N	1.054558	-1.026482	7.846059
N	-0.883156	-2.142227	6.405949
N	-0.657366	0.870866	6.220903
N	-0.831300	1.267218	8.800699
S	-1.328946	-3.707819	11.334955
S	-5.702686	0.242285	6.858276
Ru	-0.986187	-0.505841	7.733617

(9) 2COOH-diff(cis,trans)-1row 2MH

203

Ti	0.783915	-8.349159	-0.199181
Ti	-2.475718	8.056530	0.095738
Ti	-2.478418	-8.343871	-3.279279
Ti	0.794236	8.057845	-3.279279
Ti	0.788786	-5.366152	-0.100310
Ti	-2.473750	-6.850566	0.085348
Ti	-2.478418	-5.361740	-3.279279
Ti	0.794236	-6.852805	-3.279279
Ti	0.795251	-2.386446	-0.206054
Ti	-2.477418	-3.868306	0.079982
Ti	-2.478418	-2.379610	-3.279279
Ti	0.794236	-3.870675	-3.279279
Ti	0.802030	0.598264	-0.208280
Ti	-2.467450	-0.888515	0.092377
Ti	-2.478418	0.602520	-3.279279
Ti	0.794236	-0.888545	-3.279279
Ti	0.795281	3.581854	-0.107903
Ti	-2.477122	2.093004	0.080391
Ti	-2.478418	3.584651	-3.279279
Ti	0.794236	2.093586	-3.279279

Ti	0.789218	6.563162	-0.207771
Ti	-2.482202	5.076919	0.084793
Ti	-2.478418	6.566781	-3.279279
Ti	0.794236	5.075716	-3.279279
Ti	-5.751116	3.580564	-0.189859
Ti	4.055525	8.026442	0.099890
Ti	4.066890	-8.343872	-3.279279
Ti	-5.751076	2.093585	-3.279279
Ti	-5.764060	6.563688	-0.190621
Ti	4.059783	-6.900651	0.053629
Ti	4.066890	-5.361740	-3.279279
Ti	-5.751076	5.075714	-3.279279
Ti	7.364645	-2.372952	-0.192624
Ti	4.079577	-3.852620	0.053298
Ti	4.066890	-2.379610	-3.279279
Ti	7.339544	-3.870676	-3.279279
Ti	7.323896	0.603660	-0.189676
Ti	4.059870	-0.886209	0.099641
Ti	4.066890	0.602520	-3.279279
Ti	7.339544	-0.888545	-3.279279
Ti	-5.741178	-2.377012	-0.189606
Ti	4.067069	2.082919	0.086095
Ti	4.066890	3.584651	-3.279279
Ti	-5.751076	-3.870674	-3.279279
Ti	-5.753596	0.601808	-0.188659
Ti	4.068926	5.057584	0.075851
Ti	4.066890	6.566781	-3.279279
Ti	-5.751076	-0.888544	-3.279279
O	-2.483528	-8.338905	1.159160
O	-0.441545	8.057929	0.132390
O	2.025972	8.057685	0.129851
O	-2.494726	-8.350730	-1.411758
O	0.794236	-8.343871	-2.009489
O	-3.748208	8.057845	-3.279279
O	-1.208629	8.057845	-3.279279
O	0.794236	-8.343871	-4.549068
O	-2.469739	-5.356795	1.158072
O	-0.448371	-6.873176	0.064817
O	2.037425	-6.882139	0.068317
O	-2.496089	-5.361408	-1.414034
O	0.794236	-5.361740	-2.009489
O	-3.748208	-6.852805	-3.279279
O	-1.208629	-6.852806	-3.279279
O	0.794236	-5.361740	-4.549068
O	-2.476887	-2.383272	1.164760
O	-0.453658	-3.836248	0.045729
O	2.042518	-3.844842	0.073534
O	-2.491683	-2.371443	-1.412242
O	0.794236	-2.379610	-2.009489
O	-3.748208	-3.870675	-3.279279
O	-1.208629	-3.870675	-3.279279
O	0.794236	-2.379610	-4.549068
O	-2.471256	0.604866	1.162760
O	-0.431203	-0.887842	0.149278
O	2.032351	-0.890474	0.135673

O	-2.489767	0.593559	-1.412880
O	0.794236	0.602520	-2.009489
O	-3.748208	-0.888545	-3.279279
O	-1.208629	-0.888545	-3.279279
O	0.794236	0.602520	-4.549068
O	-2.463863	3.582171	1.153082
O	-0.448645	2.060512	0.053603
O	2.041060	2.064631	0.062051
O	-2.497876	3.584582	-1.414689
O	0.794236	3.584651	-2.009489
O	-3.748208	2.093586	-3.279279
O	-1.208629	2.093586	-3.279279
O	0.794236	3.584651	-4.549068
O	-2.480652	6.562570	1.162718
O	-0.446543	5.098165	0.074075
O	2.043346	5.112169	0.051739
O	-2.489829	6.571537	-1.411204
O	0.794236	6.566781	-2.009489
O	-3.748208	5.075716	-3.279279
O	-1.208629	5.075716	-3.279279
O	0.794236	6.566781	-4.549068
O	4.060670	-8.349266	1.158015
O	-6.983884	2.088753	0.135304
O	-4.525388	2.092303	0.124145
O	4.076462	-8.344145	-1.408988
O	-5.751076	3.584648	-2.009489
O	2.797100	8.057845	-3.279279
O	-7.753940	2.093585	-3.279279
O	-5.751076	3.584648	-4.549068
O	4.040975	-5.378787	1.155720
O	-6.988672	5.070210	0.122968
O	-4.532247	5.073594	0.135888
O	4.089548	-5.360273	-1.420033
O	-5.751076	6.566780	-2.009489
O	2.797100	-6.852806	-3.279279
O	5.336679	-6.852806	-3.279279
O	-5.751076	6.566780	-4.549068
O	4.063229	-2.395609	1.159437
O	6.103340	-3.870654	0.116853
O	-4.536200	8.048852	0.151271
O	4.076844	-2.381380	-1.407580
O	7.339544	-2.379610	-2.009489
O	2.797100	-3.870675	-3.279279
O	5.336679	-3.870675	-3.279279
O	7.339544	-2.379610	-4.549068
O	4.067572	0.602003	1.171137
O	6.109703	-0.899716	0.143362
O	-4.523520	-6.847833	0.120577
O	4.078294	0.592597	-1.406208
O	7.339544	0.602520	-2.009489
O	2.797100	-0.888545	-3.279279
O	5.336679	-0.888544	-3.279279
O	7.339544	0.602520	-4.549068
O	4.041869	3.580623	1.159770
O	6.104974	2.096510	0.120579

O	-4.530551	-3.876069	0.129732
O	4.083655	3.586638	-1.412515
O	-5.751076	-2.379609	-2.009489
O	2.797100	2.093586	-3.279279
O	5.336679	2.093586	-3.279279
O	-5.751076	-2.379609	-4.549068
O	4.049606	6.546845	1.175791
O	-6.982997	-0.891483	0.122454
O	-4.524685	-0.888013	0.129959
O	4.081343	6.580181	-1.407964
O	-5.751076	0.602521	-2.009489
O	2.797100	5.075716	-3.279279
O	5.336679	5.075716	-3.279279
O	-5.751076	0.602521	-4.549068
O	5.793669	-2.614269	7.962424
O	5.795621	-1.046281	9.618918
O	2.685551	-4.914161	3.211834
O	0.712118	-5.260167	2.119016
O	1.684894	4.683705	3.867290
O	0.840143	3.578503	2.072464
O	-0.227911	5.603906	10.091890
O	-0.986461	4.578321	11.985392
C	-1.235025	-2.761781	9.801186
C	-4.049364	-0.866839	6.487059
C	1.710640	-0.240542	8.804648
C	3.049281	-0.458871	9.113847
C	3.767687	-1.424927	8.386316
C	3.100840	-2.145132	7.386264
C	1.750565	-1.872650	7.117696
C	5.200748	-1.652020	8.736518
C	0.964020	-2.575421	6.095761
C	-1.171014	-2.927665	5.168780
C	-0.659228	-3.797689	4.205214
C	0.730322	-4.039701	4.179001
C	1.534100	-3.438040	5.158388
C	1.377926	-4.810546	3.084768
C	-0.527538	0.513801	4.592526
C	-0.098629	1.500800	3.721669
C	0.375749	2.724291	4.244161
C	0.256343	2.952525	5.628416
C	-0.274758	1.947731	6.446074
C	0.966776	3.688149	3.305025
C	-0.626422	2.101283	7.862806
C	-1.597892	1.022113	9.726332
C	-1.493822	2.177007	10.494762
C	-0.914569	3.332049	9.929944
C	-0.494495	3.289647	8.591388
C	-0.736510	4.539047	10.787590
H	1.113081	0.475711	9.370609
H	3.542632	0.092890	9.917106
H	3.636055	-2.914761	6.828853
H	-2.235868	-2.691520	5.236381
H	-1.321528	-4.267817	3.473469
H	2.610132	-3.611124	5.141069
H	-0.876588	-0.451957	4.223786

H	-0.123581	1.331258	2.645347
H	0.575996	3.907826	6.050437
H	-2.017862	0.091954	10.118276
H	-1.850497	2.193980	11.526170
H	-0.069785	4.184257	8.132685
H	6.720435	-2.658533	8.280236
H	3.151236	-5.280444	2.355294
H	2.122483	5.185601	3.141944
H	-0.031630	6.304100	10.756469
N	-1.307080	-1.995925	8.880787
N	-2.885729	-0.818702	6.767682
N	1.063917	-0.913752	7.819488
N	-0.383605	-2.291902	6.079978
N	-0.561744	0.694945	5.938286
N	-1.148020	0.963307	8.445335
S	-1.165564	-3.782951	11.051279
S	-5.615764	-0.926042	6.086521
Ru	-0.955336	-0.750240	7.330016

(10) 2COOH-diff(cis,trans)-2rows-S 1BB1M+S

203

Ti	-1.462712	5.102361	-0.200345
Ti	1.808398	6.491622	0.010709
Ti	1.816605	5.113270	-3.279279
Ti	-1.456049	6.604336	-3.279279
Ti	-1.452842	8.095872	-0.201158
Ti	1.803273	-8.201176	0.003443
Ti	1.816605	8.095401	-3.279279
Ti	-1.456049	-8.306314	-3.279279
Ti	-1.470019	-6.800445	-0.192066
Ti	1.806036	-5.265905	0.088067
Ti	1.816605	-6.815249	-3.279279
Ti	-1.456049	-5.324183	-3.279279
Ti	-1.448348	-3.839872	-0.050109
Ti	1.798640	-2.323856	0.045319
Ti	1.816605	-3.833119	-3.279279
Ti	-1.456049	-2.342053	-3.279279
Ti	-1.483131	-0.855573	-0.224343
Ti	1.825320	0.620196	0.025194
Ti	1.816605	-0.850988	-3.279279
Ti	-1.456049	0.640078	-3.279279
Ti	-1.439110	2.121832	-0.110058
Ti	1.819841	3.556667	0.085339
Ti	1.816605	2.131142	-3.279279
Ti	-1.456049	3.622208	-3.279279
Ti	5.089959	5.088197	-0.204871
Ti	-4.733227	-5.397287	0.085896
Ti	-4.728706	-6.815250	-3.279279
Ti	5.089258	6.604336	-3.279279
Ti	-8.023216	-3.845313	-0.196987
Ti	-4.720334	-2.452864	-0.015067
Ti	-4.728706	-3.833118	-3.279279
Ti	-8.001359	-2.342053	-3.279279

Ti	-7.993314	-0.850080	-0.199789
Ti	-4.721990	0.751672	-0.003982
Ti	-4.728706	-0.850989	-3.279279
Ti	5.089258	-5.324183	-3.279279
Ti	5.076188	-3.823521	-0.206787
Ti	-4.734181	3.689386	0.082560
Ti	-4.728706	2.131142	-3.279279
Ti	5.089258	-2.342053	-3.279279
Ti	5.102248	-0.848965	-0.108384
Ti	-4.737410	6.626737	0.053249
Ti	-4.728706	5.113272	-3.279279
Ti	5.089258	0.640078	-3.279279
Ti	5.085280	2.099612	-0.100530
Ti	-4.728413	-8.333572	0.078504
Ti	-4.728709	8.095402	-3.279279
Ti	5.089258	3.622208	-3.279279
O	1.812912	5.114555	1.134065
O	3.840508	6.618434	0.103476
O	-0.208689	6.613565	0.134260
O	1.815769	5.146322	-1.406828
O	-1.456049	5.113270	-2.009489
O	0.546816	6.604336	-3.279279
O	3.086394	6.604336	-3.279279
O	-1.456049	5.113270	-4.549068
O	1.849514	8.096243	1.226299
O	3.851363	-8.309098	0.109699
O	-0.201903	-8.333311	0.117046
O	1.823534	8.097742	-1.411781
O	-1.456049	8.095402	-2.009489
O	0.546816	-8.306314	-3.279279
O	3.086394	-8.306313	-3.279279
O	-1.456049	8.095402	-4.549068
O	1.815835	-6.820162	1.129164
O	3.862678	-5.340097	0.127746
O	-0.195952	-5.372021	-0.006876
O	1.834998	-6.843958	-1.407656
O	-1.456049	-6.815249	-2.009489
O	0.546816	-5.324183	-3.279279
O	3.086394	-5.324183	-3.279279
O	-1.456049	-6.815249	-4.549068
O	1.784814	-3.815959	1.148524
O	3.841109	-2.393067	0.059193
O	-0.224398	-2.299340	0.037844
O	1.830923	-3.856588	-1.408419
O	-1.456049	-3.833119	-2.009489
O	0.546816	-2.342053	-3.279279
O	3.086394	-2.342053	-3.279279
O	-1.456049	-3.833119	-4.549068
O	1.828668	-0.849034	1.111470
O	3.806073	0.637866	-0.123293
O	-0.239214	0.637774	0.089965
O	1.788685	-0.863746	-1.424313
O	-1.456049	-0.850988	-2.009489
O	0.546816	0.640078	-3.279279
O	3.086394	0.640078	-3.279279

O	-1.456049	-0.850988	-4.549068
O	1.829571	2.101676	1.131138
O	3.838263	3.662299	0.068078
O	-0.206787	3.648272	0.034364
O	1.791225	2.158464	-1.415503
O	-1.456049	2.131142	-2.009489
O	0.546816	3.622208	-3.279279
O	3.086394	3.622208	-3.279279
O	-1.456049	2.131142	-4.549068
O	-4.732870	-6.832946	1.154627
O	-2.726793	-5.391341	-0.023554
O	-6.788747	-5.312374	0.133373
O	-4.752950	-6.805493	-1.409263
O	5.089258	5.113270	-2.009489
O	-5.998494	-5.324184	-3.279279
O	-3.458915	-5.324184	-3.279279
O	5.089258	5.113270	-4.549068
O	-4.705614	-3.832382	1.120640
O	-2.738076	-2.297586	0.012137
O	-6.776398	-2.341210	0.150333
O	-4.769817	-3.815690	-1.408776
O	-8.001359	-3.833118	-2.009489
O	-5.998494	-2.342053	-3.279279
O	-3.458915	-2.342053	-3.279279
O	-8.001359	-3.833118	-4.549068
O	-4.704028	-0.854201	1.219512
O	-2.723861	0.635482	0.047735
O	-6.766026	0.614617	0.132911
O	-4.755292	-0.852847	-1.416782
O	-8.001359	-0.850989	-2.009489
O	-5.998494	0.640077	-3.279279
O	-3.458915	0.640077	-3.279279
O	-8.001359	-0.850989	-4.549068
O	-4.743021	2.130270	1.114175
O	-2.701459	3.655825	0.055159
O	6.327090	-2.380732	0.064605
O	-4.742014	2.110786	-1.411485
O	5.089258	-3.833118	-2.009489
O	-5.998494	3.622207	-3.279279
O	-3.458915	3.622207	-3.279279
O	5.089258	-3.833118	-4.549068
O	-4.754527	5.137962	1.136349
O	-2.674088	6.611130	0.108163
O	6.363927	0.658867	-0.096981
O	-4.708972	5.093905	-1.415061
O	5.089258	-0.850988	-2.009489
O	-5.998497	6.604337	-3.279279
O	-3.458915	6.604338	-3.279279
O	5.089258	-0.850988	-4.549068
O	-4.748978	8.090197	1.137278
O	-2.678377	-8.329214	0.111765
O	6.318915	3.648966	0.086452
O	-4.694330	8.112443	-1.414516
O	5.089258	2.131142	-2.009489
O	-5.998497	-8.306311	-3.279279

O	-3.458915	-8.306311	-3.279279
O	5.089258	2.131142	-4.549068
O	1.233206	-5.938001	9.621577
O	2.043435	-4.635418	11.283379
O	-1.388224	-5.849407	3.051892
O	-1.528883	-3.934025	1.866122
O	4.922205	1.712112	2.056802
O	5.033278	-0.537705	1.915600
O	4.566888	5.170025	8.057125
O	2.938870	5.910863	9.438449
C	-2.902962	0.644655	8.117571
C	-1.140950	1.935496	3.971312
C	1.059553	-1.205422	9.009673
C	1.433006	-2.290551	9.789730
C	1.162976	-3.581150	9.323275
C	0.530559	-3.735078	8.089238
C	0.178383	-2.601318	7.354957
C	1.534121	-4.740983	10.187510
C	-0.579434	-2.656074	6.089313
C	-1.961458	-1.370462	4.714434
C	-2.235051	-2.460304	3.911931
C	-1.547479	-3.661833	4.132116
C	-0.786524	-3.794348	5.295103
C	-1.497257	-4.632153	2.972862
C	2.024915	-0.932753	4.635610
C	3.101734	-0.835200	3.771311
C	3.819811	0.361575	3.709522
C	3.534093	1.354530	4.648401
C	2.491518	1.151050	5.559138
C	4.698384	0.548137	2.500309
C	2.133988	2.091163	6.639446
C	0.524094	2.638859	8.252858
C	1.264631	3.732755	8.679612
C	2.508061	3.981082	8.086195
C	2.943218	3.154779	7.048495
C	3.325613	5.117913	8.603974
H	1.243775	-0.187057	9.330781
H	1.919725	-2.156966	10.748891
H	0.284312	-4.724593	7.726298
H	-2.384166	-0.392221	4.529957
H	-2.887156	-2.356626	3.054457
H	-0.300113	-4.737479	5.520592
H	1.385673	-1.806080	4.613865
H	3.316875	-1.638141	3.080361
H	4.086021	2.287559	4.637222
H	-0.442422	2.377678	8.674683
H	0.903600	4.376944	9.473046
H	3.904863	3.326832	6.581158
H	1.491215	-6.630303	10.254374
H	1.411441	8.102069	2.085578
H	-5.159421	-0.839950	2.068441
H	5.028909	5.924167	8.463982
N	-1.822501	0.598316	7.635088
N	-0.763262	1.423328	4.959416
N	0.448199	-1.341602	7.818049

N	-1.058440	-1.444223	5.706142
N	1.687762	0.049277	5.481880
N	0.956653	1.824183	7.269854
S	-4.373216	0.720256	8.809292
S	-1.827286	2.701436	2.677748
Ru	-0.129084	0.206098	6.529510

(10) 2COOH-diff(cis,trans)-2rows-S 1BB1MH+S

203

Ti	-1.459853	5.098965	-0.198077
Ti	1.816119	6.491103	0.009464
Ti	1.816604	5.113270	-3.279279
Ti	-1.456048	6.604337	-3.279279
Ti	-1.454750	8.086730	-0.202625
Ti	1.807874	-8.196594	0.011437
Ti	1.816604	8.095402	-3.279279
Ti	-1.456048	-8.306314	-3.279279
Ti	-1.481484	-6.814235	-0.213402
Ti	1.827636	-5.258151	0.083042
Ti	1.816604	-6.815249	-3.279279
Ti	-1.456048	-5.324183	-3.279279
Ti	-1.465281	-3.829507	-0.128750
Ti	1.825911	-2.317050	0.059689
Ti	1.816604	-3.833119	-3.279279
Ti	-1.456048	-2.342053	-3.279279
Ti	-1.456934	-0.847338	-0.216416
Ti	1.838176	0.624918	0.030964
Ti	1.816604	-0.850988	-3.279279
Ti	-1.456048	0.640078	-3.279279
Ti	-1.439757	2.127007	-0.136535
Ti	1.825955	3.558970	0.085196
Ti	1.816604	2.131143	-3.279279
Ti	-1.456048	3.622208	-3.279279
Ti	5.088546	5.097284	-0.207956
Ti	-4.751010	-5.326101	0.069897
Ti	-4.728705	-6.815251	-3.279279
Ti	5.089257	6.604336	-3.279279
Ti	-8.028062	-3.835672	-0.200508
Ti	-4.736059	-2.339892	0.074418
Ti	-4.728705	-3.833118	-3.279279
Ti	-8.001357	-2.342053	-3.279279
Ti	-7.995345	-0.845590	-0.197153
Ti	-4.723981	0.645137	0.078080
Ti	-4.728705	-0.850988	-3.279279
Ti	5.089257	-5.324183	-3.279279
Ti	5.088266	-3.820954	-0.208516
Ti	-4.729365	3.626508	0.061554
Ti	-4.728705	2.131142	-3.279279
Ti	5.089257	-2.342053	-3.279279
Ti	5.117120	-0.838277	-0.110594
Ti	-4.735961	6.605847	0.047746
Ti	-4.728705	5.113273	-3.279279
Ti	5.089257	0.640077	-3.279279

Ti	5.097204	2.111707	-0.111488
Ti	-4.738190	-8.309419	0.076584
Ti	-4.728707	8.095401	-3.279279
Ti	5.089257	3.622208	-3.279279
O	1.809884	5.116888	1.137712
O	3.827384	6.624069	0.102680
O	-0.203176	6.621331	0.129307
O	1.814832	5.145482	-1.404646
O	-1.456048	5.113270	-2.009489
O	0.546815	6.604337	-3.279279
O	3.086393	6.604336	-3.279279
O	-1.456048	5.113270	-4.549068
O	1.842609	8.098767	1.237389
O	3.825515	-8.303479	0.110202
O	-0.210103	-8.317259	0.144536
O	1.814980	8.108977	-1.408314
O	-1.456048	8.095402	-2.009489
O	0.546815	-8.306314	-3.279279
O	3.086393	-8.306314	-3.279279
O	-1.456048	8.095402	-4.549068
O	1.783483	-6.811667	1.154743
O	3.841856	-5.338686	0.124466
O	-0.216205	-5.368157	0.100046
O	1.817992	-6.837251	-1.398048
O	-1.456048	-6.815249	-2.009489
O	0.546815	-5.324184	-3.279279
O	3.086393	-5.324183	-3.279279
O	-1.456048	-6.815249	-4.549068
O	1.789782	-3.821008	1.162779
O	3.836675	-2.388679	0.065049
O	-0.217765	-2.330265	0.068744
O	1.816118	-3.863696	-1.403255
O	-1.456048	-3.833119	-2.009489
O	0.546815	-2.342053	-3.279279
O	3.086393	-2.342053	-3.279279
O	-1.456048	-3.833119	-4.549068
O	1.833204	-0.849609	1.127014
O	3.809889	0.642320	-0.110940
O	-0.218644	0.633679	0.088426
O	1.787955	-0.870268	-1.419108
O	-1.456048	-0.850988	-2.009489
O	0.546815	0.640078	-3.279279
O	3.086393	0.640078	-3.279279
O	-1.456048	-0.850988	-4.549068
O	1.841178	2.103749	1.136248
O	3.835742	3.667662	0.062629
O	-0.198852	3.641554	0.032618
O	1.793015	2.154245	-1.412692
O	-1.456048	2.131142	-2.009489
O	0.546815	3.622208	-3.279279
O	3.086393	3.622208	-3.279279
O	-1.456048	2.131142	-4.549068
O	-4.725825	-6.809076	1.131117
O	-2.692302	-5.351515	0.054421
O	-6.803780	-5.305150	0.132432

O	-4.733844	-6.811376	-1.419460
O	5.089257	5.113270	-2.009489
O	-5.998493	-5.324184	-3.279279
O	-3.458914	-5.324185	-3.279279
O	5.089257	5.113270	-4.549068
O	-4.722169	-3.831473	1.130082
O	-2.692124	-2.328590	0.052000
O	-6.805276	-2.342727	0.132037
O	-4.750503	-3.837805	-1.421524
O	-8.001357	-3.833118	-2.009489
O	-5.998493	-2.342053	-3.279279
O	-3.458914	-2.342053	-3.279279
O	-8.001357	-3.833118	-4.549068
O	-4.721214	-0.858496	1.140459
O	-2.682756	0.631460	0.080317
O	-6.791055	0.620737	0.118984
O	-4.747340	-0.856907	-1.420491
O	-8.001357	-0.850988	-2.009489
O	-5.998493	0.640077	-3.279279
O	-3.458914	0.640077	-3.279279
O	-8.001357	-0.850988	-4.549068
O	-4.733294	2.128595	1.118065
O	-2.683909	3.642546	0.048374
O	6.317349	-2.378484	0.067764
O	-4.734404	2.122762	-1.422008
O	5.089257	-3.833119	-2.009489
O	-5.998493	3.622208	-3.279279
O	-3.458914	3.622207	-3.279279
O	5.089257	-3.833119	-4.549068
O	-4.749501	5.121263	1.105788
O	-2.659873	6.611551	0.113989
O	6.361850	0.650911	-0.115737
O	-4.699180	5.106129	-1.428344
O	5.089257	-0.850988	-2.009489
O	-5.998496	6.604337	-3.279279
O	-3.458914	6.604338	-3.279279
O	5.089257	-0.850988	-4.549068
O	-4.747727	8.093851	1.118829
O	-2.664688	-8.313738	0.132489
O	6.316022	3.661917	0.078683
O	-4.686843	8.116770	-1.424199
O	5.089257	2.131142	-2.009489
O	-5.998496	-8.306311	-3.279279
O	-3.458914	-8.306312	-3.279279
O	5.089257	2.131142	-4.549068
O	1.621999	-5.274196	9.893557
O	2.395138	-3.932107	11.541619
O	-0.297958	-5.184241	3.498469
O	-1.470239	-3.827883	2.120427
O	5.003852	1.777666	1.998817
O	5.033356	-0.484647	1.941826
O	4.756308	5.945279	7.197483
O	3.353754	6.734502	8.784317
C	-2.470701	1.395104	8.597093
C	-1.077638	2.334174	4.134331

C	1.324080	-0.559009	9.210676
C	1.727567	-1.621464	10.007829
C	1.458315	-2.926187	9.580359
C	0.789975	-3.115746	8.369609
C	0.413798	-2.003763	7.616035
C	1.875632	-4.064602	10.454093
C	-0.350194	-2.091388	6.355641
C	-1.737059	-0.872809	4.915171
C	-1.906219	-1.968458	4.086898
C	-1.168062	-3.131051	4.348400
C	-0.454580	-3.228818	5.548644
C	-1.015875	-4.092304	3.228378
C	2.097410	-0.574719	4.796945
C	3.143866	-0.596494	3.892799
C	3.898133	0.563119	3.714496
C	3.665259	1.651978	4.554658
C	2.646396	1.571421	5.508388
C	4.756105	0.632673	2.485302
C	2.359224	2.616843	6.508920
C	0.910938	3.308092	8.215033
C	1.663624	4.451346	8.449943
C	2.818799	4.667347	7.690283
C	3.169076	3.736945	6.711129
C	3.640639	5.886583	7.964923
H	1.502664	0.469723	9.501558
H	2.229630	-1.457197	10.954073
H	0.549654	-4.117693	8.036849
H	-2.208064	0.078322	4.709544
H	-2.534625	-1.900011	3.206543
H	0.084755	-4.135513	5.795224
H	1.442140	-1.427908	4.884685
H	3.309075	-1.456649	3.260735
H	4.252187	2.554346	4.439114
H	-0.000244	3.089110	8.760134
H	1.376460	5.165422	9.213416
H	4.062129	3.885083	6.119404
H	1.897171	-5.956385	10.529165
H	1.351598	8.087770	2.067729
H	-0.060252	-5.646001	2.673150
H	5.256703	6.737477	7.445798
N	-1.495288	1.260817	7.938515
N	-0.625988	1.939195	5.148065
N	0.690801	-0.732752	8.035134
N	-0.874064	-0.899708	5.950256
N	1.815664	0.491382	5.560042
N	1.253756	2.404918	7.275755
S	-3.790037	1.590307	9.526358
S	-1.840011	2.893412	2.788690
Ru	0.074418	0.763797	6.712397

(10) 2COOH-diff(cis,trans)-2rows-S 2MH+S

203

Ti -1.464463 -6.819410 -0.126465

Ti	8.343743	3.612710	0.093071
Ti	-4.728707	-6.815251	-3.279279
Ti	-1.456053	-8.306315	-3.279279
Ti	-1.447396	-3.834909	-0.206141
Ti	-4.732465	-5.331469	0.078327
Ti	-4.728707	-3.833121	-3.279279
Ti	-1.456053	-5.324186	-3.279279
Ti	-1.458363	-0.852179	-0.201314
Ti	-4.723715	-2.349803	0.096180
Ti	-4.728707	-0.850991	-3.279279
Ti	-1.456053	-2.342055	-3.279279
Ti	-1.460602	2.117073	-0.103652
Ti	-4.733942	0.628799	0.084157
Ti	-4.728707	2.131140	-3.279279
Ti	-1.456053	0.640076	-3.279279
Ti	-1.442163	5.111555	-0.203076
Ti	-4.711077	3.612764	0.073228
Ti	-4.728707	5.113271	-3.279279
Ti	-1.456053	3.622206	-3.279279
Ti	-1.470030	8.096520	-0.202811
Ti	-4.708992	6.597273	0.068275
Ti	8.361913	2.131143	-3.279279
Ti	-1.456053	6.604337	-3.279279
Ti	-7.992706	-0.853685	-0.191020
Ti	1.820492	-8.310528	0.073443
Ti	1.816602	-6.815250	-3.279279
Ti	-8.001364	-2.342057	-3.279279
Ti	5.084244	-3.833319	-0.202788
Ti	1.824807	-5.326145	0.086753
Ti	1.816602	-3.833120	-3.279279
Ti	5.089256	-5.324184	-3.279279
Ti	5.134203	-0.863980	-0.132001
Ti	1.811961	-2.345343	0.067350
Ti	1.816602	-0.850989	-3.279279
Ti	5.089256	-2.342054	-3.279279
Ti	5.066366	2.133067	-0.205982
Ti	1.820944	0.645005	0.069502
Ti	1.816602	2.131141	-3.279279
Ti	5.089256	0.640077	-3.279279
Ti	5.085057	5.115718	-0.191357
Ti	1.808178	3.625212	0.089116
Ti	1.816602	5.113272	-3.279279
Ti	5.089256	3.622207	-3.279279
Ti	-8.005939	-3.834666	-0.191192
Ti	1.807197	6.603614	0.097905
Ti	1.816602	8.095402	-3.279279
Ti	5.089256	6.604338	-3.279279
O	-4.721182	-6.818154	1.158497
O	-2.702044	-8.325043	0.080145
O	-0.215199	-8.336844	0.067419
O	-4.751140	-6.818694	-1.411105
O	-1.456053	-6.815251	-2.009489
O	7.092123	3.622205	-3.279279
O	-3.458917	-8.306316	-3.279279
O	-1.456053	-6.815251	-4.549068

O	-4.718664	-3.845824	1.169185
O	-2.700537	-5.304403	0.061104
O	-0.218702	-5.303251	0.101406
O	-4.739699	-3.828771	-1.410627
O	-1.456053	-3.833120	-2.009489
O	-5.998497	-5.324187	-3.279279
O	-3.458917	-5.324186	-3.279279
O	-1.456053	-3.833120	-4.549068
O	-4.725978	-0.859125	1.165272
O	-2.680116	-2.349608	0.154573
O	-0.219401	-2.346189	0.134321
O	-4.739989	-0.863945	-1.409993
O	-1.456053	-0.850990	-2.009489
O	-5.998497	-2.342056	-3.279279
O	-3.458917	-2.342055	-3.279279
O	-1.456053	-0.850990	-4.549068
O	-4.732387	2.128055	1.142905
O	-2.701699	0.604372	0.062478
O	-0.219760	0.617571	0.100992
O	-4.729056	2.125553	-1.418022
O	-1.456053	2.131141	-2.009489
O	-5.998497	0.640075	-3.279279
O	-3.458917	0.640075	-3.279279
O	-1.456053	2.131141	-4.549068
O	-4.753817	5.116318	1.146337
O	-2.696623	3.655258	0.064572
O	-0.212691	3.641326	0.072148
O	-4.724273	5.128048	-1.417537
O	-1.456053	5.113271	-2.009489
O	-5.998497	3.622205	-3.279279
O	-3.458917	3.622206	-3.279279
O	-1.456053	5.113271	-4.549068
O	8.326509	2.120175	1.180126
O	-2.687574	6.602363	0.134849
O	-0.224067	6.612465	0.132682
O	8.368032	2.139758	-1.410018
O	-1.456053	8.095401	-2.009489
O	7.092123	0.640078	-3.279279
O	-3.458917	6.604336	-3.279279
O	-1.456053	8.095401	-4.549068
O	1.792848	-6.821004	1.164110
O	3.856994	-8.309330	0.131438
O	-6.776138	-2.347790	0.144342
O	1.828556	-6.811184	-1.409608
O	-8.001364	-0.850992	-2.009489
O	0.546812	-8.306315	-3.279279
O	3.086391	-8.306315	-3.279279
O	-8.001364	-0.850992	-4.549068
O	1.824825	-3.830774	1.170157
O	3.857648	-5.340657	0.141383
O	-6.775403	0.625729	0.130032
O	1.817820	-3.838057	-1.408753
O	5.089256	-3.833119	-2.009489
O	0.546812	-5.324185	-3.279279
O	3.086391	-5.324185	-3.279279

O	5.089256	-3.833119	-4.549068
O	1.825871	-0.853401	1.144822
O	3.857124	-2.364388	0.084773
O	6.339043	-2.382001	0.034086
O	1.813202	-0.854980	-1.415214
O	5.089256	-0.850989	-2.009489
O	0.546812	-2.342055	-3.279279
O	3.086391	-2.342054	-3.279279
O	5.089256	-0.850989	-4.549068
O	1.823404	2.127096	1.158507
O	3.861772	0.649072	0.112566
O	6.334695	0.687604	0.057462
O	1.828833	2.132819	-1.409539
O	5.089256	2.131142	-2.009489
O	0.546812	0.640076	-3.279279
O	3.086391	0.640077	-3.279279
O	5.089256	2.131142	-4.549068
O	1.812482	5.115405	1.169530
O	3.852969	3.640310	0.128716
O	6.307353	3.630606	0.145360
O	1.822028	5.123176	-1.407509
O	5.089256	5.113272	-2.009489
O	0.546812	3.622206	-3.279279
O	3.086391	3.622207	-3.279279
O	5.089256	5.113272	-4.549068
O	1.801495	8.105595	1.174937
O	3.858135	6.611276	0.142987
O	-6.775695	-5.320691	0.133846
O	1.830329	8.092160	-1.409474
O	-8.001364	-3.833120	-2.009489
O	0.546812	6.604338	-3.279279
O	3.086391	6.604338	-3.279279
O	-8.001364	-3.833120	-4.549068
O	2.137331	-6.026655	9.674839
O	2.451957	-4.358326	11.196622
O	-0.055149	-7.465649	3.841722
O	-1.441885	-6.825002	2.163664
O	5.544751	1.150780	3.080348
O	5.304334	-0.900478	2.123808
O	2.360668	5.380624	6.689747
O	0.555270	5.797509	8.020360
C	-3.390876	-0.698761	7.463267
C	-1.493937	1.100024	3.495421
C	0.644496	-1.622595	8.502760
C	1.254900	-2.467705	9.420245
C	1.389459	-3.835304	9.105741
C	0.874621	-4.299737	7.886997
C	0.257215	-3.399496	7.005216
C	2.042002	-4.729468	10.102534
C	-0.365450	-3.774881	5.729735
C	-1.751349	-2.999370	3.981456
C	-1.803111	-4.266743	3.410425
C	-1.021190	-5.302719	3.968878
C	-0.326251	-5.054986	5.164291
C	-0.880083	-6.584820	3.239535

C	1.857738	-1.688443	4.280184
C	3.074669	-1.493307	3.647937
C	3.697207	-0.233998	3.732784
C	3.084484	0.773853	4.493009
C	1.852569	0.517410	5.108143
C	4.913613	-0.029358	2.920564
C	1.127940	1.479477	5.946433
C	-0.759716	1.811381	7.314594
C	-0.383327	3.121191	7.589965
C	0.794995	3.625328	7.015037
C	1.552171	2.796203	6.179760
C	1.191670	5.031988	7.306354
H	0.511209	-0.556988	8.699782
H	1.643248	-2.087018	10.367722
H	0.951090	-5.359729	7.642151
H	-2.284090	-2.143199	3.557221
H	-2.456934	-4.458822	2.554261
H	0.248032	-5.856745	5.631252
H	1.333851	-2.643149	4.198688
H	3.512800	-2.297706	3.055153
H	3.558442	1.753388	4.566082
H	-1.678639	1.374366	7.713030
H	-1.000917	3.754840	8.229791
H	2.458929	3.183694	5.714539
H	2.565820	-6.510411	10.413839
H	0.126547	-8.201945	3.206256
H	6.392323	1.143869	2.558750
H	2.530868	6.318748	6.927884
N	-2.395746	-0.795144	6.802920
N	-1.372907	0.175339	4.239679
N	0.165587	-2.060015	7.310989
N	-1.002220	-2.731836	5.084021
N	1.231540	-0.708171	4.976599
N	-0.025126	0.996625	6.516434
S	-4.720810	-0.553775	8.372911
S	-1.718844	2.442360	2.591068
Ru	-0.627096	-0.876569	5.837465

(11) 2COOH-diff(cis,trans)-1row-S 1BB1M+S

203

Ti	-4.477367	-7.666631	-0.197812
Ti	5.320992	5.814207	0.086254
Ti	5.327440	7.243189	-3.279279
Ti	-4.490524	8.734254	-3.279279
Ti	-4.495135	-4.681494	-0.196347
Ti	5.311192	8.751436	0.092716
Ti	5.327443	-7.667460	-3.279279
Ti	-4.490524	-6.176395	-3.279279
Ti	-4.502560	-1.700220	-0.204863
Ti	5.309570	-6.200418	0.079401
Ti	5.327440	-4.685331	-3.279279
Ti	-4.490524	-3.194265	-3.279279
Ti	-4.468663	1.266255	-0.091522

Ti	5.321855	-3.267381	0.058288
Ti	5.327440	-1.703200	-3.279279
Ti	-4.490524	-0.212134	-3.279279
Ti	-4.503242	4.242660	-0.204369
Ti	5.323087	-0.326963	-0.010230
Ti	5.327440	1.278930	-3.279279
Ti	-4.490524	2.769996	-3.279279
Ti	-4.491261	7.233622	-0.195512
Ti	5.315167	2.873636	-0.016903
Ti	5.327440	4.261061	-3.279279
Ti	-4.490524	5.752126	-3.279279
Ti	2.041286	-7.661668	-0.209478
Ti	-1.210741	8.621166	0.011348
Ti	-1.217870	-7.667461	-3.279279
Ti	2.054783	8.734255	-3.279279
Ti	2.055721	-4.659287	-0.097051
Ti	-1.206860	-6.079950	-0.006948
Ti	-1.217870	-4.685330	-3.279279
Ti	2.054783	-6.176395	-3.279279
Ti	2.064339	-1.707740	-0.100356
Ti	-1.210179	-3.131125	0.021068
Ti	-1.217870	-1.703200	-3.279279
Ti	2.054783	-3.194265	-3.279279
Ti	2.062038	1.280490	-0.233963
Ti	-1.196779	-0.191828	0.064208
Ti	-1.217870	1.278930	-3.279279
Ti	2.054783	-0.212135	-3.279279
Ti	2.068741	4.268471	-0.017765
Ti	-1.196996	2.745942	0.055747
Ti	-1.217870	4.261060	-3.279279
Ti	2.054783	2.769996	-3.279279
Ti	2.055271	7.233704	-0.202123
Ti	-1.210270	5.687706	0.080633
Ti	-1.217870	7.243191	-3.279279
Ti	2.054783	5.752126	-3.279279
O	5.333518	7.257000	1.157959
O	-5.702475	8.738788	0.128523
O	-3.247246	8.736180	0.101260
O	5.356492	7.244798	-1.409133
O	-4.490524	-7.667461	-2.009489
O	4.057651	5.752125	-3.279279
O	-6.493388	8.734254	-3.279279
O	-4.490524	-7.667461	-4.549068
O	5.330320	-7.670658	1.151623
O	-5.704610	-6.179534	0.121954
O	-3.247593	-6.183243	0.109080
O	5.330066	-7.672658	-1.406809
O	-4.490524	-4.685330	-2.009489
O	4.057651	8.734253	-3.279279
O	-6.493388	-6.176396	-3.279279
O	-4.490524	-4.685330	-4.549068
O	5.312554	-4.703297	1.140656
O	-5.720748	-3.210248	0.112270
O	-3.265912	-3.204185	0.109811
O	5.351167	-4.701251	-1.413253

O	-4.490524	-1.703200	-2.009489
O	4.057651	-6.176396	-3.279279
O	-6.493388	-3.194265	-3.279279
O	-4.490524	-1.703200	-4.549068
O	5.309407	-1.713901	1.102203
O	-5.736077	-0.244479	0.038411
O	-3.257084	-0.235720	0.086749
O	5.341364	-1.682398	-1.415231
O	-4.490524	1.278931	-2.009489
O	4.057651	-3.194265	-3.279279
O	-6.493388	-0.212135	-3.279279
O	-4.490524	1.278931	-4.549068
O	5.370335	1.278693	1.203334
O	-5.740172	2.785265	0.059021
O	-3.251965	2.791594	0.051519
O	5.350682	1.285789	-1.412751
O	-4.490524	4.261061	-2.009489
O	4.057651	-0.212134	-3.279279
O	-6.493388	2.769996	-3.279279
O	-4.490524	4.261061	-4.549068
O	5.309540	4.261264	1.117732
O	-5.727354	5.763419	0.098435
O	-3.268742	5.757021	0.123212
O	5.358016	4.252877	-1.408182
O	-4.490524	7.243191	-2.009489
O	4.057651	2.769995	-3.279279
O	-6.493388	5.752125	-3.279279
O	-4.490524	7.243191	-4.549068
O	-1.256343	-7.667963	1.231735
O	0.797143	8.747894	0.120534
O	3.275755	8.743532	0.110908
O	-1.238009	-7.666512	-1.410611
O	2.054783	-7.667461	-2.009489
O	-2.487659	8.734254	-3.279279
O	0.051919	8.734254	-3.279279
O	2.054783	-7.667461	-4.549068
O	-1.208225	-4.676218	1.101273
O	0.779272	-6.221796	0.075161
O	3.272040	-6.203812	0.098162
O	-1.255215	-4.714178	-1.416503
O	2.054783	-4.685330	-2.009489
O	-2.487659	-6.176396	-3.279279
O	0.051919	-6.176395	-3.279279
O	2.054783	-4.685330	-4.549068
O	-1.200448	-1.704359	1.122375
O	0.769999	-3.182160	-0.115213
O	3.327049	-3.233156	-0.082265
O	-1.258024	-1.701966	-1.420230
O	2.054783	-1.703200	-2.009489
O	-2.487659	-3.194265	-3.279279
O	0.051919	-3.194265	-3.279279
O	2.054783	-1.703200	-4.549068
O	-1.223615	1.277592	1.133456
O	0.819083	-0.190853	0.068931
O	3.314137	-0.186420	0.080408

O	-1.225396	1.274005	-1.411769
O	2.054783	1.278930	-2.009489
O	-2.487659	-0.212134	-3.279279
O	0.051919	-0.212135	-3.279279
O	2.054783	1.278930	-4.549068
O	-1.191915	4.242836	1.144483
O	0.811195	2.729517	0.027575
O	3.330366	2.725661	0.042231
O	-1.238425	4.280461	-1.408216
O	2.054783	4.261061	-2.009489
O	-2.487659	2.769996	-3.279279
O	0.051919	2.769996	-3.279279
O	2.054783	4.261061	-4.549068
O	-1.229642	7.242146	1.129822
O	0.800622	5.787408	0.022732
O	3.323830	5.821277	-0.009255
O	-1.231531	7.266192	-1.405288
O	2.054783	7.243191	-2.009489
O	-2.487659	5.752126	-3.279279
O	0.051919	5.752126	-3.279279
O	2.054783	7.243191	-4.549068
O	4.405069	-1.650476	9.115892
O	3.756050	-0.373029	10.872128
O	2.050321	-2.049652	1.961410
O	1.814976	-4.297147	2.048530
O	1.348571	5.990375	3.185160
O	2.104251	4.292921	1.907813
O	-2.970560	7.033943	7.841849
O	-4.498594	6.126755	9.238315
C	-3.767721	-1.219212	8.163719
C	-3.757330	0.880304	3.826854
C	0.189188	0.549818	8.742035
C	1.342846	0.318134	9.482053
C	2.327528	-0.522736	8.953331
C	2.111460	-1.102378	7.702394
C	0.929794	-0.829955	7.013824
C	3.553804	-0.816649	9.761341
C	0.562179	-1.503790	5.755611
C	-1.274373	-2.203508	4.516329
C	-0.469128	-3.011320	3.718817
C	0.919555	-2.862680	3.804415
C	1.444603	-2.171048	4.901774
C	1.699861	-3.138423	2.534946
C	0.395108	1.409440	4.244273
C	1.086798	2.380324	3.541189
C	0.825312	3.726716	3.791309
C	-0.100913	4.046352	4.781121
C	-0.757709	3.022409	5.467014
C	1.457315	4.798312	2.937170
C	-1.774452	3.260734	6.509362
C	-3.279504	2.264324	7.998260
C	-3.708665	3.501600	8.458474
C	-3.144905	4.660111	7.914057
C	-2.167054	4.535708	6.927707
C	-3.620833	5.986991	8.412340

H	-0.603725	1.185842	9.117550
H	1.470556	0.767529	10.460170
H	2.840397	-1.790898	7.295360
H	-2.343475	-2.126610	4.358891
H	-0.914831	-3.632809	2.954516
H	2.516621	-2.090502	5.046953
H	0.549304	0.359992	4.032421
H	1.803245	2.102332	2.780242
H	-0.305088	5.092218	4.977995
H	-3.686881	1.335912	8.382083
H	-4.468895	3.584048	9.226005
H	-1.725156	5.424417	6.495254
H	5.142180	-1.873875	9.711134
H	-0.773298	-7.671148	2.068300
H	4.978587	1.275530	2.083239
H	-3.345122	7.848766	8.227848
N	-2.937527	-0.798385	7.434206
N	-3.074626	0.534426	4.718845
N	-0.024877	-0.000255	7.532022
N	-0.759212	-1.386662	5.443248
N	-0.506978	1.709276	5.191891
N	-2.328777	2.139919	7.049585
S	-4.914822	-1.759497	9.189690
S	-4.860745	1.429559	2.713562
Ru	-1.660987	0.318036	6.258935

(11) 2COOH-diff(cis,trans)-1row-S 1BB1MH+S

203

Ti	-4.469417	-7.665641	-0.199716
Ti	5.342277	5.751439	0.071394
Ti	5.327440	7.243189	-3.279279
Ti	-4.490524	8.734254	-3.279279
Ti	-4.495447	-4.678799	-0.198038
Ti	5.323054	8.735863	0.087718
Ti	5.327440	-7.667460	-3.279279
Ti	-4.490524	-6.176395	-3.279279
Ti	-4.497948	-1.698429	-0.205535
Ti	5.315567	-6.176205	0.072966
Ti	5.327440	-4.685331	-3.279279
Ti	-4.490524	-3.194265	-3.279279
Ti	-4.481451	1.265212	-0.111535
Ti	5.324124	-3.202551	0.043168
Ti	5.327440	-1.703200	-3.279279
Ti	-4.490524	-0.212134	-3.279279
Ti	-4.489662	4.242449	-0.202287
Ti	5.321644	-0.220680	0.066184
Ti	5.327440	1.278930	-3.279279
Ti	-4.490524	2.769996	-3.279279
Ti	-4.490092	7.232105	-0.197372
Ti	5.329031	2.760165	0.074890
Ti	5.327440	4.261061	-3.279279
Ti	-4.490524	5.752126	-3.279279
Ti	2.045592	-7.653068	-0.209840

Ti	-1.211836	8.618498	0.014653
Ti	-1.217870	-7.667461	-3.279279
Ti	2.054783	8.734255	-3.279279
Ti	2.060641	-4.654988	-0.102449
Ti	-1.207859	-6.079196	-0.012407
Ti	-1.217870	-4.685330	-3.279279
Ti	2.054783	-6.176395	-3.279279
Ti	2.069414	-1.707713	-0.105808
Ti	-1.208071	-3.129255	0.019821
Ti	-1.217870	-1.703200	-3.279279
Ti	2.054783	-3.194265	-3.279279
Ti	2.056015	1.275277	-0.224545
Ti	-1.203657	-0.193062	0.068319
Ti	-1.217870	1.278930	-3.279279
Ti	2.054783	-0.212135	-3.279279
Ti	2.076038	4.258943	-0.137189
Ti	-1.211063	2.744638	0.069922
Ti	-1.217870	4.261060	-3.279279
Ti	2.054783	2.769996	-3.279279
Ti	2.064571	7.243086	-0.216928
Ti	-1.215745	5.683922	0.090561
Ti	-1.217870	7.243191	-3.279279
Ti	2.054783	5.752126	-3.279279
O	5.327640	7.238605	1.137464
O	-5.686240	8.735285	0.129616
O	-3.232692	8.732190	0.105192
O	5.342988	7.249150	-1.421765
O	-4.490524	-7.667461	-2.009489
O	4.057651	5.752125	-3.279279
O	-6.493388	8.734254	-3.279279
O	-4.490524	-7.667461	-4.549068
O	5.329800	-7.673011	1.135571
O	-5.693322	-6.185763	0.127298
O	-3.239265	-6.185920	0.106088
O	5.329534	-7.679624	-1.415959
O	-4.490524	-4.685330	-2.009489
O	4.057651	8.734253	-3.279279
O	-6.493388	-6.176396	-3.279279
O	-4.490524	-4.685330	-4.549068
O	5.310750	-4.687162	1.114565
O	-5.710224	-3.209587	0.115991
O	-3.258805	-3.205367	0.108130
O	5.351429	-4.711996	-1.424950
O	-4.490524	-1.703200	-2.009489
O	4.057651	-6.176396	-3.279279
O	-6.493388	-3.194265	-3.279279
O	-4.490524	-1.703200	-4.549068
O	5.307782	-1.713012	1.102945
O	-5.722596	-0.236925	0.038521
O	-3.247642	-0.234728	0.082299
O	5.345186	-1.687738	-1.426416
O	-4.490524	1.278931	-2.009489
O	4.057651	-3.194265	-3.279279
O	-6.493388	-0.212135	-3.279279
O	-4.490524	1.278931	-4.549068

O	5.329974	1.284631	1.129324
O	-5.711621	2.785016	0.080959
O	-3.236685	2.790945	0.057567
O	5.340091	1.289778	-1.420905
O	-4.490524	4.261061	-2.009489
O	4.057651	-0.212134	-3.279279
O	-6.493388	2.769996	-3.279279
O	-4.490524	4.261061	-4.549068
O	5.325919	4.267022	1.127409
O	-5.697303	5.761469	0.116310
O	-3.244726	5.757591	0.117390
O	5.347687	4.270677	-1.423572
O	-4.490524	7.243191	-2.009489
O	4.057651	2.769995	-3.279279
O	-6.493388	5.752125	-3.279279
O	-4.490524	7.243191	-4.549068
O	-1.255694	-7.668262	1.235076
O	0.803194	8.733314	0.149000
O	3.264287	8.727888	0.133864
O	-1.232009	-7.674905	-1.408837
O	2.054783	-7.667461	-2.009489
O	-2.487659	8.734254	-3.279279
O	0.051919	8.734254	-3.279279
O	2.054783	-7.667461	-4.549068
O	-1.206581	-4.678718	1.099599
O	0.776117	-6.231645	0.075035
O	3.264902	-6.208751	0.097122
O	-1.254002	-4.715097	-1.417430
O	2.054783	-4.685330	-2.009489
O	-2.487659	-6.176396	-3.279279
O	0.051919	-6.176395	-3.279279
O	2.054783	-4.685330	-4.549068
O	-1.196430	-1.704094	1.127593
O	0.765544	-3.187319	-0.114026
O	3.314011	-3.222371	-0.085777
O	-1.255172	-1.700383	-1.418064
O	2.054783	-1.703200	-2.009489
O	-2.487659	-3.194265	-3.279279
O	0.051919	-3.194265	-3.279279
O	2.054783	-1.703200	-4.549068
O	-1.215572	1.279780	1.145446
O	0.808634	-0.179094	0.069172
O	3.286478	-0.179755	0.074967
O	-1.219222	1.283564	-1.407430
O	2.054783	1.278930	-2.009489
O	-2.487659	-0.212134	-3.279279
O	0.051919	-0.212135	-3.279279
O	2.054783	1.278930	-4.549068
O	-1.194036	4.246155	1.165474
O	0.815123	2.766402	0.066779
O	3.290864	2.765894	0.064198
O	-1.219188	4.284813	-1.403517
O	2.054783	4.261061	-2.009489
O	-2.487659	2.769996	-3.279279
O	0.051919	2.769996	-3.279279

O	2.054783	4.261061	-4.549068
O	-1.209086	7.239327	1.147814
O	0.817147	5.778420	0.087274
O	3.294319	5.788130	0.048082
O	-1.216155	7.264113	-1.399612
O	2.054783	7.243191	-2.009489
O	-2.487659	5.752126	-3.279279
O	0.051919	5.752126	-3.279279
O	2.054783	7.243191	-4.549068
O	4.313590	-1.854531	9.212584
O	3.648739	-0.585442	10.968364
O	2.025448	-2.064227	1.974946
O	1.837686	-4.320003	2.037971
O	1.460527	5.779525	3.764478
O	2.093822	4.327303	2.164304
O	-3.097304	6.776275	7.988425
O	-4.647182	5.851291	9.349166
C	-3.799941	-1.492583	8.245585
C	-3.817256	0.725907	3.902060
C	0.084809	0.317492	8.829880
C	1.235146	0.087032	9.575275
C	2.233701	-0.732334	9.039152
C	2.038292	-1.288573	7.774160
C	0.858574	-1.017904	7.080947
C	3.454312	-1.027078	9.855323
C	0.512383	-1.664441	5.801979
C	-1.301519	-2.358396	4.523511
C	-0.471392	-3.112554	3.700991
C	0.912521	-2.937116	3.804499
C	1.416315	-2.276047	4.929979
C	1.701334	-3.165701	2.531193
C	0.260042	1.207366	4.291901
C	0.978308	2.183983	3.626702
C	0.767474	3.521189	3.964966
C	-0.158075	3.832112	4.960358
C	-0.849292	2.800474	5.593194
C	1.494609	4.559549	3.206377
C	-1.879846	3.026753	6.623230
C	-3.406740	2.006980	8.071412
C	-3.841949	3.236871	8.545140
C	-3.269231	4.403471	8.029732
C	-2.278410	4.294293	7.054946
C	-3.758392	5.722590	8.533638
H	-0.721305	0.932688	9.212235
H	1.351525	0.522109	10.561133
H	2.781634	-1.955187	7.356167
H	-2.371642	-2.300104	4.362783
H	-0.895397	-3.709457	2.905095
H	2.485543	-2.172479	5.082677
H	0.380517	0.165934	4.030745
H	1.693871	1.919288	2.859992
H	-0.347921	4.868133	5.208813
H	-3.820607	1.072925	8.433279
H	-4.614518	3.306185	9.300931
H	-1.835636	5.190755	6.640423

H	5.047517	-2.075798	9.813676
H	-0.757644	-7.654105	2.061479
H	1.953813	6.399230	3.193170
H	-3.485125	7.586935	8.370767
N	-2.994543	-1.048196	7.502069
N	-3.162712	0.309701	4.788031
N	-0.110481	-0.212494	7.608337
N	-0.810878	-1.573401	5.489620
N	-0.622964	1.492709	5.267304
N	-2.441972	1.897755	7.135481
S	-4.910992	-2.066318	9.291423
S	-4.856819	1.369092	2.788340
Ru	-1.750473	0.099467	6.326548

(11) 2COOH-diff(cis,trans)-1row-S 2MH+S

203

Ti	-3.032200	-8.345504	-0.189692
Ti	6.808071	5.091724	0.082572
Ti	6.797772	6.566779	-3.279279
Ti	-3.020194	8.057845	-3.279279
Ti	-3.016955	-5.360667	-0.192313
Ti	6.794633	8.072325	0.091940
Ti	6.797769	-8.343871	-3.279279
Ti	-3.020194	-6.852805	-3.279279
Ti	-3.028718	-2.375595	-0.198432
Ti	6.799340	-6.846911	0.081364
Ti	6.797769	-5.361740	-3.279279
Ti	-3.020194	-3.870675	-3.279279
Ti	-3.000179	0.593351	-0.113728
Ti	6.806462	-3.840374	0.068308
Ti	6.797769	-2.379610	-3.279279
Ti	-3.020194	-0.888545	-3.279279
Ti	-3.028928	3.575259	-0.195767
Ti	6.789219	-0.863562	0.089639
Ti	6.797772	0.602520	-3.279279
Ti	-3.020194	2.093586	-3.279279
Ti	-3.001174	6.564547	-0.192200
Ti	6.808847	2.111665	0.087284
Ti	6.797772	3.584651	-3.279279
Ti	-3.020194	5.075716	-3.279279
Ti	3.515664	-8.340983	-0.200854
Ti	0.261409	8.059061	0.095880
Ti	0.252460	-8.343871	-3.279279
Ti	3.525114	8.057845	-3.279279
Ti	3.533692	-5.367981	-0.117147
Ti	0.246114	-6.858734	0.077010
Ti	0.252460	-5.361740	-3.279279
Ti	3.525114	-6.852805	-3.279279
Ti	3.521176	-2.380214	-0.205973
Ti	0.243344	-3.862208	0.042085
Ti	0.252460	-2.379610	-3.279279
Ti	3.525114	-3.870675	-3.279279
Ti	3.526998	0.609004	-0.203397

Ti	0.264161	-0.881145	0.085163
Ti	0.252460	0.602520	-3.279279
Ti	3.525114	-0.888545	-3.279279
Ti	3.539444	3.592315	-0.128244
Ti	0.252808	2.094589	0.074875
Ti	0.252460	3.584651	-3.279279
Ti	3.525114	2.093586	-3.279279
Ti	3.545927	6.572228	-0.212338
Ti	0.249373	5.076787	0.073641
Ti	0.252460	6.566781	-3.279279
Ti	3.525114	5.075716	-3.279279
O	6.797720	6.574777	1.160890
O	-4.242176	8.056174	0.139857
O	-1.786113	8.066349	0.128649
O	6.812934	6.572182	-1.412449
O	-3.020194	-8.343871	-2.009489
O	5.527982	5.075715	-3.279279
O	8.067558	5.075714	-3.279279
O	-3.020194	-8.343871	-4.549068
O	6.791004	-8.328591	1.165495
O	-4.248418	-6.849099	0.129077
O	-1.794039	-6.858116	0.134105
O	6.814440	-8.347018	-1.408821
O	-3.020194	-5.361740	-2.009489
O	5.527982	8.057844	-3.279279
O	8.067558	8.057843	-3.279279
O	-3.020194	-5.361740	-4.549068
O	6.755686	-5.348605	1.185036
O	-4.253597	-3.875183	0.135008
O	-1.794048	-3.877658	0.123155
O	6.803507	-5.367877	-1.409737
O	-3.020194	-2.379610	-2.009489
O	5.527979	-6.852805	-3.279279
O	8.067558	-6.852805	-3.279279
O	-3.020194	-2.379610	-4.549068
O	6.796851	-2.375803	1.155637
O	-4.266991	-0.909934	0.059517
O	-1.778286	-0.913255	0.080160
O	6.789479	-2.380891	-1.410715
O	-3.020194	0.602520	-2.009489
O	5.527982	-3.870675	-3.279279
O	8.067558	-3.870675	-3.279279
O	-3.020194	0.602520	-4.549068
O	6.797185	0.615332	1.166851
O	-4.250996	2.103277	0.109017
O	-1.773519	2.115997	0.075290
O	6.804202	0.594655	-1.408451
O	-3.020194	3.584651	-2.009489
O	5.527982	-0.888544	-3.279279
O	8.067558	-0.888544	-3.279279
O	-3.020194	3.584651	-4.549068
O	6.788214	3.596354	1.156106
O	-4.243722	5.088206	0.131551
O	-1.786698	5.078984	0.130310
O	6.814238	3.581556	-1.413500

O	-3.020194	6.566781	-2.009489
O	5.527982	2.093585	-3.279279
O	8.067558	2.093585	-3.279279
O	-3.020194	6.566781	-4.549068
O	0.258664	-8.338441	1.163653
O	2.301079	8.049621	0.163303
O	4.763759	8.065135	0.120659
O	0.248715	-8.351049	-1.409729
O	3.525114	-8.343871	-2.009489
O	-1.017330	8.057845	-3.279279
O	1.522250	8.057845	-3.279279
O	3.525114	-8.343871	-4.549068
O	0.250904	-5.355552	1.137784
O	2.281888	-6.870333	0.058016
O	4.772221	-6.886847	0.044676
O	0.230488	-5.362945	-1.418721
O	3.525114	-5.361740	-2.009489
O	-1.017330	-6.852806	-3.279279
O	1.522250	-6.852805	-3.279279
O	3.525114	-5.361740	-4.549068
O	0.246732	-2.387935	1.148054
O	2.278615	-3.842299	0.065643
O	4.762279	-3.834731	0.082487
O	0.252616	-2.380362	-1.416479
O	3.525114	-2.379610	-2.009489
O	-1.017330	-3.870675	-3.279279
O	1.522250	-3.870675	-3.279279
O	3.525114	-2.379610	-4.549068
O	0.249703	0.608427	1.159202
O	2.296176	-0.881689	0.155124
O	4.753637	-0.878143	0.146960
O	0.263406	0.597175	-1.409246
O	3.525114	0.602520	-2.009489
O	-1.017330	-0.888544	-3.279279
O	1.522250	-0.888545	-3.279279
O	3.525114	0.602520	-4.549068
O	0.275859	3.588406	1.159579
O	2.290150	2.081015	0.087571
O	4.768477	2.078966	0.079759
O	0.249066	3.592220	-1.412449
O	3.525114	3.584651	-2.009489
O	-1.017330	2.093586	-3.279279
O	1.522250	2.093586	-3.279279
O	3.525114	3.584651	-4.549068
O	0.251527	6.562167	1.166622
O	2.288611	5.112401	0.078638
O	4.777898	5.106018	0.052256
O	0.242502	6.574864	-1.410961
O	3.525114	6.566781	-2.009489
O	-1.017330	5.075716	-3.279279
O	1.522250	5.075716	-3.279279
O	3.525114	6.566781	-4.549068
O	5.640221	-2.736414	9.751398
O	4.708881	-1.440375	11.392581
O	5.186668	-4.853071	3.551223

O	3.540101	-5.386854	2.082677
O	2.210031	5.083943	3.462029
O	3.502423	3.720583	2.167388
O	-2.652021	5.407131	7.365096
O	-4.098744	4.263479	8.705598
C	-1.999203	-2.717162	7.848747
C	-2.089103	-0.216133	3.722437
C	1.506754	-0.571526	8.706075
C	2.548479	-0.764394	9.607876
C	3.596880	-1.640549	9.266082
C	3.553578	-2.281005	8.020540
C	2.477544	-2.047436	7.154100
C	4.683121	-1.898967	10.256959
C	2.310808	-2.712012	5.857979
C	0.746079	-3.154679	4.158351
C	1.628761	-4.032303	3.538743
C	2.945895	-4.153804	4.022471
C	3.278154	-3.512821	5.228341
C	3.918871	-4.863299	3.148877
C	2.121805	0.419147	4.410912
C	2.704179	1.481952	3.737059
C	2.134927	2.760992	3.870518
C	1.021789	2.929599	4.705564
C	0.487055	1.822925	5.370416
C	2.678952	3.880338	3.078696
C	-0.644732	1.896982	6.302762
C	-2.029942	0.670546	7.752936
C	-2.726625	1.818323	8.123062
C	-2.363031	3.054360	7.561603
C	-1.303992	3.088198	6.645345
C	-3.134006	4.271586	7.950354
H	0.679705	0.104655	8.932612
H	2.553195	-0.256078	10.575618
H	4.337900	-2.991284	7.751492
H	-0.245499	-2.945822	3.754702
H	1.302133	-4.581353	2.652856
H	4.279820	-3.613855	5.652403
H	2.512052	-0.592147	4.310255
H	3.580545	1.330642	3.100979
H	0.554853	3.914181	4.785333
H	-2.297270	-0.311510	8.144292
H	-3.561007	1.755034	8.822959
H	-0.992784	4.037291	6.208820
H	6.280375	-2.934461	10.470640
H	5.785212	-5.178582	2.810694
H	2.473231	5.763969	2.809655
H	-3.253592	6.125514	7.638399
N	-1.219314	-2.271235	7.056036
N	-1.359897	-0.761458	4.498282
N	1.453595	-1.192204	7.499905
N	1.093813	-2.454578	5.261891
N	1.026337	0.564204	5.201625
N	-1.006904	0.696551	6.861569
S	-3.046436	-3.323755	8.922795
S	-3.217526	0.529379	2.791201

Ru -0.022758 -0.956088 6.078129

(12) 3COOH-2BB1MH

Ti	-5.176687	-5.897479	-0.201951
Ti	4.620756	4.589955	-0.044679
Ti	4.638683	6.015910	-3.279279
Ti	-5.179285	-7.403676	-3.279279
Ti	-5.166940	-2.911030	-0.094288
Ti	4.640322	7.516276	0.109001
Ti	4.638681	-8.894741	-3.279279
Ti	-5.179285	-4.421546	-3.279279
Ti	-5.222480	0.059422	-0.113618
Ti	4.656779	-7.492437	-0.029029
Ti	4.638683	-5.912609	-3.279279
Ti	-5.179285	-1.439416	-3.279279
Ti	-5.176272	3.024010	-0.206544
Ti	4.593969	-4.346813	-0.059181
Ti	4.638683	-2.930479	-3.279279
Ti	-5.179285	1.542715	-3.279279
Ti	-5.183806	6.014107	-0.193376
Ti	4.637402	-1.459477	0.110219
Ti	4.638683	0.051652	-3.279279
Ti	-5.179285	4.524845	-3.279279
Ti	-5.169855	9.006056	-0.199997
Ti	4.627689	1.438695	0.030398
Ti	4.638683	3.033781	-3.279279
Ti	-5.179283	7.506977	-3.279279
Ti	1.380572	-5.879966	-0.110236
Ti	-1.885544	-7.397911	0.081055
Ti	-1.906630	-5.912611	-3.279279
Ti	1.366024	-7.403675	-3.279279
Ti	1.340782	-2.899641	-0.108043
Ti	-1.894883	-4.424935	0.026118
Ti	-1.906630	-2.930480	-3.279279
Ti	1.366024	-4.421545	-3.279279
Ti	1.368209	0.051184	-0.209765
Ti	-1.938904	-1.428454	0.026441
Ti	-1.906630	0.051650	-3.279279
Ti	1.366024	-1.439415	-3.279279
Ti	1.366625	3.032682	-0.216475
Ti	-1.912705	1.544049	0.066887
Ti	-1.906630	3.033780	-3.279279
Ti	1.366024	1.542716	-3.279279
Ti	1.346729	6.021942	-0.099753
Ti	-1.916189	4.531391	0.054061
Ti	-1.906630	6.015910	-3.279279
Ti	1.366024	4.524846	-3.279279
Ti	1.379301	-8.873581	-0.207900
Ti	-1.906139	7.516006	0.078071
Ti	-1.906630	-8.894739	-3.279279
Ti	1.366024	7.506976	-3.279279
O	4.609335	5.985598	1.164689
O	-6.444774	-7.438005	0.137580
O	-3.976213	-7.411320	0.131109

O	4.661081	5.998928	-1.389594
O	-5.179285	-5.912612	-2.009489
O	3.368893	4.524845	-3.279279
O	-7.182147	-7.403675	-3.279279
O	-5.179285	-5.912612	-4.549068
O	4.663722	-8.884658	1.142178
O	-6.436080	-4.460402	0.092286
O	-3.957007	-4.461543	0.063858
O	4.604407	-8.922929	-1.394890
O	-5.179285	-2.930481	-2.009489
O	3.368893	7.506976	-3.279279
O	-7.182149	-4.421546	-3.279279
O	-5.179285	-2.930481	-4.549068
O	4.681178	-5.911576	1.191761
O	-6.494515	-1.471797	-0.136606
O	-3.932846	-1.411921	-0.082130
O	4.640161	-5.921276	-1.418355
O	-5.179285	0.051649	-2.009489
O	3.368893	-7.403673	-3.279279
O	-7.182149	-1.439416	-3.279279
O	-5.179285	0.051649	-4.549068
O	4.606328	-2.960110	1.130419
O	-6.446482	1.591949	0.045255
O	-3.961020	1.580535	0.073470
O	4.671137	-2.901789	-1.398788
O	-5.179285	3.033779	-2.009489
O	3.368893	-4.421543	-3.279279
O	-7.182149	1.542714	-3.279279
O	-5.179285	3.033779	-4.549068
O	4.642804	0.057993	1.166814
O	-6.423902	4.543779	0.128111
O	-3.967952	4.546967	0.107129
O	4.665302	0.078213	-1.387329
O	-5.179283	6.015912	-2.009489
O	3.368893	-1.439413	-3.279279
O	-7.182147	4.524847	-3.279279
O	-5.179283	6.015912	-4.549068
O	4.619011	3.036710	1.256323
O	-6.431124	7.525170	0.152688
O	-3.972301	7.504686	0.119734
O	4.654059	3.037622	-1.404788
O	-5.179283	8.998042	-2.009489
O	3.368893	1.542718	-3.279279
O	-7.182147	7.506977	-3.279279
O	-5.179283	8.998042	-4.549068
O	-1.888291	-5.897987	1.113935
O	0.150290	-7.430691	0.090049
O	2.634888	-7.420489	0.072303
O	-1.927988	-5.933505	-1.423450
O	1.366024	-5.912611	-2.009489
O	-3.176420	-7.403676	-3.279279
O	-0.636840	-7.403676	-3.279279
O	1.366024	-5.912611	-4.549068
O	-1.908307	-2.926695	1.087670
O	0.119988	-4.417742	-0.060887

O	2.687978	-4.470508	-0.137231
O	-1.907283	-2.928137	-1.435837
O	1.366024	-2.930480	-2.009489
O	-3.176420	-4.421545	-3.279279
O	-0.636840	-4.421545	-3.279279
O	1.366024	-2.930480	-4.549068
O	-1.931318	0.050022	1.113669
O	0.140506	-1.390857	0.056551
O	2.637398	-1.373962	0.030338
O	-1.878332	0.075460	-1.424699
O	1.366024	0.051650	-2.009489
O	-3.176420	-1.439415	-3.279279
O	-0.636840	-1.439415	-3.279279
O	1.366024	0.051650	-4.549068
O	-1.913031	3.042570	1.119505
O	0.163770	1.552607	0.137407
O	2.641256	1.560846	0.100961
O	-1.912276	3.033371	-1.425861
O	1.366024	3.033780	-2.009489
O	-3.176420	1.542715	-3.279279
O	-0.636840	1.542715	-3.279279
O	1.366024	3.033780	-4.549068
O	-1.897472	6.009908	1.113763
O	0.142200	4.495031	0.026405
O	2.658763	4.470578	0.020607
O	-1.922814	6.016901	-1.427120
O	1.366024	6.015911	-2.009489
O	-3.176420	4.524846	-3.279279
O	-0.636840	4.524846	-3.279279
O	1.366024	6.015911	-4.549068
O	-1.907821	-8.897038	1.129714
O	0.151863	7.502390	0.086008
O	2.622629	7.507217	0.090982
O	-1.917228	-8.901264	-1.415586
O	1.366024	-8.894738	-2.009489
O	-3.176420	7.506977	-3.279279
O	-0.636840	7.506976	-3.279279
O	1.366024	-8.894738	-4.549068
O	3.279334	5.252529	3.399203
O	1.402618	5.575160	2.193668
O	5.926144	2.517769	8.407475
O	5.592464	1.164575	10.188531
O	1.332477	-5.385817	2.187139
O	1.563535	-3.174574	1.824464
O	-5.068472	-2.501699	2.010108
O	-5.366837	-0.264132	1.932590
C	-2.030070	2.843867	7.627044
C	-1.544377	-1.933105	8.711873
C	-0.311865	2.253498	4.263327
C	0.169118	3.357339	3.571105
C	1.410755	3.902104	3.928491
C	2.084097	3.330078	5.015996
C	1.521972	2.246312	5.698695
C	2.009796	4.996550	3.109278
C	2.118258	1.651926	6.910736

C	1.761760	0.181168	8.699423
C	2.999092	0.484690	9.249477
C	3.834127	1.389283	8.583638
C	3.381300	1.986824	7.407922
C	5.186636	1.662009	9.161509
C	1.480539	-2.032638	5.641888
C	1.888043	-3.064436	4.802432
C	0.948614	-3.631290	3.933339
C	-0.378603	-3.222982	4.044798
C	-0.705229	-2.142770	4.868303
C	1.330560	-4.198452	2.576471
C	-2.024202	-1.488781	4.809176
C	-3.276098	0.392869	5.400486
C	-4.279880	0.058364	4.504387
C	-4.149180	-1.112357	3.745127
C	-3.044073	-1.929672	3.960949
C	-4.953049	-1.339753	2.507560
H	-1.255469	1.804756	3.978780
H	-0.417100	3.773042	2.763192
H	3.024735	3.750132	5.348219
H	1.068395	-0.509670	9.165912
H	3.330466	0.028183	10.175420
H	4.016807	2.690076	6.885341
H	2.185686	-1.546984	6.306194
H	2.934114	-3.347650	4.772860
H	-1.117182	-3.632562	3.370320
H	-3.325353	1.283833	6.015586
H	-5.122205	0.725499	4.366000
H	-2.939594	-2.830000	3.372571
H	3.716200	5.752056	2.659834
H	6.795101	2.592245	8.839646
H	5.328497	3.113347	1.908178
H	5.242018	-5.889505	1.979821
N	-1.418520	1.843656	7.464478
N	-1.070890	-1.039249	8.093367
N	0.337422	1.683418	5.300523
N	1.337597	0.730265	7.542188
N	0.238005	-1.511798	5.620093
N	-2.135378	-0.324324	5.502045
S	-2.892375	4.208794	7.827458
S	-2.161378	-3.162087	9.570083
Ru	-0.458147	0.236027	6.612291

(12) 3COOH-3BB

203

Ti	-5.186532	-5.907805	-0.203165
Ti	4.584045	4.643986	0.011391
Ti	4.638684	6.015910	-3.279280
Ti	-5.179286	-7.403676	-3.279280
Ti	-5.201155	-2.921958	-0.095130
Ti	4.627681	7.513858	0.123132
Ti	4.638682	-8.894740	-3.279280
Ti	-5.179286	-4.421546	-3.279280

Ti	-5.227440	0.037452	-0.117657
Ti	4.618110	-7.509856	-0.032617
Ti	4.638684	-5.912609	-3.279280
Ti	-5.179286	-1.439416	-3.279280
Ti	-5.190967	3.012927	-0.202327
Ti	4.573065	-4.413187	-0.049069
Ti	4.638684	-2.930480	-3.279280
Ti	-5.179286	1.542714	-3.279280
Ti	-5.183387	6.012269	-0.196919
Ti	4.606574	-1.548659	0.082741
Ti	4.638684	0.051653	-3.279280
Ti	-5.179286	4.524846	-3.279280
Ti	-5.176918	9.005776	-0.195946
Ti	4.585092	1.544220	-0.126337
Ti	4.638684	3.033782	-3.279280
Ti	-5.179282	7.506977	-3.279280
Ti	1.358047	-5.895744	-0.111026
Ti	-1.894797	-7.402896	0.081314
Ti	-1.906630	-5.912612	-3.279280
Ti	1.366024	-7.403675	-3.279280
Ti	1.305594	-2.910353	-0.098717
Ti	-1.927704	-4.427153	0.026130
Ti	-1.906630	-2.930481	-3.279280
Ti	1.366024	-4.421545	-3.279280
Ti	1.375075	0.048080	-0.223703
Ti	-1.950963	-1.428798	0.027879
Ti	-1.906630	0.051650	-3.279280
Ti	1.366024	-1.439415	-3.279280
Ti	1.320229	3.029499	-0.091067
Ti	-1.929094	1.536353	0.053452
Ti	-1.906630	3.033781	-3.279280
Ti	1.366024	1.542716	-3.279280
Ti	1.355969	5.996553	-0.112814
Ti	-1.924360	4.534249	0.031806
Ti	-1.906630	6.015910	-3.279280
Ti	1.366024	4.524846	-3.279280
Ti	1.363195	-8.898112	-0.205669
Ti	-1.900342	7.512230	0.080457
Ti	-1.906630	-8.894739	-3.279280
Ti	1.366024	7.506976	-3.279280
O	4.630112	6.005723	1.170191
O	-6.432646	-7.435993	0.142636
O	-3.971878	-7.421694	0.120676
O	4.682542	6.020253	-1.389584
O	-5.179286	-5.912612	-2.009489
O	3.368894	4.524846	-3.279280
O	-7.182147	-7.403674	-3.279280
O	-5.179286	-5.912612	-4.549070
O	4.679713	-8.873671	1.147021
O	-6.436018	-4.458900	0.083707
O	-3.961815	-4.463447	0.065822
O	4.595634	-8.920273	-1.393088
O	-5.179286	-2.930481	-2.009489
O	3.368894	7.506976	-3.279280
O	-7.182150	-4.421547	-3.279280

O	-5.179286	-2.930481	-4.549070
O	4.728228	-5.926422	1.228264
O	-6.500610	-1.458726	-0.158756
O	-3.941331	-1.412005	-0.055804
O	4.641207	-5.901552	-1.414020
O	-5.179286	0.051649	-2.009489
O	3.368894	-7.403674	-3.279280
O	-7.182150	-1.439416	-3.279280
O	-5.179286	0.051649	-4.549070
O	4.606636	-2.968680	1.140330
O	-6.453340	1.583626	0.054751
O	-3.970516	1.581092	0.083076
O	4.677470	-2.907028	-1.380003
O	-5.179286	3.033779	-2.009489
O	3.368894	-4.421543	-3.279280
O	-7.182150	1.542714	-3.279280
O	-5.179286	3.033779	-4.549070
O	4.636703	0.060997	1.284285
O	-6.442467	4.556155	0.175754
O	-3.982249	4.541861	0.109238
O	4.684749	0.084253	-1.375000
O	-5.179282	6.015913	-2.009489
O	3.368894	-1.439413	-3.279280
O	-7.182147	4.524847	-3.279280
O	-5.179282	6.015913	-4.549070
O	4.622568	3.040539	1.245536
O	-6.448910	7.505782	0.193605
O	-3.983217	7.502666	0.126533
O	4.682603	2.993289	-1.379847
O	-5.179282	8.998042	-2.009489
O	3.368894	1.542718	-3.279280
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O	-5.179282	8.998042	-4.549070
O	-1.896091	-5.898533	1.112051
O	0.150943	-7.426535	0.096317
O	2.637435	-7.409231	0.080462
O	-1.928898	-5.931926	-1.424208
O	1.366024	-5.912612	-2.009489
O	-3.176420	-7.403677	-3.279280
O	-0.636840	-7.403676	-3.279280
O	1.366024	-5.912612	-4.549070
O	-1.912781	-2.929833	1.088568
O	0.119409	-4.417573	-0.064584
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O	-1.912112	-2.928021	-1.434717
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O	-3.176420	-4.421546	-3.279280
O	-0.636840	-4.421546	-3.279280
O	1.366024	-2.930480	-4.549070
O	-1.931148	0.049568	1.111041
O	0.147160	-1.401767	0.053714
O	2.669144	-1.381433	0.028680
O	-1.896274	0.065824	-1.422616
O	1.366024	0.051650	-2.009489
O	-3.176420	-1.439416	-3.279280

O	-0.636840	-1.439415	-3.279280
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O	-1.904332	3.042806	1.094305
O	0.154266	1.507217	0.060824
O	2.691575	1.506151	0.014673
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O	1.366024	3.033780	-2.009489
O	-3.176420	1.542715	-3.279280
O	-0.636840	1.542715	-3.279280
O	1.366024	3.033780	-4.549070
O	-1.901568	6.002975	1.111139
O	0.116580	4.522233	-0.063216
O	2.683792	4.559165	-0.100631
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O	1.366024	6.015911	-2.009489
O	-3.176420	4.524846	-3.279280
O	-0.636840	4.524846	-3.279280
O	1.366024	6.015911	-4.549070
O	-1.915058	-8.896787	1.131565
O	0.142778	7.520435	0.079783
O	2.617932	7.518558	0.112175
O	-1.916718	-8.898443	-1.414948
O	1.366024	-8.894738	-2.009489
O	-3.176420	7.506976	-3.279280
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O	1.366024	-8.894738	-4.549070
O	1.517722	3.212935	1.856907
O	1.214625	5.404324	2.276561
O	5.441160	2.882953	8.304151
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O	1.275549	-5.351720	2.226229
O	1.545620	-3.148905	1.834957
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C	-1.087733	2.208436	4.761421
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C	0.973592	2.128547	5.820131
C	1.197920	4.208486	2.627106
C	1.690825	1.590945	6.994475
C	1.553685	0.144291	8.833775
C	2.796239	0.552710	9.300512
C	3.512423	1.510273	8.573815
C	2.946331	2.038118	7.412357
C	4.851366	1.938597	9.085840
C	1.303163	-2.009474	5.701912
C	1.766600	-2.976877	4.815915
C	0.856181	-3.584437	3.941865
C	-0.489757	-3.251175	4.068999
C	-0.873712	-2.221664	4.934019
C	1.272767	-4.161080	2.597751
C	-2.232050	-1.654078	4.923791

C	-3.666553	-0.016876	5.764875
C	-4.605529	-0.264186	4.772260
C	-4.341134	-1.263395	3.826244
C	-3.174241	-2.011797	3.957029
C	-5.065422	-1.393781	2.527397
H	-2.098103	1.824407	4.705462
H	-1.360368	3.606528	3.174074
H	2.524598	3.400558	5.018294
H	0.949942	-0.590270	9.355711
H	3.211898	0.136821	10.212069
H	3.485900	2.786771	6.847591
H	1.982317	-1.510958	6.383532
H	2.827830	-3.196808	4.771391
H	-1.214711	-3.712257	3.411961
H	-3.831871	0.732557	6.530812
H	-5.518496	0.321085	4.737492
H	-2.956443	-2.777593	3.226035
H	5.437351	0.085083	1.827947
H	6.290877	3.109038	8.720977
H	5.413578	3.066470	1.801786
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S	-3.478931	3.670704	8.385644
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