

Supplementary Information

Computational exploration for crystal structures of dioxides of group 14 elements (CO₂, SiO₂, GeO₂) under ultrahigh pressure

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The list of xyz coordinates of obtained EQs is shown below; (i) CO₂ at 1 atm, (ii) SiO₂ at 1 atm, (iii) GeO₂ at 1 atm, (iv) CO₂ at 10⁶ atm, (v) SiO₂ at 10⁶ atm, (vi) GeO₂ at 10⁶ atm.

(i) CO₂ at 1 atm

EQ-CO₂ 0

C	0.417129037206	-0.810003017473	-0.164281152129
C	-1.490017043564	0.697782013820	3.055760417850
C	4.031264342809	-0.809831860987	-0.164282556240
C	2.123642871789	0.697383434786	3.055925721372
C	7.644895502319	-0.809391197206	-0.164105841990
C	5.737900794437	0.697741904732	3.055905445111
O	-1.410103270840	-3.680187106721	2.406309119304
O	2.203446363846	-3.680565638504	2.406409151119
O	1.025433711510	-1.588901782304	0.485900968205
O	4.639357292433	-1.588859617273	0.485925676826
O	3.422953799527	-0.029440703244	-0.813117318004
O	1.480787710690	1.448361529131	3.706575325208
O	-0.191118357706	-0.029531926860	-0.813049001232
O	5.817835155928	-3.680154307714	2.406438476626
O	-2.132936770638	1.448536919499	3.706557359764
O	8.253243507238	-1.588363696740	0.485964018946
O	7.036636654698	-0.029133550315	-0.813108642266
O	5.094791807455	1.448499008001	3.706495881300
TV	10.841668210016	-0.000000000009	0.000000000003
TV	0.560848455525	3.624695304814	-0.000000000013
TV	-4.848305181512	-4.118969158692	6.437527165060

EQ-CO₂ 1

C	0.247488082864	-0.948347170134	-0.243591861038
C	-1.439628232777	0.765376652866	2.986613637874
C	3.838086432286	-0.948315405147	-0.243505789777
C	2.151094853629	0.765464207830	2.986630500908
C	7.428757474946	-0.948366980582	-0.243468856864
C	5.741676253421	0.765344683933	2.986588156450
O	-1.131545284015	-3.506851923493	2.256968833237
O	2.459091529762	-3.506808262874	2.256952789302
O	0.836387279970	-1.674679004243	0.480904288210
O	4.426997025175	-1.674684986540	0.480948216407
O	3.247232028352	-0.222148459143	-0.966803850942
O	1.520232822573	1.448345229011	3.717074237023
O	-0.343434497555	-0.222198917856	-0.966854153544
O	6.049807107747	-3.506829428257	2.256930088833
O	-2.070520127897	1.448263044219	3.717024406670
O	8.017615761469	-1.674787638292	0.480973718067
O	6.837914287261	-0.222213462312	-0.966791428556
O	5.110793957656	1.448227221979	3.717008451139
TV	10.771993034819	0.000000000006	0.000000000003
TV	0.324981928280	3.590098447922	-0.000000000004
TV	-4.143413936675	-3.780460731523	6.456599528408

EQ-CO₂ 2

C	0.631347010067	-0.499894669158	-0.523964542534
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C	-0.972959908772	1.265999565578	2.726086459497
C	1.030238092321	3.044806945634	-0.481264983836
C	-0.580339807702	4.818229683318	2.698927828738
C	1.418986205098	6.614054206530	-0.529911656674
C	-0.203297408834	8.313532997857	2.684597190529
O	-2.043306635515	-1.624187208785	3.388474038930
O	-1.634640157895	1.995859171408	3.381145886640
O	1.306711915239	-1.167478989460	0.180455855798
O	1.693778785281	2.320701420620	0.178366673384
O	0.365662636148	3.768081196208	-1.139767913778
O	0.091159010390	4.147342736380	1.993950459548
O	-0.044041405097	0.168331413327	-1.227723685379
O	-1.252390279673	5.488566696914	3.404071894053
O	-0.310308761259	0.536035567132	2.072894423202
O	2.095175579772	5.946460617645	0.173165834561
O	0.743721763556	7.284231469157	-1.232292242965
O	0.467308136160	7.639403331002	1.981492224198
TV	3.599681648090	0.000000000000	0.000000000001
TV	1.168056193011	10.608761975189	-0.000000000012
TV	0.043966407891	0.025475955534	6.430790554706

EQ-CO₂ 3

C	0.578429938757	-0.533427862249	-0.461420156093
C	-1.180520776676	1.309355181948	2.653152213028
C	0.656946842264	3.135626972067	-0.461419549436
C	-1.102002543080	4.978421901701	2.653154836328
C	0.735462179826	6.804678641383	-0.461412105799
C	-1.023485255839	8.647461721395	2.653150960082
O	-1.921261696842	-1.687616423081	3.365434852239
O	-1.842756021379	1.981433824406	3.365444739913
O	1.239929542467	-1.202392868806	0.254395797816
O	1.318447895608	2.466674710895	0.254403994562
O	-0.004470731820	3.805489404075	-1.176471888605
O	-0.438721103768	4.306987248593	1.941149984917
O	-0.082986504628	0.136437256742	-1.176469709662
O	-1.764231179227	5.650529688455	3.365424037553
O	-0.517232650560	0.637948398100	1.941129560662
O	1.396970017200	6.135715813455	0.254397359637
O	0.074043295822	7.474531565017	-1.176471065977
O	-0.360203773761	7.976045740918	1.941129882770
TV	3.582862885270	-0.000000000000	0.000000000001
TV	0.235546673324	11.007171735443	-0.000000000012
TV	-0.013829630029	0.016852044845	6.234303190525

EQ-CO₂ 4

C	2.593615350026	-1.265867397634	-0.652569184977
C	-2.405270119459	0.464961596271	2.654567104409
C	6.049662800398	-1.264408672198	-0.721122756291
C	1.026761111665	0.474823221382	2.652201219602
C	9.492282459681	-1.266259928985	-0.723159247178
C	4.487745637657	0.471542658332	2.647099989156
O	-1.817052494477	-0.299574173084	3.339024033641
O	1.614956929350	-0.291274416054	3.334157966437
O	3.208963931495	-2.013921218497	-1.331315082767
O	6.606750471222	-1.997044781465	-1.464683447178
O	5.491483438706	-0.528895511149	0.018187470819
O	0.441054556753	1.242235145201	1.969234887949

O	1.979845280676	-0.515441824787	0.024896541960
O	5.077514235566	-0.293930637963	3.328102015089
O	-2.992425685726	1.230184510654	1.970422181389
O	10.055613753925	-1.998247212007	-1.462451674458
O	8.927287584953	-0.530993475246	0.011897610003
O	3.898789319364	1.238289659211	1.966299736430
TV	10.360969989581	-0.000000000018	-0.000000000006
TV	0.417759055335	3.591738189734	-0.000000000056
TV	-3.567602735474	-0.127510470587	6.625984534151

EQ-CO₂ 5

C	0.907949325869	-1.163885567189	-0.603368474690
C	-0.870530090511	0.538644423155	2.559769022776
C	1.266210954392	2.256655037794	-0.639728260995
C	-0.453642713798	3.994948245312	2.553823581625
C	1.553811345317	5.792603965939	-0.637535124333
C	-0.284857759597	7.480804229470	2.617341694020
O	-0.183933815575	-0.156991445104	3.224004533703
O	0.231726836412	3.302571413715	3.223561856624
O	1.587045181136	-1.774445369586	-1.353795965544
O	1.959456454272	1.556546026692	-1.294442428958
O	0.576318897267	2.956772306934	0.016784251523
O	-1.138057399792	4.688749486811	1.884429090615
O	0.229561669704	-0.550947577774	0.146949636738
O	0.412646184884	6.860817536206	3.343989771414
O	-1.560384029679	1.234415524836	1.897834603261
O	2.253751530930	5.111452212582	-1.304599927497
O	0.855779173846	6.474043355315	0.030902695264
O	-0.986299415819	8.100697931561	1.894868807421
TV	3.669920125836	-0.000000000006	-0.000000000002
TV	0.831502829784	10.446111255028	-0.000000000181
TV	-3.739381576863	-0.041641268091	6.405194035257

EQ-CO₂ 6

C	0.610184793893	-0.735388124436	-0.324420954604
C	-1.236811372164	1.025427759756	2.807976905850
C	0.539879107055	2.785472141747	-0.395308009241
C	-1.404549306396	4.561996316844	2.803047163570
C	0.353684135822	6.316242527057	-0.264797860337
C	-1.617525937866	8.042792834150	2.904135333041
O	-0.386296836073	-1.821591842538	2.188175890762
O	-0.561293843105	1.665799891494	2.078833938088
O	1.306029002447	-0.045326035145	0.336092342841
O	1.245920046027	3.401421912395	0.326438327156
O	-0.165036458015	2.169415069385	-1.118117747646
O	-2.079555905859	3.918509461227	3.528481141688
O	-0.088213652287	-1.424627808697	-0.983857302141
O	-0.730205401551	5.207165454707	2.077593853321
O	-1.909661276677	0.381566964562	3.536825861781
O	1.014728594328	6.983200905345	0.454281242207
O	-0.308491831484	5.646909789901	-0.980079099418
O	-2.295658268752	7.390849569813	3.620813270220
TV	3.662161222643	0.000000000002	0.000000000001
TV	-0.554637119466	10.518043253817	-0.000000000015
TV	-3.680458829541	0.008826885229	6.368152930751

EQ-CO₂ 7

C	0.569419655621	-0.397531942736	-0.412586478226
C	-1.272516639420	1.347752207087	2.740304020094
C	0.656472449540	3.097883003244	-0.423501803235
C	-1.121353031581	4.822850863037	2.684976616678
C	0.789287673078	6.609286276105	-0.537596169255
C	-0.986340710964	8.306265166273	2.724690510146
O	-2.102906072517	-1.501929324600	3.443159647452
O	-1.954853789913	1.993482386205	3.458285743619
O	1.239656876034	-1.059286663815	0.302732231858
O	1.364442819512	2.486545456687	0.300602991843
O	-0.053642608607	3.709766792405	-1.144292783849
O	-0.423667652433	4.239605356008	1.929749505950
O	-0.099972472848	0.266134633960	-1.125854489683
O	-1.816549188157	5.405860668295	3.442909765434
O	-0.591476961263	0.699446836192	2.023813868633
O	1.462276939017	5.949868139253	0.175626770641
O	0.117715978267	7.268319189221	-1.253650384820
O	-0.305042478788	7.657242427423	2.008500890679
TV	3.686262466021	0.000000000002	0.000000000004
TV	0.435242186967	10.454856455211	-0.000000000057
TV	-3.735892822991	-0.030274778137	6.336164976701

EQ-CO₂ 8

C	0.856498348324	-1.235402343847	-0.018196763616
C	-1.131296629064	0.534159421399	2.662103653620
C	4.583567924915	-1.257197567144	0.420314975398
C	2.584131157722	0.592651580341	3.112025194476
C	10.045240472339	-1.243615578552	-1.488266662558
C	8.052942070791	0.606673207094	1.194515394941
O	-0.950798332896	-0.173933154993	3.591560359725
O	3.527444996484	-0.111223550624	3.004110033503
O	0.671893418355	-1.935947511769	-0.953614410139
O	3.642955658261	-1.966258737340	0.528713247980
O	5.524350939644	-0.549542913680	0.313418997803
O	1.641775749505	1.299362105496	3.220181404041
O	1.041198886538	-0.535835608588	0.916557012823
O	8.225329399764	-0.085907447175	2.138181746238
O	-1.311249878895	1.243196152057	1.731957538934
O	9.872028132346	-1.938684252675	-2.429129963977
O	10.220544794974	-0.548179800649	-0.547019508267
O	7.882503127925	1.301850384235	0.253111708926
TV	12.299584469224	-0.000000000088	-0.000000000018
TV	0.003684929517	3.681892347832	-0.000000000155
TV	-3.988643625045	-0.002924271904	5.374833074734

EQ-CO₂ 9

C	5.218779909611	-1.261365810115	0.853870288697
C	0.337699603049	-1.443304061937	-1.117397733002
C	-2.850133704221	-1.805281565960	1.542503294187
C	6.988773435745	1.743673336785	0.853765050964
C	2.110653977274	1.561637375526	-1.109377646266
C	-1.080532569793	1.199517539198	1.542435983568
O	-2.766715179071	-2.553578080017	0.631073526224
O	4.121026892291	-1.285248447504	0.408893038962
O	1.415601341130	-1.372902528853	-0.632526758541
O	-0.737350920585	-1.516977103579	-1.604599093826
O	1.034860488312	1.485466700964	-1.594145539090

O	6.312993298790	-1.236440952825	1.302768146313
O	-2.934784630793	-1.056457572852	2.453620225837
O	8.082785863490	1.768773826990	1.303089799732
O	-1.165547510307	1.948359917572	2.453528621511
O	-0.996787979851	0.451154695628	0.631097742890
O	5.891253705594	1.719570529772	0.408337761558
O	3.189379330622	1.634031751758	-0.626945111110
TV	12.023307206903	-0.000000000000	0.000000000008
TV	3.538348526920	6.009939095250	-0.000000000017
TV	0.739624814854	-0.859983190903	3.396553465995

EQ-CO₂ 10

C	0.685432162871	-0.230203495918	-0.380347909438
C	-1.864716095881	-0.014245300201	2.664534469064
C	2.790534102196	2.495108862929	-0.280921478571
C	0.201795685291	2.713220424370	2.731540627863
C	5.004869715598	5.270593181899	-0.320839908568
C	2.422474551089	5.430323848768	2.724219426787
O	-2.802931388858	0.031913105695	3.382396953910
O	-0.779163655113	2.753617837372	3.391882352206
O	1.634275151294	-0.270399577512	0.325253309359
O	3.751257167950	2.457920486358	0.408497568241
O	1.827044932356	2.528955935917	-0.967094852553
O	1.182560293988	2.671383897620	2.071528413670
O	-0.263334376265	-0.193085999012	-1.085731933606
O	1.439644638326	5.472927213141	3.381807500045
O	-0.923551735554	-0.060010067087	1.949723524538
O	5.987759863583	5.301264161427	0.336212538131
O	4.021863785446	5.238406289813	-0.977370481124
O	3.404988091275	5.387869681186	2.067131055478
TV	5.181484587782	0.000000000001	0.000000000005
TV	6.649788925131	8.159816064390	-0.000000000050
TV	-5.174836468774	0.310792471688	6.085281539118

EQ-CO₂ 11

C	0.522959153608	-0.433048832173	-0.551558622316
C	-1.307250163078	1.255824824136	2.677663916427
C	0.560642380392	2.977119065911	-0.484659840104
C	-1.333565224554	4.699245040028	2.744439199281
C	0.531461703698	6.426701224296	-0.553251674153
C	-1.294126655504	8.116159158539	2.679545038370
O	-2.022570611757	-1.561852285363	3.405022852473
O	-2.016582419842	1.847388915907	3.415349742584
O	1.210532485281	-1.057301386504	0.180354055757
O	1.262447006816	2.442735365242	0.303615505529
O	-0.141816514003	3.509089089427	-1.273409783485
O	-0.617256991049	4.168182850031	1.967625657214
O	-0.165253722023	0.188765618810	-1.285467352476
O	-2.047812370770	5.231118071577	3.523128227628
O	-0.596095422347	0.665877529353	1.939129263777
O	1.225850569406	5.821654685849	0.187678427217
O	-0.160258431998	7.033794603475	-1.295721792253
O	-0.593587003865	7.497446469804	1.953886821682
TV	3.699392833506	0.000000000004	0.000000000010
TV	0.030957597119	10.299110668798	-0.000000000060
TV	-3.788824270840	-0.058889846770	6.451083811047

EQ-CO₂ 12

C	0.654355606984	0.136132630178	-0.390137321796
C	-1.134748007520	1.898755286975	2.746644422766
C	4.723059769413	0.075636256197	-0.392028294826
C	2.731121961319	1.829817811431	2.661653678106
C	8.620420366905	0.078864293740	-0.390661917228
C	6.680470170105	1.833596160235	2.718654569237
O	-2.096050177056	-4.439179125715	3.437578504303
O	1.810271949610	-4.555001014276	3.430103478586
O	1.352756002344	-0.514894758367	0.307385207895
O	5.443355704104	-0.536163059028	0.318692878110
O	4.003991466695	0.688180990536	-1.102334678315
O	3.381827299283	1.216771233817	1.887824946704
O	-0.045965387511	0.787485039132	-1.087215150246
O	5.699389398678	-4.544693138021	3.425324274145
O	-0.439190422471	1.240932425286	2.052006423526
O	9.337383851579	-0.536350443529	0.320533420998
O	7.905836998236	0.695036551819	-1.102719496829
O	7.394626446647	1.210982171021	2.012114380546
TV	11.702486348845	0.000000000012	0.000000000033
TV	0.132335707222	3.499439608244	-0.000000000012
TV	-3.863322478211	0.017546817961	6.238345567478

EQ-CO₂ 13

C	-0.728404027236	-2.055121941155	-0.220486438386
C	1.142501098788	3.144059070128	2.798173479759
C	-0.764658688065	-0.603737927569	2.839313256281
C	0.915993296351	4.622234501860	5.917465846086
C	-0.904139523337	0.969979779531	5.835128465819
C	0.814936703033	6.288374430796	8.922593618783
O	-1.891131194083	-5.183260853733	2.598104360774
O	-2.122363975742	-3.725410318841	5.825493674684
O	-1.433011607802	-2.467327119679	0.635838192660
O	-1.441299988265	-1.094974760143	3.676714469477
O	-0.084856109925	-0.115555418394	2.002221025198
O	0.226315957012	5.579176540702	6.012039501645
O	-0.019614599414	-1.643538905717	-1.072953124075
O	-2.257194203390	-2.079518866851	8.804716178367
O	0.452791189834	4.083209002195	2.998170228911
O	-1.614517772111	0.564301597055	6.689779897272
O	-0.194002721700	1.376461071459	4.979130380115
O	0.162190533614	7.268052243214	9.037284502302
TV	3.668531769444	0.000000000001	0.000000000001
TV	3.726897051260	7.389973872764	-0.000000000007
TV	-0.304392145447	4.591035109082	9.193590401753

EQ-CO₂ 14

C	7.128511331070	-1.962606465256	1.767074221633
C	-0.137021926983	-1.235275433346	-1.903833276436
C	-2.498963663489	-2.205868691662	1.407653144042
C	8.868119668977	-3.134785075456	4.709127487010
C	1.584034144478	-2.423575433841	1.035921677251
C	-0.757823444717	-3.375486913353	4.349921950711
O	-2.638319228544	-2.865905108983	0.436661178164
O	5.959425754524	-2.074742169217	1.615360130943
O	-1.302028716291	-1.375234933812	-2.054281149971
O	1.030268120125	-1.095832403779	-1.756234823532

O	2.751485286678	-2.289897970709	1.185922370562
O	8.295509475005	-1.849121534917	1.920295980507
O	-2.360039572611	-1.545776007311	2.378685803806
O	10.035051287014	-3.020367924894	4.862357714637
O	-0.619433909841	-2.715296360351	5.320971285555
O	-0.896836324439	-4.035526534075	3.378839445619
O	7.699064547423	-3.247524275069	4.557535356904
O	0.418917409502	-2.558064252709	0.881754469885
TV	13.704540446846	-0.000000000009	0.000000000006
TV	1.652015542433	3.153744123148	-0.000000000006
TV	3.480988123770	-2.338867011406	5.885119964382

EQ-CO₂ 15

C	5.637281917836	-1.308957924618	0.775003540217
C	0.607584502789	-1.632162860877	-1.027377189037
C	-2.741958864830	-1.892823721889	1.580060087541
C	6.260760227160	-2.074747557694	4.120182019672
C	1.183812015694	-2.436836071914	2.272336795833
C	-2.162939066422	-2.700710213516	4.880145504132
O	-2.701951952790	-2.736001236694	0.751640238894
O	4.536848535111	-1.414334731930	0.350181129312
O	-0.488824506639	-1.742526212208	-1.456350501822
O	1.706730059922	-1.525508415006	-0.600362798490
O	2.283403713569	-2.330024739559	2.698123099311
O	6.735985819996	-1.202780628158	1.198758795621
O	-2.781890255209	-1.050845831819	2.409891428896
O	7.340161655144	-2.013786863433	4.599292087100
O	-2.199462756601	-1.859229441758	5.710152724570
O	-2.126871489354	-3.542751124080	4.050335826863
O	5.178338627379	-2.133863747109	3.644396072170
O	0.086696893952	-2.547106123304	1.844696975760
TV	12.313856411835	-0.000000000002	0.000000000011
TV	1.991069474094	3.024081021949	-0.000000000005
TV	1.150344542881	-1.609772702779	6.602098060547

EQ-CO₂ 16

C	5.314748559854	-1.576453859042	0.875614686808
C	0.378452270846	-1.960853928172	-0.950667037820
C	-3.062157356876	-2.183069006577	1.562129244723
C	5.746557596004	-2.355667254104	4.140025374307
C	0.810353561662	-2.740055082395	2.313718267958
C	-2.630358727298	-2.962372479715	4.826373706167
O	-3.026543887532	-3.040099719932	0.747721281748
O	4.206622553475	-1.636213064565	0.461446706338
O	-0.700546395270	-2.068696895806	-1.422486945305
O	1.460816178832	-1.856005149608	-0.481937226235
O	1.892684666401	-2.635238734050	2.782527537794
O	6.419837649530	-1.514839623396	1.292915083554
O	-3.097181929267	-1.326923113840	2.377678010413
O	6.851659181130	-2.294088619525	4.557307709189
O	-2.665379756611	-2.106253133241	5.641949475644
O	-2.594715298313	-3.819419965874	4.011989560242
O	4.638440203313	-2.415427934076	3.725840430626
O	-0.268612510886	-2.847966949111	1.841835490846
TV	12.278330002988	-0.000000000002	0.000000000011
TV	2.083515965196	3.027530698225	-0.000000000005
TV	0.863779777816	-1.558513352301	6.528755807654

EQ-CO₂ 17

C	0.715225480956	0.057260269569	-0.426190888610
C	-0.697672766128	1.806920308162	2.824282002533
C	1.316560006643	3.410004922242	-0.432046223306
C	-0.080050241492	5.227738116764	2.834682078221
C	1.990226169327	6.812612948807	-0.365230829573
C	0.564490132903	8.585561141697	2.888956582401
O	-2.598388942754	-4.261517486409	3.512544088791
O	-1.913435135093	-0.932703312666	3.630914866634
O	1.389644293811	-0.576275185761	0.310442684291
O	1.985728590037	2.769926561821	0.304228918493
O	0.642890996691	4.049920586465	-1.164056566976
O	0.599408929230	4.543853228869	2.150702810582
O	0.038541213594	0.694710225346	-1.158960673914
O	-1.363561897981	2.526727159895	3.485465097099
O	-0.034888960457	1.088388234565	2.157863857225
O	2.640417810073	6.086757674951	0.304186156052
O	1.334092788872	7.538486501176	-1.028751622783
O	1.205766471805	7.923710407387	2.147724485941
TV	3.671426423108	0.000000000004	0.000000000011
TV	1.835564612481	10.177733457870	-0.000000000033
TV	-3.484133714098	0.152888521483	6.605656239566

EQ-CO₂ 18

C	6.058789029906	-1.381584291993	0.835062151583
C	1.032888661688	-1.758909359898	-0.983425035740
C	-2.183452865719	-1.903309233439	1.585786380339
C	6.795727714158	-2.040234948209	4.144911263266
C	1.822698666372	-2.313935693139	2.342680764207
C	-1.451708473615	-2.557302240882	4.900768380903
O	-2.062635002281	-2.742038972873	0.760954114947
O	4.935324799495	-1.454895481577	0.468558934937
O	-0.086693254940	-1.834672730268	-1.357060637878
O	2.153459747153	-1.687231768266	-0.608438900243
O	2.946741388744	-2.235237106913	2.707404508975
O	7.180913083643	-1.306768722367	1.201071596089
O	-2.304515148472	-1.064706786454	2.410536309510
O	7.917328337120	-1.964668835059	4.511755125537
O	-1.570663991549	-1.718783767128	5.725690819717
O	-1.332736707845	-3.395872051283	4.075785031858
O	5.672504597303	-2.114363313634	3.777789032252
O	0.700443623972	-2.389907042163	1.978051976602
TV	12.191357030201	-0.000000000002	0.000000000014
TV	1.941415819955	3.039555236631	-0.000000000004
TV	1.469461233743	-1.314405695972	6.622672482382

EQ-CO₂ 19

C	5.763674454575	-1.151226471422	0.757627787839
C	0.733581222275	-1.445287493657	-1.015645304597
C	-2.596195621306	-1.640053477584	1.549627151768
C	6.425602543847	-1.810580339198	4.058389388865
C	1.398976048056	-2.225772341276	2.233968034035
C	-1.938794162750	-2.412228443179	4.798247755226
O	-2.461434416352	-2.478716833607	0.727253572722
O	4.661565819184	-1.266135838780	0.341121628965
O	-0.368511574034	-1.531966456327	-1.434552086594

O	1.838029559572	-1.361851849656	-0.597994519154
O	2.505010272665	-2.112362052398	2.640702671063
O	6.864420754970	-1.035375112862	1.174162197020
O	-2.732885600008	-0.801850134583	2.372104744649
O	7.550108588099	-1.735544969938	4.416792577907
O	-2.051775995777	-1.549935509282	5.599531350598
O	-1.832052600136	-3.276648207483	3.997921885855
O	5.298294148902	-1.884223284620	3.703278489819
O	0.294315321579	-2.343978115822	1.827760789288
TV	12.307952611088	-0.000000000004	0.000000000009
TV	1.935517987617	3.044642966535	-0.000000000005
TV	1.380781525669	-1.436443385054	6.522573967780

EQ-CO₂ 20

C	5.310968332820	-1.648563927796	0.393354239030
C	0.319969553282	-1.106096515446	-0.445487954737
C	-2.641514892563	-2.207621101697	1.170500597304
C	7.438796899393	2.215472190187	0.352935514381
C	2.448741885984	2.750649884677	-0.463573545693
C	-0.568106375944	1.691174846734	1.217275929071
O	-3.536541064770	-2.749790513996	0.617386599804
O	4.439661444885	-2.202004382937	-0.185590335658
O	-0.544629519902	-1.653221777292	-1.040170075499
O	1.184174183641	-0.558046643593	0.149883242817
O	3.349806635740	3.291484327393	0.081279383422
O	6.181560179389	-1.094277228519	0.973309737455
O	-1.745453379594	-1.667516433281	1.723190588603
O	8.277033628160	2.777650880236	0.971335130186
O	0.302021915751	2.244310076982	1.798524484020
O	-1.438753958663	1.137889402405	0.636908834793
O	6.601797982660	1.651114259248	-0.265356715688
O	1.548675266796	2.208948912269	-1.008432972769
TV	12.967789853058	-0.000000000003	0.000000000017
TV	4.203139107025	7.746851321796	-0.000000000014
TV	1.998818383732	-1.605166967211	2.465434633605

EQ-CO₂ 21

C	-0.116735645691	2.163263936300	4.365795725630
C	-2.046243096806	0.410595903792	1.149493638036
C	-1.400550012410	2.215325441913	-2.143029261866
C	0.079868229416	5.636637770371	4.366996027706
C	-1.851075601258	3.873076818932	1.203008706493
C	-1.192337001447	5.676002040705	-2.142322793811
O	-1.362889308942	-0.272336390220	1.830391616672
O	-2.278691308920	-1.792473870321	-2.951844026599
O	-0.731151420054	2.758196252142	-1.331730117233
O	-0.404757481270	0.025186706492	-4.750005990821
O	-0.211243707324	3.494868967113	-4.748494759113
O	-2.525573318467	4.507091084856	0.465865417633
O	0.549023597758	1.518000325170	3.631835008246
O	-2.313490499763	8.019551916580	0.466008180809
O	0.749701784906	4.995095165813	3.634042017334
O	-1.177770657496	3.240832081971	1.940865143995
O	-2.070733597334	1.671066466527	-2.952556435907
O	-0.522040287098	6.218332119051	-1.331179226786
TV	3.586562005891	-0.000000000011	0.000000000001
TV	0.415342895866	6.925723382642	0.000000000006

TV	-0.379965531117	2.783665678923	9.849261551701
# EQ-CO ₂ 22			
C	-0.265139606508	2.141836754332	4.335395516258
C	-2.082439190303	0.398295459482	1.082222085841
C	-1.313376856313	2.202344078120	-2.118380417165
C	3.193198218415	2.165441291281	4.466749097871
C	1.454676653457	0.405608128557	1.148443706915
C	2.116022521966	2.200583092593	-2.127768198718
O	-1.498394385992	-0.301210851880	1.834552133950
O	-2.052137482333	-2.017478999172	-2.918551661122
O	-0.721574607783	2.844560238480	-1.320107986190
O	-0.325419892014	-0.135120929601	-4.724091705689
O	3.136254720216	-0.111662492357	-4.588088755488
O	-2.518346806246	4.674950924642	0.325863561901
O	0.349573616362	1.453897796364	3.595685165762
O	0.949623038243	4.695358196431	0.464899780943
O	3.803247169327	1.476183463449	3.725339962402
O	2.108546349010	-0.304678808215	1.831163736502
O	1.353137534167	-2.010706731608	-2.917428056477
O	2.729617655119	2.833578616294	-1.338138798256
TV	6.967793428161	-0.000000000022	0.000000000002
TV	0.148035089438	3.578702105784	0.000000000003
TV	-0.553669974021	2.964866251215	9.800590188904

# EQ-CO ₂ 23			
C	1.228863272311	-0.719054992822	-0.169789101543
C	-0.493465465273	1.766314450084	2.459982492306
C	4.577592887090	-0.718961953279	-0.169792307153
C	2.855188029540	1.766325825954	2.460007163826
C	7.926182052984	-0.719015454918	-0.169724996445
C	6.203826153975	1.766389870523	2.460011893704
O	-3.785322353612	-4.001237718598	1.964341527455
O	-0.436671847050	-4.001249790805	1.964427353498
O	1.677804335435	-1.696069901647	0.323774965686
O	5.026501036436	-1.695993017706	0.323784116076
O	4.128800934176	0.258089711801	-0.662984199667
O	3.183663893675	2.786989326509	2.959585588475
O	0.780120975472	0.258016003439	-0.662996974467
O	2.911968066951	-4.001188832496	1.964417871841
O	-0.164953879282	2.786953664475	2.959577341298
O	8.375224625392	-1.695997044024	0.323809949711
O	7.477365583556	0.258049068847	-0.662899522462
O	6.532332349277	2.787030797138	2.959615210449
TV	10.046051639180	0.000000000059	-0.000000000032
TV	2.966882942446	4.743313012948	0.000000000019
TV	-3.220247488876	0.249723796478	5.267656140973

# EQ-CO ₂ 24			
C	-0.023811818132	1.196781327616	4.352587507548
C	-1.853783601143	-0.542462165254	1.118499246365
C	-1.226881235044	4.720359616957	-2.062934698237
C	-0.004371387880	4.740014588033	4.273667169580
C	-1.807223669073	2.946738718748	1.172793703753
C	-1.161673370588	8.280742549446	-2.150763124636
O	-1.203873606304	-1.136391346605	1.906802736709
O	-1.879222046397	0.547729041846	-2.882764679365

O	-0.555394403698	5.317751358991	-1.293200364384
O	-0.122515981198	-1.103365669287	-4.517178227672
O	-0.098055771621	2.494817605482	-4.637996619066
O	-2.474052306775	3.613045529184	0.457965837215
O	0.642947372417	0.595706068136	3.583669997325
O	-2.449187709486	7.132416638601	0.328125311834
O	0.657258530424	4.083703117486	3.546404311768
O	-1.142553507157	2.282252127475	1.890018250545
O	-1.897485736864	4.121611696429	-2.832384088462
O	-0.497911859061	8.934090785253	-1.420598098939
TV	3.587439966752	-0.000000000011	0.000000000002
TV	0.055023012892	7.080596554936	0.000000000005
TV	-0.569175934184	2.901402507352	9.639446440642

EQ-CO₂ 25

C	-0.236946303218	0.258568713381	-0.205886478035
C	-0.929245415341	-0.369114927701	3.143880745958
C	3.232522206138	0.255360258804	-0.210112459390
C	2.549507025171	-0.375564633616	3.134829345426
C	6.745903900086	0.307867212111	-0.271297058025
C	6.051438158792	-0.411567269906	3.087768463852
O	-1.421121021106	-4.650812353774	2.353420693947
O	2.047794966566	-4.654008729177	2.349183863474
O	0.331036644838	0.962697981448	0.559172507370
O	3.805142729251	0.956653183334	0.554256114004
O	2.660928756399	-0.445581137228	-0.975116311755
O	3.150889561648	0.274577617573	3.919913911883
O	-0.806067056447	-0.443909580989	-0.970989760668
O	5.624849170069	-4.706007013925	2.260900231321
O	-0.337930075366	0.282997807878	3.934486692832
O	7.279364370405	0.974578047917	0.549440900057
O	6.213170732973	-0.356084089534	-1.095010223391
O	6.580592522273	0.253289318096	3.913381870886
TV	10.415376975393	-0.000000000009	0.000000000003
TV	-0.101384497965	3.630679121264	-0.000000000015
TV	-4.739933724410	-5.061843361391	6.716193979196

EQ-CO₂ 26

C	0.789359370283	-0.716439095261	0.006038323031
C	-1.432483040583	1.461797227607	2.182441772165
C	5.152571048571	-0.607333273380	-0.007058910967
C	2.927331595734	1.503635844848	2.186794949891
C	9.512269584935	-0.670060445593	0.016264616472
C	7.322677787899	1.571731801200	2.192987595353
O	-1.526422788752	-2.057854322892	3.016145033362
O	2.896544506202	-2.001804665602	3.009084477788
O	0.765884355612	-1.554964629424	0.839267364272
O	5.071898928604	-1.444981961616	0.823478695668
O	5.234777084010	0.232677930075	-0.835759612733
O	2.934222757248	0.653721633401	1.364576811557
O	0.817646173920	0.120096680437	-0.828834635552
O	7.288561329501	-1.940494240456	3.022572529139
O	-1.360715996098	0.625679930872	1.349128704477
O	9.493520503931	-1.519852465753	0.838819974743
O	9.530394469688	0.177872531172	-0.807806277541
O	7.338867147259	0.732400330132	1.360562332934
TV	13.118986478232	-0.000000000000	0.000000000003

TV	0.022540611889	4.354917452501	-0.000000000004
TV	-0.075216204975	0.002903320113	4.363923581358

EQ-CO₂ 27

C	0.748341498014	-0.658220249384	-0.571396062787
C	-1.150617755498	0.016449386422	2.685544752727
C	0.618871015516	2.740088761492	-0.642619550957
C	-1.330161136344	3.426473820778	2.679888328493
C	0.399716616774	6.132760480976	-0.571507968491
C	-1.498157695398	6.841427961349	2.677819444110
O	-1.836077375954	-0.610773843966	3.419285322990
O	-2.025960274353	2.821586082370	3.421757635343
O	1.474163067010	-1.204418458846	0.185700518406
O	1.296338028461	2.202262702328	0.164912136577
O	-0.058668261510	3.277588654385	-1.450347791062
O	-0.632588371072	4.033756117577	1.941386818207
O	0.023122767101	-0.109288978207	-1.327856033569
O	-2.200628036177	6.253889003189	3.426505534072
O	-0.462018854363	0.642115786560	1.953159474158
O	1.115859037696	5.557286842573	0.174164228841
O	-0.318780106640	6.705168779052	-1.317035730724
O	-0.793982773536	7.428045733810	1.929321750457
TV	3.723117703221	-0.000000000006	-0.000000000003
TV	-0.538789290198	10.244558916470	-0.000000000189
TV	-3.953715640358	1.417862471073	6.511786135401

EQ-CO₂ 28

C	0.319800347272	-0.611241950445	-0.574186797992
C	-0.271668093543	1.166624269278	2.735930957199
C	3.729811299375	-0.620565935805	-0.575266652986
C	3.109933200008	1.040300998096	2.741432173635
C	7.169693621871	-0.648896252833	-0.573407528028
C	6.556899487729	1.130790324637	2.735381068842
O	0.297949101922	-1.758885426996	3.496386841294
O	3.678250512139	-1.886803100078	3.503792600070
O	0.899122914326	-1.311458540402	0.183059277694
O	4.312782289248	-1.318129082369	0.181868098252
O	3.148131638456	0.080620211694	-1.330493455584
O	2.519966238850	0.353809968511	1.979357272231
O	-0.259810629312	0.089766065824	-1.330977999847
O	7.133767697704	-1.798870671569	3.494061995839
O	-0.863913645160	0.481083791057	1.975356419300
O	7.767502839736	-1.332923527630	0.184644554290
O	6.572380854863	0.035644892400	-1.331473180808
O	5.958191974841	0.450409034259	1.974613084028
TV	10.269945975438	-0.000000000001	-0.000000000000
TV	0.021776686551	3.612367488279	-0.000000000000
TV	-1.236866261205	-0.067316403813	6.619373110519

EQ-CO₂ 29

C	5.876091493070	-1.618650851760	0.996004968547
C	0.609347893352	-1.637244965770	-1.174885856788
C	-2.552265916448	-2.106230097255	1.513454626613
C	6.751610262298	-2.581604598796	4.212287380210
C	1.484879259141	-2.599971388884	2.041501469849
C	-1.676782337218	-3.069145700891	4.729880278472
O	-2.488485090606	-2.889150571293	0.629825220487

O	4.763316405446	-1.732333462115	0.606613952240
O	-0.500781038700	-1.750198377904	-1.568839628216
O	1.721310926777	-1.523204299204	-0.783525620844
O	2.596798816417	-2.486019196459	2.433027192409
O	6.985982948970	-1.504520874554	1.389974401428
O	-2.616680822277	-1.322688244308	2.396544902130
O	7.861488562955	-2.467497991761	4.606301774505
O	-1.741111623997	-2.285496409901	5.612875170423
O	-1.613042460697	-3.852169431312	3.846337303260
O	5.638828674230	-2.695260989408	3.822904022736
O	0.374833525656	-2.712908810959	1.647309647436
TV	12.460638216783	-0.000000000008	0.000000000004
TV	1.762555708140	3.143617166452	-0.000000000004
TV	1.751006098999	-1.925926983298	6.432882984626

EQ-CO₂ 30

C	0.496014015063	-0.953462281376	-0.165533178217
C	-1.180514411318	1.278113085222	2.728329905612
C	3.776016490232	-0.913123631439	-0.098070232700
C	2.157703299853	1.282726863936	2.804927311797
C	7.132770441877	-0.928550187709	-0.162305049848
C	5.459925106661	1.278652016910	2.729788119949
O	-0.997453138220	-2.359480613452	1.933900044834
O	2.393151630968	-2.334316167671	2.065381487308
O	0.884779989950	-0.178670931039	0.638378287776
O	4.204580672997	-0.085324198005	0.628764733460
O	3.343123641532	-1.738544428927	-0.824999049528
O	1.641934381116	0.519457388160	3.546030632360
O	0.108747965543	-1.730353288269	-0.967351112968
O	5.644756155517	-2.362910872223	1.932990236900
O	-1.647059059832	0.537205069491	3.523584479455
O	7.613604754265	-0.072267577715	0.495851622450
O	6.653253109554	-1.782991515964	-0.822652835753
O	4.992948966287	0.540511802203	3.526988667625
TV	9.958759262873	0.000000000012	0.000000000003
TV	0.283455171120	4.379132410615	-0.000000000003
TV	-3.640837779129	0.074399813215	5.793136855927

EQ-CO₂ 31

C	0.313641376966	-0.742468100033	-0.406091684170
C	-0.373668351411	1.139915015664	2.799220782192
C	3.693424582062	-0.659868444931	-0.423311893296
C	2.993765016654	1.159944489119	2.791206153517
C	7.058808450018	-0.658207628240	-0.421941783378
C	6.354562406956	1.178100155568	2.792490137031
O	0.150250335663	-3.305836555833	3.547588155360
O	3.521601899878	-3.279924355910	3.542095577338
O	0.885905902311	-0.022472137429	0.337661945905
O	4.260083943898	0.056433491302	0.329194868995
O	3.127071778969	-1.374720629578	-1.177110885030
O	2.433068042476	1.881551128289	2.039854894873
O	-0.258406730856	-1.463393714134	-1.149722178830
O	6.877138561832	-3.272989065523	3.536424206475
O	-0.930524554003	1.867480243838	2.050584642671
O	7.630583932302	0.054772868400	0.329826920280
O	6.487011172538	-1.369443565536	-1.175050539776
O	5.797940269961	1.912508115240	2.050266213268

TV	10.097072936833	0.000000000008	-0.000000000026
TV	0.033455723866	3.718346744387	0.000000000007
TV	-1.423336458584	-0.042648032880	6.425872221208

EQ-CO₂ 32

C	-0.579988993545	0.578747582620	-0.047567561139
C	-2.530630132984	2.962331468228	2.206337221647
C	3.236560267031	0.578822366899	-0.048109250927
C	1.286271445613	2.962366929040	2.206262804510
C	7.054180433630	0.578744793298	-0.047661301971
C	5.103351230780	2.962250903786	2.206293964463
O	-1.307449721619	0.593309140284	-0.979680199084
O	2.509025925527	0.593862608586	-0.980148377529
O	0.606417543631	-1.777121923884	-1.364915895075
O	4.423375200213	-1.776980114390	-1.364990722625
O	2.021547454280	2.943240897231	1.279917104071
O	3.963825051227	0.565636319804	0.884172354491
O	-1.795361907760	2.943375439420	1.279986596898
O	6.326459970033	0.593666552868	-0.979573942392
O	0.147239008829	0.565901984052	0.884777661451
O	8.240906452751	-1.777332502675	-1.364762480342
O	5.838902046790	2.942846189832	1.280175329451
O	7.781735459705	0.565594388621	0.884422954908
TV	11.451293162623	-0.000000000000	-0.000000000000
TV	-0.044604216774	4.738538160779	0.000000000000
TV	-0.011842768095	0.019707674602	4.496808153335

EQ-CO₂ 33

C	2.791309483873	1.526199560182	2.406252103616
C	-0.887707485647	1.674730218337	0.631916395837
C	-4.541257698707	1.817038992593	-1.123193075999
C	0.039189513882	4.841415985169	2.406175979178
C	-3.627098191493	4.990955703696	0.626892801642
C	-7.281039438062	5.122932467711	-1.140840310094
O	-0.323423997954	1.011100737566	1.432650043254
O	-4.000650785110	1.120592070694	-1.912840005961
O	-1.453446742892	2.338236857489	-0.168130608614
O	-0.062379304632	0.669442928287	-2.171607033133
O	-2.808545614701	3.982741744142	-2.165811933861
O	-5.082780470238	2.514039395502	-0.335604671342
O	3.333803141415	0.821300962193	1.626322373764
O	-7.824296955220	5.826293985867	-0.360181718372
O	0.575792842731	4.138944488001	1.620126997668
O	-3.058849530977	4.324726301701	1.422562873679
O	-6.738915809754	4.419928075894	-1.923809630270
O	-4.197518954581	5.656997192428	-0.167741710708
TV	7.010747286308	-0.000000000014	-0.000000000011
TV	-5.490617550195	6.626281492149	-0.000000000004
TV	2.307320178867	1.560410875810	5.357580715338

EQ-CO₂ 34

C	0.376163874691	2.120415122020	2.942506125986
C	0.280212675316	-0.540052601355	0.794239041208
C	-1.691719397518	2.139887134219	-1.420123114258
C	0.356329744005	7.292513983569	2.949005344941
C	0.246195401364	4.734106252119	0.724121341149
C	-1.708660152543	7.376982762206	-1.417032959989

O	-0.416397042719	-0.526064058991	1.751981924402
O	-2.376120520979	-3.036548466523	-2.369389511169
O	-0.993462272535	2.086177908632	-0.466398551874
O	-0.670918945414	-0.475402217604	-2.579708010372
O	-0.696670669700	4.754126244012	-2.577683539346
O	-2.672440947220	4.782431309351	-0.216868264026
O	1.070605702158	2.158509568205	1.983837717990
O	-2.686379869988	9.907987404475	-0.159350575514
O	1.055947018592	7.271011786644	1.993678581372
O	-0.467093198969	4.684757667648	1.667118267070
O	-2.387513990771	2.193032712366	-2.376353026592
O	-1.006933185460	7.325212202711	-0.465821621759
TV	3.633084476971	-0.000000000008	-0.000000000007
TV	-0.033342991822	10.464693815025	0.000000000007
TV	0.349785296288	2.557369732477	6.477500335161

EQ-CO₂ 35

C	-1.571693254565	0.650361609240	4.434359669192
C	-2.127732614615	1.196720139469	1.086440384764
C	-2.735677218131	3.007269004103	-2.080805439724
C	1.860853737456	0.633325618707	4.445690665987
C	1.291547604834	1.207218985335	1.091865117075
C	0.662376610329	2.910230510740	-2.143547236254
O	-1.012418564858	-0.019738805391	3.634178694330
O	-2.108656528878	3.680750370773	-2.824387743883
O	-1.538305654575	0.492727962427	0.340110932704
O	-0.626022185381	1.827980524095	-4.633804233741
O	2.822916680355	1.817063787032	-4.616164531031
O	-3.362256065596	2.335438391681	-1.335885460684
O	0.702355549701	1.913402874144	1.837044915807
O	0.098555118161	2.244557906882	-1.344510093280
O	4.132890523863	1.900528960826	1.832975449952
O	2.404074459778	-0.042888530265	3.639490959219
O	1.224956829390	3.575453761677	-2.943679363472
O	1.880084657869	0.500920398761	0.347323070941
TV	6.850584327374	0.000000000016	0.000000000114
TV	0.122178504873	3.603820075356	0.000000000043
TV	-1.505280034108	-0.505105555152	9.865185211273

EQ-CO₂ 36

C	0.934310770590	-0.637881331659	-0.087295671849
C	-1.495065975976	1.170799186533	2.473507473182
C	0.961716442491	2.783137853882	-0.087473565951
C	-1.468044653642	4.591640636668	2.473364928400
C	0.989197556195	6.203911731765	-0.087781114044
C	-1.440975053943	8.012505682421	2.473439511336
O	-0.542946744761	-2.815177509919	2.124469343243
O	-0.515578396092	0.606077550892	2.124487039449
O	1.904097156505	-0.062867014637	0.269894601548
O	1.931631120065	3.357961928822	0.269670293631
O	-0.008844491733	2.207640406815	-0.441562847985
O	-2.447049315801	5.156118586446	2.824489965268
O	-0.036131433671	-1.213561365656	-0.441430217725
O	-0.488735950041	4.026590342371	2.124379212734
O	-2.474236456861	1.735033105789	2.824569997612
O	1.958983714008	6.778865431286	0.269486994745
O	0.018603880655	5.628432502068	-0.441819826642

O	-2.420031103837	8.576936425991	2.824508328063
TV	4.741557748402	0.000000000002	0.000000000001
TV	0.081398283594	10.262808808241	-0.000000000012
TV	-4.883377940279	0.192244186400	5.119508698048

EQ-CO₂ 37

C	4.461227880365	-2.244481038551	-0.156355897887
C	-7.072460507886	3.388967009199	2.567902081325
C	2.816171737500	0.638590471699	-0.144191778908
C	-8.732797215135	6.313247563127	2.525867899004
C	1.161645314477	3.522280273780	-0.152562143675
C	-10.387525010800	9.195878113820	2.523664812580
O	-0.595325101224	-0.391273756559	2.080810945536
O	-2.253569091757	2.489975881036	2.073686802754
O	5.552451946670	-2.097318162081	-0.589807881077
O	3.903116585874	0.783584286836	-0.588703670856
O	1.729604584124	0.494822093139	0.300314341020
O	-8.174494933222	7.259492145007	2.965596520721
O	3.370086843487	-2.390471803928	0.277534652937
O	-3.883035493206	5.368785242577	2.083209794396
O	-6.482662165764	4.286327383950	3.063675991427
O	2.251631319516	3.667000619323	-0.589740691476
O	0.070851056880	3.378652798059	0.283463761478
O	-9.825265510605	10.139253086792	2.964538905002
TV	5.407380997971	-0.000000000028	0.000000000033
TV	-4.948957829021	8.646656216867	-0.000000000177
TV	-1.973451045797	2.734364361884	5.375099592421

EQ-CO₂ 38

C	0.861363409459	-0.653653525153	-0.064362686384
C	-1.581348187540	1.097724064301	2.453105163866
C	0.881318806440	2.892608524223	-0.066832464013
C	-1.606622681927	4.636032820532	2.452611698064
C	0.812000842987	6.423541671848	-0.064148339035
C	-1.634890716709	8.174579051488	2.453043005375
O	-0.568421518130	-3.053294978377	2.660645658223
O	-0.590159726421	0.485822206434	2.660599018526
O	1.853642936964	-0.043004774583	-0.270497300757
O	1.875449147901	3.501474200402	-0.272494834803
O	-0.110002646443	2.280968644957	0.140084158781
O	-2.599196780379	5.245806526131	2.244393222857
O	-0.129465592998	-1.266979048143	0.141037160071
O	-0.615085050139	4.024812699604	2.660565802669
O	-2.573630991442	1.707921914406	2.245225785793
O	1.801329380933	7.038839958936	-0.270462938804
O	-0.175980383753	5.805778214949	0.141426867445
O	-2.626718240136	8.785304546598	2.244965467162
TV	4.697796145595	0.000000000002	0.000000000001
TV	-0.075186366587	10.616054669673	-0.000000000012
TV	-4.858514927479	-0.043043730221	5.037965844032

EQ-CO₂ 39

C	0.474808446793	-0.705710936073	-0.161336929811
C	-1.296661311585	2.626726241436	2.512446136937
C	1.146781341761	2.624595769076	-0.088334499613
C	-0.630365671033	5.960411443125	2.515814488623
C	1.813965691311	5.958204263403	-0.091427325316

C	0.027993647791	9.292970805767	2.445258513039
O	-3.556195064164	-3.304254929155	2.588228918103
O	-2.892190560653	0.026639518652	2.578385730965
O	1.364825834307	-1.475077753607	-0.030217551406
O	2.040952828153	1.852657112485	-0.015642161042
O	0.251197918487	3.396168851530	-0.157812534948
O	0.294451655521	5.223639829116	2.448415606518
O	-0.416791363526	0.063304755571	-0.289021272405
O	-2.221546540102	3.361598008486	2.589794632928
O	-0.371092262259	1.891570748025	2.439624994551
O	2.710268501825	5.189061349595	-0.015921766391
O	0.916316161632	6.727146266396	-0.163773979556
O	0.948091901704	8.558228849846	2.317940174260
TV	4.674844213818	-0.000000000004	0.000000000002
TV	2.001715744461	10.001081961133	-0.000000000032
TV	-4.988944537745	0.096238657340	5.213009989104

EQ-CO₂ 40

C	0.754856143802	-0.691217830906	-0.205944276089
C	-1.044094903388	2.668449627043	2.478791449472
C	1.439310497082	2.662002700716	-0.205979104278
C	-0.359618506026	6.021679107840	2.478806391980
C	2.123804742165	6.015253026411	-0.205910331765
C	0.324839303532	9.374928140761	2.478738329531
O	-3.316740909912	-3.283598153214	2.608637682386
O	-2.632350812457	0.069564784314	2.608553468364
O	1.645952139920	-1.466961098713	-0.126480513699
O	2.330456948706	1.886321433888	-0.126503299598
O	0.549277373516	3.438127103767	-0.287441949803
O	0.544373063707	5.267769348173	2.351014383018
O	-0.135126782138	0.084964398685	-0.287455691964
O	-1.947778224736	3.422878913203	2.608604942490
O	-0.140139500225	1.914488534171	2.351015903609
O	3.014934933750	5.239550789094	-0.126450073664
O	1.233761147942	6.791369216362	-0.287417023063
O	1.228888234142	8.621073480643	2.350963472718
TV	4.643937371786	0.000000000001	0.000000000005
TV	2.053396289458	10.059662821996	-0.000000000048
TV	-4.884614436910	-0.031342473019	5.286463439064

EQ-CO₂ 41

C	6.846162180985	-0.948363263645	2.482617889528
C	-0.621284223376	-1.671909246597	-2.561340572729
C	-2.390048972743	-1.762534415209	1.550317213332
C	8.306782687858	-1.776444636282	5.502325575415
C	0.818838920422	-2.527375604814	0.414007753620
C	-1.036307250126	-2.632718467436	4.528504898009
O	-2.325902336220	-2.501134352941	0.627979202192
O	7.090002428987	-1.753702800416	1.650118779666
O	-0.486727147340	-2.422125093161	-3.467368595909
O	-0.755604282649	-0.922489807378	-1.653966127632
O	0.676549698093	-1.774344449322	1.317279066434
O	6.601882157799	-0.142255245771	3.314009972112
O	-2.453238460277	-1.025454929697	2.473507573246
O	8.252739029653	-1.035966156325	6.423934265426
O	-1.179760009235	-1.881752175615	5.432446097777
O	-0.898785707969	-3.383663013713	3.624463689860

O	8.363904539689	-2.518029456478	4.581992481429
O	0.961970892584	-3.280440037587	-0.488774204268
TV	12.466263328381	0.000000000000	0.000000000000
TV	1.301786324373	3.326018356966	-0.000000000009
TV	2.860246182966	-1.707151501110	5.950691718470

EQ-CO₂ 42

C	-0.265516938631	0.912972678075	-1.411602015631
C	-2.070163414598	3.635647419356	2.120760743810
C	3.206959855719	0.872270751555	-1.386319856156
C	1.460110579203	3.637913648173	2.141447864904
C	6.748673657908	0.927646884207	-1.396375587224
C	5.002817421128	3.596380223492	2.142061654671
O	-0.858216859232	0.248335021361	-2.189711052232
O	2.618929974078	0.201837175612	-2.164296370144
O	0.827586815683	-1.758836130721	-0.620578474157
O	4.438520599860	-1.741228142831	-0.615141829359
O	2.117912409574	3.027905073074	1.370278410445
O	3.800478139917	0.973726898451	2.925902722183
O	-1.472569510386	2.974884742331	1.343009889195
O	6.093865405584	0.311677018906	-2.165185296541
O	0.339577204164	1.006920246953	2.899519688566
O	7.896392460932	-1.712187230770	-0.636264405268
O	5.593668384686	2.926168767487	1.365966166491
O	7.411330384181	0.973953551393	2.907297398861
TV	10.543905022403	-0.000000000000	-0.000000000003
TV	-0.032073235497	6.577761034684	0.000000000001
TV	0.008563262527	-0.569635782122	3.533845663167

EQ-CO₂ 43

C	-1.853278399930	-0.496318526287	0.563561561010
C	1.008649392182	1.188850431715	2.152346690668
C	-3.070750112322	-0.727441833106	3.806397094343
C	-0.223885417715	0.965213940045	5.457700845768
C	-4.317266643517	-0.954409134176	7.104844405121
C	-1.461288774622	0.692018886749	8.818256937537
O	1.892077417726	-1.714052624472	1.832049629186
O	0.659766125437	-1.940668502144	5.131280955171
O	-0.953020764381	-1.154036350632	0.165738582168
O	-2.158982631997	-1.402800544541	3.470711395570
O	-3.982094637486	-0.051074070906	4.140900896269
O	-1.126278402302	0.272457811356	5.783415713695
O	-2.753307518909	0.161111916882	0.963383287589
O	-0.546187256434	-2.227594305002	8.560346739721
O	0.105967241552	0.493891078247	2.471927870409
O	-3.405123547046	-1.626362598363	6.763031418801
O	-5.228698241682	-0.281037599019	7.445834339766
O	-2.393826563338	0.012779606248	9.079799001983
TV	6.916255860969	0.000000000000	0.000000000001
TV	0.018521924799	3.598674902351	0.000000000000
TV	-3.715526939895	-0.695160137001	9.909754641363

EQ-CO₂ 44

C	0.732358966368	-0.725050926573	-0.217688149511
C	-1.438716793624	1.379677486761	2.605705994711
C	0.845639413829	2.541657939355	-0.222845000711
C	-1.326293136129	4.668764739560	2.606938689763

C	0.960169703273	5.868799193871	-0.218739314392
C	-1.215929047549	7.956547498322	2.608839414061
O	-0.682566022368	-2.379990178472	1.972413612799
O	-0.565060794615	0.899967015164	1.968474108860
O	1.634350728442	-0.292936509302	0.413989971486
O	1.746512461904	2.978546546385	0.407082213759
O	-0.055536421779	2.104885012528	-0.852615581329
O	-2.202454887655	5.134526692740	3.251138647880
O	-0.169430012813	-1.157086072263	-0.849638393020
O	-0.450035858731	4.203080635104	1.962907511130
O	-2.312216700050	1.858742930133	3.243618261212
O	1.861096492422	6.301743329908	0.414057322861
O	0.058866630905	5.435729781626	-0.850521635177
O	-2.089290342511	8.437303913120	3.245786770618
TV	4.406091438229	0.000000000002	0.000000000001
TV	0.340734663144	9.856822846469	-0.000000000011
TV	-4.457746886240	0.928814292752	5.653275174038

EQ-CO₂ 45

C	6.695481258780	-1.234008661217	2.545561875980
C	-0.900667378480	-1.815625504523	-2.713934237002
C	-2.774497201669	-1.920566130598	1.476734669079
C	7.979238645897	1.902387538020	2.535896223696
C	0.452376978515	1.287202875952	-2.715048149481
C	-1.505828979360	1.232267375944	1.437711513144
O	-2.617288178712	-2.555840088576	0.490082352142
O	6.770783009385	-1.913792015895	1.579442756415
O	-0.745301282902	-2.497987552140	-3.669395844438
O	-1.059775652439	-1.134148865974	-1.758246894795
O	0.280817467680	1.954214985338	-1.751459315060
O	6.621382588112	-0.553129241543	3.511069251324
O	-2.936569162046	-1.285938015984	2.462873131291
O	7.807054164699	2.552875307269	3.509912571523
O	-1.579882960863	1.915237361535	2.401455456683
O	-1.435029612996	0.548727985716	0.474356800403
O	8.153010319619	1.253812460792	1.560975518607
O	0.621727984048	0.619097317172	-3.677996080886
TV	12.658486734329	-0.000000000000	0.000000000009
TV	2.716657431970	6.204622036411	-0.000000000020
TV	1.390425611734	-0.868106724774	3.179600543004

EQ-CO₂ 46

C	1.009496951024	-1.449568893170	-0.362352041413
C	-0.506318766285	0.979023405192	2.356909063889
C	4.344009645473	-1.432697249785	-0.320617810680
C	2.828902774470	0.976098381383	2.395811804183
C	7.714560218194	-1.446509057359	-0.357892008178
C	6.197688938331	0.974806998574	2.360761540872
O	0.015281003133	0.068640525028	2.902738012425
O	3.326413306759	0.078803782848	2.983905556689
O	0.590122246134	-2.411961315309	-0.907867407164
O	3.949076975670	-2.381176294940	-0.907520773245
O	4.738352174245	-0.484898125451	0.267771410084
O	2.328624331455	1.872603129385	1.808597578009
O	1.430998197872	-0.488501577828	0.183726588425
O	6.725254449369	0.061955711006	2.896321849861
O	-1.029055674702	1.887336502345	1.809021487292

O	7.290829530285	-2.410673047028	-0.896640881095
O	8.139351139608	-0.482746396187	0.180752461600
O	5.668612870453	1.885182204138	1.822707925035
TV	10.057439211677	-0.000000000010	-0.000000000012
TV	-0.261005164634	4.563836901055	-0.000000000079
TV	-2.779518748646	0.279579315265	5.434829459822

EQ-CO₂ 47

C	-1.926933066214	-0.484398995214	0.418525048251
C	1.624606535784	1.538821765832	2.062227590669
C	-1.025399910495	2.850591311497	0.479418948366
C	2.534980762040	4.883588984354	2.132152687788
C	-0.144600770807	6.181412352810	0.489527716854
C	3.400887558888	8.212389785480	2.127656131511
O	1.875556887749	-1.463444830546	1.778359320272
O	2.690036666973	1.856688192863	1.657136939925
O	-0.860172690154	-0.171841201900	0.012559901108
O	0.061152440273	3.166461135243	0.131144454909
O	-2.110642539707	2.534298826434	0.830833901990
O	1.448773117767	4.569740928900	2.482352109469
O	-2.994711592274	-0.796699596980	0.822787009540
O	3.621839804527	5.197652784705	1.783198803945
O	0.558186494421	1.220689995634	2.466102470462
O	0.942140623006	6.493537610085	0.139000083659
O	-1.231046395064	5.869254575258	0.840766484243
O	2.312485396579	7.906117090883	2.477892356477
TV	7.444488521694	-0.000000000001	0.000000000001
TV	2.614051570686	9.982554636431	-0.000000000009
TV	-1.213083604078	0.730944293130	3.288164513343

EQ-CO₂ 48

C	0.561737484126	2.707904678010	3.022155840878
C	-1.232758973524	0.204648106323	0.782338227645
C	-3.080138063991	2.824222498160	-1.468278859479
C	4.074662651146	2.721534306673	3.069884832483
C	2.324423529424	0.203380159641	0.785683360035
C	0.475951732966	2.823904758292	-1.473574940047
O	-0.584370688109	0.135180550554	1.769888184411
O	-2.441144353020	2.815619232532	-2.465432546811
O	-1.879727778135	0.272332556334	-0.206613294669
O	-0.414505779831	0.320378494948	-2.737230229014
O	3.055919478765	0.323056623412	-2.716512083125
O	-3.718976340803	2.836140778232	-0.473077913394
O	1.200874760047	2.621956727867	2.030576847207
O	-0.172130290766	2.834952677722	-0.484381497008
O	4.756519656001	2.646980522853	2.106946712300
O	2.978136064389	0.134305883400	1.769934941959
O	1.123462226557	2.816022623379	-2.464800693380
O	1.672258073936	0.271106682998	-0.199518694421
TV	7.112004342467	-0.000000000000	0.000000000000
TV	-0.058029744375	5.060847623918	-0.000000000000
TV	0.338976125650	2.471048637853	6.753631915549

EQ-CO₂ 49

C	6.866079998911	-1.120326570019	2.541636026201
C	-0.841597462370	-1.719026060608	-2.725102728844
C	-2.697730403034	-1.866263870099	1.438179361597

C	8.148168437809	2.018210886898	2.534586098707
C	0.518280344358	1.388272417086	-2.729282095861
C	-1.373555469367	1.263926707128	1.505319367293
O	-2.625393230603	-2.556137783566	0.479336205361
O	7.045602446714	-1.772336705553	1.569657095048
O	-0.662540684050	-2.378075082972	-3.691856221080
O	-1.025015979697	-1.062809921206	-1.756658871298
O	0.347062271202	2.051320496879	-1.763664164974
O	6.687793401231	-0.471004273570	3.514942607736
O	-2.770797166450	-1.176918852221	2.397485722479
O	8.068388306463	2.706941833164	3.494345959231
O	-1.536789754669	1.894350947259	2.494425717030
O	-1.212323008792	0.635781806302	0.515148131019
O	8.228797612705	1.329840068113	1.574767207880
O	0.686108677432	0.722372589185	-3.693273818936
TV	12.720618007877	-0.000000000001	0.000000000009
TV	2.718479455792	6.213597654872	-0.000000000018
TV	1.385707394459	-0.864199346568	3.175880272474

EQ-CO₂ 50

C	0.748744843410	-0.714326613941	-0.154326667733
C	-1.003241685190	2.661691641523	2.483630652303
C	1.508471321496	2.587482892118	-0.156549094562
C	-0.253598538524	5.955273950152	2.414193201222
C	2.249872654178	5.892769646167	-0.222387864556
C	0.511178773520	9.271634482996	2.479293602541
O	-3.419603416185	-3.222801234731	2.619142492966
O	-2.652981946864	0.110077090775	2.625952264028
O	1.627246894259	-1.494973646395	-0.006842343898
O	2.398079074566	1.820519255767	-0.006850688830
O	0.621436085263	3.357056884767	-0.304139727296
O	0.650870763480	5.219940015833	2.208055210440
O	-0.129707332763	0.065571789903	-0.299069754789
O	-1.909351835422	3.410981196556	2.626226577591
O	-0.098285867319	1.912032858946	2.341664318957
O	3.133877897534	5.133233644868	-0.013041345722
O	1.366557173713	6.652344909517	-0.431336407260
O	1.417551544192	8.524227397204	2.334198127948
TV	4.710711998917	0.000000000001	0.000000000005
TV	2.258920144265	9.911173881381	-0.000000000042
TV	-4.907499956661	0.057571658488	5.271708706322

EQ-CO₂ 51

C	3.740226634278	-1.771878543455	0.490474771771
C	0.567675668217	-1.684571270574	-1.161167293144
C	-0.678020824341	-1.899922041098	2.036456979538
C	4.312076889819	1.611083302089	0.553085465606
C	1.160649016931	1.667178919897	-1.157731622862
C	-0.070083887109	1.436124560636	2.043680762561
O	0.151538720928	-2.633506492089	1.619051092100
O	4.563764662739	-2.472086650168	0.006757563831
O	1.478028681665	-2.419033426002	-1.342503999512
O	-0.342520395984	-0.950690887105	-0.975753344739
O	0.238285363122	2.385644292760	-0.973797750167
O	2.919006592317	-1.072425433132	0.977793331308
O	-1.509335868133	-1.167272854997	2.453520479277
O	3.500237423183	2.358317412559	0.982491492701

O	-0.889132999081	2.180431268122	2.463876219002
O	0.747467725117	0.691214234893	1.621715790621
O	5.126813146754	0.864094730789	0.129381200373
O	2.083703869892	0.948703610025	-1.339280626001
TV	7.438821398750	-0.000000000001	0.000000000000
TV	1.182440878918	6.699393158923	-0.000000000000
TV	1.930585563458	-0.292195725858	4.913343897082

EQ-CO₂ 52

C	0.764472695233	-1.464521716180	-0.398986977103
C	-0.434405688070	0.809462624746	2.419282642017
C	4.074479110069	-1.402873793235	-0.394533920450
C	2.878287642692	0.696863622892	2.426097029247
C	7.385453803831	-1.416359202007	-0.398571449572
C	6.171281912635	0.819610854123	2.413773734735
O	-0.010007029113	-0.061973395992	3.097982024988
O	3.367129065804	-0.207144506799	3.012281560559
O	0.311594549411	-2.309744113797	-1.091387690065
O	3.592091392209	-2.310315612060	-0.979853622852
O	4.555003224209	-0.493782816317	0.190309203381
O	2.388347785070	1.598867782942	1.839205285013
O	1.216389322676	-0.619761915172	0.294257264125
O	6.668483170458	-0.084604416560	2.991715882768
O	-0.859147339118	1.681045326970	1.740864680519
O	6.902183547519	-2.330515618384	-0.973020828085
O	7.868886491238	-0.502480522198	0.176485722135
O	5.673385720335	1.723762551131	1.835836881401
TV	9.926774488603	-0.000000000012	-0.000000000009
TV	-0.015441363246	4.418567911295	-0.000000000076
TV	-2.393986867413	0.020466161130	5.634551764202

EQ-CO₂ 53

C	0.393972844521	-0.835518665211	-0.069360154464
C	-0.864466616588	1.557869464859	2.625621555912
C	3.783284639255	-0.704103373534	-0.084773199244
C	2.520556301832	1.505510912209	2.606856557506
C	7.155575459981	-0.701539006802	-0.085990790762
C	5.946703517129	1.427876741466	2.635863604962
O	-0.485904104427	-3.968300260523	3.150193000806
O	2.887083838816	-3.998537166005	3.177868174636
O	0.902859064185	0.099949761093	0.445284809591
O	4.279362098063	0.224644998647	0.455064005325
O	3.286525368978	-1.631378903153	-0.625096195490
O	2.011387805970	2.406852478949	2.034730544932
O	-0.115545578823	-1.770913961527	-0.583872328849
O	6.263752592724	-4.131566254164	3.158410145266
O	-1.385400845017	2.483364621903	2.102555988227
O	7.667529957896	0.230924911989	0.432232545428
O	6.642401770180	-1.631586844691	-0.605696707739
O	5.491766560986	2.386902236758	2.114117133501
TV	10.118841375068	0.000000000009	-0.000000000027
TV	0.141183783826	4.601810375556	0.000000000007
TV	-2.842187660917	-0.081636960288	5.401411345046

EQ-CO₂ 54

C	-0.841988570940	-1.295699151043	0.138810514928
C	0.934491016109	2.883633920499	1.808815634828

C	2.653623720989	-1.283916953952	0.146133685350
C	4.398200394276	2.867357543970	1.800464229542
C	6.149840413187	-1.338498356640	0.148600369444
C	7.888643139111	2.878310089725	1.804895581802
O	1.558193468125	-3.264952987552	2.151775438744
O	5.003025432250	-3.271739934361	2.149141540966
O	-0.208216738461	-2.234862647201	-0.202261225049
O	3.282471511391	-2.225811078043	-0.196039444149
O	2.024488989196	-0.343233764120	0.491709754674
O	3.787671459843	1.914316777565	1.454734986115
O	-1.475322483698	-0.356858322746	0.482237226982
O	8.513940994862	-3.271863235560	2.148912361288
O	0.306344952161	1.940640288845	1.468031110858
O	6.731206072851	-2.316097634800	-0.178324978340
O	5.568776791797	-0.362338759011	0.479400770043
O	7.257155209567	1.937791746287	1.463751806065
TV	10.474767620204	-0.000000000001	0.000000000001
TV	0.005037408177	7.090892632055	-0.000000000004
TV	-0.005927324144	1.239582085688	3.315515327288

EQ-CO₂ 55

C	0.590960472425	2.930306783610	3.002283732858
C	-1.340486217559	0.314676747044	0.782673396799
C	-3.112558079783	3.133305006506	-1.446035726351
C	4.104665535651	3.017605238980	3.000433488857
C	2.174261243562	0.316632039233	0.784254262642
C	0.398714644605	2.978996544364	-1.439179906154
O	-0.702643819965	0.172139787847	1.769842715900
O	-2.469815196913	3.110825280508	-2.440213613182
O	-1.979356694991	0.453146873668	-0.204674394271
O	-0.366194865134	0.355698146412	-2.676717880379
O	3.153268849422	0.524420513288	-2.680962947127
O	-3.756512852275	3.158440699731	-0.454115755948
O	1.231604418886	2.895170649883	2.008096460542
O	-0.242735975500	3.008387500026	-0.445527384675
O	4.738841934141	2.899590766580	2.008459535213
O	2.810165266968	0.176737631946	1.772821905562
O	1.040354934292	2.949130390459	-2.433855465551
O	1.537355613755	0.453843141280	-0.204443554248
TV	7.029863693902	-0.000000000012	0.000000000001
TV	0.039657273876	5.289538644906	0.000000000067
TV	0.317490105662	2.607373489701	6.674881715604

EQ-CO₂ 56

C	0.610585448562	0.827569949857	3.107448528174
C	-2.082024580446	1.240043493825	0.803935896422
C	-4.454797980977	2.950093898319	-1.483801493863
C	0.692511248792	4.270353517505	3.107226284772
C	-2.000788573513	4.682490063111	0.804704652711
C	-4.369397563530	6.387710347667	-1.468152674335
O	0.427854707634	0.229427828081	2.101914627290
O	-4.206188015620	3.525057621398	-2.487720409275
O	-2.119512334076	0.639133330429	-0.214444649967
O	-1.656906928615	1.821454928016	-2.812518917250
O	-1.574826671782	5.264626848216	-2.812965383113
O	-4.702792566244	2.374976666572	-0.479611581582
O	3.069512097676	1.841262986219	1.823540159284

O	-4.621443271092	5.807472899572	-0.468012355940
O	3.151443157962	5.283805386778	1.824298506057
O	0.509678758536	3.671830003028	2.101937534341
O	-4.115802929302	6.968181563793	-2.467291269608
O	-2.039026697732	4.081830300257	-0.213791696418
TV	5.117200527627	0.000000000008	0.000000000088
TV	0.163645051764	6.885225522689	0.000000000068
TV	2.456671852128	-0.395469964670	6.922413053890

EQ-CO₂ 57

C	0.674251008588	-0.796114953337	-0.157117370129
C	-1.056695303157	2.509238402231	2.487582939600
C	1.476631530074	2.463051985546	-0.155022835073
C	-0.228798098607	5.786546125383	2.555985944951
C	2.298094242225	5.695970043489	-0.086699787172
C	0.569257540971	9.022625342586	2.490764762833
O	-3.572141150643	-3.219064886705	2.778703146351
O	-2.755513613698	0.018344484462	2.774488703535
O	1.517899360492	-1.573313531919	0.135186873212
O	2.317740991444	1.682066371247	0.134019726221
O	0.634616644116	3.244401860347	-0.441045429723
O	0.683901931357	5.064877437277	2.336072228902
O	-0.169320859974	-0.018077674148	-0.446737669426
O	-1.949280425206	3.232740646582	2.773283967145
O	-0.164267546514	1.784397272611	2.203695855207
O	3.165868695649	4.924220353066	0.142775160169
O	1.429920314187	6.467854318007	-0.313199489831
O	1.461925302677	8.297358581072	2.209684448598
TV	4.818067597014	0.000000000002	0.000000000005
TV	2.432318201301	9.729019044980	-0.000000000045
TV	-5.070154238489	0.125340713075	5.289173816889

EQ-CO₂ 58

C	0.587017229156	-0.724736491051	-0.110284948640
C	-0.850382718281	1.534288440925	2.485901203843
C	3.932796303610	-0.729104800975	-0.108562756486
C	2.492755700855	1.542783545286	2.480561528033
C	7.300879676002	-0.727736838068	-0.098997722932
C	5.851513796480	1.550576521926	2.479457312434
O	-0.582275518706	-4.212202260707	2.895237088581
O	2.755217121425	-4.206158175368	2.890195359175
O	1.120720775129	0.247605475792	0.299929990959
O	4.459543911249	0.248059646877	0.298835224295
O	3.405776452979	-1.707126092516	-0.514280248475
O	2.019129731284	2.547432821032	2.073035813094
O	0.053102686334	-1.697660046279	-0.518680764833
O	6.112145892379	-4.198002453582	2.891514337761
O	-1.330555278107	2.535383302715	2.077428256317
O	7.849796262300	0.238771431260	0.305575419134
O	6.752648361220	-1.695290828634	-0.501806492749
O	5.380373844450	2.554498111628	2.068126933908
TV	10.083454251741	0.000000000009	-0.000000000027
TV	0.210885348452	4.745074825432	0.000000000007
TV	0.266021510557	-0.212582186861	5.173490407109

EQ-CO₂ 59

C	0.703976210528	-0.562088723273	-0.151368565249
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C	-1.732340043795	1.304511858299	2.542784802794
C	0.325682282577	2.701046496396	-0.156875841025
C	-2.111924628091	4.592488516285	2.545001820059
C	-0.050415504852	5.983780395389	-0.167633437541
C	-2.489684663939	7.850929504257	2.549985658388
O	-0.357513894264	-2.381639176102	2.027299979968
O	-0.747859691576	0.891417536620	2.033381951419
O	1.617388387252	-0.041631447487	0.390942757522
O	1.238345069833	3.218523516736	0.389293285355
O	-0.588055127259	2.183895919079	-0.701784962184
O	-3.096757374989	4.985452481335	3.069530260794
O	-0.207749635339	-1.082816901359	-0.695730851750
O	-1.126756063771	4.198625915233	2.021872164655
O	-2.716703820190	1.716958662837	3.053154055969
O	0.865546976913	6.483629748964	0.389370582830
O	-0.967429205356	5.484045334707	-0.722895026556
O	-3.473986666766	8.248036880171	3.072575809549
TV	4.668751031668	0.000000000002	0.000000000001
TV	-1.147477960391	9.836618375976	-0.000000000012
TV	-4.485874739448	0.469847238377	5.414939450912

EQ-CO₂ 60

C	6.889212389403	-1.398925585650	2.521922710253
C	-0.994665894856	-2.021507464093	-2.702749366949
C	-2.882825001607	-2.116344952746	1.488049996600
C	8.263901712941	1.704234235006	2.523158333364
C	0.372749743993	1.075445160308	-2.703158719585
C	-1.429979863775	0.938189976319	1.531609374082
O	-2.735860154942	-2.762798512723	0.507768440091
O	7.060464155098	-2.072315211835	1.563186490571
O	-0.823369638625	-2.699292843804	-3.658483441300
O	-1.167468655339	-1.346421041067	-1.745249169707
O	0.198652594720	1.751522089365	-1.746187017192
O	6.716931546305	-0.727867892318	3.481764227989
O	-3.033147036989	-1.468334033370	2.467606673012
O	8.083819773039	2.367335954571	3.487283871625
O	-1.510861096727	1.613746384323	2.499970235233
O	-1.349807492698	0.261635874627	0.564217654477
O	8.443455936577	1.038569445065	1.560652890677
O	0.544227765435	0.397089457918	-3.658155539496
TV	12.964395087432	0.000000000001	0.000000000008
TV	2.732218423672	6.190633106429	-0.000000000024
TV	1.436458142440	-0.829315704632	3.153351274980

EQ-CO₂ 61

C	5.984349986793	-2.309106311674	-1.090739334529
C	1.438729107973	-1.706820717943	0.299371315995
C	-2.663376171463	-0.051938662600	1.984659316704
C	6.060851724781	1.103926254725	-1.089805395739
C	1.512523701094	1.712139293410	0.296398299638
C	-2.563811507298	3.357160584748	2.045408828528
O	-1.600788224141	0.447852594035	2.133422756051
O	6.894211707283	-2.915549323905	-1.548009313794
O	2.270429906614	-2.286797400753	-0.309585501077
O	0.596583265382	-1.128692946516	0.901102045793
O	0.668084526922	2.276989480539	0.907321323498
O	5.086310396468	-1.701211869436	-0.618845577525

O	-3.726198730091	-0.551830465185	1.837668757792
O	5.162734982381	1.709082324399	-0.614477463605
O	-3.615855835572	2.821311283660	1.964733619603
O	-1.513009046442	3.894244682600	2.132418170903
O	6.970563067575	0.499609145884	-1.550186770854
O	2.346334763437	1.145692930592	-0.321901401549
TV	7.418868429677	-0.000000000030	0.000000000069
TV	0.153421690913	6.817617433707	0.000000000131
TV	2.256593484480	3.908405112670	4.915017002564

EQ-CO₂ 62

C	2.933384287471	-0.988169037249	-0.907994121502
C	0.331858666261	1.723283539638	-2.552410138658
C	3.452633436652	-0.968029379489	2.384232577027
C	0.851192178576	1.743344748291	0.739834305114
C	3.971871178574	-0.947889939141	5.676569978634
C	1.370245352278	1.763482379133	4.032168398798
O	-0.112286885110	1.105913475327	0.486293422651
O	0.406749289856	1.126083975250	3.778618296952
O	1.295653433561	2.360612596862	-2.299519035871
O	1.815028008448	2.380610809202	0.992773952935
O	2.485666106399	-0.335868174711	2.130702928530
O	-0.277722487221	-1.599125733287	2.637978237050
O	1.966406950220	-0.356048859516	-1.161568858738
O	0.926001510443	1.146131374949	7.070978098459
O	-0.796919770803	-1.619205504414	-0.654254782713
O	2.334087261889	2.400742156853	4.285091948056
O	3.004915742988	-0.315724726717	5.423015800568
O	0.241488536462	-1.579037368505	5.930289917572
TV	4.698019678678	0.000000000000	-0.000000000000
TV	0.003588354001	5.432239538718	-0.000000000000
TV	1.557601412779	0.060299043203	9.876914465112

EQ-CO₂ 63

C	7.458003932061	-0.910331550280	2.523963828453
C	-0.835199134158	-1.654759926971	-2.512512938644
C	-2.614485572358	-1.686355399632	1.531937084781
C	9.003097036638	-1.646223097524	5.554203791364
C	0.712258082096	-2.425562837988	0.401533423090
C	-1.066974559157	-2.449690637076	4.442365820989
O	-2.465332632861	-2.443869389023	0.634803354955
O	7.601955840104	-1.687167399246	1.640736477467
O	-0.680623777248	-2.414134780537	-3.407036488659
O	-0.987856082736	-0.895167141167	-1.616997849252
O	0.558366163323	-1.665302456034	1.296522867165
O	7.309797158659	-0.132736407639	3.404222593153
O	-2.766259617500	-0.931913380947	2.431479073088
O	8.942263920900	-0.886279957340	6.459810335698
O	-1.217672576519	-1.688361324891	5.335761710772
O	-0.918722271760	-3.213922984479	3.550810657229
O	9.064015802494	-2.407359913566	4.649984574820
O	0.869111449372	-3.185119694884	-0.492974575593
TV	13.288785767747	-0.000000000001	0.000000000009
TV	1.364204077896	3.298757841331	-0.000000000008
TV	3.099020847349	-1.525696753453	5.835808346852

EQ-CO₂ 64

C	0.206862894171	-0.802826511516	-0.144900002017
C	-0.186553432472	1.807761290945	2.067569135364
C	3.789369641362	-0.802343535414	-0.130813390538
C	3.395900853028	1.808417925465	2.081725814765
C	7.328384925924	-0.799782287393	-0.115194214091
C	6.934931055850	1.810848144902	2.097206518979
O	0.469464810960	-3.366401927925	3.055755225921
O	4.023621600508	-3.366668538890	3.087342720989
O	0.859213953302	-0.793031566297	0.843239850236
O	4.413688647940	-0.793471917775	0.874596867171
O	3.167859222897	-0.812549191461	-1.137998807031
O	2.774579958986	1.798376675614	1.074437469133
O	-0.447094390812	-0.813824168683	-1.132105832818
O	7.569489793911	-3.365530079264	3.099204016932
O	-0.840328523265	1.796980387198	1.080257207705
O	7.959222165955	-0.792428747020	0.886774809746
O	6.700726296194	-0.809394012441	-1.119369603815
O	6.307248520577	1.801197687047	1.093061577466
TV	10.673990009303	0.000000000000	-0.000000000000
TV	-0.003748490357	5.183810941901	-0.000000000005
TV	-0.782977749541	0.037592294510	4.425028809422

EQ-CO₂ 65

C	0.923672028498	1.159171945571	3.096592461565
C	-1.839034843642	1.608484699464	0.827679643581
C	-4.211810705227	3.139647665404	-1.507585515268
C	1.027510864970	4.567745250548	3.120879915199
C	-1.783532224542	5.019028758281	0.873921228031
C	-4.105893582570	6.542107527831	-1.492461639027
O	0.747991000886	0.582495335800	2.077326052431
O	-3.844472262280	3.651477159047	-2.509346350146
O	-1.955322038625	1.037341714886	-0.201894910724
O	-1.282386896336	1.836696539265	-2.882814268527
O	-1.176624162039	5.236994102552	-2.853650265920
O	-4.578975793505	2.628950482515	-0.504787137231
O	3.452871310574	2.180433404552	1.859083988223
O	-4.484165259371	6.022347905444	-0.498748090080
O	3.564479960206	5.598803170268	1.892919422413
O	0.851871933423	3.999938437784	2.096440012521
O	-3.726335783773	7.062813315343	-2.484841207271
O	-1.960460635673	4.440770841001	-0.142017582793
TV	5.182412434161	-0.000000000001	0.000000000001
TV	0.205730408397	6.806823309151	-0.000000000002
TV	2.389488805913	-0.101365250768	6.995503812055

EQ-CO₂ 66

C	0.671458004576	2.712968698533	3.175702906485
C	-0.965035160151	0.275769295641	0.790352965140
C	-2.474088753695	3.121529032863	-1.534945591472
C	4.090512399674	2.706937242551	3.145487945640
C	2.452495439550	0.274370703957	0.794633227063
C	0.938266437395	3.058280549123	-1.520817683787
O	-0.448481459037	-0.067465339811	1.798742630169
O	-1.888301926433	2.954700994374	-2.550612836197
O	-1.483877219364	0.619309971432	-0.216829168318
O	0.023726247844	0.418209927563	-2.738108702803
O	3.450086103559	0.414885684299	-2.764489645803

O	-3.059821884711	3.299673924920	-0.522828186622
O	1.261532591808	2.537251165167	2.166504457160
O	0.351888335255	3.165028533001	-0.498839602557
O	4.675189041047	2.527535559526	2.133370718381
O	2.964632665869	-0.063742168717	1.806797747574
O	1.525818152879	2.958191354836	-2.544296715351
O	1.938368280292	0.613063455960	-0.216685594130
TV	6.836747102490	0.000000000006	-0.000000000004
TV	0.034778282222	5.254754896791	0.000000000002
TV	0.056598965198	2.459965963362	6.926209523712

EQ-CO₂ 67

C	-0.238827825940	1.480590479038	1.325119747208
C	-1.848830044042	-1.321472167509	0.335471563249
C	-1.871810256990	3.743128451107	-0.583555177099
C	-2.225199536406	2.072380501318	4.312706517859
C	-3.814189448107	-0.756452722362	3.385648226199
C	-3.912076909271	4.339278672967	2.399094600178
O	-0.665590912680	-1.358191804309	0.334131270734
O	-4.659767651960	-4.179916710896	-0.500000913316
O	-0.689927788910	3.759505640714	-0.664482913755
O	0.502073044529	0.865009183327	-1.657124390026
O	-1.423366629062	1.447016288642	1.325545262209
O	-1.424382623399	6.625091680819	0.337883818705
O	0.944017952287	1.515531858512	1.325133396708
O	-3.386064566412	7.217752720471	3.311976638954
O	-1.042528600068	2.123894265209	4.310543468894
O	-2.634553329034	-0.822073298135	3.463989527269
O	-6.700635440006	-3.591410848697	2.317460163450
O	-2.731517388728	4.363395290467	2.483259143022
TV	5.209485234286	-0.000000000010	0.000000000001
TV	1.607858583095	7.906546698350	-0.000000000002
TV	-3.910506053847	1.154807951129	5.970851699255

EQ-CO₂ 68

C	0.803257146596	3.086789662465	3.017740312071
C	-2.332466514365	0.262764242246	0.780496067180
C	-2.057805066102	3.043072755255	-1.412444735879
C	4.308120055622	3.070519025979	2.967152510058
C	1.203397195789	0.271622832738	0.797912615668
C	1.531461528118	3.009547856463	-1.470499463235
O	-1.744129397796	0.415475030976	1.797070836590
O	-2.600177429802	3.114492247223	-2.463082349654
O	-2.922256578121	0.101616896369	-0.233513639676
O	-1.005475814200	0.333490437502	-2.526722516258
O	2.646338004052	0.279802979397	-2.660938200201
O	-1.517657056153	2.966512686051	-0.360700627366
O	0.293223668726	3.067367133984	1.949036185055
O	2.157388195720	2.910528378380	-0.470209113584
O	3.646119787309	3.087250034208	1.985245844118
O	1.856337579663	0.250460719934	1.786104700139
O	0.907553611235	3.100154829736	-2.473320558657
O	0.548725098439	0.283924795686	-0.188679158571
TV	7.052606227570	-0.000000000003	-0.000000000005
TV	3.419810682699	5.505377419799	-0.000000000005
TV	2.322476180337	2.770830733188	6.611581176131

EQ-CO₂ 69

C	-1.750513449172	-0.691411222016	0.179516072698
C	1.947758943952	1.205534044786	1.908654963271
C	-2.733211796756	-0.284654446774	3.564075292060
C	0.994597637298	1.601018808578	5.213782959094
C	-3.735521399719	0.129557309528	6.829937852010
C	-0.037781859939	2.015727720929	8.550229591092
O	1.948941248945	-1.824318182867	1.655341103537
O	0.956500210649	-1.432356927093	4.823364458154
O	-0.655191631272	-0.382438174891	-0.147683299348
O	-1.663126456299	0.035887170261	3.171758755803
O	-3.801920791173	-0.606101886937	3.958112932083
O	-0.076313958272	1.281019835788	5.603114768639
O	-2.848862210226	-0.996309917539	0.502457550223
O	-0.076582980605	-1.023004558058	8.153778925521
O	0.837671122722	0.882028053618	2.162864304548
O	-2.650094724215	0.459056393976	6.494091439828
O	-4.821602236076	-0.200400421310	7.163353698359
O	-1.108032017714	1.700914396541	8.946817814533
TV	7.358503071075	0.000000000000	-0.000000000000
TV	1.108796063196	3.354317956998	-0.000000000001
TV	-3.094527369424	1.213046526811	9.962056542303

EQ-CO₂ 70

C	-0.091403950527	2.815583895642	3.189962857462
C	1.579509911053	0.026319840471	0.796103081809
C	-4.689350608832	3.043247318091	-1.519155216783
C	3.261216227587	2.739232139889	3.169146041865
C	4.934270999662	0.028958204278	0.796281461655
C	-1.329776570600	3.053379431923	-1.500866771280
O	2.118894707241	-0.225797933658	1.818546445695
O	-4.144972106822	2.811880283716	-0.493023187075
O	1.040295474396	0.266734952357	-0.230816974184
O	-0.267795011703	0.723258849666	-2.836633058082
O	3.089200450817	0.581953626853	-2.828851108847
O	-5.234011873483	3.286413936785	-2.541064674911
O	0.393487296335	2.381656010738	2.201967800089
O	-1.872582432221	3.302300911215	-2.522053493101
O	3.743758426028	2.367524207378	2.154701870424
O	5.473140814044	-0.221725196459	1.819182608119
O	-0.786828944876	2.816088977852	-0.475483259020
O	4.395471206210	0.267354570135	-0.231248666867
TV	6.709096449381	0.000000000004	-0.000000000002
TV	-0.097918547289	5.268824422728	0.000000000010
TV	-0.309366399754	2.525096714440	7.014838225981

EQ-CO₂ 71

C	0.682088798476	3.018823756344	3.005229682470
C	-2.063433601066	0.319945701197	0.771654075343
C	-1.927762264345	2.893986479716	-1.452104315477
C	4.163643540012	2.954285877796	3.025470660762
C	1.366227633372	0.309102593340	0.772189093866
C	1.493053491622	2.837392965285	-1.405046506860
O	-1.480303263031	0.542150693475	1.778417904904
O	-2.513934101273	2.674219582432	-2.457388264990
O	-2.644298370325	0.101432233045	-0.236400648114
O	-0.784408499903	-0.042096298422	-2.695787416249

O	2.669755991680	-0.019819519229	-2.633279989347
O	-1.339295610135	3.101432696929	-0.446327715241
O	0.150899118703	3.393481185700	2.014929873219
O	2.042320146266	2.985540926094	-0.365875412378
O	3.663284850735	3.241019636471	1.992175709141
O	1.949352105434	0.536068293025	1.777251275624
O	0.942754232093	2.676223186984	-2.441487241729
O	0.782944253956	0.090825204401	-0.235159092869
TV	6.873908401071	-0.000000000002	0.000000000000
TV	3.120438212215	5.550309404831	0.000000000000
TV	1.995695930531	2.687858702744	6.692571661043

EQ-CO₂ 72

C	1.592088073067	-2.324119039672	-0.055662390462
C	-1.817093386046	4.479174969210	2.685472193884
C	3.225517527991	0.850193333531	-0.287260708858
C	-0.217616533955	7.639993570203	2.401970701902
C	6.093923030986	3.914964391681	0.090577066712
C	2.196621474612	10.406288665442	2.304532651503
O	-8.044598163903	-0.654924758714	2.202724260641
O	-4.027982522451	2.059320194693	3.068567775146
O	2.551898655022	-2.978184572642	0.185304918271
O	3.664206579615	-0.160561746995	-0.718144073723
O	2.786075616548	1.861179645222	0.142550908723
O	0.725388543739	6.959654294722	2.607980822716
O	0.643256533881	-1.665337925559	-0.301642267583
O	-2.260086583160	5.484294214995	3.124722063495
O	-1.371138173953	3.473694922787	2.249743877629
O	5.442186826728	3.312706739063	-0.689514161504
O	6.745835737499	4.508835246001	0.880778301035
O	1.547139392564	9.789761573835	1.529719235993
TV	5.445067450838	0.000000000001	0.000000000006
TV	6.873840411380	8.972575956143	-0.000000000032
TV	-5.068051716088	1.189606763629	5.131255137545

EQ-CO₂ 73

C	4.138385037626	-0.328964954344	0.360461150739
C	0.269137597046	-2.064066438003	-1.002494620439
C	-1.660969460971	-1.563652184817	1.814534234863
C	5.341356739767	2.975296585701	0.356471641702
C	1.412265799534	1.253712422278	-1.002503519195
C	-0.510919139419	1.753141846286	1.813213927669
O	-2.098371127905	-2.056177337361	0.829870705160
O	3.708978986079	-0.811596828794	-0.631512021861
O	-0.307230371956	-2.488320798441	-1.945464227057
O	0.845260906317	-1.640527339645	-0.058060747570
O	1.989288895675	1.681825129345	-0.060558590436
O	4.568325403792	0.153167659296	1.353467375237
O	-1.222886880883	-1.071510661065	2.797097804433
O	5.715636628486	3.470949462903	1.364903259412
O	-0.071395820509	2.250232170408	2.792586053710
O	-0.950619220491	1.256300317607	0.831714459605
O	4.971729812570	2.477887065051	-0.651644619156
O	0.835300298460	0.825478107246	-1.943280280948
TV	8.665205265550	-0.000000000004	0.000000000008
TV	2.286905207282	6.627182314249	-0.000000000010
TV	0.823829344570	-1.104051411476	4.279163818135

EQ-CO₂ 74

C	1.379950724782	1.719191150371	3.117319856407
C	-1.456338880476	0.130792725606	0.868919517760
C	-3.620258455872	2.958937363256	-1.499881455462
C	1.517285925371	5.166509341645	3.117302869986
C	-1.318998017172	3.578121394762	0.868900224751
C	-3.482948912106	6.406281281051	-1.499939819454
O	-1.419746651363	-0.494319900102	1.872952554447
O	-3.392902260575	0.017877041773	-2.504456054268
O	-1.501282726716	0.756469732633	-0.135224888766
O	-0.785384368928	1.690195314157	-2.939431653362
O	-0.648088440647	5.137490309223	-2.939425363742
O	-3.978995262333	2.454066908320	-0.490870269312
O	1.114117708029	1.134023409850	2.123240943586
O	-3.841688238993	5.901498760899	-0.490882916009
O	1.251487008645	4.581356192821	2.123193200311
O	-1.282447013257	2.952945552689	1.872892950344
O	-3.255556115519	3.465307954327	-2.504354376102
O	-1.363829327898	4.203878389219	-0.135197384789
TV	5.085150562603	-0.000000000009	0.000000000001
TV	0.274647228764	6.894711640489	-0.000000000001
TV	2.437840910450	0.613128771824	7.048628258321

EQ-CO₂ 75

C	0.667019179887	3.144888139388	2.978214777129
C	-1.301716582391	0.144053216979	0.759153213205
C	-3.098460151391	3.076041356482	-1.463098913761
C	4.143534982251	3.069257547509	2.979408219271
C	2.181873903771	0.227217077318	0.774232627621
C	0.299546893194	3.055884693543	-1.346913778826
O	-0.655046335838	0.175618867516	1.749990779707
O	-2.487471624511	3.307141509702	-2.451115986229
O	-1.949300474190	0.100676153527	-0.231182575315
O	-0.528851491893	0.702191235599	-2.718704907751
O	2.964846439835	0.560190450302	-2.694951289414
O	-3.706633507484	2.843190028929	-0.475528727943
O	1.309872696448	2.947512559982	2.004119856296
O	-0.291699971461	2.739643558435	-0.370745860193
O	4.770655227509	2.935697125809	1.984986779850
O	2.821460744442	0.333927435367	1.765205273028
O	0.887852885154	3.370898294272	-2.324356563253
O	1.542580945657	0.112162546544	-0.215574053056
TV	6.950618078564	0.000000000006	0.000000000000
TV	0.129868022421	5.363762831350	0.000000000003
TV	0.553652662352	2.642491568813	6.671373528918

EQ-CO₂ 76

C	1.185804115528	2.716071385949	3.120000062603
C	-1.390775236944	1.026118678743	0.789975579956
C	-4.024879646927	2.689407532018	-1.489119193392
C	1.148369243438	6.236440575225	3.119849421251
C	-1.428288759481	4.546431314327	0.790159137722
C	-4.062747066574	6.207723774892	-1.492226300115
O	-1.206092306557	0.424116496283	1.791848281840
O	-3.923544128635	-1.465706716053	-2.491138604597
O	-1.575600620335	1.633063302112	-0.209346744503

O	-1.414921550534	0.191190463671	-2.762325376685
O	-1.452373870849	3.711309111617	-2.762349893946
O	-4.093944511893	3.321195088625	-0.491387406472
O	1.266656175927	2.132620015640	2.094299154736
O	-4.131055197236	6.839231672140	-0.494368803858
O	1.229170012050	5.653230169981	2.093996006497
O	-1.243924759649	3.945363370639	1.792669274015
O	-3.960321184197	2.055941978893	-2.487682856668
O	-1.612938772120	5.152517300815	-0.209712868141
TV	5.055080959621	-0.000000000005	-0.000000000004
TV	-0.075195323023	7.040473947102	-0.000000000000
TV	2.522327890736	3.107195160142	6.910418582002

EQ-CO₂ 77

C	0.326233371965	3.724954467242	2.362664284346
C	-1.285334764360	0.499508394371	0.617980696792
C	-3.019089525134	2.567213536402	-1.108631833254
C	4.052978937662	3.726138694666	2.361886995670
C	2.442500875725	0.499906891638	0.617555958959
C	0.707928028169	2.565673328222	-1.110190511499
O	-0.573774306605	1.149636372803	1.305833274330
O	-3.731693093205	1.915648769450	-1.794287920112
O	-2.004199243018	-0.128871156918	-0.080031713267
O	-0.190685625854	-1.342012914348	-2.234860510942
O	3.536114729539	-1.340425348434	-2.235367951193
O	-2.299127434016	3.196795114229	-0.412527930361
O	-0.396509719164	4.416120864454	1.731353181660
O	1.427397474749	3.196367744470	-0.414553692813
O	3.330282171476	4.416962506423	1.730161539151
O	3.154071161236	1.150073135918	1.305373436328
O	-0.004282032528	1.912934049827	-1.795266622616
O	1.723607075475	-0.128508808285	-0.080394924186
TV	7.455968956012	0.000000000000	-0.000000000001
TV	-0.112187618709	6.347875131093	-0.000000000007
TV	1.239856349396	4.375823838715	5.228637786000

EQ-CO₂ 78

C	0.441790512816	2.327375038731	3.255085612032
C	-0.874525447107	0.135189076776	0.809474801714
C	-2.200416422442	3.038719595021	-1.583271763261
C	3.869203392533	2.315100880272	3.167837426709
C	2.533785219866	0.129204231989	0.809104288823
C	1.204799689559	2.986190994125	-1.541689133455
O	-0.533786133090	-0.343892928764	1.836558896949
O	-1.628748903997	2.849049048410	-2.602402488194
O	-1.215637132026	0.617299144906	-0.215871343342
O	0.162361706628	0.370902523610	-2.738258399490
O	3.595550181341	0.360121606555	-2.822420271651
O	-2.771123998084	3.240771090978	-0.567709996467
O	1.011083119547	2.205709942979	2.225964254180
O	0.644820136298	3.125107301170	-0.508847640023
O	4.433638258590	2.188211896357	2.135870760376
O	2.865789714531	-0.344070057380	1.841551557562
O	1.766429717364	2.856012458005	-2.576170036543
O	2.201712970058	0.606264070062	-0.221667655357
TV	6.829152986891	0.000000000006	-0.000000000004
TV	0.004350014697	5.156249122981	0.000000000001

TV	-0.293431625737	2.071326440086	7.023068622617
# EQ-CO ₂ 79			
C	1.710226537566	1.999430412563	3.146756906557
C	-0.648788579345	0.392639202456	0.793187725473
C	-3.293735661242	2.137113032548	-1.478572680068
C	1.625292610761	5.486685410794	3.146692952585
C	-0.733692681772	3.879771039869	0.793149871861
C	-3.378734165174	5.624408912649	-1.478632524086
O	-0.539674513134	-0.190586551966	1.817103561453
O	-3.321244275867	1.506361963237	-2.480018065848
O	-0.756589971297	0.976794226618	-0.230354292748
O	-0.759904985469	-0.234220953309	-2.848710767627
O	-0.844922483773	3.253001681422	-2.848759939477
O	-3.269421132057	2.768317416405	-0.478126171857
O	1.965828139661	1.489125241739	2.110496241056
O	-3.354421288564	6.255593171877	-0.478181476462
O	1.880931755269	4.976408261216	2.110419559879
O	-0.624567514903	3.296599143074	1.817089161853
O	-3.406189959237	4.993543757103	-2.479998917659
O	-0.841446142307	4.463918654997	-0.230402274525
TV	5.019734301183	-0.000000000006	-0.000000000004
TV	-0.170214719134	6.974467379359	-0.000000000002
TV	2.218129731984	2.744397220342	7.033383452200

# EQ-CO ₂ 80			
C	0.898982731515	0.587797316244	3.112279886548
C	-1.980644988783	1.209460378828	0.843839129783
C	-4.150689275345	2.547376931918	-1.485994833436
C	1.095377545530	3.992460429474	3.112514887248
C	-1.784349078832	4.614336593483	0.843723948629
C	-3.954521440278	5.952330775082	-1.483790430440
O	0.549915585230	0.072538002439	2.104736047265
O	-3.588370649239	2.920447447352	-2.457524127785
O	-2.106485947467	0.631217514899	-0.180879028204
O	-1.102259048587	1.091523082177	-2.916537411742
O	-0.905957145893	4.496632054271	-2.916507698122
O	-4.709955911166	2.175694074958	-0.511374604982
O	3.323479880928	1.788137555193	1.871331304715
O	-4.513996211731	5.580602457632	-0.509255313745
O	3.520021342840	5.192887863245	1.871240068022
O	0.746643659189	3.477024829229	2.104958017035
O	-3.391594581974	6.325238833790	-2.455041602619
O	-1.910196878688	4.036129491723	-0.181022481156
TV	5.194061319757	-0.000000000001	-0.000000000000
TV	0.392814052462	6.809753600176	-0.000000000000
TV	2.361932650884	0.010382754101	7.030684226102

# EQ-CO ₂ 81			
C	0.471141600017	0.123696768664	-0.193064962084
C	-0.557721418426	2.354548892056	2.571763845765
C	3.776578789255	0.123678263621	-0.193040227793
C	2.747187096252	2.354567179177	2.572044586259
C	7.081906150157	0.123719935884	-0.192993562096
C	6.052480751375	2.354596593012	2.572026077983
O	-1.306637336216	-5.922250547744	3.135586407883
O	1.998319124180	-5.922306654002	3.135969436895

O	0.954096352936	-0.748362212743	0.443776218424
O	4.259561499538	-0.748354099301	0.443809993783
O	3.294421973505	0.999060500587	-0.826618471550
O	2.314565970083	1.408747673820	2.008911635234
O	-0.010940597407	0.999076031575	-0.826706621224
O	5.303643378866	-5.922293874097	3.135946180113
O	-0.990509892329	1.408713130700	2.008793599958
O	7.564891835064	-0.748301457346	0.443869812528
O	6.599771740086	0.999094065721	-0.826592155591
O	5.619866703024	1.408746564217	2.008939381304
TV	9.916163036205	0.000000000003	0.000000000013
TV	0.591103632761	4.610904388933	-0.000000000033
TV	-2.652558063292	-0.093473018192	5.553208223415

EQ-CO₂ 82

C	0.784100078374	3.149569795968	2.993792826720
C	-1.316100568280	0.379186591049	0.823786561074
C	-3.077182468568	2.986966465744	-1.469843963762
C	4.293016149344	3.222865141510	2.990089457721
C	2.184321269605	0.375502619256	0.822561656941
C	0.427595509964	2.981544130945	-1.473834826427
O	-0.681401526116	0.282028483489	1.819145464840
O	-2.451978058858	2.905196774738	-2.472354544181
O	-1.953088298574	0.475100093378	-0.169857246977
O	-0.344067543365	0.271452040875	-2.649866410636
O	3.160898541270	0.270510964344	-2.653153328313
O	-3.706086236567	3.068141391057	-0.470880800507
O	1.408080760593	3.070095849448	1.991149037364
O	-0.201133659257	3.065295590520	-0.474978827810
O	4.920881130797	3.219305272482	1.986625387804
O	2.816186447147	0.276565946962	1.819307709776
O	1.052569334759	2.899251312918	-2.476460397696
O	1.550306341532	0.472528835229	-0.172806613844
TV	7.006777281404	-0.000000000012	-0.000000000006
TV	0.358740809629	5.440748570926	-0.000000000006
TV	0.503949417069	2.952055224658	6.647330242919

EQ-CO₂ 83

C	1.112578667659	-1.555890198234	-0.392415439713
C	-1.129143017743	0.903024692262	2.414768913071
C	4.527275918825	-1.555881117081	-0.392428942669
C	2.285544980998	0.903022334232	2.414746686401
C	7.941905169933	-1.555865327145	-0.392416964474
C	5.700237591292	0.903048649308	2.414788593145
O	-0.550418819057	0.024626296634	2.956284315415
O	2.864275592562	0.024629923229	2.956272595363
O	0.619290929109	-2.555857632868	-0.789855646696
O	4.033999916986	-2.555861256185	-0.789856901886
O	5.018810139912	-0.554487783266	0.005118368322
O	1.706059130135	1.780394543624	1.873320139490
O	1.604110259996	-0.554497575145	0.005126689093
O	6.278956466122	0.024643241070	2.956302360993
O	-1.708621140972	1.780399158911	1.873338258036
O	7.448656299452	-2.555848040833	-0.789864872758
O	8.433417113296	-0.554478946760	0.005169846921
O	5.120763575183	1.780414172374	1.873339424673
TV	10.244058156768	-0.000000000011	-0.000000000011

TV	-0.856299399818	4.517827825677	-0.000000000081
TV	-3.643756215931	0.490812300102	5.616983608381

EQ-CO₂ 84

C	1.856473124026	2.628444760781	3.168525042710
C	-0.781855651321	0.865909441685	0.801505949343
C	-3.600970826405	2.475868179146	-1.530256386474
C	1.746507884894	6.032427940364	3.169597987559
C	-0.891959537555	4.269632764716	0.801476358069
C	-3.710915975184	5.879428415443	-1.530272962888
O	-0.412742059230	0.326765900725	1.788278337829
O	-3.445179265679	1.916209603600	-2.562700550300
O	-1.149278955195	1.405196898794	-0.186127378303
O	-0.845191805146	0.099146520049	-2.794857570511
O	-0.955447997871	3.503565902747	-2.794142541888
O	-3.765773933439	3.035412115399	-0.500762852564
O	2.115524618591	2.056035201535	2.166354069143
O	-3.875687982016	6.438856603605	-0.500701646922
O	2.005991012668	5.459441106060	2.167945335246
O	-0.522767835759	3.730388265009	1.788164602335
O	-3.555193641933	5.319847075975	-2.562768115900
O	-1.259426684268	4.808956679186	-0.186118806101
TV	5.219835474954	-0.000000000006	-0.000000000003
TV	-0.219933470026	6.807059932299	-0.000000000000
TV	2.453967674767	3.099940134121	6.971468694172

EQ-CO₂ 85

C	1.119384218721	-1.569405052963	-0.391130592336
C	-1.057251671141	0.969166172756	2.507927363760
C	4.504733563787	-1.593857195367	-0.325249269586
C	2.297450539010	0.966661974481	2.506897501798
C	7.828522791148	-1.541443516438	-0.392551697407
C	5.682784400990	0.845717421222	2.511658497503
O	-0.509022320882	0.088578828921	3.076900720386
O	2.837732004623	0.082770352486	3.077371389331
O	0.628209152443	-2.562975176943	-0.806387439571
O	3.984724082212	-2.541679798959	-0.807580009541
O	5.026684971911	-0.646493243099	0.155710254879
O	1.759670354737	1.854373720858	1.937952664062
O	1.607626859790	-0.572124717135	0.018758488298
O	6.228710554263	-0.038256575873	3.077213954168
O	-1.603251118966	1.852900745457	1.940444197694
O	7.345820037745	-2.540771566349	-0.806184402936
O	8.307354103490	-0.538084403340	0.014431477014
O	5.139772085264	1.729260288207	1.943040253076
TV	10.070187057266	-0.000000000012	-0.000000000009
TV	-0.834329194843	4.511214893769	-0.000000000077
TV	-3.825806809533	0.370363977610	5.824057612494

EQ-CO₂ 86

C	-1.660881918084	0.575681722062	-0.747293409028
C	-2.750611300731	3.042389277746	2.242597344532
C	-0.141660840586	0.490107512817	2.241406457539
C	-1.393490516064	2.807636066834	5.308434927653
C	1.209055783412	0.265016023013	5.311949914527
C	0.187299371250	2.847257241485	8.231754621412
O	-2.696880566062	0.063382042055	-0.496863054353

O	-1.173618398266	-0.029010777125	2.497195681673
O	0.326938090440	-1.499794289829	0.187310446658
O	1.842700570103	-1.624235636015	3.153878193295
O	-0.733856921431	2.330012671207	4.450918590700
O	2.207770776845	0.809226662964	4.984720463779
O	-2.135063288933	2.600734238113	1.332691011923
O	0.210561789652	-0.276670288480	5.640745417383
O	0.890136653291	1.008941614992	1.986424216851
O	3.152715429929	-1.823955731328	6.166908695265
O	0.738414546948	2.362612245996	7.305308929105
O	3.889242758424	0.806747349541	7.971220999562
TV	5.599219128800	0.000000000001	-0.000000000001
TV	0.393584335171	5.108779133053	0.000000000002
TV	4.512294595429	-0.278268363995	8.970786433688

EQ-CO₂ 87

C	1.308658684128	1.953985213237	3.163196731210
C	-1.562400954792	0.287197930915	0.882846858213
C	-3.560512715059	2.856266846168	-1.545219198760
C	1.469584654056	5.408402222439	3.156990486314
C	-1.398930900985	3.744189261462	0.882681770260
C	-3.396516871977	6.312983639510	-1.547331267264
O	-1.480243350959	-0.335936464093	1.885516617775
O	-3.174054159305	-0.308530812914	-2.553539504070
O	-1.655557883033	0.909410996479	-0.119435987648
O	-0.626275686302	1.340629432398	-2.898553536976
O	-0.465039622066	4.796174842156	-2.905565285462
O	-4.103121313266	2.565049528446	-0.534623926542
O	1.059348294767	1.407229650261	2.143599427533
O	-3.940178859654	6.021372702988	-0.537393218043
O	1.220516072349	4.860221279748	2.138059547163
O	-1.317011240497	3.121002950373	1.885342322638
O	-3.012158242041	3.148514966702	-2.551932341043
O	-1.491915776602	4.366501750341	-0.119581558963
TV	5.065365731842	-0.000000000008	-0.000000000003
TV	0.326719485325	6.914133785467	-0.000000000000
TV	2.190968795574	1.158222732295	7.080448078031

EQ-CO₂ 88

C	-1.453618110320	0.670693794976	-0.663377610060
C	-2.421486905213	3.418959271198	2.306259446858
C	0.092841438666	0.682150928575	2.238310410495
C	-0.977987438732	3.379073758353	5.276916121573
C	1.543874440043	0.663331800481	5.274762952798
C	0.595815673873	3.486669922581	8.238099136532
O	-2.464944385348	0.057774247651	-0.647382414216
O	-0.971522032533	0.173634464263	2.328380867201
O	0.491562212955	-1.430138838693	0.187802832197
O	1.861573577080	-1.543188205410	3.155567218666
O	-0.373073572466	2.830546067427	4.421038252052
O	2.586276463426	1.221469102651	5.258441428204
O	-1.746153136920	2.945012679653	1.458000639794
O	0.501316843924	0.105450779990	5.289197207467
O	1.158745628897	1.187851736256	2.143324757139
O	3.371269873467	-1.508310091351	6.130426316481
O	1.131944429265	2.866915446262	7.385572673230
O	4.086704631487	1.384421162277	8.225819499250

TV	5.370023673118	-0.000000000000	-0.000000000001
TV	0.411299754894	5.435359615436	0.000000000001
TV	4.528094902761	0.101410689179	8.903380068938

EQ-CO₂ 89

C	1.513706289303	3.527438180034	3.147765269026
C	-1.404700871201	0.649354270616	0.872430749429
C	-3.869711987982	2.282186608105	-1.559725522793
C	1.589948096929	6.924812912156	3.149727863482
C	-1.331238595645	4.042124314268	0.871518890220
C	-3.800219004896	5.671856422859	-1.529623554119
O	-1.077885373251	1.183381230884	1.877421080909
O	-3.452381428131	2.767711781863	-2.555847438998
O	-1.742172165530	0.115789616909	-0.127126021129
O	-0.962797815066	0.955228791390	-2.841171694646
O	-0.885600364415	4.352351959118	-2.839117355543
O	-4.290411066251	1.797809329075	-0.565501632817
O	1.490501497581	2.959759966415	2.108445542040
O	-4.215466841266	5.187383405788	-0.532893062446
O	1.566147242239	6.357053102161	2.110568411015
O	-1.004450531433	4.575601974810	1.876788055992
O	-3.387264415881	6.157617311472	-2.527223512632
O	-1.668397215045	3.509155795516	-0.128467621362
TV	5.199238885959	-0.000000000006	-0.000000000003
TV	0.150128724733	6.789776160721	0.000000000002
TV	2.508818540327	3.138355997873	7.027516672404

EQ-CO₂ 90

C	1.084032833222	2.520127889877	3.161435503536
C	-1.265448769076	0.391494501835	0.801562629856
C	-2.953129829506	2.729044803874	-1.482519345607
C	4.578001021703	2.520252304739	3.161465080316
C	2.228117933517	0.391643797774	0.801080999553
C	0.543216465878	2.729252412986	-1.485478412562
O	-0.669703620072	0.507827409332	1.817921641583
O	-2.327078756173	2.556681733362	-2.471922365581
O	-1.865010800844	0.282516819976	-0.212810788233
O	-0.583225145418	0.055198203537	-2.862602023170
O	2.910737736099	0.055400642980	-2.862529142016
O	-3.580103529268	2.894169390818	-0.492852929519
O	1.173031024153	3.094547620032	2.130375208630
O	-0.080699608172	2.894634818038	-0.493980178330
O	4.667047800555	3.094599061818	2.130360275938
O	2.823946888849	0.507785753883	1.817416582280
O	1.165975457549	2.556386021503	-2.476904355750
O	1.628580228510	0.282800840501	-0.213322623976
TV	6.987359788264	-0.000000000002	-0.000000000000
TV	0.059711578022	5.063620703772	-0.000000000000
TV	1.580748692931	1.892219014405	7.056071186542

EQ-CO₂ 91

C	-1.879913711117	-0.618494968234	0.479670837515
C	0.940847498206	1.129743641291	2.094261331424
C	-3.487737454307	-0.722442654907	3.706058490722
C	-0.667060260181	1.025695422896	5.320920547706
C	-5.095692685512	-0.826577168697	6.932975868183
C	-2.275031755076	0.921666241692	8.547548062401

O	1.825278349519	-1.777843295765	1.778902359316
O	0.217360937730	-1.881884392037	5.005559819161
O	-0.973493865282	-1.304284068276	0.150365684170
O	-2.581353557958	-1.408309198969	3.376829481708
O	-4.392933850185	-0.035936390990	4.037043119351
O	-1.572500868504	0.332706844844	5.637149595101
O	-2.785106722153	0.068031681187	0.810598768536
O	-1.390625941888	-1.985875088373	8.232231971875
O	0.035427829844	0.436723060122	2.410497943547
O	-4.189302064968	-1.512408578938	6.603665880808
O	-6.000895330430	-0.140064085923	7.263915858393
O	-3.180500934509	0.228701953820	8.863725159019
TV	7.228835027519	-0.000000000007	0.000000000005
TV	0.021466675622	3.600453960563	-0.000000000005
TV	-4.823782880051	-0.312079049489	9.679956094644

EQ-CO₂ 92

C	1.312089155891	2.637221604551	3.230655235537
C	-1.319189596051	0.471463538633	0.814776152976
C	-2.867923428727	3.212775066439	-1.570509985032
C	4.821994632423	2.637429827883	3.230207456460
C	2.190917286052	0.470876572370	0.814990304231
C	0.642806514747	3.202873830779	-1.570244837109
O	-0.931387440970	0.047318373968	1.849673541418
O	-2.087642610089	-1.930866362318	-2.574109459114
O	-1.706476436616	0.899677214878	-0.217796844591
O	-0.479433145119	0.625822329590	-2.839993012267
O	3.030483646416	0.626125496551	-2.840480845546
O	-3.474821109193	3.366584298111	-0.566381621304
O	0.693517949640	2.547017949722	2.225500401378
O	0.033943553572	3.349793196724	-0.566306462676
O	4.203378346615	2.547277163617	2.225063200278
O	2.578408921915	0.047857207934	1.850428950180
O	1.424400659476	-1.932771947721	-2.574183992157
O	1.803831667870	0.897881549356	-0.218149312154
TV	7.020087933510	-0.000000000016	-0.000000000006
TV	-0.170810861939	4.994727643234	0.000000000000
TV	2.410247951474	2.095343957906	7.075489581361

EQ-CO₂ 93

C	1.363119298313	2.284066077065	3.107963692948
C	-1.336157780150	0.502233552244	0.887116356525
C	-3.457890585734	2.778199087434	-1.534747955116
C	1.358490251006	5.806370446974	3.130380085619
C	-1.345730574856	4.016535585659	0.888771645501
C	-3.468198183403	6.291234568722	-1.536477142660
O	-1.167670109441	-0.119073121482	1.879672106568
O	-2.890739330726	-0.945115460493	-2.558398004028
O	-1.514421062836	1.121604457329	-0.104815139682
O	-0.452851402662	0.852135886987	-2.949121062387
O	-0.453232832901	4.366385967704	-2.922156236479
O	-4.015135974653	2.992475610909	-0.513394390717
O	1.254841386951	1.668921303232	2.102618015742
O	-4.026094154416	6.504739721505	-0.515314858985
O	1.246244625699	5.200513390008	2.120107780086
O	-1.176086560645	3.393322155956	1.880004071803
O	-2.900394177600	2.566014401175	-2.557068389985

O	-1.525220789522	4.637278240488	-0.102001704318
TV	5.025000619953	-0.000000000007	-0.000000000003
TV	-0.019089925387	7.024689734383	-0.000000000000
TV	1.930544310694	2.043762894049	7.063692166616

EQ-CO₂ 94

C	1.560468600093	2.580847285078	3.146721199664
C	-1.197277348391	0.756590604261	0.853930789952
C	-3.852724580008	2.531573337125	-1.524229529951
C	1.408981182151	5.954167032354	3.145933890788
C	-1.351676556651	4.132574772225	0.859108612757
C	-3.992124758400	5.884776178407	-1.564942969722
O	-0.778125794130	0.230097693512	1.827510688251
O	-3.435260346161	2.059224097474	-2.526628614396
O	-1.622777850930	1.283269911717	-0.116014389627
O	-0.822737008858	0.395530108339	-2.842478682710
O	-0.972515882619	3.764760712116	-2.840854360513
O	-4.279229047002	3.004542756419	-0.527394553995
O	1.668191534070	2.010204614651	2.115761014749
O	-4.421943448858	6.354820742106	-0.568495208402
O	1.514422900714	5.388103621793	2.112101391869
O	-0.934027165652	3.609213096129	1.835170748397
O	-3.573166514007	5.415249470218	-2.568409806970
O	-1.775324137474	4.655555674494	-0.113651349868
TV	5.196951378738	0.000000000015	0.000000000009
TV	-0.303352843310	6.747003503268	-0.000000000006
TV	2.289454770032	2.755216872835	7.022937712483

EQ-CO₂ 95

C	1.389289973636	3.178247102000	3.192704021657
C	-1.528341998485	0.388977697505	0.736005035275
C	-3.090302232017	3.392670842903	-1.512512714434
C	4.814577506603	3.176064878023	3.193919101805
C	1.905947066678	0.401668815641	0.759911890103
C	0.334065577321	3.352670693047	-1.480864362449
O	-0.937508262857	0.145890105581	1.732315806226
O	-2.648196459281	-1.645438596307	-2.530464893390
O	-2.120100989776	0.624034613425	-0.261974066243
O	-0.640416926556	1.019494665518	-2.814823647727
O	2.781472740692	1.019714132424	-2.812661208710
O	-3.672952205684	3.238544542869	-0.493489811917
O	0.870440332985	2.751215438123	2.218184505978
O	-0.271752213878	3.126585977369	-0.489211983770
O	4.299114099392	2.745936629274	2.218925772466
O	2.496407203780	0.184442474795	1.762893679495
O	0.798622513511	-1.616324329824	-2.471227746851
O	1.315672296138	0.612379517674	-0.244490507021
TV	6.852969253815	-0.000000000016	-0.000000000004
TV	0.138786181415	5.203250979099	-0.000000000000
TV	2.548286173724	2.586809169246	6.981168980577

EQ-CO₂ 96

C	1.973005484572	2.566551562377	3.223403521647
C	-0.777299922393	0.623923008893	0.811579566084
C	-3.720571559462	1.988949188576	-1.565933053009
C	1.842759059039	5.905116597962	3.223415304801
C	-0.907569433923	3.962330485815	0.811685033026

C	-3.850835608405	5.327317174920	-1.565927030472
O	-0.227898319496	0.213329248139	1.775419584862
O	-3.479089412952	1.465028157600	-2.600215679741
O	-1.324922495338	1.034616524528	-0.153493725318
O	-0.862882766183	-0.176992931491	-2.813587375892
O	-0.993080011451	3.161436369819	-2.813486924091
O	-3.977959583390	2.514135176091	-0.537730208507
O	2.315519104769	2.057969563927	2.211943806159
O	-4.108148352727	5.852354305474	-0.537634063982
O	2.185214842732	5.396673595556	2.211868131625
O	-0.358162646612	3.551713507401	1.775513250789
O	-3.609314087047	4.803577780600	-2.600288312847
O	-1.455162158405	4.373050564551	-0.153392954667
TV	5.267681398699	-0.000000000006	-0.000000000002
TV	-0.260576837558	6.677046223042	-0.000000000000
TV	2.507831949907	3.250322443974	7.056001570788

EQ-CO₂ 97

C	-1.469170716501	0.711900517913	-0.666165395395
C	-2.570121865352	3.475915980973	2.309736020942
C	-0.128932716984	0.763600547853	2.316780344064
C	-1.064581456330	3.655423299705	5.278454839800
C	1.372492433368	0.933680324350	5.284531387422
C	0.445600937041	3.755144568660	8.248682759823
O	-2.493943210891	0.121945216657	-0.650773600399
O	-1.142499877528	0.153153433376	2.328305551273
O	0.346692154501	-1.429098581179	0.185819127186
O	1.800514412189	-1.394852169769	3.153798061819
O	-0.454402366323	3.093342461122	4.434401155666
O	2.409538306029	1.501243867150	5.267062415403
O	-1.974730508078	2.897528470181	1.465517648676
O	0.334973592927	0.366286944177	5.299277492673
O	0.883914811989	1.374362062303	2.301898498299
O	3.294275758634	-1.229930413643	6.123915246034
O	1.055626057365	3.192366161319	7.405184405190
O	4.010738928418	1.595299947668	8.227801322183
TV	5.366763566693	0.000000000000	-0.000000000001
TV	0.402820750275	5.449969445925	0.000000000001
TV	4.452487260983	0.296844009910	8.906759979363

EQ-CO₂ 98

C	1.495340170735	2.436932244395	3.131336621096
C	-1.335838203461	0.789272391631	0.880457537249
C	-3.526557457080	2.031238840280	-1.546126072122
C	1.552368593540	5.948708601555	3.143972871904
C	-1.282679522723	4.308508338187	0.880501554667
C	-3.473004284201	5.550964347452	-1.545149887574
O	-0.992725159903	1.366049131008	1.855069156680
O	-2.886575466087	2.052561216207	-2.541843298361
O	-1.688398184841	0.213960773820	-0.091214929757
O	-0.451719584187	0.326870159390	-2.899298066690
O	-0.394980326790	3.843456047545	-2.883519726118
O	-4.172292875200	2.004681601924	-0.555086982154
O	1.473412929306	3.065763971658	2.129221381769
O	-4.118102792715	5.524915535323	-0.553672944496
O	1.529434280906	6.573295017694	2.139408097772
O	-0.939746093962	4.885241438484	1.855181619082

O	-2.833621277230	5.571751194866	-2.541303521759
O	-1.634875755062	3.733078999121	-0.091237654199
TV	5.064430361736	-0.000000000001	-0.000000000000
TV	0.106603488826	7.037333306405	-0.000000000000
TV	1.982229910958	1.481424449030	7.032948346950

EQ-CO₂ 99

C	1.281012029470	2.208201074338	3.161759873298
C	-1.444371594827	0.409774082334	0.868896179501
C	-3.686854852240	2.670658504689	-1.549204940739
C	1.235824027331	5.643417794177	3.161700956257
C	-1.489540580861	3.846424929129	0.868102738304
C	-3.732105444137	6.107406383878	-1.548901705020
O	-1.187687702556	-0.182325433153	1.860296432418
O	-3.083363305740	-0.869710769418	-2.587462250613
O	-1.711012507190	1.000575031685	-0.120651182277
O	-0.612497209832	0.900690537220	-2.911460022111
O	-0.657937073052	4.335512594586	-2.911316032416
O	-4.248899119519	2.779538407281	-0.513659040810
O	1.248184487555	1.604490197524	2.144280839102
O	-4.294198267750	6.215807308133	-0.513331039172
O	1.203997181786	5.040516252560	2.143653280023
O	-1.233031355847	3.254806416332	1.859823914091
O	-3.127988431915	2.566122132687	-2.587702971235
O	-1.755410997144	4.437068896125	-0.121686158121
TV	5.081745434340	-0.000000000006	-0.000000000003
TV	-0.089885267652	6.872768281313	0.000000000000
TV	1.935368456777	1.910938693660	7.091054852689

EQ-CO₂ 100

C	6.677163943784	-1.517536122318	2.427457357345
C	-0.414856779397	-1.844197086272	-2.572568159291
C	-2.379589865585	-1.993915891533	1.490473968945
C	8.052563405208	-2.258784073983	5.490861519978
C	0.935450859730	-2.480199330576	0.558702318228
C	-1.009723583724	-2.744178982261	4.557696199842
O	-2.177531424400	-2.722706970020	0.580140802166
O	6.877242052525	-2.252979901629	1.521891295809
O	-0.219677791798	-2.575617523550	-3.482718127840
O	-0.608986868696	-1.109626384798	-1.664357889047
O	0.658462894954	-1.738297492847	1.440207441601
O	6.476475172656	-0.783549373218	3.333703042796
O	-2.583662222889	-1.266143879056	2.401254402485
O	7.861851250016	-1.524608414470	6.399011749416
O	-1.216073728997	-2.013779271720	5.465459062527
O	-0.805493276626	-3.475503685342	3.650556518090
O	8.243035233651	-2.995764784251	4.583886233045
O	1.214500743960	-3.223697301650	-0.319240215735
TV	12.296017464319	-0.000000000001	0.000000000008
TV	0.968429355051	3.408555410222	-0.000000000009
TV	2.729932228676	-1.506619449733	6.120074788637

EQ-CO₂ 101

C	0.904529499851	2.637936489982	3.247960090850
C	-1.268316126361	0.306672893239	0.805507510455
C	-2.422869410991	3.396547653511	-1.553367693361
C	4.330050027593	2.637985806846	3.248097223779

C	2.157363628193	0.306637555361	0.805454035566
C	1.002748153248	3.396515406897	-1.553224219504
O	-1.148767726665	-0.320709895913	1.801163497612
O	-1.883019633668	-1.634571337713	-2.575612537140
O	-1.388826138109	0.926579228682	-0.195774901114
O	-0.071458039627	0.971699378529	-2.917772188533
O	3.354125760129	0.971744110625	-2.917671410821
O	-3.015220219390	3.382505371589	-0.528947789717
O	0.411927865986	2.195546339968	2.268070714107
O	0.410214224601	3.382524381801	-0.528908549423
O	3.837506851091	2.195631365256	2.268157844681
O	2.276796118091	-0.320673205421	1.801172180798
O	1.542835127713	-1.634746733877	-2.575323990305
O	2.036940042235	0.926532101751	-0.195840947468
TV	6.851161802227	-0.000000000012	-0.000000000006
TV	0.054578011970	5.060925432687	-0.000000000000
TV	1.466738409043	2.101668093238	7.150359213608

EQ-CO₂ 102

C	-1.967279624192	-0.780206450587	0.570992570618
C	1.075693316596	0.945748186282	2.064184118408
C	-3.657380668326	-1.046601213915	3.872105795213
C	-0.613001280843	0.687746668051	5.359509636519
C	-5.378060593758	-1.243830702419	7.222456827008
C	-2.303639422611	0.426351848985	8.659314373110
O	1.878558550779	-1.993622700835	1.813050083993
O	0.189033297473	-2.250060535431	5.109080493682
O	-1.070655684175	-1.440347734306	0.168875334464
O	-2.762058975948	-1.705997061739	3.466238164588
O	-4.554853851727	-0.388697308866	4.277106318410
O	-1.585812161708	0.062393179012	5.609583810823
O	-2.864550788878	-0.120521594093	0.972558618321
O	-1.503925016908	-2.510416320119	8.402631650743
O	0.102534050492	0.321692697840	2.315107839213
O	-4.501073009242	-1.960496469771	6.880763515229
O	-6.255990676493	-0.528958610367	7.568476103862
O	-3.272786449983	-0.201460414826	8.914557555011
TV	7.274545036286	-0.000000000007	0.000000000005
TV	0.171259897221	3.563199616745	-0.000000000005
TV	-5.069528321994	-0.782121490138	9.885137080338

EQ-CO₂ 103

C	-1.701221044437	0.605944128875	-0.735784498627
C	-2.719271942957	3.700146447709	2.277385280796
C	-0.170685396892	0.918906709976	2.130764659823
C	-1.192397709637	3.962410737960	5.197564124928
C	1.380096617119	1.224404597569	5.056994261109
C	0.149982805474	4.274513792642	8.150153538306
O	-2.708523313603	-0.007124148173	-0.651822326238
O	-1.187114360021	0.334185638113	2.286991759972
O	0.181891828002	-1.526028220635	0.165042238688
O	1.794017338015	-1.108877639747	3.102267155333
O	-0.545488413884	3.394683469815	4.384953103795
O	2.396896279592	1.830418224492	5.038027459934
O	-2.144520752176	3.076616053827	1.452824539350
O	0.364709491215	0.618954371969	5.075312875604
O	0.846685918249	1.502578538445	1.969500302711

O	3.250131696776	-0.904818792977	6.013428531313
O	0.795017097659	3.706761009508	7.335622525229
O	3.715502828805	2.152139904126	7.977971722465
TV	5.440881973574	-0.000000000000	-0.000000000001
TV	0.354988896321	5.435407100044	0.000000000001
TV	4.407358338180	0.935354808582	8.796581612490

EQ-CO₂ 104

C	4.613608640771	-1.448572452936	3.561267314352
C	0.124620019155	-2.571436318457	-3.320280180440
C	-1.544946951041	-1.180411154740	1.026193748544
C	5.619157758059	-1.966604910590	7.277519503933
C	1.130347118697	-3.089536673819	0.395998853855
C	-0.539476069873	-1.698570203633	4.742424961316
O	-1.726379266542	-1.987143984956	0.179226415693
O	4.433070813606	-2.244846923221	2.703748838163
O	-0.042056872553	-3.396229593799	-4.153194421512
O	0.291268689769	-1.747636606174	-2.486372139023
O	1.297073593290	-2.265765344523	1.229914079580
O	4.797038808934	-0.652746326968	4.417867991846
O	-1.367634486726	-0.373467279273	1.874495001388
O	5.802724279135	-1.171157351177	8.134440835981
O	-0.362053486555	-0.891625173884	5.590703221256
O	-0.720892177599	-2.505326663425	3.895478602815
O	5.438574305831	-2.762527099193	6.419680203452
O	0.963641210218	-3.914333915624	-0.436900047252
TV	8.229185755786	-0.000000000005	0.000000000003
TV	-0.218517964026	4.051738592350	-0.000000000005
TV	2.011381398247	-1.036264510955	7.432482508979

EQ-CO₂ 105

C	1.705713079529	1.910895255468	3.177517664316
C	-0.533292760452	0.448070597668	0.751811245772
C	-3.462221039259	2.042474803869	-1.459655879420
C	1.408735102086	5.418040946071	3.177514623970
C	-0.830315545991	3.955132355374	0.751691629666
C	-3.758536975547	5.550395849140	-1.457201037325
O	-0.188275403041	-0.103060833741	1.739840582462
O	-3.464642251802	1.424354780415	-2.468562247057
O	-0.865308695800	0.999802775619	-0.241346086550
O	-0.875705816085	-0.158825096787	-2.935687291841
O	-1.172061809280	3.348392195868	-2.935335257590
O	-3.471029365837	2.661783779613	-0.450741889525
O	2.287372718809	1.496466625593	2.234966130850
O	-3.768302032762	6.169992814603	-0.448456226384
O	1.989854791319	5.003521391455	2.234682310212
O	-0.484857369677	3.403773033528	1.739435870999
O	-3.760095642836	4.932377923619	-2.466137433686
O	-1.162810017118	4.507064835038	-0.241197838469
TV	5.108263139968	-0.000000000006	-0.000000000004
TV	-0.594104892104	7.014143898991	-0.000000000002
TV	2.004797735043	2.479844142328	7.061904049895

EQ-CO₂ 106

C	1.355409496085	2.098188473461	3.131990573942
C	-1.618415236389	0.889323395104	0.878092292303
C	-3.808518766636	2.867837926238	-1.518370195736

C	1.194749495595	5.660909938822	3.135798850445
C	-1.752188091437	4.459813280949	0.876858272670
C	-3.964552913106	6.435934011738	-1.516777337053
O	-1.643952070142	0.295168213906	1.902056399243
O	-3.128842521327	-1.212354909673	-2.442973664339
O	-1.603920822013	1.489209388550	-0.141441855307
O	-0.769089472187	0.758869649429	-2.980089247042
O	-0.919629769502	4.500386033661	-2.983063420927
O	-4.322266463791	3.377376167820	-0.582279800310
O	0.770014217895	2.016087564146	2.105015068275
O	-4.479328176520	6.946337209517	-0.581830564064
O	0.607409118157	5.748752018748	2.109971926685
O	-1.780928353997	3.863933189009	1.900505514747
O	-3.286478288143	2.355229243871	-2.447797568364
O	-1.737169570360	5.059348142999	-0.142526374942
TV	5.027175099883	-0.000000000005	-0.000000000004
TV	-0.309836631235	7.134846020437	0.000000000000
TV	2.560506219134	4.814534696055	7.134162660196

EQ-CO₂ 107

C	-1.661460482621	-0.941922987325	0.012364230936
C	1.753922978812	1.267861654324	1.682528149161
C	-3.120839774614	-0.064362516290	3.146759090395
C	0.288318500496	2.114610422997	4.721539714197
C	-4.613984779892	0.775428656767	6.271221772376
C	-1.138580711756	2.998964782316	7.814749529256
O	2.019546951123	-1.834511945868	1.382196767579
O	0.556771646225	-0.967705816298	4.460899331928
O	-0.573101794407	-0.584318027548	-0.288418047448
O	-2.059253031371	0.299732144334	2.769351222755
O	-4.176621777257	-0.434574361930	3.532076564454
O	-0.802329564318	1.736947446392	4.983519652758
O	-2.751066679180	-1.297747414873	0.312003970738
O	-0.897597897122	-0.116673073442	7.424190368752
O	0.666092758642	0.910202079590	1.986942665016
O	-3.555210421484	1.168142647422	5.914021857103
O	-5.669632221043	0.379900396563	6.632145686100
O	-2.197450927939	2.649094770275	8.211155654236
TV	7.626480343462	-0.000000000020	0.000000000011
TV	0.821849875418	3.462176969667	-0.000000000010
TV	-4.500707188105	2.617656405977	9.306519746027

EQ-CO₂ 108

C	2.243647526418	2.010924999776	5.324750457504
C	-0.137952183679	1.864037073803	0.843474499556
C	-5.438468224751	2.492892821779	-3.743043116253
C	5.562855396638	1.914353443578	5.291712634800
C	3.154390420449	1.826513523522	0.784760658212
C	-2.127347931409	2.335871492655	-3.734390574701
O	0.458203490973	2.144053693057	1.828104365262
O	-5.999016254846	2.201586650614	-4.744724207655
O	-0.729767261907	1.560374405279	-0.135191595209
O	0.481173960498	-0.052230191912	-2.398536094052
O	3.774860686014	-0.254154850531	-2.480999413084
O	-4.876860295512	2.802082778494	-2.747216259804
O	2.607967858608	1.414002831892	6.280503698048
O	-1.601274059756	2.645974636072	-2.720290240641

O	5.952370876867	1.419391144446	6.294068526887
O	3.674239050900	2.122958514654	1.806262026714
O	-2.656225653675	2.037252078959	-4.751081575538
O	2.633499143004	1.512230595956	-0.231468033005
TV	6.659975915555	-0.000000000004	0.000000000004
TV	2.707406195715	5.658469449705	-0.000000000008
TV	1.397626270091	2.661630206571	6.769439335372

EQ-CO₂ 109

C	1.068603960871	2.402811738792	3.081600149205
C	-1.371216650035	0.426380060326	0.855869277807
C	-3.197326784213	3.104424525418	-1.509766883473
C	1.064997692313	6.366158866571	3.081580786539
C	-1.374839395986	4.389695141892	0.855848364889
C	-3.200938807877	7.067752470202	-1.509747232377
O	-1.281316545974	-0.302739948228	1.783279219014
O	-2.577300871737	-0.892165278705	-2.519419974566
O	-1.469439934483	1.147136433051	-0.077761442476
O	-0.258358789043	1.129345570538	-2.928482858309
O	-0.261970835858	5.092698212990	-2.928506379644
O	-3.814582737439	3.144832172823	-0.500971310531
O	0.979718340813	1.657287480445	2.167268190909
O	-3.818210316082	7.108150178900	-0.500958361055
O	0.976122720936	5.620605934558	2.167271141145
O	-1.284906215664	3.660579037162	1.783256035769
O	-2.580915011057	3.071136442659	-2.519441523514
O	-1.473096656741	5.110447879033	-0.077778328877
TV	4.670360804862	-0.000000000007	-0.000000000003
TV	-0.007224671787	7.926630310952	0.000000000000
TV	1.425468286480	2.010208872771	6.930969384653

EQ-CO₂ 110

C	0.699689758703	1.375379350053	3.022376629469
C	-2.356047506977	1.523867640872	0.809796376069
C	-4.862475258372	2.489525529156	-1.473874743441
C	0.243975108374	4.789993288428	3.027215917149
C	-2.855882417379	4.940611640411	0.849471095295
C	-5.309958253617	5.901635783372	-1.468582874988
O	0.556987375606	0.754000470799	2.024706076773
O	-4.226827507058	2.428451987385	-2.470857707065
O	-2.589910265865	0.903577509814	-0.170780467952
O	-1.159099488582	0.651941413219	-2.748813588485
O	-1.607920035613	4.061521130907	-2.742111378847
O	-5.499540586719	2.548941364305	-0.478013211728
O	3.394269548638	2.143340167940	1.794133326052
O	-5.948739730514	5.957811735394	-0.473599320514
O	2.827160777429	5.570676714423	1.840279022398
O	0.095324256356	4.173324538981	2.027389675524
O	-4.672137478165	5.843679391473	-2.464410932802
O	-3.024629911428	4.310363421383	-0.137628135905
TV	5.530269611755	-0.000000000003	0.000000000000
TV	-0.891224439345	6.823591949125	-0.000000000002
TV	2.019546654860	1.343845559679	6.766496576775

EQ-CO₂ 111

C	-1.728190229599	-0.932745098693	-0.087306774638
C	-0.867588652078	1.027409401167	2.959604930530

C	1.590641000243	-0.945736233988	-0.022224589828
C	2.449291092751	1.026041767236	2.960425905952
C	4.937917529458	-0.962851055664	-0.052938033781
C	5.776355740765	1.069103381164	2.922211666129
O	0.962121241301	-4.199467905237	2.298487325363
O	4.213101526199	-4.226973187217	2.287671398069
O	1.072631782141	-1.821493263122	0.581348269750
O	4.452472078868	-1.819329299272	0.602375069844
O	2.110113070866	-0.068061945712	-0.625164618843
O	2.009911861304	1.892526227048	3.633392681614
O	-1.183254393619	-0.087045873490	-0.712481599248
O	7.589189564307	-4.183435713863	2.281878008242
O	-1.369838732185	1.868218840819	3.621855416017
O	7.722319810404	-1.776352098024	0.534125610112
O	5.423783275518	-0.106099541497	-0.711452263391
O	5.286310117035	1.935724708335	3.560414648019
TV	9.999131831442	-0.000000000009	0.000000000009
TV	-1.325698767521	4.383589897701	-0.000000000010
TV	-3.663274687849	-4.338015400617	6.031844307356

EQ-CO₂ 112

C	0.146509352549	1.325112509897	2.929999443838
C	-2.712473798128	1.152746343882	0.790853086833
C	-5.417502409689	3.120758001158	-1.418892614697
C	-0.168904659117	4.864801730663	2.929942338837
C	-3.028018060584	4.692093239768	0.790176899550
C	-5.731886551586	6.659297287278	-1.420332392196
O	-0.089676225505	0.686486863685	1.961202462610
O	-5.191705542923	3.785279903143	-2.372226780515
O	-2.564697475960	0.514449687645	-0.194568779822
O	-2.384269073894	2.286414144275	-2.621833053182
O	-2.699381281189	5.825970706194	-2.621887888562
O	-5.636234620569	2.452368279453	-0.466548430368
O	2.696897375073	1.786965461213	1.778645204745
O	-5.951209938949	5.993146957899	-0.466517563034
O	2.381186651094	5.326199174029	1.778006532393
O	-0.405420717755	4.226273561329	1.961152213572
O	-5.505884979520	7.321555065028	-2.375203749937
O	-2.880093650177	4.053853455959	-0.195271172582
TV	5.566094650814	0.000000000011	0.000000000105
TV	-0.630753043556	7.079359972061	0.000000000060
TV	2.773001279138	-0.321891511683	6.517937888333

EQ-CO₂ 113

C	-1.166455949406	-0.822586073640	0.416013930272
C	0.430166037439	1.695277984452	2.076639709073
C	-3.177617742659	-0.774322580053	3.790261968782
C	-1.513508064885	1.739793968606	5.376303735166
C	-5.057580304375	-0.729399464541	7.023392387383
C	-3.369154964144	1.791566077929	8.734276227505
O	1.602903521478	-3.284365147855	2.146452292702
O	-0.341498507555	-3.245015093479	5.291431208863
O	0.015002514396	-0.822936911790	0.336566937898
O	-1.993142541216	-0.772352943215	3.789537150880
O	-4.362078313527	-0.777053053580	3.790545589104
O	-2.695205732081	1.738856028296	5.456606179940
O	-2.347852926931	-0.823001104363	0.498322779890

O	-2.194314803411	-3.190695728410	8.729755586640
O	-0.751681696157	1.688648663213	1.999821176594
O	-3.875931439484	-0.728185884689	6.947386394457
O	-6.239849467788	-0.730373392427	7.093584422095
O	-4.553353246136	1.787697304728	8.738642746672
TV	5.204616240605	0.000000000007	0.000000000013
TV	0.009638027545	4.985837166835	-0.000000000004
TV	-5.714275523756	0.141791651914	9.890326088476

EQ-CO₂ 114

C	-2.283811495264	-0.280588113461	0.411807861392
C	2.373574747848	1.339395333752	2.067836101368
C	-1.394709101565	-0.346958132700	3.797470212224
C	3.276822068934	1.501604280938	5.483251981505
C	-0.415507816037	-0.163573231393	7.151943002319
C	4.239445867955	1.563134464165	8.893107816283
O	2.380309189703	-1.710449105309	2.375709939302
O	3.247509641338	-1.526836301602	5.877741932936
O	-1.224820338481	0.076595830116	0.801413643162
O	-0.309159452271	0.011938307861	4.103299715112
O	-2.481000428430	-0.705173941349	3.493693584729
O	2.228712508229	1.120938747974	5.087099362608
O	-3.341385683039	-0.639412728765	0.019966349230
O	4.249833304601	-1.496905341244	9.201411003983
O	1.289770085800	0.979736524278	1.757787530025
O	0.675807864919	0.183321914670	7.451089355577
O	-1.505357590543	-0.512193956629	6.849159137895
O	3.150796088054	1.215229720823	8.584998529614
TV	7.270708153135	0.000000000000	0.000000000001
TV	1.077954956366	3.408459997784	-0.000000000001
TV	2.871428965960	0.143107610967	10.152501708845

EQ-CO₂ 115

C	4.427339195847	-0.916383853224	0.611621491390
C	0.329990629193	-1.740511067779	-1.224467956233
C	-1.425396375113	-1.856428847556	1.720044317729
C	5.135097705431	2.504800664432	0.612074648490
C	1.037709851721	1.681118255053	-1.224574901965
C	-0.717714209006	1.564939413060	1.720053499962
O	-1.834619904599	-2.396713839114	0.748806201789
O	3.939418076704	-1.441912718366	-0.329543225499
O	-0.222641320092	-2.238276499145	-2.146895037683
O	0.886522241947	-1.243094133698	-0.307515963140
O	1.594272253606	2.178464268778	-0.307590462825
O	4.907646663559	-0.391598307906	1.560827086826
O	-1.016110414315	-1.316358129153	2.690487362419
O	5.615356516770	3.029891575557	1.561138653825
O	-0.308655726772	2.105029864099	2.690580375371
O	-1.126762021914	1.024679349698	0.748725443660
O	4.647226474426	1.979019996074	-0.328999921098
O	0.485141574298	1.183517116665	-2.147126409299
TV	9.068645894465	-0.000000000004	0.000000000008
TV	1.415317535854	6.842941014498	-0.000000000010
TV	1.430033385332	-1.002337432656	4.103058584329

EQ-CO₂ 116

C	2.163265378444	1.498707990586	1.875012583262
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C	-1.480162373449	0.496629588194	0.590198285902
C	-3.677613803405	3.436534803772	-0.747432700180
C	3.620121310311	5.492234960684	1.871402292510
C	-0.008712868261	4.471442610427	0.542786641942
C	-2.224755430212	7.426187202019	-0.740476807121
O	-1.679157448404	-0.269911369643	1.468429131314
O	-4.078677372397	-0.046706087696	-0.595833397420
O	-1.282288921675	1.264573166625	-0.287386133686
O	-0.318209247363	2.953801339663	-2.809036881164
O	1.148400255331	6.926955082096	-2.813582170951
O	-4.733996770411	2.920224898038	-0.882980421031
O	1.102368192901	0.980379261804	1.787632953287
O	-3.280452977970	6.908377775226	-0.876547492482
O	2.549396797607	4.993882165186	1.784646413365
O	-0.206083185292	3.646489939272	1.366681107891
O	-2.621421806932	3.951113187258	-0.602885793906
O	0.186786248949	5.294247482468	-0.284124618721
TV	6.780612496926	-0.000000000008	-0.000000000003
TV	2.909475764739	7.988700117468	-0.000000000000
TV	3.540970914290	-0.932579545353	4.760995398893

EQ-CO₂ 117

C	-1.303838375446	0.240848528551	-0.817390332100
C	-2.457075748433	3.954319271369	2.127918247097
C	-0.106653708326	1.046052984235	2.144783352950
C	-1.127160809179	4.630616493912	5.074218031572
C	1.226435567049	1.740853233820	5.150047050220
C	0.264093291235	5.187265518354	8.025942039921
O	-2.267775159528	-0.444713930474	-0.806932472686
O	-1.077039425800	0.368626251183	2.149938988919
O	0.355441544988	-1.976176584033	-0.153647366597
O	1.610830971812	-1.193222753299	2.790047293448
O	-0.440600849570	3.938372848260	4.403097904907
O	2.200653576582	2.406961925155	5.069189473125
O	-1.764259515041	3.259331917895	1.466214217945
O	0.252802113906	1.073504700231	5.233088856822
O	0.863951727510	1.722042277674	2.135307953344
O	2.947555143364	-0.519669955995	5.745896624482
O	0.945364997542	4.486711929373	7.359086945452
O	3.643008514764	2.945675930920	8.016113438866
TV	5.140253072445	0.000000000000	0.000000000001
TV	0.381560780652	5.843325913729	-0.000000000002
TV	3.982969818234	2.018698077979	8.846089457729

EQ-CO₂ 118

C	-0.430527709352	-0.796274320950	0.435516770295
C	0.797409467901	1.849743181523	1.930522938008
C	-3.117855802687	-0.752481118908	3.415750597707
C	-1.889743881215	1.893468493609	4.910684985389
C	-5.798144359851	-0.707639224685	6.395959946143
C	-4.576927910717	1.938289202914	7.890899004857
O	-0.579933401849	-3.398310841034	1.934622749294
O	-3.267083333392	-3.354345934277	4.914710520224
O	0.753071052601	-0.777349982757	0.438878351008
O	-1.934260465734	-0.733663796427	3.419321982859
O	-4.301972919503	-0.767448915683	3.416018113030
O	-3.073437263851	1.904301572714	4.907806529411

O	-1.614642808305	-0.811340916890	0.435979303062
O	-5.954277825300	-3.309728048380	7.895105206843
O	-0.386282644538	1.860640542887	1.927558677238
O	-4.614498339044	-0.690764858100	6.399629405293
O	-6.982247952931	-0.720328763642	6.396277782564
O	-5.760633086908	1.948760310143	7.887833024800
TV	5.216242456258	0.000000000057	-0.000000000018
TV	2.561278946081	5.235139459682	-0.000000000002
TV	-8.062138991471	0.131908688196	8.940671814331

EQ-CO₂ 119

C	1.676275475684	1.637714268792	3.052907853120
C	-1.492634259135	1.959453868629	0.747832198843
C	-4.647025325521	2.354688367726	-1.491176260092
C	0.400670534103	4.797009274169	3.027485857894
C	-2.769174837182	5.161721655505	0.748516414825
C	-5.934277108513	5.554356605564	-1.489339007347
O	-0.861422921861	1.547234747916	1.659684849209
O	-4.175661680781	1.893585729972	-2.475488209635
O	-2.123259406626	2.372421575093	-0.163942119354
O	-1.007379278141	1.043308440389	-2.504602803913
O	-2.330895285950	4.275213504147	-2.587342344001
O	-5.127848752119	2.810564054634	-0.510278633758
O	2.151377917048	1.242454376760	2.043724982574
O	-6.409472449407	6.011113591154	-0.505794541661
O	0.921508901889	4.325073114788	2.075322479729
O	-2.128874840637	4.759649909899	1.658524457951
O	-5.469382902049	5.092812139439	-2.476347195157
O	-3.408412178701	5.564659602768	-0.161699783667
TV	6.117577678354	0.000000000001	0.000000000000
TV	-2.558524894332	6.407744817338	0.000000000000
TV	2.221082085481	0.995914671820	6.572024412393

EQ-CO₂ 120

C	1.694457032257	-0.339666334568	-0.525826592994
C	-1.113287090445	-0.034478443701	2.788013491032
C	5.156651824278	-0.349477805250	-0.527372943975
C	2.342152771143	-0.039708535950	2.775991986438
C	8.600478017652	-0.342093428723	-0.530145696878
C	5.797272136147	-0.035932583516	2.777688413993
O	-5.147177386721	-0.787822598033	3.483243218572
O	-1.695712958144	-0.780240125067	3.499228770385
O	2.332615805621	0.417619020865	-1.173653295160
O	5.678818076282	0.396244464416	-1.283830987086
O	4.632003117135	-1.097160719083	0.226175330577
O	2.924817647876	0.711258545854	2.069233204097
O	1.055490791212	-1.097444357723	0.122509381560
O	1.763090127170	-0.791012312994	3.483088058178
O	-0.528720730667	0.712753705988	2.079128845049
O	9.123786541597	0.401984789946	-1.286715789484
O	8.074586070449	-1.087362723359	0.225648938381
O	6.382416553937	0.716788089758	2.075220840734
TV	10.364054383022	0.000000000014	0.000000000044
TV	-0.491552471867	3.547206444772	-0.000000000021
TV	-4.116140832139	0.656130537371	7.039225247207

EQ-CO₂ 121

C	-1.118100047090	0.411535059756	-0.905264264375
C	-2.087038096239	4.136766662079	1.978032195364
C	0.187715831424	1.174268115223	2.063870056985
C	-0.741049327258	4.848968807725	4.944278055974
C	1.543767759451	1.888597614939	5.021866175337
C	0.639498540611	5.502955062708	7.912185216124
O	-2.077390742999	-0.277668948956	-0.971163578857
O	-0.805310838392	0.535249668812	2.147308316673
O	0.523816566004	-1.869928118862	-0.317042411081
O	1.798330053692	-1.134530639903	2.647525604741
O	-0.053176705821	4.159629094493	4.272039505030
O	2.534472464112	2.530334100085	4.939529496706
O	-1.394531839613	3.449506225044	1.308053552750
O	0.551670143644	1.247576612957	5.104882910630
O	1.180763144539	1.813036905430	1.983057452014
O	3.148060129741	-0.422140424760	5.617798387456
O	1.278040859128	4.763722221554	7.244161948060
O	3.894413590842	3.255736468425	8.057764507556
TV	5.019427249839	-0.000000000000	-0.000000000003
TV	0.441689951764	5.958199921236	-0.000000000008
TV	4.054348218658	2.153200545720	8.896713480157

EQ-CO₂ 122

C	-0.980020063700	0.310231527172	-1.167342229692
C	-2.033860773986	4.189991846730	2.248801134765
C	0.172957508290	1.085130764373	1.824489907683
C	-0.860823696301	4.975469161860	5.296030173164
C	1.346159260098	1.837575922133	4.816950080785
C	0.302511908393	5.614955732458	8.237418268120
O	-1.994801397041	-0.297478732181	-1.166580413327
O	-0.817673302833	0.438740875795	1.825552320422
O	0.524042058588	-1.906062201865	-0.146410545562
O	1.685920142468	-1.160459637653	2.838893851623
O	-0.150272252502	4.297057762671	4.638219017029
O	2.338805930893	2.483476914234	4.812717271011
O	-1.310660798431	3.466197096938	1.655970616118
O	0.355364046479	1.191101029999	4.819800354412
O	1.162563121074	1.735124570534	1.822522869558
O	2.879186448591	-0.415551485249	5.956845064566
O	1.025638303048	4.892575570029	7.642838614962
O	3.534380864564	3.091023876239	7.804448281498
TV	4.840487380847	-0.000000000000	-0.000000000001
TV	0.394486366980	6.075081002738	0.000000000001
TV	3.499205973766	2.171546582207	8.973843896674

EQ-CO₂ 123

C	1.724612535366	2.188197160531	3.100380140327
C	0.050924102784	-1.130926593662	0.746106054647
C	-5.337450903701	3.818333479942	-1.490218182513
C	0.409254100484	5.366671052891	3.102776275798
C	-1.431590101055	1.982522829252	0.751675595070
C	-6.788111232590	6.989425707296	-1.587490359202
O	0.772675955869	-1.435359940111	1.632844824466
O	-5.388127900007	3.153437268769	-0.511256700468
O	-0.668077312489	-0.826787049930	-0.143451852007
O	-0.928223798173	0.903751553820	-2.485124509925
O	-2.306115717095	4.026156970722	-2.488064179684

O	-5.300493612199	4.475406827834	-2.475166460883
O	2.185228454726	1.727736142742	2.112050739804
O	-6.759166285893	7.653081052789	-2.568489376218
O	0.930218398315	4.962748012781	2.119351089396
O	-0.762241741257	1.603313998125	1.650788910443
O	-6.833244369627	6.314467036692	-0.616157471273
O	-2.101864837016	2.360620818647	-0.147415667007
TV	6.303781612168	-0.000000000007	0.000000000033
TV	-2.805420690004	6.289570466094	0.000000000043
TV	2.207460815163	1.748647623620	6.580425732526

EQ-CO₂ 124

C	-1.150327576264	0.248276311685	-1.477800880770
C	-1.734892673406	4.307576043443	2.482211119793
C	0.052631595778	0.969347494706	1.571335293476
C	-0.403700538253	4.999480632490	5.460279205341
C	1.457603651446	1.653409924977	4.490484055597
C	0.889623479420	5.706009144226	8.451939321487
O	-2.183098884027	-0.304814329550	-1.320367648181
O	-0.984141168881	0.406664826698	1.655771621933
O	0.447145900169	-1.704304897603	0.152029535714
O	1.730622995230	-1.004683394665	3.139259118263
O	0.165924642898	4.197945884867	4.803269125307
O	2.491899335292	2.206124212296	4.326340463336
O	-1.156598908432	3.513120751051	1.823969573917
O	0.423577467840	1.103897578783	4.651587659156
O	1.089559886106	1.535177262398	1.484054792642
O	3.070875828781	-0.305399019793	6.116747558374
O	1.462419785642	4.902025934146	7.799873770445
O	3.795499899931	2.912270958156	7.309583945816
TV	4.867191612417	0.000000000000	-0.000000000003
TV	0.821211897462	6.108151993276	-0.000000000008
TV	3.913127898757	2.107786570061	8.950333372329

EQ-CO₂ 125

C	1.515529243370	1.231485241959	2.928702130251
C	-1.732778624819	0.916137252968	0.711547546709
C	-3.845415389031	2.748464256416	-1.350930828905
C	2.779215639811	4.434817026792	2.930083255832
C	-0.471578103034	4.120481571506	0.716954175613
C	-2.582005111256	5.954525237454	-1.352595923201
O	-2.050575664045	0.393334420557	1.725230067117
O	-3.317258920735	3.185835031102	-2.315708014879
O	-1.429041927119	1.443652582758	-0.304800387636
O	-0.237934372809	2.674325010413	-2.667982318120
O	1.026223003975	5.878235752684	-2.667106025666
O	-4.364845627953	2.312732180210	-0.379787307691
O	0.960116854508	0.814484981905	1.970590165383
O	-3.103563516185	5.515717312490	-0.383909866470
O	2.223167804186	4.018106311338	1.972182892619
O	-0.786366899757	3.599419454760	1.732533184316
O	-2.052306851933	6.394942500683	-2.315222119770
O	-0.170412118504	4.644446246371	-0.301792429877
TV	6.163534228426	0.000000000003	-0.000000000007
TV	2.528337731509	6.409162788699	-0.000000000000
TV	2.311621909264	-1.030063762518	6.554804517013

EQ-CO₂ 126

C	-0.503403185837	-0.837018372422	0.486477298770
C	0.760087468395	1.820330207774	1.923851200756
C	-3.433299118211	-0.846692842099	3.541356165117
C	-2.213041822635	1.785244100441	4.976871162641
C	-6.337290856567	-0.856632144616	6.547996264029
C	-5.122721927288	1.778546432681	7.981285460485
O	-0.803486230037	-3.422299463045	1.981699606935
O	-3.775700721723	-3.472987021226	4.975732530983
O	0.678950396305	-0.856265342841	0.543821065188
O	-2.249252775368	-0.882853861267	3.541867242500
O	-4.616392113726	-0.802636962981	3.542095336455
O	-3.396883015202	1.807577920969	4.978327605132
O	-1.686180012249	-0.814038630889	0.429619858984
O	-6.685965506293	-3.489070568386	7.982230637316
O	-0.422508334942	1.833788452419	1.866884139639
O	-5.153414733250	-0.882744609824	6.546854207472
O	-7.520937680401	-0.821784384803	6.548898092284
O	-6.306769944412	1.810503566264	7.980292881473
TV	5.212128827299	0.000000000058	-0.000000000019
TV	2.746459139849	5.225878493422	-0.000000000002
TV	-8.836803377934	-0.057457319954	9.112064073799

EQ-CO₂ 127

C	-1.707270987980	-0.644359693605	0.581054262064
C	2.324668533350	1.983031214066	2.122344080787
C	1.094476507061	-0.607658213481	3.663582339749
C	5.117121839207	2.008399405338	5.252471833451
C	3.910517905602	-0.575228561367	6.794146210608
C	7.939191334461	2.038354970463	8.333115225460
O	0.917708651534	-3.179520724102	2.054411432357
O	3.711717927464	-3.164115293873	5.248287274044
O	-0.522852554479	-0.624694188546	0.578577291014
O	2.278912135314	-0.592242117591	3.660162922745
O	-0.089681006820	-0.617641704380	3.663999314355
O	3.932512257214	2.019320345860	5.256700233372
O	-2.891680049619	-0.658744399408	0.583980403565
O	6.534168132915	-3.129484608836	8.325841658089
O	1.142199217217	1.985707506853	2.188800947156
O	5.092677419104	-0.572406554841	6.723809758299
O	2.728297148127	-0.572115981971	6.863035699109
O	6.754980985718	2.039174307970	8.338734113905
TV	5.208903257425	-0.000000000000	0.000000000001
TV	2.589239699913	5.158258813961	-0.000000000002
TV	8.477529062908	0.101347478419	9.343563147406

EQ-CO₂ 128

C	-0.535812584884	-0.861396799017	0.547731670724
C	0.831442466569	1.774749446840	1.871334633722
C	-3.499959287390	-0.925776428325	3.547979746563
C	-2.091503855583	1.701778605483	4.948102588715
C	-6.438266793077	-1.008493584536	6.593112613516
C	-5.069069931214	1.641334379993	7.952478270638
O	-0.895975153486	-3.539468019153	1.878700712403
O	-3.818278493378	-3.606320911012	4.956402667422
O	0.647857352345	-0.893749211249	0.547126621825
O	-2.316597613072	-0.964154613985	3.545097080315

O	-4.683401882282	-0.883314930428	3.548754890558
O	-3.274870136101	1.750477788109	4.944026920530
O	-1.718887067625	-0.820170442437	0.548674200603
O	-6.795448780942	-3.653373662652	7.958106915625
O	-0.352076108813	1.828177493136	1.863519871717
O	-5.255431030759	-1.042177242534	6.648657583941
O	-7.620150183987	-0.969343837334	6.535037073120
O	-6.252588876744	1.675682290100	7.949770289565
TV	5.215406510882	0.000000000058	-0.000000000019
TV	2.909701018634	5.252347856259	-0.000000000002
TV	-9.009046257463	-0.230668258356	9.085718537051

EQ-CO₂ 129

C	1.628264033579	3.809430573392	3.042351744342
C	-0.310870025030	0.656061386495	0.911688824650
C	-4.979320944822	2.660068172070	-1.563581369308
C	0.790211055728	6.985582071500	3.039473627653
C	-1.161928087781	3.904834261639	0.912231983398
C	-5.829409301886	5.931866698652	-1.695142688087
O	-0.039270203840	1.331415818418	1.845430451819
O	-4.357870210479	2.234315504882	-0.650278028157
O	-0.572582114256	-0.017413499731	-0.025492985269
O	-1.946363984827	1.251780195662	-2.477156433329
O	-2.772019276599	4.357252583942	-2.459912341213
O	-5.610518753935	3.078943009714	-2.474238058383
O	2.118429817536	3.549395792363	1.996274744150
O	-6.513793348206	6.283428505325	-2.596809745711
O	1.271002439210	6.788221917620	1.975047320956
O	-0.888639002114	4.583862927881	1.842860413675
O	-5.151317995307	5.576922672377	-0.793072887904
O	-1.424302224075	3.227573142415	-0.021706127598
TV	6.020897681839	-0.000000000005	-0.000000000006
TV	-1.699038540778	6.487905003585	0.000000000010
TV	3.077610745964	2.821978112298	6.562818383881

EQ-CO₂ 130

C	-0.027113660745	-0.600688780929	-0.426816055148
C	-0.573455955595	1.169926189844	2.833985303440
C	-0.099645353668	2.961044848837	-0.389395791048
C	-0.768784898739	4.709520116683	2.865115851820
C	-0.212027433600	6.448997346477	-0.393152805306
C	-0.707759811192	8.247860087238	2.863338083401
O	0.152775237617	-3.017503355765	3.602881342919
O	0.083591308251	0.561043768821	3.606100513941
O	0.639941012162	0.068056284735	0.287031796985
O	0.561035901960	3.613599824267	0.345864207340
O	-0.754507094807	2.309622991868	-1.127501941775
O	-1.419107870983	5.378377278798	2.136183058323
O	-0.688395931089	-1.269861048299	-1.143704173121
O	-0.123530395218	4.041260263549	3.597091002950
O	-1.235474260916	1.779760190056	2.065001967748
O	0.441504358166	7.109856967635	0.340248222036
O	-0.859773956532	5.787401488299	-1.129572746649
O	-1.369530271874	8.897318762000	2.126634910084
TV	3.528752742241	-0.000000000000	0.000000000000
TV	-0.204063980623	10.616713056192	-0.000000000009
TV	-6.268499897874	-0.009335205665	7.047998107195

EQ-CO₂ 131

C	-1.140588749167	-0.985761350230	0.406054605673
C	0.390907055285	1.521281347479	2.131175072880
C	-3.291662817732	-0.942769970781	3.804177492207
C	-1.724949543241	1.566721550987	5.513773445412
C	-5.455979927906	-0.897141775407	7.117592259107
C	-3.937241521788	1.611249539470	8.833954974797
O	1.550457929846	-3.444744674393	2.199960086988
O	-0.563034057407	-3.400065780779	5.510492150445
O	0.042373844187	-0.984530253575	0.339807226342
O	-2.107259133197	-0.939134824362	3.801796452338
O	-4.476193769874	-0.946205809459	3.801313356441
O	-2.909507699226	1.563543954034	5.516985921965
O	-2.323781600254	-0.987515713116	0.472349308334
O	-2.775755878000	-3.355314627538	8.832208450056
O	-0.791805887888	1.517160739638	2.060792872951
O	-4.271397304579	-0.893428626554	7.119588263764
O	-6.640630015913	-0.901206735973	7.112109992609
O	-5.121811006258	1.607735881908	8.834234720356
TV	5.218886841047	0.000000000000	0.000000000008
TV	0.023175342063	4.969667109823	0.000000000010
TV	-6.423297296619	0.133600359703	10.086126015746

EQ-CO₂ 132

C	-1.727492198004	-0.946187208674	-0.001193793836
C	1.397145249325	1.637985685353	2.308110234576
C	-3.592236966160	0.018501466419	2.853212119347
C	-0.467548408972	2.602444756385	5.162604341411
C	-5.456940465284	0.983258407759	5.707296943884
C	-2.332641584135	3.567959903075	8.016713395173
O	1.602165649949	-1.410321507565	2.098624506228
O	-0.262599619730	-0.445780003723	4.952923291969
O	-0.614078514799	-0.570238251644	-0.152958216512
O	-2.478891530827	0.394625072871	2.701329233752
O	-4.704449164351	-0.358376730385	3.000965878859
O	-1.558710608922	2.191733161443	5.374411749420
O	-2.839691421197	-1.323058369221	0.146644513253
O	-2.127708637771	0.519868133724	7.807189826497
O	0.306017951639	1.227176438730	2.519935542533
O	-4.343611499202	1.359506006170	5.555567268212
O	-6.569192255281	0.606471095367	5.855112493296
O	-3.423751023842	3.156996190864	8.228427653431
TV	8.861157464031	-0.000000000013	-0.000000000000
TV	0.885411011101	3.458742638205	0.000000000015
TV	-5.594593813301	2.894866577038	8.562727422520

EQ-CO₂ 133

C	2.525323492993	2.095130973107	1.970389024506
C	-1.486502948393	0.406270235304	1.104507504693
C	-5.223489954511	3.208647087237	-1.169094044679
C	2.697080231570	5.505976004208	1.970053023646
C	-1.315292355605	3.816966667648	1.104543711286
C	-5.051406100793	6.619073433909	-1.169274258599
O	-0.799445744733	-0.214501288234	1.842762234489
O	0.382965744394	0.051332529129	-1.044810249767
O	-2.179799102500	1.028439111833	0.375067686811

O	-1.785828001017	1.077508086056	-2.694362139746
O	-1.613806768129	4.488321190304	-2.694939594536
O	-4.073667654922	2.953711575626	-1.294576759510
O	1.789919922675	1.531492855897	1.232172751922
O	-3.901510000830	6.364215953143	-1.294215656553
O	1.961474221349	4.942479020991	1.231939040142
O	-0.628152871930	3.196534284684	1.842994465587
O	0.554114875486	3.462369076374	-1.044024305940
O	-2.008715488938	4.438783963756	0.374952684772
TV	6.926566330009	-0.000000000009	0.000000000002
TV	0.343155644478	6.821477361030	-0.000000000002
TV	5.051963084302	1.583057281135	5.393080540650

EQ-CO₂ 134

C	1.221893333404	2.327847131342	3.231658057737
C	-1.218523738574	0.455824087014	0.833301377803
C	-3.671468377699	2.322853567128	-1.545219568993
C	1.192334418536	6.009535148352	3.231175242851
C	-1.247775029274	4.137663385702	0.833268515315
C	-3.700579058700	6.004711106149	-1.545390595778
O	-0.522578684634	0.413775065037	1.788677006881
O	-3.035660788203	2.297815321976	-2.544586737082
O	-1.914710884210	0.497320397609	-0.122146933675
O	-0.660677357235	0.494864350765	-3.008882158952
O	-0.689616869357	4.176540225661	-3.008959435253
O	-4.314191617540	2.350648673479	-0.552946202598
O	1.865683003253	2.224837147364	2.245251226971
O	-4.343440279351	6.032686172621	-0.553214690259
O	1.835428980012	5.906587499192	2.244296770682
O	-0.551748660775	4.095584548693	1.788589845094
O	-3.064708450915	5.979519726632	-2.544707269343
O	-1.943970002441	4.179216594036	-0.122176255813
TV	4.846053500672	0.000000000003	-0.000000000002
TV	-0.058245077128	7.363615606427	0.000000000002
TV	1.245069327231	1.933746612807	7.234326721274

EQ-CO₂ 135

C	-0.579864741579	1.453226931849	-1.136440815691
C	-1.009372469734	-1.231585612116	0.731028291790
C	2.940875332974	0.480185329879	0.578196689146
C	-2.095525171895	7.166991440388	-0.986429540335
C	-2.552124589368	4.360684686073	0.576500987219
C	1.394715693289	6.108882584265	0.725788365065
O	-0.273501452809	-1.441888285657	-0.173310070917
O	-1.741734050937	-0.995850449654	1.629187601133
O	2.437853252289	-0.567840666385	0.352669729760
O	-3.608060057715	1.528081308152	0.807314639820
O	-5.139167714919	7.147890387539	0.961165722101
O	-1.660336304104	1.086061646769	-1.461289444385
O	0.501248437922	1.799029724133	-0.805545932389
O	-3.189690964647	6.856026048886	-1.319282511830
O	-1.000910416186	7.455039228115	-0.645564882308
O	-1.814681552801	4.217122041807	-0.339750852409
O	-3.287583478286	4.530381883064	1.487075192326
O	0.878336342881	5.070013129187	0.492110723106
TV	7.047526068945	-0.000000000022	0.000000000001
TV	-3.145784061728	11.164977359818	0.000000000023

TV	0.940614419367	1.153329288815	3.290293020009
# EQ-CO ₂ 136			
C	1.678685362166	2.086421945917	2.933558818860
C	0.183173483604	-1.089643239112	0.690747760425
C	-5.804467781579	4.035164492786	-1.321266761479
C	0.032641315172	5.473676972062	2.955631068379
C	-1.515628464685	2.208884159914	0.706091548768
C	-7.516695799806	7.534837170906	-1.497682550199
O	0.904036894686	-1.456820538734	1.553745261895
O	-5.426289320553	3.418861096303	-0.382903815263
O	-0.529125195748	-0.714838005735	-0.178071163337
O	-1.347200185852	0.839219770281	-2.512593106801
O	-2.990475928119	4.224790707795	-2.487993199813
O	-6.202096376088	4.643597013869	-2.255666316617
O	2.261147096942	1.583734544976	2.034382621364
O	-7.836329388134	8.127820622547	-2.472623098468
O	0.610328275148	4.969855756485	2.053261518173
O	-0.847985954141	1.747942775466	1.567147922686
O	-7.218617503760	6.933052847440	-0.523191496056
O	-2.175988856230	2.674926529651	-0.159436141779
TV	6.317259072087	-0.000000000007	0.000000000033
TV	-3.325889399187	6.749067913270	0.000000000042
TV	2.450545273184	1.748848135551	6.350757112892

# EQ-CO ₂ 137			
C	1.657996287571	1.971573939444	3.008047687330
C	0.175478302787	-1.265042188465	0.705629927939
C	-5.829442091779	4.303168315737	-1.509641149504
C	-0.015205049529	5.368708079744	2.970354434435
C	-1.528720253561	2.199741224671	0.677702915368
C	-7.486851541032	7.717293720467	-1.501750127340
O	0.958871242342	-1.662915974207	1.496911043042
O	-5.627424676943	3.574852078810	-0.599801694077
O	-0.605252392627	-0.864876145041	-0.087682164099
O	-1.213715140978	0.965798531031	-2.253543007933
O	-2.899308667892	4.367398692947	-2.302328037895
O	-6.048812161655	5.021380530090	-2.426369025247
O	2.175185279511	1.405787901508	2.106186839332
O	-7.707812783931	8.424053240214	-2.427166496311
O	0.511384692975	4.798204082164	2.076750325060
O	-0.732086166932	1.710163249095	1.402080794870
O	-7.283470111365	6.999374540367	-0.583693871899
O	-2.323313970961	2.693468246307	-0.048549522266
TV	6.324228049505	-0.000000000007	0.000000000034
TV	-3.333498930396	6.824173091822	0.000000000046
TV	2.367315458852	1.571817654196	6.172089203655

# EQ-CO ₂ 138			
C	-0.812130773221	0.520421153202	-0.978201237884
C	-2.135907409063	3.619874295589	2.043154588813
C	-0.057803847447	0.597115758806	2.273618868195
C	-1.071565050282	3.716676419354	5.275161299760
C	1.026823080819	0.690170653048	5.447658424968
C	-0.118602935309	3.793070643535	8.515472887672
O	-1.744014378402	-0.133681861609	-1.298941472631
O	-1.017355816195	-0.070304991409	2.092432858356

O	0.546955450838	-1.930044851083	-0.475988602996
O	1.349689542964	-1.877391697494	2.784331782749
O	-0.397304391898	3.090187066893	4.530214286755
O	1.975823596855	1.353063938072	5.689149949554
O	-1.441178100102	3.011862447447	1.300841458057
O	0.076697880696	0.028980887458	5.202991426185
O	0.899678279151	1.266306114057	2.453145118824
O	2.433264468599	-1.762309994098	6.019668789701
O	0.566609570101	3.168832159934	7.778196349126
O	2.947871407622	1.416050642082	9.072325846557
TV	4.567385629080	0.000000000000	-0.000000000001
TV	0.387030565713	6.104105314455	0.000000000001
TV	2.827721719550	0.242406197513	9.726817451589

EQ-CO₂ 139

C	-1.022562980192	0.627566013783	-1.203497492848
C	-2.121543100159	4.036866197770	2.019638434362
C	-0.012264172994	1.002774834406	2.020421646278
C	-1.111443653749	4.412313315957	5.243667392879
C	0.998096743605	1.378093761529	5.244393959779
C	-0.101018989493	4.787714894017	8.467627507975
O	-1.945596437892	-0.076098718821	-1.432851557785
O	-0.935253748153	0.299058808331	1.791068374151
O	0.404887031638	-1.785135338852	-0.470961126100
O	1.415241492791	-1.409902458262	2.753092232047
O	-0.426997258009	3.783765595843	4.509828742894
O	1.921330570848	2.081383929006	5.473591698464
O	-1.437142357693	3.408368486622	1.285695819895
O	0.075081057231	0.674439875478	5.014948243417
O	0.910895106599	1.706174058390	2.249579391683
O	2.425341951152	-1.034485856861	5.977134091424
O	0.583263227480	4.159071519867	7.733700332647
O	2.931652281722	2.457135967632	8.697724626732
TV	4.640363711435	-0.000000000000	-0.000000000001
TV	0.419351583756	6.075852634234	0.000000000001
TV	3.031022319311	1.126218106632	9.672052698571

EQ-CO₂ 140

C	-0.924120139632	0.696749791304	-0.994125394815
C	-2.141925061773	3.864097936344	1.918759002333
C	-0.091732753411	0.768292747512	2.318988703271
C	-1.309524434067	3.935685553519	5.231876386902
C	0.740547450539	0.839932208965	5.632020384132
C	-0.477155522169	4.007246568769	8.544918147269
O	-1.824634318149	0.007805307371	-1.331903538803
O	-0.992289271463	0.079409260899	1.981199331700
O	0.372361485189	-1.896284654551	-0.649019586937
O	1.204671157141	-1.824852841032	2.664038220427
O	-0.636932184676	3.309965467555	4.484168589353
O	1.639992416875	1.530008859389	5.970234206402
O	-1.469258807711	3.238458593871	1.171054041383
O	-0.159971379679	0.151007482624	5.294220340590
O	0.807716577891	1.458381287106	2.657177225182
O	2.037119378575	-1.753165288940	5.977128077012
O	0.195407727651	3.381489100938	7.797220378372
O	2.472422178432	1.601564737974	9.283254743488
TV	4.305051591364	0.000000000000	-0.000000000001

TV	0.283885122745	6.313292168491	0.000000000001
TV	2.497127175206	0.214674236005	9.939192231331

EQ-CO₂ 141

C	-1.293012837988	-1.008343623647	0.493963494521
C	0.288223886970	1.424278687864	2.199229226562
C	-3.346091652572	-1.104484244187	3.893092200736
C	-1.813591306980	1.332467181454	5.598917353336
C	-5.542422843596	-1.196553110748	7.373746399976
C	-4.017037174988	1.234682747360	9.150591909054
O	1.408370398762	-3.550792862034	2.261490916320
O	-0.693545535636	-3.641503584192	5.666473014718
O	-0.108715165991	-1.014294401631	0.486493470675
O	-2.161180685474	-1.114247836974	3.888355857176
O	-4.530325550919	-1.094332207194	3.896638034800
O	-2.996080366919	1.346007707036	5.527061926323
O	-2.477767365810	-1.001804730875	0.498395332129
O	-2.896967818240	-3.740153384249	9.218567513859
O	-0.894324744541	1.438641898659	2.131873348893
O	-4.359980546713	-1.212099025196	7.447611036417
O	-6.724495505966	-1.181105453650	7.294978431073
O	-5.199291021037	1.248724341356	9.076904474238
TV	5.189989156752	0.000000000000	0.000000000008
TV	0.062723417573	4.960461163448	0.000000000011
TV	-6.405186966911	-0.279965358484	10.352768829582

EQ-CO₂ 142

C	1.754373219957	1.872064026784	3.104996632551
C	-0.085103963418	-1.103852220739	0.765024257938
C	-5.403914645419	4.419082314394	-1.572262746438
C	0.467820108855	5.232845053226	3.135792785556
C	-1.428497525021	2.250051163517	0.691383375087
C	-6.708716547568	7.761506610276	-1.583427626211
O	0.709590853211	-1.502945481217	1.545112356992
O	-5.385179329927	3.705142062223	-0.628669106495
O	-0.880807702450	-0.704058584686	-0.014319058889
O	-1.095959897516	0.972872541237	-2.396417380880
O	-2.409837092467	4.349814953885	-2.388695799094
O	-5.442470465839	5.120793552791	-2.526999271450
O	2.216760138516	1.335690635093	2.156709680290
O	-6.744809967982	8.459271937985	-2.541209329821
O	0.961336523549	4.680736276604	2.213160254627
O	-0.631990946228	1.844027039337	1.465238620484
O	-6.690290363564	7.052647475019	-0.636070418866
O	-2.222655392909	2.657941173743	-0.086208354936
TV	6.141727948601	-0.000000000009	-0.000000000003
TV	-2.598684104635	6.700068982523	0.000000000000
TV	2.403033912140	1.436709698939	6.457701362669

EQ-CO₂ 143

C	1.607924361624	2.042935666106	2.898537094215
C	0.093387910297	-1.100583360148	0.687193513463
C	-5.916128311672	4.065498061714	-1.357853304721
C	-0.127188429404	5.435327622918	2.897605044278
C	-1.630191016918	2.286705108105	0.693688497542
C	-7.628582577165	7.519539144930	-1.433276330299
O	0.876133542064	-1.494494086141	1.481497435750

O	-5.564329258713	3.428671543982	-0.424619504144
O	-0.684426895061	-0.699435601964	-0.110446523976
O	-1.259235801752	0.913876801019	-2.408273640881
O	-2.991774682436	4.306905253500	-2.408122003338
O	-6.292475513207	4.689416580774	-2.291682894549
O	2.213265002065	1.550975783145	2.007504480110
O	-7.938302919779	8.217671190457	-2.339361548781
O	0.476525553142	4.944784680154	2.004689685672
O	-0.848381087436	1.892153021937	1.488423902121
O	-7.339035198464	6.813346948595	-0.528427618125
O	-2.405178204045	2.689052831367	-0.106072913276
TV	6.419527087612	-0.000000000007	0.000000000035
TV	-3.450486190397	6.782265082428	0.000000000040
TV	2.270760796660	1.616945609436	6.206298098351

EQ-CO₂ 144

C	1.977849518785	1.655498821897	3.158556348197
C	-0.051528936827	-1.122056676104	0.736249906444
C	-5.150774004006	4.572870897955	-1.618311090502
C	0.868203440162	5.027125557497	3.165522628793
C	-1.221066205523	2.241076345669	0.765167510410
C	-6.273434207126	7.950698721106	-1.617459123053
O	0.782284934912	-1.537899399144	1.465120186368
O	-5.165024401315	3.906263641687	-0.641553591701
O	-0.881600461449	-0.704814278438	0.002605673555
O	-1.043715463406	0.880805413181	-2.431229035731
O	-2.164454265715	4.254878587997	-2.431428747019
O	-5.157685236017	5.228022595493	-2.606277495770
O	2.489698421859	1.134009946579	2.227739517533
O	-6.283412148773	8.616215333758	-2.598002638296
O	1.390305517109	4.502795714422	2.242357910919
O	-0.436160256528	1.823105754696	1.545085031716
O	-6.284685693926	7.274219608290	-0.647405948479
O	-2.007565271570	2.660733081233	-0.013598172957
TV	5.993869038174	-0.000000000008	-0.000000000003
TV	-2.240740026059	6.740408404369	-0.000000000000
TV	2.533910196230	1.296093714372	6.534881405125

EQ-CO₂ 145

C	0.554765358771	-0.601426931243	-0.193995531471
C	-0.790961413689	1.447189342099	2.697287088525
C	3.973153202436	-0.533982234415	-0.186988019747
C	2.567614458899	1.549330927586	2.700012211291
C	7.353390854758	-0.560966431718	-0.187024491180
C	5.987601403434	1.526568995826	2.627211811261
O	-3.460259567909	-4.055738706072	2.262327465961
O	0.051899246009	-4.034131862884	2.265266906870
O	1.177196567582	-1.474788274121	0.307360547202
O	4.476155999442	-1.484644029542	0.305408591845
O	3.468104018314	0.418402531315	-0.676112344204
O	2.991667173061	2.567683562658	3.128554581356
O	-0.075967787759	0.272047195282	-0.686681179218
O	3.438584035148	-4.008977318027	2.121877173616
O	-0.208421027284	2.381370334333	3.131908953484
O	7.741146769927	-1.558611914957	0.316143899651
O	6.959240739583	0.436978120155	-0.685339520076
O	6.443931617890	2.497008677996	3.128517596783

TV	10.274195131911	0.000000000030	0.000000000054
TV	2.086135441812	4.568946258054	-0.000000000041
TV	-3.748533225699	-0.321928253974	5.883587960989

EQ-CO₂ 146

C	1.949618853408	1.483991028666	3.129376886040
C	-0.111201860139	-1.378621927671	0.730978822815
C	-5.426515282836	4.421782544051	-1.597228656887
C	0.728035359019	4.836681027499	3.129139520174
C	-1.332398884780	1.973345935144	0.730985913335
C	-6.646508379769	7.772109262745	-1.597067744398
O	0.745007026481	-1.761813933777	1.451828518332
O	-5.530955544141	3.704255822099	-0.663476263229
O	-0.969804053193	-0.995971568463	0.011973506015
O	-1.039306205949	0.913773651572	-2.331868655241
O	-2.260386479872	4.265725691999	-2.331432758595
O	-5.342378852032	5.128419837535	-2.544728640306
O	2.408075097139	0.926668681642	2.191715077910
O	-6.562443856733	8.479041633668	-2.544338845479
O	1.186142443838	4.280016730969	2.190920775478
O	-0.476055565526	1.590271653187	1.451723387687
O	-6.751222611247	7.054724377763	-0.663213856164
O	-2.191189279954	2.356162907262	0.012323503363
TV	6.158453600229	-0.000000000016	0.000000000076
TV	-2.442686899013	6.704720866915	0.000000000153
TV	2.559355252466	1.130691432967	6.412916429981

EQ-CO₂ 147

C	6.470849734329	-1.279592396859	0.733740903602
C	0.398834457446	-1.507501940625	-1.079610434154
C	-2.302298260159	-2.181013192415	1.740390561017
C	8.000674551043	-2.450228304756	3.699985520819
C	1.928693423898	-2.678158658566	1.886645546150
C	-0.772456729945	-3.351673356339	4.706654326389
O	-2.318004552852	-2.929489524267	0.823826290840
O	5.333281317084	-1.499619252754	0.487930121223
O	-0.739406779933	-1.713631308103	-1.331046043655
O	1.538441952759	-1.305865571545	-0.828908759497
O	3.068301458129	-2.476525905466	2.137344277522
O	7.608020741954	-1.058457460679	0.980056734979
O	-2.298361229235	-1.427057176321	2.653599150265
O	9.137850334717	-2.229139549254	3.946309959612
O	-0.768520768994	-2.597711142965	5.619856581783
O	-0.788155250438	-4.100143385056	3.790087856837
O	6.863100154170	-2.670232878936	3.454169951107
O	0.790446155180	-2.884280645663	1.635214123846
TV	14.027447245667	-0.000000000002	0.000000000014
TV	1.499987735474	3.275229976820	-0.000000000004
TV	3.059698022787	-2.341342747558	5.932503482102

EQ-CO₂ 148

C	1.802284790764	2.033236008536	2.439225679679
C	-1.758742777162	0.587857095068	1.123408972729
C	-4.747741703452	3.434476569661	-1.362127710092
C	2.263993274450	5.515906582651	2.497097565900
C	-1.510176012204	4.286814398455	0.911724520145
C	-4.196400377967	6.972303679626	-1.335640550434

O	-1.360655098052	-0.132997577660	1.976369935005
O	0.258553151724	-0.509257186654	-0.750886741370
O	-2.184162679617	1.305574420557	0.284867128193
O	-1.280363098992	1.308692641461	-2.737360403445
O	-0.995840308297	5.082866484340	-2.739783999053
O	-3.713093807424	3.784624045719	-1.815915753843
O	1.137866847649	1.636879939921	1.541868429907
O	-3.321763619376	7.513310165665	-1.921070812581
O	1.789209422460	4.830727069609	1.656045841614
O	-1.181771811600	3.590664676107	1.812107157625
O	0.425865405474	3.082174032176	-0.907714529942
O	-1.862794328415	4.995880272871	0.030924140459
TV	6.208907669770	-0.000000000004	-0.000000000004
TV	0.879137048705	6.938941017553	0.000000000008
TV	3.767828860494	1.116066021231	6.059646601473

EQ-CO₂ 149

C	-1.834942951439	-0.470653387913	0.538489392912
C	1.936919071304	2.031746066735	2.031868784986
C	0.563036633788	-0.438910381473	3.784267631323
C	4.338029738359	2.070300078708	5.285849559322
C	3.081064704563	-0.410338779224	7.108428553820
C	6.811053486001	2.101095413119	8.727837245228
O	0.720277786403	-2.959819458494	2.028879777120
O	3.121102063287	-2.921809223846	5.280631541773
O	-0.652974885275	-0.440275258749	0.605958668975
O	1.745338026201	-0.411243921751	3.852288954759
O	-0.619060330096	-0.470811434969	3.716619684946
O	3.153653154282	2.030113565138	5.285566350557
O	-3.017111453291	-0.502757590607	0.469870116819
O	5.592422090217	-2.906529208127	8.799257611136
O	0.753258280656	1.992251934404	2.030602485015
O	4.266024002342	-0.389098480025	7.103486064883
O	1.896718398576	-0.434773427031	7.111346701117
O	5.628750609319	2.078714128978	8.656172451567
TV	5.206613496167	-0.000000000000	0.000000000001
TV	2.400694702758	5.033676463166	-0.000000000002
TV	7.298751801253	0.101146739756	9.887067317974

EQ-CO₂ 150

C	-1.192522956230	-1.079801096041	0.343475704846
C	0.266954193265	1.316211033705	2.207985116292
C	-3.611443316323	-1.164750710261	3.943516345365
C	-2.070073729917	1.238593657038	5.659784944461
C	-5.948505598864	-1.242162809465	7.388526807762
C	-4.408556703671	1.162092639802	9.104476039948
O	1.329118021718	-3.568686857678	2.287883851702
O	-1.007782753304	-3.643816152821	5.734275320943
O	-0.008093783484	-1.107638949343	0.349092142141
O	-2.426665959540	-1.197553559414	3.942392015681
O	-4.796018402639	-1.134066003457	3.940084455043
O	-3.252315674410	1.250877033604	5.586715445949
O	-2.377087166124	-1.052808995692	0.333553073984
O	-3.346143163886	-3.720333797626	9.181278377599
O	-0.915108246188	1.331105431161	2.129884535994
O	-4.763652267422	-1.274864665921	7.387215719019
O	-7.132913573331	-1.211340704297	7.385957124118

O	-5.590584594016	1.174222575124	9.030093273925
TV	5.246532135507	-0.000000000000	0.000000000008
TV	0.119907070247	4.870756215707	0.000000000011
TV	-7.121462058619	-0.236556261648	10.498177408606

EQ-CO₂ 151

C	1.853383606084	1.547459683822	1.731672610860
C	-1.941718220718	0.604490387702	0.474172499844
C	-3.763078336195	3.056447743909	-0.898483498625
C	3.015863564495	0.970327785137	5.676541071886
C	-0.755907192247	0.081637320455	4.367193944137
C	-2.620351583851	2.455876684702	3.037528419322
O	-2.535369888159	0.001292626870	1.304288377481
O	-3.254423413012	3.691169278026	-1.759767015395
O	-1.349376572616	1.213906522871	-0.348918063680
O	1.169178158478	2.792345367219	-1.373096490553
O	2.344247667981	2.216700532173	2.574476576872
O	-4.272793925445	2.419222306230	-0.041691291113
O	1.362627243198	0.879428029468	0.889186648993
O	-3.112766088941	1.825856052829	3.910133260079
O	2.520441820308	0.293097293864	4.843429272956
O	-1.300993783105	-0.488935253941	5.250817014832
O	-2.126426033763	3.080736891060	2.160775840291
O	-0.210977610302	0.658113793007	3.489149753323
TV	8.173946331338	0.000000000000	0.000000000000
TV	2.972924660228	4.323515027257	-0.000000000001
TV	2.342819935201	-1.142713508912	7.880827455000

EQ-CO₂ 152

C	0.047485497044	-1.371416635770	0.516393141085
C	1.708650968441	1.774862311877	2.084509070025
C	-1.617926163254	-0.712092838865	3.561741354590
C	0.963831385221	2.614307275318	5.126403867803
C	-0.752630203849	0.191618378296	6.620708850821
C	0.193371153759	3.427693968524	8.180627535612
O	-1.649787355540	-3.506647602151	2.670283183519
O	-2.404260303553	-2.736862920263	5.770355210440
O	1.192793338320	-1.637388692448	0.375854476774
O	-0.457713024508	-0.668275331670	3.784039116000
O	-2.781676172159	-0.753181733127	3.342894962940
O	0.035021924352	2.259821007787	4.481322270446
O	-1.097127982421	-1.107355162044	0.657189873690
O	-3.178474425538	-1.845531516771	8.776383951525
O	0.775053575821	1.347213335634	1.496577291910
O	0.420235700088	0.211193785286	6.785737217485
O	-1.923059754661	0.171092111553	6.456674078230
O	-0.739073032844	2.997142572637	7.587591461883
TV	5.025438000688	0.000000000103	0.000000000002
TV	4.297686929506	5.706039006370	0.000000000011
TV	-2.230367997474	2.224620809287	9.136888977491

EQ-CO₂ 153

C	1.369282255391	2.196851844542	1.216079524186
C	-2.178394107849	0.515403337758	1.145664139236
C	-3.706763804833	2.434693706945	-2.167204966757
C	1.656461467772	5.489819819425	1.075764685102
C	-1.880021160849	3.841572835412	1.144795754902

C	-3.402790618796	5.753702249521	-2.167524080645
O	-1.821288963535	0.013045280341	2.155633429470
O	-3.236846123783	-1.468299753194	-2.834794118733
O	-2.537207648609	1.017204191910	0.136688734483
O	0.433879792242	1.750274594248	0.644358401925
O	0.736306050573	5.018381451197	0.498714869665
O	-4.491898832411	3.008390637491	-1.490983989305
O	2.302350439369	2.643013205627	1.793602482198
O	-4.183115285611	6.341059104345	-1.497782849818
O	2.576327435832	5.959390543884	1.654025624042
O	-1.528902275171	3.357978646837	2.165423644521
O	-2.923256235690	1.856893421854	-2.841234708995
O	-2.234951051275	4.326029920267	0.126083483046
TV	6.794791537916	-0.000000000008	0.000000000004
TV	0.612859701760	6.630679361204	0.000000000025
TV	3.636269015861	2.809434813223	6.630294028537

EQ-CO₂ 154

C	1.030331163139	2.419531542766	3.161962301294
C	-1.426784796059	0.527626863549	0.868885113086
C	-4.738912041915	2.380720323383	-1.556436435832
C	-0.328994399257	5.453823424683	3.167048786676
C	-2.779259124745	3.565782566817	0.879239865368
C	-6.150102289500	5.403589065160	-1.555670501369
O	-1.571885648187	-0.107366982204	1.857429963219
O	-3.443309287128	-0.114633668474	-2.604841935068
O	-1.287686045920	1.160289370566	-0.123295640967
O	-0.478565885632	0.907981534262	-2.951650580900
O	-1.838913890582	3.943008600056	-2.946905117479
O	-4.653069216779	1.839532164091	-0.505861287936
O	0.789368163386	1.716579484805	2.241186472826
O	-6.134738051344	4.860034812272	-0.503020028934
O	-0.569530949345	4.750057221875	2.247110945489
O	-2.921863141727	2.926140662583	1.864915079860
O	-4.812850998682	2.926900217058	-2.604158403708
O	-2.643833624283	4.202197782873	-0.110880659236
TV	6.473284280340	-0.000000000010	-0.000000000002
TV	-2.714460421173	6.067246850624	0.000000000001
TV	1.750316057145	2.214883949042	7.034155308949

EQ-CO₂ 155

C	-2.623838034851	-0.403746725973	0.544057944706
C	1.578978604456	1.309397126736	2.101854220138
C	-2.714488575238	2.938022067497	0.538474032051
C	1.501797161639	4.637305672093	2.093364306266
C	-2.793445559072	6.279974420741	0.541106564975
C	1.495802995635	7.982078744384	2.149201368402
O	2.700082079295	-1.495108679442	2.605330901929
O	2.557438732442	1.851040156670	2.491565175588
O	-1.615904327617	-0.900426074556	0.918223139611
O	-1.708846186027	2.442615580716	0.920263322004
O	-3.717840357119	3.434803102577	0.151936011024
O	0.514337460265	4.114804531440	1.700968469890
O	-3.630285237705	0.092518610405	0.165454242583
O	2.487785265859	5.159220616418	2.489927333960
O	0.599337362681	0.768530853969	1.715245643398
O	-1.784480091596	5.789713367450	0.920776237722

O	-3.800466171638	6.771656049034	0.157080849898
O	0.534845854650	7.458310532100	1.697464868852
TV	7.224534176308	-0.000000000000	0.000000000001
TV	-0.246762795076	10.004232918715	-0.000000000003
TV	1.566995986533	-1.635602843997	3.709171716479

EQ-CO₂ 156

C	1.398170975299	-1.623860568996	-1.161044234361
C	-0.545787356620	-4.132626916127	-1.535242377927
C	2.907319003250	0.542641667112	-3.080768125405
C	2.570607792957	-1.463389489483	3.493041672901
C	0.747545734372	-3.791282018024	2.167961147956
C	3.864044798544	0.359102443039	1.088761578156
O	-0.154110997110	-3.785882721533	-2.598086647646
O	0.598604345346	2.282739149107	-0.467230256677
O	0.382258757950	-1.110995795848	-0.841584145841
O	1.969133245898	0.082529789899	-3.637781826782
O	2.836645005202	0.252464208792	0.504298229547
O	2.407494525948	-2.142559113192	-1.495142367002
O	-1.076223443392	1.006898721356	-2.497050853829
O	3.525209293904	-2.073367188490	3.146570262076
O	-0.025989626781	0.473054711830	1.690854121899
O	1.124549275229	-3.049817118026	1.323928446272
O	1.901156295094	2.231135150138	3.014786567575
O	1.611329245671	-0.859240727549	3.826543460526
TV	4.900254316167	0.000000000030	0.000000000007
TV	1.506607089176	6.766627138303	-0.000000000002
TV	2.127137255259	0.624637482818	8.285547845074

EQ-CO₂ 157

C	6.141851354842	-1.392702209512	0.838959553749
C	1.784544870203	-2.249614788964	-1.819370297702
C	-4.306090154336	-0.902269436456	2.534184418828
C	6.103923201063	-1.880825862879	4.203525424236
C	1.745610340511	-2.734098096279	1.544180004476
C	-4.284649364134	-1.239262209267	5.890571513455
O	-3.250472695792	-0.753454075210	2.017247686875
O	5.155850000559	-1.599967256866	0.216925686049
O	0.798999114508	-2.458767125778	-2.441376911542
O	2.769372722786	-2.036715521904	-1.196248910788
O	2.730506160288	-2.521239572942	2.167246354900
O	7.125386417260	-1.181758229087	1.462533144593
O	-5.361520452429	-1.053301269459	3.051075242941
O	7.088241459686	-1.671565894456	4.826663489184
O	-5.344679392525	-1.392338198679	6.396734941247
O	-3.224369476359	-1.087694301678	5.383382772277
O	5.117418630736	-2.085799652180	3.581400169909
O	0.759994204377	-2.943317733081	0.922339456454
TV	14.899438622599	0.000000000453	-0.000000000144
TV	1.633356190261	3.139771828996	0.000000000064
TV	-0.079373727220	-0.970306943722	6.725275002947

EQ-CO₂ 158

C	-0.017129056194	-0.939789849477	0.474699895334
C	-0.344054091342	1.867186033258	2.076414595970
C	-1.784622132884	-0.684729996630	3.668638239470
C	-1.966746523689	2.120195571601	5.265938586633

C	-3.395002444947	-0.437228490183	6.862391581443
C	-3.739325492857	2.373172011638	8.458692793111
O	-0.325510800516	-3.793295700936	1.923205404194
O	-1.949691084650	-3.546533344683	5.108887190977
O	1.120671328435	-1.232616171747	0.327493289826
O	-0.650234879477	-0.987817151410	3.513446767120
O	-2.918720563841	-0.382076719371	3.827028569133
O	-3.101068285236	2.423527421881	5.420805885120
O	-1.155745744818	-0.650561449457	0.625374970093
O	-3.695773880534	-3.165379639931	8.304028372963
O	-1.480773321051	2.163414735545	2.229716175412
O	-2.257570024306	-0.731817488896	6.708975316372
O	-4.530253432384	-0.138810300612	7.015578202202
O	-4.900035269218	2.548432720915	8.611902911221
TV	5.095443588643	-0.000000000000	-0.000000000005
TV	1.117429611796	5.364263892028	-0.000000000004
TV	-5.309667944667	0.753303561753	9.577341827202

EQ-CO₂ 159

C	1.987232710371	2.022493206930	-1.426816406378
C	-3.940379359205	-2.334876063538	4.361137421456
C	5.604555852655	2.056361652665	-1.366891537663
C	-0.354722672656	-2.336922165852	4.364243359965
C	9.183527152391	2.062188061315	-1.367911132622
C	3.217887974638	-2.333367126703	4.343702133827
O	-4.194597103284	-6.552742674973	3.638121539548
O	-0.608744426771	-6.553801866312	3.640104918121
O	2.632303617441	2.735738320896	-2.116841705955
O	6.211251889137	2.751283992568	-2.108548458450
O	5.001478252920	1.363527694771	-0.619982001939
O	0.268632093039	-1.627814285945	5.078232755565
O	1.344983330218	1.311118245051	-0.731888541990
O	2.968411191721	-6.557899115726	3.623835590404
O	-3.318009356596	-1.624964508358	5.075136069711
O	9.784517173951	2.760548334838	-2.110734045508
O	8.585906273268	1.366449545190	-0.619096131963
O	3.836306901605	-1.616814934041	5.053586777896
TV	10.756067009009	-0.000000000009	-0.000000000001
TV	-0.365462250378	3.514361361052	-0.000000000010
TV	-7.489562987922	-6.219474408950	9.025203957651

EQ-CO₂ 160

C	0.364010182665	0.224043714599	-0.417740137163
C	-1.286782952674	1.878166232551	2.895391218745
C	0.731726207345	3.571852121286	-0.415586564953
C	-0.915007522134	5.256394199689	2.895414289096
C	1.099008044277	6.957261212017	-0.417168669321
C	-0.532842088872	8.672428607380	2.890393295648
O	-2.690857290241	-4.267359579513	3.649066399034
O	-2.299947280146	-0.836707596565	3.639707251269
O	1.017616120460	-0.419117444513	0.330008116282
O	1.386356500161	2.931373401634	0.333794979525
O	0.080527627740	4.209514779878	-1.170936111741
O	-0.253448092290	4.621232793955	2.147628494265
O	-0.286118989825	0.865610077491	-1.171172195782
O	-1.938310432079	2.524681781727	3.643678796659
O	-0.632081664336	1.228863103370	2.153299547990

O	1.745718368755	6.301872317494	0.326701779940
O	0.455601123316	7.609536393025	-1.167292667810
O	0.120187718738	8.021951042948	2.147844345229
TV	3.595277450062	0.000000000004	0.000000000011
TV	1.117009960586	10.156077287984	-0.000000000039
TV	-5.434299867574	0.136983682947	8.938260805044

EQ-CO₂ 161

C	0.339107291908	0.171875366129	-0.403162675750
C	-1.442630579930	1.823213831255	2.888265177228
C	0.637852085391	3.561182043314	-0.415675261548
C	-1.140724276998	5.210737007306	2.885953842564
C	0.892632231970	6.966449594844	-0.330477689114
C	-0.763763162592	8.624018461727	3.034112209076
O	-2.711622234542	-4.321907469072	3.632329412706
O	-2.338228995175	-0.929613043193	3.794911108369
O	1.010772131550	-0.449085475940	0.347831817117
O	1.309200388008	2.936500453350	0.332264141424
O	-0.029509428228	4.185483868179	-1.168288738452
O	-0.477824494055	4.569681645839	2.144029718836
O	-0.327217486257	0.788381581256	-1.163659710409
O	-2.112636443976	2.448474400891	3.638019151389
O	-0.770753035871	1.195299562375	2.143345004477
O	1.594069216405	6.295649461360	0.346553300991
O	0.195385125991	7.633390375158	-1.015513969082
O	-0.094812667446	8.001048939944	2.282810114675
TV	3.601093901201	0.000000000001	0.000000000005
TV	0.910459262483	10.172307505559	-0.000000000048
TV	-5.197046518445	0.899452239864	8.903123421570

EQ-CO₂ 162

C	6.299908655151	4.203406738264	4.179929251027
C	-2.342516490016	-0.691531436452	0.210765363124
C	-4.288617399878	2.298705364338	-1.665654170303
C	7.685840339949	7.492299946621	4.193539282046
C	-1.095441368889	2.597804488439	0.203850991958
C	-3.001945335981	5.634380316475	-1.676903774814
O	-1.962605566257	-1.477054688428	1.007798805499
O	-4.065149119686	1.878676004385	-2.751297610154
O	-2.736469519174	0.092225363398	-0.587230141772
O	-2.245904248700	0.316259020093	-4.513737072647
O	-0.854569175129	3.598465181940	-4.499646969992
O	-4.518160543778	2.717254991636	-0.581879062250
O	6.959900569284	4.646953595813	5.060746544177
O	-3.279400643059	6.001888175195	-0.585341664380
O	8.344178818456	7.943362188387	5.072439291660
O	-0.715625279627	1.810098006833	0.998741157665
O	-2.727265471747	5.268656074667	-2.769918889928
O	-1.488678450508	3.383118852116	-0.593062460442
TV	6.280835420941	-0.000000000004	-0.000000000003
TV	2.494014997487	6.566434448813	0.000000000002
TV	7.893031635163	3.433930070745	7.818960325786

EQ-CO₂ 163

C	2.139485445385	-2.276473554662	-1.397668940233
C	-3.986187891062	2.322849281082	4.186725380553
C	5.613416175045	-2.312781009202	-1.389353008073

C	-0.462098559167	2.372671045465	4.040153335735
C	9.097197568890	-2.319074542031	-1.395860899281
C	2.967201494032	2.324300239294	4.186994614529
O	-0.300203504980	-1.831090023685	3.288103162511
O	3.130996127529	-1.883005911210	3.441106938366
O	2.719014470261	-2.981378340038	-2.152345933044
O	6.183604569671	-3.034921924111	-2.135165945361
O	5.042964571610	-1.594596560773	-0.641366688253
O	-1.032777016772	3.092588313846	4.787735088941
O	1.559561770219	-1.577185210376	-0.638852467100
O	6.605557224986	-1.882785379320	3.437888376746
O	-4.557388960810	3.042590980154	4.934354279186
O	9.669342444141	-3.038891578830	-2.143144064714
O	8.524971564985	-1.602391291613	-0.647427035464
O	2.393845106912	3.045436889229	4.931725188369
TV	10.429944113730	0.000000000006	0.000000000003
TV	0.406884659839	3.487181618214	-0.000000000004
TV	-2.922177022091	-2.768295288944	8.888200642084

EQ-CO₂ 164

C	2.436890655780	-0.631463461888	0.189841795998
C	-1.027914684129	0.622063678301	-0.654153604240
C	0.057059239816	-0.947085245495	2.655981634526
C	2.846953848859	2.677080980289	0.189355928037
C	-0.617623562298	3.930781152106	-0.654189668282
C	0.467343046200	2.361547894026	2.655931108717
O	0.462621610343	-0.471261724265	3.658991348293
O	2.488039360029	-0.108461465528	1.254380725419
O	0.002122377295	0.933649367454	-1.147377010878
O	-4.842499416703	-1.160290510242	-0.866312154643
O	-4.432519215723	2.148262057137	-0.866809557998
O	-0.355661415204	-1.421467648564	1.653233971333
O	-2.054223281823	0.311618498523	-0.154025235448
O	0.054575083062	1.887160153144	1.653196171432
O	-1.643929638328	3.620320146744	-0.154059644921
O	0.872894156457	2.837435846327	3.658917009768
O	2.898220760909	3.200054304141	1.253896849094
O	0.412419037325	4.242372717437	-1.147379678168
TV	7.218976085217	0.000000000000	0.000000000002
TV	0.820451647848	6.617439394473	-0.000000000004
TV	2.887250792235	0.333102942498	6.472518254490

EQ-CO₂ 165

C	0.064527190743	-0.711515520928	-0.465454698168
C	-0.676649717308	1.075152864990	3.003068108675
C	3.440457456131	-0.699567946257	-0.325472446634
C	2.689880167708	1.075378660215	3.004099431533
C	6.842614281995	-0.704033122083	-0.387435257061
C	6.065972316217	1.076266347403	3.003838629144
O	-0.088165726297	-3.149829275957	3.810857730278
O	3.280355433018	-3.148303230790	3.811358641807
O	0.582899155009	-0.025538063722	0.347564189032
O	4.025521029167	-0.030376275643	0.457493890187
O	2.858154393387	-1.365300962019	-1.113175273567
O	2.146590592203	1.755981721414	2.202459838928
O	-0.451496091375	-1.392692883917	-1.284227761286
O	6.649257771888	-3.150026625575	3.813511579983

O	-1.218067131611	1.757558778001	2.202237309136
O	7.475894262836	-0.024398436619	0.346699271384
O	6.213584015844	-1.379673517364	-1.127883823352
O	5.529434687408	1.758639460434	2.199344575610
TV	10.108372087789	-0.000000000000	-0.000000000000
TV	-0.048335185944	3.548787076951	-0.000000000003
TV	-5.395865570615	0.905289635152	10.146508743047

EQ-CO₂ 166

C	-0.047002336773	-0.471200195906	-0.340263935787
C	-0.901369570972	1.234735974028	3.053913346676
C	-0.397452683073	2.849535866961	-0.260216735193
C	-1.167627134833	4.730954691484	2.971954289599
C	-0.740665313701	6.235046532287	-0.497460857775
C	-1.549563569076	8.048673755566	2.974424503730
O	0.078009656374	-2.658166329896	3.813364710104
O	-0.223982975131	0.638962458713	3.820311483850
O	0.571508150442	0.106814623735	0.488915512670
O	0.250483102001	3.499716739322	0.488015310976
O	-1.042394018186	2.198661102356	-1.010209114556
O	-1.808385705148	5.280376727899	2.141041608271
O	-0.664474159007	-1.044331610223	-1.171290198918
O	-0.531503358900	4.186930454124	3.808829486481
O	-1.582654418818	1.832936878639	2.293576308207
O	-0.066646228613	6.945735180966	0.168356649317
O	-1.410032666522	5.524657796483	-1.168879932918
O	-2.234173444001	8.533436322829	2.139176810048
TV	3.578832043994	0.000000000021	-0.000000000040
TV	-0.948646674165	10.219063485682	-0.000000000143
TV	-6.150164846898	1.171820208701	9.935891638666

EQ-CO₂ 167

C	1.596347779199	-0.071775793588	-1.986350820674
C	-3.003177451381	-1.184234415120	4.831288002774
C	1.699150470136	3.488666084453	-1.912792608919
C	-2.890083707572	2.341536740875	4.831831304902
C	1.831242179186	7.002608635041	-1.913550468619
C	-2.776210844160	5.868622412868	4.830333477672
O	-2.326204752519	-1.828951399810	5.558217584574
O	-2.213511481648	1.695886111789	5.558269775083
O	0.927593883145	-0.713591453370	-1.250311456298
O	1.035898955108	2.911310137746	-1.119344384870
O	2.364206687366	4.070395605858	-2.701804419025
O	-3.562730129351	2.981458813934	4.097132586713
O	2.268740647388	0.571082854823	-2.718920915223
O	-2.098748054196	5.224831740831	5.557961981494
O	-3.676340926692	-0.545462135233	4.096230564850
O	1.166400915960	6.434109326267	-1.115026160645
O	2.498500214096	7.575289459147	-2.706774976490
O	-3.450259490424	6.506842121635	4.095833982245
TV	3.552245067089	-0.000000000003	0.000000000001
TV	0.338405993420	10.580385360483	-0.000000000039
TV	-6.481738043508	-4.013128065723	10.125983285030

EQ-CO₂ 168

C	-1.744894527437	-0.493558342327	0.080975510882
C	1.529954790626	1.414333176173	2.208680499662

C	-0.561717754036	2.752935284622	0.081015669113
C	2.712886587920	4.660854847524	2.208710013512
C	0.619254562480	5.999064308541	0.081262666381
C	3.896096603214	7.907222995055	2.208775605016
O	1.485722382131	-1.613145628650	1.970441300689
O	2.669060217536	1.633300703327	1.970351688627
O	-0.604321477076	-0.273187687997	-0.155230085587
O	0.578854743872	2.973344224894	-0.155164910449
O	-1.701118671338	2.532970274958	0.317375018556
O	1.572356934498	4.442932280148	2.446884115372
O	-2.884294355314	-0.713490032747	0.317371973151
O	3.852003543536	4.879774943634	1.970406156659
O	0.389421270047	1.196399226684	2.446851998852
O	1.759696466561	6.219153721369	-0.155348456345
O	-0.520106105350	5.779405920136	0.317848726092
O	2.755553684880	7.689337261175	2.446918122170
TV	6.484850052032	-0.000000000008	0.000000000002
TV	3.549483339977	9.739355193737	0.000000000036
TV	-0.901233384074	2.582710933962	4.585657209127

EQ-CO₂ 169

C	4.044117493758	-1.781961721366	-2.274963064161
C	-4.088862116726	1.256944603236	4.550817248644
C	4.393836417876	1.598609147350	-2.349997669722
C	-3.885806658197	4.706331038985	4.634437169364
C	4.903747084874	4.864503558330	-2.035338224841
C	-2.905301518232	7.953824184037	4.614442497974
O	-4.729700296165	0.678393791695	3.739577779966
O	-4.542769749339	4.266790907819	3.752265328105
O	4.676239869114	-2.355550730017	-1.454929736557
O	5.047346703222	0.944323430058	-1.610723088602
O	3.738286972558	2.256335287379	-3.085288569907
O	-3.229010958584	5.150360805958	5.514057887560
O	3.408299260281	-1.204471546776	-3.091431711117
O	-3.555382361257	7.521594295927	3.724115753139
O	-3.442925870252	1.835986738028	5.357193695310
O	5.542985962402	4.190473272892	-1.299884847461
O	4.260254677684	5.537989681620	-2.765812356978
O	-2.252532906301	8.384064420909	5.503883084601
TV	3.544618959134	-0.000000000001	0.000000000007
TV	1.439341110159	10.044519992898	-0.000000000062
TV	-5.308625960017	1.279326074509	10.373969564835

EQ-CO₂ 170

C	-1.249713871847	-1.112039131680	1.069375236097
C	0.870186428216	1.784167462575	1.797577790417
C	-3.445394384714	-2.695918469365	4.491343824072
C	-1.302871155942	0.179138833297	5.307098937625
C	-5.585366411619	-4.344000588543	8.077705659561
C	-3.513025849678	-1.445547314910	8.813447662295
O	1.423154118208	-3.911709818099	1.798424022738
O	-0.750124306491	-5.550483745240	5.388660895211
O	-0.068329615682	-1.169541999756	0.990251269966
O	-2.263802792163	-2.751430361734	4.413602455762
O	-4.626186122226	-2.643535980015	4.568553311508
O	-2.484427058656	0.129635082082	5.222521561868
O	-2.430689766925	-1.061292869178	1.144158396523

O	-2.959399930664	-7.140251827841	8.814376538852
O	-0.312374331187	1.703324848562	1.795849797444
O	-4.403273819032	-4.400970052052	7.998974638601
O	-6.765544579835	-4.290408172607	8.157416267774
O	-4.695679450742	-1.526136649455	8.810493354989
TV	5.171807056192	-0.000000000001	0.000000000008
TV	0.627752044966	5.779135242337	0.000000000005
TV	-6.681925849752	-4.803311899509	10.438889060211

EQ-CO₂ 171

C	1.469910161285	2.387108907845	3.156290079508
C	-1.369340393364	0.902656518793	0.904521945741
C	-4.092148285520	1.856071903637	-1.637195733788
C	-0.776511208341	6.745902073860	3.156412433188
C	-3.615773589887	5.261426748844	0.904538928311
C	-6.338334893634	6.214946149272	-1.637089404610
O	-0.940389311848	1.188462818226	1.970214545842
O	-3.488355602216	1.746845953682	-2.651075320977
O	-1.799116830596	0.624890528027	-0.163505881966
O	-0.638913159514	0.390262297319	-2.766828858511
O	-2.885339951191	4.748999506530	-2.766745541157
O	-4.698868838495	1.968613978122	-0.625766645135
O	1.232110905976	3.036274660138	2.196377782077
O	-6.945075210185	6.327442031895	-0.625668532113
O	-1.014284533208	7.395058440295	2.196482283125
O	-3.186846429454	5.547233530216	1.970235669717
O	-5.734629462933	6.105667781083	-2.651014781025
O	-4.045542676795	4.983651811725	-0.163487211233
TV	5.978979523901	-0.000000000002	-0.000000000003
TV	-4.492794160391	8.717575763928	0.000000000032
TV	2.365908903397	1.350209227797	6.881357864276

EQ-CO₂ 172

C	3.047013987593	-1.493119731726	-2.243425896710
C	-3.735302268071	0.984042608932	4.693195895886
C	7.031275066531	-1.498518211719	-2.386295354152
C	0.169046715733	0.983033488402	4.689219400607
C	10.980640708005	-1.559341117322	-2.309589478523
C	4.246965817161	0.981236580332	4.695087568021
O	-4.503646657716	0.938276101439	3.794460043260
O	-0.604520803993	0.937905179140	3.795150404494
O	3.788810654360	-1.470751141593	-3.167383445644
O	7.770358555201	-1.476653613425	-3.312835146501
O	6.299494111443	-1.519741673150	-1.456404154200
O	0.950483485884	1.027179074029	5.578513389087
O	2.317724707230	-1.514555666487	-1.310976548341
O	3.476696597794	0.938863891800	3.798621845065
O	-2.960789445935	1.028730258844	5.588378615458
O	11.786754672144	-1.462947432499	-3.172684076191
O	10.184372999928	-1.655951685152	-1.439241389312
O	5.024257620584	1.022426121468	5.588629503549
TV	11.892086726470	0.000000000003	0.000000000014
TV	0.033378157705	4.153942974089	-0.000000000016
TV	-4.789541173383	0.437555670492	9.573644202383

EQ-CO₂ 173

C	0.827519585964	1.568784457937	2.528325856791
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C	-1.211437031575	0.624421330008	1.521379037982
C	-3.845452708271	2.857866750467	-1.568458980055
C	4.907446808677	1.568613905885	2.528269942453
C	2.868316624647	0.624397552419	1.521517118275
C	0.234316115081	2.857935638624	-1.568292928738
O	0.175140934299	0.726193837534	1.671351489313
O	-3.300370367038	3.702974068108	-2.191138577798
O	-1.642205953153	-0.113965683418	0.676713548275
O	-1.429044915049	2.143368794590	-3.778018120557
O	2.650871768633	2.143238639478	-3.778077432603
O	-4.392840828996	2.014309505603	-0.944679094049
O	2.218702784358	1.407898299184	2.435713351426
O	-0.313188816594	2.014370109225	-0.944631473678
O	6.298626278833	1.407622731332	2.435790379053
O	4.254952929473	0.726141411150	1.671361468555
O	0.779396281593	3.703038075586	-2.190986222783
O	2.437563362255	-0.114178906776	0.676999508563
TV	8.159658078083	-0.000000000002	0.000000000000
TV	-0.751842311907	3.785754966482	-0.000000000000
TV	1.836426850965	0.244408599595	7.079407167060

EQ-CO₂ 174

C	0.522156700394	1.845641193098	-0.185251058451
C	-1.347012945924	0.093582712084	1.951797381453
C	-3.115857175268	0.932231733516	-1.652247592872
C	0.596626656402	6.359231282642	-0.204415221368
C	-1.238821550498	4.601330621932	1.952028318435
C	-2.978578439603	5.436491939741	-1.627931129704
O	-0.557972311031	0.060488328464	2.831113178371
O	-2.593787744961	0.371148782798	-2.562114914562
O	-2.136136162437	0.127741988712	1.072607481775
O	0.222066318671	0.643226788810	-0.867835373838
O	0.337735087724	5.142042212928	-0.877343138119
O	-2.815878995772	2.134834533173	-0.969653641254
O	-0.000228319615	2.406871859248	0.724341276506
O	-2.719979120873	6.654159611365	-0.955618193504
O	0.034011827028	6.925095281707	0.677779773910
O	-0.452127929425	4.576167400486	2.833833561007
O	-2.414758322695	4.869062971042	-2.508247936946
O	-2.025513662832	4.627277341355	1.070296099564
TV	4.470623191002	-0.000000000004	-0.000000000005
TV	0.216369874590	9.017967973069	-0.000000000001
TV	4.586054560275	6.426417530448	5.740715685508

EQ-CO₂ 175

C	0.914891117020	3.142025489129	3.470680252415
C	-0.478237295833	1.099319706606	0.136608472737
C	-2.554749316627	1.125080343575	-0.916231028975
C	5.012376025441	3.149954126288	3.481441113244
C	3.586412192142	1.115700430842	0.220057221422
C	1.579111618962	1.104912176761	-0.964952149041
O	-0.787453930170	0.309016221098	0.987554013013
O	-2.915667076898	0.402331138682	-1.806306726093
O	-1.249998390206	1.651534051060	-0.836736952078
O	-0.799743066945	-1.329825895989	-3.608988621096
O	3.143964415017	-1.358106028246	-3.726255214826
O	-3.267944495515	1.607134468695	0.142546502024

O	1.534711066625	2.421163524541	2.764658918239
O	0.816031743005	1.645570156584	0.021493667575
O	5.786751353022	2.467110411955	2.901621276592
O	3.214822500032	0.390595574033	1.103802382860
O	1.262328871656	0.344518795365	-1.840172370972
O	2.883293797843	1.629586824058	-0.827681886693
TV	8.175860147262	-0.000000000014	-0.000000000008
TV	0.136565216093	3.627316903821	-0.000000000001
TV	1.096485517181	5.190366202972	7.791867461529

EQ-CO₂ 176

C	0.220991754585	1.801898971943	2.481760911251
C	-1.819188655833	0.795441978259	1.537226602919
C	-3.227543390274	2.916937112416	-1.491707486283
C	4.294840579385	1.783493888374	2.508917979835
C	2.259371419950	0.856821986889	1.469646583891
C	0.858247364749	2.925093596205	-1.552781094116
O	-0.431496982214	0.955070213144	1.631534311119
O	-2.555467309125	3.607434616817	-2.179091921329
O	-2.242235961848	-0.034570792319	0.778139736233
O	-0.683167696600	1.952627121865	-3.752344888827
O	3.389555459352	1.953048991421	-3.743937287178
O	-3.894941138883	2.228632903678	-0.798004401718
O	1.605590777139	1.718694346751	2.306113372228
O	0.217038105708	2.250846330098	-0.820709558813
O	5.681143193661	1.658272860592	2.376455016792
O	3.645324430039	0.957106172587	1.636131259378
O	1.502207883245	3.599199263949	-2.282980409440
O	1.840515832540	0.072066079428	0.662327031065
TV	8.149628630443	-0.000000000002	-0.000000000002
TV	0.404072780290	3.943458700010	-0.000000000002
TV	0.478759760082	0.614029858549	7.060474507242

EQ-CO₂ 177

C	3.707876301527	-2.125932177039	-0.223040529883
C	1.946775882420	-1.339594619785	-0.061908480999
C	-2.340643571506	-1.963018041957	1.582062167089
C	4.149234995842	1.456753598408	-0.229901731030
C	2.368814014914	2.197169785929	-0.075013247024
C	-1.970553428977	1.669449597095	1.577852327935
O	-1.495869637312	-2.626263752201	1.082697083436
O	4.781734407072	-2.615335800148	-0.342382212213
O	2.493481047840	-2.297546450812	-0.943701182378
O	0.878567906271	-0.836134570159	0.053205791919
O	1.283657527971	2.661581674573	0.041217679296
O	3.158234740208	-1.172442561161	0.660881971728
O	-3.184936497969	-1.300365413226	2.081923445312
O	3.574418320379	2.399232321561	0.649981693796
O	-2.744521236361	2.404305178892	2.090761180688
O	-1.199916208073	0.933026872432	1.063431740976
O	5.232559563458	0.986278578494	-0.342081135670
O	2.945126857663	1.257509978503	-0.956667754132
TV	9.281545141121	-0.000000000001	0.000000000000
TV	0.859731239439	7.165785976532	-0.000000000000
TV	-1.072206250729	-0.396067081510	3.442947842380

EQ-CO₂ 178

C	0.709479049987	-0.313269814858	0.050841846491
C	-1.849416788582	2.130814312002	1.453878671627
C	-0.901515446504	-2.262276382600	3.575693957578
C	-3.383718220132	0.208605935645	5.049622331162
C	-2.323501923951	-4.224816176306	7.215841802145
C	-4.856370420612	-1.750909613062	8.684554437684
O	0.879290427627	-2.645803448020	1.624386205328
O	-0.654388711416	-4.581952358245	5.145963893358
O	1.652598615170	-0.070194741269	0.757510857211
O	0.036816919720	-1.933542705353	4.255251489033
O	-1.935599614399	-3.091655237350	3.921615837397
O	-4.402585606504	0.369103294186	5.950549105225
O	-0.327058970998	-1.171086307414	0.305071135331
O	-2.096073298543	-6.496759532156	8.793362765812
O	-2.930013473427	2.288315713653	2.280538782056
O	-1.331905220432	-3.964980670961	7.846478770925
O	-3.391823947939	-4.997647276767	7.597589463471
O	-5.936337398775	-1.696431962056	9.528338199021
TV	5.021568818363	0.000000000002	0.000000000001
TV	-1.765005995075	4.076514868044	-0.000000000004
TV	-4.620473154394	-6.075256037477	10.709533393352

EQ-CO₂ 179

C	0.306972584600	-1.013218981558	-0.181947693470
C	-1.168275850864	1.930953550663	1.747812168612
C	-1.118455034545	-2.661061806477	3.639233446947
C	-2.593682280158	0.283103467350	5.568952455622
C	-2.543872495885	-4.308906344205	7.460383304821
C	-4.019123084402	-1.364734685724	9.390112903282
O	-0.003196026498	-3.355313485550	1.287743848634
O	-1.428566596763	-5.003157203027	5.108871451870
O	0.763193912932	-1.182967698655	1.100303967528
O	-0.662216156084	-2.830810127456	4.921474135535
O	-2.133662725339	-3.089102778111	3.154297432630
O	-2.935667816652	0.723972684429	6.821544123255
O	-0.708216650096	-1.441279269406	-0.666906765786
O	-2.854021426896	-6.650992104514	8.930027416467
O	-1.510261176926	2.371814932768	3.000428283916
O	-2.087654443657	-4.478645417217	8.742633316610
O	-3.559061185732	-4.736969373571	6.975428822190
O	-4.361091264552	-0.923867169071	10.642707957758
TV	4.538251869200	0.000000000002	0.000000000001
TV	-1.301275212240	4.182435138772	-0.000000000004
TV	-4.276258701913	-4.943543744728	11.463516285749

EQ-CO₂ 180

C	-0.073120236433	-0.417502674521	0.403680876938
C	0.042477820353	1.640197760787	1.463922139454
C	3.721185054736	-0.414572773737	0.517960432444
C	3.790291653529	1.641873246365	1.552280022075
C	7.444805461715	-0.418080628598	0.439339091521
C	7.578468761315	1.639354111630	1.479386882895
O	-0.976718348156	-2.130473043376	2.291437535777
O	2.709473622159	-2.136339898061	2.319228825074
O	0.425139975129	-1.734553944524	0.492584552484
O	4.228669576497	-1.726636133507	0.623902416056
O	2.925606605423	-0.069045556265	-0.316369654134

O	4.316208503232	0.333453695853	1.490963540411
O	-0.879174076486	-0.066909422550	-0.418360675098
O	6.560016949352	-2.135414084652	2.308488395042
O	0.540180271693	0.323240074342	1.370896204082
O	7.955940114036	-1.730526765422	0.508207192382
O	6.603251669327	-0.069372440041	-0.346542083874
O	8.087135267193	0.327486018030	1.379783670466
TV	11.225579735512	0.000000000000	0.000000000000
TV	0.217237682052	4.117856293113	-0.000000000005
TV	-1.761317712534	-0.020643984322	4.602777536438

EQ-CO₂ 181

C	-0.450145251288	-1.336372299262	0.735733453246
C	-0.022770231104	2.090071155841	2.344112584899
C	-2.462883690568	-2.990150644892	3.943096765536
C	-2.035499071808	0.436298062233	5.551478679975
C	-4.475609942944	-4.643941375805	7.150464250769
C	-4.048228820387	-1.217508329823	8.758835603787
O	-0.616240289799	-3.866683608700	1.585799276893
O	-2.628974617338	-5.520462623925	4.793171713577
O	0.878523295682	-1.477695007706	0.497100078099
O	-1.134214869547	-3.131467127743	3.704463719063
O	-3.331192307669	-2.662371241875	3.178007176045
O	-1.935022591956	1.766326922075	5.305797413567
O	-1.318449751290	-1.008586460725	-0.029359840478
O	-4.641692040547	-7.174264668196	8.000527044200
O	0.077702632465	3.420097620506	2.098431342156
O	-3.146937411415	-4.785227397448	6.911835992059
O	-5.343921088582	-4.316171418966	6.385371301895
O	-3.947755753241	0.112517368212	8.513162865758
TV	5.136613166501	0.000000000002	0.000000000002
TV	0.774333256532	5.040158824353	-0.000000000006
TV	-6.038195451726	-4.961350758420	9.622091685208

EQ-CO₂ 182

C	0.599304896559	-1.033955203890	0.554318112776
C	-1.432225706195	-0.046190383220	1.531898613134
C	0.529361218671	2.766966334555	0.554317713186
C	-1.502164751944	3.754775800005	1.531877116960
C	0.459450952002	6.568001734536	0.554297288852
C	-1.572084787813	7.555784196726	1.531886947952
O	-1.855880725212	0.758452774082	2.320968633068
O	-1.925803157555	4.559506523194	2.320876694872
O	1.974740356595	-0.808715237518	0.599939956852
O	1.904813625906	2.992164432958	0.599977263679
O	0.105379113943	1.959410117201	-0.232048717166
O	-0.126270783508	3.532503547519	1.484521715118
O	0.175324732277	-1.841528680367	-0.232036641389
O	-1.995727311148	8.360422075420	2.320971727446
O	-0.056333255634	-0.268433052190	1.484523070622
O	1.834886218727	6.793251953956	0.599928193078
O	0.035476824044	5.760415191886	-0.232045484140
O	-0.196197425368	7.333533672597	1.484510601951
TV	4.063749244308	-0.000000000005	-0.000000000030
TV	-0.209811268212	11.402932962162	-0.000000000177
TV	-3.969049519050	0.242065205957	4.302894403968

EQ-CO₂ 183

C	-0.311146986138	0.395507337536	1.286868354206
C	1.555169344425	-3.161837109035	2.582716239969
C	0.891040641924	-2.886510310341	-0.919441013584
C	3.130591826512	0.413189680504	1.807864315717
C	5.406255526987	-3.812297723908	3.150237893714
C	4.305263802740	-2.903107071820	-0.615419999807
O	2.221519473057	0.462284379555	-0.856720347398
O	0.253681669608	-0.556168783584	0.864532512862
O	-0.709551027368	3.622929396765	-0.334485455275
O	-0.869686803520	1.343794558407	1.720019065007
O	2.629395142602	1.486822017128	1.822149146595
O	2.284949063900	-3.210700500166	1.695752071359
O	1.549198079050	-2.096961027232	-1.509286251532
O	5.331214971536	-3.091291880038	2.214287785400
O	4.721957459480	-1.796416751910	-0.637130207585
O	4.985282923236	0.943196233854	-1.250836730832
O	3.637327428889	-0.656127360428	1.819334493520
O	2.942747051239	3.286308111242	-0.615804242611
TV	6.824142392629	0.000000000000	-0.000000000027
TV	-0.941950995456	7.296997523598	0.000000000055
TV	-0.453087218152	1.824553523342	5.340364246048

EQ-CO₂ 184

C	0.539393705870	-0.440670611385	2.266368204799
C	0.943341589781	2.825554257420	5.163950151794
C	4.340498699377	-0.265876604729	2.676242312148
C	4.728328177911	1.773389143285	6.147475216324
C	7.787780686788	-0.571193675141	2.325701801956
C	8.572921406135	0.783382791589	5.515505454867
O	-1.285820118745	1.448521337881	-0.638524527006
O	2.538112315994	0.530218744760	-1.507405760013
O	-0.032097913713	2.398534206016	-0.615516353367
O	3.133548615528	2.013083705422	0.233964662262
O	3.612981489063	-1.041971394561	3.189175396163
O	5.079100239536	0.506329425574	2.164682995211
O	-0.263534888572	-1.242834208811	2.603367592293
O	7.645181112533	-0.192529825697	-1.765199516835
O	1.328280011941	0.361188055181	1.900608211688
O	5.721098914559	0.756632682812	-0.767468437729
O	7.579094665383	-1.161854729716	3.330282129170
O	7.999334667534	0.023637904086	1.325401922823
TV	10.840872422712	0.000000000005	0.000000000005
TV	-0.569109697427	3.507107908751	0.000000000001
TV	1.891768361231	0.503050731238	6.780884204015

EQ-CO₂ 185

C	0.326590392872	2.563823458747	1.225911399318
C	3.115102678589	-2.387509549326	-1.576916255005
C	0.678819860034	-0.561494260651	-3.707305497882
C	0.596257728365	6.833166296716	1.225909149531
C	3.384771938736	1.881839363754	-1.576891564664
C	0.948479902039	3.707843112485	-3.707287640663
O	-0.315858406988	-0.985804111069	0.132918834200
O	-0.561467404342	0.479023455482	0.516900347940
O	0.232941703676	-1.347558902563	2.367198408631
O	1.752081732262	0.641275094937	0.754741203152

O	2.021743259831	4.910617050883	0.754758477644
O	-3.169669195038	-1.506032490609	-0.834598207617
O	3.345806881618	-1.612716078283	2.148622081410
O	-2.900028433680	2.763305643434	-0.834571765168
O	3.615510919603	2.656641593468	2.148649035313
O	-0.046195258084	3.283535175934	0.132928604102
O	-0.291810657934	4.748354280241	0.516918348516
O	0.502640784335	2.921779156449	2.367198164858
TV	6.017145342900	-0.000000000000	0.000000000000
TV	0.539349069419	8.538681337862	-0.000000000001
TV	-0.043994631061	1.656342325875	4.468137751796

EQ-CO₂ 186

C	1.300329813020	-0.164541052900	0.776749709156
C	2.430467634059	0.877870306882	0.560093950345
C	-2.521805256995	2.761755783532	0.653455927268
C	0.422373591759	4.626138567837	0.776743300290
C	1.552519282243	5.668548598589	0.560084387629
C	-3.399174662391	7.552726798607	0.653436101928
O	3.391217508179	0.666608902762	-0.397925712200
O	-2.207022602714	1.838769099177	1.321954733878
O	-2.836151665723	3.684889518164	-0.015724200940
O	1.135855215662	-1.194288261478	0.147428120137
O	0.257898960071	3.596390033955	0.147426603362
O	3.218427851262	-0.606788980051	-1.235751268518
O	-5.346400608494	1.914844503238	1.179571237614
O	2.340486262447	4.183878490687	-1.235752581093
O	-6.224341020734	6.705533251529	1.179541197354
O	2.513276324695	5.457273375358	-0.397931123676
O	-3.084500765241	6.629669385011	1.321888745039
O	-3.713617917172	8.475852996073	-0.015710931539
TV	7.931995871366	-0.000000000003	-0.000000000002
TV	-1.755897999388	9.581323536276	-0.000000000006
TV	-1.989599784997	-4.147382035082	2.984851216716

EQ-CO₂ 187

C	-1.151360590570	1.447636901770	1.604585487312
C	-1.876148111993	0.473067739670	0.636198574568
C	-1.617253717596	3.988243754375	-0.881874622370
C	-2.400184342292	1.726990741938	5.636413869840
C	-3.124980138553	0.752384028724	4.668061956975
C	-2.866156254083	4.267912428027	3.149853600414
O	-2.816016731206	-0.247071370455	0.918727458188
O	-0.815597692690	4.485088665509	-1.595898715768
O	-1.468446935066	0.353719239692	-0.674704839114
O	-0.317505449863	1.288203418532	-1.117730723954
O	-1.566383568823	1.567536125776	2.914119572818
O	-2.418679343237	3.492567865726	-0.166509387972
O	-0.214923571590	2.173609341314	1.326028622337
O	-3.667516584708	3.772004066477	3.865137681230
O	-1.463768498484	2.452994002581	5.357849776921
O	-4.064809092927	0.032205388403	4.950638405678
O	-2.064566995627	4.764948039389	2.435888254582
O	-2.717367881030	0.633126232372	3.357109284045
TV	4.228107724832	-0.000000000001	-0.000000000002
TV	-1.531979461642	6.268713025819	0.000000000008
TV	-2.497777962135	0.558751818969	8.063638569477

EQ-CO₂ 188

C	-0.866754291667	1.463987995708	1.014235716002
C	-1.996370759377	0.459562352752	0.616421788894
C	-2.380556662020	3.605089661004	-1.024452388243
C	3.987969028745	1.334713595679	0.914991517886
C	2.774467355587	0.419108201441	0.556268631737
C	2.568215027316	3.610690116103	-1.008277507566
O	-2.927135768996	-0.151734963875	1.065038469188
O	-1.685591712581	4.074076113531	-1.858185243416
O	-1.540165398548	0.488067032219	-0.707972573692
O	-0.437806587000	1.481612412572	-0.323282430767
O	4.381510574372	1.311057238980	-0.436293310218
O	-3.070259589757	3.139153782081	-0.179551837791
O	-0.410241401488	2.069688769733	1.940372629833
O	1.879737949261	3.153428802543	-0.157657068541
O	4.510077241036	1.909178239690	1.825137452829
O	1.826224168868	-0.136294814837	1.041746911270
O	3.264518650696	4.071028949366	-1.846458532279
O	3.177556738583	0.426568928565	-0.784094030299
TV	9.561884136171	0.000000000062	0.000000000215
TV	-2.756284464513	5.318551015265	0.000000000033
TV	-1.651217443862	0.203572441865	4.693271874766

EQ-CO₂ 189

C	-0.608804152451	1.780122857890	0.782862007532
C	-1.753801186053	0.916451306735	1.370073114391
C	-1.649315479154	2.548226492232	-1.975694569600
C	-1.029266411072	5.660433438050	1.197496845788
C	-2.176911957093	4.735537796446	1.700086383602
C	-3.323741276116	7.265927301719	-2.200055330944
O	-2.681707562889	0.982556554630	2.127163141616
O	-0.738926714891	2.997116557118	-2.581864502753
O	-1.316375849541	-0.171300623017	0.599761234701
O	-0.175462669235	0.682007441966	0.023828410270
O	-1.467936026066	5.467315301154	-0.121455396826
O	-2.543845837080	2.087446861163	-1.346136996088
O	-0.167896604531	2.894604588318	0.802162896575
O	-4.216745746351	6.732978579836	-1.641337433833
O	-0.110370760798	6.322816890109	1.592241061605
O	-2.650044928729	4.267609965828	2.698891417459
O	-2.421217430532	7.805192972919	-2.752530863128
O	-2.605431459740	4.572648436546	0.372496775206
TV	4.552664409971	0.000000000002	0.000000000002
TV	-1.292959738971	8.260479685035	0.000000000001
TV	0.218472672216	-0.476595755008	6.413525741618

EQ-CO₂ 190

C	-0.225473330153	1.882337796674	1.525052636870
C	-1.603354751707	1.232592852774	1.217709137698
C	-2.410914040482	2.038352819940	-2.257070769477
C	-0.631843974045	5.268071278958	1.525151936182
C	-2.009542636129	4.618096997983	1.217829590226
C	-2.817014591918	5.423508285630	-2.256997201061
O	-2.717878058692	1.122512022297	1.637608185604
O	-1.501359876493	2.682877400629	-2.659122920918
O	-1.063840378062	0.686987506286	0.030890868785

O	0.284890428719	1.347195560360	0.331017920893
O	-0.121136257631	4.732605193633	0.331543500968
O	-3.309328494630	1.393958076935	-1.831844472013
O	0.319523464580	2.583111292261	2.329241482658
O	-3.715734303305	4.779689919443	-1.831698339691
O	-0.087080977126	5.969135391397	2.329294341660
O	-3.124215210492	4.507876679589	1.637309309718
O	-1.907106655332	6.067402809599	-2.659278255661
O	-1.469661207017	4.071983055935	0.031351243120
TV	5.562787755751	0.000000000000	-0.000000000001
TV	-0.812846923322	6.770484456805	-0.000000000000
TV	-0.673086326147	0.237966339187	6.643852915262

EQ-CO₂ 191

C	3.865764042072	3.244729192004	3.332258853110
C	1.447566086793	1.837626066652	1.658342694775
C	-4.200354321493	1.557682049298	-0.656186504001
C	5.390700471669	5.703671580995	3.381982356782
C	-0.723857679779	3.862789949756	0.296588909966
C	-6.001529397789	4.427392632702	-1.274903373421
O	0.484817256123	1.219639169301	1.777311157226
O	-5.176689927421	1.754682399613	-1.298553793374
O	-0.934853620708	0.801355929230	-1.882540840224
O	-3.256610566860	0.330686535791	-3.145256561506
O	-0.584275487684	2.688471073760	-3.038090513779
O	-3.220438182976	1.352646251872	-0.027580726023
O	4.831052739619	2.808094298473	2.455947027318
O	-5.812511712380	4.425201518456	-0.103556642200
O	4.423712401638	5.451912159140	2.422174064065
O	-1.189465156577	4.383583199087	1.209691496619
O	-6.178326882222	4.430598318296	-2.444234822820
O	-2.882056518676	3.600308967148	-1.960253912177
TV	8.120679132243	-0.000000000016	0.000000000005
TV	0.476544220602	5.159689682286	-0.000000000007
TV	6.671143928829	4.190588950143	6.178002303963

EQ-CO₂ 192

C	5.135460090322	-1.328759496971	1.076469204192
C	-0.212539506499	-1.250444512161	-1.823403942986
C	-3.113902498238	-1.815720818565	1.076371292087
C	6.240138763922	-2.299595506362	4.378617684743
C	0.892201551701	-2.221043254773	1.478703116601
C	-2.009122896024	-2.786411933718	4.378577139389
O	-3.158902678758	-2.569552590606	0.164397819224
O	4.346161328972	-1.826388961050	0.164278209313
O	-1.318537714644	-1.294772425258	-2.137093760907
O	2.955896529730	-4.216691648900	2.232581199815
O	4.060537032004	-5.187568212876	5.534726344429
O	6.375311009129	-1.182773915269	0.824876268415
O	-3.068517215812	-1.060091093558	1.985096897226
O	7.480004438832	-2.153652247260	4.127046594190
O	-1.963740802491	-2.030726852022	5.287265706579
O	-2.054137958786	-3.540279600200	3.466636681138
O	5.450795931764	-2.797098638624	3.466399478283
O	-0.213823600892	-2.265555284781	1.165150790374
TV	12.374114125315	-0.000000000003	0.000000000010
TV	1.671806309119	3.204127389842	-0.000000000005

TV	2.209504273969	-1.941294151935	6.604416241807
# EQ-CO ₂ 193			
C	1.587213644979	1.274536287237	1.887333459331
C	-1.224814175329	-0.043486314877	0.717366185082
C	-3.846556911107	1.867725897069	-1.601860124164
C	1.591419713582	4.886925833059	1.887255961115
C	-1.220287497617	3.568692760392	0.718150889727
C	-3.842346277625	5.480014858245	-1.601860389433
O	-0.963760173850	-0.720568243292	1.652290004839
O	-2.904663548243	2.013284474356	-2.436708013630
O	-1.506007616697	0.633992859435	-0.212259185409
O	0.929817321512	0.864870626332	-1.799168803582
O	0.933996533633	4.477185472902	-1.799171177234
O	-4.084507040775	2.678950623548	-0.611511525553
O	2.035987885934	1.882356153466	2.754918190760
O	-4.080348748227	6.291283037128	-0.611556260943
O	2.040226004754	5.494635373038	2.754910349171
O	-0.959273035247	2.891371449397	1.652941858808
O	-2.900374276019	5.625516346898	-2.436630829455
O	-1.501541563307	4.246401884006	-0.211301718983
TV	5.604534576174	-0.000000000007	-0.000000000004
TV	0.008396738289	7.224633899728	-0.000000000002
TV	2.359724628803	2.806692654038	6.517451265786

# EQ-CO ₂ 194			
C	-0.082785849638	1.787499783016	3.098272006366
C	-1.927529060836	0.535283887809	1.090311319843
C	-1.598831913998	2.094279280951	-3.092112289351
C	-0.073968205195	5.510413998700	3.235759850241
C	-1.832599313078	4.196536193700	1.130918927146
C	-1.571358083162	5.845932923720	-2.986409050557
O	-2.351001675926	-0.182237857905	1.931538895391
O	-1.805231935197	-2.172584631162	-3.950972160630
O	-1.404177457425	2.797915345395	-2.159373306797
O	0.697863883083	0.546565430842	-1.219006171009
O	0.768245956173	4.123439016871	-1.291680530127
O	-1.334052827412	4.796336240090	0.240390836158
O	0.070483179787	1.959556678536	4.225077246988
O	-1.444471470552	8.619112213971	0.257281160771
O	0.124114568956	5.695943232849	4.354125242572
O	-2.335831237708	3.605378795320	2.024854275421
O	-1.787721285339	1.398470508443	-4.030617605634
O	-1.392886036900	6.516835894228	-2.025644474928
TV	4.335950565265	-0.000000000010	0.000000000001
TV	0.058639743521	7.356459732371	0.000000000004
TV	-0.355749296158	2.299561639351	9.119273208514

# EQ-CO ₂ 195			
C	-1.435555035454	0.970895124090	-1.629194608218
C	-0.719556049144	2.961141433203	-0.431708178403
C	-0.710450477184	-0.019298778274	-0.671134398392
C	-0.728359174968	5.270311091988	-1.725832951542
C	-0.129559301142	7.232285766543	-0.425289279840
C	-0.000407751318	4.292280741851	-0.761169555477
O	-1.017246919060	2.603740064369	0.685182286042
O	-0.963121551841	2.289972234081	-1.622982506401

O	0.231757194115	-1.332372145793	-3.925805842171
O	-2.246242849725	0.626028259200	-2.456946057141
O	-1.461651852928	4.907321905710	-2.615780816480
O	0.382247691232	0.220575705279	-0.185327995262
O	0.039199029155	-0.157975222368	-4.276688605056
O	1.123496349309	4.518422056599	-0.342543582208
O	0.670417164430	4.112453765755	-4.425949798280
O	-0.424824462042	6.804436292330	0.667617062551
O	-0.329555349890	6.613559581249	-1.650948937776
O	0.722654698929	2.977815765948	-3.928289159275
TV	4.316788695711	-0.000000000002	0.000000000000
TV	1.268208756765	8.618850692528	0.000000000001
TV	1.083867255867	1.452486989285	6.566013210163

EQ-CO₂ 196

C	1.012300067803	-0.032923206338	-1.068829196161
C	0.449263520152	1.262851307902	-1.710059126158
C	4.590665103193	-0.066552738554	-1.067379566195
C	4.020789359234	1.220230955301	-1.714090731633
C	8.237433489010	-0.021658527162	-1.057255562350
C	7.634073920469	1.259972705022	-1.695146890824
O	1.704774260100	-0.976383841241	-1.332135532777
O	5.286046011195	-1.007496314739	-1.330386820348
O	3.359340851119	1.522197755029	-0.504911304132
O	6.933086392716	1.511741488284	-0.498087758589
O	4.024815754394	1.829006107656	-2.743893466462
O	3.940150586510	0.251997425215	0.133649613401
O	0.463364395735	1.884629297390	-2.732399269789
O	8.976341723133	-0.931473125381	-1.316423356880
O	0.357615236012	0.280666599614	0.130370060657
O	10.653073056848	1.553543729761	-0.503638033748
O	7.630057813143	1.889318610600	-2.713087533655
O	7.535721920607	0.246465442350	0.128693602886
TV	10.873418891484	0.000000000000	0.000000000000
TV	0.239898934397	4.919243928460	-0.000000000002
TV	1.027287693649	1.043851393284	4.205256432520

EQ-CO₂ 197

C	-2.488293083341	-3.408325600521	-3.101733729704
C	-0.004275610558	-1.082538776939	-2.900617360140
C	-0.007712477620	1.470906077188	0.131920833184
C	-2.514521415829	2.033506627147	-3.155545800503
C	-0.033459011613	4.392497295585	-2.904163033253
C	-0.038090997068	6.948064761495	0.134001350227
O	-2.476650192198	-4.374759907225	-2.477209769098
O	-2.480605691478	-2.083791978009	0.157519161347
O	-2.490156639350	-1.031341561483	-0.498389182902
O	0.003208257872	-1.972722795962	-2.120609983905
O	-0.025482050411	3.501030560552	-2.125407143202
O	-0.011605662733	-0.183796373662	-3.668577422182
O	-0.007019522597	0.805312837501	-0.804882847951
O	-0.041191528610	5.291810386218	-3.671614185115
O	-0.036184828623	6.286668526678	-0.805674573122
O	-2.505826393739	1.101148172327	-2.480811804199
O	-2.510101881614	3.396600567170	0.018509531876
O	-2.519559707982	4.521803041836	-0.502573533061
TV	4.984354361215	-0.000000000002	-0.000000000000

TV	-0.058527794702	10.953933426451	0.000000000002
TV	0.021139955303	-0.936125362059	5.313178649308

EQ-CO₂ 198

C	0.500165644181	0.306985212608	3.084582882373
C	-3.017977827850	0.430932688608	1.050717626643
C	0.141106818033	0.506485860921	-0.875392077176
C	1.584082223873	3.581709974306	3.060910747633
C	-1.930204277423	3.748454042573	1.082718544529
C	1.237444280974	3.820089074630	-0.909198650840
O	-3.591171491158	1.291366535455	1.626936246199
O	-0.418355517186	0.619709159515	2.464660690374
O	-2.206872357731	2.422825985231	4.024612632333
O	1.079134539678	0.113523343853	-0.334879992045
O	2.154360699810	3.428961777620	-0.332895305018
O	-2.445708770528	-0.428972909644	0.473353714434
O	-2.627993502496	1.651245256422	-1.784878485137
O	-1.290381756932	2.907270117865	0.550213130843
O	-1.639812824071	4.810395945388	-1.794541356696
O	-2.569491633153	4.589612008756	1.616252010778
O	0.749461235237	4.071739675702	2.436425687262
O	-1.189655318802	5.745437291244	3.898114055788
TV	6.651408536435	0.000000000000	-0.000000000000
TV	2.164424717004	6.632133118621	0.000000000000
TV	1.387873538772	1.196285173934	6.462747410953

EQ-CO₂ 199

C	-0.115531761567	2.109308339843	4.381145225245
C	-1.968119243090	0.368247991454	1.252975061127
C	-0.181517657507	6.129762122364	-1.901735892230
C	3.396917989856	2.119454086421	4.444336921464
C	1.588592089167	0.320488061701	1.234637908632
C	3.343335849473	6.052573179488	-1.949644640854
O	-1.369384546119	-0.364288245593	1.962915277572
O	-2.375971514149	-7.365853363594	-3.891766583800
O	-0.698887888202	6.798013857771	-1.120742521352
O	-1.697979656560	-2.629688437313	-4.412050777440
O	1.687202166616	-2.605444825134	-4.477138186586
O	-2.497863473675	4.891667465871	0.543014609299
O	0.507631369733	1.485256594125	3.641796006829
O	1.017661561398	4.851026485557	0.569241790465
O	3.943802715460	1.477994648587	3.661202895289
O	2.230142619293	-0.418829975351	1.899318519137
O	1.134983830903	-7.363391860003	-3.872898030758
O	2.815524918562	6.755483101146	-1.206848413069
TV	7.033773074068	-0.000000000032	-0.000000000005
TV	0.068814416038	3.790452079137	0.000000000028
TV	-0.001798848053	2.987647654098	10.803241991971

EQ-CO₂ 200

C	1.333546632635	-1.311161975179	-0.645930608365
C	0.667805553478	-0.222730696621	2.952377161477
C	3.884804365550	-0.309541419009	2.864448215160
C	3.111458821744	2.150737757797	-0.625585441264
C	2.563436349975	3.289610217366	2.977210407436
C	5.720082928094	3.165251315076	2.803286758137
O	-1.056638292804	0.790908684508	-0.203726697930

O	1.820949752908	-0.644670458044	0.155026667291
O	3.733455580462	0.578504124280	2.097336412304
O	4.048426410343	-1.204720893116	3.622776730631
O	5.809784291576	2.275225436553	3.580372337205
O	-0.343514812256	-0.503659305745	2.479330387488
O	-0.358691877549	1.659239525658	0.339544086537
O	1.490979265953	3.073801798364	2.619666787603
O	1.398349201824	5.130419391428	0.346656802599
O	0.707627694778	4.255669760549	-0.195729403538
O	3.591951309901	2.822133215597	0.175316933246
O	5.645199409730	4.046301566237	2.016061246009
TV	7.132605629921	-0.000000000000	-0.000000000000
TV	3.523798964582	6.934871364270	0.000000000000
TV	0.263944027088	-0.656540038160	5.914955575576

EQ-CO₂ 201

C	0.222905000708	-1.813245818812	-2.203925242880
C	0.131406568053	0.330600430520	1.074438751940
C	1.562016355709	-2.028706820755	-1.450534285288
C	3.816159695240	-1.256157980426	-1.616133414773
C	3.794785034045	0.588917627177	2.573381811011
C	4.437486421242	-2.599066140001	-2.099886516002
O	1.462282602990	-2.371436630812	3.617064614424
O	0.031742837018	-1.002075571891	-3.082606397080
O	0.564384745948	-2.383551591920	2.762703039963
O	1.759699130766	-2.809665824524	-0.544007840733
O	3.814011966653	-3.493354634721	-2.615041703892
O	2.469858433451	-1.120604133371	-1.960843047790
O	0.676214391880	0.186221665779	0.071093073362
O	5.783196246574	-2.750692191988	-1.745429462892
O	3.207882466400	0.700891828094	1.589695962499
O	4.752139427498	-2.321719273851	1.011145375195
O	4.422938882200	-0.377303212717	-1.057118791273
O	3.938432159775	-2.254355409009	1.942995293832
TV	6.472838757628	0.000000000000	-0.000000000000
TV	0.992413823746	5.422572865122	0.000000000000
TV	0.257434183145	1.715896680764	7.380553278802

EQ-CO₂ 202

C	-0.089842849060	1.044695799642	2.107543081338
C	1.175352117088	1.237833791877	1.197657206991
C	0.586565545765	0.021808781030	0.400938050780
C	-0.691046584102	0.283523251839	6.498610549458
C	0.583261385508	0.465443697398	5.599412117153
C	-0.003661330550	-0.750654071943	4.803181713401
O	0.735422846412	-3.042210384969	1.148657918142
O	-2.799656688381	-0.700320487065	3.267965264582
O	2.636047103566	-1.045504737786	2.127289014654
O	-0.532632374461	-0.043603569917	1.302078778089
O	-1.135817534869	-0.803793013316	5.690695875125
O	-0.610565445925	1.468868973514	3.105243435554
O	0.806590048472	-0.687938856008	-0.538641225342
O	-1.216279773376	0.713838526954	7.491179590501
O	0.225407203484	-1.464440973451	3.868575383246
O	0.144856726190	-3.816265572019	5.551081012444
O	-3.429227146290	-1.340739830332	7.765824303394
O	2.016952083379	-1.806738255363	6.664947467733

TV	5.769784896189	0.000000000002	0.000000000002
TV	1.408237696469	4.990399016926	-0.000000000002
TV	-1.204597054765	-1.529510606924	8.797655517550

EQ-CO₂ 203

C	1.825399658542	2.517086379791	1.591346248410
C	-2.321550887533	0.094124249337	1.172782443669
C	-3.308529854570	2.420809572803	-2.010409617580
C	2.239305807581	6.069300013651	1.749927536750
C	-1.902994389936	3.672461925002	1.127710335657
C	-2.992573289962	6.017280432953	-2.011478938062
O	-1.924604729440	-0.425138603287	2.157954556851
O	-2.764472365300	-1.300380257955	-2.500700089710
O	-2.747539897194	0.611676939136	0.197156445802
O	0.103878660247	1.310784583519	0.186992950360
O	0.539312808919	4.878770632155	0.310286043594
O	-4.339094579914	2.766064252945	-1.541639621429
O	1.019821343589	1.938715838318	0.940704222062
O	-4.035209422853	6.296713256688	-1.526390133243
O	1.438601346691	5.506700918207	1.080050205404
O	-1.494908073275	3.063643042887	2.054836116606
O	-2.277133925698	2.074497890792	-2.481678261518
O	-2.333032342635	4.278801367152	0.205688426726
TV	6.575990808314	-0.000000000006	-0.000000000003
TV	0.816179916991	7.041251367977	-0.000000000012
TV	2.976721379801	2.342055266456	6.242915941154

EQ-CO₂ 204

C	0.423042053602	-1.179188123699	-0.239077108472
C	-1.327848698271	0.086088281662	2.888468391377
C	0.834054257076	2.200642646867	-0.087619597432
C	-1.065029011085	3.520977768724	2.892896652160
C	1.165699148584	5.635810008964	-0.085403567937
C	-0.749961168907	6.898694917576	2.893110370562
O	-2.073153808111	-0.425968851270	3.601692223329
O	-1.885118386676	3.118458437198	3.594155289717
O	1.773067742050	-1.248571219631	-0.134862171727
O	2.183614386298	2.125008561897	0.015392661129
O	0.103179486370	2.733940707555	-0.973504720198
O	0.871289834578	5.004192599648	0.975104928815
O	-0.307934312273	-0.674634492862	-1.141635212579
O	-1.457154918992	6.567334858317	3.739881405191
O	0.541160157122	1.553844622549	0.965017677735
O	2.515345626559	5.564226985772	0.017978254666
O	0.433773249607	6.157399291919	-0.977562178899
O	1.120339782676	8.478696360464	0.834649509338
TV	3.652257993256	-0.000000000006	-0.000000000003
TV	0.992700847409	10.263694394160	-0.000000000183
TV	-3.445538915519	2.266397494557	6.523644320305

EQ-CO₂ 205

C	-2.533586926924	0.026105856497	-0.330730288758
C	0.913481053139	1.383459517869	0.679746700347
C	-2.132624629358	-1.529115861191	2.980638991433
C	1.262803361169	-0.188403806457	4.114978308301
C	-2.027335845637	-2.735291629851	6.426162001657
C	1.534162961790	-1.377148183600	7.603739180377

O	4.916898012439	-6.464930550282	3.806263017965
O	5.173328210002	-7.542789834391	7.118972406340
O	-2.315551443006	1.212837733340	-0.811245627336
O	-1.851060945983	-0.348675425104	2.533376202370
O	-3.163786979886	-2.205447284129	2.669533487882
O	0.480846132659	0.157952961303	4.884636797525
O	-3.618133678801	-0.620974687272	-0.490228878609
O	5.534858460642	-9.027256201146	10.463290831969
O	0.159594786711	1.821708514106	1.427950489704
O	-1.905366843475	-1.568486659823	5.849394855156
O	-3.082462151582	-3.435579576530	6.310867330099
O	0.615596578175	-0.874396327630	8.077457599603
TV	6.157398301115	-0.000000000023	0.000000000005
TV	-0.027284606329	4.382832656981	-0.000000000007
TV	0.895883389628	-4.127193505513	10.129015777393

EQ-CO₂ 206

C	0.229700583790	-1.799584925887	0.751518295433
C	-2.551562095469	-0.034807979302	-0.813812805136
C	0.308251618725	1.939915336183	0.727537819928
C	-2.532627732136	3.698921135290	-0.786082883552
C	0.299812134779	5.672554189975	0.766582375596
C	-2.502577908384	7.433660894124	-0.804114443972
O	-2.419355014641	-1.370747977985	-0.927354407074
O	-2.386079753083	2.361252541401	-0.840847353133
O	-1.442116661897	0.178291528061	-1.421921698114
O	-1.424426803971	3.893764904611	-1.404244016593
O	1.022158184495	2.667000708908	1.261732748858
O	2.895835983349	4.448603963161	-0.299610210923
O	0.968691494093	-1.077600036100	1.257271286363
O	-2.357523879954	6.095293134228	-0.840714546189
O	2.877713402742	0.702344638746	-0.307445441144
O	-1.385989070690	7.621932845940	-1.408252930794
O	1.045530996527	6.397028274565	1.259167376935
O	2.918798280667	8.191619618711	-0.341892876137
TV	6.314390614456	-0.000000000000	0.000000000000
TV	0.063937021631	11.197925314307	0.000000000000
TV	-0.310477528225	0.029722095803	3.520456366097

EQ-CO₂ 207

C	-1.725751912310	-0.273393725312	-1.918109464932
C	2.141715130588	1.277939434254	0.087100357770
C	-1.216127438989	3.566845207072	-1.841669884449
C	2.612620849683	4.966115398138	-0.011941450873
C	-0.701357169700	6.903951289474	-2.127723454131
C	3.062548502340	8.596229392276	-0.073483550621
O	1.184531168963	1.690246235008	0.827755688542
O	1.600093484877	5.309965115150	0.692906736395
O	1.788300642824	-0.016621723068	0.210831946035
O	2.359613093445	3.655708837145	0.084796123889
O	-0.267234295860	3.252243820940	-1.272882871655
O	3.518406342492	5.630917397707	-0.602054451064
O	-0.880759396802	0.121322357124	-1.245948488988
O	2.024697884365	9.028443595635	0.526704295229
O	3.087408894877	1.856565254016	-0.522192263459
O	2.668502821121	7.307186701085	-0.080163095840
O	0.091025393338	7.340583894178	-1.418037670341

O	4.105069332607	9.156504680269	-0.530922365770
TV	6.495483751012	-0.000000000001	-0.000000000000
TV	1.730971508356	10.917760554196	-0.000000000009
TV	-0.136204277275	0.403790055373	3.582890541616

EQ-CO₂ 208

C	-0.185784682563	-0.173740433019	-1.034642113492
C	-0.940728079222	1.298751931449	2.579681082004
C	3.507671009855	-0.316112530461	-0.910709451094
C	2.848068054418	0.893286280830	2.707186859983
C	7.144987939017	-0.582640994799	-0.792657757833
C	6.284186542034	1.288195727076	2.631623624050
O	-0.108047182370	-3.544393084875	5.462874099552
O	3.519192404737	-4.036661428866	5.748413235034
O	0.541138183717	0.358474697547	-0.142820832987
O	4.247533608402	0.090493275253	0.037150636843
O	3.756342160271	-0.927748937719	-2.004592949921
O	2.087749188561	1.527267498139	2.118796882385
O	0.060498743946	-0.768847657304	-2.136871718595
O	7.149758551536	-3.567456841696	5.425093883437
O	-1.459576435544	1.952205817619	1.785932643105
O	7.884792120190	0.095340710450	-0.013791784946
O	7.377562348194	-1.357509948606	-1.779294540646
O	5.751988624338	1.942059493124	1.847607988948
TV	10.965716150786	0.000000000002	-0.000000000000
TV	-0.365311952075	3.565608100321	-0.000000000000
TV	-2.657390151417	0.281056859265	6.576973921371

EQ-CO₂ 209

C	-0.193423759342	-0.741261764443	-0.768954065859
C	-0.687448806917	-5.890897277174	-1.218639976123
C	2.398359824339	-0.565028308555	-0.472315864290
C	1.906730392274	-5.736297995710	-0.963623241718
C	5.027293486086	-0.646309908988	-0.602239322004
C	4.527798683106	-5.846080499668	-1.123163397053
O	-0.177231186156	-1.874610389917	-0.321236578409
O	2.398455612582	-1.474857481985	0.332029233000
O	0.640897327566	-2.669606559559	-3.188577617158
O	3.523414769632	-1.816726503978	-3.789245477466
O	3.572322910286	-2.193774632755	-2.600894915119
O	1.895081988702	-4.610315313118	-1.428888483572
O	0.736738381186	-1.436311976674	-3.337411700543
O	5.046754290682	-1.565370748737	0.190954269033
O	-0.692148305536	-4.923809157316	-1.953655919063
O	5.656812081363	-1.923558135415	-3.910239322056
O	5.702295274523	-2.294455328276	-2.720430179430
O	4.510692695314	-4.936288537029	-1.927194284152
TV	7.844426903445	-0.000000000000	-0.000000000001
TV	-0.824068303001	5.878153338700	0.000000000000
TV	0.330479626249	-2.374234805164	4.774411759781

EQ-CO₂ 210

C	0.912629388461	0.281004744326	1.388399301746
C	-1.777145726896	-1.881688933135	1.456606870006
C	-0.085411172059	-0.317899667238	4.943531835221
C	-2.797987337382	-2.320365628349	5.222931076496
C	-0.876288183873	-1.508448417224	8.835561376936

C	-3.589879897976	-3.670532153207	8.885048539873
O	-2.839130553835	-1.446728530091	0.745460247234
O	-3.699724845389	-1.519453921797	4.611896269926
O	-2.476983178925	-0.997800182492	2.211991334644
O	-3.261119301683	-1.428187877574	6.128613188743
O	0.386766366922	0.308909640226	5.828049971233
O	-0.531566613002	-0.963898232545	4.057945797050
O	1.292521778158	0.875807798631	2.338817770872
O	-4.547971383692	-2.938300462215	8.270574373488
O	0.563984751677	-0.334174782592	0.438589017587
O	-4.104904142402	-2.796951278172	9.778309463427
O	-0.429521648817	-0.868839021673	9.724554827400
O	-1.296060642283	-2.161025948193	7.942168911860
TV	6.279217461921	0.000000000001	-0.000000000005
TV	0.048898978601	3.580963102410	-0.000000000002
TV	-2.588433923114	-2.488282065118	11.281894585249

EQ-CO₂ 211

C	1.048405035796	0.223164475474	-0.935012413704
C	3.011366384057	-2.216399585808	1.703882730741
C	1.531991608176	3.856241714872	-0.942636665938
C	3.453709168144	1.440569317258	1.700258691600
C	2.002837552523	7.519648374386	-0.947294931207
C	3.945622932987	5.090674140194	1.703206312910
O	0.766626390871	1.021395826539	-0.153287100914
O	1.362898130425	4.678509177212	-0.153462910448
O	0.404805612744	-0.572710901833	2.310060603692
O	0.868818732240	3.083120594554	2.307163962687
O	-1.194622299227	2.833776166251	-1.972105477193
O	-1.816996631819	2.162141999494	0.816225391004
O	-1.658902733326	-0.824106704961	-1.970695473027
O	1.829143015927	8.335164227928	-0.152145463920
O	-2.262740808006	-1.495346906680	0.818816833602
O	1.339375989322	6.736481299962	2.308528827503
O	-0.722866682560	6.486689592771	-1.970726483621
O	-1.328739492951	5.813316576274	0.819333321895
TV	5.426058006932	0.000000000006	0.000000000042
TV	1.400528420765	10.963544128392	0.000000000011
TV	1.796289527274	-0.452305220175	5.267053422886

EQ-CO₂ 212

C	1.854546527904	1.873962363532	2.390222304111
C	4.355980832175	1.420592373933	-0.065856365622
C	1.454614786468	5.412390582431	2.371701210088
C	3.933808530124	4.978103823576	-0.092347904349
C	1.001153058904	8.933471874441	2.371702776119
C	3.505826137737	8.472977387639	-0.090519796886
O	1.168585060770	1.062869689902	-1.942505979646
O	0.726962013432	4.583043165006	-1.931157637815
O	1.595277177124	0.411904866129	-0.976371076679
O	1.167821383189	3.935004485369	-0.969673439407
O	1.469844114480	2.449959902416	1.469436662892
O	-1.410524805325	4.390419946711	0.820784018953
O	1.892556741222	-1.035384795499	1.464745999945
O	0.313732607081	8.135984178781	-1.944339962732
O	-0.969236401833	0.811989711590	0.824916245932
O	0.737806002458	7.480610575809	-0.979978637285

O	1.037297901456	5.972434037118	1.455422302397
O	-1.830267649296	7.887521650189	0.820436864455
TV	5.729343043054	-0.000000000000	0.000000000000
TV	-1.285337134440	10.560079868468	0.000000000003
TV	-1.845717180310	-1.697661550803	5.205682112285

EQ-CO₂ 213

C	1.135623303860	1.447281126664	0.408973599120
C	0.843562391534	0.472388753861	-0.560966905492
C	-0.063240184042	-0.709724123036	-0.309004350181
C	1.992307316533	0.563243047261	5.669990723639
C	1.701157164708	-0.411943573527	4.700133646886
C	0.793726187077	-1.593606361180	4.951587316986
O	-1.072057319788	1.195465562767	-3.437760404768
O	1.325572576235	0.707716604842	-1.784751889459
O	-1.218417501803	-0.771899120128	-0.671311686853
O	0.622465529975	1.384653796482	1.637288992046
O	1.478255718956	0.501087878232	6.897966277957
O	1.104055067525	-0.262546343084	-2.687173375721
O	1.921655522285	2.525179595219	0.168158960850
O	1.963663232270	-1.147479613208	2.574431788332
O	2.778134582986	1.641283237062	5.429165266113
O	-0.213099156623	0.311970962261	1.823829998437
O	2.183967220014	-0.176741398033	3.476628592196
O	-0.361329426590	-1.655693118798	4.588907558081
TV	4.625680288222	-0.000000000001	-0.000000000003
TV	1.248925239365	4.350627233061	0.000000000008
TV	1.714989214408	-1.767079854892	10.522327613413

EQ-CO₂ 214

C	0.655510489965	1.013323409325	-0.255218195750
C	-3.376308184849	-1.028251919131	-2.023050689594
C	-2.206086624328	-0.052735735629	-1.759976107589
C	0.359248870097	0.875381265149	3.960689388899
C	-3.672566703290	-1.165996843451	2.192916502923
C	-2.502429894303	-0.190467125243	2.456106980356
O	-1.712596661050	-0.904023198948	-0.771886297957
O	-0.379184634776	1.849925976047	-0.283405379728
O	0.805100111498	1.715471346335	0.871468141695
O	-2.869711483147	-1.879879343396	-1.024935874681
O	-3.165834681271	-2.017761990121	3.190878033854
O	0.434504068319	-1.194852311999	-2.741129020138
O	-1.696516798255	0.958915110030	-2.197107704214
O	0.138397626869	-1.332752675929	1.474666993631
O	-1.992960448646	0.821200179071	2.018943746581
O	-2.008855320658	-1.041809751700	3.444127824337
O	-0.675393633789	1.712107632254	3.932528007921
O	0.508992977365	1.577546346201	5.087305073823
TV	4.757365556944	-0.000000000007	0.000000000044
TV	-0.220708460789	5.722459630318	0.000000000103
TV	-0.592460501627	-0.275606423846	8.431980802505

EQ-CO₂ 215

C	1.042595752042	1.501067482103	0.374507277540
C	1.693937826505	0.392828657965	0.570188631000
C	0.569868621400	2.709977328034	0.328133036816
C	1.731335040734	3.635974683667	3.380281936643

C	2.417685456348	2.546228327759	3.202649497257
C	1.209376779817	4.819981364248	3.237069584728
O	-2.857433130936	2.844348989535	0.354081344388
O	-0.684333811048	-1.634378886947	0.989814102268
O	2.257168660060	-0.638569638413	0.721538479796
O	0.108928543256	3.802057968501	0.263072432723
O	0.709032896775	5.890332898631	3.158037327570
O	-1.557682992413	-1.077847564973	0.306066431525
O	-2.438430743800	1.741902657280	-0.032580291563
O	-0.093931989148	0.768139916931	3.292917902155
O	-1.713116319032	3.901309231704	3.006720853742
O	-2.131620250322	5.016489086036	3.356028535952
O	-1.102243663239	1.004763255852	2.608946882570
O	3.016126437744	1.529574154374	3.081191718867
TV	6.923025661005	0.000000000000	0.000000000006
TV	-3.208798413355	7.142704734237	-0.000000000004
TV	1.181484985480	5.447181925729	5.483866177750

EQ-CO₂ 216

C	1.069378487139	3.913439276769	-1.409062394011
C	0.580493067572	5.093032334737	-1.161200327875
C	-1.825465314925	2.747082330544	-1.244732136543
C	4.507344004911	3.915790244796	-1.409696196434
C	4.021434662880	5.096153525671	-1.158717563678
C	1.615642148959	2.743989501657	-1.242754401391
O	0.313409172142	1.199355368810	1.296792239794
O	0.987342189853	0.974045947156	2.314499252298
O	-0.824957803035	4.029093451705	1.477087551037
O	-1.325626771517	1.678286281955	-1.152211218560
O	2.114486430289	1.674863744691	-1.149154773315
O	-0.366567652766	5.075102376537	1.964635619575
O	0.139663509115	-0.710024557726	-0.990240162062
O	2.941908435784	5.228821588156	1.969088412718
O	3.582542392825	-0.706122242933	-0.986367622715
O	3.767956070674	1.334336965634	1.308770197240
O	4.415375640242	0.974670761450	2.305071375424
O	2.616980844421	4.137349812678	1.474767634538
TV	6.881599540932	-0.000000000000	-0.000000000000
TV	-0.029062131266	6.876288428847	0.000000000000
TV	0.505837602548	-0.193595808852	5.910191557187

EQ-CO₂ 217

C	1.430301363464	-0.101583432742	-0.886528176747
C	0.922848006329	-1.432681414326	-0.365797535804
C	0.670305668925	-1.878074827997	0.887036240764
C	0.808784006199	-1.211124696052	2.237388292341
C	0.301240805142	-2.542208059969	2.757809476849
C	0.048649486644	-2.987527306300	4.010648216494
O	-2.199303179126	-2.441352792442	-0.439793967123
O	1.761252701799	0.981109483562	-0.445645050903
O	-2.219462383050	0.374875872291	-0.772652913834
O	0.183206532594	-3.080380625183	1.455939604839
O	-0.438435447148	-4.189697144139	4.579795911832
O	-3.122316139768	3.236845680668	-1.249715663631
O	-1.400894310747	0.508290054752	0.151779197373
O	-3.743916945002	2.127666437742	1.873726585511
O	-2.021967381161	-0.601440714016	3.275132046911

O	-2.822590902836	-3.550619036924	2.685574505952
O	1.139771784198	-0.128566178053	2.678548618278
O	-2.841193215619	-0.734355293029	2.351195470131
TV	6.860658225008	0.000000000004	0.000000000000
TV	0.016484139389	5.705772548162	0.000000000007
TV	-1.243062652527	-2.218690072946	6.247399929329

EQ-CO₂ 218

C	2.437858767239	0.807731878416	-0.534596404803
C	5.701410626914	1.733463987222	1.604849527869
C	2.650608825370	1.976071197559	-1.265144785576
C	0.922964668702	4.355219518666	-0.543683183012
C	4.215199851660	5.378930156328	1.679311486323
C	1.152234351378	5.528604170927	-1.261227526596
O	4.714526217359	1.317914348437	-2.134026857154
O	3.685445313171	2.213578311154	-1.998962296449
O	1.864548763606	0.081162009470	0.186664344925
O	-0.822264960663	0.381274785063	-0.648858290698
O	-2.359342632886	3.977977553055	-0.807185827054
O	4.745979245381	1.590641141468	0.980254666485
O	-0.497494479944	1.362217211577	-1.334632828087
O	3.333103101698	5.147675209231	0.978969010713
O	-1.972704186087	5.044816010138	-1.308099794926
O	3.260941449961	4.989748283049	-2.125398708170
O	2.186873654058	5.829325820923	-1.972690604697
O	0.295591396650	3.655664685029	0.166100980148
TV	7.974162873167	0.000000000000	0.000000000000
TV	-3.261065420282	7.255831256930	0.000000000000
TV	-1.802216285890	-1.871691382926	4.968780656649

(ii) SiO₂ at 1 atm

EQ-SiO₂ 0

O	-5.066345139082	-0.311255880109	0.012262618204
O	0.555938052959	-2.460483463813	0.219081400968
O	1.793591436244	-0.275713819303	-0.582531143028
O	7.976331352671	5.288818083464	0.291810692031
O	-6.155151922787	-4.811327708675	2.066989350238
O	-0.532619016547	-6.960904469291	2.273576928748
O	0.704824518546	-4.775939130243	1.472158917528
O	6.887844512787	0.788162932053	2.346974134157
O	-7.244047627250	-9.311606499647	4.121588899401
O	-1.621648937379	-11.460794086202	4.327902890834
O	-0.383817592551	-9.276232866367	3.526544705467
O	5.798906541422	-3.712051429629	4.401453017024
Si	-13.005319908634	-8.090534669691	3.074711721560
Si	0.824839877647	-6.035313840154	2.543330680987
Si	-0.264000607650	-10.535522484224	4.597800605075
Si	-10.827645032080	0.910061298995	-1.034591197922
Si	-11.916617079284	-3.590310923550	1.020080844567
Si	1.913445378186	-1.534966137153	0.488683689405
TV	11.553055294360	0.000000000012	0.000000000011
TV	-3.481779053152	3.790149355328	0.000000000046
TV	-3.266725438038	-13.500368987228	6.163709658005

EQ-SiO₂ 1

O	-3.311461122391	2.983340494323	0.540250614344
O	5.677520922150	-3.047900015225	-1.716886753247
O	-1.926122412771	1.108974317154	0.534212312992
O	-0.773157743127	-0.338189075541	-1.257659084963
O	-4.785190203322	1.886179761085	2.567581819794
O	4.201911319143	-4.145478741048	0.308080631486
O	-3.400843605085	0.010956898283	2.560405917533
O	-2.249002644418	-1.435536095229	0.767466163301
O	-6.262442587939	0.785818951747	4.589834804521
O	2.726948425280	-5.243261224257	2.331263396484
O	-4.878398850112	-1.088928035530	4.582769924429
O	-3.724298904585	-2.535454539114	2.791040795931
Si	-6.308661783625	-0.701686880680	5.599024763126
Si	-2.295732402576	-1.471186944255	2.562102042593
Si	-3.773163366310	-2.571039144512	4.586193577183
Si	-3.356294872991	1.497433303763	1.550019363798
Si	-4.832391478702	0.397008775003	3.574149809118
Si	-0.820696828910	-0.372461053130	0.536827706911
TV	5.064757769057	0.000000000011	0.000000000010
TV	-3.594435883825	4.836716891629	0.000000000061
TV	-4.428188321652	-3.296432883664	6.074032934469

EQ-SiO₂ 2

O	-4.435267514480	-2.167310119317	1.136479706496
O	1.560255431117	0.018502761567	-0.783328960738
O	-0.672545763905	1.510910022994	-0.862715570033
O	6.149155117487	2.425680669988	1.146295617851
O	-5.617640094888	-6.490865196934	3.609046678615
O	0.377844101754	-4.305047771935	1.689220976693
O	-1.854923699830	-2.812618846852	1.609842486730

O	4.966781683520	-1.897868078615	3.618866249092
O	-6.800013442379	-10.814388823133	6.081630912099
O	-0.804536870733	-8.628594302041	4.161819363721
O	-3.037295120118	-7.136153041076	4.082422665804
O	3.784389359052	-6.221422197159	6.091438365220
Si	-9.788079018033	-10.169525480920	4.483651174233
Si	-0.238659611110	-2.793247084016	1.998458123629
Si	-1.421031144764	-7.116788343809	4.471043044667
Si	-7.423313959285	-1.522425661843	-0.461492867073
Si	-8.605696986021	-5.845980316276	2.011074512167
Si	0.943717164301	1.530294292362	-0.474102925054
TV	8.447057875356	0.000000000011	0.000000000010
TV	-2.922703326656	4.081558734153	0.000000000051
TV	-3.547127796083	-12.970638247093	7.417718263976

EQ-SiO₂ 3

O	-4.082098847071	-1.502294524801	0.807643002734
O	1.415619243739	-0.027209520969	0.297362091719
O	-0.048687136893	2.010619527925	-0.992610480056
O	6.923867384868	1.440774751160	0.807008208059
O	-7.018002432024	2.578954319336	0.807500648451
O	-1.520783192805	4.053916461539	0.296956724064
O	-2.984981192008	6.091737926746	-0.993039518173
O	3.986978931429	5.520957460820	0.806393884662
O	-9.954211425728	6.659853089105	0.807530585502
O	-4.457071310084	8.134778376963	0.297100718552
O	-5.921338808923	10.172541080861	-0.992797116352
O	1.051727626392	9.602257450981	0.807193989751
Si	-13.286245546400	6.609403767166	-0.374119934649
Si	-1.528891226884	5.576634464393	-0.376172580881
Si	-4.465264644425	9.657484935106	-0.376201404821
Si	-7.413558907998	-1.552520705314	-0.373979044297
Si	-10.349945082386	2.528460504877	-0.374149453857
Si	1.407662958047	1.495489972159	-0.376031102702
TV	8.845626251763	0.000000000010	0.000000000009
TV	-8.808825816362	12.242882694362	0.000000000138
TV	-1.486681650523	-4.088755420662	2.430701362113

EQ-SiO₂ 4

O	-2.255287979582	2.239036867190	0.518056401454
O	3.335632887425	-1.012516138933	-2.447007414850
O	-1.587875884590	-0.333644967583	0.978444198655
O	0.325508087724	0.090269176889	-0.949421851257
O	-4.962468221060	6.557568995614	0.502639742889
O	0.561414585572	3.446078446424	-2.424045632230
O	-4.253047257451	3.989039794271	0.945765259812
O	-2.353207230810	4.449601525291	-1.002017146261
O	-7.663918372264	10.967791332415	0.586373906200
O	-2.107933024718	7.753152624597	-2.450878884525
O	-6.885345807214	8.403208691935	0.999532690581
O	-5.021139104575	8.754186666081	-1.013551252822
Si	-7.821196408099	9.642766205291	1.575676858992
Si	-2.656744096322	3.849435012209	0.516033360683
Si	-5.313801308606	8.182275561492	0.520179606747
Si	-2.481960171028	0.949676920295	1.536863686541
Si	-5.152925546953	5.261856643824	1.523490409340
Si	0.013803032125	-0.494721611808	0.572428592442

TV	4.964466609620	0.000000000011	0.000000000010
TV	-8.082723692051	13.070238719335	0.000000000182
TV	0.345152351001	-3.017900187858	4.052902017824

EQ-SiO₂ 5

O	-2.146531303794	-5.511802370269	2.840695911932
O	0.585430641201	-2.833566526815	1.191000360106
O	-2.146154326858	1.649716937372	0.668394906693
O	0.581599604923	-1.094426472304	-1.380269803244
O	-2.145898856961	3.332989165704	-0.962479377210
O	-3.512725596923	-0.518109412492	1.086421747920
O	0.588179273842	-5.511983301029	2.840916292909
O	3.320025849268	-2.833608713417	1.191122638685
O	0.588532227743	1.649712749217	0.668366974251
O	3.316330011419	-1.094656017597	-1.380327104453
O	0.588855971124	3.332923641368	-0.962546759459
O	-0.777997889419	-0.518269132398	1.086608982231
Si	1.956555765985	2.491333236950	-0.147195934064
Si	-3.514996938535	-2.075831935475	2.110163576465
Si	-0.781555243506	-6.268573804296	1.921868837193
Si	-0.780346205645	-2.076023392192	2.110155187080
Si	-0.778098062447	2.491335372736	-0.147258838250
Si	1.952993053516	-6.268480143101	1.921876941534
TV	5.469245989299	0.000000000002	0.000000000002
TV	-1.363768607897	6.594185110277	0.000000000001
TV	-2.729116695343	-0.138140338284	4.325104630021

EQ-SiO₂ 6

O	-1.934702529425	-4.162881440319	2.873973370840
O	0.490743010673	-3.094946878791	1.089213189464
O	-1.455822774824	0.527719171736	0.329750686517
O	1.305984924329	-1.260684213772	-1.876237821167
O	-1.460425254232	3.070140417763	-0.635748111557
O	-3.558983275342	-0.555669295462	1.571043216720
O	-4.361876963407	-4.187936689532	7.138143230911
O	-1.936383676822	-3.120282909599	5.353214990407
O	-3.883173506603	0.502764205637	4.594022894878
O	-1.121261517801	-1.286001196388	2.388065729108
O	-3.887950845292	3.044956308050	3.628617058121
O	-5.986321965990	-0.580802648745	5.835160411025
Si	-2.927300778759	1.774147973157	4.111277225680
Si	-4.439551358268	-1.830793042056	2.166743682333
Si	-1.990235187764	-5.425614748634	1.796109431604
Si	-6.866782120638	-1.856070752814	6.430805903133
Si	-0.500029082424	1.799318997996	-0.152815057501
Si	-4.417477638409	-5.450809351683	6.060327520109
TV	4.866430379421	0.000000000001	0.000000000001
TV	-0.020736462875	5.411521420490	0.000000000001
TV	-4.854535710362	-0.050627846951	8.528383500884

EQ-SiO₂ 7

O	-2.854243850932	-5.546257395540	3.840614651551
O	-0.418829460159	-3.061454097080	0.628016504114
O	-2.392890262301	0.535338579581	1.269100656824
O	1.725241104776	-1.132543766081	-1.723623670626
O	-2.388087482266	1.729694907764	-1.108582499506
O	-3.118204174377	-2.024338077762	1.884372657794

O	-5.284825640215	-5.578499414044	8.152098498212
O	-2.849424913110	-3.093716956901	4.939396746273
O	-4.823365636066	0.503158546131	5.580788628809
O	-0.705368609275	-1.164690839062	2.587673321872
O	-4.818626008308	1.697419538074	3.202931576420
O	-5.548675452621	-2.056615377557	6.195651215916
Si	-3.829594307736	1.099158324553	4.392754879317
Si	-4.692761588915	-2.503949251576	2.081690077755
Si	-2.276562651983	-6.101061370568	2.392544431996
Si	-7.123283644892	-2.536153022933	6.393011999941
Si	-1.399009195706	1.131498347722	0.081256628682
Si	-4.707079255155	-6.133376573891	6.704079496825
TV	4.832065802012	0.000000000001	0.000000000001
TV	-0.002608774109	5.418696937902	0.000000000001
TV	-4.861109302892	-0.064479040728	8.622833623304

EQ-SiO₂ 8

O	-2.525387506156	2.231707194191	0.393354443416
O	2.996017983332	-0.875477491795	-2.442506542593
O	-1.798463564476	-0.300818889004	0.922394092383
O	0.033598913667	0.242793668515	-1.059301966254
O	-2.018175413160	-0.728231212275	4.405115175780
O	3.461675935890	-3.739888925605	1.535959539822
O	-1.285711807559	-3.260099586189	4.980327276654
O	0.511740871032	-2.712504733683	2.970024390053
O	-1.526505125538	-3.667328156666	8.416983598699
O	3.975447022899	-6.704706616089	5.570645483709
O	-0.784563073924	-6.202836531043	9.011924206990
O	1.012162786603	-5.629460305450	6.995203011813
Si	-1.705998043159	-4.909980243084	9.507154320082
Si	0.299441841248	-3.353269783796	4.486613557932
Si	0.798154108653	-6.289969857690	8.508618154642
Si	-2.711382185632	0.977765681662	1.465049371975
Si	-2.201330345723	-1.970711865873	5.495271487552
Si	-0.206432622012	-0.394889470604	0.454692348973
TV	4.991043912097	0.000000000013	0.000000000012
TV	-2.765932917828	4.223092710011	0.000000000060
TV	1.481662100968	-8.786042391020	12.049935814610

EQ-SiO₂ 9

O	1.476417774772	1.336990347040	0.452902577128
O	-0.448243252745	-2.915740463049	-3.013977986453
O	-0.954498764853	0.598190996936	1.568374748052
O	-1.484571051068	0.097469580115	-0.994173487074
O	1.340937762597	-1.338456286229	4.417450241930
O	-0.539074620754	-5.642899258326	1.026237681214
O	-1.083869338857	-1.997737262273	5.597480446842
O	-1.574921418842	-2.614208413140	3.039591171713
O	1.334858783515	-4.167453203409	8.498979561277
O	-0.613890893869	-8.272652855508	5.121584852899
O	-1.096908054062	-4.915265021018	9.641234804400
O	-1.617030493240	-5.378260085836	7.050985719895
Si	0.126238678773	-3.788323790472	9.573237382604
Si	-2.273479151049	-2.457607533161	4.538727944419
Si	-2.303464850851	-5.314380550340	8.564981389293
Si	0.265335711368	1.722754697900	1.519652718520
Si	0.182721671681	-0.932124420529	5.543392212041

Si	-2.169868706176	0.186251076368	0.514211949100
TV	4.839890553327	0.000000000033	0.000000000070
TV	2.507238528301	4.411010287156	0.000000000063
TV	-0.219276633372	-8.233675652939	12.084446064847

EQ-SiO₂ 10

O	-2.835844446871	-5.276188877616	3.280039512223
O	0.003567146324	-3.862944971040	1.299141565478
O	-2.073949793743	0.251728999122	0.592866969354
O	2.016855759704	-1.181117149691	-2.049987747562
O	-1.397877399762	2.546659983628	-0.617591333893
O	-3.333759393338	-1.878627814059	1.506656759624
O	2.275998425779	-5.305785022279	3.306103773219
O	5.139338054417	-3.857402148176	1.300796228034
O	3.040330115449	0.268381619979	0.622560719424
O	7.147820700770	-1.175408048944	-2.046668394721
O	3.733626056367	2.539793882209	-0.616699370657
O	1.806507328449	-1.893849593540	1.506155910857
Si	4.323419250974	1.139752455044	0.037225457003
Si	-4.698274595267	-2.527364788761	2.183242749225
Si	-2.405896315223	-6.106109606329	1.917848705085
Si	0.437623840494	-2.535084920738	2.182552153198
Si	-0.798551088871	1.143468640422	0.022344721874
Si	2.718367395689	-6.110183782229	1.933126469026
TV	10.268188651532	0.000000000002	0.000000000002
TV	0.193215520969	5.370897845308	0.000000000001
TV	-2.756199705885	-0.208314426128	4.341294081108

EQ-SiO₂ 11

O	-2.658764176200	-4.784775687884	3.195030421388
O	0.079564388060	-3.326969425446	1.136951433566
O	-1.970327843472	0.664654652152	0.507105300128
O	2.151727017057	-0.564353055451	-2.192146590923
O	-1.505171724402	2.976040200436	-0.740393780743
O	-3.064389092787	-1.527085509485	1.577226787014
O	2.392444436331	-4.784864295963	3.195255557877
O	5.130815772371	-3.326944719213	1.136953875399
O	3.080810105837	0.664690715696	0.507211829074
O	7.203101086006	-0.564332835479	-2.192145455604
O	3.546054499374	2.976052731096	-0.740307999722
O	1.986932961832	-1.527072378003	1.577350733956
Si	4.279551305414	1.641133401106	-0.094807442231
Si	-4.518670679871	-2.091162436660	2.129208708854
Si	-2.210459784444	-5.670688164512	1.877031546766
Si	0.532610848565	-2.091164182223	2.129247983236
Si	-0.771621050981	1.641134989518	-0.094909404453
Si	2.840836723107	-5.670655567314	1.877167270582
TV	10.102619897955	0.000000000002	0.000000000002
TV	0.169801569314	5.402833893180	0.000000000001
TV	-2.672840444776	-0.265704881627	4.402591813850

EQ-SiO₂ 12

O	-2.010325750928	1.527924071514	0.035383615788
O	3.353681452490	-2.009486283699	-2.871568452315
O	-0.247175633265	1.534479510425	2.199096557053
O	-0.221790917917	-0.244869773279	-0.702199698820
O	-2.041139363805	5.069446352128	0.035332641438

O	3.322825387312	1.532082820271	-2.871558641331
O	-0.278039856280	5.076028325194	2.199119457405
O	-0.252639577516	3.296678894422	-0.702210662560
O	-2.072144659676	8.610997976836	0.035367009417
O	3.291916907645	5.073608261288	-2.871601283670
O	-0.308908769861	8.617612844994	2.199086518423
O	-0.283473979714	6.838141822779	-0.702198341695
Si	-2.094033464308	8.611101571679	1.834521794705
Si	-2.031818042483	3.296831002331	-0.336798569402
Si	-2.062645317647	6.838374029506	-0.336771826167
Si	-2.032297056313	1.528032648415	1.834540225456
Si	-2.063153218064	5.069548363070	1.834507676132
Si	-2.000964346399	-0.244716643524	-0.336749645453
TV	3.565142274898	0.000000000010	0.000000000009
TV	-0.092582502617	10.624633539681	0.000000000162
TV	-1.776914938296	-1.775057662594	4.335037354484

EQ-SiO₂ 13

O	-1.211909300525	-4.452089312571	3.043707423995
O	0.403643775834	-2.815254802370	1.585877145581
O	-2.185004279151	0.895590813112	0.361272128181
O	1.723043717386	0.014632808366	-1.816207210364
O	-3.604972621084	2.646607184340	-1.178949852425
O	-2.210933429761	-2.175728213562	1.921186707596
O	3.985285397729	-4.452039266332	3.043634148078
O	5.600903028122	-2.815243961390	1.585862715840
O	3.012221056726	0.895619986804	0.361197733718
O	6.920327904714	0.014619987096	-1.816172407722
O	1.592297586140	2.646742904351	-1.179008097285
O	2.986366940634	-2.175652126518	1.921151784558
Si	2.569699665417	1.298381684762	-1.180286000634
Si	-3.675440663105	-2.309973066647	2.703525347768
Si	-1.124909552202	-3.430711335294	1.730267001064
Si	1.521811182452	-2.309898620041	2.703437495062
Si	-2.627496154741	1.298323206988	-1.180230485111
Si	4.072338114466	-3.430670890062	1.730198825780
TV	10.394503583238	0.000000000002	0.000000000002
TV	-0.720860707342	5.204272008657	0.000000000001
TV	-0.673681520555	-0.861209841627	5.127171838905

EQ-SiO₂ 14

O	-3.918487134906	-2.429703273084	6.353895139132
O	-1.761632630511	-2.302668853634	-0.051218754487
O	-1.972427867678	0.333988690007	0.435241551412
O	3.513833590250	-2.390283814573	-2.918961800793
O	-0.260701804505	1.229381714561	-1.461100446457
O	-3.455282222080	-1.278979680083	1.871980718903
O	-4.032970880604	2.803044651741	6.353749341032
O	-1.876115579609	2.930194721669	-0.051422579962
O	-2.086879926051	5.566909005061	0.435060019326
O	3.399453649174	2.842794687661	-2.919254194419
O	-0.374817500556	6.462027323900	-1.460883097325
O	-3.569487602981	3.953750794694	1.871991699122
Si	-1.054585013429	6.787509618384	0.017835819539
Si	-4.715925983444	-2.272999983285	2.253180976431
Si	-1.870221199597	-6.392046910505	1.136162688700
Si	-4.830350597839	2.959920239277	2.252934562658

Si	-0.940495702212	1.554747703987	0.017651380710
Si	-1.984365085373	-1.159296168661	1.136401526793
TV	5.277393847098	0.000000000006	-0.000000000008
TV	-0.228555400940	10.465662966334	0.000000000000
TV	-4.317195945664	1.069839652080	5.217287883229

EQ-SiO₂ 15

O	-4.005605988644	-2.929079510213	6.402521687681
O	-2.071091840620	-2.672365195974	0.046246699778
O	-2.296325632789	-0.076665691077	0.737011432749
O	2.885493835552	-2.937606111029	-2.737207277901
O	-0.649073785281	0.583213354034	-1.329074076364
O	-3.808426078276	-1.786660186456	2.020526560744
O	-3.959107554643	2.208888691297	6.443539723417
O	-2.007369908899	2.474237289712	0.075111402865
O	-2.243659328843	5.069351830064	0.743686538926
O	2.937233918749	2.211063052090	-2.713177227980
O	-0.624379593189	5.704506636282	-1.355535551919
O	-3.759813130375	3.365137401386	2.024952260963
Si	-1.153601361967	6.164925752795	0.151664096677
Si	-5.050166920745	-2.814972422424	2.374853494734
Si	-2.373061991089	-6.759185367836	1.334837249722
Si	-4.995580446141	2.337308573045	2.400103233229
Si	-1.194479247663	1.024128592792	0.177200475754
Si	-2.328822214682	-1.623241555729	1.314478289330
TV	5.262772346381	-0.000000003432	0.000000000774
TV	0.099710943037	10.287039101583	-0.000000000396
TV	-4.051903323656	1.051160989203	5.210977655725

EQ-SiO₂ 16

O	1.106219465656	-5.645959490561	3.959070320624
O	-0.056448132862	-2.404517375558	-0.112595898025
O	-2.677510892512	1.072730905836	1.672967792951
O	-0.504020917890	-0.005532068970	-2.804224279497
O	-4.720888224451	0.304940465853	0.040534480480
O	-3.440172848556	-1.503498451090	1.617641699781
O	0.820553357173	-6.713648807668	8.914272113568
O	-0.344977593856	-3.526432678729	4.843742350833
O	-2.891303292837	-0.091218707975	6.570155985602
O	-0.813950355588	-0.949780498689	2.066954292211
O	-5.030741270090	-0.810871537505	5.059421514638
O	-3.746524917358	-2.634375841848	6.604263272812
Si	-3.639114654173	0.118705907924	5.092175885500
Si	-4.894359113358	-1.125355094832	0.887435324660
Si	1.286427346600	-5.690051019420	2.318186258987
Si	-5.194582572892	-2.264922943951	5.868622071994
Si	-3.343727515868	1.246184457735	0.148892001335
Si	1.003877272980	-6.832688058208	7.275724276035
TV	5.233427633074	0.000000000001	0.000000000001
TV	-3.652043277728	5.252686466900	0.000000000002
TV	-0.619864098883	-2.166604302233	9.849118306557

EQ-SiO₂ 17

O	-3.904600954998	-3.233698434467	1.584463677238
O	0.912994345936	-1.137716872522	1.564841532160
O	-3.067440499509	0.967943888985	-0.067998655493
O	1.313837609948	-0.893936215028	-1.064531585731

O	-2.881760199414	-0.762284404164	2.025431217807
O	-1.232040289239	-1.083812407035	-0.109739975917
O	-3.097273604868	-4.142754488287	6.548507247182
O	1.720108699062	-2.047149480065	6.528682109107
O	-2.260556400307	0.058628664145	4.895622645493
O	2.120980870666	-1.802846926432	3.899526061480
O	-2.074303637550	-1.671244180193	6.989916978421
O	-0.425051358302	-1.993280118836	4.854706835696
Si	-1.227604740538	-0.884094782314	5.805078492467
Si	-4.191537570701	-1.736012297107	2.260226771505
Si	0.339042083179	-1.604501225271	0.067279299589
Si	-3.384226845933	-2.645029050883	7.223973450829
Si	-2.034581553220	0.024951066549	0.841000116820
Si	1.146073378652	-2.513754047665	5.031182846990
TV	6.497066328121	0.000000000001	0.000000000001
TV	-3.495539163029	4.234016930599	-0.000000000000
TV	1.614228509748	-1.818285940472	9.927724549687

EQ-SiO₂ 18

O	-2.479361961871	-2.380886884637	2.300488179854
O	0.136776191905	-2.554948080005	1.634652848787
O	-1.327603772661	0.941375383307	0.490996125453
O	2.087433723947	0.330093594816	-1.477616354116
O	-3.697446052580	-0.238986920731	1.135265857747
O	-1.725451450736	-1.610208868058	-0.167546770561
O	2.711915154189	-2.381250049514	2.300223021150
O	5.328220177049	-2.554909076746	1.634370290064
O	3.864199800765	0.941176582134	0.490645941263
O	7.278508776431	0.330198623120	-1.477690702286
O	1.494125123285	-0.238931883686	1.135388221465
O	3.465782232595	-1.610393360911	-0.167624434215
Si	2.708559164952	-0.134405247267	-0.004638661522
Si	-3.898718404728	-1.514620684848	2.192532136966
Si	-1.404002450056	-2.681946821069	1.066661103843
Si	1.292712082800	-1.514695257033	2.192535032551
Si	-2.482988515147	-0.134314120754	-0.004672018346
Si	3.787416430451	-2.682138038962	1.066494585554
TV	10.382681624219	0.000000000002	0.000000000002
TV	0.187418554876	5.165985981214	0.000000000000
TV	-1.205828941335	-1.293043616160	5.186254538007

EQ-SiO₂ 19

O	-2.437019267449	-2.486007660440	2.259227615298
O	0.193800469128	-2.581786727713	1.639468347961
O	-1.466708483508	1.128443943181	0.306485060600
O	1.870029535660	0.166631251969	-1.421585425544
O	-3.635404264308	-0.245982915705	1.248136480172
O	-1.608519133463	-1.482574315148	-0.123016827589
O	2.766481738200	-2.487444038170	2.258708985659
O	5.397208799044	-2.581454969247	1.639036989856
O	3.738243037114	1.125418663235	0.306200330273
O	7.073101457164	0.166700232887	-1.421564453748
O	1.568663326963	-0.246763327073	1.248236870702
O	3.593630104802	-1.485973601681	-0.124594813176
Si	2.676501984890	-0.103260499508	0.009644956944
Si	-3.834483189877	-1.581998071247	2.227551534617
Si	-1.333603673075	-2.653773072563	1.025729199991

Si	1.369340877519	-1.582755408516	2.227651407606
Si	-2.527326315589	-0.101111103991	0.010053849606
Si	3.869857846281	-2.656099491134	1.025094294492
TV	10.406728922724	0.000000000002	0.000000000002
TV	-0.041833564382	5.264239516896	0.000000000000
TV	-0.880692295446	-1.263228286162	5.191460915516

EQ-SiO₂ 20

O	-2.978251373863	0.410991161595	-0.407659695395
O	1.697285527611	-0.591689684456	-0.278674076367
O	-0.389735692186	0.183090309101	-0.652257300917
O	1.071688826725	2.183585077053	0.243987789246
O	-5.621006158678	4.811718410797	-0.408043812112
O	-0.944385878322	3.810926066985	-0.278893136891
O	-3.031849691958	4.584432589136	-0.651994017125
O	-1.570506612037	6.585521069048	0.244062565065
O	-8.263494764556	9.214084024862	-0.407599118909
O	-3.587411102065	8.211819788672	-0.278493732095
O	-5.674760143322	8.986487975798	-0.651839630407
O	-4.212122621363	10.987123745938	0.244025018295
Si	-9.086940913030	8.165495712817	0.574577844991
Si	-1.837800768892	5.005404431039	0.688257714885
Si	-4.479600550909	9.407143387786	0.688446093270
Si	-3.802008600561	-0.637377897403	0.574687023996
Si	-6.444444394998	3.764115729285	0.574907398199
Si	0.804845268143	0.603575952915	0.688092290111
TV	7.142216931700	0.000000000012	0.000000000010
TV	-7.926990270089	13.204500407605	0.000000000165
TV	-1.787716207841	-4.296775439556	2.348192453160

EQ-SiO₂ 21

O	-4.810283533627	-2.832168727421	2.702254517626
O	0.367327574772	-2.438893599177	0.453226125282
O	-0.217656947639	0.152240162981	1.063993900481
O	1.898817119905	-2.178541288230	-1.875350569436
O	0.769190520685	2.454146962485	-0.246518906284
O	-3.823324756914	-0.536886880438	1.389480817647
O	-2.044653731099	0.900989357191	2.702249317373
O	3.132921605810	1.294251283568	0.453231568543
O	2.547938306570	3.885422985170	1.064049368505
O	4.664408707706	1.554617607965	-1.875327377226
O	3.534730218022	6.187291893866	-0.246525172028
O	-1.057732974936	3.196258199393	1.389447622999
Si	4.083787149686	4.655123460135	0.540218952726
Si	-5.359246914594	-1.302380924503	1.915510810541
Si	-4.787231101742	-3.924275423647	1.227386105671
Si	-2.593651006934	2.430776789760	1.915525005542
Si	1.318204844433	0.921957597994	0.540228283302
Si	-2.021641424287	-0.191124173379	1.227384032446
TV	5.786075029130	-0.000000000000	0.000000000002
TV	5.531183317243	7.466316514561	0.000000000004
TV	-3.287439937691	0.501340414013	3.877122207520

EQ-SiO₂ 22

O	-3.091793167918	3.513272226806	0.328312602050
O	6.424976974035	-3.937871491591	-2.229106419730
O	-2.123738091372	1.162274263399	1.332441961290

O	-0.927035539145	-0.119882254185	-0.766931387258
O	-4.479326025392	2.038205605482	2.313928410785
O	5.051319209015	-5.382313406900	-0.260537580006
O	-3.488414443703	-0.284366069094	3.304976649515
O	-2.315133985705	-1.582133126476	1.215383222962
O	-5.850471453108	0.577079304710	4.316792077031
O	3.657642809167	-6.879822776922	1.766707224295
O	-4.903087412991	-1.782534395614	5.328313288655
O	-3.712118656020	-3.027557121358	3.204190143854
Si	-6.274287359153	-0.933273527425	4.928008512974
Si	-2.750887153719	-1.697880894307	2.835757072549
Si	-4.139359959989	-3.168595603898	4.825123811718
Si	-3.505454327182	2.000043416233	0.940597188347
Si	-4.886992803099	0.531297061109	2.937056282068
Si	-1.366769197289	-0.238953653241	0.852167235175
TV	5.652894194691	0.000000000011	0.000000000009
TV	-3.643142671245	6.504476499823	0.000000000077
TV	-4.150764260754	-4.394674209943	5.973271623471

EQ-SiO₂ 23

O	-2.881364847571	-0.033925647155	-0.548587880464
O	1.757599659971	-0.506052700490	-0.361713138674
O	-0.300030145276	0.335562426579	-0.763026645597
O	0.824665012592	2.235094293654	0.605963236965
O	-5.421973928298	4.548437047517	-0.557273089688
O	-0.784193905629	4.099477688392	-0.358991122957
O	-2.840449838310	4.942638338756	-0.762902262876
O	-1.716187909669	6.843153155239	0.606899673004
O	-7.962258725861	9.155783815966	-0.558199361528
O	-3.323738827443	8.709195532568	-0.359646771789
O	-5.380942518220	9.550429207442	-0.761315943917
O	-4.239552255818	11.455198815559	0.586359491804
Si	-8.953344535489	8.495501677043	0.571426578817
Si	-1.717645626425	5.191087975686	0.676047449809
Si	-4.254623343264	9.803986787302	0.674081003795
Si	-3.871733817361	-0.717009907609	0.568942884991
Si	-6.414106627467	3.887311188229	0.571713957247
Si	0.822673667470	0.583172140766	0.675811158876
TV	7.216081098595	0.000000000011	0.000000000010
TV	-7.618423154717	13.824799399171	0.000000000162
TV	-1.974736563160	-4.584572005392	2.375914685289

EQ-SiO₂ 24

O	-0.644248739486	1.601311535972	1.503526961588
O	5.828089531657	-0.049706591978	-3.223235810571
O	-3.533554725296	-0.398866371698	0.808607568363
O	-0.825488947462	0.125568808527	-0.754485003317
O	-1.164541931227	4.384270757707	1.503684213311
O	5.307417633169	2.733126659531	-3.223205812576
O	-4.054134234314	2.384281468270	0.807843501986
O	-1.345620711258	2.908716484292	-0.754632648533
O	-1.685572893786	7.166874571028	1.504192280458
O	4.787357389824	5.516248413662	-3.223667441805
O	-4.573960217370	5.167254025423	0.808774668267
O	-1.866016375653	5.691485330180	-0.754548065273
Si	-5.656306994501	6.405356451227	1.151371247438
Si	-0.527977021682	3.063663036624	0.682637443264

Si	-1.048447753613	5.846592824806	0.682851423672
Si	-4.615656094917	0.839440011797	1.151164208302
Si	-5.136082605015	3.622491208021	1.151215087697
Si	-0.007940809336	0.280166859286	0.683017847810
TV	7.583061110383	0.000000000012	0.000000000009
TV	-1.561094555650	8.349057510197	0.000000000116
TV	-3.730784215900	-2.157088652691	3.502242075455

EQ-SiO₂ 25

O	-3.656221867873	-3.539519369011	2.072743754466
O	-0.040761273746	-0.822076141358	1.416742863856
O	-0.048720879083	1.634859908489	0.179005049421
O	-0.025259945914	-1.891607524387	-1.402215793183
O	-1.855497013394	-1.887346239921	2.995164029391
O	-1.831756250390	-0.232325040292	-0.483131913248
O	0.021589631860	-3.539533253816	2.072665311657
O	3.637131907710	-0.821991379643	1.416838995585
O	3.629268085676	1.634632583499	0.178763869403
O	3.652595198320	-1.891394819976	-1.402236703856
O	1.822252232551	-1.887343249870	2.995167634532
O	1.845782153882	-0.232450705940	-0.482939466198
Si	2.700372013284	0.404778706620	0.799427327183
Si	-3.726512552417	-1.967491725538	2.613422706034
Si	-1.892378911101	-1.806400639955	-1.020890280719
Si	-0.048799757932	-1.967520189938	2.613415181258
Si	-0.977461471660	0.404799135316	0.799469800918
Si	1.785391195748	-1.806479007871	-1.020947962885
TV	7.355610563510	0.000000000002	0.000000000008
TV	1.812567857548	4.582590812339	0.000000000001
TV	0.009171054271	0.325355687867	5.714000783698

EQ-SiO₂ 26

O	-1.574924625348	1.122263425775	0.716177851530
O	-0.678015023954	1.394908749294	3.176037197779
O	2.231829821172	2.101315300511	2.600774368076
O	1.039146645879	0.405205120405	0.273347222785
O	-2.383485740360	3.846916204968	0.721759118780
O	-1.483742116810	4.087913096061	3.181584827985
O	1.429888783853	4.817870081439	2.606598149186
O	0.230773645812	3.118988637972	0.283700930675
O	-3.183621767433	6.536609401603	0.712624700501
O	-2.287085844525	6.813383802301	3.170822098141
O	0.625884884789	7.532573003484	2.602574925002
O	-0.567021873151	5.836594190820	0.270592203715
Si	-1.780369602473	6.949905885223	-0.072642969324
Si	-2.844240066845	3.703079292508	2.310178485433
Si	-3.647649919389	6.417270865133	2.302817258777
Si	-0.169720057614	1.524463921364	-0.068090956530
Si	-0.975631328667	4.238960377404	-0.063592002794
Si	-2.035841097929	0.992332056257	2.306292189422
TV	5.495443565659	-0.000000000000	-0.000000000000
TV	-2.412837306863	8.139085297403	0.000000000000
TV	-0.145706234444	-0.033594789044	4.860711713442

EQ-SiO₂ 27

O	0.524126579869	2.129516767552	2.475540844027
O	1.120981384392	-0.233921719511	1.563779808387

O	-1.401881748043	0.697751029268	1.221861626870
O	0.351118250489	2.655733370788	0.293679107260
O	-2.149489651422	6.429900674509	2.475997744485
O	-0.248761167180	5.021944109945	1.229536208279
O	-2.788764746989	4.068291013182	1.529011295820
O	-2.036542152958	6.950188198109	0.286026328039
O	-4.646874491811	10.747489139691	2.486480581925
O	-3.924969341305	8.390719903651	1.559942049430
O	-6.465085935563	9.305630291587	1.198457818565
O	-4.647190875217	11.252651856020	0.285144234089
Si	-2.312845072429	8.037637431007	1.744860247221
Si	-1.863153570883	5.346025652106	1.018308339920
Si	-4.851382009765	9.649407392299	1.015653488405
Si	2.737797948562	-0.564420910748	1.755776838677
Si	0.667674068289	3.738176909176	1.743519378922
Si	0.210444492942	1.043889285538	1.025984095229
TV	5.068291033017	-0.000000000002	-0.000000000004
TV	-7.600446255335	12.914335736055	0.000000000004
TV	-2.527226625172	-2.836737870500	3.260600570970

EQ-SiO₂ 28

O	-1.632078516332	-4.010604005684	2.674286122472
O	0.320537763242	-2.108208026660	2.328452739287
O	-2.325048344026	1.822742730481	0.436802768786
O	2.274437800776	-0.196951598064	-1.633215268963
O	-3.938421881556	-0.263370466395	0.419945433687
O	-1.945368300177	-2.105988589599	0.811529106679
O	-1.640520803334	-4.013378948227	6.975169418509
O	0.311958310614	-2.110437579248	6.629732715042
O	-2.333391606721	1.820174622955	4.738121943984
O	2.266076014859	-0.198956929151	2.667784726078
O	-3.946962739747	-0.265709985824	4.720999967434
O	-1.953468770985	-2.108244238325	5.112881311200
Si	-3.140308103310	0.786886723386	3.701822922473
Si	-3.089021614744	-1.159914553165	1.557777084684
Si	-0.807234115091	-3.059794996714	1.559936832926
Si	-3.097537824540	-1.162288944581	5.858881240936
Si	-3.131810745492	0.789121694846	-0.599347039803
Si	-0.815603761210	-3.062231937772	5.861184923866
TV	4.537700732329	0.000000000001	0.000000000001
TV	-2.364139053569	5.802759269000	0.000000000001
TV	-0.016929712799	-0.004641217590	8.602320920920

EQ-SiO₂ 29

O	-2.602839259217	2.284241046901	0.374998083732
O	4.117511223841	-0.594203473077	-1.598900329223
O	-1.995443036958	-0.358010945190	0.762058773346
O	0.817991118474	0.419311269350	-0.533103417732
O	-3.673856123185	-1.383436086318	3.638179454057
O	3.047975667607	-4.268024514548	1.670677685399
O	-3.068059854991	-4.024991880224	4.026919526285
O	-0.258630165663	-3.240656667684	2.735791533598
O	-4.741958346895	-5.034499465484	6.918883823734
O	1.978299857864	-7.935976487046	4.941137710241
O	-4.141264652324	-7.677966334523	7.294994044363
O	-1.328632246755	-6.895626858514	6.001346860226
Si	-5.288877981443	-6.492567983237	7.474048584818

Si	-1.526629529790	-4.232821320762	3.468922495280
Si	-2.599222566256	-7.886208128913	6.737652692069
Si	-3.144483133637	0.826462243002	0.936660231343
Si	-4.215309448727	-2.839221089298	4.204118580758
Si	-0.455215753058	-0.565655394880	0.201355524332
TV	5.008218393081	0.000000000012	0.000000000011
TV	-2.647688625119	4.423227829169	0.000000000055
TV	-3.219661310639	-10.983079944315	9.805115746379

EQ-SiO₂ 30

O	-2.762607527481	0.295913205773	-2.697573745928
O	-4.097403057786	-1.467514777543	-1.098091664718
O	-4.833568122417	-0.138186423686	1.407528168247
O	-0.119049401485	0.794546861173	1.261285369685
O	0.061891194907	-0.612819726946	-1.062223357459
O	-2.326977959881	0.351033781807	-0.099166499566
O	-3.345198093904	3.076301961362	-2.697598375078
O	-4.679963982573	1.312865623767	-1.097998588819
O	-5.416155814532	2.642290422255	1.407475674013
O	-0.701701578706	3.574812686610	1.261118161619
O	-0.520802383521	2.167542411404	-1.062083598549
O	-2.909726169907	3.131523483326	-0.099191283032
Si	-6.468779882802	3.871681180623	1.863305451041
Si	-3.516126422127	0.104301810981	-1.235453064201
Si	-0.706304776331	0.676268687344	-0.296074873136
Si	-4.098832297397	2.884699941279	-1.235513570311
Si	-5.885996313246	1.091403511768	1.863279463662
Si	-1.289000470365	3.456673101225	-0.296161592106
TV	7.285758952323	0.000000000002	0.000000000002
TV	-1.165371756839	5.560749970887	0.000000000003
TV	-2.593488841960	-1.975913305377	6.210219913395

EQ-SiO₂ 31

O	-2.330625669235	-2.400300684504	1.993460860522
O	0.454161578422	-7.214530393725	3.125256063664
O	-3.746830803697	2.720204296416	-0.004833987027
O	2.000294189152	0.665416834244	-1.697634533594
O	-2.304407872677	0.512792040488	0.613392523204
O	-0.931442610617	-1.903421787032	-0.298912968907
O	0.513463079128	-2.401017255780	1.993398856770
O	3.298855261038	-7.214785549528	3.125358857755
O	-0.902216638573	2.719442980664	-0.004075465631
O	4.845014462574	0.665208504006	-1.697721474189
O	0.540656857444	0.512135616217	0.612971722965
O	1.913496072170	-1.903307283683	-0.298676196882
Si	1.961967954266	1.078812003516	-0.095081239066
Si	-2.341534067504	-1.252099749337	3.191142382921
Si	-2.354530711411	-2.533280709715	0.343238891505
Si	0.503309401984	-1.252467009498	3.190967045710
Si	-0.882885316761	1.078299341008	-0.095008909661
Si	0.490419501474	-2.533844212642	0.343221973721
TV	5.689957850244	-0.000000000000	0.000000000014
TV	-1.372494314472	6.861247523829	0.000000000001
TV	-1.488695180567	-2.821433298980	6.284120082578

EQ-SiO₂ 32

O	-3.800128880481	3.417777111101	1.173983635938
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O	4.598566842162	-3.231020156137	-0.398973930910
O	-2.426139512403	2.131383560157	-0.398991591717
O	-0.879646439731	-0.834723365270	-0.913969717276
O	-5.174706823274	2.311785692927	3.257549089181
O	3.223849467376	-4.341724701053	1.687031785144
O	-3.800852182452	1.020738721880	1.687051562653
O	-2.256363965511	-1.944664463704	1.173960940806
O	-6.551063645391	1.206183362004	5.344446507315
O	1.846467127290	-5.446575050047	3.775797987305
O	-5.178209955579	-0.084139997814	3.775812945220
O	-3.630951467387	-3.050642594277	3.257532126719
Si	-5.183098461949	0.008361026624	5.602798930854
Si	-0.886838648377	-3.142674335758	1.429235961619
Si	-2.263044941393	-4.248541779115	3.515570898415
Si	-2.430613788448	2.219750607421	1.429229415716
Si	-3.806807187927	1.113938361090	3.515603403111
Si	0.488323670856	-2.032573183390	-0.655630517118
TV	5.480939283598	0.000000000011	0.000000000010
TV	-4.284230832907	5.362423263397	0.000000000072
TV	-4.127655529905	-3.321488989530	6.258440447000

EQ-SiO₂ 33

O	-1.725859634903	-5.100400897740	3.344355991710
O	-0.306872222419	-4.125275698002	0.791076758553
O	-1.733332540813	1.292983157344	0.864943512147
O	1.096523068699	-0.348350231616	-1.588394542413
O	-1.737804342254	4.036154610503	-1.212398529540
O	-1.725257012842	-1.876853816458	1.235257881765
O	1.112898896323	-5.100405141837	3.344336633829
O	2.531864304221	-4.125261955212	0.790949766939
O	1.105398918611	1.292990741359	0.864944614529
O	3.935298248767	-0.348194059608	-1.588241310475
O	1.100976539212	4.036176969537	-1.212380491826
O	1.113494382638	-1.876834655580	1.235257825537
Si	1.106387637430	2.662859126680	-0.174232106371
Si	-3.145370619278	-2.646933851491	1.678703211592
Si	-1.731492563239	-6.577490744694	2.456173777964
Si	-0.306611899008	-2.646890675441	1.678737464001
Si	-1.732357008029	2.662854169425	-0.174237543305
Si	1.107251884067	-6.577488614778	2.456177859557
TV	5.677501712912	0.000000000002	0.000000000002
TV	-0.007901227546	7.549780375341	0.000000000001
TV	-1.416521151455	0.548773024351	4.484509448038

EQ-SiO₂ 34

O	-1.522304823515	-1.123472221060	2.558903382556
O	0.269335675447	-2.441290367859	1.803300529045
O	-1.546845077283	0.732319347233	-0.864116816403
O	0.323520988827	-1.147901374397	-1.838829864649
O	-3.265576543181	0.065439862291	1.027795703509
O	-1.563792062536	-1.823071772716	0.056758366328
O	2.059327594061	-1.123516420558	2.558913179069
O	3.851040113178	-2.441241279662	1.803449029271
O	2.034877623248	0.732332095048	-0.864180301733
O	3.905135067083	-1.147913839491	-1.838827629956
O	0.316115069241	0.065447397662	1.027807947637
O	2.017869710868	-1.823055992999	0.056767218575

Si	1.109325045133	-0.539619671168	-0.403510778975
Si	-3.309458724842	-0.931171272407	2.800024286121
Si	-1.519779988997	-2.634363046175	1.562231318495
Si	0.272199371649	-0.931152245628	2.799991051442
Si	-2.472371578609	-0.539682840796	-0.403521208383
Si	2.061900432132	-2.634378670601	1.562223701439
TV	7.163296439152	0.000000000000	0.000000000002
TV	1.802976970408	4.392112800466	0.000000000000
TV	-0.004031283704	1.909252091100	5.168060994537

EQ-SiO₂ 35

O	-1.630611631252	-5.609300526776	2.899805144092
O	-0.207102807568	-3.577666348183	1.381503139548
O	-1.641631593798	1.760279600322	0.157360865500
O	-0.197987126177	-1.014723764752	-1.730020777886
O	-1.634322106788	4.072401479958	-0.646584264831
O	-3.060700486495	-0.191703617335	1.233182403684
O	1.212319673558	-5.609333359593	2.899834216161
O	2.635718775752	-3.577612286065	1.381476562990
O	1.201290956509	1.760266807463	0.157296156048
O	2.644898919910	-1.014712069098	-1.729912050922
O	1.208526170734	4.072459453164	-0.646619970259
O	-0.217797241222	-0.191693997059	1.233148612001
Si	2.622504759330	2.913540722351	-0.244583644781
Si	-3.045003613214	-2.806805194361	2.789711628200
Si	-1.628689687694	-6.374725617913	1.488404742056
Si	-0.202101290992	-2.806787493406	2.789692828432
Si	-0.220381939626	2.913499958207	-0.244577938498
Si	1.214206716441	-6.374703864923	1.488396888777
TV	5.685785405205	0.000000000001	0.000000000004
TV	-0.010997072591	7.034204038569	-0.000000000000
TV	-1.425332371875	-0.940472951737	4.769937924412

EQ-SiO₂ 36

O	-0.860687968351	-3.918990978488	1.735009118642
O	1.611656603320	-3.182772716944	0.803499750402
O	-1.936657761446	0.215635429077	0.203635655688
O	-0.963761734694	-2.167824717427	-0.005601686989
O	-3.987022963774	1.485450617730	-0.609319250175
O	-3.838997142696	-0.684331580585	1.849812450663
O	-1.047201121766	-2.502312248284	4.770249716499
O	0.636244000024	-2.555547188549	3.242759615735
O	-2.639512686978	0.650363774294	3.847146997254
O	-1.122386275563	-0.917973344390	2.430715361251
O	-4.317574379321	2.856901728280	3.017398860978
O	-4.929877746775	-0.475414890845	4.874648875117
Si	-2.672185197148	3.223758058414	2.963895156910
Si	-4.033043789167	-2.303766665923	2.158352682966
Si	-0.856788484815	-5.623512268799	2.223815577142
Si	-5.340309259812	-2.054125999304	5.256019046953
Si	-2.439426398783	1.891410728466	-0.071236680056
Si	-1.858771458698	-5.607665118271	5.198068778735
TV	5.943406883464	0.000000000001	-0.000000000001
TV	-1.561178630925	5.743019013426	0.000000000001
TV	-1.578043492942	1.217883456152	6.075203161344

EQ-SiO₂ 37

O	-3.784701582681	-0.526008648100	-2.151646087473
O	-5.198374779118	-1.946337210070	-0.350555097313
O	-5.502870572026	-0.537257649908	1.973033473234
O	-0.076653878511	0.874222833291	0.852595091215
O	-0.531368867965	-0.530780626054	-1.463340412239
O	-2.489567060714	0.886732419724	-0.195608770614
O	-3.775227089583	2.301838440600	-2.151412330261
O	-5.188878773283	0.881399745956	-0.350518721715
O	-5.493251579728	2.290324192386	1.973046657317
O	-0.067086488521	3.702064337431	0.852484576252
O	-0.521578594946	2.296736937202	-1.463731616117
O	-2.480010204685	3.713979215354	-0.195545737456
Si	-5.881214239810	3.706905493555	1.151326583376
Si	-3.791968362636	0.889910682765	-1.239386258406
Si	-0.868843841124	0.885808295113	-0.608243774186
Si	-3.782425493002	3.717657083399	-1.239401014875
Si	-5.890749964844	0.879251088937	1.151205419860
Si	-0.859319011071	3.713265003183	-0.608325019528
TV	7.454434709706	0.000000000000	0.000000000001
TV	0.019161671534	5.655305472300	0.000000000002
TV	-4.718240069084	-0.054488801863	10.575163515769

EQ-SiO₂ 38

O	-2.086878990847	-2.224007312412	3.576959655366
O	0.637144044007	-2.225890777144	0.302281485974
O	-1.751124667200	0.520938931678	1.269505595052
O	2.006982802740	-0.850137162610	-3.139150402244
O	-1.697789124738	1.892123803655	-0.824335655152
O	-3.763853793453	-0.850955967282	2.065563995431
O	-2.089286545349	0.519591625585	3.576955612206
O	0.634785868884	0.517642636902	0.302235754556
O	-1.753514683004	3.264540914221	1.269508608178
O	2.004527029348	1.893397163522	-3.139267203538
O	-1.700198253934	4.635704054339	-0.824353965899
O	-3.766273977928	1.892637072575	2.065590852387
Si	-0.868546129427	3.264224250728	-0.435857898329
Si	-4.945780946989	-2.221584069690	1.940109714053
Si	-1.917965271022	-3.594793980685	2.415226368538
Si	-4.948178347770	0.521980511925	1.940086276969
Si	-0.866154475194	0.520632300018	-0.435850041007
Si	-1.920333313462	-0.851209382935	2.415255651119
TV	5.915138794390	0.000000000001	0.000000000001
TV	-0.004785505319	5.487166119772	0.000000000002
TV	-2.059592902752	-0.001149191226	5.730891657093

EQ-SiO₂ 39

O	-2.734703089123	3.279381895582	0.090426504344
O	4.539927976796	-4.898507514815	-1.946531288481
O	-0.915468556700	1.717299804069	1.191046201322
O	-0.904675450891	-0.445286920705	-0.845416846866
O	-2.733691588998	2.558844943857	2.906461080724
O	4.540995253543	-5.618904842923	0.869550124812
O	-0.914466205547	0.996891631147	4.007200824434
O	-0.903646504689	-1.165633377979	1.970713909637
O	-2.732648214744	1.838577526987	5.722528698170
O	4.542003013095	-6.339258899135	3.685677800394
O	-0.913406130569	0.276622613230	6.823392926583

O	-0.902660259144	-1.885975308887	4.786865284336
Si	-2.728193397209	0.664993191249	6.923011056892
Si	-0.909695997771	-0.717957962684	3.585717537097
Si	-0.908728517302	-1.438198448428	6.401842153613
Si	-2.730198241669	2.105591403834	1.290712603992
Si	-2.729216119105	1.385192597469	4.106831761110
Si	-0.910561191598	0.002401012714	0.769590750285
TV	3.631870498765	0.000000000010	0.000000000009
TV	-3.640599400915	6.007846555304	0.000000000083
TV	0.003106361033	-2.160950771961	8.448350565094

EQ-SiO₂ 40

O	-3.204272087377	-5.873696532064	1.839850937079
O	0.071931823429	-2.771533170247	0.439700691292
O	-2.319001760660	0.851397131499	0.435116265740
O	1.465257088858	-2.806278131426	-1.771121680427
O	-1.572482902562	3.570283893313	-0.733085500870
O	-1.366882996435	1.807752895325	2.697313897292
O	-3.206347960263	-1.228543160915	1.839852068906
O	0.069840383413	1.873629154166	0.439691322807
O	-2.321079782771	5.496559782290	0.435106080863
O	1.463171780131	1.838879161792	-1.771117140111
O	-1.574565932275	8.215445134175	-0.733085499473
O	-1.368968695470	6.452899345659	2.697323090581
Si	-0.632657164221	4.936148685007	0.023632135376
Si	-4.883322398693	-2.031705919563	2.088327767335
Si	-2.362213327026	-4.354568813422	2.097624180773
Si	-4.885413383576	2.613461712226	2.088328968509
Si	-0.630571789489	0.290996551567	0.023626818796
Si	-2.364309005371	0.290597543327	2.097623121524
TV	5.008402272631	0.000000000001	0.000000000001
TV	-0.004164388114	9.290311479952	0.000000000002
TV	-2.150039385310	2.323784163294	3.396155177027

EQ-SiO₂ 41

O	-4.794268145607	-4.748477118531	3.604543997700
O	-2.384243119105	-4.189739753203	4.195795265691
O	-1.710303249667	-0.063635993178	1.481045490374
O	3.276224395207	-0.041210937829	-5.365842060482
O	0.587265901991	0.936488385097	1.137558730895
O	-3.974602591150	-1.723764507987	1.473977013306
O	-0.014482759594	-4.748496550285	3.604550095741
O	2.395536376768	-4.189740019928	4.195791101891
O	3.069463961329	-0.063603656808	1.481045767163
O	8.055999146918	-0.041225593701	-5.365838014027
O	5.367042631313	0.936443092582	1.137548093627
O	0.805192539955	-1.723756531832	1.473973663631
Si	4.005638207509	0.343377289047	0.077110710018
Si	-4.649763341819	-2.491325503474	0.067321167829
Si	-4.679575228352	-4.892581158963	1.945649838813
Si	0.130031112845	-2.491307612644	0.067327219336
Si	-0.774143119203	0.343399391860	0.077110735858
Si	0.100200883680	-4.892573885575	1.945648954632
TV	9.559573865846	0.000000000002	0.000000000002
TV	1.437351958907	4.539547015172	0.000000000001
TV	-3.954852721596	-1.147721459165	4.781701334191

EQ-SiO₂ 42

O	-1.056887433143	1.337630959442	1.537795027442
O	4.760550507934	1.158836797763	-6.291462723782
O	-1.053026768604	-0.476600189071	2.916434668842
O	-3.910415709400	-0.663376794141	-2.444697829465
O	1.834709375237	1.337626780787	1.537798116484
O	7.652143082065	1.158841053678	-6.291456571334
O	1.838566410022	-0.476605419025	2.916434370000
O	-1.018825360909	-0.663373230152	-2.444698774185
O	4.726297298839	1.337638126509	1.537802154029
O	10.543740684872	1.158840032346	-6.291455130927
O	4.730145625890	-0.476595723246	2.916430634114
O	1.872766910637	-0.663384327534	-2.444706181809
Si	4.725529518945	1.335202177429	3.308700745621
Si	1.835651474183	-0.474297871120	1.145303880843
Si	4.727234009396	-0.474283901965	1.145300497888
Si	-1.057655325454	1.335192775927	3.308694532364
Si	1.833937866740	1.335185056520	3.308696998108
Si	-1.055943056467	-0.474292624678	1.145302388963
TV	8.674771006921	-0.000000000021	0.000000000009
TV	-0.006272869326	3.622442671877	0.000000000050
TV	-1.478689096595	-1.627380542070	6.594988428201

EQ-SiO₂ 43

O	-2.096396605594	-2.970478868245	3.569190188724
O	0.973713388975	-2.330878253348	0.311685435465
O	-1.811081213860	-0.064360264526	1.480536456317
O	3.038290298172	-0.473130658399	-2.949887434920
O	-2.196649167354	1.283314442975	-0.647819980205
O	-3.762074137693	-1.888897587986	1.685401815196
O	-2.656224489947	-0.241477922352	3.569264092159
O	0.413829746350	0.397833949757	0.311555967696
O	-2.371021562413	2.664572104224	1.480452703195
O	2.478364755007	2.255696807832	-2.950031165950
O	-2.756581198597	4.012197658297	-0.647875819815
O	-4.322200595526	0.839915108589	1.685064745921
Si	-1.657290590784	2.815053566055	-0.318176893237
Si	-5.357163328276	-2.218696512400	1.883796217754
Si	-1.728973924306	-4.315774277500	2.381078883197
Si	-5.917282522175	0.509980860106	1.883756146297
Si	-1.097222311800	0.086318969557	-0.318109614399
Si	-2.288823971885	-1.586991784010	2.381149030810
TV	6.875603012934	-0.000000000000	0.000000000001
TV	-1.120035116871	5.457562243142	0.000000000004
TV	-2.288869374812	-0.481447556895	5.629488098777

EQ-SiO₂ 44

O	-3.786646319607	-4.646579317211	4.095105412909
O	-1.242020313909	-2.659332309800	0.686718504690
O	-2.182372117865	0.863085894144	0.772106307079
O	1.806434024516	-1.241595941911	-2.310130097115
O	-0.779849143643	0.570556822828	-1.397275642785
O	-3.317960435392	-1.421945451018	2.010152455919
O	-2.086128491200	-0.208497488356	4.095092938811
O	0.458438883425	1.778527914264	0.686920311548
O	-0.481983119954	5.300944673917	0.771967565936
O	3.506804555482	3.196277527840	-2.310158233321

O	0.920679993728	5.008291990367	-1.397391766478
O	-1.617661860574	3.015927209552	2.010131141831
Si	1.200639881983	4.954467156838	0.376574785869
Si	-4.785735979021	-2.037824481321	1.348738805163
Si	-4.064733702630	-4.593042818674	2.319035579831
Si	-3.085442570470	2.400129082732	1.348880839062
Si	-0.499831783754	0.516619227932	0.376547470468
Si	-2.364210865997	-0.155132569775	2.319059769599
TV	5.008279518406	-0.000000000000	0.000000000001
TV	3.400896278472	8.875770774944	0.000000000003
TV	-2.488512520460	0.740794270861	4.236042982972

EQ-SiO₂ 45

O	-3.465750448041	-2.466622533100	1.972807691451
O	-1.102729851925	-1.825260632065	2.293737211826
O	-0.108216120978	0.212118399769	0.284302734616
O	3.210972938408	-0.203633562107	-1.787557376920
O	-2.826782826104	0.842442733940	0.613946909007
O	-2.076588510302	-1.755837824899	-0.080903608452
O	1.614212314242	-2.466620872282	1.972783279131
O	3.977220211640	-1.825291985959	2.293731319853
O	4.971686916263	0.212082210701	0.284276086395
O	8.290909042451	-0.203654215079	-1.787567024491
O	2.253153914986	0.842500490534	0.613971555489
O	3.003335049209	-1.755864509515	-0.080922557656
Si	3.396646052184	-0.045230161187	-0.037961334346
Si	-4.606943208153	-1.573771356249	2.623149985152
Si	-1.956106081712	-3.029053595976	1.288778233936
Si	0.472991896016	-1.573776499636	2.623101118664
Si	-1.683254345916	-0.045215778455	-0.037975604916
Si	3.123829369013	-3.029101419323	1.288765784912
TV	10.159833023087	0.000000000002	0.000000000002
TV	2.702128372859	4.444308738935	0.000000000000
TV	-2.340536938472	0.338180101830	4.456830701561

EQ-SiO₂ 46

O	-4.203630487831	-3.290822299184	2.608687117212
O	-0.285543585528	-3.462636613066	0.240945928219
O	-0.548797496010	0.260451367348	0.502263952391
O	0.977965284189	-1.026060792772	-2.114277637590
O	0.109518860490	2.941992705215	-0.020221904576
O	-3.532197648694	-0.602676759270	2.101468006374
O	-6.374247206401	-3.621109580887	7.045390472967
O	-2.456369507579	-3.793685713844	4.676598122172
O	-2.719505719639	-0.070536786666	4.938934116713
O	-1.192685708357	-1.356280887631	2.322374860652
O	-2.061639034030	2.611596505999	4.416822911445
O	-5.703175627165	-0.932734143126	6.538435815820
Si	-1.616996007803	0.915781663497	4.354564445935
Si	-4.641208096723	-1.592541942863	2.669326307589
Si	-4.456594195321	-4.630671089309	1.293031119456
Si	-6.812052235686	-1.922867774225	7.106159148011
Si	0.554031517140	1.246256560638	-0.082170165940
Si	-6.627616585038	-4.961162376530	5.729667794535
TV	5.017579101211	0.000000000001	0.000000000001
TV	2.412548491274	4.456549250085	0.000000000001
TV	-4.341719213741	-0.660541033861	8.873846419746

EQ-SiO₂ 47

O	-1.520141958989	-2.123940445401	2.440978228295
O	0.263815372420	-3.008291334899	1.340648350409
O	-1.583992308936	1.171113648851	0.120803369295
O	0.310802130062	-0.074025810019	-1.399246265390
O	-3.260699993329	-0.328207836088	1.478207681796
O	-1.581056436408	-1.687995325622	-0.208430585632
O	2.071817054363	-2.124259420184	2.441026062139
O	3.855808857749	-3.007777374686	1.339844627017
O	2.007804962607	1.171460446440	0.120351667381
O	3.902887497347	-0.074148343667	-1.399346349449
O	0.331547572204	-0.328208652501	1.478503692062
O	2.010360219677	-1.687585723435	-0.208505260849
Si	1.160455928106	-0.258933463246	0.021369937647
Si	-3.317616168006	-1.656217478814	2.503950284665
Si	-1.528706359521	-2.972259334650	0.872565583520
Si	0.274251376673	-1.656256407395	2.504145118728
Si	-2.431250185592	-0.259322873691	0.021314177954
Si	2.062924814161	-2.971966738826	0.872284084133
TV	7.183757359717	0.000000000002	0.000000000002
TV	-0.111408942372	5.608589938851	-0.000000000000
TV	-0.094128203307	-1.144555533055	5.491848898253

EQ-SiO₂ 48

O	-1.901243265748	-2.705364693205	3.493195815822
O	0.016388545016	-0.962016875206	-0.079863504045
O	-1.841775771545	0.089259976282	1.235909562106
O	2.012266628840	-0.821406584932	-2.834517210195
O	-2.586969859457	0.603930223545	-1.113700217537
O	-3.711035401240	-1.627743697435	1.964145004417
O	-2.348941314063	0.049629594278	3.493196128853
O	-0.431259084560	1.792947780911	-0.079897965133
O	-2.289462020633	2.844204434223	1.235916015493
O	1.564615443323	1.933597484148	-2.834561459186
O	-3.034654157576	3.358877351125	-1.113695577266
O	-4.158724423278	1.127203516275	1.964200459725
Si	-1.472202174486	3.046589192188	-0.459487945200
Si	-4.782873605654	-2.249009507097	3.029122770620
Si	-1.590937617884	-4.097514453135	2.315772181785
Si	-5.230619089141	0.505935366662	3.029130163546
Si	-1.024511363648	0.291625570567	-0.459518033065
Si	-2.038682189886	-1.342532340133	2.315815441287
TV	5.952933704323	0.000000000002	0.000000000000
TV	-0.895415768049	5.509941652791	-0.000000000016
TV	-2.063065983703	-0.203766429499	5.688229364845

EQ-SiO₂ 49

O	-3.790118977779	-5.771256481763	3.416080387815
O	-0.373242927778	-4.459264262764	1.572928583893
O	-2.478665671486	0.254287437771	1.031194310313
O	1.696023435190	0.021659879458	-2.110558446926
O	-0.831855841839	4.017904704633	-0.696720699630
O	-3.944040514576	-2.071214185782	1.137659348259
O	1.237893021367	-5.771287414496	3.416073099541
O	4.654694216460	-4.459250111850	1.572954264462
O	2.549351733343	0.254286693765	1.031201176915

O	6.724065172607	0.021749777156	-2.110530825411
O	4.196153648764	4.017912226778	-0.696712041220
O	1.083976574619	-2.071254685347	1.137667930037
Si	4.040976024487	0.290088177516	0.250484481530
Si	-5.035885440973	-2.922417322692	2.088892533066
Si	-3.165528359122	-6.230645501240	1.927154299595
Si	-0.007875912243	-2.922439238366	2.088910545039
Si	-0.987018373572	0.290074812418	0.250482996783
Si	1.862500877147	-6.230665171367	1.927155827262
TV	10.056039745964	-0.000000000032	0.000000000040
TV	0.353400274592	5.110242319163	0.000000000280
TV	-3.096420096033	-2.016881957740	4.279916098597

EQ-SiO₂ 50

O	-4.091052865453	4.326101044088	2.681320037276
O	4.033413372874	-2.406927273385	-3.358274511926
O	-2.039371677555	0.080677060692	0.677931486852
O	2.021043006597	-2.366336923437	-1.355275517631
O	-4.086817197334	4.407427025289	6.687203886330
O	4.037592737819	-2.325556623466	0.647483503285
O	-2.034941729019	0.162754954177	4.684108141784
O	2.025251224886	-2.284656692887	2.650290086100
O	-4.082994671776	4.488226394010	10.692561104009
O	4.041872564329	-2.244108709876	4.653457856198
O	-2.030735045223	0.244400908661	8.690416296130
O	2.029417876307	-2.203461254466	6.656459266096
Si	-3.037101604662	1.164039261601	9.673700359273
Si	-1.028897258676	1.041992607367	3.664518142682
Si	-1.024643451269	1.123274963604	7.670622108006
Si	-3.045283160834	1.000836347690	1.661545740109
Si	-3.041206268744	1.082442471101	5.667590731858
Si	-1.033014033416	0.959973288417	-0.341392028352
TV	4.028782046137	0.000000000013	0.000000000011
TV	-4.068365037626	4.204015681792	0.000000000049
TV	0.012513344879	0.244329213852	12.017757370576

EQ-SiO₂ 51

O	-2.906519247647	-4.979506420429	4.211917354118
O	0.852819630213	-8.661725056781	-1.798447667810
O	-1.347107279558	3.430565875843	0.489629109688
O	0.952947971109	-0.770268428175	-1.015800483338
O	-2.992301325900	2.089683573696	-1.123966329584
O	-4.194854024127	-1.201486585935	2.249425752483
O	-5.348884692613	-5.060907405382	8.248178778178
O	-1.610930974204	-8.758707294028	2.244477773874
O	-3.788200634925	3.355694712193	4.528307267383
O	-1.529247984100	-0.839365683948	2.949691307100
O	-5.454222402456	2.006025185857	2.921882339789
O	-6.633773361171	-1.279922572178	6.289463865475
Si	-3.879440110191	1.975047202241	3.388003499402
Si	-5.683055018947	-2.192607353134	2.301540605220
Si	-2.519857436364	-6.378434003961	3.403171214978
Si	-8.124498616976	-2.272544768266	6.346852162800
Si	-1.416550446133	2.058531190231	-0.659293006959
Si	-4.964348748438	-6.469494686156	7.456196539223
TV	4.965247989034	0.000000000001	0.000000000001
TV	-0.587456645741	5.562896993219	0.000000000001

TV	-4.909833986257	-0.172833439934	8.075189734338
# EQ-SiO ₂ 52			
O	-5.445430737560	-1.465729749076	0.954932553522
O	2.139181649488	0.119242119702	-0.090285937598
O	0.143404217586	1.875180613817	-1.215570931419
O	7.967118862332	1.837692549625	0.740348588422
O	-8.910477702193	2.568556888386	0.979922572958
O	-1.205750103542	4.276084568619	-0.130636736609
O	-3.296846042527	5.952279094818	-1.230776815381
O	4.541082427272	5.959431091660	0.728415395718
O	-12.307111308080	6.689863346714	0.934626603514
O	-4.592161802153	8.387794040753	-0.130254194763
O	-6.728904996648	9.999404990298	-1.178192584339
O	1.217195055265	9.924640785740	0.883947695371
Si	-13.773638362676	6.834940603228	0.058523383755
Si	-1.828599544184	5.813638689900	-0.357752225838
Si	-5.231457659031	9.916266329820	-0.346335959804
Si	-6.947592381365	-1.390845354622	0.127809057368
Si	-10.359806671810	2.732761439927	0.078872191687
Si	1.586658616246	1.689857232683	-0.302003438863
TV	9.771801572706	0.000000000010	0.000000000009
TV	-10.248194571010	12.255317024670	0.000000000147
TV	-1.177159741442	-4.860238751230	1.798494390686

# EQ-SiO ₂ 53			
O	-1.433099234273	-1.708755638650	3.225791745594
O	0.013865556391	-3.155634394044	1.464466395668
O	-1.439312128989	0.849480391045	-0.304071313295
O	0.007218871602	-0.489077744033	-1.937167468294
O	-2.881662295688	-0.298117273963	1.454362187775
O	-1.434825226891	-1.686769661954	-0.159528292717
O	1.456890664233	-1.708827976859	3.225794487571
O	2.903943138902	-3.155452714947	1.464420943611
O	1.450771060826	0.849470466332	-0.304003736315
O	2.897262434804	-0.489093814181	-1.937120696341
O	0.008344646121	-0.298099466355	1.454294878392
O	1.455172053397	-1.686729978770	-0.159444967611
Si	0.009135081966	-0.423864543674	-0.242581167885
Si	-2.877948880028	-0.853566489757	3.001924002047
Si	-1.430908587021	-3.172179063983	0.666978038347
Si	0.012074921005	-0.853562744967	3.001850582546
Si	-2.880869810173	-0.423933468377	-0.242524066366
Si	1.459094379010	-3.172108350691	0.667022851011
TV	5.780055243673	0.000000000000	0.000000000002
TV	-0.012372299391	5.424992601412	-0.000000000000
TV	0.007387878267	0.909948663973	6.000491483508

# EQ-SiO ₂ 54			
O	-2.763529335781	0.703736384200	3.462264278642
O	-1.058344835578	-1.535746599988	2.845994498789
O	-1.089479744900	0.032366055118	-1.090934267825
O	0.611120095988	-2.061607686878	-1.426716365111
O	-4.461319584538	0.642593769524	1.510954536109
O	-1.065227572415	-2.664848760313	-0.028693419949
O	0.609946062036	0.706689280691	3.461725825614
O	2.296303919159	-1.540534560174	2.848237498861

O	2.275351230994	0.032961854082	-1.093503850085
O	3.976443873900	-2.057319316411	-1.405844140718
O	-1.095452855391	0.648319399901	1.514062440693
O	2.292198070305	-2.665893894020	-0.028267508932
Si	2.295251613938	-1.729051473041	-1.710344980130
Si	-4.440574417376	0.100642067489	3.093054225602
Si	0.616495087956	-3.338314010114	0.030835277085
Si	-1.074582979363	0.105766259354	3.097431424641
Si	-1.072785940249	-1.729420558815	-1.706725530285
Si	3.981463829864	-3.336630523958	0.031649170374
TV	6.731579690382	-0.000000000002	0.000000000002
TV	1.661213594494	4.647352884683	0.000000000001
TV	-1.689133869631	4.080426921511	6.078940340140

EQ-SiO₂ 55

O	-1.088466728357	-6.013546833744	4.593354052318
O	-0.839351801527	-4.159552491156	-0.241130142080
O	-1.199391832459	1.772145849837	2.709652095241
O	-0.947742825612	-1.053261868077	-1.934112182664
O	-1.002560893565	3.736802770767	-2.430496902876
O	-2.314215502359	-1.620945945300	0.180143772016
O	1.661957154613	-6.013519793973	4.593365556106
O	1.911079805791	-4.159444673122	-0.241234665707
O	1.550973030597	1.772175589563	2.709647495220
O	1.802623115686	-1.053242518045	-1.934143691208
O	1.747800770853	3.736816491663	-2.430470694359
O	0.436205362362	-1.620932153040	0.180185464144
Si	1.795841535327	2.116091734610	-0.932552156332
Si	-2.516490232985	-1.936364784747	1.741350227837
Si	-2.464574774511	-6.810172863939	3.734693475554
Si	0.233872419697	-1.936343311104	1.741378232245
Si	-0.954536665533	2.116058882136	-0.932565479673
Si	0.285815096453	-6.810158917804	3.734709519588
TV	5.500748185754	0.000000000002	0.000000000002
TV	1.260508035119	7.065136212221	0.000000000001
TV	1.126275366865	0.529497080720	4.639922657967

EQ-SiO₂ 56

O	-0.979326510231	-3.674028468877	1.558463565497
O	-0.085293344765	-0.903807213658	0.560364489323
O	-1.644283621286	1.738756735224	0.560720999999
O	-0.138325471168	-3.049911426088	-0.817195139554
O	-2.979025845561	-0.691839332154	1.544174842226
O	-2.084258700802	-0.127812552108	-0.820521911766
O	-1.601285486781	-0.392930644919	4.870077216801
O	-0.707212540360	2.377315885686	3.872100066434
O	-2.266213196113	5.019875532291	3.872404704679
O	-0.760193274775	0.231244881832	2.494466865957
O	-3.600919352908	2.589286931027	4.855886950266
O	-2.706230754085	3.153313360472	2.491188837304
Si	-2.237347573548	3.256403238767	4.238659196738
Si	-4.561959252283	-0.205979938746	1.997254652630
Si	0.141110895775	-2.659556727708	0.927504030416
Si	-5.183888166403	3.075108219638	5.308949889977
Si	-1.615431378731	-0.024730039818	0.926958393046
Si	-0.480825133129	0.621550931365	4.239186741362
TV	5.528036716650	0.000000000001	0.000000000001

TV	-3.399848595455	5.116548716130	-0.000000000000
TV	-1.243842970576	6.562241550855	6.623386520038

EQ-SiO₂ 57

O	-3.013040318804	-5.883704703669	4.083079649423
O	0.069291176988	-3.183816642917	0.610524702331
O	-2.456909315362	1.093101021065	1.461974435630
O	1.766865231916	0.138622825652	-2.837525977684
O	-2.063630565899	2.084652023725	-1.572033877515
O	-2.825198507998	-1.398736238248	1.741407808742
O	2.012163127496	-5.885999808438	3.971382259662
O	4.968067312669	-3.170087879704	0.594725565114
O	2.351175542905	1.068919658225	1.230877924524
O	6.553471313387	0.157532315275	-2.878175921741
O	2.932373965071	2.073103334212	-1.633788752013
O	2.037681354357	-1.415616401040	1.603402046700
Si	3.954337678393	0.716368961635	0.680743580217
Si	-3.510123173823	-2.864463028917	1.752600341841
Si	-3.441739283548	-5.315600861333	2.565478228411
Si	1.352734900466	-2.882715501513	1.652539471265
Si	-0.925937067264	0.698063619788	0.781883631339
Si	1.483995025516	-5.335456229017	2.475102180737
TV	9.652010578593	0.000000000002	0.000000000002
TV	-0.118688042585	5.300672817331	0.000000000001
TV	-1.974193032489	-0.463934208185	4.710780948921

EQ-SiO₂ 58

O	-0.861443833500	-4.918995972711	3.544716855773
O	-0.395133249421	-3.554403991179	0.387541417942
O	-1.718306016501	1.174040960651	1.456369220080
O	-0.455541041773	-1.749910275112	-1.530921382249
O	-1.425661741458	2.626363644555	-1.663067352830
O	-1.810256866645	-1.417914660259	0.573328703875
O	1.929247914508	-4.918964374034	3.544730530566
O	2.395517459576	-3.554420767981	0.387526820393
O	1.072359484503	1.174138528973	1.456434249237
O	2.335116804787	-1.749907658214	-1.530923722949
O	1.365000554109	2.626361470444	-1.663072795180
O	0.980414636463	-1.417908588099	0.573323353523
Si	1.535044627199	1.977218806276	0.115941054714
Si	-3.176690787657	-2.040184012889	1.548789450624
Si	-2.182012787756	-6.064982889513	2.988162769371
Si	-0.386026510094	-2.040169720302	1.548786860232
Si	-1.255625127761	1.977216606408	0.115927161310
Si	0.608667768305	-6.064971942524	2.988180780940
TV	5.581336299844	0.000000000002	0.000000000002
TV	0.463526323695	6.573965240934	0.000000000001
TV	0.125120602817	1.169336177191	4.151297495936

EQ-SiO₂ 59

O	-2.073884852910	5.053597946436	0.251828223693
O	3.369706848830	-8.413814259634	-2.453458806192
O	-0.705630688709	3.170655806571	0.916430951867
O	-0.734917902015	-1.227037202447	-1.020405600393
O	0.663029322600	5.053571473532	0.251841336674
O	6.106672659330	-8.413879979292	-2.453377930852
O	2.031415179995	3.170704485421	0.916412616660

O	2.002119136623	-1.226882106544	-1.020487299438
O	3.400101472059	5.053557024389	0.251747183094
O	8.843576911649	-8.413874066542	-2.453524890085
O	4.768386673271	3.170667822688	0.916489295717
O	4.739011030222	-1.227070677497	-1.020481387268
Si	3.356897348976	4.011107394067	1.787139758668
Si	1.957294701746	-0.456008627357	0.669411590708
Si	4.694300359824	-0.456097284162	0.669402852308
Si	-2.117150636481	4.010967190670	1.787100364115
Si	0.619860314105	4.011042099168	1.787129375326
Si	-0.779729145722	-0.455930669783	0.669422220718
TV	8.211034149242	0.000000000030	0.000000000027
TV	-1.282591785299	9.132469559385	0.000000000127
TV	-1.455553113413	-0.201367585794	2.407175291574

EQ-SiO₂ 60

O	-2.350926166385	-3.191786092664	2.506943397602
O	0.479184359682	-3.711164432609	1.591095837759
O	-2.112132793728	0.840503498072	0.114920349324
O	1.208102089871	-2.446661565271	-1.669234161213
O	-0.195145604024	2.428936319342	0.148699734590
O	-3.521118952260	-1.186001269707	1.232255935633
O	-4.485965472715	-1.259356793967	5.838732149632
O	-1.655860036358	-1.778729864081	4.922862622060
O	-4.247205191654	2.772986714501	3.446753694012
O	-0.926892922533	-0.514214497435	1.662571796293
O	-2.330167770789	4.361415481384	3.480487487312
O	-5.656153651608	0.746409444510	4.564059247915
Si	-2.482969175431	2.593991283603	3.757730389346
Si	-4.940162663016	-1.915507113991	1.672989414996
Si	-3.128171662125	-4.655734695421	1.813910080960
Si	-7.075198057486	0.016928171569	5.004801205284
Si	-0.347896862034	0.661497933117	0.425947020491
Si	-5.263198078086	-2.723333837993	5.145726380364
TV	5.139755202298	0.000000000001	0.000000000001
TV	0.445472529006	4.864500860737	0.000000000001
TV	-4.270058737444	3.864891253896	6.663627907421

EQ-SiO₂ 61

O	2.179019960935	-0.570792692418	2.111981926639
O	0.747972553300	-2.280270400920	0.653574958996
O	0.792927718722	1.842683183234	0.654946518628
O	2.225148079459	3.562622786275	-0.799894613815
O	5.038702784898	-0.570639255156	2.112066301443
O	3.607856162863	-2.280193501225	0.653630290003
O	3.652634208033	1.842674637077	0.654940158383
O	5.084828607964	3.562538047874	-0.799829743370
O	7.898462963813	-0.570676092842	2.112023409426
O	6.467523904460	-2.280192144478	0.653601896836
O	6.512303203987	1.842529482064	0.654891972342
O	7.944466571033	3.562578188118	-0.799891959958
Si	6.494499046919	-5.543271520966	2.113967635284
Si	3.609054358284	-1.452639990878	2.112601449728
Si	6.468757107635	-1.452593637464	2.112588961137
Si	0.775106168568	-5.543097359919	2.113980740951
Si	3.634810689556	-5.543176200018	2.114008133609
Si	0.749312867315	-1.452681769195	2.112546012322

TV	8.579106112254	-0.000000000000	-0.000000000000
TV	0.015729256913	8.214146190571	0.000000000000
TV	-0.004734078947	-0.009326252077	2.912653666130

EQ-SiO₂ 62

O	-2.295520272399	-2.478929763410	3.573036508073
O	0.546675008622	-2.499789064743	0.512786906325
O	-1.846849784520	0.401301340558	1.235981949261
O	1.824800192634	-1.084927474252	-2.796110858827
O	-1.803531676565	1.846049100882	-0.762772226672
O	-3.784138314894	-1.002731011736	2.006545070620
O	-2.260602438907	0.401399126341	3.573033610263
O	0.581604848513	0.380542402579	0.512784427601
O	-1.811923746876	3.281630406335	1.235982919251
O	1.859712544939	1.795407913541	-2.796126683186
O	-1.768622674270	4.726380789769	-0.762775938255
O	-3.749218702914	1.877605069625	2.006549163961
Si	-1.073180049290	3.278043255121	-0.410281206978
Si	-5.295109493949	-1.063584937371	1.574732433808
Si	-2.097741312279	-3.920174199605	2.394847955130
Si	-5.260187386903	1.816749213639	1.574729726999
Si	-1.108097993949	0.397707164714	-0.410279005218
Si	-2.062820371874	-1.039845289595	2.394849788150
TV	6.132726796540	0.000000000001	0.000000000001
TV	0.069837196612	5.760661925535	0.000000000002
TV	-2.138009214753	0.017504462734	5.498925932256

EQ-SiO₂ 63

O	-2.809730090327	-2.667715400865	2.348890304543
O	-0.588860740701	-1.854688011201	2.164449421802
O	-0.846053408320	0.873333984146	0.017449862843
O	1.863563750102	-0.011890036913	-1.562594833657
O	-3.308372819597	-0.120799352325	1.092994605392
O	-1.289268947139	-1.740963141304	-0.167668411569
O	-0.637858356376	1.560187691058	2.348876594615
O	1.583064248375	2.373388973832	2.164533341033
O	1.325917499842	5.101310929104	0.017483192993
O	4.035571940086	4.216175166009	-1.562563353247
O	-1.136388460547	4.107110759539	1.093011221153
O	0.882635111027	2.486959929060	-0.167621683054
Si	0.205376300715	3.975425601061	-0.202482159215
Si	-3.817537453378	-1.378596567163	2.386619595354
Si	-1.691142472066	-2.788634326030	1.092459709777
Si	-1.645571897199	2.849381619521	2.386681614641
Si	-1.966586788301	-0.252520992811	-0.202550350913
Si	0.480800557429	1.439320468531	1.092495731234
TV	4.745147088275	0.000000000001	0.000000000001
TV	4.343860393305	8.455865664626	0.000000000002
TV	-0.735958780421	-0.438184849983	5.304468135561

EQ-SiO₂ 64

O	-2.625577175977	-1.998863703342	1.182779327041
O	0.054798882874	-1.415484213145	2.188409490226
O	-2.214604929390	0.568243172184	0.149443418992
O	2.463324887890	-1.847369526750	-1.519548645962
O	-2.290923115803	-0.054178349950	3.259769921419
O	0.042269342289	-0.817550568853	-0.479316454699

O	-4.895333479791	2.038729149768	1.182762511339
O	-2.214917283725	2.621840639545	2.188585169972
O	-4.484738753185	4.606272101878	0.149497608282
O	0.193124759049	2.190236524974	-1.519311832051
O	-4.560646109852	3.983230043604	3.259934108200
O	-2.227886662346	3.220047232299	-0.478803098483
Si	-3.761518044493	3.609016291403	-0.970122727643
Si	-3.127673971533	-1.434863516376	2.723806469635
Si	0.522986329156	-1.958202367335	0.634489363560
Si	-5.397343386646	2.602603544831	2.723884196077
Si	-1.491435916481	-0.428568303810	-0.970419488344
Si	-1.747001304904	2.078983724411	0.634625066166
TV	4.795039374700	0.000000000004	0.000000000004
TV	-4.539529440896	8.074984170274	0.000000000004
TV	-0.566296780351	-0.320537798917	5.777902976863

EQ-SiO₂ 65

O	-2.999436855771	2.008225496836	1.518485007620
O	3.988907092761	-1.193804017494	-5.401597026665
O	-1.297641139122	0.219105380377	2.748788461258
O	-0.285007719677	1.307911194356	-4.185543680376
O	-5.563792181209	6.295487671739	1.518460208963
O	1.424518965431	3.093386364990	-5.401552419679
O	-3.861871529733	4.506401775565	2.748646811255
O	-2.849256391895	5.595225161549	-4.185568107607
O	-8.128162178779	10.582647530566	1.518446702849
O	-1.139681085855	7.380517788685	-5.401440913099
O	-6.426223450536	8.793446500716	2.748791005090
O	-5.413630432902	9.882365495150	-4.185570755289
Si	-7.983238191340	9.383602833964	2.739326327266
Si	-2.860876680972	3.206680733780	2.738942454760
Si	-5.425194971461	7.493833564851	2.738968424121
Si	-2.854658588920	0.809227565756	2.739386337182
Si	-5.418955393367	5.096430367347	2.739339666070
Si	-0.296617563062	-1.080563918488	2.738989870908
TV	5.112411686160	0.000000000012	0.000000000012
TV	-7.692962910202	12.861588301834	0.000000000204
TV	-0.162822326155	-3.587043833568	8.144271936783

EQ-SiO₂ 66

O	-0.133738256288	-3.051278949952	1.722418290364
O	1.835313976931	-3.227302187443	0.484434563214
O	-2.162894635670	-0.449551837217	0.376989662036
O	-0.021501932904	-1.631215275487	-0.521135732365
O	-3.814886833896	1.285354773177	-0.638496942709
O	-4.290587111025	-0.789358530467	1.711663325472
O	-1.149722538260	-2.161928105950	4.968250681241
O	0.820440141038	-2.337966874472	3.731212219946
O	-3.176963629994	0.438984223685	3.623396803960
O	-1.035972146443	-0.742874718849	2.724622528579
O	-4.828777392480	2.172314502477	2.607758270271
O	-5.306065847082	0.101150231673	4.957022927118
Si	-3.088490789878	2.159030835913	3.178807169386
Si	-4.389019880211	-2.410301918213	2.105842728508
Si	-0.520434937988	-5.067193172803	2.149925581570
Si	-5.404336865261	-1.519811534998	5.351637998346
Si	-2.073980258501	1.270701175905	-0.067485738166

Si	-1.535630208665	-4.177165223693	5.396172838611
TV	6.042883216108	-0.000000000000	-0.000000000000
TV	-2.109891557123	4.544724356564	0.000000000002
TV	-2.029485157747	1.778529297879	6.492492395458

EQ-SiO₂ 67

O	-1.349331783682	-0.888997616322	2.226171675926
O	0.226610149090	-2.524981385969	1.686854736047
O	-0.855752712615	0.515418446695	-0.503662855091
O	0.776716033706	-1.721849206350	-1.272234586590
O	-3.123917656704	0.308597935687	0.768593193414
O	-2.225802296242	-2.013415879525	-0.062002482442
O	-0.888051348454	2.219703108148	6.183342236297
O	0.687904465533	0.583723580129	5.644033390470
O	-0.394465796888	3.624133644490	3.453501514072
O	1.238014196432	1.386871735300	2.684962815910
O	-2.662620076829	3.417309954014	4.725766195099
O	-1.764508950545	1.095308846767	3.895174707827
Si	-1.876464652398	2.913461781316	3.247943977612
Si	-2.771831146025	0.055244215551	2.620658892241
Si	-1.420569741346	-2.554657412246	1.299275402637
Si	-2.310539018151	3.163968907393	6.577826075627
Si	-2.337743444853	-0.195269534021	-0.709230229934
Si	-0.959274793232	0.554062629272	5.256440788102
TV	5.135732623554	-0.000000000000	0.000000000001
TV	3.255945037573	4.701127228763	0.000000000000
TV	0.922579976525	6.217443757186	7.914351567847

EQ-SiO₂ 68

O	-2.403465705816	1.517571110953	0.128576233586
O	1.828263862644	-1.352495914174	-2.313658880420
O	-0.760228410702	1.012376265769	2.173076771166
O	0.303494430432	0.672256289824	-0.519537502573
O	-1.550236875993	4.335102053094	0.141859518206
O	2.694363421409	1.458267438683	-2.321847612249
O	0.113260778037	3.856370299641	2.174904111785
O	1.163937269833	3.486661886224	-0.544912923328
O	-0.665916171683	7.150236886902	0.139731492334
O	3.566965047515	4.269195100852	-2.310217267606
O	0.985862255194	6.674265162950	2.185387637036
O	2.039029836250	6.302180496518	-0.531372914166
Si	-0.496077497197	7.103489416559	1.736613324192
Si	1.296816047932	1.902448535488	-1.045807850687
Si	2.164852293417	4.720532339805	-1.044638012497
Si	-2.235119729418	1.471056470380	1.727215278512
Si	-1.370603261241	4.291777196206	1.736556195002
Si	0.433189120091	-0.906577750501	-1.036629223948
TV	4.981145130401	0.000000000010	0.000000000009
TV	2.602773414653	8.443352757893	0.000000000144
TV	-1.133191721418	-1.160517258366	4.710303110704

EQ-SiO₂ 69

O	-3.860043660706	-2.510587640353	1.513028340956
O	7.862181817552	-2.381299325980	2.085287369279
O	-3.854223610984	1.001692577012	-0.094028814269
O	7.594527680161	1.104612301550	0.189887881350
O	-4.934055736829	-0.071194910207	2.171557059203

O	-5.402540618971	-1.335538940759	-0.311256105631
O	-1.684445058323	-5.487662549340	5.629088573647
O	10.021748958464	-5.274016010576	6.112212239676
O	-1.647684436600	-1.927563540960	3.965301283978
O	9.797453641596	-1.871517616121	4.257150734239
O	-2.699303745174	-3.010014415205	6.241569271807
O	-3.127359623125	-4.275302027011	3.745143690042
Si	-2.946707513646	-2.823446541334	4.581502089968
Si	-4.810768181533	-1.674006925798	2.693214151996
Si	-5.331433784413	-2.721122453877	0.658480620685
Si	-2.647598584730	-4.615185725820	6.770192360127
Si	-5.170926941323	0.118568560379	0.512554301954
Si	-3.126836903714	-5.654504981729	4.722706148896
TV	14.108140370584	0.000000000001	-0.000000000001
TV	1.889821707083	5.137290966765	-0.000000000001
TV	4.319641172355	-5.943441568156	8.154273791594

EQ-SiO₂ 70

O	-2.365134610842	-4.870332519070	1.912083144226
O	-0.640571761189	-4.241742489631	0.206971543300
O	-0.647517472262	0.821717483271	0.211138808939
O	-0.650009007941	-1.424655502224	-1.494055184460
O	-0.651843830792	4.810790282913	0.211205465046
O	-2.372005747563	0.062885087711	1.916053793048
O	-2.362260885680	-4.862896814796	5.319049896487
O	-0.637601747914	-4.234277583664	3.613928765448
O	-0.644630613158	0.829099875070	3.618076230722
O	-0.647161616122	-1.417140756724	1.912808181682
O	-0.648988324112	4.818246974949	3.618020295325
O	-2.369127316441	0.070247206895	5.322990337410
Si	-0.644382863355	2.805074155542	3.615013627701
Si	-2.371234411730	-1.686387885538	1.914492478954
Si	-2.364886556318	-6.659483973759	1.914687724404
Si	-2.368338219562	-1.679023433553	5.321361623730
Si	-0.647380546189	2.797634644044	0.208071244935
Si	-2.361996817835	-6.652046649707	5.321594318018
TV	3.448637182648	0.000000000001	0.000000000001
TV	1.717039267061	7.219372124943	0.000000000001
TV	0.005788448197	0.014810910637	6.813815894232

EQ-SiO₂ 71

O	-0.808168713152	-0.796416882513	2.115858526444
O	-1.873324007462	-1.746290128059	-0.219963643956
O	0.230576363664	0.122275329501	-0.235778505048
O	-0.382416878741	1.959404053692	1.767658682336
O	0.794339530077	-2.215699675041	0.654202076659
O	-2.438738758295	0.595504658905	0.651221699027
O	0.119884832998	4.676659495497	2.078913702344
O	-0.982333074849	3.774130625331	-0.275163233985
O	1.133330552896	5.667974491686	-0.251529242046
O	0.522241354825	7.439122227918	1.804065437436
O	1.663698681718	3.279390641335	0.517106256135
O	-1.538490097640	6.086822000704	0.658173452426
Si	0.067540525931	3.366832399668	0.997942620802
Si	1.626231560539	-0.810504500905	0.199755734335
Si	-0.815540905586	0.521587412716	1.046127102997
Si	2.515374980824	4.702272296997	0.154300886230

Si	-0.824554221421	-2.130739564024	1.063480710833
Si	0.087783756041	6.021371244157	1.043529261375
TV	4.895938717909	-0.000000000033	0.000000000044
TV	1.813520156110	10.986309419258	-0.000000000003
TV	-1.874478010049	0.206700636760	8.142436257888

EQ-SiO₂ 72

O	-1.453330194787	-3.429899298972	0.961246607714
O	-0.567491338512	-1.339213664880	1.591861687008
O	-2.993221468525	0.537498112429	-0.761792890500
O	1.537440683412	-1.725066288223	-0.128095661103
O	-2.884154761153	0.420430171058	1.592331186856
O	-0.674634073558	-1.214762429642	-0.762390845464
O	-2.235881651357	-2.475228533112	5.222546114622
O	-1.349980438275	-0.384493911195	5.853121056014
O	-3.775793271661	1.492149127913	3.499542084637
O	0.754929242754	-0.770418535833	4.133340261964
O	-3.666763920681	1.375179807424	5.853657774028
O	-1.457237027184	-0.260049420663	3.498887043148
Si	-2.562181893080	0.554077539797	4.678212058353
Si	-4.383913683507	0.078485259430	2.546891041615
Si	0.041955044596	-2.575530068306	0.416238498030
Si	-5.166471438708	1.033196622194	6.808173379100
Si	-1.779555113552	-0.400635694076	0.416895517222
Si	-0.740644690467	-1.620775253914	4.677554892456
TV	4.426617480339	0.000000000001	0.000000000001
TV	-3.643006153347	4.350871639955	-0.000000000000
TV	-1.565105848337	1.909373101093	8.522625115413

EQ-SiO₂ 73

O	-2.542150221105	0.246994938894	-2.069827795398
O	-4.200633829985	-1.493611320173	-0.503062023064
O	-5.048208526885	-0.194002606976	1.638528855712
O	0.175714922023	0.811300116214	0.536635856575
O	-0.147160442973	-0.714016653688	-1.501787994450
O	-2.251709704935	0.382501691553	0.392658236476
O	-3.113373193400	3.069925313754	-2.069759834178
O	-4.771837757842	1.329257031230	-0.503093893004
O	-5.619476079753	2.628886814792	1.638564088407
O	-0.395472626779	3.634299126295	0.536604489115
O	-0.718328077539	2.108946813850	-1.501689181526
O	-2.822902514905	3.205394619863	0.392718628901
Si	-6.449793599787	3.929928968522	0.953333177506
Si	-3.426110221412	0.137012978130	-0.746915439094
Si	-0.980340892817	0.587574203700	-0.837747234726
Si	-3.997321168701	2.959913506114	-0.746839515820
Si	-5.878608768077	1.107002022264	0.953320811756
Si	-1.551563236666	3.410503415086	-0.837691298505
TV	7.548992504557	-0.000000000002	0.000000000001
TV	-1.142408020487	5.645816682012	0.000000000010
TV	-2.917692760476	-0.337218738680	10.770585278127

EQ-SiO₂ 74

O	-3.691425206933	-0.500491179768	1.118369549091
O	-0.315061197681	-2.397447062621	1.863330239723
O	-1.424181232551	0.727264100149	0.552641597474
O	2.302381101574	-0.467904229677	-1.516161547770

O	-4.769733395557	0.519876366149	4.278733263469
O	-0.636080177756	-3.451514422908	-1.813892638636
O	-2.981161630112	4.123507871919	1.124683296231
O	0.393591508457	2.225992713750	1.863302227685
O	-0.715446533324	5.350901952491	0.555843277906
O	3.006108754720	4.155578363627	-1.510038704156
O	-4.062311137280	5.144270658873	4.278797612121
O	0.073758656969	1.171432162212	-1.814613846626
Si	-1.658701013742	4.051262808494	0.095115614305
Si	-4.415058153840	-1.228700839618	2.419176560589
Si	-1.165518923262	-2.555190283170	0.433317866678
Si	-3.708499708807	3.394925378397	2.422556160567
Si	-2.366825239815	-0.572555271392	0.091024021799
Si	-0.457168184468	2.068036939299	0.433281784496
TV	5.129493653750	0.000000000001	0.000000000002
TV	1.415797007113	9.247315023976	-0.000000000004
TV	-0.460626484219	-1.348607298422	4.988526700957

EQ-SiO₂ 75

O	-6.019259966936	-4.826533059302	3.800924757264
O	3.534677336374	-1.416044991993	1.107797887498
O	-0.743074378556	0.627313706209	0.214778751088
O	0.719379086124	-0.241926157863	-2.948083811640
O	-1.752701210659	2.844643867135	-0.868469075412
O	-2.427333873133	-2.221315356847	2.308352141003
O	-6.026485471771	-5.481611567818	8.536839843393
O	3.527639795481	-2.071576956271	5.843842054771
O	-0.750543592438	-0.028061568433	4.950706409860
O	0.711907289510	-0.897425135113	1.787429357050
O	-1.759758319115	2.189460239913	3.867282077725
O	-2.434400217423	-2.876541396756	7.044648080324
Si	-1.684201973201	0.526709435308	3.682435176474
Si	-3.792900815295	-1.395764123196	2.963474320949
Si	-3.577454894920	-5.031722478805	1.625155817902
Si	-3.800050766073	-2.050820294108	7.699391731888
Si	-1.676902042598	1.182036923284	-1.053326428578
Si	-3.584739633347	-5.687051016560	6.361176501357
TV	5.547185988449	0.000000000001	0.000000000001
TV	2.757263961499	4.770059736200	0.000000000001
TV	-0.014527274395	-1.310253295646	9.471524118356

EQ-SiO₂ 76

O	-2.880303453238	-5.481197204960	3.870746968975
O	0.308262057636	-1.691190283240	-1.935967188913
O	-2.044001915432	0.370122934822	1.330038545700
O	2.531864470773	-0.770103118216	-1.153800056807
O	-1.763049894247	2.144143455202	-0.622675993175
O	-4.014885363841	-1.970476740941	1.318152971164
O	-5.933115008165	-6.044215607258	7.848701569151
O	-2.744355437000	-2.254134992140	2.042080721604
O	-5.096707392704	-0.192911121097	5.308017545293
O	-0.520773098326	-1.332988905370	2.824131520166
O	-4.815731026997	1.581175180195	3.355375943811
O	-7.067633421201	-2.533465689045	5.296182238373
Si	-3.973526912497	0.804075913122	4.560231561254
Si	-5.359669653085	-2.657121783158	2.153647909755
Si	-2.112329298044	-6.031798221392	2.523952000118

Si	-8.412395734351	-3.220145954344	6.131709361040
Si	-0.920834395208	1.367098303414	0.582201803207
Si	-5.165073274366	-6.594833848408	6.501958569495
TV	5.620160672329	0.000000000001	0.000000000001
TV	0.059704840371	5.267574814603	0.000000000001
TV	-6.105406065587	-1.126003101301	7.956077353969

EQ-SiO₂ 77

O	-2.298864718093	-2.813026045920	1.926411214319
O	2.663943226749	-6.490094976257	1.755304483562
O	-1.877814192222	2.647069030125	-0.151260021466
O	1.248207187104	0.424278032362	-0.915439996442
O	-6.069425468889	1.543808251187	0.789645718128
O	-1.303664756662	-1.079111401401	0.066162631850
O	2.312892334189	-2.812899697319	1.927827298388
O	7.282851343727	-6.486677328851	1.756000937372
O	2.728422667051	2.651424853038	-0.150286611629
O	5.864512693984	0.422721762497	-0.915180812242
O	-1.448930138924	1.540092406996	0.787873875217
O	3.304957803945	-1.071721009702	0.069416499033
Si	2.223184859839	0.154149242657	0.398050032184
Si	-3.629108721555	-1.833096392973	2.258839410854
Si	-0.935982819107	-2.403140130034	1.040132962122
Si	0.979429806210	-1.837214857153	2.259129833463
Si	-2.380159000438	0.150942043476	0.396664310363
Si	3.674146416551	-2.397294893575	1.041172638563
TV	9.221705982456	0.000000000002	0.000000000002
TV	-1.314366081419	6.230057037881	0.000000000000
TV	-0.530220793316	-2.257307825786	4.826149071236

EQ-SiO₂ 78

O	-2.598153413514	-3.981398823229	3.048410906931
O	0.364595514658	-2.200673806525	-0.141945464675
O	-1.808503759289	1.432403620563	1.387633307685
O	2.160873062345	-1.649676338485	-1.795817550531
O	-3.372556148545	0.090138144281	0.028683417130
O	-3.174497422599	-0.848659442149	1.209967711173
O	-5.490121260638	-3.061333384422	6.878662634568
O	-2.527678379210	-1.280425837060	3.688504232069
O	-4.700632844532	2.352630276452	5.217721264895
O	-0.731286529086	-0.729372072124	2.034250836406
O	-6.265193468510	1.010545088750	3.859103066406
O	-6.066384249127	0.071476531252	5.039948549437
Si	-4.626323600441	2.067138680910	3.468466561087
Si	-4.809229272881	-1.912447452063	1.607141687221
Si	-1.160555500572	-4.784655464192	2.537512862664
Si	-7.701149678859	-0.992230546100	5.437530552934
Si	-1.734119024696	1.146849464552	-0.361629510423
Si	-4.052420847566	-3.864296959650	6.367555317123
TV	5.099121174020	0.000000000001	0.000000000001
TV	-1.008648593284	4.861983605856	0.000000000001
TV	-5.784139880493	1.840425322498	7.660320518975

EQ-SiO₂ 79

O	-2.956080177609	-2.326204972977	-0.872645662663
O	-0.695490212415	-2.096258181079	0.588642717809
O	1.090776825170	-0.082180379324	0.412678528955

O	2.913111405184	-2.065792659801	0.550490516211
O	-1.220660988312	0.140020874153	-0.986781372850
O	-3.741903689953	-0.537128235998	2.613507836054
O	-3.443116861724	2.058007726507	-0.872274201055
O	-1.182548151287	2.287761356735	0.589004570274
O	0.603755365798	4.301972231628	0.413025212494
O	2.425840805500	2.318255151268	0.550780029619
O	-1.707645381395	4.523964944158	-0.986702180469
O	-4.229045049779	3.846952737201	2.613794449962
Si	-2.709490457998	5.494193230955	-0.043170423113
Si	-4.421142733027	0.184131355564	3.944839459953
Si	-3.239947238868	-4.764209651605	0.961710860660
Si	-4.908163711551	4.568186270027	3.945178968155
Si	-2.222379029430	1.110173675238	-0.043073913927
Si	-3.727024572136	-0.380176102854	0.961459007634
TV	6.370927429563	0.000000000001	0.000000000001
TV	-0.974108069974	8.768069729482	0.000000000002
TV	-4.367800351185	1.107279178584	4.377372066243

EQ-SiO₂ 80

O	-1.325180744480	-5.946084285143	3.446869193057
O	0.378075920399	-3.071552522242	3.710430735168
O	-2.212858730273	0.579126354509	0.981678169158
O	0.964056311927	0.357243006429	-3.368426026180
O	-2.703483933014	2.318105477061	-1.163540455727
O	-2.335544366122	-2.245277229891	1.452346785595
O	3.140187768116	-5.949937370521	3.450459233890
O	4.842107562339	-3.070566358091	3.710907961181
O	2.254972996363	0.578747517896	0.986160231060
O	5.430737103202	0.355886765416	-3.365281635561
O	1.763488019190	2.316096230918	-1.161702811801
O	2.129685757243	-2.245509993898	1.452694497740
Si	2.975393446146	1.669567316053	-0.061058149556
Si	-3.800347354351	-2.199102020543	0.568987660717
Si	-1.185760968350	-6.122082095762	1.821404028732
Si	0.665721382614	-2.198523949295	0.567930716806
Si	-1.491227147828	1.671183026200	-0.063541448234
Si	3.280843193320	-6.123703412091	1.824712088301
TV	8.932054089822	-0.000000000002	0.000000000016
TV	-0.452743203929	5.390570983160	-0.000000000000
TV	-1.027678262115	-1.249284742357	4.675836700789

EQ-SiO₂ 81

O	-2.288361848908	-2.519458150758	2.162123840080
O	3.750902713448	-5.529260358443	1.463537628774
O	-2.292981213786	1.627585025743	0.302436305611
O	1.557021958707	0.047309679918	-1.215455521016
O	-6.206237841347	1.643300187017	0.910794207691
O	-1.454091044089	-1.026559168217	0.038254560880
O	3.025853930185	-2.519067953140	2.162009015772
O	9.065285177658	-5.529458058514	1.463786001558
O	3.022298586007	1.628137632000	0.301323235633
O	6.871575938508	0.046919369943	-1.215683379703
O	-0.892165401577	1.642804023898	0.912079625984
O	3.860572377272	-1.026160288141	0.038488182322
Si	2.510240312715	-0.065510186216	0.120105651502
Si	-3.979538636512	-2.035294168867	2.039724238590

Si	-0.951679375992	-1.987101777146	1.348497669005
Si	1.334455270661	-2.034938590522	2.039766775662
Si	-2.804750993975	-0.066176059319	0.120043717544
Si	4.362926338019	-1.986862270101	1.348632647764
TV	10.629069540563	0.000000000000	0.000000000002
TV	-2.121908911915	5.097529941316	-0.000000000001
TV	-0.538138272527	-2.197363242596	4.930912818159

EQ-SiO₂ 82

O	-7.754389355259	-9.455698551265	3.250150301590
O	-1.277766985772	-2.562517885913	1.067255029862
O	-1.091624354452	1.949779056513	0.623357780756
O	4.876550987300	5.935472846128	-3.076082428775
O	0.097110719357	3.473752580400	-1.489044673471
O	-2.983384688467	-3.462484111130	3.017620199033
O	-2.408621476441	-9.464643862438	3.273674019125
O	4.022966224878	-2.689395532691	1.037773479403
O	4.198058743803	1.816627478953	0.634029135945
O	10.199648386358	5.889775143258	-3.112696902748
O	5.317182157809	3.440245894888	-1.465500412739
O	2.356114067308	-3.538125601540	3.018426555384
Si	5.485649501921	2.385968357859	-0.209363963400
Si	-4.327485740465	-3.949254729284	2.077619962482
Si	-3.827035683523	-8.744983514048	2.876423848852
Si	0.987680734259	-3.999387240503	2.101964992208
Si	0.230666013556	2.472257257166	-0.188211032210
Si	1.499556740738	-8.803221121563	2.846801405657
TV	10.702393066011	0.000000000002	0.000000000000
TV	2.251068931664	6.132931199128	0.000000000007
TV	-2.481635923197	-2.947583421952	3.812618970742

EQ-SiO₂ 83

O	-1.160053743288	2.380364262546	2.032117799387
O	-3.937888403121	-0.629560437179	3.139101258612
O	-0.825744989658	-2.437905199161	1.918875692659
O	-3.610468061574	0.838187283552	3.167884704039
O	-0.034040234559	0.292675569470	0.791343234981
O	1.171169577088	-2.224930804434	0.620427603329
O	3.353178875579	2.380366662204	2.032062218551
O	0.575546846785	-0.629496521954	3.139168546355
O	3.687421279487	-2.437875509470	1.918758666151
O	0.902820408013	0.838284976137	3.167937565487
O	4.479230540673	0.292687245594	0.791243929104
O	5.684462468753	-2.224898497879	0.620452538193
Si	4.731558568305	-1.171930041181	1.519599255505
Si	0.214920837458	-3.650030282922	1.166347404726
Si	0.325295433314	1.738785721941	1.592430483807
Si	4.728169250665	-3.650001093256	1.166303393360
Si	0.218374447821	-1.171948457636	1.519688227992
Si	4.838542063364	1.738745155536	1.592455025827
TV	9.026464715421	-0.000000000000	0.000000000000
TV	-2.548113070526	6.907654110285	-0.000000000000
TV	-1.624812858887	-1.844736942262	3.797909164639

EQ-SiO₂ 84

O	-3.236673324871	-8.021964791061	2.965945900215
O	-0.035544435312	-3.471315428582	-0.456083589178

O	-2.006346820477	4.958524427188	0.480259423487
O	1.376400375228	-0.972879520192	-0.261232898509
O	-3.494086632714	3.330484278965	-0.754278969936
O	-3.725951847985	-2.458239744561	1.630243254323
O	-4.670919084585	-10.580736979758	6.201333228025
O	-1.456420547895	-5.949714047749	2.770360180472
O	-3.412365715042	2.557355970070	3.584085578594
O	-0.004664681037	-3.468582528499	2.929312440624
O	-4.882684526263	0.912908142635	2.348268402032
O	-5.227750046170	-5.036808805823	4.878916378065
Si	-3.785543356355	-0.015060407745	3.283092568640
Si	-4.133728660443	-3.763365320934	2.747344626656
Si	-0.625913421596	-10.610293173456	2.509838031599
Si	-5.683237818423	-6.330085254744	6.001104451480
Si	-2.329869542681	2.424541760214	0.125169022040
Si	-2.172079421628	-13.101519132587	5.674863849076
TV	5.761268546585	0.000000000001	0.000000000001
TV	-0.768285292134	6.339440348151	0.000000000001
TV	-2.928819210648	-4.979826198276	6.333822463761

EQ-SiO₂ 85

O	-2.033438334625	0.018444850993	0.212224084541
O	-1.136865362634	-0.174854066256	2.949993694578
O	-0.091763282259	-1.230921401265	-2.177223497444
O	0.250166954392	0.055582845570	-1.408302879374
O	-2.320731637126	-2.063212952787	1.408667430631
O	0.443101302773	-1.080064548110	1.084544543140
O	-3.406481304183	3.719823573403	0.197639038563
O	-2.514429581362	3.568721292652	2.947937608720
O	-1.473513762918	2.487473423820	-2.170073874024
O	-1.107368262753	3.776594639198	-1.416728991273
O	-3.709718156793	1.666796918918	1.439607814534
O	-0.942042154142	2.629325246093	1.084646626454
Si	0.509972032040	2.516107871953	0.265226669103
Si	1.466463778703	-1.986924356230	-1.915913252154
Si	4.022128968765	-0.826814484337	1.410386673109
Si	0.074677052270	1.711706407520	-1.906486988560
Si	1.890942290718	-1.193456128599	0.257150906284
Si	2.641242814607	2.895764276683	1.415147541586
TV	5.165480329599	-0.000000000000	-0.000000000001
TV	-2.772032277072	7.416848542903	0.000000000006
TV	-2.178739674709	-2.282399490620	6.153017346668

EQ-SiO₂ 86

O	-3.445460658137	-5.891916385814	3.811334565315
O	0.406939482007	-3.560007893470	-1.144274833028
O	-0.744049297474	3.048151496975	0.342444528820
O	1.743303876970	-1.158954767514	-1.502642848638
O	-1.154261377210	2.447372610057	-1.951537574155
O	-3.980133473709	-0.394011284823	3.645360799092
O	-5.664804607332	-6.225977702656	7.771855379735
O	-1.812527409231	-3.894092191004	2.816195257811
O	-2.963508268587	2.714279637531	4.302902784777
O	-0.476324769304	-1.492928746570	2.457757923795
O	-3.373792417370	2.113353646426	2.009002257099
O	-6.199473761547	-0.728009440898	7.605840360936
Si	-2.438047714795	1.411895962745	3.191124066371

Si	-4.140606901031	-1.937670064601	2.727710313454
Si	-2.800016504843	-8.092744683280	2.063754843111
Si	-6.359893047805	-2.271615968766	6.688144091623
Si	-0.218570741558	1.745798842394	-0.769424287392
Si	-5.019304135381	-8.426588132945	6.024233953527
TV	5.266825102201	0.000000000001	0.000000000001
TV	0.945600942463	5.742260970340	-0.000000000000
TV	-4.438867912768	-0.667917179511	7.920934133214

EQ-SiO₂ 87

O	-1.415915801322	-0.540569417148	0.732213013429
O	-1.763430776648	4.115655570748	-0.712657098453
O	-3.889149973699	-0.991471492034	1.774741743420
O	-1.731691655378	2.657824303244	-1.165872139777
O	-3.980633412710	3.327694455680	0.737176610367
O	-4.309589642435	7.966815644690	-0.701607499610
O	-6.456725254267	2.865817164187	1.749998654425
O	-4.313637829425	6.512974657675	-1.162182897843
O	-6.523785565887	7.197615833997	0.764089845400
O	-6.841541432408	11.824196566366	-0.699983298064
O	-8.990826303918	6.757060831474	1.786646902385
O	-6.848824054008	10.365512144125	-1.149185524603
Si	-7.439705522782	6.146689521432	1.685937459620
Si	-2.434904730150	3.943093852600	0.862126307627
Si	-4.976703656598	7.810727188860	0.877587265540
Si	-2.329807333973	-1.582773333637	1.670123826253
Si	-4.894321915553	2.280480887236	1.667870893943
Si	0.131109911893	0.069996363285	0.868037374992
TV	4.946131081828	-0.000000000000	-0.000000000000
TV	-7.666651812151	11.605431971483	0.000000000000
TV	0.075220385644	-4.346396559241	4.413176510536

EQ-SiO₂ 88

O	0.353778930003	2.454744630526	-0.043476574722
O	-0.776185172011	-3.424312881862	-2.022913947610
O	2.145380915668	2.419038259213	1.967192490397
O	-2.277649357417	-0.361271596669	0.674245109807
O	4.994536381151	2.454698716068	-0.043403883984
O	3.864601425096	-3.424291496720	-2.022892056246
O	6.786139421394	2.419063742273	1.967240359193
O	2.363099395009	-0.361280839863	0.674234663529
O	9.635312845963	2.454729636264	-0.043433667461
O	8.505340228253	-3.424277118731	-2.022902740445
O	11.426890753577	2.419117037252	1.967174678340
O	7.003848319915	-0.361225750167	0.674200155947
Si	11.069128873641	3.134417896596	0.497799929361
Si	-0.262791107688	-2.223094461846	-0.914490009835
Si	4.377946275918	-2.223100265690	-0.914447431041
Si	1.787594877534	3.134370788497	0.497840846746
Si	6.428354832761	3.134350692032	0.497881269449
Si	-4.903549103147	-2.223036638906	-0.914550818140
TV	13.922265191521	0.000000000075	0.000000000168
TV	3.927143997668	5.196213359503	0.000000000092
TV	-1.961758587678	-1.970337145082	3.654598468269

EQ-SiO₂ 89

O	-2.493483888296	2.022971061130	0.440035038971
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O	2.220138088039	-0.480461712039	-1.673986471596
O	-0.605719235467	0.285710335427	1.239928087160
O	-1.029587967520	-0.691924984602	-1.312350044808
O	-3.102718177574	0.875193349760	4.901596856462
O	1.611028801635	-1.628079279443	2.787425962080
O	-1.215086821377	-0.862074884902	5.701471414374
O	-1.638749916809	-1.839873537844	3.149133172404
O	-3.711996599814	-0.272578696687	9.363085802494
O	1.001717274791	-2.775901185347	7.248887525501
O	-1.824225270445	-2.009668346044	10.162686699405
O	-2.248053114008	-2.987686027065	7.610514750285
Si	-2.222037081119	-0.388292990041	10.099484340606
Si	-1.611788139630	-2.239903436917	4.835498677391
Si	-2.220994501116	-3.387539651160	9.296905244474
Si	-1.003611217017	1.907086339195	1.176621274355
Si	-1.612832403579	0.759325280609	5.638115055864
Si	-1.002550015800	-1.092117529230	0.374001960632
TV	4.710999177497	0.000000000011	0.000000000010
TV	-2.821022275720	4.131941623652	0.000000000061
TV	-1.827528999581	-3.443153053997	13.384296845748

EQ-SiO₂ 90

O	-1.331224297832	2.491338542219	0.297436657007
O	2.195233919263	-0.954431466758	-0.513051744789
O	-0.258652327724	0.082810963328	0.813899295694
O	-2.683292828071	0.052010057192	-1.605370380028
O	3.315968846447	2.507628576881	0.296641110247
O	6.782667459400	-0.999706731086	-0.516316343055
O	4.396620087335	0.094912121599	0.804958134473
O	1.969541359256	0.107039626238	-1.584189387052
O	7.861582565429	2.407950711926	0.289647040600
O	11.403407772296	-0.996869976821	-0.527032246430
O	8.971339549763	0.005655812381	0.810230700833
O	6.610452652782	0.088759633370	-1.572095648471
Si	8.448722312122	1.428870537260	1.496446244931
Si	3.920061518524	-1.023512697473	-0.344525479882
Si	8.503069108770	-1.114146472544	-0.340116923717
Si	-0.759086133223	1.510214647148	1.508183336906
Si	3.878216069794	1.514980485602	1.500245193592
Si	-0.722487259758	-1.036906883477	-0.339691187254
TV	13.848113827376	0.000000000033	0.000000000030
TV	-0.772488842630	5.059830038722	0.000000000076
TV	-0.570062099844	-2.857802821568	3.760755886609

EQ-SiO₂ 91

O	-0.026981111990	0.542945506209	1.092748008890
O	-0.860391889491	-0.699895130291	0.775337815381
O	0.601919558678	-0.167752560041	-1.230035598203
O	0.789925121206	-2.746793646568	-0.772619673705
O	4.557540130687	0.543010593121	1.092746353968
O	3.724160875439	-0.699779203319	0.775391290836
O	5.186597313969	-0.167751468762	-1.230050676734
O	5.374598303331	-2.746723645854	-0.772589063719
O	9.142423039177	0.542901777841	1.092709254860
O	8.309162840238	-0.699993967377	0.775348345697
O	9.771589021030	-0.167952212144	-1.230030271782
O	9.959384635446	-2.747015679793	-0.772779250213

Si	11.235317940405	2.952596166111	-0.755862876998
Si	4.832344661530	1.364752417685	-0.638940887446
Si	9.417190690912	1.364565187631	-0.638974799976
Si	2.065830480365	2.952642095493	-0.755805618589
Si	6.650723973265	2.952494289044	-0.755872921837
Si	0.247686706400	1.364709006711	-0.638847715488
TV	13.754150486225	-0.000000000000	-0.000000000000
TV	-2.175480928740	4.471001772657	-0.000000000000
TV	-1.298988261656	-2.691300123452	3.525693317715

EQ-SiO₂ 92

O	-2.884933996899	2.225954369185	0.429787904321
O	2.426218409258	-0.082906103250	-2.539305729036
O	-1.889507347511	-0.377767104878	0.292468601986
O	0.497036411086	0.278987003786	0.987744704869
O	-2.172113675459	-0.477303191968	3.946784924793
O	3.139000860872	-2.786162999909	0.977683836419
O	-1.176690556463	-3.081037272985	3.809453492789
O	1.209844692680	-2.424274927240	4.504740319856
O	-1.459290853462	-3.180513211176	7.463775093094
O	3.851823496279	-5.489445890086	4.494673388274
O	-0.463889155552	-5.784296407490	7.326432837862
O	1.922650932362	-5.127520284917	8.021719695883
Si	-0.252176974888	-4.159211523644	6.920250749026
Si	0.104499077692	-3.823786478116	4.635454826279
Si	0.817302509152	-6.527037477304	8.152451221876
Si	-1.677788395460	1.247303038837	-0.113728204459
Si	-0.964965775772	-1.455953641840	3.403259109319
Si	-0.608315064595	-1.120526655518	1.118465935129
TV	5.133234219855	0.000000000012	0.000000000010
TV	-3.429351246193	4.339621989670	0.000000000059
TV	2.138401129508	-8.109794829637	10.550964712253

EQ-SiO₂ 93

O	-3.314520295197	3.663013157097	1.352937146945
O	4.010692208022	-2.144707047978	-0.968166548141
O	-2.362675726709	0.748307403740	1.135519767721
O	2.289851724998	-3.854220782328	-3.999846267795
O	-4.973030754338	2.835912687122	5.377985051923
O	2.334678204676	-2.985941977899	3.082204566141
O	-4.026704909141	-0.083152543496	5.172410017739
O	0.625945248651	-4.674146029911	0.028002586368
O	-6.635313928488	2.004768314569	9.413322627444
O	0.686315305155	-3.807883839762	7.102040325250
O	-5.682301427601	-0.908324288913	9.191139471097
O	-1.040903349653	-5.506501670111	4.066959570239
Si	-7.728395092684	2.790494567899	10.428232762733
Si	-2.424786984245	-1.486934986402	3.778296100380
Si	-4.075231547542	-2.314152301894	7.808479238195
Si	-4.414512912952	4.436486163373	2.371226204309
Si	-6.066448498256	3.610820660903	6.401650401909
Si	-0.755793483912	-0.654452982444	-0.251577964737
TV	4.692702344290	0.000000000010	0.000000000012
TV	-3.080051841432	4.399228317959	0.000000000065
TV	-4.982826847518	-2.478505765837	12.085873993030

EQ-SiO₂ 94

O	-4.864628366434	5.223900708300	1.992476737877
O	4.276625758094	-2.018572014727	-1.153820258585
O	-2.217813174970	-0.143478621342	0.700499933497
O	5.891721345586	-5.942237699014	-4.063353329133
O	-1.180478455036	5.223899262840	1.992475030667
O	7.960717935380	-2.018508169517	-1.153921822022
O	1.466330553099	-0.143473259263	0.700496459846
O	9.575758935807	-5.942140075400	-4.063503011950
O	2.503654490295	5.223909346894	1.992468792258
O	11.644810269299	-2.018525335895	-1.153921032355
O	5.150474147182	-0.143503635238	0.700498906202
O	13.260006725121	-5.942181392937	-4.063415851409
Si	0.672044316754	5.285356026097	2.393878649670
Si	3.299618483299	-0.203508494556	0.298981790255
Si	6.983769127596	-0.203515229864	0.298988315801
Si	-6.696234746391	5.285343335350	2.393889958430
Si	-3.012091053011	5.285377005064	2.393878132433
Si	-0.384521512445	-0.203553271707	0.298991815568
TV	11.052430642058	0.000000000027	0.000000000036
TV	-4.489528880000	4.903600151774	0.000000000068
TV	-1.891182943926	-0.833654163563	3.953494776847

EQ-SiO₂ 95

O	-2.747875877785	1.916569432001	2.135696430738
O	-0.697676602410	1.066061520111	-2.083160874529
O	-1.107513390771	-0.765248362812	-0.004195504793
O	0.897403769055	0.367182749699	0.060842228555
O	1.916805139017	1.916569388206	2.135703800783
O	3.966988026924	1.065997076092	-2.083152505094
O	3.557185143560	-0.765208914677	-0.004165674524
O	5.562061445859	0.367214040123	0.060797131134
O	6.581417907107	1.916453998081	2.135808682457
O	8.631684977772	1.066009403861	-2.083076508085
O	8.221856703411	-0.765178902846	-0.004196080976
O	10.226730360520	0.367220922960	0.060949562190
Si	8.630624025021	1.045579944409	-0.348146699989
Si	5.153741028724	-1.444426104724	0.401764140593
Si	9.818365152796	-1.444450777937	0.401803601815
Si	-0.698692908806	1.045555566813	-0.348200214731
Si	3.965956518720	1.045502988610	-0.348232190648
Si	0.489052212187	-1.444498953631	0.401723206666
TV	13.994086049971	0.000000000039	0.000000000036
TV	-3.238718197842	3.356822762124	0.000000000039
TV	2.588599516667	-3.007570431079	4.530053755023

EQ-SiO₂ 96

O	-2.665674608119	-0.067089278375	2.708500052279
O	13.581154167136	0.372341331921	-7.066738222785
O	-4.346936472530	1.231462614757	1.834332572524
O	-3.322363879530	-0.289104558259	-1.881700520292
O	-3.953966455908	3.317856139653	2.708484908791
O	12.292892235764	3.757272113770	-7.066757427456
O	-5.635201013038	4.616417792639	1.834288530845
O	-4.610621234923	3.095865364994	-1.881726483847
O	-5.242258030027	6.702792046495	2.708489991486
O	11.004601301913	7.142261837952	-7.066746711100
O	-6.923440336329	8.001404252696	1.834313933384

O	-5.898903143987	6.480853798074	-1.881717885743
Si	-5.709765116581	8.457279485078	3.100506895063
Si	-5.130564640618	2.866365130859	1.473536619215
Si	-6.418839321895	6.251339785655	1.473513968687
Si	-3.133213227616	1.687358499488	3.100499532092
Si	-4.421498753803	5.072323136669	3.100464948793
Si	-3.842288297945	-0.518580262795	1.473566969634
TV	5.071191206311	-0.000000000011	0.000000000006
TV	-3.864845560596	10.154875939827	0.000000000137
TV	-2.207671988797	-0.856982907944	3.777268150681

EQ-SiO₂ 97

O	-3.320685649391	0.465887827980	0.174293878388
O	3.168756879961	-1.845093230159	-0.229538992196
O	0.397461117491	2.544378923239	1.402695787577
O	-1.099850380005	0.369396625615	-1.380600669166
O	-2.328669216500	3.636074898945	0.174267433988
O	4.160795373720	1.325058362996	-0.229588836058
O	1.389534299469	5.714539171114	1.402701850851
O	-0.107752961674	3.539513909017	-1.380557672051
O	-1.336574678528	6.806208123805	0.174318188018
O	5.152884235693	4.495203406765	-0.229608276196
O	2.381584860506	8.884688498539	1.402705483016
O	0.884290504796	6.709717494182	-1.380543080576
Si	2.368001733729	7.129212634940	1.202383119877
Si	-1.619883681819	2.731377017430	-1.010764543388
Si	-0.627831864058	5.901555123687	-1.010761506353
Si	0.383921884657	0.788876265234	1.202325660193
Si	1.375970307768	3.959036412522	1.202327333557
Si	-2.611925219160	-0.438816439402	-1.010756785148
TV	5.005466532285	0.000000000010	0.000000000009
TV	2.976146918894	9.510480066420	0.000000000150
TV	-1.923116998912	-1.896487344699	4.310578268637

EQ-SiO₂ 98

O	0.229151869787	1.703721843330	-0.418307716947
O	0.496544906813	-1.251244020688	-1.257078985173
O	-1.000114832581	-2.451011285261	0.558122584907
O	-1.833024763592	-1.358330859839	-0.076336662896
O	0.329384470475	2.317145854147	2.380497789675
O	0.596852992774	-0.637797703942	1.541840638951
O	-0.899815249614	-1.837650790620	3.356939772281
O	-1.732720955604	-0.744876878348	2.722606783982
O	0.429830860005	2.930510780845	5.179249873341
O	0.697257544436	-0.024352301590	4.340561679501
O	-0.799462855800	-1.224225762474	6.155807234050
O	-1.632391248560	-0.131499086381	5.521494509739
Si	-3.371370930177	-0.484209345084	5.896168551015
Si	0.176155336946	3.501571394584	3.596405801025
Si	0.276450568926	4.114961013446	6.395215755253
Si	-3.572006812032	-1.711056659560	0.298516574409
Si	-3.471622484641	-1.097650728568	3.097359386105
Si	0.075839023522	2.888183301652	0.797563930179
TV	4.530322340753	-0.000000000000	0.000000000000
TV	-2.145431289236	6.526738660649	-0.000000000000
TV	0.300965764209	1.840222566264	8.396462080822

EQ-SiO₂ 99

O	-1.984103342909	-0.935195219606	0.154101685172
O	-1.118107395803	-0.233756994618	-0.821151484226
O	0.170833765514	1.939582901739	0.347527376768
O	5.335508717249	1.897885629488	0.201722824847
O	-2.772416762472	-4.387831584329	2.306224710475
O	-1.906384158540	-3.686423637359	1.330991208452
O	-0.617452125255	-1.513072925801	2.499701292520
O	4.547239408457	-1.554764249379	2.353873907607
O	-3.560741036928	-7.840532043408	4.458277898283
O	-2.694721396339	-7.139030321880	3.483089366779
O	-1.405766039709	-4.965727704960	4.651794218886
O	3.758915760328	-5.007336341998	4.505992399994
Si	-7.881621215500	-8.574646402973	4.045794506377
Si	-0.327988060981	-3.003018398990	1.717869283145
Si	-1.116302406119	-6.455682966524	3.869995893295
Si	-6.305043334659	-1.669394745996	-0.258510991368
Si	-7.093331489024	-5.122009390392	1.893681616231
Si	0.460313260728	0.449622906668	-0.434271267934
TV	7.823630090966	0.000000000104	-0.000000000105
TV	-2.690613744527	4.472955160119	0.000000000019
TV	-2.364971751699	-10.357923630923	6.456361421105

EQ-SiO₂ 100

O	-2.198656003003	3.867626918248	1.787492409674
O	5.286962239668	-4.173437735807	-4.472862193649
O	-1.069822624555	1.869031505891	2.359963756430
O	0.589560127978	-2.379149173377	-0.197703995905
O	0.718590462283	3.868454142819	1.792144762674
O	8.155672689036	-4.183239587287	-4.490611697707
O	1.827154136280	1.871357148280	2.372363837918
O	3.509198545408	-2.374503494782	-0.185703439487
O	3.603905924342	3.873432486783	1.813591246908
O	11.069991757472	-4.180584540446	-4.483057357316
O	4.725653645562	1.869328498642	2.377331840322
O	6.371514139862	-2.381403851577	-0.199693690443
Si	3.273493817258	2.168530969892	1.519883536579
Si	0.643521163062	0.649623346139	-0.847188217809
Si	3.561542253619	0.654387073062	-0.834612808597
Si	-2.527789218776	2.161445016066	1.507027317203
Si	0.376081415925	2.164274054635	1.508733532205
Si	-2.248898901167	0.653467571948	-0.851800465418
TV	8.692854674334	0.000000000030	0.000000000028
TV	-0.334960382010	4.613247252367	0.000000000064
TV	-1.651032107514	-0.194957567147	5.424423106105

EQ-SiO₂ 101

O	0.090265527517	-0.904721680553	1.978501287153
O	0.118067979001	1.827801671625	1.594548835267
O	2.640371387521	0.281372603485	-0.840655575044
O	1.817696067487	-2.345679328254	0.351131772311
O	1.481662869867	3.337601227593	-0.859312350695
O	2.831537916833	0.314118902129	0.660588210520
O	4.799012259180	-0.904720445247	1.978528122980
O	4.826869100250	1.827816059356	1.594615157655
O	7.349198462576	0.281361072688	-0.840664304172
O	6.526519953857	-2.345656281727	0.351171630037

O	6.190508365176	3.337604828748	-0.859278911281
O	7.540382997755	0.314106156386	0.660581387482
Si	5.500375535448	-2.413211542561	1.744125325719
Si	1.033078860752	-0.322913574884	-1.034518219133
Si	-0.149684738192	0.338591962846	0.871216182294
Si	5.741893449561	-0.322898164297	-1.034524268879
Si	0.791580311482	-2.413247184781	1.744107639240
Si	4.559136238515	0.338636816250	0.871234968059
TV	9.417668584850	0.000000000000	-0.000000000004
TV	0.531625704606	5.403442569754	-0.000000000000
TV	0.789798965587	-2.603257969583	4.849643726328

(iii) GeO₂ at 1 atm

EQ-GeO₂ 0

O	1.174668930605	5.679842364884	1.932232453888
O	12.581911657204	-4.950596555415	-2.992287675516
O	-6.695175407221	2.408499448340	0.903076406987
O	1.659855516300	2.222170538604	-1.557467198404
O	-1.676464129009	8.120803042101	4.393719246706
O	9.730747710629	-2.509405344045	-0.530571580100
O	-9.546325872485	4.849580586948	3.364724981410
O	-1.191158171187	4.663314461830	0.904223386486
O	-4.527533692018	10.561893748098	6.855298625714
O	6.879532509308	-0.068167127202	1.931006063043
O	-12.397481416693	7.290802423252	5.826259110719
O	-4.042332228672	7.104547751615	3.365755567405
Ge	0.073315468294	7.705507644828	5.110418399635
Ge	-0.631599613483	5.264332092307	2.649291819369
Ge	-3.482738300174	7.705449040893	5.110879764800
Ge	5.775619674979	2.823175615043	0.187270202077
Ge	2.924421560880	5.264332930898	2.648866642706
Ge	2.219567545550	2.823019704824	0.187606240479
TV	7.110670681914	-0.000000000149	-0.000000000548
TV	3.013986803113	3.493480818939	-0.000000000135
TV	-8.553362070247	7.323507465609	7.384827293230

EQ-GeO₂ 1

O	3.727711141923	0.416378627976	2.601880592209
O	6.019921595683	-2.371614641936	-0.874983918025
O	-3.737816778968	1.936694446467	1.599319650393
O	-1.451184368212	5.270944154821	-2.345060504891
O	3.723278976879	2.030557626249	5.075180403106
O	6.015678105603	-0.757497770701	1.598533387897
O	-3.741913694347	3.550439147680	4.072778981791
O	-1.455381450642	6.885155267967	0.128406274488
O	3.719423144503	3.644617159491	7.548575301630
O	6.011211417066	0.856169282725	4.072050522039
O	-3.746280863256	5.164751908442	6.546176016644
O	-1.459646043826	8.499232279834	2.601708532348
Ge	4.564842988666	1.984503655345	3.336042258449
Ge	2.276583236682	4.678652188792	3.336009976165
Ge	2.272283169626	6.292746013566	5.809378550300
Ge	4.573425752059	-1.243493014359	-1.610888297693
Ge	4.569085576675	0.370569549710	0.862625968717
Ge	2.280899900823	3.064738794168	0.862444147288
TV	4.573200492309	-0.000000000006	-0.000000000011
TV	-0.006074998013	5.387878511609	0.000000000002
TV	-0.012826935751	4.842158764136	7.420322793569

EQ-GeO₂ 2

O	-3.018698161557	-1.155225077040	-1.355971902183
O	2.207690464070	-0.526013161215	0.773597220121
O	4.480811653241	-0.031093439613	-0.830553419175
O	1.841461273108	-0.338440785419	-1.722321982951
O	-2.118322451477	-3.288021958312	-2.964259318052
O	-0.380747707628	-0.846662710144	-0.468121613613
O	-1.643921556191	1.471051310939	-1.355552701944

O	3.582392099530	2.100550807295	0.773524125368
O	5.855512326233	2.595182942201	-0.830219944497
O	3.216185313611	2.287751354063	-1.722238975611
O	-0.743846290595	-0.661400227718	-2.964079450579
O	0.993976184681	1.779655583585	-0.468140430782
Ge	4.146936049800	3.475178472127	-0.479948625751
Ge	4.874072518799	-1.906318238515	-1.096360784062
Ge	-1.310222152460	-2.035718693084	-1.711850061883
Ge	6.248670833709	0.719959580404	-1.096206442154
Ge	2.772038172569	0.848892219748	-0.479983412246
Ge	0.064529259097	0.590493060088	-1.711859065085
TV	9.660034818633	0.000000000007	0.000000000001
TV	2.749541661728	5.252544735225	0.000000000014
TV	-3.696197257502	-1.425398171170	3.790082410865

EQ-GeO₂ 3

O	2.167389156249	5.195709704774	1.230491231054
O	5.202785490250	-9.645202855524	-3.182414012115
O	-4.695181743848	2.486483991552	0.819132209688
O	1.377124212810	3.813109169512	-1.102172129372
O	0.869627753405	8.372579558319	2.900922057524
O	3.904486405616	-6.468050837425	-1.512476737388
O	-5.993264860816	5.663806871484	2.488825547806
O	0.079131371229	6.990084657822	0.567587353798
O	-0.429245760547	11.550434944356	4.569501768577
O	2.606299060904	-3.290668617602	0.157268244144
O	-7.291190015745	8.841172379358	4.158774786844
O	-1.218908688885	10.167341617846	2.237293711930
Ge	2.562756021722	9.238935329619	2.570493049483
Ge	1.139147273728	6.577970805732	2.151668524690
Ge	-0.158947106174	9.755288381264	3.821506292912
Ge	5.158797974200	2.884607630248	-0.769306654098
Ge	3.860820668354	6.061881804795	0.900417938844
Ge	2.437023221202	3.400697031985	0.481744545610
TV	5.454163046505	-0.000000000112	-0.000000000425
TV	6.980406539172	7.557842014448	-0.000000000341
TV	-3.894265480106	9.531845802352	5.009605375781

EQ-GeO₂ 4

O	4.089253594421	1.101181867237	4.045581491445
O	7.435783011626	-1.734586388733	-7.100387394801
O	-5.369835109299	1.609769091797	1.405717912561
O	0.677056236619	1.859609205333	-0.933067275020
O	2.746053822025	4.686131290144	4.045440264747
O	6.092679789918	1.850386185038	-7.100491430729
O	-6.712963133377	5.194670705063	1.405718502849
O	-0.665989290726	5.444573896725	-0.933143246177
O	1.403033970433	8.271183485415	4.045730981373
O	4.749515510194	5.435323496738	-7.100534434262
O	-8.056077959912	8.779655891416	1.405824258636
O	-2.009186316772	9.029638304088	-0.933047985449
Ge	1.725709641977	8.385321527787	-0.199500087606
Ge	0.369862141717	5.829882623695	0.673460181470
Ge	-0.973302133800	9.414892629551	0.673567922940
Ge	4.411967140757	1.215302777553	-0.199619165299
Ge	3.068866912962	4.800286692615	-0.199645358880
Ge	1.712998793669	2.244942168400	0.673512671456

TV	5.407048495464	-0.000000000012	-0.000000000008
TV	-4.029442228388	10.754908848977	-0.000000000015
TV	1.347628268556	0.512106089824	3.526517422646

EQ-GeO₂ 5

O	-1.804464817208	-0.720354237923	-1.613875451708
O	2.417408672378	-0.543560908684	1.063091454347
O	3.692631098977	1.797603960023	-0.256710493512
O	2.310283312531	1.283914386341	-2.318356220870
O	-4.491107924286	-5.947845662177	-3.647767264622
O	1.030091297635	-1.058700739537	-1.000041017587
O	-0.265208082679	1.899400947434	2.388191783928
O	3.957421267530	2.076423494244	5.065974921385
O	5.234172494959	4.416043057780	3.745223507506
O	3.850076870891	3.903754022161	1.684653273154
O	-2.951418919411	-3.328318625033	0.355064692287
O	2.570800985360	1.560168304389	3.002715411479
Ge	3.902348441598	2.989110023033	3.374175400780
Ge	1.127277878453	-2.037803625734	0.655545857443
Ge	-0.392740644629	-2.011432824044	-1.914313956507
Ge	2.667903768122	0.581085706866	4.658242664949
Ge	2.362277342493	0.369744652587	-0.628450125203
Ge	1.147401745189	0.608537342125	2.088250171409
TV	5.489275268615	0.000000000006	0.000000000001
TV	3.989284945489	4.787433974142	0.000000000007
TV	3.080190457993	5.238967466207	8.005113400518

EQ-GeO₂ 6

O	4.060872367581	3.399020165485	1.214237051097
O	5.258309747643	-1.562950308852	-2.768094642451
O	-8.033748156008	1.227657601186	1.214130065073
O	2.461263353610	1.908084304442	-0.235576544090
O	3.269512784843	4.699040649584	3.748626223215
O	4.474061784243	-0.263574922801	-0.235564609198
O	-8.825216132616	2.527595882416	3.748756649528
O	1.674159936034	3.208461785275	2.293291410996
O	2.483744005670	5.999025808662	6.277572295380
O	3.686941902823	1.036941002058	2.293270536107
O	-9.610774491266	3.827525145692	6.277476427082
O	0.881524243212	4.509099556952	4.827157486084
Ge	3.477120389043	2.868637836697	3.020579657010
Ge	1.464424391255	5.040153380855	3.020563948509
Ge	0.675059789627	6.339373957100	5.552945492355
Ge	5.051933437885	0.267413470150	-2.042398159177
Ge	4.267357130644	1.569301216932	0.488075323357
Ge	2.254695648716	3.740864118492	0.488113361443
TV	7.053736066845	-0.000000000000	0.000000000001
TV	3.028241018162	4.342926842348	0.000000000003
TV	-2.364155382532	3.900446044127	7.595272264363

EQ-GeO₂ 7

O	3.752313848894	4.032288259225	1.874715602513
O	2.082599166533	-4.303529762218	-3.913554631726
O	-0.674442273085	1.963762669355	1.203908220553
O	0.798351383233	3.645602417117	-0.725586753800
O	6.701204393405	4.032324923847	1.874739566507
O	5.031580437869	-4.303401947809	-3.913581622056

O	2.274560762026	1.963780992347	1.203910262400
O	3.747320621742	3.645532632250	-0.725556766002
O	9.650172055899	4.032328898830	1.874737597037
O	7.980519977599	-4.303470083415	-3.913575023361
O	5.223577517452	1.963734399007	1.203912904880
O	6.696333915552	3.645475868519	-0.725577378549
Ge	8.077084019707	-1.170088011576	-1.354401122340
Ge	5.224822999813	3.838546310493	0.575026416895
Ge	8.173790112710	3.838617040582	0.575004457247
Ge	2.179093858273	-1.170192249617	-1.354384351883
Ge	5.128077120932	-1.170162529859	-1.354370072187
Ge	2.275783575292	3.838612234675	0.575028150016
TV	8.846990197137	-0.000000000006	0.000000000003
TV	1.569564778546	6.690545478808	0.000000000001
TV	1.572960390414	3.326976893439	3.858867421552

EQ-GeO₂ 8

O	3.010928159406	3.512369983664	2.322385228219
O	4.506823257530	-2.307652923701	-4.815095606832
O	-4.641806555603	2.033032567836	2.322365345995
O	2.161051118866	2.032883977826	0.323716310800
O	3.009536291399	6.471034776865	2.322344723614
O	4.505383224480	0.650980667114	-4.815114190837
O	-4.643270387940	4.991691218735	2.322353654855
O	2.159625275152	4.991536635695	0.323713594484
O	3.008107809581	9.429693675693	2.322362737255
O	4.503962672093	3.609666689873	-4.815119946380
O	-4.644714046215	7.950384138484	2.322398250181
O	2.158194951064	7.950218553126	0.323697820303
Ge	3.653469003003	5.089831771700	-3.816017535651
Ge	1.309148957091	6.471721411291	1.322809935724
Ge	1.307724290204	9.430381123067	1.322815905631
Ge	3.656330808296	-0.827491444116	-3.816005064625
Ge	3.654896990666	2.131160855449	-3.816020354456
Ge	1.310585878973	3.513052789733	1.322804647772
TV	5.102330744609	-0.000000000002	0.000000000001
TV	-0.004304155560	8.875974314656	0.000000000003
TV	0.206135489787	2.861216846862	5.138816347778

EQ-GeO₂ 9

O	2.879365382784	3.767387268759	2.315576895678
O	4.865137292414	-2.701594318426	-4.797235322844
O	-4.779751033358	2.292857904151	2.313732057667
O	2.029432181250	2.291780194913	0.314086836695
O	2.871867122019	6.719650723814	2.313453514734
O	4.857393555666	0.250563863616	-4.799306198299
O	-4.787040035387	5.243996366747	2.312806216441
O	2.022352998185	5.240573959396	0.316460783606
O	2.865381310438	9.671606376258	2.313595209717
O	4.849863360379	3.204393932016	-4.800440791458
O	-4.794321048136	8.194021835384	2.316076140842
O	2.015084516684	8.193057422775	0.315908479332
Ge	3.996160604027	4.679511229169	-3.799232546991
Ge	1.167508912070	6.719141310362	1.315146003859
Ge	1.161128768456	9.670265200756	1.315326009963
Ge	4.009699247501	-1.222868618031	-3.799837218447
Ge	4.002796987436	1.728032934220	-3.800585739793

Ge	1.175625805172	3.766985773261	1.314865125430
TV	5.108502285764	-0.000000000001	0.000000000001
TV	-0.021465977280	8.854576939047	0.000000000009
TV	-0.277099475569	3.515018688236	5.114438413928

EQ-GeO₂ 10

O	1.476883981410	3.744268769719	2.414493054806
O	10.362519169302	-6.605006010909	-4.577355313032
O	-6.200278463356	2.819784367487	1.266134493746
O	-0.236752826483	3.449465109701	-1.136311208675
O	1.484438613579	5.599739837042	4.707171142024
O	10.371128552567	-4.754172662960	-2.284776912562
O	-6.192261205387	4.673747898671	3.561425911343
O	-0.228097336265	5.300271715866	1.156226973392
O	1.492454337351	7.453723042551	7.002422033830
O	10.378037075904	-2.899925654172	0.009551241258
O	-6.183626331282	6.524235839238	5.855466248927
O	-0.221236123183	7.154515266617	3.450624364971
Ge	3.190734063513	6.377046392061	4.080460950127
Ge	0.628940210369	5.450359826063	2.932528026694
Ge	0.636179456211	7.303659792399	5.226706214667
Ge	3.174358230967	2.670370382669	-0.508502654526
Ge	3.181619745292	4.523685461199	1.785694665545
Ge	0.621113104594	3.597130599845	0.639425253392
TV	5.115085408024	-0.000000000002	0.000000000001
TV	-2.938730015319	7.274489559300	0.000000000002
TV	0.024261665317	5.559927055154	6.882032874727

EQ-GeO₂ 11

O	1.917022724603	3.208604040441	2.552937340035
O	7.976495685884	-6.002310811644	-4.641052873565
O	-5.751133982519	2.365995383242	1.344020672545
O	0.211817914576	3.162643994097	-1.014221140817
O	1.918457982191	4.893752769599	4.970872893892
O	7.977948237945	-4.317125154076	-2.223173393747
O	-5.749661166361	4.051140507084	3.761900558814
O	0.213241569539	4.847775217364	1.403691114182
O	1.919880519012	6.578950809525	7.388771605824
O	7.979320083672	-2.631993667531	0.194725314082
O	-5.748260907259	5.736328522181	6.179788385322
O	0.214655788393	6.532985197445	3.821573073307
Ge	3.622841260845	5.713293092247	4.397186676233
Ge	1.066318237343	4.870720333472	3.188230823876
Ge	1.067744544151	6.555902314740	5.606106563581
Ge	3.619987158896	2.342977946540	-0.438596601048
Ge	3.621405488265	4.028153561841	1.979273315628
Ge	1.064884763051	3.185524964045	0.770311712139
TV	5.111607061632	-0.000000000002	0.000000000001
TV	-0.099404924920	6.637199789810	0.000000000001
TV	0.004270659342	5.055521899085	7.253696292824

EQ-GeO₂ 12

O	1.908084278450	3.209155913119	2.546279955422
O	8.456574099288	-6.002952611264	-4.675698622698
O	-5.761879696749	2.382115188450	1.328722029130
O	0.204142365784	3.210076261376	-1.022979399878
O	1.909180952487	4.863294776604	4.981445978579

O	8.457709423909	-4.348832705166	-2.240560431215
O	-5.760823852971	4.036243182571	3.763873168317
O	0.205201389605	4.864164891446	1.412184107308
O	1.910295207293	6.517384950155	7.416574695769
O	8.458772390013	-2.694741318331	0.194615377505
O	-5.759694058431	5.690355515748	6.199032148166
O	0.206295288795	6.518274884849	3.847333647749
Ge	3.614278055968	5.690597269356	4.415276579563
Ge	1.057248247429	4.863543138455	3.197687887801
Ge	1.058348715423	6.517670570008	5.632833239199
Ge	3.612114584311	2.382372874470	-0.455034803774
Ge	3.613191568437	4.036468080572	1.980129756378
Ge	1.056167142603	3.209430371359	0.762530155533
TV	5.112965803413	-0.000000000002	0.000000000001
TV	-0.584633543891	6.731837532364	0.000000000002
TV	0.003267697556	4.962322076959	7.305460020104

EQ-GeO₂ 13

O	1.878039022117	3.282691947695	2.551070718386
O	8.615409674437	-6.838319890080	-4.620141776933
O	-5.797589432575	2.426390384333	1.349861036162
O	0.165475134193	3.193701631564	-1.017289645941
O	1.888318209935	4.995763130332	4.953251612251
O	8.625591339927	-5.125389957949	-2.218145578580
O	-5.787493988028	4.139204981189	3.752218933487
O	0.175188180599	4.906608170152	1.385412180273
O	1.898966529909	6.708521680016	7.355742895849
O	8.636204227569	-3.413144984883	0.184179665328
O	-5.777213534484	5.851809744942	6.154021700953
O	0.185765257862	6.619488800018	3.787419882961
Ge	3.594446344516	5.808021726395	4.371767117624
Ge	1.032318443331	4.951610533444	3.170782770123
Ge	1.042873092901	6.664542985912	5.572909497153
Ge	3.573747284428	2.382291314008	-0.432694170856
Ge	3.584030452354	4.094915026490	1.969889036146
Ge	1.022009989857	3.238780607463	0.768481690629
TV	5.113841210476	-0.000000000002	0.000000000001
TV	-0.794998439485	7.462900905667	0.000000000002
TV	0.031241862023	5.138398466952	7.206824637622

EQ-GeO₂ 14

O	2.022671575455	4.215835900264	2.444224305559
O	7.507000373600	-8.151538137081	-4.540535831928
O	-5.638381069204	3.285926111511	1.297638144826
O	0.322901530190	3.914319135581	-1.106657894433
O	2.018753187665	6.072570791495	4.731556888414
O	7.505261587328	-6.295179254056	-2.253950049765
O	-5.640461611212	5.141868512251	3.584830413307
O	0.321198982682	5.770653524841	1.179975452748
O	2.016631089555	7.928538901088	7.018753678998
O	7.500652421593	-4.439520709886	0.035261077356
O	-5.644122844379	7.002487850267	5.878190855003
O	0.316556981642	7.626287352254	3.469212864139
Ge	3.722147922950	6.848545484054	4.101925304945
Ge	1.169753812641	5.921168983259	2.955814843757
Ge	1.166324192433	7.780564236695	5.244567502226
Ge	3.728553387745	3.134547554139	-0.478138807957

Ge	3.725133830262	4.993895754160	1.810660043398
Ge	1.172964288677	4.061932669728	0.667951865198
TV	5.107962760700	-0.000000000002	0.000000000001
TV	0.482703364994	9.279174379775	0.000000000003
TV	-0.009646924200	5.573296651270	6.867864946318

EQ-GeO₂ 15

O	1.641898583242	4.595013378970	2.519850863669
O	9.099670103177	-11.096946115811	-4.818259853117
O	-6.001563311730	3.809382033685	1.265440565208
O	-0.055464521578	4.726235390588	-1.055065863510
O	1.637860647548	6.166243237189	5.028602084507
O	9.095671743064	-9.525732985705	-2.309520226905
O	-6.005562228845	5.380664638196	3.774226137201
O	-0.059517362498	6.297402466624	1.453735131203
O	1.633806121475	7.737452115736	7.537342886735
O	9.091574343531	-7.954583651046	0.199308986405
O	-6.009622485286	6.951773114770	6.282989115524
O	-0.063535822859	7.868608556799	3.962476100763
Ge	3.335198624173	7.019027420451	4.498782659677
Ge	0.788732558203	6.233428561907	3.244403025807
Ge	0.784673824200	7.804657787076	5.753148700989
Ge	3.343287365392	3.876597262471	-0.518729197717
Ge	3.339224221193	5.447823526023	1.990029144743
Ge	0.792763093782	4.662209245689	0.735648000675
TV	5.096956661083	-0.000000000004	0.000000000001
TV	-1.503660747540	13.466398115735	-0.000000000000
TV	-0.012230128872	4.713616106293	7.526240439266

EQ-GeO₂ 16

O	2.464845604793	3.693073604759	2.456504925471
O	5.947643303595	-7.747739239402	-5.010505413579
O	-5.182473400420	2.995448423719	1.153078487685
O	0.766169683802	4.065971406511	-1.100307182914
O	2.463765824123	5.088598907104	5.063438350673
O	5.946602461852	-6.352203684099	-2.403745898902
O	-5.183445152159	4.390868682859	3.759907902930
O	0.765328412976	5.461501447076	1.506546449262
O	2.462679615841	6.484196946342	7.670176200326
O	5.945601795998	-4.956756177434	0.203019184289
O	-5.184524425162	5.786472864612	6.366755884739
O	0.764173762196	6.856889645747	4.113348889529
Ge	4.163349296754	5.973735855322	4.590775091519
Ge	1.614654186233	5.275923802927	3.287401610968
Ge	1.613600701689	6.671566999226	5.894164150098
Ge	4.165354550006	3.182798397291	-0.622959352854
Ge	4.164397944656	4.578305880488	1.983877741484
Ge	1.615631138206	3.880529574430	0.680501499875
TV	5.098476472408	-0.000000000004	0.000000000001
TV	2.467797416268	9.720376307080	-0.000000000001
TV	-0.003010538500	4.186508608109	7.820544070236

EQ-GeO₂ 17

O	1.532477789454	6.207219874498	2.251706138854
O	9.123095520599	-18.496038728757	-4.699183806725
O	-6.143970152239	6.434085388547	0.799333659831
O	-0.172210555122	8.641095962237	-0.342100851736

O	1.530272192926	5.753335963196	5.156388364291
O	9.120867291313	-18.949839028816	-1.794455600873
O	-6.146206419598	5.980290736649	3.704005511258
O	-0.174420254343	8.187304669489	2.562653121617
O	1.528063449271	5.299513181733	8.061086053304
O	9.118674293851	-19.403657457745	1.110253318201
O	-6.148346441999	5.526404205729	6.608747187193
O	-0.176632347835	7.733472102714	5.467341924817
Ge	3.236542955522	6.743787604092	5.310289196954
Ge	0.678448513543	6.970706386672	3.857951536758
Ge	0.676234191091	6.516881831561	6.762651104967
Ge	3.240972583924	7.651406194570	-0.499156027030
Ge	3.238743125728	7.197689168849	2.405590847936
Ge	0.680650150385	7.424550542150	0.953230364208
TV	5.118369634217	-0.000000000004	-0.000000000001
TV	-1.614405330503	27.817876369070	-0.000000000002
TV	-0.006644687639	-1.361466408612	8.714154430564

EQ-GeO₂ 18

O	-5.766368469018	14.212375595234	2.210641075849
O	32.244033590910	-43.469104156535	-4.682198523553
O	-13.433434160773	14.471341848371	0.761635106800
O	-7.471859543149	16.703372489412	-0.335351848336
O	-5.762287720792	13.694623251325	5.108550277321
O	32.248327522611	-43.986910108493	-1.784336789183
O	-13.429184915239	13.953576622115	3.659675661361
O	-7.467593698351	16.185552600250	2.562554134238
O	-5.758107820294	13.176937447614	8.006342041881
O	32.252305848824	-44.504790540080	1.113708525221
O	-13.424917300046	13.435634088459	6.557560901167
O	-7.463289137505	15.668056572001	5.460284439792
Ge	-4.058243038291	14.681646443394	5.282022255696
Ge	-6.615176991536	14.940506598988	3.833035175787
Ge	-6.611117817382	14.422983570321	6.730899177079
Ge	-4.066753133434	15.717104424852	-0.513827182622
Ge	-4.062434997154	15.199457245479	2.384117517538
Ge	-6.619496044075	15.458265671110	0.935139092567
TV	5.109864619220	-0.000000000046	0.000000000009
TV	-32.057276681552	60.949312447350	-0.000000000070
TV	0.012581986456	-1.553298247511	8.693724448768

EQ-GeO₂ 19

O	-0.500197315886	9.097295525888	2.232817979176
O	15.629001207996	-28.245622076857	-4.686548690366
O	-8.173112055520	9.338969038280	0.783176868800
O	-2.202874320317	11.558708652560	-0.337693063535
O	-0.500802178726	8.614145796604	5.132114283043
O	15.628449681613	-28.728724640720	-1.787259877600
O	-8.173814202870	8.855739862197	3.682473673000
O	-2.203469504624	11.075485770715	2.561610775092
O	-0.501279449664	8.130987560729	8.031243028206
O	15.627852063886	-29.211857589850	1.112031456780
O	-8.174343148028	8.372591634652	6.581597907406
O	-2.204134990747	10.592406351091	5.460774678218
Ge	1.205774015295	9.603715054357	5.294202700184
Ge	-1.351663720195	9.845235779163	3.844596632874
Ge	-1.352238044120	9.362120933399	6.743794105884

Ge	1.206924739113	10.570045694925	-0.504268531111
Ge	1.206358149749	10.086834903190	2.394952905055
Ge	-1.351044736932	10.328471723881	0.945395489969
TV	5.115460089394	-0.000000000003	-0.000000000000
TV	-10.157875075885	40.529094670853	0.000000000008
TV	-0.001720148166	-1.449500657912	8.697669754516

EQ-GeO₂ 20

O	1.635587995461	4.772325154926	2.349500148527
O	8.918758643785	-15.106344071497	-4.897974698470
O	-6.023473037102	4.855465755684	0.877044853680
O	-0.065253667099	6.938519606804	-0.480527659723
O	1.633439143445	4.606049272165	5.294428348340
O	8.916623642301	-15.272633134578	-1.953011819682
O	-6.025611491103	4.689203863660	3.821965067859
O	-0.067371417537	6.772291101466	2.464407384022
O	1.631297283980	4.439787288491	8.239407294349
O	8.914476963696	-15.438887204588	0.991945386572
O	-6.027757492604	4.522878227755	6.766915994363
O	-0.069536006320	6.605979106692	5.409373854611
Ge	3.335051997384	5.606082438939	5.353069770016
Ge	0.782743534400	5.689237912681	3.880579325246
Ge	0.780600851456	5.522936370417	6.825535059712
Ge	3.339319040221	5.938629844443	-0.536850282351
Ge	3.337193842129	5.772373912318	2.408118831238
Ge	0.784877030788	5.855490233742	0.935638954140
TV	5.106750126938	-0.000000000019	-0.000000000001
TV	-1.320688706489	22.294310272306	0.000000000014
TV	-0.006405384186	-0.498800930813	8.834884256825

EQ-GeO₂ 21

O	2.049015913015	3.921546698648	2.559468334235
O	7.549316049800	-10.268727528317	-5.073219011564
O	-5.630089163896	3.531858721282	1.138325663118
O	0.335708617696	5.074299520460	-0.809351369307
O	2.055713669438	4.701134302105	5.402037204989
O	7.555986558989	-9.489165766039	-2.230689083848
O	-5.623431768367	4.311439629212	3.980891165052
O	0.342402041081	5.853812284719	2.033176586660
O	2.062375731024	5.480733522158	8.244603578132
O	7.562638258832	-8.709584960936	0.611812668170
O	-5.616774574440	5.090959447004	6.823460365808
O	0.349054929906	6.633367999442	4.875678325638
Ge	3.761562649433	5.667411707003	5.139028061309
Ge	1.199669385212	5.277549849713	3.717772484618
Ge	1.206332867143	6.057092862894	6.560313848113
Ge	3.748254195635	4.108368442662	-0.546001381163
Ge	3.754892195013	4.887890756539	2.296497949678
Ge	1.193022044885	4.498008954668	0.875243402553
TV	5.117155133961	-0.000000000004	-0.000000000001
TV	0.451989786980	14.173769809863	-0.000000000001
TV	0.019978770654	2.338634407296	8.527544151414

EQ-GeO₂ 22

O	1.993957009589	4.683368909429	2.568535060710
O	7.832306905235	-13.087694168639	-5.063923323823
O	-5.660253621217	4.280420627834	1.150572406404

O	0.297402006799	5.806422820451	-0.810330376510
O	1.992222465564	5.489192114325	5.403722670591
O	7.830400422524	-12.282141477265	-2.228256893919
O	-5.661937334614	5.086336337478	3.986106209490
O	0.295566889999	6.611724856721	2.024905270817
O	1.990127862571	6.294820290147	8.239049814885
O	7.828573663573	-11.476789600246	0.607287766114
O	-5.663906081257	5.892080253125	6.821335691589
O	0.294137063096	7.417565630418	4.860187186476
Ge	3.694259002434	6.453472167745	5.131749128730
Ge	1.143390645105	6.050515901799	3.714181081900
Ge	1.141550234513	6.856337978840	6.549651368773
Ge	3.698033898082	4.842089751957	-0.538926751848
Ge	3.696188038165	5.647545423587	2.296539172212
Ge	1.145319629980	5.244777236742	0.878871714737
TV	5.103408772277	-0.000000000004	-0.000000000001
TV	0.123301126110	17.685566025319	-0.000000000001
TV	-0.005748783365	2.416913197938	8.506192613015

EQ-GeO₂ 23

O	1.641888794459	4.328593486095	2.549606146143
O	8.901194156493	-11.392255944757	-5.088673743825
O	-6.013123038993	3.950847847823	1.123502004431
O	-0.054626358470	5.510012202879	-0.810284169884
O	1.636973634508	5.084052497268	5.401900063330
O	8.896315014910	-10.636847847819	-2.236430895738
O	-6.017948460088	4.706327556469	3.975823268149
O	-0.059572469161	6.265369413759	2.041952608966
O	1.632074152559	5.839428147825	8.254134506180
O	8.891390892117	-9.881458991478	0.615823634810
O	-6.022889951939	5.461744574732	6.828048656464
O	-0.064444836642	7.020812037820	4.894242190420
Ge	3.338546971458	6.052690197611	5.148228341546
Ge	0.788508714218	5.675010483283	3.722074659999
Ge	0.783607863436	6.430423932741	6.574324918585
Ge	3.348341612265	4.541887952026	-0.556318012323
Ge	3.343449334106	5.297234177028	2.295962414629
Ge	0.793388226798	4.919575170164	0.869797865419
TV	5.104992563514	-0.000000000003	0.000000000001
TV	-1.291008806927	15.769127729855	0.000000000001
TV	-0.014698350990	2.266200519076	8.556797994972

EQ-GeO₂ 24

O	1.704102226146	5.210340671767	2.591307729192
O	8.739835755299	-14.696509930272	-5.037026630165
O	-5.964841198315	4.789971851572	1.179630489399
O	0.000594214664	6.288861333965	-0.802042337202
O	1.703955655829	6.051109050433	5.414691423722
O	8.739603673128	-13.855703004243	-2.213658188362
O	-5.965008005992	5.630682552805	4.003009120687
O	0.000384948519	7.129627445225	2.021391737624
O	1.703731214770	6.891917048356	8.237991327276
O	8.739496765986	-13.014922796443	0.609679028735
O	-5.965185604578	6.471481033892	6.826313810434
O	0.000252064890	7.970368867414	4.844610096112
Ge	3.408826738323	7.010725660501	5.129742837499
Ge	0.852569344999	6.590252127320	3.718102112059

Ge	0.852377129784	7.431101270495	6.541413218842
Ge	3.409141743986	5.329146259803	-0.516921576226
Ge	3.408999258144	6.169929948731	2.306400928092
Ge	0.852708157668	5.749576108638	0.894745701422
TV	5.112699555842	-0.000000000004	-0.000000000001
TV	-1.069933213292	19.724187892931	-0.000000000001
TV	-0.000495721709	2.522352471448	8.469998731822

EQ-GeO₂ 25

O	-1.136044397583	9.783335291152	2.285460041529
O	17.344876726874	-30.274186324189	-4.824569023843
O	-8.800297254518	9.943297503833	0.819669466495
O	-2.840707820457	12.093694815671	-0.427160458345
O	-1.135522145253	9.463419168839	5.217068829823
O	17.345362862178	-30.594074400672	-1.892947676780
O	-8.799790642410	9.623357285447	3.751219346441
O	-2.840208470728	11.773771819070	2.504443256250
O	-1.135023578527	9.143518318344	8.148653628550
O	17.345884726861	-30.914014652140	1.038629231755
O	-8.799254061336	9.303452553831	6.682837898250
O	-2.839698265654	11.453864250121	5.436024949994
Ge	0.566557390232	10.458616871376	5.328218017669
Ge	-1.988375434785	10.618566674924	3.862396803952
Ge	-1.987844295337	10.298671388070	6.794000275761
Ge	0.565553347654	11.098478759820	-0.534988943847
Ge	0.566037538116	10.778547386104	2.396603823283
Ge	-1.988863763035	10.938495522387	0.930803377375
TV	5.109324575851	-0.000000000003	-0.000000000000
TV	-12.522365497003	42.847764313120	0.000000000009
TV	0.001504266951	-0.959772391090	8.794827379935

EQ-GeO₂ 26

O	-3.104999926309	11.775801274978	2.358208575317
O	23.547606707289	-36.573978021188	-4.897120078579
O	-10.773168263999	11.851166220309	0.886387721946
O	-4.810376807145	13.926995511583	-0.481733327039
O	-3.100813988952	11.625097147526	5.301701008125
O	23.551950463490	-36.724721664550	-1.953521095104
O	-10.769024220112	11.700475106073	3.829975183363
O	-4.805997875717	13.776291765610	2.461743664025
O	-3.096464789860	11.474376097797	8.245172411968
O	23.556268831147	-36.875388074617	0.990022026351
O	-10.764761220881	11.549611405663	6.773515986960
O	-4.801816901849	13.625563758407	5.405246574784
Ge	-1.395819221427	12.625248753207	5.353882180376
Ge	-3.953289285435	12.700594152749	3.882104039901
Ge	-3.949038099149	12.549877303217	6.825608158805
Ge	-1.404365435975	12.926708209181	-0.533197077279
Ge	-1.400066680933	12.776005380564	2.410351794751
Ge	-3.957541178779	12.851314066071	0.938576507253
TV	5.110708145760	-0.000000000009	0.000000000005
TV	-20.698442471039	50.727067643948	0.000000000013
TV	0.012905351913	-0.452146741165	8.830594040124

EQ-GeO₂ 27

O	1.647160527791	5.465100572393	2.301387689936
O	8.722841857505	-16.935714077802	-4.851382851543

O	-6.018305359690	5.610451893858	0.831454068904
O	-0.057703181354	7.743138660193	-0.441539183045
O	1.646983896640	5.174448860095	5.241280545369
O	8.722679187654	-17.226379641072	-1.911500131730
O	-6.018492809608	5.319782573721	3.771340899913
O	-0.057886364498	7.452454346140	2.498350001078
O	1.646800812275	4.883760810965	8.181161076338
O	8.722479245478	-17.517060165808	1.028395767799
O	-6.018666311799	5.029087475378	6.711224212816
O	-0.058070910753	7.161792511952	5.438250176192
Ge	3.349623014151	6.167992744867	5.341717366956
Ge	0.794522850516	6.313311566597	3.871770879814
Ge	0.794339589731	6.022643003439	6.811661188802
Ge	3.349986701523	6.749327054780	-0.538083212362
Ge	3.349790517531	6.458658984316	2.401820747859
Ge	0.794704322356	6.603977230740	0.931875233270
TV	5.110367077121	-0.000000000004	-0.000000000001
TV	-1.114724318271	25.114866592581	-0.000000000001
TV	-0.000545797517	-0.872036379708	8.819679450219

EQ-GeO₂ 28

O	-4.227021068936	12.815663416019	2.333653650624
O	27.202800303428	-39.305875989374	-4.895465319581
O	-11.889040634729	12.915860923480	0.860312543943
O	-5.932508464501	15.011307574684	-0.475426998832
O	-4.229049590552	12.615241181384	5.280340949486
O	27.200763909512	-39.506301856653	-1.948788286864
O	-11.891109272643	12.715461103747	3.806993108455
O	-5.934543419194	14.810878282623	2.471239213367
O	-4.231094791065	12.414800549039	8.227015745768
O	27.198750400222	-39.706748037922	0.997920206098
O	-11.893121684497	12.515002759370	6.753667553757
O	-5.936561453705	14.610445391201	5.417935569314
Ge	-2.528297127386	13.612825794908	5.350925599660
Ge	-5.081638086493	13.713063209602	3.877578400280
Ge	-5.083675126379	13.512632004136	6.824269049464
Ge	-2.524226107250	14.013665526682	-0.542448810191
Ge	-2.526260306153	13.813245131831	2.404242554505
Ge	-5.079593834300	13.913471200284	0.930883850998
TV	5.108728974917	-0.000000000047	0.000000000016
TV	-25.469165552333	54.617831621312	-0.000000000055
TV	-0.006093150603	-0.601296916514	8.840058906286

EQ-GeO₂ 29

O	-1.100193972725	-0.458288061369	-2.031042142620
O	1.001247000895	-1.243839020828	2.237607800722
O	3.162530730692	2.059476749901	-0.579293005513
O	3.162100629121	2.015126548059	-3.410070856171
O	-3.251525389605	-6.201998057291	-3.392770743534
O	1.007580371271	-1.314960150632	-0.580725601338
O	3.157812637750	-0.458287115871	-2.031063444361
O	5.259211688887	-1.243834460126	2.237626699729
O	7.420509731846	2.059476582752	-0.579273320534
O	7.420086770615	2.015134502767	-3.410085348578
O	1.006364193359	-6.202069059108	-3.392864297472
O	5.265573055977	-1.314971341842	-0.580734087013
Ge	6.332859039142	0.383350454002	-0.580282472493

Ge	-0.054807578496	-2.091949233764	0.846964124629
Ge	-0.055099414281	-2.095153035665	-2.007153127810
Ge	4.203152677233	-2.091951039857	0.846988951907
Ge	2.074893981969	0.383358357691	-0.580287374547
Ge	4.202859902120	-2.095151153162	-2.007145218579
TV	8.515960515928	0.000000000012	0.000000000002
TV	4.263180852675	4.952006679678	0.000000000007
TV	-0.000553142088	2.481011435655	4.280170029010

EQ-GeO₂ 30

O	-2.106244700193	-1.444722516062	-1.895546116913
O	2.380833019674	-1.765754578551	1.056424844049
O	2.803955300798	0.908888361110	0.040781802723
O	2.820307847666	1.574551762244	-2.838580303267
O	-2.713198548884	-4.495130594605	-3.843089491183
O	0.457712681467	-0.456055162272	-0.909897219022
O	3.005980717137	-1.444721444100	-1.895636796670
O	7.493070752171	-1.765790186247	1.056496024677
O	7.916171094544	0.908875579538	0.040878564405
O	7.932516304118	1.574562074252	-2.838466748781
O	2.399068063103	-4.495126990768	-3.843128578852
O	5.569927671261	-0.456045697122	-0.909879113605
Ge	7.300156697648	-0.734561459624	-0.432177191657
Ge	1.265469708921	-3.123390855702	1.521699130617
Ge	-0.369609803567	-1.166445922025	-2.366074556086
Ge	6.377655955761	-3.123381965566	1.521795018651
Ge	2.187968478442	-0.734554947345	-0.432265581238
Ge	4.742626291725	-1.166399252405	-2.366099079139
TV	10.224432703059	0.000000000014	0.000000000002
TV	2.540524739159	4.372184494175	0.000000000007
TV	-0.034749448849	0.003386833864	5.831417019260

EQ-GeO₂ 31

O	-2.044944569997	-1.315904083176	-2.007521377513
O	2.472245578664	-1.772833886497	0.943115354152
O	2.795682699383	0.977146384204	0.013671048783
O	2.825530082151	1.678105128896	-2.931308601517
O	-2.560092682581	-4.439194771052	-3.898735197213
O	0.459703439915	-0.427604130676	-0.929524025116
O	2.950942146892	-1.315960334115	-2.007462337048
O	7.468228153436	-1.772599038504	0.943135695260
O	7.791680177317	0.977330635695	0.013625253206
O	7.821550493484	1.678155586048	-2.931293924775
O	2.435787486534	-4.439189748806	-3.898672311747
O	5.455695925029	-0.427459983044	-0.929541798681
Ge	7.199909831580	-0.667166403133	-0.478343612913
Ge	1.325143264093	-3.088382892368	1.453974438242
Ge	-0.296454964738	-1.090136702642	-2.448057393764
Ge	6.321156038316	-3.088242884312	1.453947855602
Ge	2.203912348735	-0.667314811323	-0.478277785477
Ge	4.699442157186	-1.090138127723	-2.447980796585
TV	9.991805601595	0.000000000014	0.000000000002
TV	2.528256970337	4.413883099687	0.000000000007
TV	0.005366318149	0.002836612788	5.848946163898

EQ-GeO₂ 32

O	3.493221324293	1.851531516489	3.466137813172
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O	5.220146046287	-2.661571876184	-2.868319042987
O	-4.759715695724	3.083952841923	2.055385473183
O	0.477580102262	3.598034856903	-3.625583423087
O	8.715582307722	1.851063882593	3.465591917455
O	10.442301244735	-2.661273734872	-2.869272532757
O	0.462637757483	3.083985615491	2.055377788392
O	5.699693088331	3.596974360864	-3.624214649294
O	13.938275631611	1.850743130236	3.465582736305
O	15.664776583825	-2.661305812819	-2.869461531210
O	5.685242243011	3.084024949979	2.055400115110
O	10.922883840959	3.597935960532	-3.625411551558
Ge	14.799124859955	-1.139612369179	-2.372717190235
Ge	6.997023182244	3.332122933825	0.816665612905
Ge	12.219374224807	3.332176462887	0.816220669058
Ge	4.354248927517	-1.139760070152	-2.372004367580
Ge	9.576739381413	-1.139548883631	-2.372521278441
Ge	1.774264010326	3.331889399337	0.816364468630
TV	15.667635038966	-0.000000000000	-0.000000000003
TV	2.650287372600	4.505360523460	0.000000000000
TV	0.019999354339	2.972481282447	4.244942278743

EQ-GeO₂ 33

O	-2.904834432078	-1.064091851256	-2.376035296332
O	4.158478726127	-1.308988775927	1.427677871801
O	2.302300895184	0.678751110468	-0.172036912201
O	1.604126531054	0.854649074147	-2.745387609466
O	-1.709473302225	-2.861986964066	-3.811895957611
O	-0.285545606754	-0.196633280580	-1.305482787219
O	-2.205469533377	1.789408141793	-2.375890698222
O	4.857806099273	1.544459773247	1.427663286412
O	3.001558609502	3.532326048904	-0.172114814919
O	2.303505446818	3.708159592680	-2.745295110503
O	-1.010190366728	-0.008440518158	-3.811833071285
O	0.413858925783	2.656871405587	-1.305497078438
Ge	2.354506074192	2.179148650301	-1.218546592611
Ge	4.094980041408	-2.806092284655	2.478278778765
Ge	-0.998914109420	-1.528583442133	-2.559398691831
Ge	4.794234940766	0.047407412438	2.478378034107
Ge	1.655018655051	-0.674391240107	-1.218504260038
Ge	-0.299577850570	1.324951229461	-2.559328607454
TV	6.153075897934	0.000000000007	0.000000000001
TV	1.398650313349	5.707031798465	0.000000000012
TV	1.591234900684	-0.433248161737	6.381607266345

EQ-GeO₂ 34

O	2.782717901486	2.299274944857	0.526129147442
O	2.558586017664	-1.304523677349	-3.158592598411
O	-1.765136781837	0.353679670615	2.383965167466
O	1.496950231873	3.989432149506	-1.313163282527
O	5.805870769569	2.299151497810	0.526180727780
O	5.581692941872	-1.304368847893	-3.158638153780
O	1.257867425655	0.353712798620	2.384220684794
O	4.520180067877	3.989424620916	-1.313164040071
O	8.828772281610	2.298788690006	0.526319906722
O	8.604724895380	-1.304431456869	-3.158663627062
O	4.280933374371	0.353781760835	2.384074479738
O	7.543022606699	3.989506770111	-1.313275881426

Ge	8.828705855293	-0.669886338781	-1.310227041902
Ge	4.282383216040	3.338684726014	0.531872405987
Ge	7.305447455686	3.338689404134	0.531861104959
Ge	2.782582192533	-0.669912476450	-1.310216157869
Ge	5.805637727888	-0.669859788126	-1.310166972492
Ge	1.259173340356	3.338617613823	0.531879586752
TV	9.069150074139	-0.000000000006	0.000000000003
TV	0.794813289326	6.410806651650	0.000000000001
TV	-0.003386082021	-0.008837864921	3.693722952638

EQ-GeO₂ 35

O	3.287639058946	3.355495708969	1.839739826572
O	2.926224668731	-2.847452515194	-4.004660735642
O	-1.616132346697	1.543801857914	0.300776395819
O	0.689580127238	3.331616796108	0.610927847204
O	4.711508326050	5.202978369092	4.914972081580
O	4.349919077054	-0.999843957259	-0.929278352256
O	-0.192414223485	3.391090860207	3.375943306388
O	2.113369518813	5.178995655964	3.686040641370
O	6.135202009134	7.050455296209	7.990226337954
O	5.773569942585	0.847495096749	2.145923957354
O	1.231406329100	5.238723130432	6.451219634387
O	3.537078960654	7.026518206570	6.761293477949
Ge	6.334847700983	4.218785409770	4.750938708809
Ge	3.797106095213	4.714889352499	3.207372965441
Ge	5.220816494989	6.562403181179	6.282642456470
Ge	3.487464277766	0.523935311751	-1.399541944630
Ge	4.911045668769	2.371250348552	1.675690266147
Ge	2.373294275368	2.867516702619	0.132170370306
TV	5.345081371622	-0.000000000001	0.000000000002
TV	4.034454727588	5.190380250986	0.000000000003
TV	4.271077502177	5.542401933249	9.225754746988

EQ-GeO₂ 36

O	-1.392277653671	-0.847036940168	-0.719531194521
O	2.959822270223	-1.599180827665	0.758005705470
O	3.207129089534	1.241446318074	-0.683472800284
O	4.506776497086	3.349788884455	-2.194071130672
O	-5.029682920401	-4.598998307498	-2.198903686230
O	1.052130895524	-0.328326722284	-0.728865402010
O	-1.379803728212	-0.831880253885	2.231329724661
O	2.972322318272	-1.583997032180	3.708870332788
O	3.219624807444	1.256600139412	2.267390025785
O	4.519211064234	3.364959911285	0.756811370578
O	-5.017225126980	-4.583830731594	0.751932108860
O	1.064609787973	-0.313160354009	2.221989985966
Ge	3.087195262308	-0.560422380111	2.227403845297
Ge	0.421343825848	-3.814818673482	-0.719080693842
Ge	-0.172094092893	-0.611413785679	-2.200211277732
Ge	0.433844152066	-3.799678163541	2.231780678893
Ge	3.074724768372	-0.575582089492	-0.723448674003
Ge	-0.159620739200	-0.596243949195	0.750651073046
TV	6.480482955679	0.000000000006	0.000000000000
TV	4.386702698293	5.930389388167	0.000000000009
TV	0.024946142302	0.030331785032	5.901714830566

EQ-GeO₂ 37

O	-2.110359442910	-1.412621256046	-2.016154287908
O	2.725869216263	-1.201937633004	1.192105272761
O	2.908783845842	0.829917757348	-0.131538789435
O	1.897487073061	1.163416464418	-2.949983885220
O	-2.048721575622	-3.498206220219	-3.973116622719
O	0.434236262326	-0.289277989194	-0.987602994247
O	-0.650253851286	2.210276624440	-2.016108727180
O	4.185924545720	2.420981894775	1.192103630944
O	4.368783358633	4.452834443361	-0.131537476886
O	3.357537169474	4.786335031402	-2.950007869986
O	-0.588673333043	0.124698766938	-3.973122887867
O	1.894332750276	3.333668570363	-0.987627120862
Ge	3.561294036484	2.710813581140	-0.564466673260
Ge	2.091120271121	-3.012216249540	1.628494244950
Ge	-0.415680381694	-0.916655277230	-2.480357077858
Ge	3.551169466888	0.610693931805	1.628502121869
Ge	2.101231810725	-0.912097012495	-0.564472839181
Ge	1.044396984957	2.706261936168	-2.480357534952
TV	5.183938884940	0.000000000007	0.000000000001
TV	2.920094478179	7.245818989292	0.000000000012
TV	0.587969567228	-0.229461890299	6.015577688712

EQ-GeO₂ 38

O	-2.717170706620	-1.605589053762	-1.756950689059
O	2.251256929670	-0.812857042623	0.594322777105
O	4.343004478373	0.836984297499	-0.587564940513
O	1.843726575526	0.809320430177	-1.836669077415
O	-3.161060149694	-4.376266916289	-2.903875130446
O	-0.213658624529	-1.579492129344	-0.479382211197
O	-1.546054000711	-0.603020000204	1.767445574785
O	3.421075085913	0.189045255141	4.117022263562
O	5.515994420483	1.836574166851	2.938218035192
O	3.013462369795	1.810815201027	1.685970561169
O	-1.992606667073	-3.374570674537	0.617445500567
O	0.959634604385	-0.578882441069	3.042496010593
Ge	3.744172761465	1.973325838232	3.493494637400
Ge	3.029226994442	-2.329099206551	-0.227265263451
Ge	-0.940906299071	-1.742792521872	-2.292146230178
Ge	4.200251844063	-1.327064609415	3.297017025770
Ge	2.572610887345	0.972250175265	-0.029075500999
Ge	0.229258651591	-0.741047191862	1.230812051794
TV	6.352179104471	0.000000000006	0.000000000001
TV	2.546795570632	4.421869722588	0.000000000007
TV	2.339419817232	2.003847562729	7.045250214393

EQ-GeO₂ 39

O	3.525435638018	2.742042193476	1.019906122711
O	3.899657978763	-1.487318167688	-3.343806459011
O	-4.111096481972	1.532450069482	1.632735458555
O	1.413051340449	2.627900506391	-0.993885223260
O	3.564094830219	4.342803652069	4.592712473212
O	3.971167577120	0.079768700756	0.156837262394
O	-4.072469655627	3.099609593992	5.110087934608
O	1.490776868309	4.207653874558	2.510751367370
O	3.625014020891	5.891864287157	8.069603025485
O	3.990214672861	1.661593213834	3.667931474726
O	-4.011333240409	4.656958592240	8.606759265292

O	1.510854872507	5.785454249584	6.024703291923
Ge	4.310834302147	2.832240880102	5.253978629473
Ge	1.767668819858	4.608430739651	4.443468358669
Ge	1.829792342047	6.169287775906	7.954538280470
Ge	4.209815131892	-0.319587668780	-1.773963182063
Ge	4.271948977946	1.256220091712	1.740081240418
Ge	1.729190949943	3.024414836971	0.925576384230
TV	5.089776408136	-0.000000000000	0.000000000000
TV	2.586461521163	4.668423642234	0.000000000000
TV	0.162937391999	4.713094939580	10.538172670668

EQ-GeO₂ 40

O	-1.696326214720	-1.291968862864	-1.468092247549
O	3.265256913206	-0.388816102202	1.182499353939
O	4.265307814886	1.113885960070	-0.953202234039
O	1.569457476004	0.681453027419	-2.180459979406
O	-5.266378248794	-4.710036445636	-3.726559342809
O	0.879486463463	-1.035744240467	-0.292305791464
O	3.445244639522	-1.291962061998	-1.468085360776
O	8.406786899663	-0.388912692438	1.182544199918
O	9.406859393819	1.113885822006	-0.953166753534
O	6.711036418981	0.681456728748	-2.180435193151
O	-0.124750843628	-4.709986931631	-3.726498878865
O	6.021050092650	-1.035718259202	-0.292247653432
Ge	7.722221687341	-0.024908723193	-0.478990573279
Ge	0.793610541744	-2.788490153872	0.351483391161
Ge	-0.104883022372	-0.503646986066	-1.931283617636
Ge	5.935171889177	-2.788475146895	0.351493265705
Ge	2.580655880219	-0.024884856208	-0.479031626613
Ge	5.036707732342	-0.503658609953	-1.931264421797
TV	10.283162975742	0.000000000012	0.000000000002
TV	4.341784763752	4.870879129807	0.000000000007
TV	2.693733088882	1.434667707265	4.180189339330

EQ-GeO₂ 41

O	-1.400605933020	-3.766850833519	-1.830210184865
O	0.299150560192	1.374274894713	1.368303593430
O	3.056488132515	2.276204826557	0.798531199682
O	2.054260240545	2.896936317356	-2.753867483130
O	-2.166195282709	-6.482171954714	-2.751750949098
O	-0.004038807248	-1.632476888948	-0.255789679194
O	4.098686857615	-3.778667439689	-1.832727440157
O	5.794079925652	1.368965135204	1.357365311514
O	8.553877933927	2.274044283206	0.797489397525
O	7.547412037503	2.893931833378	-2.765261106741
O	3.327849789802	-6.489808791182	-2.760277238669
O	5.493245717920	-1.638257648134	-0.266607749952
Ge	6.865217632530	2.833840358299	1.134146447643
Ge	4.031159861577	-4.903555616126	-3.275033378909
Ge	-0.362320102447	-2.274100112074	-1.911741040703
Ge	9.527367181563	-4.895604294742	-3.269390099368
Ge	1.370245200946	2.838750182096	1.143411273385
Ge	5.131639188418	-2.282169663215	-1.920194335867
TV	10.993159177849	0.000000000018	0.000000000020
TV	0.828614046800	5.500922733256	0.000000000012
TV	-0.712323403980	1.008517670407	5.372203343778

EQ-GeO₂ 42

O	-1.775645857157	0.667202233194	-2.215146348082
O	1.134980495718	-5.287552299750	0.932708451741
O	2.699905279010	1.890152947235	0.480506446568
O	3.286565015738	3.590315141817	-1.871756546143
O	-3.533991038636	-6.031205596187	-3.664204041538
O	0.808114096971	1.851967036269	-1.537596642296
O	3.502923241113	0.667360679635	-2.214682174421
O	6.412814020759	-5.287553392001	0.932133112595
O	7.979468049329	1.888890771269	0.481660994104
O	8.566427480849	3.589856936158	-1.870749676074
O	1.744546631861	-6.030191094810	-3.662777817078
O	6.086045125397	1.851897887420	-1.534932620932
Ge	7.880613273740	1.984715632646	-1.325253508522
Ge	1.383592449804	-6.593643367867	2.185310774343
Ge	-0.325559436778	-1.880813234389	-3.605922122706
Ge	6.659765194621	-6.594660935940	2.183841977509
Ge	2.602286555451	1.984593089529	-1.326647725486
Ge	4.953930024596	-1.880365218189	-3.604874756133
TV	10.554783861018	0.000000000012	0.000000000006
TV	4.136819516374	5.723637007439	0.000000000005
TV	0.398781487654	-2.028988436830	5.095502710165

EQ-GeO₂ 43

O	-1.741059068088	-0.695560361568	-1.554157722189
O	2.775719479725	-0.513700005103	0.631914087594
O	4.066899106833	1.978847419431	-0.436157071382
O	2.666859728270	0.971708712070	-2.834505797658
O	-4.524099691350	-6.361114361183	-3.837874520075
O	1.332643088225	-0.723138659742	-1.459423897293
O	-0.146112153213	2.675609698932	2.004483198069
O	4.371950380727	2.858399408091	4.190718315509
O	5.663123083621	5.350842841553	3.122864330167
O	4.263091653030	4.343910114632	0.724475230446
O	-2.927851252392	-2.988749162869	-0.278968179991
O	2.927992748306	2.649233188797	2.099700350447
Ge	4.330169186958	3.903844627116	2.588116430622
Ge	1.305169372517	-1.893483264653	0.088710742168
Ge	-1.612444269025	-1.683957202539	0.193836074449
Ge	2.901348305943	1.478608795739	3.647694492565
Ge	2.734305794956	0.531839646154	-0.970776292872
Ge	-0.016202517339	1.688085368529	3.752847538035
TV	5.848392328488	0.000000000006	0.000000000001
TV	4.393097150499	4.908144448578	0.000000000007
TV	3.192436915833	6.744348347117	7.117978117711

EQ-GeO₂ 44

O	-2.184317705152	-0.851229828735	-2.024436969410
O	2.491383312982	-1.150852712902	1.000888552901
O	3.679316686792	1.038205979083	-0.274641591889
O	1.684974416916	1.314710002460	-2.072765997119
O	-2.997567131912	-4.700431302028	-3.661614623280
O	0.515176418790	-0.902167513730	-0.800038402506
O	-0.559100287737	0.260231282723	2.586164996534
O	4.116597953139	-0.039592440735	5.611506430891
O	5.304371901299	2.149622323266	4.335995335219
O	3.310288781588	2.426139988560	2.537841277890

O	-1.372367400999	-3.588991384008	0.949020260053
O	2.140273444593	0.209136046614	3.810621702027
Ge	3.713849862558	1.192980135680	4.073658328166
Ge	1.987989439151	-2.997053470487	1.186344029005
Ge	-0.343364724060	-1.444110472350	-2.261504647661
Ge	3.613082651315	-1.885700907553	5.796959186415
Ge	2.088745196502	0.081631143553	-0.536970636588
Ge	1.281772210079	-0.332670075095	2.349102000890
TV	5.205327502344	0.000000000006	0.000000000001
TV	2.531892455674	4.606022001645	0.000000000007
TV	3.250322413681	2.222854230905	9.221224320128

EQ-GeO₂ 45

O	2.693862677700	4.135406665178	4.899872825869
O	7.658797535975	-7.618760013658	-5.121983811495
O	-4.868903713427	2.375649436906	0.488221777841
O	0.212056007388	3.562289003919	-2.309612179568
O	2.709698734413	5.986010069357	7.301900962742
O	7.680765404460	-5.775252131022	-2.730163260273
O	-4.854119505608	4.233324063291	2.895724030141
O	0.215747226720	5.404168228412	0.090707359575
O	2.737903565217	7.831840515996	9.695001166814
O	7.706909398523	-3.908116192930	-0.312399536178
O	-4.833223217242	6.100940062053	5.314091704872
O	0.245200343076	7.256547224608	2.486255388793
Ge	3.119228363543	5.808071575089	5.521983043272
Ge	0.661702464045	5.588742005291	1.856858561365
Ge	0.683144562186	7.440537141861	4.254873064848
Ge	3.083791956621	2.108097298072	0.723493602383
Ge	3.097583576249	3.957147855074	3.119952746208
Ge	0.646478968604	3.739606038927	-0.539589721007
TV	4.870854843864	-0.000000000002	0.000000000001
TV	-0.395666127852	7.371378797237	0.000000000002
TV	0.062244462784	5.549519839556	7.192812323406

EQ-GeO₂ 46

O	2.923901976993	2.314026504249	0.938822771752
O	2.945337862790	-1.017288744211	-3.817260654750
O	-1.565560221603	0.586697636027	3.231447816321
O	1.404375044413	3.518396931313	-1.322521471463
O	5.946037830925	2.314087470702	0.938902399991
O	5.967498808056	-1.017263838189	-3.817242925128
O	1.456592766864	0.586686717595	3.231447563749
O	4.426539984336	3.518388772483	-1.322543481939
O	8.968196842079	2.314104185011	0.938896553537
O	8.989652787275	-1.017277439445	-3.817240340548
O	4.478737955740	0.586635208027	3.231492704637
O	7.448654678037	3.518379566820	-1.322519062761
Ge	8.986600052091	-0.582922467863	-2.042374546320
Ge	4.434328173236	3.244857779637	0.482870308809
Ge	7.456476020539	3.244876546879	0.482903185844
Ge	2.942290989305	-0.582942958219	-2.042389456548
Ge	5.964452233475	-0.582939746108	-2.042368864202
Ge	1.412190487854	3.244861039500	0.482898526117
TV	9.066456585255	0.000000000000	0.000000000000
TV	1.471231307919	5.778054978646	0.000000000000
TV	0.025391874111	0.213079025299	4.880379155150

EQ-GeO₂ 47

O	3.576676761729	2.448309754264	0.959819858258
O	3.761111773689	-1.269698841538	-2.776033335927
O	-3.755145674901	1.136763226775	1.278438063915
O	1.349020008422	3.313834757814	-0.844778264695
O	3.603639997629	3.218396700149	3.884805653385
O	3.787879878510	-0.499561748704	0.149010957058
O	-3.728200527806	1.906918552075	4.203422701143
O	1.375922588356	4.083979781444	2.080269893948
O	3.630444953130	3.988662558507	6.809893323927
O	3.814898086743	0.270576544755	3.074031370978
O	-3.701415895862	2.677088851431	7.128531895463
O	1.402819413109	4.854100116279	5.005291061258
Ge	4.254564284103	1.564329454767	4.292799790125
Ge	1.812022119710	3.555916222844	3.779265019955
Ge	1.838820167714	4.326077287056	6.704322552517
Ge	4.200733483520	0.024060425454	-1.557263990982
Ge	4.227629677874	0.794216167742	1.367744834008
Ge	1.785051812450	2.785768713822	0.854236073179
TV	4.887300858735	-0.000000000000	0.000000000000
TV	0.076878045719	6.053949994240	-0.000000000000
TV	0.080622821600	2.310467212678	8.775105818013

EQ-GeO₂ 48

O	-2.146652171269	-0.908258414756	-1.616392045809
O	2.535394652830	-0.614687182795	1.074980510913
O	3.809041285240	1.663914751680	-0.546597264030
O	1.903276226434	1.435523905098	-2.213909463369
O	-4.647977853586	-4.725695671233	-3.957201571530
O	0.636573329842	-0.868599290602	-0.589462402408
O	3.053403195627	-0.908035601601	-1.616070766323
O	7.735683082313	-0.614034960359	1.073816929997
O	9.008957698069	1.664536149930	-0.547819807903
O	7.103189700335	1.436923776083	-2.214975338250
O	0.551556429552	-4.725705041316	-3.957460336933
O	5.836294839522	-0.867889299398	-0.590014573169
Ge	7.416507078672	0.400994039520	-0.569189353685
Ge	1.350465781625	-2.289947461939	0.500844050183
Ge	-0.642232712902	-1.881031784753	-1.635040236451
Ge	6.550356893265	-2.289191541871	0.500006097240
Ge	2.216638655597	0.400035015413	-0.568128031992
Ge	4.558258039010	-1.880089057148	-1.636294955695
TV	10.399074387262	0.000000000012	0.000000000002
TV	3.719597677147	4.966798930103	0.000000000007
TV	2.355556699892	1.555434790637	4.360976343254

EQ-GeO₂ 49

O	0.939853111954	3.991333656050	2.452551866846
O	9.266207477838	-11.194531740455	-4.687369419958
O	-6.185948565270	3.966432352170	0.467751109395
O	1.188303879025	4.981742197233	-0.435596107316
O	0.966316501315	5.990330248425	4.712961508677
O	9.292654458056	-9.195570904522	-2.426993996166
O	-6.159403252475	5.965371500269	2.728128153704
O	1.214776007217	6.980753333156	1.824808793875
O	0.992758106819	7.989278452291	6.973318841700

O	9.319144862142	-7.196597151091	-0.166603655460
O	-6.133038131915	7.964358909229	4.988509041677
O	1.241223319780	8.979683375748	4.085175114652
Ge	3.038748171520	9.233849310542	3.859418940884
Ge	0.553862421613	5.709705959913	2.952138946728
Ge	0.580228189366	7.708688213126	5.212510231467
Ge	2.985824849906	5.235906200027	-0.661339894127
Ge	3.012328341915	7.234862612350	1.599058872324
Ge	0.527321468986	3.710749607482	0.691740524874
TV	4.915410903594	-0.000000000004	0.000000000001
TV	-1.001938713017	14.144708060017	-0.000000000000
TV	0.079449339007	5.996906343542	6.781150055292

EQ-GeO₂ 50

O	-6.576312583512	-0.917731936593	-1.895908422544
O	3.557793779091	-0.822829199415	0.465982835271
O	6.772473738053	-0.301330849776	-0.166095358067
O	1.721962115091	-0.205924019968	-1.274307699516
O	-4.277650969571	-3.196535237719	-2.380069465865
O	-1.476378956277	-0.904791454523	-0.642868641322
O	-7.067677544526	-2.371091499754	0.636687982250
O	3.066408318354	-2.276152972991	2.998637908641
O	6.280989135177	-1.754700876009	2.366500818985
O	1.230582513140	-1.659269014865	1.258283364338
O	-4.769043998536	-4.649944106977	0.152560664446
O	-1.967698736903	-2.358065286625	1.889714124872
Ge	2.631866356418	-0.516155262340	2.127510703457
Ge	7.211670884932	-2.063961924067	-1.031357659849
Ge	-2.877766744948	-2.052982196546	-1.512812526381
Ge	6.720222724601	-3.517258253970	1.501247303499
Ge	3.123239997505	0.937189690871	-0.405095127533
Ge	-3.369140254218	-3.506382657719	1.019807435687
TV	15.195474389708	0.000000000007	0.000000000001
TV	0.967636213242	2.906097592337	0.000000000007
TV	-0.982749414154	-2.906668974295	5.065176921294

EQ-GeO₂ 51

O	-2.548571498286	-2.639387270920	-1.035148998830
O	2.730649892024	-0.794903789240	-0.161754831930
O	3.816704556278	1.485801757546	-1.611138811858
O	1.107032604341	1.169431013075	-1.828213070791
O	-2.620058753524	-5.470123906694	-2.407325300225
O	0.312238752272	-2.014657652448	-0.281049743108
O	-0.916928008491	-0.480294491024	1.807474360367
O	4.327501132274	0.100957450547	3.187273410272
O	5.831155389402	2.613068151661	1.879180421707
O	3.877586587321	1.619688004937	0.862809970054
O	-0.218822967173	-4.172062127909	0.896541030294
O	1.815688839421	-1.412375919171	2.485897340863
Ge	3.780705759688	1.897692696372	2.814244928046
Ge	3.828218587441	-2.205936783880	0.139278082572
Ge	-0.951240766355	-2.102133543170	-1.838324633509
Ge	5.510972333983	-1.261417927081	2.842049243287
Ge	2.439244561996	1.141418195647	-0.360105016845
Ge	0.739737393757	-0.836215707706	1.090690080694
TV	7.631252373654	0.000000000006	0.000000000001
TV	1.322411487093	5.081057533948	0.000000000007

TV	3.519080047030	1.700548675787	6.075643088623
# EQ-GeO ₂ 52			
O	-1.219446100467	-1.935593730351	-2.922380386092
O	-1.399772777418	-5.444078196470	6.009425397034
O	2.964238372326	3.659026817771	-0.744856905386
O	4.853072233397	4.143758395098	-2.926096106647
O	-3.239199186750	-7.454270529989	-3.233674245332
O	0.688760183274	-1.452324487587	-0.751877668984
O	2.626515616627	-1.935670919163	-2.922405431215
O	2.446221241539	-5.444054105230	6.009645331669
O	6.810330034585	3.658868068492	-0.744902415751
O	8.699145094703	4.143842484502	-2.926165477725
O	0.606771061659	-7.454253018938	-3.233731361280
O	4.534766555496	-1.452382955578	-0.751919299296
Ge	6.794272749832	3.752905437276	-2.576798503109
Ge	-0.253150094496	-2.672473222367	0.230982433497
Ge	0.687250635272	-1.545114440998	-2.581501591928
Ge	3.592949884949	-2.672626839383	0.230917725873
Ge	2.948222671074	3.752982963320	-2.576719519629
Ge	4.533265494627	-1.545070254655	-2.581545439200
TV	7.692053230269	0.000000000032	0.000000000010
TV	4.136225496518	7.577448495692	0.000000000013
TV	0.153535371409	3.806771106818	4.630727132413

# EQ-GeO ₂ 53			
O	-2.205064678137	-1.348850856141	-1.992437923891
O	2.790345835306	-1.304566358324	0.771899707653
O	3.893323672475	0.876492688433	-0.766309396436
O	1.734852564338	1.123644310845	-2.343687676348
O	-3.104348716818	-3.782999673375	-4.189682145830
O	0.625620625442	-1.049026281860	-0.803642056465
O	-0.120770337765	3.303291737215	-1.992536992271
O	4.874967084334	3.347669603666	0.771694149733
O	5.977150717413	5.529373862060	-0.765990883555
O	3.819105389001	5.776112324104	-2.343480241850
O	-1.019319110185	0.869706156301	-4.189412907763
O	2.709849989443	3.603617877433	-0.804242432389
Ge	4.346627137197	4.560220766345	-0.782577567287
Ge	2.875320994809	-3.234323011106	0.535768465436
Ge	-0.436496739208	-1.600123687841	-2.107403817398
Ge	4.960261857344	1.417975974955	0.535641438527
Ge	2.262280917228	-0.091973740523	-0.782378353516
Ge	1.647830337978	3.052201225031	-2.107810808678
TV	5.250213447303	0.000000000007	0.000000000001
TV	4.169223951648	9.304738960546	0.000000000014
TV	2.497396217674	0.287377204563	4.625438454008

# EQ-GeO ₂ 54			
O	2.527011918534	4.714975019384	2.525150109605
O	6.933828552486	-7.803607435484	-3.760185982295
O	-7.001354257778	3.655363277800	1.670990892602
O	-0.854731532624	3.387726587527	-1.197786678759
O	1.133751362068	6.834201276243	4.233330229633
O	5.540579748036	-5.684453113550	-2.051865707113
O	-8.394667373738	5.774585068668	3.379230497396
O	-2.248016374372	5.506773878268	0.510622816005

O	-0.259521060967	8.953313383973	5.941696057026
O	4.147214531009	-3.565260867439	-0.343608775064
O	-9.787998724424	7.893870685703	5.087529080561
O	-3.641182102253	7.626051466341	2.218797319373
Ge	5.259360433072	3.801287383360	0.455874197670
Ge	-0.238888633799	6.980094705779	3.018180232201
Ge	-1.632145593759	9.099295663725	4.726539158788
Ge	8.045870633778	-0.437070400329	-2.960655256050
Ge	6.652618145029	1.682166622904	-1.252464972962
Ge	1.154387877986	4.860910929068	1.309960201427
TV	6.816690662555	-0.000000000002	0.000000000001
TV	4.526455089662	8.012498379203	0.000000000001
TV	-4.179808128981	6.357614992214	5.124788785275

EQ-GeO₂ 55

O	2.361221625639	4.897270752984	2.239369604581
O	4.516376063407	-3.614299817715	-4.610585034234
O	-4.120355813720	2.768863826081	2.239399223226
O	2.360274670307	2.762512029128	0.162636688640
O	6.681989673506	4.897264022901	2.239380252045
O	8.837139607886	-3.614292153957	-4.610583851129
O	0.200429368011	2.768881086518	2.239380240480
O	6.681045508230	2.762493972331	0.162657153279
O	11.002741815104	4.897266725894	2.239382069884
O	13.157893950029	-3.614290541595	-4.610603320853
O	4.521177043973	2.768876301835	2.239372426665
O	11.001817064436	2.762493390615	0.162665945529
Ge	12.080883329944	-2.546549133589	-3.571964813516
Ge	5.604038970603	3.830263532169	1.201287064181
Ge	9.924804961866	3.830254101217	1.201292222421
Ge	3.439343397489	-2.546536847563	-3.571988805192
Ge	7.760116025807	-2.546539860280	-3.571974852896
Ge	1.283272413510	3.830272942545	1.201273242960
TV	12.962307800619	-0.000000000007	-0.000000000002
TV	0.000821491474	4.256802755224	0.000000000001
TV	0.003890670080	4.248403441998	4.773260408914

EQ-GeO₂ 56

O	2.654452241011	4.237725440708	1.637145553383
O	2.650066740356	-3.592774383675	-3.818096145785
O	-1.908900403779	1.761604718667	0.917018640583
O	1.130835635111	4.233037110456	-0.931170394544
O	5.694209254361	4.208006843362	1.665754505734
O	5.689823199732	-3.622311782522	-3.789298113283
O	1.134203053441	1.795266170289	0.887170881981
O	4.180300128275	4.203565200200	-0.904108474725
O	8.733414987618	4.236057395034	1.639115585809
O	8.729025618478	-3.594474011970	-3.816079746684
O	4.183527585257	1.765691421766	0.914250203170
O	7.204398085101	4.199446501930	-0.901388241229
Ge	10.251374503014	-1.504479751052	-1.014694125250
Ge	4.176259699541	3.600077347888	0.830529111738
Ge	7.212293871678	3.596017780765	0.833339390645
Ge	4.175709436855	-1.534041564847	-0.987842599082
Ge	7.211670992940	-1.538111746314	-0.985002038009
Ge	1.135296082512	3.629738055964	0.803751461633
TV	9.116651082787	-0.000000000006	0.000000000003

TV	-0.002777375485	7.571983792230	0.000000000001
TV	0.003812242257	2.696323899908	3.636746940759

EQ-GeO₂ 57

O	4.459077517199	3.072110318448	3.407385561474
O	1.224880593854	-0.440984688016	-4.985252657650
O	-0.136786479054	0.574376798182	2.804723352558
O	-1.132074415074	2.910797081144	-5.588197042795
O	7.499390014505	3.071780918412	3.407528673529
O	4.264608915259	-0.441119363607	-4.984819260165
O	2.903050862744	0.574611833692	2.804306622885
O	1.907539384221	2.911132760476	-5.588333951912
O	10.539055270165	3.072079916822	3.407955947398
O	7.304909848499	-0.440388832867	-4.984647435457
O	5.942816137586	0.574483106893	2.804081784180
O	4.947411479975	2.910677643740	-5.587934239123
Ge	7.334703446262	-0.811433703213	-3.185384319442
Ge	7.528513460392	2.701402986717	5.206601654931
Ge	10.568448863047	2.701302571521	5.207142053289
Ge	1.254596781972	-0.811325308748	-3.186049418190
Ge	4.294795330547	-0.811873934322	-3.185603431295
Ge	4.488520222535	2.702131956486	5.206891561911
TV	9.119847102001	-0.000000000007	0.000000000004
TV	2.239330047299	5.849023171894	-0.000000000001
TV	3.169514386281	2.341938480986	5.595057996003

EQ-GeO₂ 58

O	2.851366419136	1.745462746106	0.948518281632
O	4.490423896658	-2.359297718331	-1.195414047981
O	-1.702819894626	3.163715702571	-1.195697665387
O	-0.186546995384	1.745671440990	0.948638266615
O	2.862096324870	2.807953667427	3.787583093837
O	4.501352979796	-1.296968306316	1.643318220627
O	-1.692433361884	4.225918098833	1.643180613870
O	-0.175695942106	2.807833349971	3.787248674611
O	2.872805932047	3.869794893103	6.626036809726
O	4.512183755526	-0.234567646534	4.482143068718
O	-1.681193466847	5.288002759917	4.481874826645
O	-0.165099135592	3.870197454324	6.626270730996
Ge	4.381030323284	3.781320656185	3.426944361248
Ge	1.343122214582	3.781497442747	3.427086683319
Ge	1.353837491303	4.843477817011	6.265899754050
Ge	4.359462722947	1.656900427672	-2.250845724123
Ge	4.370269075931	2.719130037698	0.588168061326
Ge	1.332393447228	2.719035871895	0.588312878487
TV	6.075709168800	-0.000000000001	0.000000000001
TV	2.919980091827	5.522703139150	0.000000000003
TV	0.032109294165	3.186633138291	8.516473347689

EQ-GeO₂ 59

O	7.510761016888	5.221090062446	4.649313766590
O	0.853644189447	-4.690970409675	-4.966421425462
O	-0.112995927064	3.687697155561	2.584996790213
O	-0.304763153736	3.287049304235	-2.223509224653
O	10.547579414039	5.220472202804	4.649036394042
O	3.890826652084	-4.690331646184	-4.966189356626
O	2.922870468460	3.687785616920	2.584562725497

O	2.733245676898	3.287252623533	-2.223720536375
O	13.584363606512	5.221249612215	4.648892407818
O	6.927520152946	-4.690030873045	-4.967083413044
O	5.960872689642	3.687941243398	2.584668649883
O	5.770043711987	3.287408384393	-2.223148263613
Ge	8.704001295850	-1.267886443679	-1.191904806876
Ge	2.697002548672	1.768920745597	-1.191836428439
Ge	5.733630011310	1.768885805962	-1.191713579903
Ge	2.630180220852	-1.267749321982	-1.192202451634
Ge	5.667178261023	-1.267767482151	-1.191410712222
Ge	-0.340224119884	1.768745481454	-1.191935078974
TV	9.110638464934	-0.000000000006	0.000000000003
TV	0.133001962790	6.073361100053	-0.000000000006
TV	3.295226035463	3.437240205990	4.807950847346

EQ-GeO₂ 60

O	3.574616209359	3.777214870350	2.372376042852
O	8.548160846728	-6.942792393161	-4.314550700630
O	-5.538287921106	1.967303969737	1.003268531863
O	-1.565097523705	1.834946623218	-2.941816171673
O	4.535688175810	5.852446130838	4.685637032290
O	9.509133923091	-4.867540268976	-2.001347208912
O	-4.577379629973	4.042520302810	3.316484904341
O	-0.604130673990	3.910214769503	-0.628579460750
O	5.496587286031	7.927626255860	6.998852662873
O	10.470083443708	-2.792351968590	0.311891016567
O	-3.616353507409	6.117770613970	5.629782452384
O	0.356836359379	5.985410060097	1.684643193925
Ge	5.804501052543	7.162876230685	5.268721783620
Ge	2.840126739546	7.009790448082	4.354041678538
Ge	3.801065151788	9.085011246122	6.667240619884
Ge	3.882557659095	3.012427827827	0.642259835305
Ge	4.843503309377	5.087663968563	2.955483858826
Ge	1.879133870755	4.934554605186	2.040788942566
TV	5.472386510691	-0.000000000003	0.000000000002
TV	-2.810633664832	6.963251769782	0.000000000001
TV	2.882868578938	6.225662422161	6.939692751525

EQ-GeO₂ 61

O	4.081867755715	3.885507615391	2.714975510577
O	7.321290757174	-8.326559073065	-4.727606183890
O	-6.784812391164	3.188421215842	1.561238125455
O	0.660942849724	3.915958553495	-1.266002454089
O	5.452674874018	5.280125823342	5.022674925180
O	8.692032254787	-6.932063486135	-2.419579785059
O	-5.413976741922	4.583133045149	3.869239579748
O	2.031512780914	5.310403916361	1.042256110394
O	6.824103201126	6.674658545385	7.330521686262
O	10.063348358592	-5.537453087095	-0.112053499433
O	-4.042692418937	5.977421028573	6.176575508166
O	3.402902019815	6.704777325920	3.349555153574
Ge	6.796527544701	5.811662980790	3.888673306737
Ge	2.717281340997	5.114537397970	2.734796535725
Ge	4.088300235012	6.509287925136	5.042330138865
Ge	4.054686244945	3.022835821830	-0.727059381086
Ge	5.425563426093	4.417134052024	1.580842342644
Ge	1.346252062804	3.720309151461	0.426796539515

TV	6.787655007893	0.000000000020	0.000000000020
TV	1.464692300316	10.150376803925	-0.000000000047
TV	4.113126933442	4.183336766754	6.923446089333

EQ-GeO₂ 62

O	-2.763750185428	-1.860671879646	-1.810766715788
O	2.138436702784	-0.893257592094	0.558613951623
O	4.159046872089	0.358236417200	-0.433320163548
O	1.879236331083	0.790512763764	-1.943334668256
O	-3.286074108298	-4.389505304648	-3.045409239400
O	-0.508378058615	-1.571710406225	-0.505314571581
O	-1.619970870877	-0.837610712266	1.759653442359
O	3.282166164096	0.129838149986	4.129046282147
O	5.302790486353	1.381261026782	3.137174530457
O	3.023002127254	1.813610800262	1.627155998475
O	-2.142299336610	-3.366402660284	0.525001754632
O	0.635366553430	-0.548569012253	3.065120920058
Ge	3.582315289379	1.924294275819	3.529115162861
Ge	3.973771874187	-1.444676416767	0.135888378338
Ge	-0.912272473428	-1.778447211542	-2.430363350986
Ge	5.117492222297	-0.421622516944	3.706344935044
Ge	2.438578113804	0.901193082770	-0.041345907984
Ge	0.231501676365	-0.755347475588	1.140089521804
TV	6.584879055556	0.000000000006	0.000000000001
TV	2.668360834267	4.414360745145	0.000000000007
TV	2.287500290837	2.046154388909	7.140882284743

EQ-GeO₂ 63

O	4.024110200639	5.100473692601	4.059205046323
O	8.261743027196	-10.392267316812	-3.438341202088
O	-5.141879940956	3.686759178667	2.195553846917
O	-2.098974416423	3.304871828284	-4.387770542780
O	5.005246765482	6.476962761326	6.872099021576
O	9.242796124581	-9.015735785874	-0.625434114063
O	-4.160851773637	5.063243875068	5.008434577708
O	-1.117935126515	4.681430368043	-1.574937107643
O	5.986416465927	7.853676894665	9.684945957507
O	10.224109241265	-7.639217691477	2.187549097848
O	-3.179525326597	6.439872020498	7.821384524441
O	-0.136651641215	6.058000338167	1.238032417703
Ge	5.291224873605	6.222175075705	4.982150540048
Ge	2.328730378745	6.274468815111	4.076199329313
Ge	3.309846603524	7.651153214852	6.889057302797
Ge	3.328847027255	3.468912132875	-0.643710283551
Ge	4.310056710885	4.845539248358	2.169256911249
Ge	1.347528344837	4.897971277577	1.263204549365
TV	5.468839278362	-0.000000000004	0.000000000001
TV	-2.141142814962	13.657680365443	0.000000000000
TV	2.943493729219	4.129698579598	8.438781362696

EQ-GeO₂ 64

O	3.232861304245	2.609641541733	0.382057165874
O	6.413008475584	-2.612179002154	-4.523048253347
O	-4.319233166990	2.049196538002	1.497110305257
O	-0.131384108609	4.862628738291	2.323927243682
O	4.434977086941	7.441923908721	0.406089570076
O	7.620063724313	2.142688282664	-4.502584809485

O	-3.122736167997	6.855750523926	1.500826844636
O	1.069090499460	9.688251915683	2.335654516636
O	5.635873261508	12.277064546252	0.422998059995
O	8.822999914343	6.965314122484	-4.488207470570
O	-1.924010152146	11.671200332255	1.511205367062
O	2.276493348677	14.436206913504	2.349113199436
Ge	7.727314395429	8.985701467208	-2.219452922798
Ge	2.640038862284	7.664451610013	0.066584330991
Ge	3.839558980633	12.457172197184	0.069125439106
Ge	5.329442636845	-0.632103043287	-2.241490650593
Ge	6.527720130960	4.158840572766	-2.233844985146
Ge	1.438532943479	2.842595873191	0.053307575444
TV	5.050894493673	-0.000000000000	0.000000000000
TV	3.582665923933	14.356630693133	-0.000000000000
TV	-1.341881358313	2.488983739384	4.061330828447

EQ-GeO₂ 65

O	-7.410011768532	1.356504926728	-2.814506086298
O	3.930089535323	-0.549815085483	1.361256704029
O	4.294896766346	0.870837401643	-1.218911610636
O	2.879359057931	3.067361818666	-0.761247229431
O	-4.657079964911	-7.795052524629	-4.491230358061
O	2.686003905644	-2.253892121209	-0.758169561373
O	-4.616251852640	3.711918540891	1.857769586957
O	6.726569049906	1.834451853812	6.002128856872
O	7.047225557123	3.441573552270	3.544642822865
O	5.573920922910	5.622318570027	3.827337324912
O	-1.884322705902	-5.616004682657	-0.028998474890
O	5.386950688916	0.328940170048	3.829767258946
Ge	5.215944162868	3.803172185240	3.604606696180
Ge	2.343366758005	-1.195130333639	0.719297318337
Ge	1.270049320560	-3.157610330539	-1.425141429248
Ge	5.094996028451	1.306060472166	5.369807777651
Ge	2.471301794219	1.276338673544	-1.091911800380
Ge	3.981799394318	-0.610820399419	3.202134769234
TV	9.208287277922	0.000000000007	0.000000000000
TV	3.325442958374	5.855251433574	0.000000000007
TV	5.554453359570	4.764837848773	9.250847814745

EQ-GeO₂ 66

O	-1.288456145754	-2.001529806418	0.212863497354
O	5.028996898881	-0.436799269499	3.348308912270
O	3.733991948450	0.857624261610	-0.241697170762
O	2.205829252043	2.237180384612	-2.562349887841
O	-11.030222713904	-6.982189141069	-12.594381971406
O	1.397711142618	-0.674666683465	-0.777007672643
O	4.107850091514	-1.990273805887	0.240539771219
O	10.455292542331	-0.736384316102	3.426239523028
O	9.126221255547	0.836825667917	-0.199201165715
O	7.584340593945	2.170141254545	-2.534178173538
O	-5.621298564429	-6.861481435412	-12.601003576035
O	6.801320656778	-0.707026098128	-0.768279122305
Ge	8.282569380631	-0.700878257096	0.291507318865
Ge	3.367192411132	-0.737268374063	3.378591775446
Ge	0.199660360355	-2.041001965731	-0.833274655477
Ge	8.775615280403	-0.915485737042	3.397635363222
Ge	2.870935340185	-0.653809369765	0.291609588385

Ge	5.591621435250	-2.068181099792	-0.808687745986
TV	10.838906504660	0.000000000056	0.000000000024
TV	2.586451374204	4.337570544368	-0.000000000014
TV	2.613719351596	0.915106443801	7.293226179627

EQ-GeO₂ 67

O	-1.389677723261	-2.054922378215	-0.890215754250
O	5.325686679692	0.118829739752	3.224131673946
O	3.330663760995	0.828227376185	0.313958158194
O	2.916363729874	1.316682220718	-2.565243421940
O	-11.689892251026	-5.524696001180	-12.520723717271
O	1.195846617628	-0.933468778874	-0.441135651683
O	3.746738354532	-2.067021977472	-0.941746732739
O	10.470883043711	0.226254581824	3.206297884792
O	8.439066448798	0.865208446219	0.368501392629
O	8.167290256529	1.313561001450	-2.510840875689
O	-6.555947185302	-5.466286515730	-12.461348603120
O	6.285440618776	-0.896992982898	-0.370864655470
Ge	7.996701500263	-0.896747824366	0.271472640023
Ge	3.862041446748	-0.726477402545	3.254753184250
Ge	0.374048262171	-2.487770304286	-0.908830631080
Ge	9.038995215541	-0.667107340879	3.284846705517
Ge	2.904600124394	-0.940273551470	0.209540505976
Ge	5.518280890661	-2.464314791927	-0.882084887330
TV	10.166522857331	-0.000000000044	-0.000000000040
TV	2.379496833350	4.543136071105	0.000000000013
TV	2.282573119911	1.953738504513	7.208109194206

EQ-GeO₂ 68

O	-2.231781674293	-1.585330785325	-1.519570709933
O	3.065849135352	-0.396091907774	0.809061187148
O	2.857581388364	1.831899648000	-1.512535312780
O	2.753123379452	-0.752083694405	-1.921560473649
O	-3.986089275560	-4.289867589687	-3.333259068831
O	0.301462273975	0.068715623241	-0.817528432507
O	0.407204093343	-0.467146030651	2.919072933132
O	5.704938774794	0.722369095753	5.247658418033
O	5.496406115752	2.950169346709	2.926084447393
O	5.392021833584	0.366009582189	2.517174719187
O	-1.347291956616	-3.171716939504	1.105257231349
O	2.940423934920	1.186952688087	3.620809590760
Ge	4.718179901624	1.621106670631	3.949013849763
Ge	2.857110280484	-2.759940502420	0.916636370980
Ge	-0.494443081671	-1.020031133998	-2.054009876877
Ge	5.496056896915	-1.641723459157	5.355165213506
Ge	2.079269065098	0.502882744837	-0.489549456699
Ge	2.144438709133	0.098141208283	2.384486542934
TV	6.116971019243	0.000000000006	0.000000000001
TV	2.795353840249	4.669619028019	0.000000000007
TV	5.277708578617	2.236383521648	8.876993986207

EQ-GeO₂ 69

O	-2.402006181051	-1.035604127935	-1.897334605775
O	2.523208994235	0.099280307124	0.807672679265
O	2.867282392841	1.867339067389	-1.525356267140
O	3.148492624361	-2.229377438001	-1.239021424392
O	-4.114011080448	-4.237317533936	-3.397137011962

O	0.573617601720	-0.305467556933	-0.854776836371
O	-0.301759917266	0.672780412311	2.652866756693
O	4.623381006656	1.807482315795	5.357823796500
O	4.967572981327	3.575892769321	3.024658952411
O	5.248900258723	-0.521096515821	3.311123855564
O	-2.013690089003	-2.528685071271	1.153087430377
O	2.673802595791	1.403000601663	3.695324326158
Ge	3.632892856702	2.934313204805	4.080786194403
Ge	2.105837531771	-1.920770804832	0.701279682381
Ge	-0.509651607584	-1.003362142480	-2.158080939241
Ge	4.206091621846	-0.212428688239	5.251379076020
Ge	1.532486479015	1.225953544970	-0.469303032876
Ge	1.590604340897	0.705186870480	2.392030557143
TV	6.119016824240	0.000000000004	-0.000000000004
TV	3.116521489563	4.673343959137	0.000000000002
TV	4.200652748241	3.416981905180	9.100286968967

EQ-GeO₂ 70

O	0.961590599108	-1.709910214219	-3.206445231876
O	2.684782523337	-0.925168079220	1.252101541771
O	3.978759944142	0.092935379945	-1.189681302975
O	1.429738865473	-0.251014924441	-0.937021416549
O	-1.735856224985	-3.685610815592	-2.878289210811
O	-0.268668579883	-1.063531074841	0.848428378080
O	2.387164381859	0.948550950988	-3.206444024200
O	4.110328123773	1.733314473589	1.252132231027
O	5.404340338363	2.751394247507	-1.189646356876
O	2.855260005011	2.407477882098	-0.937026411404
O	-0.310257727933	-1.027110412469	-2.878224450604
O	1.156885941251	1.594960544182	0.848386246802
Ge	4.196818700534	3.398673865543	0.367918336029
Ge	2.679159185179	-0.919941047407	-2.260864189463
Ge	-1.684035266561	-2.012073021837	-1.591665380664
Ge	4.104702204230	1.738549946381	-2.260866525039
Ge	2.771264493854	0.740183561841	0.367898280319
Ge	-0.258468621766	0.646390757652	-1.591591148770
TV	9.886338940857	0.000000000008	0.000000000001
TV	2.851152515852	5.316964253336	0.000000000014
TV	-2.383842961677	3.021751257464	4.625449729838

EQ-GeO₂ 71

O	-2.479646381155	-1.469451154798	-1.581929189918
O	3.098444724216	-3.740695300840	2.554930876241
O	4.465082204704	0.604028040213	-0.123795513964
O	0.249061360989	3.689084943524	-4.697680056172
O	-3.270339330520	-4.221060005518	-3.013009023132
O	0.084058510383	-2.135760823603	-1.432104424066
O	0.179280255220	3.055223887273	-1.604383398046
O	5.735716490160	0.808698858857	2.576806762107
O	7.121488501801	5.130017995293	-0.176541575598
O	2.878992255019	8.208215604576	-4.670447542900
O	-0.726641138557	0.348894467030	-2.982704665532
O	2.727748843914	2.378398625315	-1.420092073454
Ge	5.214227194594	5.422016591552	-0.397056285750
Ge	3.199154985481	-2.622467644117	0.514742433149
Ge	-0.764893841320	-0.510593077564	-1.351700857670
Ge	5.864416255918	1.916701210265	0.549496106066

Ge	2.566643505372	0.897038714530	-0.355683710792
Ge	1.893640133886	4.009894377809	-1.382451324110
TV	6.232589018122	0.000000000006	0.000000000001
TV	5.282263276206	9.063939282579	0.000000000014
TV	3.061702012460	1.305046069574	4.325023030405

EQ-GeO₂ 72

O	-1.445915242752	0.155318875563	-1.968765654937
O	4.369924683359	1.040235125543	0.789852378998
O	2.181372045354	2.258507798918	-1.044310294435
O	1.484486319948	-0.601210148632	-0.583724271786
O	-5.332732312858	-6.827827530708	-3.598614739155
O	1.258944277884	-1.184220630883	-1.902444733135
O	3.918263029832	0.155296090815	-1.968770080322
O	9.734119061438	1.040204202540	0.789843292052
O	7.545510480714	2.258480763864	-1.044337516033
O	6.848692768979	-0.601227819518	-0.583732796690
O	0.031456459857	-6.827838687091	-3.598572551840
O	6.623196438614	-1.184260607457	-1.902428519140
Ge	8.300586684672	0.680414685931	-0.452413655679
Ge	2.790234581922	-2.547574059864	1.123355404590
Ge	-0.648092520449	-1.475310187114	-2.387399444790
Ge	8.154447055306	-2.547589325781	1.123355141711
Ge	2.936403665981	0.680414776696	-0.452418632400
Ge	4.716113793495	-1.475326454128	-2.387403120325
TV	10.728397103530	0.000000000012	0.000000000004
TV	3.246440232825	4.911776482412	0.000000000009
TV	4.033185036859	2.729222800675	4.856513348995

EQ-GeO₂ 73

O	-1.146135502376	0.677810473957	2.157620170317
O	2.466334880746	-2.990245009044	0.637176785139
O	3.077209215278	0.558514993298	-2.633087799125
O	1.255333272973	1.549631696642	-0.932582302299
O	-1.283551199590	-3.611227684922	-3.415533569775
O	-1.829813962476	-0.074681695914	-1.258969490070
O	1.259397933452	2.954228729160	1.658026149396
O	3.635732993171	1.272044889710	0.745365254728
O	4.554090146627	2.782093925452	-1.562460576589
O	2.747726079113	4.244871830435	-0.001879684043
O	0.820985659036	-1.180720876418	-2.256898461925
O	-0.608644700562	2.260117197907	-2.944052514570
Ge	4.129492868572	2.986172233701	0.342320336642
Ge	3.056439309377	-2.674758605261	-2.168263953900
Ge	-0.846642382510	-1.559462310850	-1.533946537657
Ge	5.014403338281	1.216581904947	-2.532136707005
Ge	2.371168426019	0.135724427130	-0.391936597528
Ge	1.239910185039	1.514965251884	-2.751904736589
TV	7.269553582966	0.000000000005	0.000000000001
TV	3.317262751718	6.750026043606	0.000000000013
TV	-2.533181545099	-3.614332708653	4.945600865291

EQ-GeO₂ 74

O	-1.963669794164	-0.394730321157	-1.004912591454
O	2.915761483192	-0.217228271196	1.022714798551
O	2.388258569554	1.577518798781	-1.953033502490
O	3.310610501460	-0.971363029711	-1.361018276064

O	-4.292480538639	-4.479984331839	-3.590351868961
O	0.626230896550	-0.611968726150	-0.731858697839
O	0.204788575517	1.183915664518	3.408068423902
O	5.084243215720	1.361404787572	5.435736365490
O	4.556751509309	3.156162350655	2.460001919245
O	5.479072860188	0.607249657836	3.051976222990
O	-2.124000462738	-2.901358417698	0.822672389507
O	2.794706678703	0.966656803935	3.681151089295
Ge	4.274377398387	2.036805575019	3.852622533305
Ge	2.590927027985	-2.238988655559	0.482439184122
Ge	-0.531099404692	-1.107968152615	-2.062905176781
Ge	4.759404850689	-0.660353073862	4.895437931207
Ge	2.105905949322	0.458175425808	-0.560390927249
Ge	1.637375747447	0.470658562234	2.350103871437
TV	6.615729962449	0.000000000006	0.000000000001
TV	3.373709399301	4.512575410939	0.000000000006
TV	4.336925158302	3.157216296417	8.826027841493

EQ-GeO₂ 75

O	-0.497701960179	-0.630302033855	-0.834065600985
O	0.433807195277	-1.146194316291	0.209168883319
O	2.708214439308	0.787326538100	-0.051667162168
O	3.690170311156	1.950546107809	-3.203227027692
O	-3.961319769352	-3.902112627386	-3.507528393065
O	2.159837652952	-1.027292196281	-2.097979655433
O	-1.739699449392	0.143394145439	4.598582021134
O	-0.811708452544	-0.372167018765	5.644834786334
O	1.462449971446	1.560297666018	5.381054352915
O	2.452384897128	2.722756741118	2.228246608372
O	-5.195973834796	-3.129479750621	1.927330269946
O	0.919549743888	-0.268226230371	3.339879799233
Ge	1.440628998016	-0.398844973682	5.193563635420
Ge	-0.426872841164	-2.615269725258	1.112258154626
Ge	0.419091560948	-0.936752430440	-2.468798453431
Ge	-1.673026797287	-1.842407636822	6.545574567541
Ge	2.684688799164	-1.169985514439	-0.245904253178
Ge	-0.820037586809	-0.165582009323	2.965937385129
TV	6.311597229896	0.000000000006	0.000000000001
TV	3.996586263344	4.412193522667	0.000000000008
TV	-2.480028405531	1.546690784322	10.867154981560

EQ-GeO₂ 76

O	-3.124497010281	1.128223522398	-6.015835787843
O	3.936834124406	-4.364187329806	4.213458057949
O	2.379372443599	1.669984067037	-0.133984786600
O	3.070701063389	1.734064348666	-3.023683923787
O	-4.070395428069	-3.768089417563	-4.368474921353
O	2.274714892505	-1.134780027246	0.659672811108
O	0.187960628404	5.382819241700	-6.016415530309
O	7.246894090233	-0.107938790668	4.213309097722
O	5.691853807632	5.924574773783	-0.135545774695
O	6.380701929118	5.989866232570	-3.024517682752
O	-0.760978626059	0.486705891877	-4.368405942431
O	5.585024533215	3.120198992445	0.659741172485
Ge	4.495221018161	4.434349875779	0.022796958819
Ge	1.417595032055	-2.645047412495	1.247521146819
Ge	-1.152201985144	-1.081856128351	-2.096953192447

Ge	4.727164088878	1.610263740005	1.247732355925
Ge	1.184190647211	0.178825843490	0.022946944441
Ge	2.158012367515	3.174172855941	-2.096964466540
TV	6.133610223134	0.000000000006	0.000000000001
TV	6.620562211480	8.511514302896	0.000000000014
TV	0.720194193555	-0.090424709096	5.766362459576

EQ-GeO₂ 77

O	-3.468913037488	-1.432327504808	-1.311527231354
O	2.613996972852	-1.351849176589	0.654623834450
O	4.996820936485	-0.533765342976	-0.989314513044
O	0.172422185554	-0.266764066183	-2.323370106452
O	-1.197599747990	-0.628563634471	-2.858548811668
O	-0.943461717463	-0.799497053137	-0.003052901570
O	-2.438457903561	1.433253415320	-1.311491554290
O	3.644582783961	1.513734132747	0.654705494600
O	6.027293711173	2.331825997655	-0.989086117377
O	1.202918081615	2.598847031400	-2.323432382714
O	-0.167137996674	2.236976541108	-2.858612863156
O	0.087108464557	2.066080319852	-0.003118800260
Ge	4.083336616148	2.983167730309	-0.627479425955
Ge	5.616641227780	-2.388526711918	-1.112188321426
Ge	-1.734163157431	-2.089323750730	-1.024719846754
Ge	6.647076381435	0.477070252610	-1.112207269067
Ge	3.052946105459	0.117576380138	-0.627427495777
Ge	-0.703717799890	0.776263092655	-1.024652323389
TV	10.807027362513	0.000000000007	0.000000000001
TV	2.060889406734	5.731170765804	0.000000000014
TV	-2.863300974045	0.985695985972	3.710586803505

EQ-GeO₂ 78

O	-2.126397942290	-1.806424563843	-2.011570297092
O	2.617969630280	-1.187458813322	0.945021499099
O	2.963569498051	0.976393550129	-1.004489448537
O	2.716359157534	1.262803190011	-2.466959018515
O	-2.389883707127	-5.384464189179	-3.994148704248
O	0.430234612419	-0.683442064341	-1.023704631871
O	0.208472163150	2.777802863778	-2.017720604084
O	4.937691007271	3.353578540496	0.950389361219
O	5.288055695592	5.546788121740	-0.985509014298
O	5.002833313785	5.826959619663	-2.442331253157
O	-0.118440178440	-0.908568475810	-4.015258302377
O	2.764832150159	3.892920315967	-1.017806043059
Ge	4.564601622133	3.833310818421	-0.735816841900
Ge	1.388037782951	-2.365622683761	1.854928599008
Ge	-0.350829708062	-1.611135727127	-2.385550712591
Ge	3.692940396534	2.162397253308	1.827203962554
Ge	2.231889964577	-0.732341654452	-0.744471494709
Ge	1.982185027195	2.994213044564	-2.397024406170
TV	5.119819179530	0.000000000007	0.000000000001
TV	4.605331374396	9.158742619480	0.000000000014
TV	0.166332393619	2.126757895319	6.640432954021

EQ-GeO₂ 79

O	-4.002166529538	-2.714207390120	-5.630424087447
O	5.032635936701	-1.225563488969	1.875986983864
O	2.430911733995	0.320172591835	0.853635477658

O	2.251562383750	2.520618765950	-1.994134455310
O	-2.959457791812	-3.451324702615	-2.796449386033
O	0.388535374719	-1.302422645360	-0.628472380997
O	-1.853279057917	1.636728945065	-5.630422370397
O	7.181537094900	3.125399075481	1.875984977249
O	4.579838799256	4.671137682352	0.853638727616
O	4.400453256599	6.871568670235	-1.994097764506
O	-0.810539899916	0.899620579048	-2.796473277511
O	2.537501570681	3.048565444398	-0.628515012198
Ge	4.393817545400	3.352795456704	-0.394030489246
Ge	4.217171531116	-2.812993957774	1.487065991717
Ge	-1.407133192506	-0.796907704474	-2.439540849243
Ge	6.366067405203	1.537967014759	1.487051324481
Ge	2.244874795073	-0.998170853215	-0.394033416565
Ge	0.741788308609	3.554077914460	-2.439535384324
TV	5.128330137076	0.000000000007	0.000000000001
TV	4.297832606604	8.701943918009	0.000000000014
TV	1.674785129876	0.139180179954	6.012693675486

EQ-GeO₂ 80

O	-1.261289452167	0.469419204024	-3.089063617624
O	1.432070943212	-0.644996607979	1.805287818837
O	1.382917564573	0.758199943286	-0.972287748551
O	1.305385789629	-0.416502724119	-1.905512462127
O	-1.999335911767	-9.464203833782	-2.402937903132
O	-0.919153891893	-0.708082030908	-0.191785697358
O	-0.636534973444	4.431060639688	2.425798418710
O	2.534943983283	1.086571006003	5.750016067320
O	2.141819566258	3.722817417998	4.141444707698
O	2.034449402272	3.225601646425	2.713952866496
O	-1.344365290016	-5.095846940830	1.101883954513
O	0.012521990154	1.838139546152	4.105476550072
Ge	1.399725746055	2.332799263887	5.221118787190
Ge	1.979227697556	-2.413089475491	1.158908414397
Ge	-0.600930669380	-0.760469466564	-2.002843730294
Ge	2.702675024533	-0.740251822866	5.161878846966
Ge	0.457382877988	0.243484393853	0.589277475469
Ge	0.158126025453	2.839905884640	2.584903847447
TV	5.200902445522	0.000000000003	0.000000000003
TV	1.132771261889	6.956696234088	0.000000000007
TV	1.652277654357	5.708651287670	9.105568814060

EQ-GeO₂ 81

O	-5.097372953906	-3.035208849078	-1.713933268587
O	1.868949028379	-2.014247756104	0.078418674337
O	2.342576276946	0.657608731430	0.324915489062
O	8.829022396067	2.916452926671	-2.411319995011
O	-2.735059641961	-4.164073869289	-2.662861328253
O	-0.148925571980	-0.227578285172	-0.493608384772
O	-0.120245109740	-3.035569297426	-1.713117505593
O	6.847480938599	-2.013444384280	0.077016252947
O	7.320896565513	0.657297205418	0.322361040597
O	13.806946789181	2.915771203820	-2.410835472821
O	2.242263162641	-4.164088755915	-2.660565071988
O	4.828290490424	-0.228000197328	-0.493334272921
Ge	6.645321868449	-0.604364545123	-1.136535359245
Ge	0.692311773722	-3.388531201686	0.130916416893

Ge	-0.989807106733	-0.285275088530	-2.399195752712
Ge	5.670651381149	-3.387828697264	0.129349763539
Ge	1.667404108934	-0.605308423760	-1.135461280644
Ge	3.987219593348	-0.285000778911	-2.397459461909
TV	9.955176049050	0.000000000018	0.000000000012
TV	3.462574002833	4.784607771143	0.000000000007
TV	-1.513385859421	0.486443232043	4.654934084998

EQ-GeO₂ 82

O	-5.234749060151	-3.513380628749	-1.246929673834
O	4.145676132736	-0.488526559245	-0.607840741402
O	3.298262249587	2.248567760555	0.167962557061
O	3.398264196694	1.529441218799	-2.686410365563
O	-7.312811197101	-5.892186212450	-4.312830223244
O	1.060528533949	-0.724109626957	-0.857911901942
O	-2.660383823780	-0.663027039174	3.154084728724
O	6.718771732188	2.362630156153	3.791088331945
O	5.871820635518	5.099472011410	4.568308445885
O	5.974088377050	4.379668855802	1.714398558871
O	-4.741313369159	-3.040330617574	0.082831175699
O	3.630747280200	2.125781316287	3.538608286598
Ge	6.775935246247	4.166568942280	3.340219334716
Ge	2.569454940497	-1.161387288509	0.007412164371
Ge	-0.419304150437	-0.886262488517	0.417640451901
Ge	5.141029769071	1.691275887921	4.403583385704
Ge	4.200818680161	1.314854656625	-1.060657879448
Ge	2.152805729176	1.964780938984	4.816575013235
TV	7.444419260051	0.000000000006	0.000000000001
TV	3.861735449978	5.031669470278	0.000000000007
TV	5.145690725193	5.704801603381	8.796230871173

EQ-GeO₂ 83

O	-4.272351338248	-1.677386636754	-2.090657825618
O	2.773819265470	-1.565092940744	-0.747907338306
O	4.421486932203	-0.005655189546	0.187290316421
O	1.199090536745	0.659344874464	-1.738877286540
O	-1.572772505868	-4.376092269169	-1.160254174936
O	-3.335083005427	-2.720879722051	-2.494688559515
O	-2.846580955457	-2.185959865053	0.037205401629
O	2.238788378224	-1.629397711819	2.718228653777
O	4.001521196776	-0.082780069279	3.491928364852
O	1.465597861949	0.390312040923	1.052195786531
O	-0.447904465617	-3.082559050478	3.083776969103
O	-2.308028507002	-2.417118400349	1.342266665889
Ge	2.046772656410	0.246688890077	3.070349047806
Ge	4.676960017720	-1.887931551260	-0.212225410524
Ge	-1.520377163513	-2.553447909891	-1.802873448381
Ge	4.294833333727	-1.959399531097	2.790689388191
Ge	2.475205630605	0.321565573818	-0.452528864882
Ge	-1.143117856667	-4.127784688610	1.325000867517
TV	9.445182363572	0.000000000005	0.000000000001
TV	0.588401879671	3.584642407404	0.000000000007
TV	0.475697672228	-0.430522160329	6.702309025537

EQ-GeO₂ 84

O	-3.738644527236	-0.705104820346	-1.764134496776
O	4.107061794874	-2.118217244605	1.477279521912

O	5.752953992222	-0.644548126998	-0.416868465089
O	2.427592133891	0.718361660878	-2.950947648194
O	-2.186141117438	-2.250466873049	-3.641404543502
O	-0.263823308572	-1.924806948976	0.692417959368
O	-3.641864861797	2.337973581566	-1.764017042954
O	4.203769925643	0.925092954815	1.477363814669
O	5.849274603460	2.398498131231	-0.417867916013
O	2.524398894838	3.761451042733	-2.950774273249
O	-2.089147304900	0.792549858413	-3.641499577440
O	-0.167125293378	1.118014868568	0.692612591998
Ge	3.952840643714	2.457545974666	0.226455906045
Ge	6.757152169883	-2.195282090295	-1.085264941095
Ge	-1.836043381852	-0.738479899844	-2.392671804619
Ge	6.853886747962	0.847686356961	-1.085331704406
Ge	3.856338325603	-0.585501625048	0.226637061233
Ge	-1.739428272768	2.304560982659	-2.392531226960
TV	11.591321975752	0.000000000007	0.000000000001
TV	0.193470777069	6.086096139363	0.000000000014
TV	-1.639886774277	-3.020658572597	4.190147327532

EQ-GeO₂ 85

O	-1.674903631194	-1.735432146733	-2.695317010371
O	0.812701660238	-2.657241872885	-1.387589307625
O	1.922589010957	0.114851255510	1.116851615632
O	4.312124370475	2.797181906203	-3.816470950120
O	0.192230350650	-3.915559319153	-1.873685013747
O	0.015124752518	0.177851740362	-1.131457606634
O	1.667588056932	1.999795714082	-2.694770819297
O	4.155643036667	1.077999366665	-1.387998865686
O	5.265226362988	3.850160704874	1.116693465397
O	7.655187976001	6.532694563474	-3.815600216118
O	3.535182874256	-0.180364043338	-1.873873601287
O	3.358184361683	3.913020162987	-1.131845924146
Ge	3.489779588630	3.680241894907	0.683482256434
Ge	-0.487836252612	-2.213773379245	1.809935360339
Ge	0.005589295207	-1.208612459751	-2.294570547780
Ge	2.854903768297	1.521297325518	1.809655428620
Ge	0.147041278069	-0.054698321255	0.683851711242
Ge	3.348356064009	2.526539686816	-2.294958730684
TV	7.793183811309	0.000000000006	0.000000000001
TV	6.685303280212	7.470227263392	0.000000000014
TV	-1.798043694929	2.328831179399	5.074773027346

EQ-GeO₂ 86

O	-3.604450262900	-1.136181970141	-1.020272693085
O	2.492122161728	-1.576910972793	0.175805109214
O	4.819026177539	-0.533900341814	-1.212310704871
O	1.911407753304	0.033715272017	-2.224389312302
O	-5.264494500976	-2.524458353772	0.903433110145
O	-2.884296779313	-1.251674092550	0.230829484579
O	-2.802482548284	2.443850508583	-1.464064568778
O	3.152553121476	1.614359998675	-0.132043701762
O	5.536625886461	2.940201203669	-1.554507977821
O	2.724658250479	3.522934668513	-2.344860758085
O	-4.229564031764	1.090309610936	0.513102399349
O	-1.768636947558	2.283998113360	-0.431747981060
Ge	3.818873780780	3.163283058413	-0.912337147786

Ge	5.686729945408	-2.238526565184	-0.909442052964
Ge	0.955859631296	-1.160652922084	-3.412162949902
Ge	6.659991996676	0.842946669033	-1.470867715254
Ge	3.067372815215	-0.112787654328	-0.841959811881
Ge	0.980478168713	2.230404585016	-2.852205443547
TV	10.975798275075	0.000000000005	0.000000000001
TV	1.324824165104	6.248196727646	0.000000000014
TV	-5.064611278599	-2.895929300305	4.584135004547

EQ-GeO₂ 87

O	-1.808202939482	0.879730328723	-2.338640872473
O	2.244886450732	-0.733286014224	1.167573017364
O	1.364981548947	1.340686293849	-1.022576175803
O	1.238340316673	0.668336445197	-2.359037655674
O	-1.644764089402	-7.255128948496	-3.752110779289
O	-0.174093901486	-1.078910218283	-0.685380476803
O	-1.371625511141	3.342774393955	2.620338723915
O	2.703257930426	1.750568643968	6.133194509157
O	1.839760280866	3.772164231733	3.839779658889
O	1.669988834634	3.069293578812	2.526556834546
O	-1.302631888950	-4.918018562280	1.310938644216
O	0.274964290564	1.405951562723	4.305169594636
Ge	1.399373231614	2.542521846966	5.218121801697
Ge	2.416206283372	-2.672799549888	1.122010743931
Ge	-0.444181157582	-0.266028349474	-2.304996637025
Ge	2.827535116526	-0.194246075072	6.140908731133
Ge	0.909853761486	0.046763211123	0.290772081367
Ge	-0.029671437503	2.172020010083	2.669935529449
TV	6.042977408909	0.000000000003	0.000000000005
TV	1.037061298279	5.927770489132	0.000000000009
TV	0.886093660728	4.944326450004	9.939633452584

EQ-GeO₂ 88

O	-1.539531590826	-1.479742957216	-2.211731596447
O	0.691602584927	-0.947824101905	1.998158488800
O	2.435836609253	1.511426429609	-0.345491702426
O	0.934391921205	-0.580351501811	-3.210915489354
O	0.002942221717	-0.582441582566	-4.359922159975
O	0.886077917633	-0.825517841780	-0.756499026982
O	3.245662927225	-1.479705322031	-2.211731550780
O	5.476846151988	-0.947946780489	1.998189527602
O	7.221070701832	1.511416716335	-0.345509558353
O	5.719655597328	-0.580458006899	-3.210907162650
O	4.788202445614	-0.582415368952	-4.359882807515
O	5.671328865855	-0.825597246300	-0.756534597454
Ge	7.434387461852	-0.749891550625	-0.139584837953
Ge	0.333572050874	-2.662410601233	1.407244206138
Ge	0.222505130169	-2.085687120885	-1.878077120944
Ge	5.118768068060	-2.662467701444	1.407209033951
Ge	2.649129015658	-0.749767785489	-0.139523929278
Ge	5.007686082281	-2.085759458421	-1.878093179960
TV	9.570466990735	0.000000000014	0.000000000002
TV	2.561337019328	4.748806961302	0.000000000006
TV	-0.049138545055	2.391194684791	5.112242449421

EQ-GeO₂ 89

O	-3.243758453654	-0.972592018050	-0.707632660551
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O	1.931571460204	-1.724438325712	0.205260793047
O	4.187117617882	-1.030210151155	-1.473266715789
O	1.427469920842	-0.031029216699	-2.190665401214
O	0.459230810868	-1.735074873638	0.100907176145
O	-1.467466481876	0.055524748083	-2.038315086497
O	-0.657403599039	1.947275757364	-0.707633583381
O	4.517815027975	1.195749196490	0.204751353374
O	6.773687729846	1.889642349640	-1.473493349852
O	4.013831276189	2.888912593368	-2.190747417042
O	3.045458341358	1.185138122776	0.100803064277
O	1.118666127493	2.975747051319	-2.038459566160
Ge	5.208028270701	2.556390891258	-0.874215008642
Ge	5.392362210943	-2.053926270480	-0.549035474919
Ge	-2.455505304762	-1.658239199145	-2.327793457317
Ge	7.978863142589	0.865876378054	-0.549256489211
Ge	2.621485475542	-0.363523890100	-0.873917640900
Ge	0.130907081222	1.261672124267	-2.327837320455
TV	10.366357489692	0.000000000006	-0.000000000000
TV	5.172851022283	5.839747926785	0.000000000014
TV	-2.429515913802	-0.470481987106	4.325390186004

EQ-GeO₂ 90

O	-1.471249715577	-3.666121998252	-3.398644358234
O	1.195699561002	0.303771785738	1.691631766087
O	3.188791523067	1.340727857630	0.182204910120
O	3.260619625531	-0.013205742849	-2.300169776712
O	-2.321987343656	-3.885027572663	-4.560168410298
O	0.811461595164	-0.637814084557	-0.644786994503
O	3.281802680650	-3.666084825402	-3.398727951738
O	5.948888317776	0.303685759942	1.691591550855
O	7.941982064885	1.340686796183	0.182157066774
O	8.014001151203	-0.013218396347	-2.300424479396
O	2.430902287137	-3.885087553356	-4.560230004338
O	5.564746508364	-0.637909771666	-0.644864668038
Ge	6.142703675277	1.114488459767	-0.212934437182
Ge	0.989067362857	-1.574939347382	1.193153801142
Ge	-0.477200879321	-1.483510338937	-1.974498371992
Ge	5.742274872547	-1.574956406194	1.193059526307
Ge	1.389518600861	1.114520155991	-0.212795016166
Ge	4.276035885170	-1.483517908913	-1.974483945994
TV	9.506599663020	0.000000000012	0.000000000002
TV	2.409875227694	4.469536143408	0.000000000007
TV	0.581471689198	2.266057189485	5.176435668801

EQ-GeO₂ 91

O	-3.159103299765	-1.019960181526	-1.459870717035
O	1.778981821119	-0.619772063218	0.962611867923
O	4.455428333204	-0.090331082684	-0.335649601453
O	1.835741487159	0.153242183886	-1.725543404952
O	-1.730225312536	-3.352028969254	-3.157752799047
O	-1.956865646961	-1.493443730768	-0.735473585430
O	-1.692614823352	2.447066201727	-1.514146348527
O	3.633604423101	2.678308505740	1.319907419415
O	5.994394785440	3.377604473805	-0.431311843785
O	3.308743319268	3.480199643593	-1.349182845207
O	-0.617778438006	-0.298156729569	-3.149543888341
O	-0.529948559421	1.788697553272	-0.881039405086

Ge	4.315049685106	3.908177993899	0.148284292576
Ge	4.907494419722	-1.827723814924	-0.969338880593
Ge	-0.850471342086	-1.963346546080	-2.199829680080
Ge	6.228001632260	1.208435446008	-1.003012434882
Ge	2.712976152194	0.780502038554	-0.104768508877
Ge	0.465637929286	1.117560535725	-2.371128432515
TV	9.827925139594	0.000000000007	0.000000000001
TV	2.700197154582	6.147408745950	0.000000000014
TV	-3.454654581188	-1.916721755180	4.135350837146

EQ-GeO₂ 92

O	-3.295180103256	-0.710984460846	-1.174586125812
O	2.731899569634	-1.621039812314	0.674370287829
O	4.749335918282	-0.303307763167	-1.049877228071
O	1.754296747497	0.133064146230	-1.611981012349
O	-1.565257378396	-2.579754970176	-2.809335826455
O	-2.272952295882	-0.878906697791	-0.187568035203
O	-2.780886418872	2.449324849243	-1.174883297886
O	3.246206806630	1.539224317117	0.674174154118
O	5.263645130999	2.857157440006	-1.049688466869
O	2.269148224109	3.293441109235	-1.612128689700
O	-1.051035633974	0.580637652149	-2.809105555535
O	-1.758372206541	2.281367047755	-0.188113687923
Ge	3.510569862912	3.119700492975	-0.385815573905
Ge	5.775224517507	-2.084571900378	-0.886260989043
Ge	-0.136169468665	-1.201863955925	-2.046684231061
Ge	6.289481998478	1.075892409237	-0.886426474057
Ge	2.996263956775	-0.040650210130	-0.386095680705
Ge	0.376929130137	1.958743028601	-2.046782363267
TV	10.603724182470	0.000000000008	0.000000000001
TV	1.028478904527	6.320789675251	0.000000000014
TV	-3.510360547683	-2.713345118372	3.740329908121

EQ-GeO₂ 93

O	-3.266309006002	-0.937008232699	-1.447558503580
O	1.574761529152	-0.579929235734	0.985524088701
O	4.259395216575	-0.045985843883	-0.339523464680
O	1.604529405540	0.171656377717	-1.671686784836
O	-1.807950417515	-3.417990443096	-3.191341322263
O	-2.048307146873	-1.438882124727	-0.787545228137
O	-1.862396936426	2.537416375228	-1.548755467345
O	3.300220545355	2.794816419043	1.397492256266
O	5.692541732174	3.418394541751	-0.383661142121
O	3.030338267015	3.461314266849	-1.322048839136
O	-0.732750143466	-0.343681289815	-3.196917098360
O	-0.739937783790	1.838419871891	-0.874623939817
Ge	4.014241293089	3.953631144962	0.177738123307
Ge	4.715231393501	-1.800852998659	-0.958965014318
Ge	-0.967502702230	-2.003267155403	-2.229885320947
Ge	5.940535209290	1.212618582502	-1.034296464286
Ge	2.496314900725	0.834108511263	-0.075153686576
Ge	0.237726811447	1.112295451923	-2.341936426745
TV	9.735194008585	0.000000000005	0.000000000001
TV	2.565699618713	6.161426032705	0.000000000014
TV	-3.439783940386	-1.804024355020	4.190077049727

EQ-GeO₂ 94

O	0.779429691327	8.154462693682	0.749248345000
O	0.995432500542	-3.446656596099	-0.402207124498
O	1.853957161536	-0.642081803298	-1.616379895219
O	1.765862669312	2.424640384348	-2.498103908004
O	2.287899699840	-17.685093155753	-4.374017395900
O	0.276502882067	1.615128889487	-0.194285337102
O	3.865610843630	8.154487442294	0.749242182081
O	4.081706427245	-3.446667729051	-0.402231955221
O	4.940155206828	-0.642072862099	-1.616386451820
O	4.851998573531	2.424705645849	-2.498109472830
O	5.374096045450	-17.685064220275	-4.374055491942
O	3.362685154267	1.615183981596	-0.194381827696
Ge	3.397139225927	-0.056012203060	-0.792303006040
Ge	-1.138208879560	-2.501601076738	0.939893611573
Ge	0.230259862932	3.188846938265	-1.308513711587
Ge	1.947962187063	-2.501602101600	0.939886143838
Ge	0.310962087666	-0.056038763860	-0.792297495025
Ge	3.316430212778	3.188906001925	-1.308600673242
TV	6.172361181271	0.000000000008	0.000000000008
TV	0.484261878311	9.334392260093	0.000000000008
TV	-2.502490276580	4.502626011076	5.286970167857

EQ-GeO₂ 95

O	-3.060702586563	-0.969412070389	-1.187265798675
O	1.937840060986	-0.923915665237	0.870172449679
O	4.497487205349	-0.081273049763	-0.447682668385
O	2.045259540868	0.818509910400	-1.672872512680
O	-1.512970172653	-3.168988543670	-3.242142464234
O	-1.685859202580	-1.405294319761	-0.727310018891
O	-1.969245375415	2.166407082194	-1.299777962516
O	3.078983829493	2.192838742138	0.868422290610
O	5.644357097267	3.035046584951	-0.475125780396
O	3.197061284916	3.913285243006	-1.683215957028
O	-0.401215421383	-0.114759368059	-3.238303505147
O	-0.623203000367	1.733079848218	-0.804999792340
Ge	3.943151944873	3.625591456761	-0.032680327927
Ge	5.139878117966	-2.048171437144	-0.910136243775
Ge	-0.688823053380	-1.744196683072	-2.278657715770
Ge	6.273616891749	1.041990417987	-0.935653751893
Ge	2.800997758076	0.527899864878	-0.023712435754
Ge	0.437093640099	1.364199114463	-2.322062903126
TV	10.054978607345	0.000000000005	0.000000000001
TV	2.259700050645	6.200676490287	0.000000000014
TV	-4.004231845683	-2.165232406165	4.414113280568

EQ-GeO₂ 96

O	-0.471438358377	-0.037495027372	-0.235108036576
O	-3.466407381897	-0.151856817613	-1.777501207857
O	-2.657101753203	0.128548866725	-2.691166451530
O	-1.925306774207	-2.543761632724	-0.337339918916
O	0.000470521262	-1.677535646256	-2.681518266468
O	-4.815869091849	-2.655928541820	-0.159173417911
O	-3.187791824647	4.899021597258	-0.260184146276
O	-6.193896127764	4.775686736730	-1.788459297740
O	-5.380048327653	5.057536874608	-2.697315413248
O	-4.639916125448	2.390923836067	-0.336908806511
O	-2.714900952048	3.243847393785	-2.691685813410

O	-7.534015371996	2.276612500107	-0.159057853342
Ge	-4.851951311834	5.421502786134	0.870468310425
Ge	-3.324722071881	-3.286585119997	-1.466256144224
Ge	-0.417744265012	-1.757339605517	-0.932180420128
Ge	-6.040385064669	1.634640836107	-1.456094617176
Ge	-2.137959854461	0.495749468661	0.883711699497
Ge	-3.132978894358	3.172982636071	-0.942267476346
TV	5.830857828367	-0.000000000000	0.000000000000
TV	-5.434399783493	9.864329238780	-0.000000000000
TV	-1.014736451296	2.549934068673	5.102114924915

EQ-GeO₂ 97

O	-3.143443724175	-0.965160007659	-1.183468783229
O	1.864820631771	-0.890619822630	0.762938992756
O	4.436291317818	-0.062617826652	-0.574909118570
O	1.979467867125	0.839966123434	-1.758132585653
O	-1.742577107478	-3.190240837018	-3.175050442034
O	-1.785195198111	-1.391922265473	-0.711654931654
O	-2.002816021305	2.101463349072	-1.121104849392
O	2.982811581118	2.184063284482	0.766521808784
O	5.589583964500	2.992596387980	-0.444450637417
O	3.122064277640	3.935535600000	-1.741118545772
O	-0.583578353643	-0.030418281271	-3.178997394331
O	-0.627368669496	1.667939110550	-0.639332239945
Ge	3.879762805413	3.622599138381	-0.096449633837
Ge	5.093305881696	-2.080650132385	-0.920072916072
Ge	-0.803851945467	-1.737030113964	-2.286373822380
Ge	6.219737612485	1.020820166833	-0.889397716272
Ge	2.742166263219	0.530953491035	-0.120268759335
Ge	0.308695256455	1.359081524073	-2.231683523818
TV	10.078875088358	0.000000000005	0.000000000001
TV	2.267295191803	6.194633303380	0.000000000014
TV	-3.983280030238	-2.169922770312	4.378681703382

EQ-GeO₂ 98

O	-5.324067913506	-3.398207410449	2.465707244159
O	2.775627177539	-0.278609893756	-0.494372015019
O	3.822663125885	2.287418174068	-0.478988088610
O	5.014303884418	1.723627192375	-2.826982205634
O	-3.084251101943	-5.415260734930	-4.562381716018
O	0.366626659589	-0.706570698807	-1.887405024163
O	-5.505384448529	-0.840596331021	6.377135890153
O	2.595216588862	2.288043846732	3.420035522392
O	3.642322884751	4.854520229112	3.430836944691
O	4.830848751272	4.288540735685	1.081932692223
O	-3.266429543529	-2.857366275171	-0.647700976068
O	0.186856473832	1.863671930365	2.028333391279
Ge	3.514991856077	3.477577187764	2.157469265145
Ge	1.251646795592	-1.665505480631	-0.531409376055
Ge	-1.895344671615	-1.777606757681	-0.011387742734
Ge	1.071571327074	0.900592845473	3.381710920607
Ge	3.696616560832	0.912007108773	-1.754361715917
Ge	-2.075608737662	0.788697732072	3.901530912244
TV	5.932967651005	0.000000000008	-0.000000000001
TV	4.107007897967	5.295411246126	0.000000000008
TV	-0.361873918479	5.124892128666	7.825083050933

EQ-GeO₂ 99

O	-3.030151044739	-1.059344625315	-1.212537338350
O	1.641625274606	-0.836331177942	0.676461416955
O	4.353987934356	-0.189770167389	-0.320873678896
O	2.026398876752	0.812799851443	-1.809059832818
O	-2.061616768307	-3.099475449990	-2.882078716209
O	-1.748828996101	-1.539856261234	-0.578847535229
O	-1.809597068871	2.246368501235	-1.209617098956
O	3.074451104160	2.193152462908	0.725634007918
O	5.591417711560	3.180613949855	-0.320641186652
O	3.185167809485	3.959161847920	-1.806986717137
O	-0.985613114742	0.073062098118	-2.761843791896
O	-0.523891463960	1.774198861992	-0.578051894681
Ge	3.853900118756	3.727242655930	-0.106836102709
Ge	4.927792910178	-2.057055074940	-0.905578534223
Ge	-0.781827009120	-1.775196567004	-2.354620282100
Ge	6.262258982564	1.016467682606	-0.934367340681
Ge	2.676389504277	0.522865314950	-0.109970195708
Ge	0.374352573307	1.344755873204	-2.353329413496
TV	9.823431036900	0.000000000006	0.000000000001
TV	2.319531791651	6.275168334426	0.000000000014
TV	-2.793754719192	-2.538767967928	3.809251660094

EQ-GeO₂ 100

O	-0.557123194113	1.618561481036	1.456088134686
O	3.483720644893	-3.107293629403	-2.973075887910
O	4.164643031332	-1.403572206735	-0.637308247771
O	1.850397049577	-1.414131181440	-4.035794633191
O	3.677008405129	-1.910982390215	0.487726978787
O	1.359493831641	-1.609011083196	-1.207829002953
O	-3.934138814176	5.057676673421	1.275469058636
O	3.382418069260	0.203766906163	-2.702243118330
O	1.878208539044	3.260447088758	-1.611732410738
O	0.998481107010	1.528756228791	-4.026110381796
O	2.251249453055	2.737946959490	-0.316922943869
O	-0.116079634503	1.009936061708	-1.162427758815
Ge	0.549697665043	2.145790753693	-2.349021478176
Ge	0.864846814965	0.615502603507	0.489718727783
Ge	-1.307117697763	1.153396894200	2.988155279599
Ge	-2.892437691677	3.756967057666	0.280403064341
Ge	2.832868089148	-1.506164931319	-2.232555338755
Ge	-5.417360339433	4.227711306555	2.217553192060
TV	6.859854475914	0.000000000002	-0.000000000000
TV	-4.135197406162	6.532973735665	-0.000000000001
TV	-3.706891899125	0.787323734400	7.253814771947

EQ-GeO₂ 101

O	-3.482928221982	2.488172031951	3.654765814872
O	0.784219851630	0.001123952043	1.532898319818
O	-3.565212769664	0.738055193582	-0.610696232292
O	-3.102504455230	1.368248426124	4.030873032589
O	-0.572326884825	-0.584727754604	-1.171364798336
O	-0.840760733015	2.064042231611	-0.124365553696
O	-6.422166093333	6.647068035117	3.678178999863
O	-1.974336645270	4.175910595221	1.527856571505
O	-6.324301136362	4.910375312131	-0.617487353024
O	-5.870406976891	5.564370389737	3.931027108803

O	-3.330638823604	3.586275856372	-1.174033247772
O	-3.599638564131	6.237136072089	-0.130763708200
Ge	-5.794315223177	3.714483637725	1.008327665543
Ge	0.250211994591	0.596370866072	-0.097095136681
Ge	0.388760846452	-2.205721686124	-1.693376257714
Ge	-2.508418984332	4.769213676115	-0.102588530036
Ge	-3.037006941931	-0.462646378581	1.010629999119
Ge	-2.367768657270	1.963080664149	-1.689997531213
TV	5.629814222569	-0.000000000000	-0.000000000000
TV	-5.516164023478	8.345842078939	-0.000000000000
TV	1.731776196943	-0.786662177516	7.534261981417

EQ-GeO₂ 102

O	-2.082225750981	-1.404585797210	-2.619897824701
O	1.795137516940	-0.735641659059	-0.201850668447
O	4.565950804160	0.091153797244	-0.157107568617
O	1.453860741883	2.036383921224	-0.107560765359
O	0.612658830572	-3.102378188828	-2.374063549969
O	0.753549920483	-1.975271617727	-2.887213272356
O	-2.400744094803	0.698834114399	2.495599244476
O	1.476744384505	1.367907881386	4.913576429968
O	4.247521969022	2.194521769390	4.958399775449
O	1.135293257993	4.139792082663	5.008099521030
O	0.293968070756	-0.999254588382	2.741314627100
O	0.434924692755	0.127915271021	2.228318269274
Ge	0.437752303498	2.610451185759	3.848610571530
Ge	0.385227052420	-3.205074272595	0.931821528844
Ge	-2.133237994785	-1.219059207851	-0.812566767879
Ge	0.066691943473	-1.101733556863	6.047571349579
Ge	0.756256682783	0.506896303528	-1.266858854459
Ge	-2.451685768492	0.884321752322	4.302936216980
TV	5.563780170346	0.000000000005	-0.000000000002
TV	3.190556733969	4.917379286096	0.000000000006
TV	-0.637125358768	4.206687771834	10.231108982387

EQ-GeO₂ 103

O	-4.096904672869	-2.249804878889	-0.331184396186
O	2.827779022853	-0.140130560045	0.562737963986
O	4.505438792635	1.293214000480	-1.521602883562
O	1.675806083699	0.781887476196	-1.910327382910
O	-1.540883253205	-3.182607379031	-1.187281468029
O	-1.249897463075	-4.204460665451	-0.531464604330
O	-3.996578104954	2.213265255121	-0.208176898313
O	2.623006363171	2.822848658911	0.263083669706
O	4.743389233926	4.231585967081	-1.363614859386
O	1.795504767197	4.743257126793	-1.804028755579
O	-1.429769658421	1.021200700868	-1.077439616374
O	-1.466015025764	-0.218772581564	-0.879798778761
Ge	2.933500252852	4.780133220742	-0.314462266431
Ge	5.391375112174	-1.968655796548	-1.518525253712
Ge	0.528804562615	-1.963627385153	-2.328751973623
Ge	5.726910055541	2.675362470563	-1.461721141135
Ge	2.878745543167	1.245453758191	-0.647881246195
Ge	0.373784249934	1.958670274048	-2.696348905027
TV	10.928636616537	0.000000000007	0.000000000001
TV	0.090900152766	8.092321835320	0.000000000014
TV	-3.920429057118	-2.851040026617	3.565386986114

EQ-GeO₂ 104

O	1.041866264567	1.985266135559	1.673545801433
O	5.193429061043	0.397644734555	-5.954566186325
O	-6.024555558768	2.138459309894	5.261386453717
O	2.561281398265	1.785461009856	-0.767894152388
O	1.392042073415	5.319515847735	1.677288230942
O	5.533312208643	3.745453860985	-5.960617265220
O	-5.675892960281	5.503735863340	5.261121457175
O	2.911094038414	5.107913416157	-0.754566923904
O	1.762543546362	8.647478480732	1.681266704557
O	5.901722956533	7.085670221331	-5.953608589454
O	-5.309999261288	8.833898943541	5.269037202544
O	3.278922584240	8.462086880147	-0.756394322464
Ge	7.545337480375	6.653401528004	-2.467345012208
Ge	0.971142354092	5.344398701342	-0.099337409908
Ge	1.336305519440	8.683108880386	-0.093327088859
Ge	6.840796395265	-0.027557936258	-2.457511663731
Ge	7.188653323666	3.322910031845	-2.475791316924
Ge	0.622260095168	2.004857623906	-0.102290462975
TV	4.711879742716	-0.000000000001	-0.000000000002
TV	1.064042018938	10.024084548822	-0.000000000001
TV	-0.063856185014	-0.054736259043	4.927093029025

EQ-GeO₂ 105

O	6.925443714241	3.557604936055	0.266957782695
O	0.436483785781	-2.415363331580	-3.000321701936
O	-7.659085853611	0.668060908937	0.511797247747
O	3.270215483698	2.890748006924	-0.420915503875
O	8.222738550181	5.977124039404	3.118936014583
O	1.733672302026	0.004237870117	-0.148399319076
O	-6.361755100279	3.087570639532	3.363564805701
O	4.567418434896	5.310196928450	2.430993950144
O	9.519904671545	8.396422303432	5.970617369743
O	3.030920935666	2.423650930192	2.703424549873
O	-5.064631280843	5.506922124598	6.215578740397
O	5.864679934480	7.729662481269	5.282757261397
Ge	6.868444039713	4.456783937360	4.862699850727
Ge	5.672554263826	6.352796207021	3.788219479630
Ge	6.969737621652	8.772213348818	6.640156126586
Ge	4.273945711840	-0.382207035110	-0.840997054178
Ge	5.571179429343	2.037298939094	2.010881406524
Ge	4.375278931178	3.933332353341	0.936408365658
TV	6.522113939780	0.000000000000	-0.000000000000
TV	4.135109311404	4.500196509173	-0.000000000000
TV	3.891679682396	7.258402723320	8.555642033487

EQ-GeO₂ 106

O	2.426566777147	6.101349536952	1.214632172387
O	4.453409317286	-4.575822754897	-3.136730056605
O	-1.678911829251	3.021714104997	1.153583112824
O	-1.629472765091	1.923871400393	0.212524707076
O	6.406755925683	6.131813058731	1.165761683369
O	8.427895947741	-4.494591320808	-3.238763890593
O	2.380993278683	3.039801732250	1.166339965615
O	2.448012727413	1.937975589860	0.190079199349
O	10.346495443530	6.042226771075	1.274387377658

O	12.372985374122	-4.586722509557	-3.116592336881
O	6.541442425052	3.072648668167	1.161483285324
O	6.557151962708	1.965209794475	0.193790838708
Ge	12.369471715075	-3.140156118723	-1.892081672148
Ge	6.409670490893	4.662761004038	-0.031487795806
Ge	10.350226696167	4.643518140695	-0.013440203646
Ge	4.454279483987	-3.113575051473	-1.931202814711
Ge	8.426170219149	-3.083898035836	-1.964090377227
Ge	2.428593345577	4.643239153909	0.005027832394
TV	11.895639410130	0.000000000000	0.000000000000
TV	1.975764262482	6.197354654928	-0.000000000000
TV	-2.014289294446	3.449625853828	3.302694609490

EQ-GeO₂ 107

O	1.452585030589	3.665347257608	3.431089260843
O	4.088213877868	1.293660021187	-6.169306043223
O	-3.659327849019	0.027339380156	1.516084500956
O	1.441319901342	2.243533404230	-0.421600629529
O	6.584936785870	3.667344700311	3.433451266012
O	9.220439202730	1.298156349499	-6.117238249479
O	1.471538773157	0.024303009064	1.485245982337
O	6.572754259779	2.245390327735	-0.418127888783
O	11.716345378719	3.669383815731	3.459523109341
O	14.351275286270	1.293477070110	-6.169188880087
O	6.604434310215	0.026044683132	1.491344784204
O	11.704797298827	2.248231208593	-0.392097868474
Ge	15.092585436796	-0.394767816521	-2.339204797138
Ge	7.379852198008	1.685074745620	1.524490164710
Ge	12.512029866491	1.686420630924	1.529827034029
Ge	4.830774339780	-0.393654004023	-2.340235828724
Ge	9.961924467375	-0.390380000671	-2.303893511187
Ge	2.248057088353	1.683059661648	1.509208120480
TV	15.394582871591	0.000000000000	0.000000000003
TV	2.637212624524	4.606680570366	0.000000000003
TV	-0.023602494977	-0.027215771943	3.843461461014

EQ-GeO₂ 108

O	2.113272794397	2.827181635875	1.385235797586
O	6.510710557939	-1.656493566777	-2.068745946602
O	-2.667052151170	3.369829933072	0.752914882664
O	-0.288809784995	2.395331078870	0.022225832896
O	2.958527164304	3.920265503101	3.357747143085
O	6.943511042904	-0.726220234383	0.535721879508
O	-2.403383596879	5.056232774264	4.081603850988
O	-0.185095774944	3.612366410099	2.784705479720
O	2.760459575821	3.997270653964	6.374579459709
O	7.024176494453	0.232948668316	3.455267557356
O	-2.279048505277	4.621663036086	7.227005879954
O	0.465737339926	4.432824313056	5.579869179622
Ge	7.777168324787	-0.321790181967	5.092635814519
Ge	-0.983380283095	3.463962523332	4.643844152833
Ge	0.984564116553	3.376135232595	7.316083553052
Ge	7.037025305920	-2.387008893701	-0.368874139709
Ge	7.182752549179	-1.252612926886	2.332479159543
Ge	-1.364096065959	2.223789139076	1.722230320260
TV	6.065605991768	-0.000000000000	-0.000000000000
TV	0.285606524362	5.773428979350	0.000000000003

TV	1.528240209504	2.667551098804	8.390325888196
# EQ-GeO ₂ 109			
O	4.717592187014	6.703250690461	0.913538491031
O	4.330828075483	-4.875268875139	-4.230289490615
O	-4.542980872639	-0.343026064867	0.288569197296
O	0.083378567179	3.223877761974	0.850483329229
O	8.387024896308	6.701176021914	0.912178499910
O	8.000631627354	-4.877188184030	-4.231684977629
O	-0.882074843010	-0.338570479123	0.289385091472
O	3.749346878050	3.222297656650	0.847518478036
O	12.049354881930	6.702272183091	0.914269384655
O	11.664845991738	-4.875515878319	-4.231794093674
O	2.782445021649	-0.338954143672	0.287692438491
O	7.400879019945	3.218576344653	0.848417170383
Ge	10.450809154880	-1.299243140464	-1.421598072326
Ge	5.917903820868	4.596802391370	1.264113763725
Ge	9.587186690250	4.600424927597	1.261770368105
Ge	3.120465874295	-1.299045160241	-1.422761568191
Ge	6.784132681841	-1.302266542447	-1.421323389103
Ge	2.259464816782	4.600162552401	1.261910835330
TV	10.994349811261	-0.000000000006	0.000000000003
TV	0.734653421465	6.476165213250	0.000000000001
TV	0.601471036957	3.100417641841	3.398045105191

# EQ-GeO ₂ 110			
O	-0.821604512145	2.951890370455	2.972815501982
O	5.724987825520	-3.715922887965	-4.534809564921
O	-1.956993389092	2.662477857479	2.121848984428
O	0.392475187374	2.818009728621	0.249207604575
O	-0.779455058652	6.918001319825	2.972822692501
O	5.767009549581	0.250356168391	-4.534760273161
O	-1.914814763049	6.629027469361	2.121764751135
O	0.434633169732	6.784224279858	0.249409054914
O	-0.737464478385	10.884251784850	2.973019624508
O	5.809048651905	4.216815191163	-4.534779776639
O	-1.872800334645	10.594993689451	2.121950405197
O	0.476586359874	10.750498669556	0.249772811184
Ge	5.953233058409	6.127856378386	-4.886225032505
Ge	0.714029913384	8.339266862017	1.653827572743
Ge	0.756372593508	12.305338380995	1.654624852134
Ge	5.869042680199	-1.804978287886	-4.886318051038
Ge	5.911198713503	2.161277828284	-4.886133224571
Ge	0.671943831190	4.372811241633	1.653845050017
TV	3.922244415790	-0.000000000001	0.000000000003
TV	0.125928464466	11.898875646658	-0.000000000006
TV	-3.471271388940	4.356758371638	4.886044916347

# EQ-GeO ₂ 111			
O	3.549902827976	3.791777137933	0.762345501678
O	9.000656275804	-14.096470306713	-5.178536528108
O	-4.117670070208	11.422480905387	3.709842240614
O	0.768946003310	2.601342941024	-1.025844809930
O	3.558413748776	6.940421676154	3.109044855049
O	9.004418456035	-10.845721435181	-2.757834948234
O	-4.127614785764	14.598050716729	6.082776064643
O	0.804364835693	5.770596712532	1.345553504289

O	3.579525150963	10.075582162522	5.458112345941
O	9.025553796735	-7.709248202064	-0.408051771928
O	-4.120047329862	17.767911813532	8.446569862998
O	0.812371411779	8.945863441171	3.708850242405
Ge	1.675516045316	5.832176849987	4.588471478030
Ge	0.497098206693	7.127031717317	2.835168889183
Ge	0.517733612729	10.301607102290	5.202351633827
Ge	1.665147634506	-0.522505817449	-0.152835643677
Ge	1.671728553054	2.646840305694	2.210314408344
Ge	0.487476600382	3.957738558221	0.470334832096
TV	4.910914419843	-0.000000000002	0.000000000001
TV	4.308988077813	7.411417710270	0.000000000001
TV	0.030405884270	9.525606547139	7.108728125077

EQ-GeO₂ 112

O	2.625116061830	3.537987762547	0.330668742691
O	2.805411038528	0.017658952389	-1.653094703650
O	-4.776542746695	2.028630034695	1.752731680834
O	3.283245648170	0.987030315290	-0.601177826837
O	4.671588977847	6.914169754258	0.330693502232
O	4.851844056516	3.393864244310	-1.653103430451
O	-2.730202400352	5.404981379144	1.752657104793
O	5.329691194287	4.363258800934	-0.601203722496
O	6.717897236979	10.290432986871	0.330626667840
O	6.898274791375	6.770118920743	-1.653090287105
O	-0.683782450997	8.781183580802	1.752675369694
O	7.376108137532	7.739501811285	-0.601186139805
Ge	8.482824561744	5.873628436826	-2.071764627859
Ge	3.729614064784	5.189430812507	-0.097168406063
Ge	5.776003245379	8.565631291404	-0.097169519534
Ge	4.389954347601	-0.878849144701	-2.071790697999
Ge	6.436412091286	2.497389423117	-2.071768822350
Ge	1.683159869769	1.813174630107	-0.097139427875
TV	6.086132814215	-0.000000000002	0.000000000001
TV	6.139275591051	10.128684045324	0.000000000003
TV	1.882277313375	1.260663122480	4.247821679363

EQ-GeO₂ 113

O	2.656127788862	3.522304894968	0.302102776671
O	2.915454014780	-0.104583389537	-1.550027389009
O	-4.929413570203	2.034052755949	1.702878524870
O	3.327763341879	1.013482008389	-0.631302854303
O	4.607838380427	6.950221888310	0.302254985330
O	4.866723185921	3.323812729677	-1.550434643645
O	-2.977832406363	5.462507027662	1.703071375231
O	5.278866802011	4.441481063055	-0.631128656587
O	6.557481279762	10.378517390174	0.301931772089
O	6.818020596231	6.752335352339	-1.550239400695
O	-1.027755160435	8.890751494704	1.702993012778
O	7.229635793270	7.870806074901	-0.631333856418
Ge	8.441583570741	5.964059975919	-2.025489044209
Ge	3.660553009255	5.229548653028	-0.137851491883
Ge	5.610845644345	8.657732505280	-0.137925405306
Ge	4.539052827065	-0.892587271419	-2.025716058370
Ge	6.490432106528	2.535719426924	-2.025614072135
Ge	1.709331997799	1.801119590430	-0.137774118340
TV	6.212274565927	-0.000000000002	0.000000000001

TV	5.852956413107	10.284548431318	0.000000000003
TV	1.937205376232	1.222430232364	4.163547637962

EQ-GeO₂ 114

O	2.738528797767	3.529704664305	0.243322760987
O	5.784576675161	-2.770858137738	-2.760107288888
O	-2.978861773604	2.861294588069	1.329556541608
O	0.294389854177	2.582152033309	-0.784949911324
O	4.269215672978	8.247219710080	0.242980334923
O	7.346595703984	1.937624722250	-2.722469729184
O	-1.446719259687	7.587708831844	1.335279518423
O	1.819227097767	7.304591909731	-0.781195034915
O	5.795958753912	12.937898065787	0.222544565162
O	8.862540992843	6.659166401813	-2.726893856853
O	0.076394228644	12.292105125761	1.317539718409
O	3.353206782751	11.988368842971	-0.798015509749
Ge	8.380351773387	7.932689602625	-1.512777364986
Ge	1.426261589681	7.771755490295	0.959558219877
Ge	2.954239662134	12.472274886600	0.938201490887
Ge	5.311215313245	-1.510752771809	-1.530210999515
Ge	6.854704505681	3.213121743206	-1.514472252413
Ge	-0.106706165089	3.051102051087	0.955329824685
TV	4.993411242928	0.000000000000	0.000000000003
TV	4.601818021870	14.133161081469	0.000000000012
TV	-2.145523215798	2.951657953182	3.679725685987

EQ-GeO₂ 115

O	2.437603877124	3.260143422103	1.440828188228
O	6.329189559980	-0.802619023845	-2.490347798054
O	-6.210733727124	1.950415260921	1.718575520316
O	-0.865566957997	3.490735013136	-0.707686443103
O	3.732426293778	4.657139358368	3.720651606407
O	7.624070410410	0.594773705136	-0.211119036638
O	-4.916011632100	3.347187787629	3.998200175251
O	0.429548532753	4.887710783326	1.572088758838
O	5.027196825683	6.054579024113	6.000164474822
O	8.918987269230	1.991277749464	2.068505717823
O	-3.620833494960	4.744387210048	6.277788139795
O	1.724218949615	6.284587780795	3.851690073634
Ge	7.402453508100	1.516524896862	3.186783925837
Ge	1.836839326913	4.720202592753	2.813407390339
Ge	3.131665019232	6.117376568884	5.092920838079
Ge	4.812458283523	-1.277300830223	-1.372353302909
Ge	6.107586375472	0.119758865132	0.907131017877
Ge	0.541800743264	3.323408683092	0.533664853176
TV	6.162761395383	-0.000000000001	-0.000000000005
TV	-2.791280680693	6.423306867608	0.000000000004
TV	3.884528484897	4.191000686629	6.838943686423

EQ-GeO₂ 116

O	6.464347183071	0.633531250233	3.896683634851
O	3.709255975072	-1.339784927053	-4.442128931279
O	-4.908976722511	1.703459313518	1.482755026085
O	-2.023460657135	4.432809672116	-3.006680703529
O	9.248823739885	4.619766125475	3.892194321213
O	6.483057856755	2.598976140105	-4.445199084559
O	-2.121890797288	5.670541641823	1.484960119480

O	0.741694161412	8.421719484597	-3.014018675972
O	12.025400111168	8.587079679521	3.902340479453
O	9.267032930921	6.594020792530	-4.430800362175
O	0.632905640874	9.622795641230	1.470108925774
O	3.493322546197	12.352728807619	-2.998498720126
Ge	10.432774512956	7.543902072419	-1.306477784218
Ge	5.903129872073	6.394170505884	1.049958245141
Ge	8.650838422003	10.365881014139	1.038608368331
Ge	4.874342586579	-0.389596211056	-1.317508525302
Ge	7.653980595483	3.575169109662	-1.319185249063
Ge	3.118168271932	2.418714436617	1.043284372039
TV	6.404953128257	-0.000000000002	0.000000000004
TV	8.307770185862	11.904350993427	0.000000000006
TV	2.810472119307	0.606743933488	3.847635641479

EQ-GeO₂ 117

O	0.657250903232	1.252364823858	0.604593381780
O	4.195076117850	-2.841685433795	-2.030443122447
O	-0.462888889292	1.668092645129	-0.312586352490
O	1.770324107334	3.664738643772	-1.040445197796
O	1.140784307606	3.257185601348	3.915105100324
O	4.679831198119	-0.781837775231	1.302987408209
O	0.029069776701	3.652554187378	2.977980118259
O	2.224542488115	5.717015435980	2.307631241592
O	1.621932881601	5.456240759431	7.317180451842
O	5.104371974365	1.267472525626	4.657835400294
O	0.525974827696	5.783156573486	6.337945665444
O	2.791490993319	7.803304126893	5.616278056723
Ge	5.242152682518	4.959973226350	7.060864467397
Ge	2.645919299425	4.111189765019	3.211829508919
Ge	3.154075426868	6.195773036546	6.543443355914
Ge	4.259273591000	0.822867720347	0.398717552852
Ge	4.734346166949	2.876733418724	3.733646516991
Ge	2.174828429378	2.058518906261	-0.128643080890
TV	6.228308561637	-0.000000000006	0.000000000004
TV	4.123293623277	4.265974407785	0.000000000008
TV	1.455867282048	6.197733537003	10.002372542280

EQ-GeO₂ 118

O	2.712411370022	1.756111406909	-1.461424079291
O	2.785751168707	0.291073892034	-1.807265799395
O	-5.095497400821	2.097009605005	3.359986618046
O	0.343495600274	3.339462342444	-0.298320424045
O	2.299227068083	3.559056371215	1.753963491922
O	2.370929458325	2.094314239578	1.407345166616
O	-5.509515263674	3.901872892797	6.575203679189
O	-0.069618393444	5.143702419894	2.916549734227
O	1.884242391684	5.365245107590	4.968734323433
O	1.957706574180	3.900375707012	4.622869599227
O	-5.923740052307	5.706257455667	9.790189316955
O	-0.484643006836	6.948610720279	6.131769596775
Ge	4.537523812897	1.962887886330	5.326807064352
Ge	0.929072996451	3.672979306001	3.051395381280
Ge	0.514337117546	5.478086735699	6.266549496736
Ge	5.365496960066	-1.646626466413	-1.103312657285
Ge	4.952388168422	0.157834329193	2.112199017759
Ge	1.342138064321	1.868736480693	-0.163939153035

TV	5.169702987397	-0.000000000000	-0.000000000000
TV	-1.463058601378	5.602724127072	0.000000000000
TV	-1.242324999771	5.413720146845	9.645086726963

EQ-GeO₂ 119

O	3.741481228577	1.849560734717	-1.091969767292
O	3.886595993493	0.584209152131	-1.855495562749
O	-5.689570483508	1.241990473565	3.257292800674
O	1.370464510102	3.397684572629	-0.361599666541
O	2.428289896190	2.814373323368	2.480738350901
O	2.563893127084	1.545565061257	1.720298106055
O	-7.000426810829	2.213282012968	6.832491475635
O	0.058585295257	4.372142812631	3.214640524513
O	1.114757885109	3.794825488154	6.060609366994
O	1.259416608861	2.528928681253	5.298318349836
O	-8.311119639337	3.179174796402	10.396619554879
O	-1.255697463127	5.344682950641	6.793066685923
Ge	3.225428486917	1.201478609869	5.417665986164
Ge	0.784996248910	2.755699853057	3.434237383289
Ge	-0.528920639723	3.728498230314	7.012412954359
Ge	5.846153744312	-0.748774700350	-1.742590046102
Ge	4.540040732710	0.228970446148	1.840498158871
Ge	2.095341503233	1.780046719628	-0.145280898673
TV	5.546147141030	-0.000000000000	-0.000000000000
TV	1.884895210294	5.299188638079	-0.000000000000
TV	-3.940747455830	2.916175384724	10.731285563678

EQ-GeO₂ 120

O	3.921387557380	2.052552167132	-1.089365064608
O	4.107781448925	0.804206439271	-1.873064945715
O	-5.516807978023	1.308588429063	3.176760442850
O	1.449100159617	3.523388459016	-0.457994537419
O	2.498751894408	2.973074687704	2.460133820584
O	2.684871086188	1.724460052304	1.676748485468
O	-6.939200256776	2.229367012065	6.726361660303
O	0.026315054750	4.443840133146	3.091377324064
O	1.076144670487	3.893858066886	6.009933726218
O	1.262403143734	2.645312446797	5.226543680362
O	-8.361901779083	3.150025943552	10.275867161822
O	-1.396319871626	5.364872117262	6.641232089750
Ge	3.151473256835	1.260903036420	5.298383073797
Ge	0.822568995710	2.866027437871	3.353979308273
Ge	-0.600047248327	3.786959970356	6.903623447265
Ge	5.996601467123	-0.580727358352	-1.801071859078
Ge	4.574022692221	0.340113414314	1.748675670430
Ge	2.245147714441	1.945383689678	-0.195736777315
TV	5.486477340978	0.000000000000	-0.000000000000
TV	1.768987935426	5.287645189393	0.000000000000
TV	-4.267921030224	2.762149965757	10.649141254893

EQ-GeO₂ 121

O	3.375849724990	4.785565026538	1.364931594987
O	2.160866503056	-2.470755817533	-2.597051960988
O	-1.072922869647	2.226878272531	0.662693131767
O	0.155892729806	2.523602253639	-0.017222386022
O	4.760713768009	5.896362468969	4.068295827904
O	3.550124755219	-1.390155009457	0.138782576052

O	0.335372594541	3.327137559879	3.400775663107
O	1.561238975014	3.613482226154	2.710248502182
O	6.108420290449	6.972019175438	6.801082609214
O	4.954839362770	-0.322428305255	2.773284641817
O	1.725584269062	4.410924459317	6.053684104053
O	2.932091093648	4.775568530721	5.360087758377
Ge	6.680116012838	0.646331246131	3.445483872417
Ge	3.196451509067	4.932094819980	3.322684219276
Ge	4.559905635002	6.001010867046	6.036025468313
Ge	3.889732573169	-1.507229825516	-1.934637482183
Ge	5.318407786388	-0.447224902349	0.726274731691
Ge	1.782699650815	3.839679767610	0.650270399058
TV	4.035706675721	-0.000000000002	0.000000000001
TV	1.858068049980	7.153869561958	0.000000000001
TV	4.143127363554	3.225769722452	8.107221616936

EQ-GeO₂ 122

O	-1.730279196727	0.717581937180	0.453816028357
O	1.152980281260	-0.305229246448	-0.319909893672
O	1.414269534486	0.888402192413	-1.163631082602
O	0.262427065136	2.127887035892	1.005769003294
O	-0.647944669658	4.410722883048	0.453786845671
O	2.235300225321	3.387923592478	-0.319918132101
O	2.496600464747	4.581549212506	-1.163639870891
O	1.344748343243	5.821033151490	1.005773724314
O	0.434363703291	8.103858822478	0.453815960626
O	3.317619117167	7.081066733774	-0.319923127173
O	3.578931779074	8.274697430038	-1.163629108679
O	2.427069363120	9.514155380604	1.005773812935
Ge	2.102857579521	7.589978409858	1.114870255079
Ge	-0.109243130114	6.231397913939	-0.478600904329
Ge	0.973056676107	9.924526973095	-0.478586205536
Ge	-0.061793746948	0.203691539129	1.114866472771
Ge	1.020534499203	3.896840744384	1.114863889544
Ge	-1.191581521733	2.538254808525	-0.478592936576
TV	5.651947128949	0.000000000001	-0.000000000004
TV	3.246961687510	11.079421956935	-0.000000000015
TV	-0.836547143427	-0.551037017084	4.056910644287

EQ-GeO₂ 123

O	2.037905761014	1.534779584503	1.155136743268
O	2.732008609075	-1.359770584185	-3.312804829223
O	-0.845475430922	1.477249489106	2.227911120064
O	0.945126339480	3.978845780536	-1.383426640259
O	3.073845370191	2.472039702170	4.702317251190
O	3.768103254416	-0.422541326475	0.234267261436
O	0.190454892229	2.414624859908	5.775043388394
O	1.981455176036	4.916088133116	2.163571666911
O	4.109868780126	3.409208738067	8.249615614088
O	4.804273909669	0.514792592115	3.781581379870
O	1.226419671708	3.351577502893	9.322466244826
O	3.017434904485	5.853304717672	5.710959059647
Ge	5.611537330406	1.336157437575	5.355700261946
Ge	1.680474324628	4.936709641930	4.368352376376
Ge	2.716457520903	5.873829012705	7.915586450734
Ge	3.539351747047	-0.538347775668	-1.738733264546
Ge	4.575578054269	0.398905934611	1.808448438189

Ge	0.644155741354	3.999525381830	0.821162199826
TV	3.901398618115	-0.000000000002	0.000000000001
TV	0.831052750488	6.329268145536	0.000000000001
TV	3.108166828196	2.811713354814	10.641614688125

EQ-GeO₂ 124

O	1.663058059209	2.327794332761	0.856953579620
O	7.844365781070	-2.422187640856	-3.049789273781
O	-5.991233253968	6.623786118774	3.557087366420
O	0.431544302772	0.456836146058	-1.067130761067
O	6.523502135306	2.332399845367	0.846783314069
O	12.696500277947	-2.436991225065	-3.039233410709
O	-1.134893728074	6.622972134479	3.563607161908
O	5.293401970372	0.456267837584	-1.068541191639
O	11.389158061718	2.325534995107	0.848027498904
O	17.551640935881	-2.432758258469	-3.031718123107
O	3.720906085654	6.622342704179	3.572640645708
O	10.155331686796	0.462584211496	-1.087744666702
Ge	15.739508318542	-1.158309435269	-1.484891244216
Ge	5.606643480685	2.240111151923	-1.330555038530
Ge	10.472697626014	2.245675318004	-1.346752623895
Ge	6.020749865733	-1.158606063797	-1.492899178241
Ge	10.886136655011	-1.154456575363	-1.495606575694
Ge	0.749397850920	2.238367567314	-1.337016451950
TV	14.578221046374	0.000000000000	-0.000000000000
TV	1.716723006958	4.741606946626	0.000000000000
TV	-0.574883510496	3.474466163083	3.962994460857

EQ-GeO₂ 125

O	1.157654490904	1.885825526463	1.328249445794
O	4.201645544366	-1.396508910417	-3.547716402583
O	-2.779828853218	0.897350017461	2.000877648490
O	2.242515818951	2.810872770845	-1.139982534793
O	1.348722984506	3.471120817219	4.905798222717
O	4.112671790883	0.200960785771	0.050583155622
O	-2.585193073573	2.525817672542	5.626335934698
O	2.202858445219	4.423441549439	2.456770472860
O	1.440007228744	5.177259329215	8.593806175817
O	4.243045701283	1.819762473692	3.646545096219
O	-2.498258612626	4.082439430795	9.034121001006
O	2.406309383407	6.033181936899	6.048568489743
Ge	4.099893442999	2.965414541066	5.292444540598
Ge	2.697822956539	4.920365060309	4.363554545582
Ge	2.844976021795	6.559561971372	7.950730413709
Ge	3.945783126390	-0.266645581181	-1.898926022096
Ge	3.910868571612	1.358258899027	1.711561942090
Ge	2.527436083345	3.309762515831	0.808684063096
TV	4.770686324485	0.000000000000	-0.000000000000
TV	2.622714557034	4.772588764273	-0.000000000000
TV	0.252273785774	4.856363269015	10.755374703751

EQ-GeO₂ 126

O	3.787161470126	1.963584547236	-1.211117406433
O	3.258670686466	0.935162770562	-2.128358460053
O	-2.012789603449	0.466193291552	2.738725863334
O	1.617641307548	3.967727219632	-0.205475794544
O	6.854103313226	1.963578138593	-1.211154757846

O	6.325557598187	0.935161607877	-2.128394948246
O	1.054130912750	0.466247652496	2.738761404205
O	4.684547313902	3.967723407925	-0.205477734372
O	9.921002744737	1.963574244199	-1.211109579078
O	9.392491709559	0.935124046122	-2.128348395874
O	4.121048909685	0.466255869180	2.738800438337
O	7.751479293597	3.967752846281	-0.205465654734
Ge	9.980882564912	-0.878747623414	-1.971243215517
Ge	5.305588595468	2.251637246536	0.354058943955
Ge	8.372459163905	2.251598320076	0.354025322652
Ge	3.847020101167	-0.878713134011	-1.971223110983
Ge	6.913986455288	-0.878713663319	-1.971250690453
Ge	2.238655716162	2.251561532894	0.354022852429
TV	9.200781200570	-0.000000000000	-0.000000000000
TV	0.244549680955	4.868823997602	0.000000000000
TV	-1.237419529750	1.676655785519	5.721327684929

EQ-GeO₂ 127

O	0.155562539046	1.081599085289	-1.687193956085
O	-2.698482835822	1.110418252107	2.707295937617
O	-1.803095533393	1.774459259243	0.172470318328
O	-1.002136063337	0.179827137789	-5.829342763813
O	0.328977505122	0.227102443318	-0.683698414184
O	-1.253349358673	1.462603699479	2.826687520282
O	5.883227914794	1.202517128552	-1.232652292590
O	3.018293750014	1.149302232207	0.375533842382
O	2.792529716144	2.582813209362	2.559945121316
O	4.147961758027	-0.199420479199	-6.419931650789
O	5.554321701014	-0.068276074297	-1.337995669020
O	1.029064337437	0.191365940663	2.195980234521
Ge	2.853968696122	0.448812055921	2.416237617639
Ge	-0.175083876930	-2.436418239031	0.829414582730
Ge	-2.237158493148	-0.811000830668	3.250182295301
Ge	5.776769552153	-1.011680291271	0.707534730230
Ge	-0.340223409693	0.880837988418	1.203509425567
Ge	2.705938569498	-0.590800670823	-0.848416340647
TV	10.176945240688	0.000000000000	0.000000000000
TV	-3.358073160584	3.894450366006	0.000000000001
TV	-0.267981575879	-1.094337937367	7.110322966242

EQ-GeO₂ 128

O	2.863757418400	2.579546950916	1.041912582603
O	0.980366907083	-0.494177006312	-0.718871075210
O	0.988229797285	0.923337389795	-0.344468527168
O	1.002995453588	3.634978816672	-0.804405012421
O	2.879458828308	3.715638214002	4.116076256422
O	0.995687069138	0.641902253454	2.355631734844
O	1.003940452346	2.059488951101	2.729748606083
O	1.018809734125	4.771074815595	2.269800538303
O	2.895184735069	4.851555865302	7.190362998151
O	1.011394046302	1.778010604111	5.429761890220
O	1.019776231358	3.195617378758	5.803968939657
O	1.034461383671	5.907208639099	5.344011654954
Ge	2.875477495903	1.631005316551	4.199878286568
Ge	1.022294944005	4.426844709756	4.189545579023
Ge	1.037975131549	5.562851861566	7.263749074230
Ge	2.843988083459	-0.641180138665	-1.948586109688

Ge	2.860407337950	0.494902729073	1.125834020746
Ge	1.006550931829	3.290708139314	1.115340272177
TV	3.719553967546	-0.000000000002	0.000000000001
TV	1.897473713466	6.797441570341	0.000000000001
TV	0.047212565600	3.408183271381	9.222645360829

EQ-GeO₂ 129

O	5.887319501521	1.120415224716	4.137327324230
O	3.964835161303	-1.689875429376	-4.767020263899
O	-4.372983410900	1.931187682835	1.480884239519
O	-1.405958719699	3.949612944362	-3.200697509064
O	8.208805519572	2.089102288330	8.435020305046
O	6.274764026313	-0.753291500543	-0.461946855377
O	-2.041442632032	2.926035300659	5.787085226114
O	0.849997066142	4.811254823214	1.115402587070
O	10.507413667113	3.013943564056	12.708329818576
O	8.587197870608	0.215907669957	3.823028001463
O	0.289306062078	3.899385352672	10.100995849608
O	3.182860720286	5.822318725947	5.369529048533
Ge	9.458612616911	1.671379284718	7.079267082035
Ge	4.601970681820	4.583336823960	5.592599053496
Ge	6.938801409052	5.547805564856	9.869311429334
Ge	4.856501365404	-0.221530157904	-1.484570409668
Ge	7.147946449063	0.688196665019	2.792983979821
Ge	2.286890709250	3.585512149088	1.308761315702
TV	5.904614625506	-0.000000000000	0.000000000001
TV	2.479631829067	4.316111452201	0.000000000001
TV	6.930461391509	2.847889221791	12.855726418971

EQ-GeO₂ 130

O	9.858122720095	4.081220038477	2.608338889658
O	4.055398642325	-2.592564708445	-4.629123507728
O	-11.290839564846	0.137964358221	0.131655253048
O	1.473174594653	3.110649280634	0.171202199399
O	11.441309817630	6.946596372610	2.591777800053
O	5.622475601769	0.234714274408	-4.749053675620
O	-9.731993213220	3.013975159442	0.012422234018
O	3.038279607164	5.952355800954	0.168341023155
O	12.984785636640	9.776646943991	2.627627348162
O	7.183173567371	3.074271632044	-4.630623280773
O	-8.158205208193	5.799863943798	0.121982761999
O	4.614769252977	8.800962999756	0.164928116418
Ge	6.264880593800	4.256170323198	-1.405363208380
Ge	4.441856218345	7.044326383101	0.804956796343
Ge	6.010113870803	9.888044214346	0.835155409570
Ge	3.104328580202	-1.451066791095	-1.319602916777
Ge	4.693051406350	1.369210428074	-1.344197450205
Ge	2.878134872715	4.197698955469	0.819971663737
TV	6.930098913356	-0.000000000001	-0.000000000006
TV	4.710972682693	8.521224488949	0.000000000006
TV	-0.039693953239	2.985892283804	4.945464036685

EQ-GeO₂ 131

O	-2.075693557499	-0.875671978069	-1.782610429618
O	2.648511390273	-1.799729162346	0.006863018492
O	3.776310999936	0.271552656315	-1.613553665791
O	0.780773330362	-0.183944395227	-1.736653329904

O	-2.618607477928	-2.381699028454	-0.078723983024
O	-2.073919491330	-1.010797702590	-0.329454896991
O	-2.856031465474	2.954253505799	-1.506145122161
O	2.018283895335	1.188142178349	0.545228473695
O	2.622844054526	3.034297819385	-1.773319957495
O	-0.066607177798	3.178085019598	-1.193632882596
O	-4.087275169254	2.340206886335	0.273837270522
O	-2.868284551943	3.094623875707	-0.040068532618
Ge	1.507177450258	3.357715007174	-0.217573369545
Ge	4.831017190861	-1.564233485996	-2.436733950752
Ge	-0.091433703664	-1.852802470314	-2.323681474007
Ge	4.156816630877	2.123278041028	-1.716322360789
Ge	2.202440438581	-0.201064079881	-0.650859078963
Ge	-0.888985761194	1.924089683279	-2.269739963175
TV	8.753770895282	-0.000000000000	-0.000000000000
TV	-2.145958142437	8.227011253275	0.000000000000
TV	-2.562846646040	-1.093734061606	4.135617563046

EQ-GeO₂ 132

O	-1.995793000036	-1.131757997842	-1.815138424986
O	2.554064587223	-1.905209469249	0.126239419573
O	3.787586867898	0.133620728394	-1.568706508785
O	0.810478405169	-0.244548730713	-1.684444999059
O	-3.161509193000	-1.563600543642	0.138598163523
O	-1.934604153467	-0.956121476208	-0.337896671152
O	-2.938588231471	3.026450611568	-1.511372876678
O	2.051403001805	1.117335002470	0.594972561654
O	2.699920736364	2.917206771789	-1.777216712063
O	0.012898526628	3.128061613024	-1.189483364696
O	-4.013467210144	2.143946168164	0.257814986210
O	-3.058364947060	3.220036011738	-0.057879263205
Ge	1.596547914677	3.301292007966	-0.222444366621
Ge	4.852149258331	-1.761075983050	-2.264529166106
Ge	-0.045448035789	-1.857929944037	-2.440386241770
Ge	4.212930160505	1.972683585347	-1.712354388034
Ge	2.220485200895	-0.297586927938	-0.573434193946
Ge	-0.934269564338	1.803355382842	-2.041375798758
TV	8.796268313949	-0.000000000000	-0.000000000000
TV	-1.968298277649	8.153412733348	-0.000000000000
TV	-2.629273991633	-0.883360496063	4.166967555473

EQ-GeO₂ 133

O	-1.924768239135	-1.307630787560	-1.788014018346
O	2.642136369062	-2.002204190025	0.173984751715
O	3.833628459948	-0.017451612953	-1.608826178390
O	0.841761051339	-0.371272869629	-1.622292484593
O	-3.105843290738	-1.511328083817	0.199016260912
O	-1.828763040299	-1.070867679505	-0.313257019355
O	-2.871099706861	2.963694817213	-1.565844317399
O	2.158411598400	1.030202263355	0.575008518757
O	2.829777849807	2.788572273906	-1.800276341445
O	0.124963578533	3.001869075639	-1.228019560948
O	-3.774070166595	1.846896356300	0.158327206027
O	-2.950177579121	3.053016322782	-0.105411052011
Ge	1.709748972688	3.203164793814	-0.262662246640
Ge	4.923010431084	-1.905534934664	-2.199236202879
Ge	0.023417814353	-1.976946504349	-2.436983143066

Ge	4.327622359406	1.820030245134	-1.740339724997
Ge	2.292003722316	-0.412096428685	-0.562496958097
Ge	-0.880948663351	1.644642922176	-1.951715334187
TV	8.813931586871	0.000000000000	0.000000000000
TV	-1.708412576142	8.154827654814	0.000000000000
TV	-2.645355209589	-0.785838906322	4.167025688173

EQ-GeO₂ 134

O	-1.439490973673	-2.036362513591	-1.148329357290
O	2.999179040968	-1.623179545360	-0.923634058182
O	3.621338565756	1.025731493723	-2.303836039605
O	0.687379480843	-0.153818598469	-1.766173428605
O	-3.304656214049	-1.202178184314	0.029245284570
O	-1.952177165264	-0.839158263071	-0.398946268930
O	-3.181306363448	2.980851654446	-1.630873055263
O	2.676563487631	1.356224682100	0.086559376826
O	3.085294517830	3.833343253817	-0.708797523474
O	0.509650879133	2.688308122489	-1.438721866786
O	-3.514881845901	1.871392668538	0.325815310611
O	-2.551727868005	2.856452210907	-0.294495869528
Ge	1.341822472614	3.082601244181	0.179193185062
Ge	4.780449395130	-2.114866261684	-1.666373214599
Ge	0.167698807719	-2.058871198377	-2.296971902638
Ge	4.055066090565	2.282132604436	-0.989955977278
Ge	2.426234401329	0.048598314433	-1.242203377828
Ge	-0.786592865383	1.425261943256	-1.890539061988
TV	8.941275241751	-0.000000000000	-0.000000000000
TV	-1.437040921244	7.747733503445	-0.000000000000
TV	-3.044870002027	-0.020868994711	4.384094651421

EQ-GeO₂ 135

O	-0.956033948198	-2.487878410903	-1.181689081436
O	2.494534620440	-1.492867871617	-0.602553374812
O	3.510502310272	0.970201886974	-2.011435598576
O	0.455927924129	0.053392731727	-1.812216788374
O	-2.784372177530	-2.318135860548	0.319827894459
O	-1.708197869678	-1.540135970906	-0.283886211488
O	-2.413302525466	2.834635981315	-1.469068669449
O	2.277980341326	1.645558673865	0.176095301630
O	2.977864618822	4.015421851742	-0.896092208559
O	0.582022461722	2.881584818042	-1.868402931109
O	-3.071924835988	2.345827891558	0.667000801350
O	-1.923995673690	2.926727187943	-0.076762839670
Ge	1.047142966261	3.487933940898	-0.169987148827
Ge	4.041776098432	-2.408245855687	-1.395169899403
Ge	0.260981138306	-1.833185631909	-2.560289934747
Ge	3.808375575837	2.375157741167	-0.855946643584
Ge	2.100922232493	0.211075560751	-1.040335157559
Ge	-0.683572700151	1.795332908161	-2.679758114129
TV	8.062857128120	-0.000000000000	0.000000000000
TV	-0.122819993465	8.187898077292	0.000000000000
TV	-1.907089609364	-1.443144246741	4.629713502697

EQ-GeO₂ 136

O	-0.940418991169	-2.525783860525	-1.120567093067
O	2.401223603780	-1.469842881081	-0.608054232573
O	3.427144110668	0.986695062203	-2.005677348884

O	0.352973038646	0.080064609815	-1.739278103086
O	-2.803668965110	-2.398873444133	0.351909078085
O	-1.695761751455	-1.617842196089	-0.185463143541
O	-2.340033397810	2.729571767417	-1.432805046517
O	2.236635838368	1.663862325781	0.209476787847
O	2.978959998375	4.028451797123	-0.911392376185
O	0.614692251297	2.884713109720	-1.894171136276
O	-3.051078351883	2.337500720702	0.704813305358
O	-1.846003566993	2.778800524887	-0.038691256462
Ge	1.013911664818	3.547498639389	-0.201592546235
Ge	3.952609595827	-2.394287538287	-1.380602811919
Ge	0.213186522352	-1.799743345804	-2.527707539192
Ge	3.765419157771	2.369659057438	-0.833021147147
Ge	2.021736881695	0.247536614605	-1.013839330099
Ge	-0.662547002677	1.819334445468	-2.727439895384
TV	7.980551045726	0.000000000000	0.000000000000
TV	0.004501481227	8.161973973699	-0.000000000000
TV	-1.887593654513	-1.540759242586	4.657699953998

EQ-GeO₂ 137

O	-6.023484424841	2.129619645871	-3.173979786012
O	1.425143080305	-2.414543163503	2.650086263295
O	3.989156293507	1.485379730280	0.127333247066
O	1.831857481427	1.945096793797	-5.022950036174
O	-4.030443091454	-8.351711993771	-4.245771803160
O	4.121377055684	-2.532838021875	1.417325340454
O	-2.749427916579	7.799176530582	-3.180233915875
O	4.737495217760	3.262471004022	2.648349972439
O	7.285661781242	7.164385601286	0.126000522772
O	5.119568042359	7.619885097507	-5.025857159356
O	-0.752070004009	-2.671129339737	-4.247230419896
O	7.429623268747	3.152307141049	1.422272199615
Ge	6.829089685230	5.285777804415	-0.156846773107
Ge	0.480474026520	-2.721190615286	1.138269799779
Ge	-0.188606149370	-3.134084853237	-2.225981334049
Ge	3.787297901401	2.956767943722	1.139417294549
Ge	3.515689440127	-0.390695751098	-0.159921434924
Ge	3.122576022859	2.544896886871	-2.223885441816
TV	5.494857344738	-0.000000000284	0.000000000071
TV	6.591638658113	11.355092042944	-0.000000000292
TV	2.372664795237	2.469738533597	5.019371517572

EQ-GeO₂ 138

O	-3.282278315988	-1.198036651300	-1.190545771341
O	3.284144636855	-1.816523708147	0.056293055331
O	4.706984858039	-0.301979727623	-1.568572944888
O	1.768294855222	0.473899471182	-1.296708424248
O	-2.925921972581	-1.254373856352	-2.536195042833
O	-2.204803018322	-1.906205451748	-0.375327694143
O	-2.262157690441	2.230107694508	-1.146995985080
O	4.311939497887	1.755914129078	0.109039429215
O	5.682184205922	3.184776558686	-1.620636159206
O	2.746702687383	4.011407174775	-1.175047421807
O	-1.737007660911	2.132018716866	-2.449118426384
O	-1.364357265604	1.450288023573	-0.208389261706
Ge	4.256653427056	3.721214411213	-0.228306440208
Ge	5.219908500122	-2.251287759576	-0.636988068111

Ge	-0.236798618496	-1.515316240018	-1.869252391029
Ge	6.215794146023	1.313143485699	-0.708643615169
Ge	3.188245182298	0.163039849440	-0.240678124742
Ge	0.852751175974	2.091549856607	-1.870715509515
TV	10.862651646217	0.000000000007	0.000000000001
TV	2.135855493576	7.143883528343	0.000000000014
TV	-3.040899578222	-2.973650514800	3.283189004653

EQ-GeO₂ 139

O	-2.983519321258	-1.570347157506	-1.107246292100
O	3.179728806959	-1.802076430187	0.010826181268
O	4.642669571659	-0.307285144338	-1.626492047802
O	1.647478934135	0.567352521189	-0.942197143969
O	-2.305059549206	-2.008803674487	-2.272936426296
O	-2.413536901036	-2.287361394505	0.031547818242
O	-2.018828434481	2.438692573819	-1.264106133367
O	4.401835565864	1.794439062609	0.070380598213
O	5.807008886251	3.301258581480	-1.547942131302
O	2.812118602262	4.044011535623	-1.208536775110
O	-1.880251279488	2.408495674033	-2.658763155559
O	-0.861888068976	1.653371682760	-0.597053143858
Ge	4.334358915661	3.779589961991	-0.287135232647
Ge	5.090028766520	-2.247443164625	-0.772752349947
Ge	-0.210207363731	-1.535168217930	-2.049105567242
Ge	6.245000740979	1.174151252403	-0.763984758103
Ge	3.204355246154	0.188544061135	-0.149829340155
Ge	0.917730180001	2.125526425956	-1.821462896156
TV	10.734667133357	0.000000000007	0.000000000001
TV	2.285052309060	7.217852996118	0.000000000014
TV	-2.953823633227	-3.038596574769	3.330249400885

EQ-GeO₂ 140

O	-1.247034619652	4.365777771508	8.105232523583
O	10.372834132513	-12.513882481198	-6.342419317129
O	-4.751498453339	2.632249396752	2.436258774049
O	1.879364047157	6.314477806039	0.372821598592
O	1.900539036008	4.409940294355	8.269189529780
O	13.505720007974	-12.514474915015	-6.343110500803
O	-1.515095807243	2.796046479359	2.447284571940
O	5.010851957759	6.317539147108	0.372445128688
O	5.037760370720	4.339343882770	7.990966598563
O	16.638416974465	-12.516445280346	-6.341700084478
O	1.581472399365	2.988182098422	2.576584957852
O	8.142915154365	6.317663068104	0.372116568554
Ge	11.286854156118	5.331455336213	-7.137588394730
Ge	3.447815794682	5.031772833329	0.149963716028
Ge	6.578723582235	5.032184492765	0.149561117903
Ge	5.020143700266	5.332300439561	-7.137034686863
Ge	8.153307225310	5.333573970239	-7.137894477350
Ge	0.311348754505	5.033604672944	0.149511141964
TV	9.398916435501	-0.000000000012	0.000000000002
TV	-3.785893364015	16.814687133594	0.000000000003
TV	-0.003073809939	1.126169487466	4.528481870686

EQ-GeO₂ 141

O	-2.003989118316	-0.968516548563	-1.715395088855
O	2.237103241102	-1.687266658947	0.792424269474

O	3.454938902045	0.258311296041	-1.102267726664
O	2.161000988794	-1.680113526815	-2.145919668708
O	-2.463029289917	-0.940539943444	0.667525199369
O	-1.442837222458	-0.742154356952	-0.324802799857
O	-2.750119040104	2.391624870274	-1.715380475917
O	1.490988270203	1.673086228680	0.792373308905
O	2.708797460476	3.618577194942	-1.102196700511
O	1.414893253502	1.680052375744	-2.145993596423
O	-3.209117225152	2.419803907515	0.667582580278
O	-2.188949357740	2.618046161867	-0.324799894938
Ge	0.755915385146	2.983818973730	-0.565786911459
Ge	4.052056848565	-1.387391240694	-2.032382718964
Ge	0.201463262814	-2.328898248916	-2.612911404336
Ge	3.305931682664	1.972899901612	-2.032417420373
Ge	1.502082720176	-0.376412058312	-0.565669287002
Ge	-0.544699424641	1.031395347195	-2.613019508958
TV	7.950894927323	-0.000000000000	0.000000000000
TV	-1.492277077815	6.720575249509	0.000000000000
TV	-2.349881145414	-0.306585829023	4.581636530381

EQ-GeO₂ 142

O	-2.895374887605	-0.916710484723	-1.454957156937
O	1.211684815103	-0.197209295032	3.423799968365
O	3.628365936788	-0.465147354353	-0.339099451638
O	1.710687232061	1.375265435904	-1.614091255547
O	-0.737289199088	-2.917488599629	-3.565890953604
O	-1.495574133231	-1.229133997767	-1.113524000415
O	-2.387615021131	2.137173941908	-1.454931188094
O	1.719522188011	2.856748512798	3.423759321753
O	4.136211138179	2.588849354996	-0.339054253543
O	2.218423092642	4.429164867807	-1.613993506219
O	-0.229475062491	0.136379959308	-3.565827193223
O	-0.987779162565	1.824763299437	-1.113570589199
Ge	2.249455549739	2.863934917847	-0.201952769030
Ge	5.087736332922	-2.200291967477	-2.419275198988
Ge	-0.352014062664	-1.411532745727	-2.570277847622
Ge	5.595658409706	0.853633448854	-2.419316014147
Ge	1.741658494013	-0.189968260521	-0.202022554239
Ge	0.155781464247	1.642443760598	-2.570322142795
TV	9.355692335588	0.000000000000	-0.000000000001
TV	1.015601293051	6.107884675839	0.000000000014
TV	-3.379052831065	-2.778113424822	5.180964887079

EQ-GeO₂ 143

O	2.445447281399	0.283640637003	-2.207053271845
O	-0.592942664597	2.648690922718	-0.617982361583
O	1.501193565761	0.917797704164	-3.096108194540
O	-0.745379773882	2.624240117174	-3.363155493938
O	-2.363709215715	3.837727500998	1.018166210372
O	-0.309314190631	1.933812482601	0.617536872412
O	6.830778649217	0.281209403118	-2.209333883829
O	3.792486952564	2.648895459075	-0.620245972517
O	5.886699211092	0.915160585045	-3.098207672201
O	3.641787152220	2.621703743012	-3.367518257744
O	2.021414064479	3.835628711445	1.012273432260
O	4.075023630777	1.933560864978	0.615255176873
Ge	4.153867844303	1.312924167767	-2.179672347808

Ge	2.682241577145	0.686999673119	1.448820679756
Ge	0.709427040484	0.036052434145	-0.107409191914
Ge	7.065730751608	0.689201506379	1.451900745666
Ge	-0.231268672520	1.313120667495	-2.178338315276
Ge	5.096156463852	0.036318975988	-0.109373675987
TV	8.769255202764	-0.000000000000	-0.000000000000
TV	-1.807643532243	4.566283993032	-0.000000000000
TV	-0.331844488841	-1.397441134857	6.459362319480

EQ-GeO₂ 144

O	-0.457587813257	5.060634941208	-1.769330302331
O	-0.522471298255	-0.537507090090	-0.305669181773
O	-1.539050857381	2.804801651486	0.458206255981
O	-1.904620197314	2.100818836102	1.410939838506
O	2.551969952720	5.060835868298	-1.769391989952
O	2.487029922924	-0.537318367702	-0.305994267408
O	1.470857221570	2.804897999247	0.458105683494
O	1.105533076058	2.100767058938	1.410833103080
O	5.561330467275	5.060547009932	-1.769156853666
O	5.497117450414	-0.537650934983	-0.306049077789
O	4.480416447682	2.804866769847	0.458226654766
O	4.114863978424	2.100680271176	1.410820165048
Ge	6.989084479260	-3.473374687899	-0.900285314829
Ge	3.991987512895	-1.079350682226	0.720485301074
Ge	7.001744545844	-1.079918617443	0.720852195119
Ge	0.969804857372	-3.473176955804	-0.900089890240
Ge	3.979363954708	-3.472948037679	-0.900185550277
Ge	0.982337221022	-1.079793196799	0.720825744040
TV	9.029044201647	0.000000000001	-0.000000000000
TV	0.077153254320	9.304623312461	0.000000000003
TV	0.013466679818	0.442755224780	3.751882354157

EQ-GeO₂ 145

O	2.274307272873	1.180450094507	-1.012986095600
O	-0.619305489465	-0.366016059354	0.971377624756
O	-1.494565557069	-1.213199075860	1.262802124311
O	-0.408874577340	2.751857787646	0.115555873048
O	2.014404914846	2.627807736339	-1.406933654347
O	-0.181980596238	1.165338801601	-2.371099515065
O	7.292120625881	1.199937554618	-0.855086900075
O	4.576712452828	-0.333725820791	0.907131564473
O	3.726361585609	-1.223187947309	1.145213001003
O	4.611215804191	2.859368356655	-0.010743027715
O	7.149852211798	2.637565365605	-1.329458006995
O	4.989574750942	1.251630516908	-2.447148122251
Ge	2.912464671208	2.579510351065	0.625317797902
Ge	0.020032310389	3.014384563256	-1.731814108262
Ge	0.950347213048	-0.087310063062	-1.698068582601
Ge	5.203452445057	3.089273871951	-1.815106359850
Ge	-2.123866609670	2.602415625983	0.762601536313
Ge	5.996337443781	-0.034685131259	-1.654110514055
TV	10.063612009650	-0.000000000001	0.000000000000
TV	-0.164914238594	7.066235427052	-0.000000000001
TV	-0.786676177187	0.985809423129	5.505944035016

EQ-GeO₂ 146

O	-0.989226017011	-0.619612203402	-0.635707698894
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O	-0.926090229854	1.433970123079	-0.606855780081
O	1.164464528190	2.467097071270	-1.946801505050
O	2.512661427493	2.386914395993	-2.312900161503
O	-1.311759378034	-1.864562261737	1.740018685921
O	-1.233444103267	-0.804097514723	2.801133050053
O	1.280513876598	0.373261524477	0.963851285356
O	2.714782767670	0.307688026152	1.097052154461
O	-1.211423357155	-3.883780975924	5.843523144562
O	-1.120474957498	-1.812163575874	5.839116738119
O	1.087580652136	-0.387545182329	4.692212690606
O	2.496634753917	-0.808285453863	4.379763342355
Ge	-2.758773935496	-0.670263540999	6.279641767298
Ge	0.450125111314	-1.764317603379	0.301523399106
Ge	-0.039148921547	-2.015290040977	4.155986583502
Ge	-2.481809576016	2.606164047026	-0.043792079445
Ge	-2.619741679371	0.663725902158	3.008800786542
Ge	0.081043102601	0.480219771906	-2.374738694300
TV	6.085303080385	0.000000000007	-0.000000000003
TV	0.095525212265	4.300737809084	0.000000000008
TV	0.104459837307	-5.148951337986	9.412993712822

EQ-GeO₂ 147

O	0.230308248939	6.406373638016	3.734779474230
O	3.817838619751	-3.963250945755	-6.709931973948
O	-1.473611477022	4.012566469591	3.923134290127
O	2.018136425321	2.473008615596	-0.097593123008
O	3.589138619040	6.412463168957	3.735354702084
O	7.168985570919	-3.960481647635	-6.709307123873
O	1.914073024186	4.005328380806	3.905323705659
O	5.388372700641	2.473827395160	-0.094307630251
O	6.965542280377	6.410176610750	3.739302033793
O	10.533509423619	-3.961671986176	-6.712249257542
O	5.273335235414	4.010984458346	3.907182893813
O	8.754454986683	2.481013417367	-0.094050839968
Ge	12.213928326468	-6.351817694722	-6.155237889355
Ge	5.279553939744	5.479292572409	2.790694172879
Ge	8.663615389126	5.475823299122	2.800969292680
Ge	5.465900082317	-6.344585237625	-6.171206006901
Ge	8.836976684955	-6.342554397480	-6.169315718897
Ge	1.914852616888	5.474867047515	2.789680025573
TV	10.128854116623	0.000000000001	0.000000000000
TV	0.017048078130	5.078511969183	-0.000000000001
TV	-1.788881120586	5.103576860327	5.958552043599

(iv) CO₂ at 10⁶ atm

EQ'-CO₂ 0

C	-0.061105537805	0.425836979961	0.187382860209
C	-0.775453729146	-1.109586782780	1.726500117641
C	-2.201601704674	-2.838116926731	1.236747738056
C	-2.919303994948	-4.375416846371	2.769166955118
C	-4.353751618379	-6.100243137487	2.279306996746
C	-5.062520087775	-7.634320413761	3.816441331379
O	-2.534744137186	0.841801919992	0.936625520054
O	-4.691774025264	-2.426489892106	1.981041624465
O	-0.450869238051	0.195398675687	1.450174685897
O	-2.564052715490	-3.068877721139	2.506589593291
O	-3.984413396599	-4.795072758669	2.050830839510
O	-1.859753099536	-5.164236833156	2.524490821391
O	-1.836273138939	-1.533878667189	1.011233285219
O	-6.803189273039	-5.657564451335	3.028689776039
O	0.284659555117	-1.895562501861	1.485599830353
O	-4.726952582302	-6.327126923928	3.548419488575
O	-6.117948890674	-8.046837169301	3.090662832995
O	-3.996680903920	-8.417065697133	3.579312798545
TV	7.059965140184	0.000000000002	0.000000000001
TV	-1.366535795140	4.484387591299	0.000000000003
TV	-6.430182266363	-9.780744303834	3.127432006394

EQ'-CO₂ 1

C	-0.735621277394	-1.105859754871	0.212120702737
C	0.492600857796	-0.521324373757	1.982188071046
C	-3.276098298222	-3.726229383693	1.622790723524
C	-2.038268984964	-3.134589106569	3.385102828837
C	-5.817452688505	-6.329023256752	3.029808379169
C	-4.577857313789	-5.753985744005	4.793658569558
O	-0.378170263999	1.495378684751	0.337859450497
O	-2.930400821930	-1.131288110974	1.747553641152
O	-0.729268988761	-0.513145867339	1.416195909803
O	-3.264896725377	-3.139031099714	2.829008143526
O	-4.536134170238	-3.742930103799	1.156309060430
O	-1.634697443104	-4.401105902020	3.587421852026
O	-1.996551013335	-1.135621116121	-0.257031816636
O	-5.475958929470	-3.732168469816	3.158416504715
O	0.892091926042	-1.789897275251	2.183878693686
O	-5.805172950533	-5.740366856945	4.237068984756
O	-7.074388661338	-6.349434810502	2.554907194397
O	-4.180312865826	-7.022402960131	4.994924931040
TV	6.015224624587	0.000000000003	0.000000000001
TV	-0.116541357820	3.855933766816	0.000000000002
TV	-7.610124872851	-7.837638416948	4.222796890052

EQ'-CO₂ 2

C	0.671188990165	-2.154148914266	0.669190451547
C	-0.659981636616	-0.720435054259	1.740019597068
C	-0.939037502583	-4.679399098479	2.097567471910
C	-2.270211281364	-3.245701726207	3.168427507547
C	-2.549271970086	-7.204620903506	3.525962444966
C	-3.880422381584	-5.770915123869	4.596819660753
O	-2.193340336628	0.514750420329	0.100247349897

O	-3.803553529605	-2.010495320589	1.528628039575
O	-0.911541075858	0.594139855326	1.855792533104
O	-2.521732400807	-1.931125174622	3.284181845974
O	-3.329531935322	-3.926547517547	2.695177042584
O	-1.242145766834	-3.389262176295	2.310089840727
O	-1.719306622089	-1.401286135841	1.266784778175
O	-5.413793218837	-4.535723414105	2.957006824746
O	0.368077906523	-0.864007981822	0.881694084699
O	-4.131960753207	-4.456332915553	4.712594220855
O	-4.939752367320	-6.451741009303	4.123549799757
O	-2.852381084154	-5.914474962785	3.738459941506
TV	6.891533121007	0.000000000001	-0.000000000000
TV	-1.839724889181	3.327196678905	-0.000000000000
TV	-4.830663406280	-7.575720847435	4.285164093581

EQ'-CO₂ 3

C	0.047449292778	-1.663324938306	1.254425647602
C	-1.862198876168	-0.753041081370	0.537631371263
C	-1.354347412223	-2.344849107170	4.131725853330
C	-3.263998890855	-1.434560331397	3.414933708323
C	-2.756144039086	-3.026368279321	7.009020059521
C	-4.665788027008	-2.116084911750	6.292231701368
O	-1.290803227298	0.426298327616	0.233634222294
O	-2.692606639132	-0.255220580624	3.110934862874
O	-0.783154444705	0.733986933873	2.332149134033
O	-2.184949651302	0.052461709616	5.209445183145
O	-2.630649649352	-2.043671187552	4.434454808945
O	-0.722498504506	-1.212552543334	3.775278787002
O	-1.228852736118	-1.362137038414	1.557161899757
O	-4.094391260696	-0.936745509338	5.988238345992
O	0.679297477556	-0.531027999469	0.897972865439
O	-3.586747042473	-0.629061182729	8.086742747292
O	-4.032451754397	-2.725190588923	7.311759491419
O	-2.124291963741	-1.894073122663	6.652574853335
TV	3.818139631749	0.000000000000	-0.000000000000
TV	-1.405274958536	2.961197648831	0.000000000000
TV	-4.205383775070	-2.044561864928	8.631892990193

EQ'-CO₂ 4

C	-2.063673962209	0.418417369225	0.172139968039
C	0.800944002890	3.465050447340	-1.316214448585
C	-0.631409905600	1.941605981712	-0.572292455026
C	-2.062956022057	-1.915919455016	2.404099275228
C	0.801658834899	1.130710083332	0.915741074392
C	-0.630695100002	-0.392738236346	1.659644669690
O	0.693171985069	5.776655185864	0.033391882501
O	0.360293073624	-0.150907704856	0.780298511756
O	-1.623188302592	0.495227838874	1.459174484863
O	-2.507544051763	-0.826746625970	-0.062034094714
O	-2.506825903188	-3.161085846525	2.169921161661
O	-0.164128651250	2.063853991585	0.685268531116
O	-1.098406854633	0.690050801282	-0.750022494293
O	-0.163417758308	-0.270502549654	2.917207685734
O	-1.097701356930	-1.644293755899	1.481933438200
O	0.693885839842	3.442317359458	2.265337382399
O	0.361003127560	-2.485262636544	3.012247267359
O	-1.622461555464	-1.839111928228	3.691131781733

TV	4.856252696229	0.000000000000	-0.000000000000
TV	-1.103680513957	4.469242481608	0.000000000000
TV	0.001424063965	-4.668692786232	4.463889123592

EQ'-CO₂ 5

C	0.036410723006	-1.736039179538	1.449869488243
C	-1.809129208830	-0.559070382778	0.792515100165
C	0.054729889007	-0.673341500311	3.364197778348
C	-1.790811059490	0.503623624784	2.706845384952
C	0.073091614436	0.389362620652	5.278516605379
C	-1.772454119049	1.566304175862	4.621163936982
O	-1.410385519128	-0.494556477364	-0.497810225333
O	-1.392026423183	0.568171689650	1.416527483573
O	0.469211590640	2.764886249601	2.734912275494
O	0.487576853481	3.827587444872	4.649238834078
O	-1.294028878108	-0.591647568475	3.326357085105
O	0.550507069736	0.422014862039	2.745679830173
O	-1.312349476380	-1.654336482667	1.412021674552
O	-1.373692163723	1.630857564001	3.330842483710
O	0.532205853155	-0.640686799370	0.831356965062
O	0.505958505328	4.890279103650	6.563553985604
O	-1.275667981947	0.471048705904	5.240681825779
O	0.568862753465	1.484725030898	4.659999979196
TV	3.690130391324	-0.000000000000	-0.000000000000
TV	0.015014461493	4.568256760385	-0.000000000000
TV	0.055093524826	3.188093773256	5.742981126551

EQ'-CO₂ 6

C	0.055714122007	-2.050743522369	0.944609859705
C	-1.744190746406	-0.655204436721	1.287990363142
C	0.060854179719	-2.562301772607	3.068491503155
C	-1.739084435923	-1.167492817144	3.411164062190
C	0.066378364096	-3.075087035607	5.191846457715
C	-1.733234122975	-1.679985959207	5.534862703915
O	-1.384220281298	0.296350395627	0.394282231175
O	-1.378289459222	-0.215843300861	2.518570150250
O	0.417520328233	1.263506791425	1.836547420259
O	0.422682924270	0.752308732277	3.960332749917
O	-1.272617096515	-2.392860985903	3.119568985883
O	0.527961150539	-1.337344440979	3.360413955696
O	-1.277915964247	-1.879747881305	0.994380797950
O	-1.373429830153	-0.728225829927	4.640893499487
O	0.522685978537	-0.826042517770	1.239048411584
O	0.428287456527	0.238625561516	6.082809458433
O	-1.266924990138	-2.905061420424	5.243293961829
O	0.533537368323	-1.850957942921	5.486132519604
TV	3.600474684375	0.000000000000	-0.000000000000
TV	-0.003529876307	4.266016922122	-0.000000000000
TV	0.017196667299	-1.536285239068	6.370594452450

EQ'-CO₂ 7

C	-2.134918359911	2.141098514014	1.099940796605
C	0.736356110533	2.155875146426	-2.399881544983
C	-0.698681111457	2.744212001251	-0.649418595773
C	-2.132714323109	0.317602890782	4.237336793275
C	0.738548057547	0.332379109222	0.737520827462
C	-0.696486795163	0.920711299617	2.487977640537

O	0.384400697539	3.529288194893	-0.470962753092
O	-0.342196956168	0.089877395056	1.511627113355
O	-1.774181044037	1.714607580183	2.310471082687
O	-2.513772138585	-2.016734275362	-1.807129796234
O	-2.511588558907	-3.840233593349	1.330275694143
O	1.102577520910	1.590807147514	0.504139139622
O	-1.056308614170	1.907335353894	0.323389353244
O	1.104772199645	-0.232690907050	3.641534441075
O	-1.054106898152	0.083844422213	3.460792322860
O	0.386594297050	1.705783329765	2.666431977768
O	-0.339995500997	-1.733621412197	4.649027186611
O	-1.771979024650	-0.108890700657	5.447867075200
TV	4.317640084767	0.000000000000	-0.000000000000
TV	0.010109037286	3.620919234856	0.000000000000
TV	0.004390253845	-3.646998334741	6.274793710807

EQ'-CO₂ 8

C	-0.573860589086	-0.927932150877	1.562741860662
C	-2.77326437235	-0.927944325978	1.562731008615
C	-0.571714309487	-0.917151347507	3.760442728949
C	-2.775186349197	-0.917144832274	3.760432775593
C	-0.569572797087	-0.906381355137	5.958132072121
C	-2.773035508940	-0.906329720409	5.958142886135
O	-2.777814745905	-0.130931310415	0.460346738605
O	-2.775670229325	-0.120169210297	2.658049485500
O	-0.572194885472	-0.120167083522	2.658041332209
O	-0.570064234022	-0.109365920880	4.855748736885
O	-1.672751114697	-1.717556166550	3.763535110378
O	0.530709163629	-1.717572226879	3.763515955877
O	-1.674902493140	-1.728345083478	1.565822497091
O	-2.773542973943	-0.109350670454	4.855740044189
O	0.528559735424	-1.728356597516	1.565799315936
O	-0.567898763409	-0.098581459776	7.053451355395
O	-1.670596776298	-1.706756658755	5.961233203229
O	0.532866768885	-1.706762926199	5.961214097543
TV	4.406930866707	0.000000000000	0.000000000000
TV	-2.207270973206	3.284084609633	-0.000000000001
TV	0.006450075737	0.032364093552	6.593109511806

EQ'-CO₂ 9

C	-0.146044081898	-2.085732186484	0.927872690808
C	-1.094896657175	-0.474089112573	1.347445624089
C	-0.148275828414	-2.634313854872	3.041702455777
C	-1.096486554095	-1.022061412769	3.460628034415
C	-0.149625846909	-3.183862992461	5.154535786737
C	-1.098293169916	-1.571885449008	5.573593276233
O	-1.465036493872	0.471121258515	0.464005280748
O	-1.467297030831	-0.078423587863	2.576343471813
O	0.440204187048	1.306882313099	1.812149841211
O	0.439447031946	0.758576288942	3.925920444372
O	-1.483820367736	-2.295839601474	3.132174406171
O	0.238026495355	-1.360370646004	3.370466079442
O	-1.481337975023	-1.748412769780	1.016593164077
O	-1.468624240436	-0.626472415141	4.690332190540
O	0.239598777217	-0.813077394088	1.258901604164
O	0.437570859710	0.208651422371	6.037716476322
O	-1.485175472069	-2.845554906823	5.243698494657

O	0.236663188564	-1.910537070864	5.484917320295
TV	3.572712008934	-0.000000000000	0.000000000000
TV	0.214451907100	4.335981846733	0.000000000000
TV	-0.006848649666	-1.649078918218	6.339200703518

EQ'-CO₂ 10

C	-1.840234374025	0.243854989561	0.747059859985
C	0.672983300146	3.887926057245	-1.129794949489
C	0.075269548888	0.191784726552	-0.407835382898
C	-3.186745712598	-1.549742354647	3.086175709139
C	-0.673567961000	2.094286094328	1.209358169239
C	-1.271259685214	-1.601857381567	1.931273898886
O	1.467620059737	8.995290481199	-0.328691293940
O	-0.704091209310	-2.183961958268	0.874990567383
O	-1.828334700381	1.581607653752	0.796497398541
O	-3.108217463369	-0.156141882110	0.735173880223
O	-4.454723195161	-1.949765196820	3.074282849463
O	0.119046095506	1.540952260236	-0.483050961104
O	-1.188458915850	-0.255712896525	-0.333299696521
O	-1.227492897407	-0.252688951106	1.856090784013
O	-2.535007861285	-2.049313349051	2.005787063331
O	0.121034427709	7.201636616152	2.010483069967
O	-2.050604172277	-3.977521862317	3.214120680482
O	-3.174834986235	-0.211992034426	3.135636454658
TV	3.835341765842	0.000000000000	0.000000000000
TV	0.090720532232	5.581497298846	-0.000000000000
TV	-2.693053162527	-3.587226293933	4.678235470934

EQ'-CO₂ 11

C	-3.438386406527	2.011604023270	-0.153592586861
C	0.402841238640	2.797891296430	-1.655616255846
C	-0.691865075340	2.215140589113	0.238624635820
C	-4.474471586639	3.936653022355	-0.153589070590
C	-0.633243969078	4.722937567624	-1.655616803627
C	-1.727949503037	4.140187873190	0.238625548325
O	0.432030651995	2.824374573000	0.683141978123
O	0.488434061655	0.384188932007	2.579377530590
O	-5.348802410557	2.260307341186	2.412175182344
O	-2.266372819992	-1.100905048537	-3.110991123571
O	-3.302458749573	0.824142729015	-3.110993273708
O	3.918494620732	2.189536066731	-1.259126245042
O	-0.749666201199	0.943027018070	0.703242544399
O	2.882411874334	4.114582336136	-1.259122702929
O	-1.785757753095	2.868074176089	0.703236646459
O	-0.604055076137	4.749421507821	0.683141710373
O	-0.547649782210	2.309234574308	2.579380421889
O	-6.384889635257	4.185354185089	2.412177521545
TV	7.025446631368	0.000000000000	0.000000000001
TV	-2.072174860877	3.850095863426	-0.000000000002
TV	1.181231588434	-1.828925483842	3.684185363305

EQ'-CO₂ 12

C	-2.394252875146	1.529875356799	0.082235551434
C	1.261400361343	1.836846390044	-0.385904744006
C	-0.506409442814	2.121249664985	-0.818120863145
C	-3.308761920898	-0.129318642286	2.605840030002
C	0.346879351670	0.177571987223	2.137675873829

C	-1.420924318354	0.462066149976	1.705471615266
O	0.718315665282	4.393654280175	-0.008248977593
O	-0.321177962047	0.091646984105	0.962396183334
O	-1.917304522919	1.636072961420	1.332418650544
O	-1.868343685745	-1.022219754264	-0.321463565282
O	-2.782849487572	-2.681431006108	2.202154289278
O	0.190486190354	2.228395204061	0.348857904414
O	-1.451441482438	1.168059060901	-0.778913852637
O	-0.724016975410	0.569167531544	2.872449123578
O	-2.365961831589	-0.491122479959	1.744674923272
O	-0.196161368253	2.734422972249	2.515326706037
O	-1.235678946507	-1.567507335170	3.486008637112
O	-2.831824007749	-0.023078259661	3.856025128736
TV	5.411027415231	-0.000000000000	0.000000000000
TV	-1.207219922167	3.678473123310	-0.000000000000
TV	-1.829002830783	-3.318333458769	5.047188833754

EQ'-CO₂ 13

C	-1.548798473325	1.092193940975	0.447829782167
C	-0.306842375271	3.476708730310	-1.160882048207
C	0.962863488984	-0.542964801090	-0.110452973051
C	-1.581615282655	0.465852137094	2.602241418265
C	-0.339663754458	2.850371062178	0.993536997032
C	0.930029418113	-1.169299553050	2.043957636225
O	-1.993733748314	8.525406896816	-0.176245915198
O	1.963684753051	-1.573290298748	1.334044819977
O	-1.609273280566	2.386172579926	0.824839671503
O	-2.843732461688	0.687416274726	0.340018283014
O	-2.876550889676	0.061077750911	2.494424383900
O	-0.892716204710	0.969135301771	-0.743149049947
O	-0.033100798081	-1.130504429023	0.040692985737
O	-0.925540175692	0.342791770626	1.411263433786
O	-0.065942591267	-1.756837210374	2.195113764539
O	-2.026564407469	7.899061913714	1.978153489574
O	1.930868009163	-2.199630533035	3.488448204533
O	-1.642097012611	1.759831966656	2.979240349438
TV	3.992273669622	-0.000000000000	-0.000000000000
TV	-2.352393667067	5.738036478346	0.000000000001
TV	-0.065638895652	-1.252691624215	4.308805019319

EQ'-CO₂ 14

C	-1.873158588111	0.375554581767	0.563883497735
C	1.053444260076	3.230499379748	-0.394310356223
C	0.007983922288	-0.506664302813	-0.512812637606
C	-3.901111788510	-1.534302842110	2.922985803572
C	-0.974541131272	1.320651213025	1.964782626357
C	-2.019964995843	-2.416516896840	1.846309167450
O	4.465644839651	9.323115278158	-0.471074055120
O	-1.579456802325	-1.865792592126	0.730527048960
O	-1.543789009789	1.708051074860	0.764716521906
O	-3.151781518449	0.017530475174	0.585399633554
O	-5.179738717300	-1.892308258916	2.944517757269
O	0.686732617730	1.941105434405	-0.581846450610
O	-1.288053884208	-0.076835235442	-0.529649334471
O	-1.341239372940	0.031243879248	1.777244298753
O	-3.316002667964	-1.986707147965	1.829471477406
O	2.437669411263	7.413265007929	1.888039629279

O	-3.607487838909	-3.775633385672	3.089583889322
O	-3.571747753667	-0.201805493525	3.123810979556
TV	3.753961146805	0.000000000002	0.000000000001
TV	2.155107028998	5.595056728832	0.000000000000
TV	-4.055934066849	-3.819682435080	4.718204160564

EQ'-CO₂ 15

C	-1.786929300814	-0.353837451981	0.835406820025
C	1.329090947084	4.696555975859	-2.237843033290
C	0.152414996223	0.363764312633	0.061451429841
C	2.086573425473	-0.353929334331	0.835314985114
C	5.202657354827	4.696352461777	-2.237910104507
C	4.025908323504	0.363627316508	0.061375859934
O	2.911399017352	7.228001907559	0.098113153790
O	-1.186262348140	-1.569289015129	1.338134907652
O	-3.698809790847	1.376699532288	0.878929428944
O	-3.038690641723	-0.702870568066	0.454908371202
O	0.834776180000	-0.702836897263	0.454865133973
O	0.180992878214	2.876092569251	-0.734760921219
O	-1.101066440854	-0.039446290982	-0.256877231546
O	4.054538027635	2.875986393205	-0.734854406245
O	2.772466188188	-0.039561068716	-0.256965883049
O	6.784858370631	7.228113211773	0.098191654246
O	2.687254887784	-1.569471916508	1.337979572547
O	0.174633655378	1.376817420194	0.879015920307
TV	7.746990761129	-0.000000000000	-0.000000000000
TV	0.804737528036	5.070199008947	0.000000000003
TV	-1.950118487292	-2.340366304330	2.521400510340

EQ'-CO₂ 16

C	0.534519711330	0.370636885595	-1.969268900079
C	5.583261661250	2.407621185640	0.192455520078
C	3.641569020821	1.346694715774	0.189652511143
C	4.441642858569	0.370622273154	-1.969213434447
C	9.490391392393	2.407626454380	0.192438257502
C	7.548698738892	1.346679407234	0.189664466706
O	2.404829811302	1.400976544012	-0.341689967646
O	-1.501298988373	-1.003250552895	-0.315057092397
O	0.320747225935	0.199718512422	-0.292776805950
O	-0.218152922199	-0.924752819063	1.507693842823
O	3.688956993427	-0.924769885287	1.507694717568
O	-4.747240254945	-2.023182338624	-2.189245382530
O	-2.800604556280	-0.843868289669	-2.223141211022
O	-0.840066227970	-2.023179782078	-2.189261940960
O	1.106517314153	-0.843872590338	-2.223162136700
O	6.311962953178	1.400989347896	-0.341661123556
O	2.405844850426	-1.003217163235	-0.315055471223
O	4.227911225701	0.199730730362	-0.292816645133
TV	7.814271426095	-0.000000000000	0.000000000000
TV	1.950437623683	3.390797897058	0.000000000000
TV	0.597221916079	-1.179741482864	3.745741633390

EQ'-CO₂ 17

C	-1.795204529382	2.446794421501	1.279605702608
C	0.648103369216	2.180298485011	-2.506230944167
C	-0.120382489992	2.219603143694	-0.345060995129
C	-1.575708449258	6.106908623870	1.279665065268

C	0.867486897113	5.840415228491	-2.506295336904
C	0.099098278866	5.879697903359	-0.345102007992
O	0.382282379140	3.463138138698	-0.467594400520
O	-0.314734665574	-0.026579838206	1.565274718426
O	-1.786883903955	1.854656689763	2.285398843155
O	-2.752802311148	-1.795374806774	-1.952804746255
O	-2.533327007015	1.864749342165	-1.952753753167
O	0.844819051686	1.607570696395	0.384871508119
O	-1.291220056305	1.907781713749	0.193794439376
O	1.064401340899	5.267636785039	0.384696284729
O	-1.071586917300	5.567875248621	0.193927246091
O	0.601810277809	7.123204415959	-0.467571260828
O	-0.095357237120	3.633606879226	1.565213852871
O	-1.567597985825	5.514764903004	2.285441442031
TV	4.347087516526	0.000000000000	0.000000000000
TV	0.438881425386	7.320157146777	-0.000000000000
TV	0.004975413885	-1.870300303101	3.184158281580

EQ'-CO₂ 18

C	1.297941054891	-1.309011243528	1.304851623258
C	-2.517513786026	-1.312038974914	-0.912519877338
C	-0.905860524063	0.149611473566	1.094860103183
C	5.077255301542	-1.309010921545	1.304863631775
C	1.261797141443	-1.312032429643	-0.912536050870
C	2.873454184661	0.149620170427	1.094861305667
O	-1.240596498984	0.706049374389	-2.141698101480
O	-1.205688678843	-1.302729354088	-1.058484591797
O	0.745732190612	-0.030799582636	1.413943301178
O	0.748700951800	-0.079502720430	-0.998533535647
O	4.528011881619	-0.079503261941	-0.998525715337
O	-1.104521650027	-1.318226080689	-3.277929411065
O	0.784847398512	-1.875451871815	0.206249006218
O	2.674791860433	-1.318225767270	-3.277933585892
O	4.564158892005	-1.875455637147	0.206263378483
O	2.538716825320	0.706052969778	-2.141696303279
O	2.573617343431	-1.302710219418	-1.058496412488
O	4.525046798075	-0.030795984563	1.413955776316
TV	7.558627502200	0.000000000000	-0.000000000000
TV	-0.033308541802	3.930644814956	-0.000000000000
TV	0.071325855952	-1.893890335015	3.365023343238

EQ'-CO₂ 19

C	-3.437872391676	-0.334947535761	0.832479367295
C	1.868778197040	3.245588748275	-1.308549072041
C	-0.170097057656	2.667231318011	-1.523488622309
C	-4.519724180594	3.064681816236	0.832455903875
C	0.786926348588	6.645182519706	-1.308533082385
C	-1.251959167697	6.066845158915	-1.523461614732
O	0.166248493598	3.632892219611	0.368681304675
O	-0.586101523928	1.344244183627	0.725729918797
O	-2.702139827380	0.662359440483	1.377353299024
O	-2.928281473367	-0.958475190469	-0.237860058033
O	-4.010120690557	2.441166415697	-0.237871300968
O	1.192966262648	2.089028549651	1.729705596724
O	0.186405620663	1.554455852658	-1.526835705867
O	0.111132943968	5.488623640782	1.729709946420
O	-0.895474612174	4.954059405217	-1.526812558743

O	-0.915558869908	7.032514712164	0.368680887368
O	-1.667947035772	4.743841451339	0.725757090255
O	-3.783995550833	4.062005248578	1.377334358309
TV	5.826316166354	0.000000000000	0.000000000000
TV	-2.163665910153	6.799237386886	-0.000000000000
TV	-1.276521137667	-2.282244007079	2.575909938399

EQ'-CO₂ 20

C	0.702865193677	-1.202143341618	0.851534186406
C	-2.486572929545	-1.226277036467	-1.159897301894
C	-2.226552797790	0.199363231560	1.475267795984
C	-1.039796522832	-3.137014116581	3.748535736684
C	-4.229208107477	-3.161155376667	1.737091459530
C	-3.969221777353	-1.735511219611	4.372268088530
O	-0.757383775356	0.789914911743	-1.440695121752
O	-1.338397006587	-1.222080320004	-0.525102243709
O	0.169595733374	0.014533997515	0.596444295525
O	1.479758365704	0.015415585751	-1.445589826606
O	-0.262877023078	-1.919462820309	1.451408548577
O	-0.162569687235	-1.206100933335	-2.406743128800
O	0.876031883095	-1.812748937257	-0.397193568847
O	-1.905179586282	-3.140978848881	0.490263467839
O	-0.866623627894	-3.747611920782	2.499800589573
O	-2.500023957998	-1.144960915635	1.456313561722
O	-3.081040698294	-3.156957230568	2.371892164498
O	-1.573077772905	-1.920333661862	3.493463760551
TV	4.388693486823	-0.000000000000	0.000000000000
TV	-0.031597732966	3.910499237742	0.000000000000
TV	-3.485287284582	-3.869768519127	5.794002548697

EQ'-CO₂ 21

C	1.885286676062	-1.203344960424	1.381539471536
C	-2.598314802540	-1.351599198161	-0.795391635268
C	-0.867863106330	0.403901561054	0.788636973923
C	2.951941749698	-2.952503189147	4.637438381849
C	-1.531625855452	-3.100687942048	2.460507185200
C	0.198816300044	-1.345214127361	4.044607285757
O	-1.880596451322	0.829845163744	-2.318779629101
O	-1.347563341730	-1.140125272740	-1.282802808324
O	1.215671525842	-0.030109027499	1.603896251640
O	0.735229472132	-0.166097459661	-0.734419157886
O	1.801958823454	-1.915174311022	2.521535680907
O	-1.754117431416	-1.222761313824	-3.443052127070
O	1.264574813440	-1.907808914871	0.427624947862
O	-0.687674234863	-2.972111077043	-0.187209850584
O	2.331245369317	-3.656945191736	3.683494113609
O	-0.813937853790	-0.919310146360	0.937227571160
O	-0.280876671339	-2.889226967405	1.973086071471
O	2.282307628455	-1.779316175379	4.859862707977
TV	3.951329442014	-0.000000000000	-0.000000000000
TV	-0.529970752851	3.900895188177	-0.000000000000
TV	2.133285126828	-3.498276152030	6.511857981507

EQ'-CO₂ 22

C	-2.214950297986	1.510754506527	0.066230329034
C	1.445312545212	1.512545742274	-0.451397615363
C	-0.308487172132	1.511965887472	-0.977508159046

C	-3.097349152531	1.507245299433	3.025750021083
C	0.562914954814	1.509037046645	2.508114099439
C	-1.190883962263	1.508452524589	1.982010760325
O	2.100793499772	3.914429248241	0.478183332127
O	-0.098301718290	0.782894340566	1.575873852681
O	-1.698508427323	2.290508182786	1.022356584521
O	-2.896600085164	-0.889919378376	-0.869243736875
O	-3.778999607211	-0.893428694729	2.090257882416
O	0.378499280754	2.236616190812	-0.034506131348
O	-1.262647381607	0.731099437519	-0.460345933326
O	-0.503899218239	2.233101771577	2.925011647849
O	-2.145039515651	0.727590890034	2.499184597991
O	1.218393839799	3.910927624923	3.437687841660
O	-0.980698605701	0.779368538147	4.535395759567
O	-2.580902887421	2.286994749272	3.981869076470
TV	5.416998016508	0.000000000000	0.000000000000
TV	-0.010023748154	3.128519430074	-0.000000000000
TV	-1.764794446946	-0.007018571497	5.919025355554

EQ'-CO₂ 23

C	2.114639153045	2.361847527659	-4.201317378544
C	5.490507235235	1.970440789410	-0.103309663011
C	3.723175431260	1.000490482361	0.804031632191
C	5.856651431975	2.361872010849	-4.201310821925
C	9.232507147572	1.970413868672	-0.103369995267
C	7.465201670352	1.000538859124	0.804022135560
O	3.033826253021	1.590852796713	-0.164367846347
O	-1.909446315325	-1.942926077528	1.067863327313
O	1.192498048473	1.206091549210	-1.085765429161
O	-2.145081188970	-2.981731664450	3.038116350751
O	1.596871768542	-2.981714807353	3.038190286919
O	-5.257421808419	-1.532547036796	-3.046107096034
O	-2.988769816485	-0.741926620279	-1.750544598076
O	-1.515462425704	-1.532530134218	-3.046119794615
O	0.753136284571	-0.742002678288	-1.750540911478
O	6.775796957526	1.590872386843	-0.164356545201
O	1.832497304791	-1.942953603289	1.067906127803
O	4.934527223517	1.206114986658	-1.085770576683
TV	7.483945440203	-0.000000000000	0.000000000000
TV	2.996260177886	3.798883143484	0.000000000001
TV	-0.890096664566	-2.431481293610	3.530040085848

EQ'-CO₂ 24

C	-2.206492117876	2.349308622572	0.841963411952
C	0.781890173648	1.256984461093	-1.026174572547
C	-0.759637902856	2.885668178892	-0.846111719019
C	-2.202866447735	0.743978194969	3.938796416805
C	0.785515526340	-0.348340183921	2.070668944370
C	-0.756014332370	1.280332557673	2.250716666340
O	0.202701092703	3.774867705965	-0.703157096263
O	-0.258732212628	0.300505467648	1.462030350399
O	-1.965640364753	1.771659341863	2.041491729458
O	-2.130243941507	-2.404886513859	-1.906484697411
O	-2.126635128183	-4.010240891082	1.190343857197
O	1.074127961136	1.722756977573	0.195648954420
O	-0.998524567707	2.237379057432	0.317746726570
O	1.077756373771	0.117461461385	3.292470586632

O	-0.994917559495	0.631990833286	3.414546126627
O	0.206279866500	2.169566501821	2.393782588287
O	-0.255142307519	-1.304877750929	4.558896891883
O	-1.962001475635	0.166330586065	5.138335391068
TV	4.243650846533	-0.000000000000	-0.000000000000
TV	-0.287510665144	3.784725250835	0.000000000000
TV	0.007245534538	-3.210676478808	6.193681353442

EQ'-CO₂ 25

C	-0.923869510799	1.006849166917	0.332250314519
C	-0.923066695020	3.818143509907	-1.047921980711
C	0.893558687817	-1.068938034228	-0.357733185257
C	-0.923958495542	0.310766293025	2.416568997230
C	-0.923256827775	3.122024221123	1.036230432416
C	0.893534360799	-1.765086720938	1.726312443433
O	-3.418026655396	10.421525080562	-0.008670206473
O	1.627456870491	-2.808926140026	1.380278965408
O	-1.718544125442	2.065952493935	0.683046384452
O	-1.675619340032	-0.018583985004	-0.007130135926
O	-1.675949400559	-0.714683440928	2.077356539634
O	-0.123953990049	1.360829555440	-0.707800203920
O	0.088970975791	-1.421557227174	0.682412964863
O	-0.124172296817	0.664345064494	1.376345245291
O	0.089044483680	-2.117450487599	2.766713678398
O	-3.418101527424	9.725525837794	2.075596092166
O	1.627232661892	-3.504821966461	3.464562076837
O	-1.718756668898	1.369878353332	2.767146178357
TV	3.291356086161	-0.000000000000	-0.000000000000
TV	-3.295041312304	6.960364357802	0.000000000001
TV	-0.000338011505	-1.392017836819	4.168431876240

EQ'-CO₂ 26

C	1.299011355825	-1.261278918922	1.409245633197
C	-2.551514562416	-1.260869096581	-0.870526757001
C	-1.036195166374	-0.426079058821	0.268807669412
C	5.148454922109	-1.261274317655	1.409265578671
C	1.297945094056	-1.260875662406	-0.870547981814
C	2.813262825249	-0.426102418320	0.268788940093
O	-1.234349548499	0.755764703922	-2.028017308654
O	-1.209105942802	-1.178138510036	-0.829364413791
O	0.800925189568	-0.000097158838	1.494096703031
O	0.799957116063	-0.000105282460	-0.954455510232
O	4.649404317017	-0.000095108412	-0.954421709431
O	-1.021548859458	-1.194299978604	-3.128708618838
O	0.780082103092	-1.806948836981	0.269676517492
O	2.827873065816	-1.194320554514	-3.128729703222
O	4.629530677694	-1.806950021591	0.269699060892
O	2.615105549048	0.755753821487	-2.028033669801
O	2.640358471830	-1.178152890383	-0.829398241337
O	4.650359817170	-0.000090772357	1.494118352202
TV	7.698898735144	0.000000000000	0.000000000000
TV	-0.048407112680	3.867166805772	-0.000000000000
TV	0.025986399588	-1.933474355069	3.396124408107

EQ'-CO₂ 27

C	-1.240357225343	-1.245493983332	0.823851972245
C	0.775473896333	-0.713113410651	1.548962276837

C	-3.544922898902	-3.682235564503	2.508442563031
C	-1.396805020601	-3.283989854878	2.843578780019
C	-5.510932499452	-6.385920819606	3.403742289669
C	-3.448063428034	-5.622698516764	3.707138037333
O	-1.845987006002	1.286016648007	0.692639954012
O	-4.152569651310	-1.323792078894	2.529000366053
O	-0.418647414880	-0.276659168013	1.181440394811
O	-2.484374692989	-2.880188830692	2.193814240289
O	-4.477722072679	-3.423693072432	1.554756440145
O	-1.123247866209	-4.430781547342	2.947208091381
O	-2.510613413041	-0.880946227663	0.797992021693
O	-6.118511835963	-3.855328899457	3.292474614204
O	1.047840531805	-1.861396983611	1.651169031050
O	-4.757420962639	-5.483966326875	4.025988197638
O	-6.723924966671	-5.958971574490	3.104746476753
O	-3.103099103889	-6.921918034754	3.692871730683
TV	7.129743610357	0.000000000002	0.000000000001
TV	-0.945558386570	3.659701930310	0.000000000002
TV	-6.441481944380	-7.734781552277	3.877655113314

EQ'-CO₂ 28

C	-2.122705917810	0.463681497080	0.712540009060
C	1.205706827445	3.472550781779	-0.951151093055
C	-0.413107841246	0.409645773447	-0.736539471588
C	1.332428267011	0.463682777015	0.712531849465
C	4.660830886363	3.472557289832	-0.951163582832
C	3.042033031988	0.409645588003	-0.736537602685
O	3.031152269857	8.153235496759	-0.060370276698
O	-1.319542421941	-2.160336452251	1.426562158022
O	-1.587869860816	1.404540456852	1.452934377344
O	-3.048381539671	1.189620594803	0.003865787030
O	0.406745766782	1.189619928443	0.003857105421
O	-1.199458912499	1.234138890407	-1.440252637997
O	-1.266683475821	-0.291697389655	0.029676582460
O	2.255682471070	1.234146181587	-1.440246839387
O	2.188447581641	-0.291698819759	0.029667838700
O	6.486215712244	8.153206212664	-0.060372667902
O	2.135610115986	-2.160332323960	1.426575216680
O	1.867257184646	1.404562074949	1.452898905653
TV	6.910263362146	0.000000000000	0.000000000000
TV	1.253329168298	5.168054653035	0.000000000000
TV	-1.642131607317	-1.681729618463	2.844817234202

EQ'-CO₂ 29

C	1.048631459759	1.092572307457	-2.151241972348
C	5.444231965623	2.083276842823	0.177915590089
C	3.506424067670	0.948566835475	0.196106646124
C	2.996490956655	4.452108459397	-2.151256904123
C	7.392056505167	5.442812722460	0.177907649569
C	5.454248074681	4.308109077328	0.196100368953
O	2.253738051726	1.021169253657	-0.302530313737
O	-1.646154826663	-1.344133805726	-0.307343812213
O	0.170341246879	-0.145647189337	-0.326751248288
O	-0.328050772938	-1.205851496590	1.520221775200
O	1.619793940469	2.153685572991	1.520229932435
O	-4.215264322289	-1.255716504034	-2.240426267866
O	-2.275840254504	-0.109415105691	-2.277791429733

O	-2.267446887309	2.103806668571	-2.240350231596
O	-0.328001669606	3.250118714076	-2.277786392608
O	4.201566251092	4.380716407789	-0.302549255696
O	0.301669797076	2.015390667635	-0.307340734776
O	2.118165689193	3.213890693453	-0.326751762850
TV	3.895869587377	-0.000000000000	-0.000000000000
TV	3.895654422174	6.719069995057	0.000000000000
TV	-0.046315070397	-2.199932548660	3.837313568200

EQ'-CO₂ 30

C	-1.839704113951	0.445833677829	0.699803863926
C	0.494082450402	2.751766799016	-1.696284069506
C	0.521151493517	0.551929369762	-0.822300914391
C	-3.763501762073	3.762741376351	0.699713654196
C	-1.429706556020	6.068727412699	-1.696424964751
C	-1.402635993448	3.868919286911	-0.822314129318
O	-0.153893739372	6.102349726417	-1.258158756675
O	0.107481214575	-0.392688801471	2.556827722078
O	-1.259891003328	1.614369435434	0.891217335815
O	-3.142017440876	0.525574345305	0.506705968792
O	-5.065841413472	3.842524214392	0.506681077663
O	-0.153170196217	1.679090602788	-1.151389975848
O	-1.250854503197	-0.567192780098	0.706532617707
O	-2.077005129277	4.996040629850	-1.151531051737
O	-3.174761924225	2.749662915307	0.706616894018
O	-2.077628315853	9.419258777047	-1.258055135009
O	-1.816261671292	2.924191897029	2.556902936935
O	-3.183612416689	4.931285990465	0.891029139636
TV	3.846312918958	-0.000000000000	-0.000000000000
TV	-3.847544072005	6.633806898146	-0.000000000000
TV	-1.671290196545	-0.973430215864	3.916858033490

EQ'-CO₂ 31

C	0.563884290716	1.343652468216	-0.101903496840
C	-0.039296219114	-1.589934345531	-2.040850672265
C	2.836600414461	1.345920505984	-0.102451058271
C	2.234562573229	-1.587750100053	-2.039995540654
C	5.110035440091	1.341781613952	-0.102068695624
C	4.508876464754	-1.588546273218	-2.038761331949
O	0.879071342563	0.332114727612	-0.595998047024
O	3.148738247924	0.333550053015	-0.596739896267
O	-0.411800241871	-0.496960517214	1.247454989802
O	1.862980227705	-0.496088191088	1.251722123502
O	2.949290759069	1.545848860400	1.191041545771
O	4.479465555648	2.357505114468	-0.675829093195
O	0.678744264153	1.545503748253	1.191588133013
O	5.422517794265	0.331110869972	-0.599502691480
O	2.202400151866	2.359776589512	-0.677321739040
O	4.136351776987	-0.498600902702	1.249012330898
O	5.226352784768	1.543339971684	1.191466001803
O	6.752320078308	2.356804820556	-0.678316916353
TV	6.821822057370	-0.000000000000	-0.000000000000
TV	-0.018794806684	3.978936498430	0.000000000000
TV	-1.523081453123	0.437170368278	3.683475096756

EQ'-CO₂ 32

C	-3.355007028196	-0.135797119240	0.928322119089
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C	1.669581744966	3.724611801768	-1.397192369024
C	0.234186241447	2.144384352183	-1.509597788889
C	-4.648769986498	3.424037080253	0.928307336324
C	0.375816430835	7.284421458484	-1.397183914420
C	-1.059574300013	5.704203600779	-1.509563461373
O	0.167916103700	4.545001290803	0.720810268721
O	-0.683209759784	0.580300849980	0.322331988129
O	-2.306230201210	-0.014761278286	1.761705974022
O	-2.747014995626	-0.539018556473	-0.235476487985
O	-4.040777032342	3.020827630224	-0.235487967465
O	0.003727920012	2.470352123408	1.357995233983
O	0.627941980201	1.051444997983	-1.511684400037
O	-1.290028126683	6.030164618975	1.358006880272
O	-0.665804220208	4.611269311367	-1.511674966835
O	-1.125829535985	8.104817264260	0.720800193303
O	-1.976969854418	4.140119520436	0.322343450071
O	-3.599997574331	3.545062661155	1.761713569803
TV	5.506387869727	0.000000000000	0.000000000000
TV	-2.587511853591	7.119640758186	0.000000000000
TV	-1.474153150340	-2.559007928910	2.552265491129

EQ'-CO₂ 33

C	-1.489464552292	-0.034366052018	-1.255576258069
C	-0.390524321273	1.345790784656	1.003129966036
C	0.136063572006	1.487470902963	-1.637824985408
C	2.326232972749	-0.034379761897	-1.255583634012
C	3.425180950012	1.345793249103	1.003159497256
C	3.951737465073	1.487467291515	-1.637831218449
O	2.225543072359	8.566281858985	0.240101031576
O	-1.009715202259	0.282496991414	1.500250696262
O	-2.902549687538	1.218047589572	1.057378471961
O	-2.212179985096	-0.488870547450	-0.261357305727
O	1.603501519218	-0.488872203765	-0.261375470334
O	-0.930045048490	2.311654091276	0.628135095614
O	-0.357630555152	0.520206469811	-0.831642184260
O	2.885635282046	2.311640495730	0.628162896641
O	3.458045483475	0.520227224602	-0.831642216923
O	6.041259148751	8.566284017947	0.240106748198
O	2.805984852589	0.282520567839	1.500275017312
O	0.913139004444	1.218043049546	1.057396334020
TV	7.631390234764	0.000000000000	0.000000000000
TV	1.280983097043	5.094385642916	0.000000000001
TV	-2.374363870004	-1.443729214434	2.618670320003

EQ'-CO₂ 34

C	-1.670977165528	-0.365940339553	0.791804121850
C	0.864248563003	3.890239893253	-1.731081170043
C	0.294000518492	0.403568940477	-0.010557045600
C	2.228080583674	-0.365949032727	0.791800046994
C	4.763300061293	3.890238088660	-1.731076711900
C	4.193048399829	0.403567223521	-0.010562652755
O	2.738002194743	7.652895698714	0.075386697102
O	-1.078527214837	-1.420424716043	1.371084766366
O	-3.758373647692	1.500694206916	0.761786455455
O	-2.944101628116	-0.682272637426	0.453832026952
O	0.954944991868	-0.682261569769	0.453845209395
O	0.279239953151	2.990633839916	-0.943445201823

O	-0.955802284962	-0.094015452219	-0.331584504729
O	4.178299272189	2.990634020893	-0.943439087589
O	2.943242778188	-0.094005336844	-0.331581415363
O	6.637046161936	7.652909453665	0.075397054945
O	2.820520500630	-1.420433554414	1.371073797250
O	0.140665410134	1.500689831049	0.761793271223
TV	7.798095067731	-0.000000000000	-0.000000000000
TV	0.576772966898	5.223318914241	0.000000000003
TV	-2.045422472430	-2.224113465755	2.484880366549

EQ'-CO₂ 35

C	-0.659689645246	-0.880422878363	0.223202078709
C	-0.426419289256	-0.817707024730	2.045799787865
C	-2.870728932542	-3.445274052673	1.800362382029
C	-2.668634935671	-3.371196611777	3.625819757357
C	-5.108477184258	-6.020332761456	3.382576240609
C	-4.880038395275	-5.941456384358	5.205381554733
O	-1.488232444371	1.269657694455	0.082739819745
O	-3.680435788652	-1.293089676710	1.662684888497
O	0.328283844314	-0.297142358651	0.995725546618
O	-1.902964957627	-2.845674835094	2.588038517424
O	-3.799077405213	-3.368383427705	2.830944108556
O	-2.097443459490	-4.585950738758	3.764551481984
O	-1.566202615233	-0.797347228662	1.267706536023
O	-5.913766709365	-3.868278977469	3.244990437752
O	0.149135494499	-2.031503550846	2.182603653982
O	-4.138271649133	-5.413516416120	4.157187375671
O	-6.025103125000	-5.954357801722	4.427469729240
O	-4.279590175599	-7.145016756019	5.342299381477
TV	6.172280985106	0.000000000005	0.000000000006
TV	-0.887308903267	3.495139926962	0.000000000002
TV	-6.669509625530	-7.688500962458	4.738618116878

EQ'-CO₂ 36

C	-0.141507856810	-2.027395690822	1.082846596556
C	-0.572156619513	-0.252652508800	1.096045893282
C	-2.487568907070	-4.733284764170	2.741816412137
C	-2.917895606231	-2.958476066468	2.754694939445
C	-4.828894583607	-7.425240491639	4.396504090159
C	-5.259254914583	-5.650148433712	4.409188811226
O	-1.036797174833	0.568149747293	0.119794285363
O	-3.375172538214	-2.136224684705	1.776451703612
O	-0.553214592585	0.700295542609	2.060208839673
O	-2.899913845485	-2.006815425598	3.718950033779
O	-3.653513125059	-4.088662356270	2.952711684517
O	-1.752207744937	-3.603584178107	2.546303016897
O	-1.305544096900	-1.382074362953	1.295483984068
O	-5.726291752645	-4.829922547442	3.433674153941
O	0.593921898660	-0.896998100656	0.883814896770
O	-5.231501988576	-4.695744026279	5.372779775827
O	-5.992410320738	-6.779411690882	4.612064634593
O	-4.096582320761	-6.295936786610	4.192585598309
TV	5.856053760389	0.000000000001	0.000000000000
TV	-0.870851368313	3.549763215491	0.000000000000
TV	-7.025128163719	-8.089162765206	4.964519182427

EQ'-CO₂ 37

C	-2.197068078534	2.804356932337	1.159788117002
C	0.379036445448	1.293911032663	-1.748205518434
C	-0.909721534179	2.773839271108	-0.462898563025
C	-3.832476315413	6.270023211229	1.159790292732
C	-1.256422227866	4.759567477474	-1.748197416390
C	-2.545159702534	6.239510031527	-0.462885237771
O	0.048275514729	2.534794531620	0.456815523710
O	1.085425300329	0.904205878406	1.549125915553
O	-1.699637091406	2.387994426186	2.136557713010
O	-1.302387706586	-1.675931376573	-2.064254449604
O	-2.937799970237	1.789733415841	-2.064275912564
O	0.489572017943	0.642242194150	-0.571656189765
O	-2.060161613339	2.223707537323	-0.018028033226
O	-1.145863798180	4.107896092885	-0.571653035630
O	-3.695595258639	5.689387463670	-0.018031741035
O	-1.587124077044	6.000446420595	0.456804591160
O	-0.550023844878	4.369874519696	1.549130071647
O	-3.335037793660	5.853660313361	2.136549530305
TV	4.533560041740	-0.000000000000	0.000000000000
TV	-3.270851965869	6.931315690682	0.000000000000
TV	1.630558066333	-1.361392566875	3.200890430555

EQ'-CO₂ 38

C	-2.417155040853	1.330531837877	0.057624526222
C	1.192548438981	2.690509873346	-0.396521124798
C	-0.472023649895	2.067893537956	-0.823773113777
C	-3.473382391533	-0.582157879051	2.649035038434
C	0.136313354933	0.777820937509	2.194897923003
C	-1.528253782440	0.155205953218	1.767641912208
O	0.885406575847	4.005963924807	-0.118141849273
O	-0.322206112151	0.099130242616	1.056935957876
O	-2.029041842191	1.367766124845	1.354762984469
O	-1.783407818733	-1.017969954275	-0.270028122300
O	-2.839635606457	-2.930669886468	2.321366709050
O	0.181703573798	2.149177517223	0.357561220250
O	-1.395406444952	1.121271146917	-0.800683445640
O	-0.874529896350	0.236483804992	2.948976290607
O	-2.451633784043	-0.791422128161	1.790728994801
O	-0.170822822973	2.093274356752	2.473279865257
O	-1.378424129588	-1.813556499198	3.648349412316
O	-3.085258202225	-0.544912495853	3.946170406308
TV	5.387982579095	-0.000000000000	-0.000000000000
TV	-1.121599932218	3.565045118819	-0.000000000000
TV	-2.112448743411	-3.825371455882	5.182822489542

EQ'-CO₂ 39

C	-2.302939302236	0.915248039160	0.018093983898
C	1.483622792703	2.485415358440	-0.528040363583
C	-0.413167731822	2.477018977831	-0.557819527882
C	-3.696459092442	-1.952106688616	2.378280404889
C	0.090098916248	-0.381936377682	1.832149098066
C	-1.806687968989	-0.390335119997	1.802365375034
O	0.749950053923	5.094456037759	-0.215530463782
O	-0.846055253130	-0.733338205029	0.887765456989
O	-2.478444378726	0.646672537949	1.366979280401
O	-2.131630680360	-0.147654586120	-0.852230782458
O	-3.525169815547	-3.014996400870	1.507934114830

O	0.522062142022	2.798718547034	0.397210236223
O	-1.064087984256	1.428021149835	-0.097921124294
O	-0.871468555596	-0.068614661880	2.757390757673
O	-2.457605471186	-1.439321106207	2.262317652559
O	-0.643576384802	2.227112582891	2.144655570067
O	-2.239590207723	-3.600691146032	3.247945459878
O	-3.871980840741	-2.220678883685	3.727161607327
TV	5.674870183217	0.000000000000	-0.000000000000
TV	-1.383306913320	3.708460945120	-0.000000000000
TV	-2.787059505859	-5.734702110570	4.720364450463

EQ'-CO₂ 40

C	-0.377325023425	-2.158836608310	0.891031479673
C	-0.614561326826	-0.566970014801	1.781055595268
C	-2.523355946335	-4.719130138519	2.434384279692
C	-2.760652469557	-3.127300778374	3.324425593651
C	-4.669463833058	-7.279444030870	3.977741275458
C	-4.906715177057	-5.687594036386	4.867826769304
O	-1.501361163433	0.522438203317	-0.048260536349
O	-3.647471435334	-2.037877272867	1.495119398057
O	-0.666234837919	0.725875084141	1.888609850548
O	-2.812339949815	-1.834460982195	3.431938216738
O	-3.669625329519	-4.032979955486	2.796655927989
O	-1.790098792944	-3.540573057864	2.429036541807
O	-1.523565152379	-1.472651814683	1.253294578751
O	-5.793546971191	-4.598195785770	3.038468257659
O	0.355947241570	-0.980278849180	0.885673058249
O	-4.958460457688	-4.394750658877	4.975358579226
O	-5.815686704650	-6.593239148090	4.339989811878
O	-3.936166301205	-6.100904669772	3.972448560082
TV	6.186226839341	0.000000000001	-0.000000000000
TV	-0.912681833937	3.548148266556	0.000000000000
TV	-6.438256780820	-7.680957764268	4.630094190000

EQ'-CO₂ 41

C	-1.702691281769	0.384555294875	0.075474891228
C	-0.350454463052	3.659623063039	-1.022424208305
C	0.209877187326	1.546079970600	-0.543312320446
C	-1.624335836371	-2.302010446015	2.564653339165
C	-0.272007218280	0.973051005598	1.466667787954
C	0.288277401485	-1.140479601145	1.945792932690
O	-0.267796993973	6.287339989466	-0.323746556274
O	0.338459202787	-0.173197212247	1.011925605688
O	-1.555540656854	0.608240158679	1.496668413892
O	-1.921956460756	-0.930078452246	0.033023865343
O	-1.843511429056	-3.616650007259	2.522109859271
O	-0.263906252098	2.033291118636	0.600890588820
O	-0.598417393402	0.527575211265	-0.877532387316
O	-0.185461588648	-0.653225022734	3.090012808253
O	-0.519967561993	-2.158997461426	1.611599129978
O	-0.189395090589	3.600768445009	2.165353850645
O	0.416893544463	-2.859750440959	3.501015100388
O	-1.477096726939	-2.078316714436	3.985756265375
TV	4.027197113585	-0.000000000000	0.000000000000
TV	-1.782697230209	4.976897478251	0.000000000000
TV	0.156899898978	-5.373111296564	4.978186369477

EQ'-CO₂ 42

C	-0.815348946245	-0.070203004432	0.706420804516
C	-0.941116863981	3.498221116919	-0.268943264491
C	0.692707549201	0.001553913694	-1.454140331290
C	2.314378904540	-0.070194334474	0.706411738155
C	2.188613409080	3.498234259558	-0.268949464316
C	3.822459790566	0.001565937834	-1.454156838662
O	-3.479900774642	11.435396030172	-0.294636500505
O	1.592758974668	-3.349764509467	0.814226942767
O	-1.527737827890	1.109935784019	0.851332918953
O	-1.602012319707	-1.121077247395	0.810413297412
O	1.527712063370	-1.121065179694	0.810432740739
O	-0.228765998428	2.342846328297	-0.387986441205
O	-0.023834271686	0.008293605012	-0.340969188667
O	2.900979868580	2.342844986309	-0.387968332525
O	3.105880339944	0.008292112158	-0.340999115028
O	-0.350134257023	11.435390216237	-0.294630790132
O	4.722505498190	-3.349758324874	0.814213548816
O	1.602000338683	1.109950136086	0.851339886575
TV	6.259464723054	-0.000000000000	0.000000000000
TV	-3.320162749903	6.848996045053	0.000000000001
TV	0.118347433817	-2.235725517739	2.271544652941

EQ'-CO₂ 43

C	-2.482343693685	1.329978504778	0.043630181008
C	1.428929866121	2.918598407634	-0.972009901717
C	-0.396446264579	1.939287622189	-0.658129692930
C	-3.877955980611	-0.335859327907	2.597077149541
C	0.033323405695	1.252723884162	1.581470038429
C	-1.792078046875	0.273435795150	1.895353236233
O	0.993976918307	3.917172356560	-0.026480443042
O	-0.621149570581	0.100687982799	1.191949507746
O	-2.208089163018	1.493474302406	1.385812141011
O	-1.840218262694	-1.022832142645	-0.401901783930
O	-3.235563189468	-2.688705224628	2.151180351801
O	0.102441758065	2.107654230717	0.565121445028
O	-1.334463404323	1.031369892370	-0.695860656157
O	-1.293230126754	0.441814157977	3.118611435390
O	-2.730039744672	-0.634534863067	1.857691898334
O	-0.401617433474	2.251245114883	2.527060953011
O	-2.016951410998	-1.565165427624	3.745404718293
O	-3.603960924665	-0.172377112925	3.939294801124
TV	5.398337380131	-0.000000000000	0.000000000000
TV	-0.997988778054	3.555891925641	0.000000000000
TV	-2.791377583712	-3.331791739618	5.106976327006

EQ'-CO₂ 44

C	0.122209154740	-1.843599546414	1.336156036215
C	-0.930912411202	-0.607000946525	0.478768265449
C	3.720955322326	-1.839849439189	1.334284554650
C	2.670525091843	-0.602137663946	0.477075436700
C	7.306591435237	-1.841885652340	1.336579159130
C	6.262971962136	-0.597516585618	0.478264155931
O	-1.400027594502	0.580438483457	0.254002563660
O	2.202913445267	0.585673222711	0.252113391091
O	-1.243832310783	0.698420866024	2.367326554477
O	2.360912029682	0.705585298464	2.364164264057

O	2.381450332850	-1.506031764058	1.483070559734
O	4.010516360874	-0.583725488918	0.840453312688
O	-1.216483690551	-1.510183671001	1.486187811575
O	5.791150985058	0.588245533931	0.250426628125
O	0.411386856551	-0.585365890433	0.841381883241
O	5.933046243531	0.694496115431	2.368446066677
O	5.966838830158	-1.508446537830	1.476456266531
O	7.600239142882	-0.580308302241	0.855661828575
TV	10.783521413364	0.000000000000	-0.000000000000
TV	-1.833686169751	3.171239367964	-0.000000000000
TV	-1.767580320401	-1.120271021560	2.969089198142

EQ'-CO₂ 45

C	0.090903677887	-1.595015833812	1.504627756375
C	-2.110432413721	-0.378549616469	0.691585617709
C	0.107910449099	-0.379469457175	3.327608761060
C	-2.093228183071	0.836986056269	2.515021778925
C	0.123130192534	0.835791609343	5.151174538226
C	-2.078080329082	2.052404013915	4.338714767949
O	-2.120182479523	-0.317948192384	-0.666215848272
O	-2.104187412563	0.898565142875	1.157087361284
O	0.111698355629	2.299531401373	2.862646608067
O	0.126944996314	3.515471661461	4.685867619711
O	-0.987175755993	0.236166591309	2.921244525710
O	1.214300369319	0.219958061071	2.922496896755
O	-1.012534374731	-0.986913643524	1.102249823565
O	-2.088735859332	2.113468904885	2.980474858927
O	1.188315279648	-0.987599482315	1.094042317185
O	0.143858811195	4.731102688133	6.509645076723
O	-0.974102284455	1.450803109219	4.746044516885
O	1.225530810824	1.441103480013	4.744300616659
TV	4.401524682310	0.000000000000	-0.000000000000
TV	0.013377641947	3.955920669853	0.000000000000
TV	0.047485699837	3.647430209367	5.470484928259

EQ'-CO₂ 46

C	0.358809731149	0.452239296894	-1.794705594736
C	5.181252782419	2.272318165456	0.489415583412
C	2.759571659531	0.454144299879	0.065442620382
C	4.025586472847	0.452238015225	-1.794713430295
C	8.848046703734	2.272317138670	0.489430328653
C	6.426351284847	0.454141034539	0.065446922615
O	2.250774148991	1.596436392605	-0.368894880435
O	-1.175284873995	-0.805526031209	-0.373382717884
O	0.391027880080	0.553768626481	-0.445629998815
O	0.573175569837	-0.756263117729	1.270282955171
O	4.239957974865	-0.756251182583	1.270272141984
O	-4.470046276145	-2.123895644709	-2.161438930331
O	-2.625624813892	-0.712618148951	-2.122469116264
O	-0.803257515113	-2.123884117450	-2.161442802604
O	1.041168323140	-0.712619888369	-2.122463518570
O	5.917552946018	1.596427228862	-0.368893992069
O	2.491502904099	-0.805529706270	-0.373370672099
O	4.057808803359	0.553760273910	-0.445635693942
TV	7.333575274961	-0.000000000000	-0.000000000000
TV	1.782447382340	3.786073307023	0.000000000000
TV	1.449338301994	-1.261386901619	3.525166658601

EQ'-CO₂ 47

C	-0.377160942107	-1.904611296039	0.488976259789
C	-2.668733823812	-0.495221202435	1.181622255794
C	-1.441453841509	-2.728958078688	2.207598130096
C	-3.734800723532	-1.320964120627	2.899349968717
C	-2.507271449346	-3.554900707609	3.925215029591
C	-4.800773581369	-2.144386816899	4.615702505369
O	-2.128435740115	0.607214210839	0.660455343951
O	-3.192899870966	-0.220538603494	2.379864494575
O	1.963151057497	1.959682359000	2.389406941525
O	0.893531917923	1.139140241851	4.100713118020
O	-1.975584140642	-3.832961782145	2.730579097710
O	-1.427020496972	-1.676006614663	2.724780478355
O	-0.915576513873	-3.006428036030	1.009787869936
O	-4.263522976201	-1.041789752353	4.092340911700
O	-0.366186388666	-0.849485100524	1.001216557314
O	-0.170941977036	0.312643557194	5.816155750162
O	-3.045486133718	-4.658726157868	4.446528114302
O	-2.497785977170	-2.501484862989	4.441171712671
TV	4.610762567067	-0.000000000000	0.000000000000
TV	1.094825556217	4.337230654406	-0.000000000000
TV	-3.195723654884	-2.476150360449	5.152106220685

EQ'-CO₂ 48

C	1.032217631952	2.582548230132	-4.254675791085
C	4.305281064474	2.063672382831	-0.203143587144
C	3.675732167348	0.789227483938	0.920290585367
C	4.785254941303	2.582621397647	-4.254734975018
C	8.058295123735	2.063656655924	-0.203146569081
C	7.428739387850	0.789181715239	0.920303412296
O	3.071904217811	1.508252914246	-0.044759207362
O	-0.828100116374	-1.990994064159	1.083197078611
O	1.167504303799	1.275144165917	-1.114483568929
O	-1.050365167360	-3.045388450648	3.000402596115
O	2.702603148000	-3.045365245783	3.000452697898
O	-5.105689514396	-1.471159864830	-3.083694090200
O	-2.953733944971	-0.780694393324	-1.744586569866
O	-1.352730415378	-1.471304620784	-3.083560648698
O	0.799310448520	-0.780751808667	-1.744600982273
O	6.824915152283	1.508258530617	-0.044732097058
O	2.924905108236	-1.990927071444	1.083201318684
O	4.920563090991	1.275224678438	-1.114480398067
TV	7.506015845418	-0.000000000000	0.000000000000
TV	1.792256269955	3.771058207951	0.000000000001
TV	0.183221697611	-2.587729284817	3.572558312849

EQ'-CO₂ 49

C	-2.315120814774	0.631293978551	0.298375918418
C	1.265665596032	3.886083041666	-0.683815831050
C	-0.415858604953	1.735363912823	-0.449655949290
C	-3.136252195062	-0.501073615315	2.200503578905
C	1.471621048344	1.803377690835	1.368666002537
C	-0.762639278047	-0.605047289726	1.790691140588
O	1.641084836772	7.402731044041	-0.303456315089
O	-0.002258658138	-0.617474142060	0.889728466908
O	-2.441653873134	1.718781030675	1.031877299356

O	-3.424077726437	-4.008740557005	-0.332809853770
O	-3.773965623040	-6.197681069655	2.136034576749
O	0.170682616294	1.703897809528	0.755858951619
O	-1.239979937470	0.602683135216	-0.459937594338
O	-0.941745002409	0.620619725988	2.471239699934
O	-2.250165952716	-0.518191815797	1.143713225685
O	1.310242479255	5.150478901990	2.125712724202
O	-1.010254672504	-1.714646532795	2.529169515884
O	-2.577052576936	-0.493037929384	3.451430233876
TV	5.271150254353	-0.000000000000	0.000000000001
TV	-0.078534215546	4.536012124259	-0.000000000000
TV	-1.337215832983	-3.321089417081	4.097986491010

EQ'-CO₂ 50

C	-1.394476733623	-0.140022125191	0.556947884723
C	0.659307774378	-1.073264069897	1.879070537066
C	-3.483710429563	-3.415597149747	1.730499179532
C	-1.472743139159	-4.307726482052	3.112404620431
C	-5.572310899603	-6.718536422434	2.866178417065
C	-3.569634995021	-7.581726218741	4.289815725830
O	-1.672182000172	1.170395355090	0.874187371365
O	-3.847438898378	-2.116622458040	2.020994061188
O	-0.342449695156	-0.668882189804	1.132761979957
O	-2.545545027322	-3.743179685873	2.596935090515
O	-4.447430555054	-4.341948534135	1.690346410418
O	-1.190940797745	-5.618556680050	2.797202491277
O	-2.503737678519	-0.853832765111	0.803213755986
O	-5.886654362125	-5.410887194027	3.174651420329
O	0.971854616084	-2.382907928593	1.570237859957
O	-4.517195026812	-7.237440490200	3.451193129915
O	-6.578385032298	-7.591577929931	2.918973967154
O	-3.207727212283	-8.881383768460	3.998508148432
TV	6.890162324636	0.000000000002	0.000000000001
TV	-0.700372891353	4.032852108285	0.000000000002
TV	-6.313487480608	-9.812744787875	3.544016516637

EQ'-CO₂ 51

C	-2.611937771585	1.885848790389	-0.442044781496
C	0.945869142315	1.127996616355	-0.402433617286
C	-0.427149466249	2.354358043201	-0.707251320129
C	-3.610079950525	-0.401014013628	2.181196994633
C	-0.052277059791	-1.158803928751	2.220787018330
C	-1.425294377250	0.067621102135	1.915933007325
O	0.972830613693	4.424513581771	0.020042906247
O	-0.327886937071	-0.294044936177	1.172929731102
O	-1.832374746889	1.278203610413	1.719413770239
O	-1.877421645644	-0.579072877132	-0.491781665907
O	-2.875557401621	-2.865945708812	2.131366192411
O	0.156391643843	1.877263766456	0.454634775433
O	-1.464994609626	1.499254827063	-0.905465598392
O	-0.841799123651	-0.409453708185	3.077836988475
O	-2.463113716672	-0.787605835064	1.717848986010
O	-0.025343030373	2.137661725967	2.643287982233
O	-1.326285540985	-2.580792323382	3.796095892225
O	-2.830663581611	-1.008501391322	4.342649735023
TV	5.528370318375	0.000000000000	-0.000000000000
TV	-1.187570580844	3.543666676108	0.000000000000

TV	-1.996506418076	-4.573464814008	5.246433094172
# EQ'-CO ₂ 52			
C	-1.660908097885	2.040086304475	0.476116735597
C	4.355474610456	3.042452688840	-1.425718276601
C	-1.393372286192	0.074525909288	-0.639980460665
C	-2.632091473613	2.968829174731	3.388082147823
C	3.384301644701	3.971195478540	1.486236692991
C	-2.364539428383	1.003292172749	2.271976022685
O	5.755634195806	6.237083910543	0.818358879713
O	-3.802871243104	-0.623391476754	-0.167896204943
O	-1.206018829772	1.637760852748	1.716672926741
O	-10.127808079734	-4.234434959923	-1.088409559367
O	-11.098972594297	-3.305673753851	1.823555081918
O	4.086451429831	4.644329718659	0.846388007340
O	-2.215875062526	1.006900764326	-0.155315989371
O	3.115287680668	5.573100053043	3.758367497603
O	-3.187063753334	1.935653265517	2.756641492866
O	4.784455721911	7.165844699651	3.730337499275
O	-4.774052083106	0.305354595992	2.744063650966
O	-2.177187945602	2.566511061787	4.628639631535
TV	5.272484816507	-0.000000000002	-0.000000000004
TV	3.123272927741	3.288823999515	0.000000000002
TV	-1.942327696467	1.857495309551	5.823924624734

# EQ'-CO ₂ 53			
C	0.231711237919	-1.285786596942	0.917263676147
C	-1.364097199536	-1.299272202292	1.925157632678
C	4.301064855128	-1.284779303360	0.931157554386
C	2.685624054037	-1.296199808059	1.904941892250
C	8.354778505161	-1.291982441474	0.930259746781
C	6.754130954896	-1.302600599784	1.927348830930
O	-1.778162520532	1.975118352277	-0.383671634301
O	2.287198791004	1.981943741859	-0.366602224378
O	-2.518696751142	0.979397282892	1.440690145855
O	1.511690613671	0.921248230884	1.435638362638
O	3.502654814754	-2.295378480810	1.413430554915
O	5.515210945371	-1.319214674642	1.494551640805
O	-0.565425506268	-2.297453019877	1.409246474403
O	6.337422978728	1.984939464952	-0.383969741280
O	1.462126334206	-1.296169807910	1.385066064061
O	5.485225523126	0.951348848994	1.404617147628
O	7.560152948236	-2.304581796740	1.425694366600
O	9.575478185075	-1.273769158422	1.469998248364
TV	12.175590829803	0.000000000000	-0.000000000000
TV	-4.073297590846	4.495814381355	-0.000000000002
TV	-2.853615130609	-2.268591026529	1.798946133158

# EQ'-CO ₂ 54			
C	0.234366968311	-1.648889895724	1.123015986040
C	-0.999661704566	-0.303854674229	1.121638337528
C	-1.716455817968	-3.019365336562	3.275885784700
C	-2.950490466806	-1.674338640787	3.274500675705
C	-3.667312196487	-4.389860105891	5.428749540560
C	-4.901342853095	-3.044827462585	5.427372920803
O	-1.547051291061	0.432836128056	0.117941649239
O	-3.497885014482	-0.937641420188	2.270808583657

O	-1.683346623142	0.307442281710	2.126848436585
O	-3.634188160911	-1.063050658576	4.279713059772
O	-3.077592264568	-3.026708178016	3.277301856136
O	-1.588601282365	-1.665831367068	3.271713962169
O	-1.126776531715	-1.656222412819	1.124443734363
O	-5.448730375265	-2.308138526344	4.423674454060
O	0.362214876215	-0.295364272185	1.118851495692
O	-5.585052459927	-2.433551543393	6.432579227638
O	-5.028449578854	-4.397192373734	5.430178266395
O	-3.539456713084	-3.036328409061	5.424582275939
TV	5.884909852936	0.000000000001	0.000000000000
TV	-2.463348908430	2.693807453056	-0.000000000000
TV	-5.852558242405	-4.111468351996	6.458600236263

EQ'-CO₂ 55

C	-1.687436393190	1.039874730533	-0.237260433929
C	0.313031775132	3.872677607167	0.022249249838
C	0.417829601542	0.248517938122	-0.853600149162
C	-3.308145779738	-1.539164930001	1.571100322188
C	-1.307675840571	1.293658929376	1.830614832172
C	-1.202883961768	-2.330511216058	0.954752746959
O	-4.590663270214	11.834239142604	0.388274453810
O	2.957465743427	-7.275197823452	2.293468270739
O	-0.966823019568	1.737860840314	0.587920092320
O	-2.599256746259	0.209056430160	0.380290376821
O	-4.219974668170	-2.369987480081	2.188645774365
O	1.029543505823	1.440896691258	-1.169351338160
O	-0.868992314092	0.358358039112	-1.090656848109
O	-0.591167235800	-1.138135816130	0.639010950081
O	-2.489704235905	-2.220666787015	0.717691343705
O	-6.211368748976	9.255211723613	2.196660676568
O	1.336748502741	-9.854226859815	4.101865972134
O	-2.587526109767	-0.841192290074	2.396287432199
TV	3.678407693066	-0.000000000006	0.000000000004
TV	-3.684589013016	7.668640628048	0.000000000020
TV	-3.241434648318	-5.158045627145	3.616734514587

EQ'-CO₂ 56

C	-3.582857048447	1.949823097021	2.080435415021
C	0.827349023872	0.458655078458	-2.779213262051
C	-1.002418526111	3.201310543569	-0.970157482019
C	-4.720198458970	5.481701858814	2.080421185716
C	-0.310054682290	3.990549215046	-2.779200951273
C	-2.139756432315	6.733183833112	-0.970165134203
O	0.258402608185	3.324394801291	-0.548597026780
O	0.593016365815	-0.621312786777	1.720394687110
O	-2.411162956209	2.261924279971	2.554323825145
O	0.167429705895	-0.682554166834	-2.281759128721
O	-0.969966851531	2.849335014783	-2.281751361439
O	0.378850039879	1.423896735368	0.778835080535
O	-1.680123269721	2.434990748592	-0.117020856308
O	-0.758457348873	4.955782588375	0.778842054155
O	-2.817466731460	5.966879300495	-0.117019165301
O	-0.878935994379	6.856277001039	-0.548606236342
O	-0.544356909312	2.910568244207	1.720402724319
O	-3.548505313974	5.793788759219	2.554311290147
TV	3.947841722016	-0.000000000000	-0.000000000000

TV	-2.274731353877	7.063755815375	-0.000000000000
TV	-0.605073854809	-2.087486537805	3.585085752461

EQ'-CO₂ 57

C	-2.513342963072	1.441076094472	-0.288440844357
C	0.570231189036	3.432693973951	-1.129384062462
C	-0.439715154001	1.976394214850	-0.654323024136
C	-3.526394002210	-0.743302481675	2.359017084258
C	-0.442917675264	1.248437113362	1.517735803015
C	-1.452961224128	-0.207635195520	1.993134808950
O	0.966462646943	4.007779761275	0.034927728952
O	-0.301055776467	-0.123578502279	1.262837537789
O	-1.808563911103	1.113499748955	1.681228646513
O	-1.683546591686	-1.005150827022	-0.264999447550
O	-2.696433625647	-3.189474315530	2.382621711047
O	0.117121169072	1.934585513711	0.579479736017
O	-1.350758644298	1.056026661296	-0.802728951627
O	-0.896677485518	-0.248513480390	3.227228507594
O	-2.363745003938	-1.128420950876	1.844964150209
O	-0.046829732496	1.823574121686	2.682034832042
O	-1.315061995606	-2.306397207058	3.909948875061
O	-2.822445707900	-1.069454769756	4.329095626562
TV	5.440107406521	-0.000000000000	0.000000000000
TV	-1.146025788892	3.568554939461	0.000000000000
TV	-2.027010313132	-4.367190940619	5.294862402731

EQ'-CO₂ 58

C	-4.025094967428	-0.387306178327	0.873266255590
C	2.671339314445	3.139420734934	-1.276640723855
C	0.537694556132	2.859166335724	-1.098094711273
C	-4.971816539764	2.724667544262	0.873256266736
C	1.724666424548	6.251442106110	-1.276646785942
C	-0.408967035419	5.971234196702	-1.098095504616
O	0.301662640833	3.378801760537	0.095210786644
O	-0.638221566506	1.367955117356	0.626257464592
O	-3.740339973601	0.672841983038	1.290939051133
O	-3.612496115622	-0.889934897575	-0.274514188897
O	-4.559193606874	2.222036797376	-0.274526207930
O	1.333740931647	1.879311072987	1.571826265954
O	0.365625332189	1.733609289012	-1.370968004451
O	0.387104263768	4.991321236164	1.571839039340
O	-0.581147723989	4.845739611290	-1.371077202782
O	-0.644987087164	6.490778087058	0.095239485512
O	-1.584867434954	4.479997859480	0.626252173135
O	-4.687082363978	3.784805956027	1.290952198795
TV	7.030073962727	-0.000000000000	-0.000000000000
TV	-1.893363555814	6.223995843543	0.000000000000
TV	-2.105292833945	-2.243734800798	2.312454331312

EQ'-CO₂ 59

C	-2.023018580013	3.046738678867	0.711808222857
C	-1.967937600336	-2.280648481057	2.390252328067
C	1.704955393957	-1.636375571510	1.599406041226
C	-4.662551877851	0.369734923156	2.386563579558
C	-3.953383222156	-3.494992560801	3.827352299262
C	-0.262390407805	-2.914962964050	3.492330490841
O	3.903119725807	-0.106139363372	0.726225019733

O	0.676741024682	-0.886301613672	2.069066218913
O	-2.174552369923	1.933322835100	1.300594808928
O	2.123539176724	-1.321047873914	0.307002931948
O	-0.311066972947	-3.910699042331	2.827927039982
O	-3.364770340416	0.555276334187	2.224575597176
O	-0.227357558607	0.981651486099	-0.550260410676
O	-5.506407579288	-0.496723562249	4.351228370346
O	-2.986709684978	-1.475707000257	2.547442592548
O	1.277418378739	-2.893388328024	1.551704155451
O	-1.209762258036	-2.003986083433	3.473006371119
O	-3.758239813308	0.765137166742	4.512801352164
TV	5.661085106306	0.000000000001	0.000000000001
TV	-0.995345063489	4.095889202538	0.000000000000
TV	-4.491631934035	-3.383155373127	4.418004205419

EQ'-CO₂ 60

C	-1.624533187399	2.530439772548	1.258745060771
C	0.722246257285	2.643354392709	-1.917096222127
C	-0.193392804168	2.036529125846	-0.369995716659
C	-1.148767304076	6.293064124455	1.258718495483
C	1.198042012361	6.405969339780	-1.917094661048
C	0.282380289020	5.799150341885	-0.369996479639
O	0.452117238694	3.230026041739	-0.678924476007
O	-0.140282091065	-0.474470495276	1.573601616070
O	-1.652018216925	1.877906659651	2.226488663606
O	-2.742451161969	-1.630975154256	-2.082058547472
O	-2.266682997035	2.131644270225	-2.082047250211
O	0.701352305476	1.406574317567	0.360679200457
O	-1.400170057074	2.001453471622	0.065830167980
O	1.177120995240	5.169214209891	0.360698064469
O	-0.924422644784	5.764111695103	0.065780190997
O	0.927902681636	6.992645402359	-0.678918844054
O	0.335518613025	3.288135882731	1.573602068074
O	-1.176195825387	5.640525930796	2.226464327011
TV	4.209265447861	0.000000000000	-0.000000000000
TV	0.951564426538	7.525237004994	0.000000000000
TV	0.011539907650	-2.077844062808	3.260951039952

EQ'-CO₂ 61

C	-2.071826529931	0.843294351770	0.607636446785
C	2.346505871785	3.305151820228	-1.837532634902
C	-0.412307024350	2.179098076500	-0.502056838806
C	-2.912678929044	4.399431176227	0.607620711336
C	1.505652711449	6.861351844183	-1.837560382465
C	-1.253149029282	5.735276714736	-0.502044075553
O	1.132380297782	4.318132754311	0.156222179629
O	-1.434871139909	-0.365873382314	0.916441588492
O	-2.094463465358	1.225429485600	1.928108696979
O	-2.525478324713	-0.912253324508	-0.971376640663
O	-3.366276118136	2.643919749952	-0.971348910927
O	0.338298563577	2.146179758208	0.541678208295
O	-1.513314517206	1.450975640228	-0.401881743681
O	-0.502477269909	5.702443630626	0.541637740908
O	-2.354164216412	5.007167010973	-0.401853004080
O	0.291622197266	7.874364155985	0.156247549127
O	-2.275748486908	3.190253873784	0.916455781586
O	-2.935268600719	4.781614118462	1.928080985628

TV	5.295779889897	-0.000000000000	0.000000000000
TV	-1.681623638911	7.112352971851	0.000000000000
TV	-1.400222960524	-2.282020058305	2.732302143874

EQ'-CO₂ 62

C	-2.160682272210	0.745281579017	0.623907131133
C	2.489826762691	3.355895373985	-1.894559564579
C	-0.429383293022	2.177945647712	-0.424726932324
C	-3.056936225224	4.352860110276	0.623891472786
C	1.593566858568	6.963464086865	-1.894558457442
C	-1.325630996456	5.785525477726	-0.424746182119
O	1.066615112163	4.330741556449	0.028267678912
O	-1.584284220993	-0.477687945839	0.959943694768
O	-2.357615338754	1.096265764665	1.943149622572
O	-2.400855650154	-0.933157537946	-1.067869252831
O	-3.297134006651	2.674401263813	-1.067882759845
O	0.457231015786	2.180839093379	0.507653813458
O	-1.478876196924	1.419050976466	-0.238494029095
O	-0.439041091815	5.788398322587	0.507654038710
O	-2.375140276499	5.026642674659	-0.238500879740
O	0.170351799023	7.938300126903	0.028274871518
O	-2.480538224671	3.129886622804	0.959933442474
O	-3.253863957267	4.703835400437	1.943137949336
TV	5.319463527469	0.000000000000	0.000000000000
TV	-1.792524628040	7.215139078206	-0.000000000000
TV	-1.547707185887	-2.372332048604	2.691136612146

EQ'-CO₂ 63

C	0.242781409446	-2.044976342703	1.072441632101
C	-1.814278516260	-0.460606423576	1.459854669159
C	-1.798273965178	1.375152157879	1.072450809592
C	-3.855333147268	2.959475885631	1.459889396974
C	-3.839314727929	4.795229790850	1.072474709063
C	-5.896329223269	6.379611497857	1.459871335037
O	-2.173294210277	0.271642646368	0.341316883899
O	-4.214307955810	3.691706566380	0.341335713039
O	-1.446864922063	0.652857779115	2.186309468583
O	-3.487924186651	4.072977703850	2.186335558763
O	-2.830552960867	2.170782281648	1.260103428682
O	-0.785037521096	2.036357326550	0.571731011946
O	-0.789534631076	-1.249348352605	1.260077465758
O	-6.255345597497	7.111825078031	0.341330045595
O	1.255977707114	-1.383769481970	0.571765004007
O	-5.528930301847	7.493077156603	2.186316540664
O	-4.871568105527	5.590915478334	1.260046181440
O	-2.826086300889	5.456477006674	0.571781419443
TV	6.967491862918	0.000000000001	0.000000000000
TV	-6.123083236697	10.260347852902	0.000000000000
TV	-2.059790609926	-3.141686941414	1.373857801679

EQ'-CO₂ 64

C	-2.261324185490	0.303786736432	0.630515055315
C	1.202885312569	3.343607371064	0.075570795429
C	-0.672419424127	0.819016485072	-0.156421997808
C	1.441100773558	0.186167645704	0.543272067056
C	4.902818027897	3.355623897008	0.086186698921
C	3.029972488132	0.792127316885	-0.176380838224

O	3.993006156629	9.024265055426	-0.428665926413
O	-1.541367533335	-2.388622142778	0.637799015172
O	-1.551408341532	1.500138263818	0.676589411023
O	-3.537609288766	0.271925142708	0.749040406053
O	0.164633777427	0.077924711066	0.604257677557
O	0.047000825088	1.498820815770	-0.972993773232
O	-1.646581971404	-0.088552828658	-0.551699269984
O	3.749402097116	1.381118643663	-1.060754960715
O	2.152712557198	-0.202495771148	-0.588450355982
O	7.693505594143	9.221954906745	-0.280743737743
O	2.159208252732	-2.553436571803	0.519943289625
O	2.054674271679	1.431572288330	0.578198925681
TV	7.405017901001	0.000000000000	0.000000000000
TV	1.782299510244	5.454318878215	0.000000000001
TV	-1.780770955485	-1.934578991799	2.604153474663

EQ'-CO₂ 65

C	2.068834896773	-2.410368841797	0.817079202564
C	-1.322552362551	-0.163353912805	1.416555573870
C	1.564943950004	-3.638817787982	2.542275565513
C	-1.826457382898	-1.391765715266	3.141785600071
C	1.061036486053	-4.867244197002	4.267476738412
C	-2.330371375995	-2.620231193068	4.866931984238
O	-1.410170843758	1.057505154073	0.887494126548
O	-1.914089884310	-0.170922866730	2.612704529340
O	1.026206166586	0.691647934925	1.345465715780
O	0.522280807178	-0.536802574385	3.070648682036
O	-3.721457656071	-2.758734771963	2.987264475873
O	-1.193971347442	-2.276376605990	2.704439007107
O	-3.217523935064	-1.530284594636	1.262106600539
O	-2.418018765252	-1.399352793481	4.337924925475
O	-0.690069009500	-1.047974955937	0.979211528652
O	0.018327755793	-1.765224580135	4.795839216673
O	-4.225357660676	-3.987176931927	4.712485248969
O	-1.697890567378	-3.504847042186	4.429578057329
TV	4.652644111447	-0.000000000000	0.000000000000
TV	-1.129815403306	4.322849180245	-0.000000000000
TV	-1.511768970671	-3.685310892926	5.175574479857

EQ'-CO₂ 66

C	-1.679572358017	1.865101446023	0.713198289283
C	0.648310095357	3.351585337233	-1.719699117752
C	-0.294609040161	1.644355198652	-0.895484276822
C	-3.264655800591	5.430749812837	0.713179881041
C	-0.936728625397	6.917137019459	-1.719781174474
C	-1.879654145079	5.209919562428	-0.895530659916
O	-1.401081883663	4.215049301654	-0.445623530220
O	0.574547622016	-0.760049968229	1.341757276977
O	-1.309067575629	0.575629547870	1.270690487743
O	-1.987114977794	-0.654353629786	-0.590223246824
O	-3.572229614448	2.911196435996	-0.590141994640
O	0.987605108279	1.739339065281	1.314458964782
O	-1.627862859640	1.921369478954	-0.551748493696
O	-0.597481143098	5.304882901773	1.314393924040
O	-3.212861362996	5.487052025857	-0.551755016454
O	-2.986153548439	7.780630363233	-0.445572686592
O	-1.010537706338	2.805493339584	1.341716454578

O	-2.894096142231	4.141249228759	1.270640576611
TV	3.943744642828	0.000000000000	0.000000000000
TV	-3.170151529310	7.131122400684	0.000000000000
TV	0.884002094747	-2.616545515746	3.648713929925

EQ'-CO₂ 67

C	-2.002857443211	1.216279400678	-0.285576818632
C	1.655033292350	1.690618071184	-0.444025265921
C	-0.249807807357	2.340498024619	-0.488129074491
C	-2.699062589921	4.972017276452	-0.285528005607
C	0.958824598026	5.446349130692	-0.443998003388
C	-0.945978386953	6.096239887297	-0.488117093368
O	1.627360734700	4.286353778982	-0.699107940895
O	-1.661664371662	0.677052170100	0.932166805671
O	-3.310868778697	1.861701454971	2.177356204359
O	-2.021413062474	-1.375419997495	-0.014910144626
O	-2.717483847045	2.380337865922	-0.014975945164
O	0.616988587908	1.690239947875	0.365734086364
O	-1.037278842895	1.398715152979	-1.106312931554
O	-0.079202868099	5.445996815249	0.365776005207
O	-1.733467773984	5.154481830049	-1.106270417252
O	0.931255925772	8.042090449698	-0.699135912344
O	-2.357836043579	4.432747330876	0.932170260121
O	-4.007059857240	5.617435411819	2.177359849222
TV	5.447629910860	0.000000000000	0.000000000000
TV	-1.392287845070	7.511479410705	0.000000000000
TV	-2.662149483229	-1.565798499674	2.477586890948

EQ'-CO₂ 68

C	-2.162059016613	0.756301738396	0.108020726762
C	1.102071103937	2.831402492295	-0.436488201291
C	-0.605824348663	2.324619951776	-0.715920030860
C	-3.508018921086	4.194354765782	0.108021781326
C	-0.243887054239	6.269473587935	-0.436506275513
C	-1.951775056610	5.762649022839	-0.715938573169
O	0.909390714014	4.156619444107	-0.068609216391
O	-0.255611180804	-0.255286301457	0.966084602826
O	-1.877830704660	0.961521788638	1.407614853751
O	-2.007226283783	-0.561203169901	-0.363651121793
O	-3.353157416782	2.876831804437	-0.363615531872
O	0.193535517009	2.156121353923	0.363163524512
O	-1.589766113001	1.497011894617	-0.822934243031
O	-1.152407992184	5.594158551076	0.363135255620
O	-2.935739868894	4.935065313471	-0.822939462384
O	-0.436558753696	7.594737382822	-0.068632817171
O	-1.601544039681	3.182729267769	0.966076733106
O	-3.223707999670	4.399592799374	1.407593653273
TV	5.776441103099	0.000000000000	0.000000000000
TV	-2.691903611951	6.876084433088	-0.000000000000
TV	-0.789335706902	-2.622674059498	2.535450667823

EQ'-CO₂ 69

C	-2.338738602788	0.233577615354	0.888940909580
C	0.170240713434	2.810183191207	0.422895980391
C	0.288978460344	0.866698539259	-1.227416997911
C	-4.160597172205	-2.115345749683	3.310875825151
C	-1.651622094597	0.461246776074	2.844824963304

C	-1.532917488459	-1.482261418765	1.194523416464
O	0.887905381239	8.195093471163	0.374158119656
O	0.261233786194	-3.342480114872	1.071140969911
O	-2.272690960770	1.147178451586	1.858283102064
O	-2.963816007704	0.592633464776	-0.151860748919
O	-4.785686127918	-1.756273420557	2.270075840107
O	0.759299886254	2.056103051331	-1.754605163454
O	-1.007855380532	1.370302046414	-0.997799369377
O	-1.062622739014	-0.292857092883	0.667317701251
O	-2.829754613060	-0.978638046863	1.424146803136
O	-0.933969303626	5.846181449266	2.796085151454
O	-1.560647702196	-5.691412145976	3.493056803283
O	-4.094579350929	-1.201740423247	4.280214410188
TV	3.911873168270	-0.000000000000	-0.000000000000
TV	-0.637120497726	5.345765938257	0.000000000001
TV	-3.643759062099	-4.697860924140	4.843855550425

EQ'-CO₂ 70

C	-1.833986092874	0.314537425272	0.712126934782
C	0.872799958383	3.894390325531	-1.482588718930
C	-0.053820385127	-0.849110638711	0.334434866745
C	-3.195792148896	-1.643034715465	2.959470801152
C	-0.489013762604	1.936855841127	0.764755917426
C	-1.415609137153	-2.806714664692	2.581785226622
O	0.964275839345	9.333130827730	-0.460458816865
O	-0.248393357919	-1.945415910747	0.733801425467
O	-1.834161231577	1.681786340574	0.621825044377
O	-3.086740769743	-0.068412235912	0.649135238435
O	-4.448546699818	-2.025998705207	2.896491814952
O	0.132271681759	1.865727315336	-0.390724190790
O	-1.002216966574	-0.142803601808	-0.279043319066
O	-1.229535262728	-0.091810404550	1.856631521239
O	-2.364008380630	-2.100376419707	1.968315355829
O	-0.397544234108	7.375604043361	1.786894119625
O	-1.610220224917	-3.903009261976	2.981161609766
O	-3.195959694636	-0.275784510412	2.869174304706
TV	3.997029861469	0.000000000000	-0.000000000000
TV	-0.451643484857	5.663865031931	0.000000000000
TV	-2.723620306736	-3.915097401129	4.494715819982

EQ'-CO₂ 71

C	-0.600438648651	0.321237184481	1.026606014041
C	4.701173245785	1.089032809337	2.231577034309
C	-2.382245384201	1.216434066552	-1.246374193492
C	-0.335566438314	-2.295063258894	3.522589187949
C	4.966032977524	-1.527256562946	4.727568282138
C	-2.117375168661	-1.399855256045	1.249608221038
O	6.835631614378	7.827735645091	0.700728870368
O	-2.559806361817	-1.414348541485	0.004143866610
O	-0.785821795369	1.156237883614	0.051533247601
O	-6.020705329574	0.376156533727	-1.054587255217
O	-5.755835929161	-2.240126096802	1.441372280746
O	-2.064896490184	2.486725963080	-0.988831835186
O	-3.288951034521	0.781080536429	-0.320380180235
O	-1.800028438624	-0.129564976990	1.507158714027
O	-3.024060992896	-1.835216578359	2.175624137081
O	7.100498918941	5.211434122856	3.196713635339

O	-2.294921468296	-4.030635880735	2.500133577534
O	-0.520947321019	-1.460062006696	2.547511948661
TV	4.711949293895	-0.000000000001	0.000000000000
TV	3.295445620751	4.249333540116	-0.000000000004
TV	0.529739965285	-5.232584241397	4.991974256802

EQ'-CO₂ 72

C	1.112746732267	-0.362105257147	2.289593270710
C	-2.014990107354	-0.924919679248	-0.496403555512
C	-0.882882177119	-0.732998678734	0.501012615162
C	4.360692038095	-0.362122518249	2.289607265659
C	1.232952259230	-0.924902998448	-0.496413278702
C	2.365067001101	-0.733002778809	0.501007710988
O	-0.877083811484	0.021124053881	-2.495509953979
O	-1.477443627253	-1.880422327176	-1.269200028205
O	0.521098864543	0.621337937176	1.533664681543
O	0.818064222893	0.222858463902	-1.060120650734
O	4.066004088610	0.222836908948	-1.060115272592
O	-0.790791136861	-1.875018400140	-3.518012556409
O	0.187939014434	-1.461904103434	0.145690277008
O	2.457161786312	-1.875025444770	-3.518024654209
O	3.435895847673	-1.461920952606	0.145707480559
O	2.370849994937	0.021119480108	-2.495519368083
O	1.770495338394	-1.880411947686	-1.269202671250
O	3.769012286610	0.621318180953	1.533733228926
TV	6.495885754282	0.000000000000	-0.000000000000
TV	0.670177260056	3.678752122597	-0.000000000000
TV	-0.491595534255	-1.267252246756	4.164730475491

EQ'-CO₂ 73

C	-3.261910265238	-0.476803635307	0.854577860709
C	1.215219167005	3.674781078732	-0.870413644923
C	-0.283102613047	2.608418696907	-1.600803650227
C	-4.243926618708	-2.916293973536	3.418532513610
C	0.233181249917	1.235284245285	1.693542599626
C	-1.265138616449	0.168932265347	0.963134626090
O	0.340976077072	3.735863151521	0.236870477002
O	-0.450974105774	1.197025292088	0.591006001104
O	-2.453492704761	0.490462797347	1.383342714441
O	-2.809220526342	-0.978941902427	-0.337039116034
O	-3.791238278127	-3.418434190380	2.226905174109
O	1.232198862385	2.098469750905	1.751563749077
O	0.121973065629	1.514174259283	-1.608459155597
O	0.250172506069	-0.341022113553	4.315512650140
O	-0.860029318548	-0.925299598256	0.955481937495
O	-0.641061991941	1.296340214997	2.800833549791
O	-1.433001839074	-1.242472107873	3.154956373018
O	-3.435518581397	-1.949019667101	3.947291270997
TV	5.840770600987	0.000000000000	-0.000000000000
TV	-1.234740733198	3.494455234079	-0.000000000000
TV	-1.964057129054	-4.878978645683	5.127905334713

EQ'-CO₂ 74

C	-3.349550009689	-0.661023480578	0.648299636523
C	3.083519277720	3.471605370065	-2.012988912331
C	0.490028821555	2.589192285908	-2.000115586759
C	-4.357320872691	2.878778376660	0.648276156302

C	2.075743290851	7.011417519170	-2.012926424173
C	-0.517712035385	6.128926702717	-2.000092746083
O	0.328539170030	3.549637010476	-0.011058707441
O	-0.904719111511	1.200626803565	0.031589527731
O	-2.849800677525	0.445863365394	1.280069666435
O	-2.395946096495	-1.330056605123	-0.051054733847
O	-3.403713426522	2.209752642232	-0.051076987711
O	-1.367726785196	2.971407708584	3.952791519882
O	0.640586408063	1.622607591132	-1.400328958401
O	-2.375544615304	6.511198321220	3.952694011064
O	-0.367205786294	5.162364928888	-1.400237154422
O	-0.679222832100	7.089441618769	-0.011102413350
O	-1.912576318172	4.740364475089	0.031634745999
O	-3.857570925742	3.985617759631	1.280103018227
TV	5.666013348358	0.000000000000	0.000000000000
TV	-2.015596364791	7.079606773834	0.000000000000
TV	-1.245702387380	-2.355329711546	2.632717983975

EQ'-CO₂ 75

C	-0.930359065926	-1.381093744517	0.547391930104
C	0.335449396587	0.485732934895	1.879197119413
C	-2.880749382301	-3.552324291768	1.732297254945
C	-1.630888855811	-1.749654141090	3.132906950997
C	-4.841318864294	-5.705421418457	2.887530023602
C	-3.583510356822	-3.921695095750	4.317223821825
O	-1.967678963436	1.112694887945	0.849435552374
O	-4.004668384813	-1.091240695261	2.004677950948
O	-0.292981973869	-0.401562552077	1.145124340975
O	-2.250311244105	-2.781381791146	2.597589251015
O	-4.169449369724	-3.302086913256	1.679963667831
O	-0.590873667383	-4.242656815545	2.831547257590
O	-2.224844863591	-1.383752401854	0.798386105669
O	-5.906009089170	-3.223122023925	3.182238516204
O	1.396170461546	-1.997140883500	1.583052514950
O	-4.206618732490	-4.709723554310	3.471476778659
O	-6.139820661575	-5.543123174024	2.953390987628
O	-2.462172144163	-6.383024490123	4.042920492094
TV	7.295825272026	0.000000000000	0.000000000001
TV	-1.487741938160	3.755753070354	0.000000000002
TV	-5.877439333995	-6.558606192673	3.593790848777

EQ'-CO₂ 76

C	-2.032854829432	1.198624118540	0.052000649004
C	1.012620561057	2.179240061389	-0.354650354240
C	-0.618855890426	2.319055295648	-1.086814236061
C	-2.382282519954	-0.947138654702	3.051963038128
C	0.663180169015	0.033468690211	2.645352592020
C	-0.968277095884	0.173299380748	1.913200121210
O	-0.544857733046	4.545205293306	-0.475903845064
O	0.242824702851	0.450197628533	1.409325804267
O	-1.944370516340	0.745619756710	1.282015924400
O	-0.542117151484	-1.132147472393	0.171785112886
O	-0.891551260251	-3.277903501410	3.171792634756
O	-0.151200850920	2.540268100713	0.271371112111
O	-1.047117254000	0.973040568191	-0.824549652156
O	-0.500643391817	0.394435647763	3.271432342052
O	-1.396564332789	-1.172714335688	2.175403942126

O	-0.894292571338	2.399421756203	2.524061596170
O	-0.106627620026	-1.695585329063	4.409322758548
O	-2.293803586434	-1.400123797478	4.281990884334
TV	4.581424231288	-0.000000000000	0.000000000000
TV	-1.874013102797	3.681712053343	0.000000000000
TV	-0.698872316596	-4.291536577438	6.000000612890

EQ'-CO₂ 77

C	0.167884639797	3.162362541193	0.553950189117
C	2.417815302349	1.483513817704	-0.220529664520
C	-0.599131983980	1.410664108849	-1.212461801007
C	-0.898055655445	2.846970811119	3.639254195579
C	1.351805386752	1.168135613272	2.864740702171
C	-1.665105401984	1.095224272615	1.872862955679
O	1.253568181366	3.626301992706	0.506262714579
O	-0.740552885016	0.224925189460	1.484269733395
O	-2.172978220715	1.936600130181	0.992232693581
O	-3.127975780679	-1.147337195092	-0.980595646022
O	-4.193922623360	-1.462689274162	2.104634561285
O	-0.203532184828	2.086159409017	-0.071084699129
O	-1.586873990825	0.593642876806	-0.660052367458
O	-1.269481328889	1.770756786369	3.014237525477
O	-2.652830276670	0.278243267624	2.425306229586
O	0.187639190053	3.310880822102	3.591547669448
O	-1.806504731176	-0.090430010777	4.569535610750
O	-3.238964936250	1.621253045608	4.077503776443
TV	4.913919586191	-0.000000000000	0.000000000000
TV	0.036911002705	3.299094210705	0.000000000000
TV	-2.131933298067	-0.630783106186	6.170576372768

EQ'-CO₂ 78

C	-1.235575536350	0.440450946752	1.151548742838
C	-0.237328956824	3.006040201594	-0.439501057816
C	-0.218031503022	0.538159568770	-1.089716491870
C	-0.757735652609	-0.809359423955	4.312666192556
C	0.240433613237	1.756419481141	2.721613659116
C	0.259691221823	-0.711445131561	2.071376724527
O	-0.295753555866	8.805459733830	-0.757897254979
O	0.951464995359	-2.188895211319	0.281950742237
O	-0.851700004464	1.525664294062	1.996881896243
O	-2.527041611765	0.304746968705	1.388438602618
O	-2.049166117841	-0.945020239732	4.549654922649
O	-1.207177836693	0.389720042813	-2.021864740676
O	-1.079166101304	0.913008714801	-0.059197808637
O	-0.729522761045	-0.859782267662	1.139320759233
O	-0.601395447094	-0.336677370517	3.101987981877
O	0.181991801115	7.555855901201	2.403212178938
O	1.429219902240	-3.438571650630	3.443028169007
O	-0.373877328873	0.275942178678	5.158000877630
TV	3.453902572143	0.000000000000	-0.000000000000
TV	-0.464812427939	4.586913614915	0.000000000001
TV	0.955537421600	-2.499340880882	6.322237674936

EQ'-CO₂ 79

C	-1.903606829200	0.547486616269	0.932361482988
C	1.401088693680	3.351328181435	-0.993953311373
C	-1.857801969754	0.503484067234	-0.941386213171

C	1.332264208339	0.547488078711	0.932374811216
C	4.636982799048	3.351291393191	-0.993928495559
C	1.378056121820	0.503487931675	-0.941375800740
O	3.178399440882	7.595728396329	-0.066719489242
O	-1.004772371580	-1.802433749957	1.599267105297
O	-1.250150012521	1.395962614968	1.672731037150
O	-2.638131855622	1.202189542807	-0.042715149483
O	0.597726009202	1.202171454754	-0.042679672856
O	-1.137882546789	1.214033691287	-1.746464620441
O	-1.136133184935	-0.132344080697	0.023982764166
O	2.098023123984	1.214133193234	-1.746296392103
O	2.099679048576	-0.132395865544	0.024000249701
O	6.414375606257	7.595646415932	-0.066765999048
O	2.231072967818	-1.802467646122	1.599279499903
O	1.985719327072	1.395978322470	1.672763851271
TV	6.471706113649	0.000000000000	0.000000000000
TV	1.240356737245	4.713621652216	0.000000000000
TV	-1.600694598978	-1.487335933094	3.295117381109

EQ'-CO₂ 80

C	-1.169047935368	2.117379816083	0.733118305496
C	0.525795653741	0.957195487695	0.485704264394
C	-1.810487170794	0.330181871154	-1.401929439585
C	-2.968962739466	0.959301500369	3.980822471888
C	-1.274144000653	-0.200911741578	3.733398286652
C	-3.610433889655	-0.827928706620	1.845766940405
O	1.275454075368	6.304433521180	0.863491670620
O	-0.746821623766	-0.224220814490	2.532904466112
O	-0.797922366788	0.804321670284	0.478992564449
O	-1.652774195569	2.709922695645	-0.181240842615
O	-3.452716107312	1.551827509039	3.066458864438
O	-1.026307100583	1.401125649462	-1.821645695755
O	-0.761025301093	-0.572751937751	-1.250350815464
O	-2.826259304342	0.243023731488	1.426056629385
O	-2.560957699142	-1.730842966084	1.997349715614
O	-0.524492582666	5.146335857546	4.111189957368
O	-2.546766849987	-1.382327958774	5.780606384749
O	-2.597864518709	-0.353771569375	3.726692142418
TV	3.891590308996	-0.000000000000	-0.000000000000
TV	0.880114723962	3.887756274760	-0.000000000000
TV	-3.599885759332	-2.316205191293	6.495396449544

EQ'-CO₂ 81

C	0.293664052782	-1.757596175463	0.910423830363
C	-0.742728791796	-0.588777774549	1.931368815364
C	-0.654203670732	-4.156857692480	2.728817049390
C	-1.690584707145	-2.988025353601	3.749760305928
C	-1.602070852002	-6.556073452354	4.547183602763
C	-2.638466675982	-5.387278841563	5.568143594908
O	-2.296143631278	1.229536270465	-0.398545369957
O	-3.244034794873	-1.169648729593	1.419843077381
O	-1.526354937738	0.321238403261	1.415184352732
O	-2.474238055672	-2.078025173601	3.233583731139
O	-1.931546797281	-4.240191127784	3.235995851022
O	-0.411948600328	-2.905426771436	3.242193665970
O	-0.983676311531	-1.840958246498	1.417608625636
O	-4.191944964455	-3.568898489847	3.238211862053

O	0.535908474847	-0.506156245447	1.423786630884
O	-3.422123450318	-4.477281981304	5.051913813433
O	-2.879399330457	-6.639436647263	5.054398964638
O	-1.359840322677	-5.304637871288	5.060566592193
TV	6.039666218924	0.000000000001	-0.000000000000
TV	-2.610721728524	2.988449657300	0.000000000000
TV	-2.843641924546	-7.197722697668	5.455156065682

EQ'-CO₂ 82

C	-1.292337367139	-1.223108499177	0.606655596248
C	0.545919420731	4.315523556254	-1.651788118575
C	0.364673558370	0.392010467362	0.426787099181
C	-3.093339778547	-3.702346698712	2.724390987793
C	-1.255052673373	1.836288240111	0.465942611630
C	-1.436299314916	-2.087246079184	2.544517590793
O	1.956367465874	8.579338578437	-0.347429241789
O	-0.568545553381	-2.026319617264	1.406422629373
O	-3.974370353526	1.784563136378	0.417296344304
O	-2.468182738188	-1.333273503447	0.477753982436
O	-4.269187791576	-3.812495620301	2.595503710360
O	-0.043750708417	3.649736505160	-0.858625982043
O	-0.642159086059	-0.350759300374	-0.087891186953
O	-1.844726225580	1.170506095950	1.259104643474
O	-2.443141944451	-2.830006508511	2.029855294644
O	0.155402704749	6.100094054530	1.770298779162
O	-2.369524842180	-4.505540770073	3.524152583520
O	-5.775338029659	-0.694680204695	2.535017670888
TV	4.017780782449	0.000000000000	0.000000000000
TV	-0.166839280903	5.965253926792	0.000000000003
TV	-3.601942851692	-4.958466909985	4.235458648237

EQ'-CO₂ 83

C	-2.374780354867	0.113507928345	0.747915755293
C	1.999134303159	4.098827948420	-1.095061794876
C	-0.787929127859	0.633971125604	0.001497696235
C	-4.236624651681	-1.660901633852	3.352539015870
C	0.137244311201	2.324346286896	1.509562796880
C	-2.649784135576	-1.140453226705	2.606092761196
O	3.804966102372	9.088673363126	-0.041730541991
O	-1.652534907207	-2.649178044901	0.465225615287
O	-1.718853987544	1.351099867883	0.732027920505
O	-3.655883295586	0.149155586749	0.963716398694
O	-5.517721122587	-1.625253889318	3.568335605567
O	0.000324098560	1.088365126958	-0.910062943072
O	-1.719605439062	-0.310085535927	-0.405907619335
O	-1.861528220411	-0.686067174049	1.694529833594
O	-3.581447087279	-2.084531031929	2.198714754589
O	1.943180637798	7.314223194839	2.562912326689
O	-3.514350642543	-4.423596850389	3.069793148006
O	-3.580706190869	-0.423311600360	3.336604910905
TV	3.706951850585	-0.000000000025	0.000000000007
TV	1.801957696357	5.452068148357	-0.000000000001
TV	-3.723689368393	-3.548845043848	5.209211099786

EQ'-CO₂ 84

C	-1.884362866112	-0.227868441477	0.660788562004
C	1.686181810062	4.320272496564	-2.210181871315

C	-0.039603119702	-0.080729570373	0.465107273066
C	-4.113269206694	-2.433335722942	3.082992254096
C	-0.542725190561	2.114795642297	0.212010523827
C	-2.268514074732	-2.286209597781	2.887326894758
O	2.780977648483	7.418259381910	0.410767496153
O	-0.834221478790	-0.988948262061	1.194409645403
O	-3.889907541850	1.213067529467	0.817385851849
O	-3.016059279180	-0.711059758992	0.178640730571
O	-5.244968088967	-2.916520233862	2.600840927640
O	0.152114915798	2.817900698008	-0.693892178349
O	-1.091259380551	0.114969140049	-0.425387966686
O	-2.076790281837	0.612419575962	1.728341123428
O	-3.320165120298	-2.090510292405	1.996823638182
O	0.552068159340	5.212794820026	2.832979490869
O	-3.063126038804	-3.194426198593	3.616620853331
O	-6.118830651333	-0.992409536948	3.239625157583
TV	4.106064469700	-0.000000000000	0.000000000000
TV	0.360177683167	5.097221365571	0.000000000003
TV	-4.457812893771	-4.410948431874	4.844433170270

EQ'-CO₂ 85

C	-1.267597149732	2.168328681195	0.618154971864
C	0.773509191250	3.827951965938	-1.993749354089
C	0.652246848296	5.004768067221	0.610007417257
C	-1.501560535797	0.483728467433	3.214292996634
C	0.539504047895	2.143333116156	0.602381680800
C	0.418264066195	3.320160134658	3.206156683284
O	1.521517795851	4.587149719917	1.245290040983
O	-2.258270432613	-0.278371868902	-0.028017763270
O	-0.371312549345	1.171786791499	0.808492842125
O	-6.023507146763	-7.326741928449	-1.007523793941
O	-6.257514242676	-9.011355903429	1.588617760537
O	1.449213743177	1.934263687307	-0.368905022417
O	-0.356770645822	3.139204621201	0.413358004662
O	1.215241439633	0.249662353204	2.227241785821
O	-0.590732575862	1.454597824890	3.009471596124
O	1.287557231534	2.902525067102	3.841395850066
O	-2.492260797357	-1.962982635170	2.568140234577
O	-0.605274419176	-0.512804983813	3.404678175446
TV	3.613984332569	0.000000000000	0.000000000001
TV	2.040064539441	5.693654850340	0.000000000000
TV	-0.467965382147	-3.369205287744	5.192290766016

EQ'-CO₂ 86

C	3.181101281551	-1.405511211757	1.554409932293
C	-2.666845668366	-1.298048643447	-0.789530184553
C	0.113612488122	0.304929392720	1.553329332095
C	6.974598178038	-1.405513929814	1.554417005760
C	1.126645808449	-1.298043955025	-0.789532950534
C	3.907112357850	0.304917858624	1.553329276863
O	-2.100815095375	0.602653203011	-2.445500826408
O	-1.362013858985	-1.162765728384	-1.026366933817
O	2.690646253277	-0.195125870281	1.097004213464
O	0.487343278524	-0.131223618410	-0.896042817330
O	4.280829100812	-0.131225801203	-0.896031172674
O	-6.043596788196	-0.732415689491	-4.299394516642
O	2.562855707031	-2.354516548450	0.882843398799

O	-2.250120075415	-0.732390725889	-4.299368177814
O	6.356358842470	-2.354532272594	0.882850202938
O	1.692635544483	0.602591173919	-2.445558229257
O	2.431479382089	-1.162776411124	-1.026361309340
O	6.484120080814	-0.195161283894	1.096998297025
TV	7.586966429352	0.000000000000	-0.000000000000
TV	-1.710717763117	3.524673403454	-0.000000000000
TV	2.806139641733	-1.557203199214	3.787897475995

EQ'-CO₂ 87

C	-1.844894011120	0.089535223764	0.872348839089
C	0.099781238912	4.655500078875	-2.634942956278
C	-0.281523256222	0.569759834555	-0.835043685632
C	-2.971312430022	-1.505627174034	3.446700083076
C	-1.026639373384	3.060317207945	-0.060603050510
C	-1.407943472507	-1.025429103650	1.739312470483
O	2.056308062636	8.218716291409	-0.045744388047
O	-0.673706261402	-1.901814740149	1.022278199780
O	-1.425754712683	1.241136649683	1.431370787872
O	-3.183734751077	-0.028265459642	0.853009374639
O	-4.310153683682	-1.623441056090	3.427379452356
O	0.411918091680	1.156279725519	0.136435230876
O	-1.399190848871	-0.061909349479	-0.376468117666
O	-0.714528781154	-0.438902344597	2.710797319993
O	-2.525656643315	-1.657046400311	2.197864904021
O	0.929927582196	6.623506204793	2.528633723326
O	-1.800081592663	-3.496970136456	3.596649452465
O	-2.552167128245	-0.354032929858	4.005728273238
TV	3.868133958409	-0.000000000000	-0.000000000000
TV	0.392661479751	5.156906171524	-0.000000000000
TV	-2.252808204256	-3.190342105066	5.148718316025

EQ'-CO₂ 88

C	-1.813491219960	0.850005107029	0.211189009917
C	3.070433231845	3.147719937476	-0.414930446898
C	0.215147708317	0.271754120899	0.205934422013
C	-3.992237362929	-0.975565211771	2.828329837553
C	0.891719601781	1.322112744760	2.202148829844
C	-1.963623491200	-1.553872581981	2.823001989291
O	-1.620745953246	5.115792199542	-1.546276719242
O	-2.535474849272	-0.270643674050	-0.106266875574
O	-1.319936076293	-0.617667238309	3.493098741993
O	-2.344482656480	2.037006742544	0.265937771838
O	-4.523187118127	0.211446831614	2.883118686534
O	0.832912770101	2.417628371738	-1.126942418810
O	-0.707142461517	0.869391712987	-0.596118918740
O	-1.345815964130	0.591934901535	1.490137935344
O	-2.885943207284	-0.956232040568	2.020958503141
O	-3.799421552951	3.290133918962	1.070873474907
O	-4.714189433715	-2.096267098122	2.510817576523
O	-3.498642654005	-2.443324956419	6.110202107138
TV	5.065049205578	-0.000000000000	-0.000000000000
TV	1.801289056875	3.769685524129	0.000000000003
TV	-4.357442220825	-3.651309740093	5.234198226280

EQ'-CO₂ 89

C	2.065735137820	2.819730529388	-3.118077559213
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C	9.866650731333	-1.153445223314	0.392252266781
C	4.257296677472	1.404786504675	0.262419933638
C	1.205143752058	0.774175270390	-0.705172557504
C	9.006023142416	-3.208104769605	2.801965843622
C	3.401963927548	-0.654839081435	2.667545229200
O	3.326777122261	2.010805392409	-0.144021009559
O	-2.801018318164	-1.749483644814	0.725922057430
O	-3.265663728697	3.964164253276	-1.034952106561
O	-2.043560660396	-3.611575521553	1.613562858663
O	-2.902421268441	-5.662135826661	4.028199834496
O	-5.288370910478	-1.440190817318	-2.470374142903
O	-3.156844019348	-1.495731562728	-1.770327420212
O	-6.122138913079	-3.489624187059	-0.097171873624
O	-4.000552286685	-3.544361803545	0.624884482063
O	2.490195457995	-0.071023545751	2.199665224250
O	-3.662161165062	-3.794443272380	3.147490457212
O	-4.136522957334	1.915784611934	1.391155739795
TV	5.726195948065	0.000000000000	0.000000000000
TV	2.415158048545	3.678550390016	0.000000000001
TV	-1.712469212150	-4.106536505453	4.825958005459

EQ'-CO₂ 90

C	1.279922884038	-0.732288997460	0.784755979001
C	-2.616076460233	-1.567013539172	-0.822396478418
C	-1.017311108502	0.554366156019	0.933786295013
C	1.434545045501	-2.371305015931	4.101224845582
C	-2.461231910498	-3.205880161144	2.494048678857
C	-0.862660316779	-1.084763984025	4.249972083073
O	-1.445467600159	0.881478682707	-2.305056998922
O	-1.369932569070	-1.204609702974	-1.264423944912
O	0.639339179829	0.024963780509	1.674073901379
O	0.804404736236	-0.316238808538	-0.485743277069
O	0.959185234129	-1.955153598244	2.830699993266
O	-0.993597660108	-1.335514727684	-3.434637654535
O	1.036338123594	-2.034930191424	0.492005344973
O	-0.838919937327	-2.974129816270	-0.118046551849
O	1.190975291027	-3.673934332546	3.808353130399
O	-1.290598063305	-0.757236486414	1.011245796867
O	-1.215002615377	-2.843400898497	2.052345875716
O	0.793930488270	-1.614107556394	4.990562933762
TV	3.878786654341	-0.000000000000	0.000000000000
TV	-0.093409069537	4.021947399310	-0.000000000001
TV	0.309521365890	-3.277800283550	6.632770817801

EQ'-CO₂ 91

C	-3.067541886245	0.279501034100	0.624991879887
C	4.545995832996	3.058896657107	-1.236086948349
C	-0.995443730055	0.650071820860	-0.285605470857
C	-4.968395955209	-0.767133768181	2.569006980744
C	2.189431654403	2.309134625840	0.986002520782
C	-2.887611885572	-0.446234614644	1.914201623389
O	2.754616552912	9.183115845031	0.315328440551
O	-0.434665476493	-2.248913080705	0.086339556735
O	-3.074625349589	1.582316253694	0.907349151844
O	-4.235155927988	-0.160683038756	0.203896902391
O	-5.915348669459	-1.112639252594	1.702830424396
O	-0.953975710356	1.810964756492	0.366389659097

O	-2.135283187584	-0.028315207034	-0.285734069803
O	-2.829086561759	0.519744686759	2.883610272998
O	-3.832793781824	-1.357492427597	2.260209613611
O	0.691159264141	8.239625484183	2.424479229890
O	-2.523991593108	-3.177049109322	2.312002601250
O	-4.913313201788	0.572009708574	2.439747970208
TV	4.167230170473	-0.000000000000	-0.000000000000
TV	0.894390813672	5.673206807577	-0.000000000000
TV	-4.346155044748	-1.769934751835	4.252893452128

EQ'-CO₂ 92

C	1.687966903257	-1.421130292852	1.638375979288
C	-3.525103455296	-0.110918339089	-0.582541151987
C	-1.365314695417	-0.006725278589	0.013463472924
C	2.781073339803	-3.643980031008	4.257495193736
C	-2.431996225057	-2.333768553948	2.036576671796
C	-0.272205621562	-2.229574720136	2.632579933432
O	-2.898434257118	0.920284005848	-2.515241918251
O	-3.245655906906	-1.062994187409	-1.448321526509
O	1.805975814363	-0.635552401805	2.718177776983
O	2.848251593666	0.695057125802	-0.314781870220
O	3.941358366841	-1.527794025243	2.304334239642
O	-2.827518705622	-1.463067813763	-3.510997885869
O	1.301881843908	-0.670631964939	0.565599791974
O	-1.734412063351	-3.685915965103	-0.891878941189
O	2.394988244018	-2.893476956489	3.184718819768
O	-1.805328530896	-1.302567224117	0.103871465834
O	-2.152554240981	-3.285850002810	1.170799945850
O	2.899082961461	-2.858395242619	5.337292033044
TV	5.296878015784	0.000000000000	0.000000000001
TV	1.336141985636	3.594984539551	-0.000000000002
TV	2.186210835705	-4.445696635149	5.238235649077

EQ'-CO₂ 93

C	-2.041477726753	2.347121254081	2.509448848199
C	1.906608430234	3.700648138422	-3.283126055253
C	0.986564608125	2.781335299358	-1.335118197944
C	-1.626963180901	6.092430604931	2.509399632902
C	2.320585661524	7.445458463114	-3.283387630442
C	1.400479492808	6.526638667214	-1.335170123494
O	1.935773694228	3.379338584110	-0.541118351743
O	-2.014700084003	-0.595526609919	1.481481102825
O	-3.082209780349	1.438136705691	2.232880763324
O	-1.671522491816	-1.937603355887	-1.445478991466
O	-1.256811385929	1.807583283222	-1.445308318303
O	0.039118754827	1.539071354417	0.406784834756
O	-2.146265922209	1.252314770833	0.411503425454
O	0.453063461165	5.284361736207	0.406788100038
O	-1.732405968813	4.997820279676	0.411578591915
O	2.350058287816	7.124153818643	-0.541251353288
O	-1.600739517557	3.149834441218	1.481445049291
O	-2.668057692761	5.183415389503	2.233124330952
TV	4.568994827396	0.000000000000	0.000000000000
TV	0.828703133096	7.490641357033	-0.000000000000
TV	-3.054054627823	-2.084415277209	2.997213535988

EQ'-CO₂ 94

C	0.297622239784	-1.836825881899	0.894658834730
C	-0.840751029588	-0.563363945772	1.638270658344
C	-0.634331680808	-4.112416730529	2.815754809372
C	-1.772715273671	-2.838957084940	3.559364992463
C	-1.566262196464	-6.388019388795	4.736853273183
C	-2.704663767474	-5.114565181725	5.480456787065
O	-2.300373821378	1.039456013398	-0.298506080779
O	-3.232312326821	-1.236135100125	1.622593049694
O	-1.658894169755	0.376163529526	1.753333132883
O	-2.590837037703	-1.899421452220	3.674417669908
O	-2.041867097076	-4.070458649950	3.358888452857
O	-0.513642983955	-2.727097441864	3.358168479327
O	-1.109907895211	-1.794865135959	1.437794753133
O	-4.164251128892	-3.511704848827	3.543687207806
O	0.418320074323	-0.451505511318	1.437075471128
O	-3.522807037888	-4.175037747300	5.595528791190
O	-2.973821903325	-6.346058806370	5.279978953211
O	-1.445593060919	-5.002698181445	5.279277808261
TV	6.032133055068	0.000000000001	0.000000000000
TV	-2.657737566112	2.960128906566	0.000000000000
TV	-2.795867734079	-6.826781077390	5.763283228216

EQ'-CO₂ 95

C	-2.502793491832	2.213712377717	0.302057552655
C	1.180686264448	1.569867868866	-0.037002750837
C	-0.432965159772	2.399953960194	-0.578860283828
C	-3.959749912194	0.656402498375	2.934498799802
C	-0.276266269122	0.012547133607	2.595424733124
C	-1.889904883905	0.842657803366	2.053583739048
O	1.138688068623	4.085148384574	0.222800609554
O	-0.857659602059	0.267301074298	1.355579364861
O	-2.128457453052	2.071523998243	1.618831483967
O	-1.208065716526	-2.522243605727	-2.620842969399
O	-2.665037287460	-4.079538971378	0.011619649002
O	0.197701603854	2.242780139617	0.641527059909
O	-1.569302458048	1.680480072069	-0.473712243535
O	-1.259255896162	0.685442182608	3.273966260960
O	-3.026243341975	0.123176612208	2.158742982340
O	-0.318280920267	2.527834234983	2.855216771301
O	-2.314661935027	-1.290030671950	3.988042752180
O	-3.585432412045	0.514218270568	4.251273858794
TV	4.990631095524	-0.000000000000	0.000000000000
TV	0.053856816672	3.812919304182	-0.000000000000
TV	-2.913939375671	-3.114608174247	5.264876991254

EQ'-CO₂ 96

C	0.012179512844	-1.934546241345	0.710232478084
C	-0.410460776569	-0.343204467236	1.495487195853
C	-1.094500500291	-4.309743396651	2.231500668823
C	-1.517140813902	-2.718395927527	3.016748588720
C	-2.201179926690	-6.684945474303	3.752765126030
C	-2.623814265322	-5.093598125165	4.538017795060
O	-2.211108690382	0.260841188898	0.191106614534
O	-3.317791280084	-2.114356192865	1.712373746526
O	-0.668828378215	0.663419703805	2.015549369686
O	-1.775512273985	-1.711771768719	3.536809202084
O	-2.262361153336	-3.787782271557	2.723127248610

O	-0.348840694411	-3.240301415724	2.524565709485
O	-1.155683803788	-1.412584738390	1.201853760371
O	-4.424471248157	-4.489559265644	3.233641224289
O	0.757840690647	-0.865103793385	1.003304270130
O	-2.882186462376	-4.086975971526	5.058076663387
O	-3.369036959055	-6.162980022765	4.244393273869
O	-1.455517526916	-5.615504311711	4.045830198097
TV	7.346695444181	0.000000000001	-0.000000000000
TV	-2.477508453278	3.203960814840	0.000000000000
TV	-3.320059522792	-7.125581631491	4.563799557572

EQ'-CO₂ 97

C	-2.579531290699	1.962182571619	0.666281737185
C	1.829806746940	1.666566169572	-0.389550540407
C	-0.379465260198	2.265022346143	-0.655743919810
C	-2.703062452395	0.143807551612	3.885068030807
C	1.706339032313	-0.151855541753	2.829180229893
C	-0.502972415668	0.446589832596	2.562953919742
O	-0.148227918048	3.557388251561	-0.984375839609
O	-0.642797420626	0.002972307705	1.299642395706
O	-2.474553359749	0.831405395526	1.403422446880
O	-1.038560956626	-0.200579731220	-1.208587786389
O	-1.162010370365	-2.018934183200	2.010213340339
O	0.570271948507	1.547194996522	0.035783833165
O	-1.351902985746	2.232842160208	0.263738116032
O	0.446793867087	-0.271253361085	3.254405623208
O	-1.475447094449	0.414456703214	3.482403600945
O	-0.271634428529	1.738964330015	2.234434757962
O	-0.766340997092	-1.815335794957	4.518375130962
O	-2.598119621980	-0.986879502876	4.622266031056
TV	5.374913865989	0.000000000000	0.000000000000
TV	-2.567685980517	2.924135891354	-0.000000000000
TV	-0.247140388176	-3.636651528457	6.437454627636

EQ'-CO₂ 98

C	0.628998900668	-1.386408771622	1.086024268018
C	-1.572225246428	-0.617959731044	1.086610282944
C	-1.435278313038	-2.703120833714	3.332682853857
C	-3.636534658829	-1.934668955546	3.333296932622
C	-3.499549101869	-4.019827196423	5.579345009734
C	-5.700765699634	-3.251377229616	5.579921066589
O	-1.482880030366	0.300457093374	0.082878078777
O	-3.547172589396	-1.016253067342	2.329551038596
O	-1.559342374620	0.294754647580	2.089979822239
O	-3.623619296094	-1.021952214122	4.336651489813
O	-3.634868899162	-3.092984313076	3.330263386650
O	-1.437633240221	-1.544889205657	3.332752598250
O	-1.570586141305	-1.776276390850	1.083609145574
O	-5.611435035632	-2.332956801842	4.576195666908
O	0.626645802710	-0.228179284683	1.086094775639
O	-5.687875445418	-2.338665960510	6.583297558229
O	-5.699129029542	-4.409693674460	5.576912333640
O	-3.501907829990	-2.861597903611	5.579414502911
TV	6.113162346793	0.000000000001	-0.000000000000
TV	-2.100490174513	2.600644137645	-0.000000000000
TV	-6.192820677115	-3.950109752502	6.739967894717

EQ'-CO₂ 99

C	1.030079840210	-0.954196885223	1.275141633854
C	-1.850461184437	-0.668653885399	-0.840434920349
C	-0.716595537318	0.038623506685	2.294609784072
C	4.541821259335	-0.954191251506	1.275149045806
C	1.661300334916	-0.668658180736	-0.840417605973
C	2.795154191302	0.038603956106	2.294624086224
O	-1.247999698808	-0.054683593220	-4.906539930472
O	-1.063934118906	-0.294296515360	-1.814993184858
O	0.526703164889	-0.247617216142	2.266613486835
O	0.677296675643	-0.137105267757	-0.444577230148
O	4.189024867833	-0.137104624647	-0.444584700475
O	-1.271165628804	-2.059688505592	-3.116486884490
O	0.617461489839	-1.994427054859	0.917377163570
O	2.240588913087	-2.059711833134	-3.116475187277
O	4.129193650308	-1.994413680876	0.917373774327
O	2.263742331255	-0.054694865861	-4.906528951445
O	2.447818077885	-0.294321232773	-1.814988199558
O	4.038453114787	-0.247622930056	2.266632364655
TV	7.023480144837	0.000000000004	-0.000000000006
TV	0.013719110700	3.522601759795	-0.000000000005
TV	0.003658821691	-1.841317685112	4.242019582415

EQ'-CO₂ 100

C	-0.756557872339	-1.235021476575	0.451777674650
C	0.405057442000	-1.334794839061	1.845732283279
C	-2.656308514228	1.458614182508	0.451856256156
C	-1.494449786033	1.360069932137	1.845670522584
C	-4.556157112132	4.152090219898	0.451910375076
C	-3.394231161905	4.053576666750	1.845723119288
O	-3.384205953931	1.468346996492	-0.455429911614
O	-5.283963496188	4.162778891372	-0.455504882149
O	1.133910975714	-1.346194510049	2.752539879868
O	-0.765608324351	1.347688510920	2.752421485880
O	-2.804763824328	1.732037198105	1.758261618957
O	-1.346885901517	1.086462843736	0.539023806510
O	-0.904931424833	-0.962052360806	1.758225774145
O	-7.183500298542	6.857199519244	-0.455414936403
O	0.552713194091	-1.608013101969	0.538987577655
O	-2.665236492691	4.041775770820	2.752358077754
O	-4.704379764584	4.425321709504	1.758506053301
O	-3.246832394365	3.780195948112	0.538786498772
TV	7.556995890578	0.000000000001	-0.000000000000
TV	-5.698898480233	8.082081902414	-0.000000000003
TV	-1.497362139817	-3.476451744503	1.755333760503

EQ'-CO₂ 101

C	2.937062759234	0.908433979689	-0.378293216985
C	1.239797438441	-1.013533409810	-1.642559641561
C	1.916460536239	0.476157284133	1.519886745522
C	0.219172162999	-1.445892661130	0.255589879814
C	0.895824142392	0.043819905347	3.418053291290
C	-0.801440133355	-1.878161522196	2.153735423160
O	-0.096059145267	1.984360254173	-0.340464806375
O	-1.116687339090	1.552041986823	1.557679964194
O	1.721361313396	0.846001403584	0.215654496454
O	0.700746316637	0.413695112453	2.113800327319

O	-1.315238051697	-0.633293109930	2.013111756674
O	-1.659625447450	-0.333496625880	-0.230020608912
O	-0.294610585743	-0.201014590383	0.114911599267
O	-2.137296360322	1.119737607771	3.455813543637
O	-0.639028399043	0.098842370360	-2.128158172170
O	-0.319888014845	-0.018635219348	4.011934882027
O	-2.335845642647	-1.065618019710	3.911264625528
O	-2.680253823405	-0.765799710520	1.668180453447
TV	5.115331453063	-0.000000000000	-0.000000000000
TV	-1.531256805913	3.378845547703	0.000000000000
TV	-3.061853100499	-1.296964555242	5.694458339809

EQ'-CO₂ 102

C	1.097589378387	1.069734764648	1.341956471814
C	-0.186545627334	0.376290663093	1.093943338671
C	0.011342621323	2.979880173519	1.341952148604
C	-1.272793522722	2.286434755199	1.093943078409
C	-1.074910681677	4.890023915813	1.341958572760
C	-2.359044470704	4.196579660290	1.093941188940
O	-1.567360494244	0.146501045845	-0.522400733031
O	-2.653601135684	2.056651844035	-0.522403265024
O	-3.359284480666	0.412154154802	0.791519172167
O	-4.445533264866	2.322296799275	0.791510538977
O	-1.306742227318	2.328229618052	-0.239334878590
O	-0.603441313016	3.970976465511	-1.555482152463
O	-0.220501024601	0.418086695128	-0.239332032887
O	-3.739846537216	3.966790760138	-0.522407260194
O	0.482811458836	2.060835886527	-1.555476282534
O	-5.531785857735	4.232443826202	0.791517531135
O	-2.392989677083	4.238379038542	-0.239334253270
O	-1.689688853908	5.881122745281	-1.555481218090
TV	5.502435953745	0.000000000000	-0.000000000000
TV	-3.258746217986	5.730434858939	-0.000000000000
TV	-1.716372473779	-1.027887524196	3.197561312518

EQ'-CO₂ 103

C	-5.627796873059	0.883609070510	0.164043257281
C	0.370161279361	2.130353027993	-0.869898651960
C	-2.060025228888	1.321587782181	-0.070672738006
C	-7.094052119796	0.751500136933	1.865189922493
C	-1.096110575929	1.998243755134	0.831223002687
C	-3.526299655602	1.189455337604	1.630455804961
O	1.958113679306	3.670397897306	0.508306649688
O	-0.513306548246	0.866801752507	1.279134572018
O	-1.751486881032	2.687792906020	1.817432059583
O	-2.164880262390	-1.444658410720	-0.585245993839
O	-3.631162083534	-1.576797472077	1.115866019007
O	2.935449809665	1.925500401208	-0.079691356006
O	-1.353123591782	0.601335261358	-0.979609187567
O	1.469192017713	1.793386076839	1.621448718994
O	-2.819386935214	0.469223039867	0.721499399824
O	0.491841346647	3.538271894363	2.209419433464
O	-1.979580459206	0.734664856442	2.980244117096
O	-3.217735128179	2.555681252405	3.518562444942
TV	7.743206418478	-0.000000000000	-0.000000000000
TV	-0.534701914265	3.834984509360	0.000000000000
TV	-2.932537563806	-0.264227065170	3.402238665572

EQ'-CO₂ 104

C	-1.334519026146	0.515311719968	0.669167335872
C	0.067745756683	3.316316122996	-1.038672254878
C	0.517445201042	0.406387047194	-0.716814866896
C	2.390454686026	0.515305802995	0.669161853701
C	3.792733087639	3.316310464293	-1.038685897576
C	4.242412567261	0.406382745877	-0.716810916061
O	1.071534598210	8.050521380840	0.117876177285
O	-1.751920284763	-2.258184951645	1.137585354637
O	-3.102136484346	1.568184097279	1.650827934948
O	-2.406049120300	-0.143633198029	0.201673793716
O	1.318913680688	-0.143633618241	0.201688032853
O	1.248264751867	1.342585455394	-1.343081011764
O	-0.570444502073	1.077917454783	-0.241302331253
O	4.973227739672	1.342566724223	-1.343098584614
O	3.154518923639	1.077914325697	-0.241316508648
O	4.796516645218	8.050506865430	0.117863367098
O	1.973048573530	-2.258186747904	1.137581213823
O	0.622846116503	1.568196866834	1.650832965461
TV	7.449941888447	-0.000000000000	-0.000000000000
TV	0.473729584465	5.020545573366	0.000000000000
TV	-1.880581357110	-1.725100541474	2.708081466274

EQ'-CO₂ 105

C	0.173572693526	-0.650255543641	3.035750643615
C	0.256317313788	-0.111640881490	-0.415150248938
C	2.370051693674	-0.650040512417	3.038783848383
C	2.452731231025	-0.110946522423	-0.413205325641
C	4.566787709696	-0.651921409764	3.036466148374
C	4.649751898267	-0.112856023370	-0.415564494085
O	1.342764945703	-0.693524486557	0.140491550955
O	3.540107932145	-0.692936592534	0.141957323063
O	2.358542820580	1.355008233957	1.171762216393
O	4.557232113380	1.351797127154	1.169610950623
O	4.661592031315	-2.121324352594	1.451928029794
O	3.479561456149	-0.064079173521	2.490516116918
O	2.466286402484	-2.117183349192	1.453584319999
O	5.737342991628	-0.694210385905	0.140116317941
O	1.283641768072	-0.064121219713	2.487567076844
O	6.753688090665	1.354749464240	1.168341774416
O	6.859055752258	-2.118565858959	1.451905357805
O	5.675963994578	-0.064967268865	2.486734398338
TV	6.590939455853	-0.000000000000	0.000000000000
TV	-0.547317141662	4.765522760567	0.000000000000
TV	-0.045724247131	-1.992946877442	3.203674887953

EQ'-CO₂ 106

C	-1.501437686441	1.552993257318	0.773221081558
C	1.848478903831	2.315008099404	-0.904119011625
C	-0.631345366826	3.016140525827	-0.663906563255
C	-2.842235205290	-1.346981238194	3.263642878579
C	0.507687383561	-0.584964996982	1.586293530906
C	-1.972193313780	0.116153583612	1.826499899675
O	0.113161826345	5.298708781987	-0.646365599447
O	-1.774348896799	-2.942473760995	1.152697026849
O	-0.905485572013	0.353487708447	0.926669113577

O	-2.156436778174	-0.909220193045	-0.111182425746
O	-3.497215064471	-3.809203098473	2.379232404073
O	0.092809362849	3.341744824787	0.423107076154
O	-1.278544996698	1.887009880653	-0.484815371789
O	-1.247977747585	0.441729307503	2.913523028325
O	-2.619334843841	-1.012977847969	2.005599354518
O	-1.227555088604	2.398677683042	1.844060164691
O	-3.115103810388	-5.842488751645	3.643128372198
O	-2.246214975116	-2.546455777865	3.417085601743
TV	5.332963266911	0.000000000000	0.000000000001
TV	-0.965556133339	4.006694142358	-0.000000000000
TV	-2.681540077347	-5.799989264876	4.980828219877

EQ'-CO₂ 107

C	-2.716842319345	0.993409477914	1.646576041820
C	0.136513380653	2.889850711993	-2.409307207696
C	-0.515266165574	2.953290128737	-0.155380984022
C	-2.312323223496	4.377235886698	1.646571820846
C	0.541029123873	6.273662566908	-2.409307684460
C	-0.110722840296	6.337114359162	-0.155385969910
O	1.990128783247	3.972507907495	-2.283785483036
O	-0.072838279475	0.282232034869	1.882144473984
O	-1.905497794577	1.495596730934	2.521142887744
O	-2.845558744578	-1.354795267290	-1.417119693559
O	-2.441037120583	2.029041339411	-1.417075924954
O	0.967300445872	0.721978032970	0.010225186208
O	-0.826508911921	1.909832752915	0.642718216879
O	1.371808490670	4.105781186026	0.010219894703
O	-0.421928037325	5.293673680043	0.642748644926
O	2.394665822297	7.356334425752	-2.283800281428
O	0.331670150665	3.666048075910	1.882142483795
O	-1.500980859696	4.879400796989	2.521149235890
TV	5.010835668222	-0.000000000000	0.000000000000
TV	0.809048239967	6.767666954298	0.000000000000
TV	-0.339743444623	-2.199011416197	3.019645576614

EQ'-CO₂ 108

C	0.934355278024	-0.205962708481	-1.697225903684
C	3.263980496120	1.851205837940	-0.123156717238
C	1.920426988260	1.385149737547	-0.513413510374
C	1.218528751761	3.237386977115	-1.697223729465
C	3.548180899626	5.294552551178	-0.123165071440
C	2.204626710839	4.828500458149	-0.513413847920
O	1.436969545667	0.659326620684	0.512779454167
O	-1.349590933671	-0.465968353164	-0.295053759917
O	0.750660732464	-1.045868353372	-0.670565187616
O	-0.240779110314	-1.278378786157	1.458088300313
O	0.043396360316	2.164974381457	1.458083625017
O	-0.961698441006	-0.505576915349	-2.499217054649
O	-2.666100049732	0.661861191988	-1.613595263345
O	-0.677525969680	2.937777319191	-2.499216794396
O	-2.381924394407	4.105210920955	-1.613601032288
O	1.721159339214	4.102685695653	0.512777247056
O	-1.065417111928	2.977384675568	-0.295067635481
O	1.034825318583	2.397483609047	-0.670563914496
TV	4.603276525302	-0.000000000000	0.000000000000
TV	0.568366722747	6.886699492061	0.000000000000

TV	-0.034110751040	-1.825082180113	3.284319310107
# EQ'-CO ₂ 109			
C	-2.441340354276	0.467330813396	0.606590291500
C	0.722423615525	3.288832786776	-2.067949437522
C	-0.330869163660	1.636965147315	-0.903792726907
C	-2.864093543663	-1.447305417056	3.064896301662
C	0.299688686934	1.374209638363	0.390368994101
C	-0.753605071915	-0.277664015659	1.554533391892
O	1.048156282623	5.747024849747	0.104572510419
O	0.144679756867	0.022109143063	0.641089176139
O	-1.678358553697	0.755931098646	1.599938957633
O	-2.468644196690	-0.771295487244	0.226982270057
O	-2.891388418957	-2.685936494891	2.685293624060
O	0.023089909704	2.229138941909	1.219285875562
O	-1.068576068007	0.555923870569	-1.179382759878
O	-0.399657688426	0.314487016705	3.677594997334
O	-1.491293979272	-1.358708466959	1.278932130049
O	0.625415067741	3.832399118655	2.562879846486
O	-0.278014215118	-1.892547845336	3.099421389218
O	-2.101088874616	-1.158709437452	4.058227607963
TV	4.824625693609	0.000000000000	0.000000000000
TV	-0.697417704364	4.343669791287	0.000000000000
TV	-0.845463791945	-3.829270380795	4.916629658094

# EQ'-CO ₂ 110			
C	0.768521197193	1.902128929154	-4.091006912976
C	5.092810332818	1.261377708292	-0.188658748244
C	3.261554383585	1.979880980079	0.883848807908
C	4.482691202155	1.902142034728	-4.091028271484
C	8.806980164393	1.261359600209	-0.188595970742
C	6.975725560296	1.979904696935	0.883847337386
O	2.736636449869	1.216825315666	-0.101987347278
O	0.159595350767	-0.609067206366	0.608191971510
O	1.025205383913	2.008161123366	-1.258276185008
O	-1.595187321203	-2.656617180086	2.987685298765
O	2.119002943078	-2.656604123605	2.987659630566
O	-4.558733169450	-3.887322585141	-2.706287166251
O	-3.635860501326	-0.284789462062	-1.574782836321
O	-0.844554965094	-3.887333900379	-2.706332184981
O	0.078325084931	-0.284808827203	-1.574768474203
O	6.450802881142	1.216839235270	-0.102008709645
O	3.873748849407	-0.609074655472	0.608157204115
O	4.739436394869	2.008200951913	-1.258408238895
TV	7.428355909464	0.000000000000	-0.000000000000
TV	2.687728820396	3.862793088759	0.000000000001
TV	0.073552138970	-2.031164654423	3.623569111708

# EQ'-CO ₂ 111			
C	-1.492369937955	2.609672222611	1.165510755252
C	-1.252122140079	1.802173561067	-2.051544089249
C	0.440416513918	3.727931745618	0.609751564826
C	0.354114776042	1.270106269131	4.023848012939
C	0.594312877566	0.462570284522	0.806790950778
C	2.286902702126	2.388367970258	3.468037817571
O	0.012292648821	3.351923580083	-0.628250739315
O	-0.079821910737	0.750787859028	1.917545799334

O	-1.624780450072	1.556865496966	0.302813890308
O	-2.394843328740	-4.117489420152	-2.172354689043
O	-0.548373726271	-5.457064948404	0.685953209266
O	0.236673968498	1.049074201416	-0.157690233408
O	-0.192381480359	2.913572505273	1.454605653547
O	2.083133772184	-0.290521538829	2.700601445629
O	1.654116137058	1.574003504998	4.312890818964
O	1.858776204744	2.012342187990	2.230045885739
O	1.766664185049	-0.588766951416	4.775830434345
O	0.221696273334	0.217274585828	3.161178466675
TV	3.889219741943	-0.000000000000	0.000000000000
TV	-0.775390666038	4.581478592152	-0.000000000000
TV	3.692954604251	-2.679149279315	5.716641277024

EQ'-CO₂ 112

C	-0.979079031864	0.817383945022	0.586580873380
C	0.477898198370	2.235011995696	-2.122325447600
C	-0.887761929860	2.808287989382	-0.451024927627
C	2.547505667501	0.817377293395	0.586567109135
C	4.004458598794	2.234979254083	-2.122329788438
C	2.638822597708	2.808296056191	-0.451011411819
O	0.128805474830	5.102708947161	0.076617331619
O	1.059879736894	0.431758535764	2.177224303062
O	-0.722458268252	1.467821034002	1.768167939507
O	-4.931425527248	-3.986642271157	-2.265083906125
O	-1.404844213065	-3.986668156476	-2.265105611549
O	1.295777590756	3.397558482155	0.988655015575
O	-1.505786813752	1.601589422550	-0.321573365319
O	4.822351571997	3.397519667563	0.988631512737
O	2.020719361212	1.601627177011	-0.321508896583
O	3.655389694890	5.102710910554	0.076590541788
O	4.586449445796	0.431617944161	2.177256140513
O	2.804195574456	1.467830330949	1.768148245413
TV	7.053168319476	0.000000000002	0.000000000000
TV	-0.094467356252	4.764602175619	0.000000000001
TV	0.746360109592	-2.239948486465	3.047336090409

EQ'-CO₂ 113

C	-3.148276125659	2.157770834454	0.589274833991
C	3.573754175659	1.984269700858	-1.611375916240
C	-0.372526736879	2.861034134955	-0.425422176808
C	-4.398025870411	0.981659116133	3.103992776988
C	2.323966074733	0.808199292509	0.903323062952
C	-1.622292130099	1.684948121110	2.089282643885
O	-0.080657760052	2.982405329365	0.870259821976
O	-0.998409370764	1.041465845840	1.339970765601
O	-2.561976389837	2.528902001016	1.724930774766
O	-1.415237394458	-2.391149063512	-2.386259932340
O	-2.665017714529	-3.567232120360	0.128446171862
O	1.041043875200	0.967935560244	0.646826613553
O	-2.241528741575	1.758443452111	-0.333363602559
O	-0.208695968632	-0.208164912705	3.161536766188
O	-3.491301767053	0.582350517756	2.181336421660
O	-1.330414900462	1.806306712051	3.384966575604
O	-2.248188130747	-0.134644456142	3.854695514645
O	-3.811718286747	1.352796854843	4.239643486217
TV	6.118439697517	-0.000000000001	-0.000000000000

TV	-0.628573794757	3.359357133606	0.000000000001
TV	-2.499521184629	-2.352206249316	5.029423191596

EQ'-CO₂ 114

C	1.640358322547	-2.556925664575	1.429619252727
C	-1.509577085592	-0.377390300138	1.429599058578
C	3.510133728366	-3.784336403864	3.361835633367
C	0.360134355005	-1.604772363270	3.361848267204
C	5.379761875168	-5.011663777259	5.294015789702
C	2.229896985797	-2.832127734729	5.294011166362
O	-4.533256541929	0.857494217262	-0.503033307430
O	-2.663604260095	-0.369918639292	1.429190110265
O	0.933399043645	1.805666350858	1.448966981611
O	2.803183951631	0.578243633067	3.381181461346
O	2.356106638063	-3.776838762684	3.361369695191
O	1.513504900022	-1.601288201920	3.381166499842
O	0.486329570720	-2.549456523527	1.429193968278
O	-0.793888368677	-1.597307749097	3.361407349633
O	-0.356195050514	-0.373942984844	1.448955942764
O	4.672803754780	-0.649106654359	5.313388401546
O	4.225728937845	-5.004206069763	5.293587302850
O	3.383278879682	-2.828641135198	5.313392050785
TV	4.439427921585	0.000000000000	-0.000000000000
TV	-1.860343517097	4.359070009728	0.000000000000
TV	5.609104741488	-3.682172567001	5.796630835039

EQ'-CO₂ 115

C	0.542223327920	2.120545045724	-3.701332866511
C	6.021358689006	1.213441623958	-0.343009630303
C	3.277633346126	2.012049320128	0.751954008379
C	1.363577345939	-0.139672012380	-0.494212901957
C	6.842399548899	-1.046333784128	2.864699671314
C	4.098894220823	-0.247816482805	3.959444868474
O	3.353723782130	1.323002362866	-0.458990596448
O	-0.581315355335	-2.216228136350	0.925362105510
O	1.371740293232	2.045586409525	-1.212864104709
O	-0.685135072448	-3.070108294219	2.879007478787
O	0.135948334026	-5.330801763381	6.086523409685
O	-6.805048816515	-2.149441526547	-2.649599579793
O	-3.398161416679	-0.302852643417	-1.615311415790
O	-5.983790213871	-4.409577136450	0.557572589633
O	-2.576824509192	-2.562887948405	1.592433941877
O	4.174743957124	-0.936499170657	2.748356486069
O	0.239926352514	-4.475954319143	4.133081770624
O	2.192235798336	-0.214514324116	1.994958577426
TV	4.059397042512	0.000000000000	0.000000000000
TV	2.548992316043	3.881931070768	0.000000000001
TV	1.642757855629	-4.520139348653	6.414862923981

EQ'-CO₂ 116

C	-2.735966388734	1.522286552988	0.293290003248
C	2.460378723420	0.591627841273	-1.957490407726
C	-0.485022924737	2.167400059746	0.765351082191
C	-3.210094768414	1.111893661997	2.458735092942
C	1.986270504991	0.181234968382	0.207968748346
C	-0.959148634771	1.756986700677	2.930796087816
O	1.385911430426	4.301943962968	0.137970514457

O	-0.004627601187	1.736304130012	1.981356844528
O	-3.359040160743	1.983547564603	1.421170324439
O	-6.751122865775	-4.801920473308	-1.388128805961
O	-7.225218008552	-5.212297426691	0.777319545946
O	3.230512731588	3.669382402405	0.988882432230
O	-1.428468822466	1.277811379709	0.436336400531
O	2.756386974482	3.258987652467	3.154332155916
O	-1.902599382531	0.867409517591	2.601784143889
O	0.911783776610	3.891555080719	2.303437998191
O	-0.478748587523	1.325901887982	4.146805210495
O	-3.833157772302	1.573145159055	3.586627187565
TV	5.355669328735	0.000000000001	0.000000000000
TV	0.557123338264	4.365555492783	0.000000000002
TV	-0.948237322053	-0.820787396381	4.330897097540

EQ'-CO₂ 117

C	-2.861053421589	1.765462881747	-0.037201884732
C	4.673728859707	2.277482067915	-2.120935027816
C	-0.565685695175	1.686261533566	0.459317172436
C	-4.616560573577	0.200030631525	1.988175597641
C	2.918238706299	0.712036716355	-0.095555827293
C	-2.321180959222	0.120819302824	2.484698224845
O	1.713348597561	3.030353110465	-0.265643171557
O	-1.352101884528	-0.256988332906	1.611908666447
O	-3.329692988724	2.370909549061	1.013613929926
O	-1.712882120739	-1.125494721934	-1.110159720054
O	-3.468394981278	-2.690948109389	0.915196521021
O	-0.694114380199	3.012601901132	0.672263081797
O	-1.703715505570	1.126756919439	0.037001998227
O	-2.449581771636	1.447160350316	2.697636654184
O	-3.459214180179	-0.438668395931	2.062381342824
O	-0.042147917797	1.464923351562	1.759742462792
O	-3.107619890776	-1.822410324713	3.637288671683
O	-5.085190393405	0.805476975869	3.038993900863
TV	6.901401943838	0.000000000000	-0.000000000000
TV	-1.329753237501	3.683491353482	-0.000000000000
TV	-3.511003913020	-3.130871953821	4.050772407619

EQ'-CO₂ 118

C	-4.614864839537	1.505401826201	2.043137558394
C	1.978875796720	2.480996084569	-1.625129599656
C	-0.132081021358	3.037718178684	-0.975394264819
C	-4.571303486614	4.310569443274	2.176507558190
C	1.940154441358	5.790651438277	-1.961050167268
C	-0.303421482835	6.002607684757	-0.871296810147
O	0.651422225268	3.936275824154	-0.260564716791
O	-0.740525623281	0.107708837079	1.246068507560
O	-4.119488847812	1.455755468702	3.105217252772
O	-2.670928484902	-1.475211174826	-1.961144910595
O	-3.050028588728	1.682665518169	-0.759135520220
O	4.830757757794	0.924515936976	-1.069204455971
O	-0.795018381009	2.050059863182	-0.231225702684
O	4.654018670483	3.868825583280	-1.644826984517
O	-1.192236865049	4.976045467526	-0.772330861747
O	0.494557968541	6.287739324878	0.137474240557
O	-0.852308196993	3.666839540668	1.114525353329
O	-4.474734049889	3.672224890477	3.182849181280

TV	5.636261199780	0.000000000000	0.000000000002
TV	-0.499211679909	6.056589467059	0.000000000002
TV	-1.401739178565	-2.212352727108	3.011247788549

EQ'-CO₂ 119

C	-2.064876484200	2.370299869967	0.654102141815
C	2.121992392196	3.002794132196	-3.944374441631
C	0.124530080202	2.694648551740	0.767910262690
C	-2.386979812592	5.290201939662	1.486341396961
C	0.870682538449	6.158257875700	-3.178651385167
C	-1.143018450302	6.687489498327	-0.039099348196
O	0.352939512955	2.095176360703	-0.446204860506
O	-0.331725231120	0.533250193754	2.391871917189
O	-3.121255309988	2.174557805376	1.482703428354
O	-1.367167914876	-1.697928242846	-3.564038963173
O	-1.495015692354	2.095070152194	-3.202454307910
O	1.131081447100	-0.037545656805	0.469534326645
O	-0.971770820172	2.393214628374	1.425350326836
O	0.122123223238	4.058848839523	0.557109479331
O	-1.199372260115	5.364250114261	1.641672444562
O	-1.332006200388	5.492021852180	-0.586000541343
O	-2.308489385949	3.737294944828	2.805196944875
O	-3.207616366258	6.052280780261	2.153506836358
TV	4.268292506401	0.000000000000	-0.000000000000
TV	-1.213151602668	6.866392389827	0.000000000000
TV	0.472633800997	-1.644503752430	3.535996685662

EQ'-CO₂ 120

C	0.259041046335	-1.915262998447	0.656811855901
C	-2.684177453677	-1.019455444457	-0.263903158469
C	-0.795748325099	-2.527097140452	3.419946312041
C	-3.741656603921	-1.629570832109	2.499568763488
C	-1.856620633418	-3.142318068340	6.183729593513
C	-4.800524509948	-2.246075598727	5.261849602915
O	-2.354774145710	0.034648208961	0.473490405766
O	-3.408000158227	-0.576649914021	3.235929615520
O	-0.122241813924	1.137318748892	1.834419321023
O	-1.179599248899	0.521350105777	4.598518399934
O	-1.809972283691	-1.913210335559	4.084430571479
O	0.415903372477	-0.813952194512	5.447980954213
O	-0.753425257102	-1.298691225192	1.322027892587
O	-4.467492628099	-1.193489675440	5.997227905722
O	1.473256611370	-0.195448699271	2.680654278341
O	-2.240300813180	-0.094412264924	7.361686526783
O	-2.871679018358	-2.529827579238	6.847686482983
O	-0.650271465374	-1.428632819679	8.210587459928
TV	3.644426119733	0.000000000000	-0.000000000000
TV	-1.038637161086	3.381204166786	0.000000000000
TV	-3.178927230391	-1.842737195316	8.289704810882

EQ'-CO₂ 121

C	-0.185768765502	-2.800045930439	1.608750490054
C	-2.430856701452	-2.256569139770	0.984471604714
C	-2.048125977205	-4.347172485363	3.332507538460
C	-4.293223681436	-3.803703387775	2.708227844861
C	-3.910476564109	-5.894293224463	5.056236868964
C	-6.155567805831	-5.350830230560	4.431974685884

O	-1.075631144324	4.618924985729	0.487542714931
O	-2.937918816266	3.071798528883	2.211267895314
O	0.508734537477	1.647129230006	0.757438295117
O	-1.353633680055	0.100010586460	2.481174071099
O	-3.132042068764	-4.392714047730	2.603737590098
O	-1.751510506721	-3.096267092939	3.789234928091
O	-1.269656629465	-2.845536412184	0.879920988927
O	-4.800300356906	1.524672711454	3.935014416808
O	0.110868617197	-1.549143004826	2.065491546926
O	-3.216007093668	-1.447075205937	4.204864510026
O	-4.994407864778	-5.939879988876	4.327498608627
O	-3.613847597720	-4.643390366300	5.512985874380
TV	4.185883784901	-0.000000000001	-0.000000000000
TV	-0.279476555611	4.811731519887	0.000000000000
TV	-5.587004894811	-4.641388677291	5.171223376707

EQ'-CO₂ 122

C	-0.908360105393	1.589089238226	2.514113576421
C	-3.289362448157	2.201952085763	-4.675889570257
C	-1.354225130746	2.601639458166	-1.005061005802
C	-1.497657690965	4.743448429860	2.514099230546
C	-3.878612662939	5.356180620297	-4.675927957220
C	-1.943563344983	5.755886637830	-1.005054187859
O	-0.056675162951	2.554289434063	-1.244883441790
O	0.001957073324	1.005525851255	0.468553631907
O	0.333788508368	1.265975102514	2.500637318984
O	-2.324394466248	-2.240808978378	-2.978581807492
O	-2.913695048115	0.913480962304	-2.978673382272
O	2.734326023894	1.502729824059	5.568282693209
O	-1.781519000601	1.400031876464	-0.709827405807
O	2.144858559408	4.656973208078	5.568238542323
O	-2.370793333212	4.554265068727	-0.709854431145
O	-0.645977166790	5.708598065484	-1.244913334935
O	-0.587308032506	4.159668993993	0.468581230281
O	-0.255472266408	4.420346324879	2.500635958586
TV	3.482660751168	-0.000000000001	-0.000000000000
TV	-1.178651438315	6.308467791133	-0.000000000004
TV	2.134637203516	-1.727882133280	4.701836363052

EQ'-CO₂ 123

C	-1.106466865651	-1.186878157190	2.010110004453
C	-1.678125117262	2.348936990126	1.883022654492
C	-1.328504485841	-1.190413247820	4.185185460764
C	-1.899834032630	2.345385888100	4.058871657222
C	-1.548697213587	-1.196506921712	6.361938977321
C	-2.120080332980	2.339301252457	6.236418524298
O	-3.027258995040	-2.099480408334	2.924196248021
O	-3.246929125588	-2.103994189531	5.100513924123
O	-0.651859723161	-1.897214838666	0.968062478256
O	-0.873957097620	-1.901988653665	3.145132588502
O	-0.608669695858	0.011033033988	2.004989247288
O	0.988601471874	-0.112664131723	1.886499148329
O	-0.385956199212	0.017507645776	-0.171336481579
O	-3.467620013390	-2.110684684397	7.276918967703
O	1.207157725328	-0.106134372163	-0.289059322252
O	-1.094217640478	-1.905779767739	5.320202069651
O	-0.826415842804	0.006641967857	4.180379080817

O	0.763324815764	-0.116260315578	4.062350579943
TV	4.172719309264	-0.000000000000	-0.000000000000
TV	1.003431423937	3.667130526268	0.000000000000
TV	-0.662992315916	-0.016405035740	6.528526925502

EQ'-CO₂ 124

C	0.580239541592	-0.638450946627	-2.444641985222
C	0.240315868200	-0.192900266792	1.259368526595
C	0.634782172955	2.455749528284	-2.444814590727
C	0.294863486678	2.901371288385	1.258249102789
C	0.689306935343	5.550147939920	-2.445557239909
C	0.349203397517	5.995677875109	1.258917494455
O	-0.155137650299	0.182631902726	0.074725332718
O	-0.100464802695	3.276939464876	0.073576801818
O	1.503141119434	-0.072426712462	-1.645094647192
O	1.557718765070	3.022164021815	-1.645699434350
O	0.090942432685	1.498332382592	-1.696401385853
O	-1.120345759278	4.444193461376	0.050196500426
O	0.036342631838	-1.596090122951	-1.696679075311
O	-0.046391349454	6.371413870749	0.074429359812
O	-1.175362016374	1.349173140033	0.051158983177
O	1.612093431274	6.116122334719	-1.645580218787
O	0.145373548873	4.592551997864	-1.697617722410
O	-1.066619115531	7.537922989245	0.051187109143
TV	2.948166632462	-0.000000000000	0.000000000000
TV	0.163288200588	9.282788470915	0.000000000000
TV	-2.189345500987	-0.740405192091	3.685948329373

EQ'-CO₂ 125

C	-0.300910542758	-0.615100873075	1.445814087291
C	-2.060917103357	-1.318044793753	1.680299315053
C	2.721987706562	-0.619158387968	1.446579663904
C	0.960132186721	-1.318209290943	1.680439299796
C	5.741205874800	-0.620466847107	1.450307774697
C	3.981328622148	-1.324428373249	1.683809130015
O	-1.573265028458	1.910065322059	-0.142680106949
O	1.449855810041	1.920854222252	-0.149029793006
O	0.010329229079	0.590047711976	0.924777427543
O	3.031569739733	0.586117118434	0.925246145640
O	1.838818832406	-1.291048416560	0.648069653202
O	3.669363647625	-2.528997805712	2.204738126308
O	-1.184564365436	-1.284755265310	0.645974498153
O	4.471758664362	1.920436656819	-0.149081951848
O	0.654515807655	-2.524540358061	2.203591764106
O	6.040134607518	0.586949420616	0.925701421146
O	4.861689167225	-1.297086989857	0.652777246937
O	6.705637766764	-2.525825018964	2.203485036473
TV	9.067029058991	-0.000000000000	0.000000000000
TV	-1.952739004703	4.336455076372	-0.000000000002
TV	-2.629586867266	-2.564116689835	2.626942448282

EQ'-CO₂ 126

C	0.320875036195	-1.101036303456	1.143561870664
C	-1.723491634626	-1.590192038030	1.456495888781
C	3.711051174167	-1.108944049552	1.148392864182
C	1.669777888438	-1.592558196314	1.477851540273
C	7.111819650379	-1.109865049791	1.138764820302

C	5.068217728473	-1.587612718334	1.462923872225
O	-2.446605921582	2.160587509905	0.383779373539
O	0.951939103528	2.171332947888	0.367127449978
O	-1.181822004673	1.670671124233	0.746335749400
O	2.209321242709	1.692923054372	0.745826985460
O	2.711797681221	-1.895853933403	0.685255827759
O	4.825857660348	-2.511077285460	2.350463589538
O	-0.671374155255	-1.879793477536	0.662057609246
O	4.354117398433	2.157104942139	0.396911728087
O	1.374302626151	-2.519964526981	2.344799083129
O	5.617051884333	1.675675412914	0.757530249684
O	6.110674430002	-1.877396365159	0.660189768268
O	8.260729065200	-2.507193015845	2.352550467983
TV	10.193331111664	-0.000000000000	-0.000000000000
TV	-3.350839085002	5.745706733469	-0.000000000002
TV	-2.302243340955	-2.576497941532	1.743140327570

EQ'-CO₂ 127

C	-0.197048957914	-1.951662104577	0.865171714524
C	-1.672082756423	-0.458776086684	1.181609450865
C	-1.846735495094	-4.239444412721	2.606287057630
C	-3.320824145114	-2.744474819899	2.928358592889
C	-3.502385344992	-6.523841881351	4.340817770511
C	-4.975907848313	-5.030000213413	4.661083553383
O	-0.490147892027	-0.182790500471	1.840837220805
O	-2.123685412063	-2.458228348121	3.567122517054
O	-2.012742659052	1.393559629166	2.203581290686
O	-3.632864837375	-0.875114751034	3.938667325537
O	-3.048518933625	-3.802819137811	2.142028392295
O	-0.868582193185	-3.615781296614	2.042983943758
O	-1.387116104665	-1.503802340963	0.381172341765
O	-3.784285466507	-4.744933072741	5.305468412694
O	0.798092212882	-1.319465354343	0.333517111166
O	-5.296489544342	-3.165672091664	5.675304441646
O	-4.706054873427	-6.089803484198	3.873225709519
O	-2.528884950196	-5.881301762322	3.783097467744
TV	6.749049778213	0.000000000001	0.000000000000
TV	-1.758343393628	2.912582493916	0.000000000000
TV	-4.958595084266	-6.858406940740	5.205855195414

EQ'-CO₂ 128

C	1.405486613263	-0.829639319056	1.397426543933
C	-3.253429382687	-0.695043384948	-0.740750585847
C	-1.460083150058	-0.049422507242	0.598346531061
C	1.853509908942	-1.843207876365	4.268767815702
C	-2.805404279132	-1.708582632761	2.130595538338
C	-1.012072196525	-1.063002893440	3.469721632932
O	-1.374928867246	-0.085318857730	-2.294663008564
O	-2.579584630900	-1.596710000675	-1.468383036051
O	1.354504464787	0.526079314420	1.453003424529
O	2.725364116645	0.239383807298	-0.214563882785
O	3.173433550594	-0.774180540909	2.656740652749
O	-1.441665906387	-1.916732159943	-3.485211135461
O	1.184686923293	-1.308760349184	0.209059035872
O	-0.993630967215	-2.930230617326	-0.613900968004
O	1.632720948192	-2.322323969873	3.080399497613
O	-0.926888833978	-1.098824140154	0.576595054919

O	-2.131555457637	-2.610243668835	1.402969523370
O	1.802588407774	-0.487484703533	4.324296216825
TV	5.162374494894	0.000000000000	0.000000000000
TV	1.033480487369	3.535054064026	-0.000000000000
TV	0.896016478875	-2.027105846407	5.742719324800

EQ'-CO₂ 129

C	-2.657669223190	1.827391080566	-0.003843602513
C	3.999658665888	2.206854619268	-2.124187721041
C	-0.531437475392	1.780082590451	0.055210202788
C	-4.627221670062	0.445411084081	2.533495749890
C	2.030164422275	0.824904305288	0.413168406225
C	-2.501022161391	0.398077125041	2.592560162467
O	1.459248330780	3.227984623060	0.116362809051
O	-1.461004977748	0.049723321239	1.811082022269
O	-2.678316591015	2.351685623771	1.265905792326
O	-1.873177606465	-0.940646855131	-1.116403181034
O	-3.842709166782	-2.322615799916	1.420926862435
O	-0.576011110796	2.783967938268	0.661967672265
O	-1.564072279754	1.005742427110	-0.119005009474
O	-2.545591918228	1.401982895645	3.199273595724
O	-3.533615336990	-0.376265107647	2.418305908333
O	-0.510363141399	1.846074147628	2.653699306651
O	-3.430524099643	-1.332320598893	4.348414441014
O	-4.647965219660	0.969658057758	3.803240910568
TV	5.790042706970	-0.000000000000	-0.000000000000
TV	-0.774223335065	3.521226055252	-0.000000000000
TV	-3.939060289750	-2.763979034852	5.074685400793

EQ'-CO₂ 130

C	-0.087442307154	0.965461823458	0.869122311054
C	4.944100756862	1.955953531023	1.673051185686
C	-2.247831864128	0.708180918685	-0.760366018338
C	1.301971126338	-1.070772642592	2.828906033191
C	6.333518979232	-0.080294565201	3.632808973741
C	-0.858410289893	-1.328020582275	1.199297386269
O	4.047616672090	8.447449707446	-0.195134470913
O	-1.549118354345	-1.324393621236	0.017459576291
O	0.489820255208	1.170058483404	-0.133363784123
O	-6.915246402480	-0.240557852701	-0.788652790946
O	-5.525844004195	-2.276786495360	1.171075382831
O	-1.858350408670	1.907954605774	-0.426426397750
O	-3.159575230866	0.343972014367	0.169659191207
O	-0.468927947716	-0.128244826365	1.533232324025
O	-1.770208069762	-1.692221415233	2.129263773766
O	5.437012719258	6.411247459453	1.764594894618
O	-0.159799487223	-3.360591957008	1.977219955565
O	1.879158656911	-0.866163409347	1.826381919222
TV	5.710584141006	0.000000000000	-0.000000000000
TV	1.641803609959	4.720280740262	0.000000000000
TV	2.778803310658	-4.072453493933	3.919378955440

EQ'-CO₂ 131

C	1.927548720597	-0.264874797875	-2.773886065594
C	4.968194033142	2.501605778813	0.654675036329
C	2.814942053534	1.579315000713	-0.001929289604
C	3.969669295212	2.961217829239	-2.773887964287

C	7.010318447425	5.727700381019	0.654670657517
C	4.857045360437	4.805410581270	-0.001921195398
O	2.254705885798	1.059212605229	-1.140864040311
O	-2.059207809919	-1.364706497306	-0.135418197117
O	0.003887454611	-0.532222758346	0.001138078564
O	-1.016535639065	-1.328895999294	1.822275748314
O	1.025586746282	1.897204083766	1.822287548820
O	-3.476196236611	-0.334872616306	-2.405693352065
O	-1.358261162975	-0.123997458985	-1.732131850877
O	-1.434074954127	2.891228663327	-2.405695696752
O	0.683860756230	3.102099114475	-1.732127972490
O	4.296823197301	4.285310763394	-1.140862116938
O	-0.017077777337	1.861367948380	-0.135408441200
O	2.046006363476	2.693852199557	0.001140749624
TV	4.120257450414	-0.000000000000	0.000000000000
TV	4.084238825677	6.452178441356	0.000000000000
TV	-1.386631273938	-2.331318954391	3.885577949220

EQ'-CO₂ 132

C	-2.388673825873	1.513420355460	0.341424033780
C	1.415334055330	2.063612674619	-1.718447767195
C	-0.606998441877	1.918694540743	-0.914671069176
C	-2.877715824226	0.981442522168	3.410426996143
C	0.926420346081	1.532301643281	1.350855219524
C	-1.096118926252	1.387436584384	2.154270057907
O	0.518914243237	2.816389494601	1.033788444803
O	-0.090511405082	0.706824301736	1.528149848317
O	-1.689531130114	2.204273813147	1.253730799440
O	-1.808037573281	-1.130518883969	-0.521240677769
O	-2.297078644082	-1.661978098629	2.548194960206
O	-0.225455760087	2.991120754007	-0.129727732579
O	-1.367003886723	0.877918830123	-0.398302812992
O	-0.714728915077	2.459537378327	2.939467178628
O	-1.855935286747	0.346391814922	2.670375347511
O	0.029542151052	2.284099949611	4.102951781396
O	-0.579818080962	0.174239393308	4.597498046805
O	-2.178514037996	1.671716682760	4.322997005641
TV	4.647904212462	0.000000000000	0.000000000000
TV	-0.985051373664	3.543830490752	-0.000000000000
TV	-0.978262744877	-1.063696220598	6.138304815731

EQ'-CO₂ 133

C	0.993226153670	-0.561645207588	0.481436119942
C	-0.809506848721	-1.428320596049	1.741607452864
C	0.148962070857	0.407807652068	-0.352860470491
C	-0.204463740781	1.633700684262	0.481430169298
C	-2.007209171186	0.767002006580	1.741632168796
C	-1.048726517347	2.603145622518	-0.352869987433
O	1.929996134693	-1.435630073166	-1.555692316662
O	1.087751861483	-0.552709550297	3.874545337913
O	2.191281274390	-0.034189777441	0.736168258875
O	0.376369615714	-0.847387898560	1.674263071762
O	-0.821324595385	1.347946199083	1.674247954777
O	0.529227543137	-2.757886087248	-0.662866406744
O	2.783130283943	-1.160462804817	2.559506589998
O	-0.668452239918	-0.562546933398	-0.662890528868
O	1.585434493522	1.034872169959	2.559524693822

O	0.732339150558	0.759684828202	-1.555671812936
O	-0.109955188331	1.642626822799	3.874559148391
O	0.993594103394	2.161145737996	0.736174163502
TV	4.393231982702	0.000000000000	0.000000000000
TV	-2.395380579863	4.390681651425	-0.000000000000
TV	-1.481090673833	-0.299164990429	5.340333135056

EQ'-CO₂ 134

C	-0.825016137552	-0.817211774134	1.096715975916
C	0.324779371401	-1.818272690231	0.927420583237
C	1.488028009364	-0.818170993582	1.095079820227
C	2.637863900287	-1.819267663943	0.926083592217
C	3.801492394649	-0.818644449336	1.095275856508
C	4.953462510936	-1.817969361218	0.927184240292
O	0.316449170700	1.842277796526	-0.393264462458
O	2.633685208120	1.840071790747	-0.393666371324
O	0.332960030717	1.332290615772	1.732672143246
O	2.640908776062	1.331341214195	1.731459005249
O	1.477538534470	0.108693709982	0.290941955778
O	2.596315676043	-1.097308117768	-1.169664560859
O	-0.830447853100	0.109296268081	0.292469374017
O	4.952132334909	1.842065196727	-0.393578376087
O	0.281221998050	-1.095556694950	-1.169526258095
O	4.964870897249	1.331883407956	1.732208977290
O	3.791969068301	0.108819804195	0.291545970981
O	4.902644045982	-1.095658787174	-1.171198109521
TV	6.941672849426	0.000000000000	0.000000000000
TV	0.000022508521	4.076390978192	0.000000000000
TV	-1.101182910980	0.693417351816	3.586965404585

EQ'-CO₂ 135

C	-0.373212199054	-1.454376018736	-2.235696322263
C	0.691240556462	-1.877196192495	1.110533934614
C	-0.144617129684	0.100646018741	0.187214818174
C	-1.671392399240	1.607456184335	-2.235705514707
C	-0.606943320470	1.184645817773	1.110530132467
C	-1.442805079621	3.162489144229	0.187222176142
O	1.208588437657	0.090320874247	-3.011884212659
O	1.672277580705	-1.258309673863	-1.335333291082
O	-1.325974251997	-0.568933610208	-0.076460780446
O	-1.656729448819	-1.583313132219	0.804493476999
O	-2.954900833936	1.478523838267	0.804489778969
O	-0.671750643063	-2.198602210167	-1.359040512992
O	0.286343368151	0.435914153145	-1.051792766598
O	-1.969935309798	0.863244659480	-1.359034343620
O	-1.011860857540	3.497757741732	-1.051788150751
O	-0.089592767263	3.152166396681	-3.011875795182
O	0.374085622656	1.803539167906	-1.335331909931
O	-2.624173957698	2.492929096498	-0.076437702415
TV	4.590923565011	-0.000000000000	-0.000000000000
TV	-2.596380085931	6.123685742441	0.000000000000
TV	-0.322916336406	-0.735430792184	3.652679780966

EQ'-CO₂ 136

C	-1.696550850466	2.828601412952	-0.487235985333
C	2.402691735503	4.951177903882	-2.319564223093
C	1.326452421660	3.185755731690	-0.605415241151

C	-2.359888578455	7.454967987727	-0.487230042437
C	1.739358757223	9.577540463325	-2.319572144081
C	0.663110656663	7.812125751305	-0.605418835099
O	0.949178733167	4.303197344190	-0.628595350443
O	-0.233434906727	-1.281579081605	0.473016425429
O	-2.036377156815	-0.707415506897	1.835880064577
O	-3.073320027721	-4.111306393704	0.948825421500
O	-3.736632112237	0.515076919877	0.948830323461
O	0.557033794342	1.887792337494	1.349698432434
O	-1.395870958126	1.535414250693	-0.129359660928
O	-0.106284670836	6.514151863083	1.349684260158
O	-2.059208652747	6.161781702388	-0.129354330204
O	0.285832108780	8.929558999191	-0.628598596529
O	-0.896768821235	3.344787161058	0.473021280228
O	-2.699727706159	3.918962850227	1.835863859224
TV	4.386071108008	-0.000000000000	-0.000000000000
TV	-1.326661539365	9.252735695819	0.000000000000
TV	-2.629565616992	-2.790989116246	2.634813570571

EQ'-CO₂ 137

C	-2.113079721413	0.396196947704	0.263209169615
C	0.793838501498	2.904511163735	-1.228637019790
C	0.536234857057	1.430642930811	-0.918252895044
C	-3.381534433827	-1.662399834528	2.858569073870
C	-0.473538204543	0.846260228681	1.368482722822
C	-0.732043606571	-0.627716695881	1.677408112569
O	1.345114013122	8.035413671694	-0.136181490733
O	-0.726169965277	-1.543210272727	0.946577035972
O	-1.818594365337	1.187411342331	1.293998611103
O	-3.122290660510	-0.430031982388	0.442267413860
O	-4.390799979124	-2.488442292942	3.038039127689
O	0.240596800787	1.499517658830	0.376305694856
O	-1.388669847366	0.237249496861	-0.637129274063
O	-1.027939582414	-0.559210292910	2.971978697306
O	-2.656989554296	-1.821887908470	1.958477955503
O	0.077586975500	5.976451790153	2.461103448202
O	-1.993529170048	-3.601249434980	3.545548045660
O	-3.087828574611	-0.870058764573	3.888851297794
TV	4.255239673896	-0.000000000000	0.000000000000
TV	-0.121559980313	4.828606324012	-0.000000000000
TV	-2.536696847836	-4.115356429828	5.193253290621

EQ'-CO₂ 138

C	1.129720443874	0.962012548224	-3.339777799139
C	5.454995978478	2.506642793033	-0.125313668241
C	3.305378687304	1.445395696354	0.716011644153
C	0.291929065021	0.245050942801	0.457613662874
C	4.617201826273	1.789689182445	3.672066323126
C	2.467587266638	0.728431762751	4.513397892506
O	2.346065382988	1.442059319514	-0.246370963134
O	-1.735994894826	-0.981095662840	0.287769306468
O	0.652326201827	0.453471953411	-0.905069235720
O	-1.309360582948	-0.991799244215	2.436760773139
O	-2.147146374487	-1.708755367289	6.234147336544
O	-4.024279421431	-2.374882713333	-2.435790253228
O	-2.213763477418	-1.177694602769	-1.914904124294
O	-4.862071550337	-3.091844611588	1.361598984257

O	-3.051544143827	-1.894638803066	1.882479284497
O	1.508272840899	0.725097595062	3.551007820165
O	-2.573789569962	-1.698063892054	4.085150458194
O	-0.185469167757	-0.263474725876	2.892313625614
TV	3.933692549329	0.000000000000	-0.000000000000
TV	2.042559208125	3.434160134711	-0.000000000000
TV	-1.675581773502	-1.433913850566	7.594770001653

EQ'-CO₂ 139

C	0.380914247454	-1.074092655840	2.651890539104
C	1.520115995455	-1.651908810941	-0.341295910181
C	-0.989812829937	-3.187101081702	0.982234637040
C	-0.417867791098	-1.897360352185	4.727446085544
C	0.757495357190	-2.498346021269	2.633016307754
C	-1.578297897912	-4.039211772480	3.082278438695
O	0.813657376866	2.075189494733	0.785060622361
O	-1.290222703949	-2.013299675610	0.471508596748
O	-0.265963433053	-0.226660478776	0.199170471304
O	0.245785595289	-3.181760875209	1.562585231575
O	-0.473626402445	-4.121814818491	3.755012963249
O	-1.628054609379	0.778098980282	1.793485466195
O	1.284894363229	-0.162122879237	1.610094737301
O	-2.102231836630	0.134771346521	4.023261168618
O	0.609511713923	-0.502113040111	3.854753236799
O	0.049508487078	1.367574224969	2.844931045046
O	-1.765127763878	-2.772486026393	2.685107631942
O	-0.772345970677	-0.924541212142	2.357474884357
TV	3.839876200068	0.000000000000	-0.000000000000
TV	-1.445116071491	6.262747709412	-0.000000000000
TV	-1.275002343121	-1.358701353373	4.353963974069

EQ'-CO₂ 140

C	-0.316286703166	0.781344847387	-0.601336258636
C	0.225307388596	1.913282941174	0.010322798446
C	-0.295222439308	3.048972446449	-0.614437884282
C	0.234570133479	4.187090884315	-0.000592520802
C	-0.274826668058	5.320395500741	-0.642840936321
C	0.264534326198	6.452990315543	-0.030179664977
O	-0.236616430655	0.722271406001	2.144744678258
O	-0.221839617871	3.042879284888	2.155564909587
O	1.120629497339	1.909626545782	0.816956782776
O	1.130449499467	4.192175865967	0.808348152900
O	0.177672434690	4.170759211839	-2.775701704780
O	-1.188972141964	3.046879369408	-1.423949546873
O	0.175580412329	1.875826013418	-2.770490025589
O	-0.212028984043	5.389229496122	2.145903210652
O	-1.206151860744	0.791096250197	-1.409623163451
O	1.155712346982	6.446644609284	0.777750814038
O	0.197867729428	6.534236593162	-2.772107028576
O	-1.169757422329	5.324690736371	-1.450935042838
TV	2.734699800149	0.000000000000	0.000000000000
TV	0.032903964396	6.817024011632	-0.000000000000
TV	-1.344730880567	-1.140502646872	5.665427859471

EQ'-CO₂ 141

C	-0.552754970592	3.221090683464	1.860168324631
C	-1.687402497442	3.414548799433	-1.275710987019

C	2.077999057241	2.800798758638	-0.021059626116
C	-0.058817977060	6.145778072060	1.859898550448
C	-1.193291345397	6.339312512152	-1.275578842276
C	2.572125180707	5.725468702118	-0.021028962281
O	2.491353879494	1.879645155997	-0.959336497000
O	-1.690841455323	-0.132685643141	0.880511318634
O	-3.164519812050	1.426659975255	1.055485461689
O	-1.754146833795	-1.583736586622	-0.671997296060
O	-1.260154308039	1.340895973024	-0.671756994817
O	0.822343424717	2.224793040343	0.072638572349
O	-3.101516659654	0.095359151245	-0.503652852787
O	1.316553017520	5.149322349938	0.072949823136
O	-2.607454572308	3.019877404747	-0.503753372362
O	2.985556742169	4.804235268587	-0.959193063548
O	-1.196597169627	2.792129356662	0.880580271492
O	-2.670519570632	4.351293523240	1.055311829593
TV	6.780681037722	-0.000000000000	0.000000000000
TV	0.988056523991	5.849264949471	-0.000000000000
TV	-2.349111251850	-0.900405474773	2.585218812826

EQ'-CO₂ 142

C	0.627196493767	0.188475828957	0.726934847340
C	0.654063601684	0.338180530176	-0.822636145074
C	0.035833789773	-1.405896584507	2.282863826770
C	0.062710751825	-1.256186299197	0.733291779377
C	-0.555535077985	-3.000267609219	3.838806111149
C	-0.528643617244	-2.850558330162	2.289241325871
O	-0.242917149977	1.737520541848	2.034100883362
O	-0.834294748194	0.143166205797	3.589997464830
O	1.714895111619	0.306540611237	1.257888760713
O	1.123534984482	-1.287850078638	2.813818550606
O	2.626820299240	-2.965226615858	1.760353294578
O	-1.080387479274	-0.665383265543	2.540778345831
O	3.218173478770	-1.370830306710	0.204380643163
O	-1.425630713564	-1.451207560430	5.145963587580
O	-0.489025646688	0.928991743512	0.984854285242
O	0.532164555892	-2.882215018171	4.369744805713
O	2.035479467469	-4.559589247369	3.316244001931
O	-1.671738755997	-2.259729784238	4.096714628524
TV	4.244899048479	-0.000000000000	-0.000000000000
TV	-0.827007250513	5.334167732012	0.000000000000
TV	-1.774086605895	-4.783103163832	4.667780881111

EQ'-CO₂ 143

C	-0.177467277774	0.229326702151	-0.327474830213
C	-0.546976034178	0.434350666494	-1.707867735049
C	3.127976554057	3.460591752674	-0.080043055030
C	-0.554104310483	-1.114065236465	1.483064828505
C	-0.904337923460	-0.920467212648	0.097440030270
C	2.783437284145	2.095381019395	1.721242768932
O	2.512000824052	2.303909991470	0.358815215718
O	1.510931304837	-0.207281533834	-1.380534742267
O	2.223275268560	0.520640094654	-0.764134905093
O	0.862304252244	2.249074904043	-1.373949589675
O	0.580341275259	0.840042088243	0.393806737312
O	-2.561107065940	1.495389337265	-1.093259770558
O	-1.534177356944	2.421055891373	-0.794659857113

O	-2.913284589628	0.130033787137	0.714153349263
O	-1.885282097652	1.054488308450	0.990029637779
O	2.165853393543	0.939327189842	2.160673040836
O	1.119276180122	-1.610348552710	0.489466142485
O	1.841954578087	-0.855184624385	1.065276114176
TV	6.630463734820	-0.000000000000	-0.000000000000
TV	-1.122489108199	4.293794166953	-0.000000000000
TV	-0.697781300740	-2.726092011490	3.600983660611

EQ'-CO₂ 144

C	-1.555341033770	0.252308829516	-0.069974122991
C	-2.320180405201	-1.014247411153	0.380256539558
C	-1.670380770569	2.663737597553	-0.069997738401
C	-2.435179574318	1.397184940138	0.380253296470
C	-1.785360061204	5.075152883233	-0.069983321339
C	-2.550185060414	3.808621087205	0.380236454333
O	-2.208039959843	0.460399828439	-1.487317357220
O	-2.323084730514	2.871795970583	-1.487380278160
O	-0.364258683396	0.165797459464	0.033885423087
O	-0.479287346328	2.577329103416	0.033844807867
O	-3.180495469807	1.207781292369	-1.040543504434
O	-0.542610387763	2.302583566927	-2.198211192620
O	-3.065491061932	-1.203640381359	-1.040541599958
O	-2.438067905060	5.283259863035	-1.487337689172
O	-0.427599491236	-0.108831214137	-2.198200670295
O	-0.594277659676	4.988623054492	0.033847517262
O	-3.295482292930	3.619259816306	-1.040721941712
O	-0.657624137622	4.714045179184	-2.198249775488
TV	4.143261634183	0.000000000000	0.000000000000
TV	-0.345023017606	7.234270895956	-0.000000000000
TV	-2.553293650438	-0.949984999020	3.561802087792

EQ'-CO₂ 145

C	-0.240129054105	-0.413646613192	1.708031450412
C	-2.045287558343	-2.618326633057	-1.763240733661
C	2.243742015132	-0.413677459530	1.708019258103
C	0.438589121797	-2.618323951079	-1.763235423594
C	4.727628234458	-0.413651386347	1.708024011677
C	2.922471574172	-2.618348939394	-1.763239138659
O	-2.265039222017	-1.914364094197	-0.670564556737
O	0.218882040919	-1.914310426780	-0.670581309905
O	2.012787306239	3.429350617290	4.699233341207
O	4.496632042714	3.429341496759	4.699229374192
O	1.634969249064	-1.508505508232	2.373116344938
O	2.062887067500	-0.225583944093	0.413706231834
O	-0.848886319333	-1.508493056135	2.373128485073
O	2.702758951344	-1.914296814970	-0.670597912912
O	-0.421003833781	-0.225576443228	0.413710612458
O	6.980522223148	3.429333906519	4.699240065016
O	4.118901727936	-1.508501589220	2.373142288995
O	4.546737182278	-0.225611129632	0.413696350062
TV	7.451639036350	0.000000000000	0.000000000000
TV	0.596528846528	3.341243676538	-0.000000000000
TV	0.576334067825	2.318771841087	4.187385314226

EQ'-CO₂ 146

C	-0.018632883011	-1.783035478201	1.050341824439
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C	-0.992582065634	-0.263054547691	1.205699836277
C	-1.920248359507	0.675589689135	1.049767369744
C	-2.894572092015	2.195140323854	1.205203128844
C	-3.822625289015	3.132792201815	1.048592256379
C	-4.796421333487	4.652743205332	1.201188751002
O	-1.834260721147	-0.111018769051	-1.082804134603
O	-3.738758226867	2.349755545370	-1.081858503814
O	-1.077808203472	0.518249729703	3.336730342228
O	-2.980260765903	2.980770734255	3.336406923359
O	-2.923883411140	1.044181600501	1.868794707369
O	-1.892044680771	1.826431113506	0.385528681426
O	-1.024397683287	-1.415678813861	1.867307626508
O	-5.639587217358	4.810380338422	-1.084975663630
O	0.010624635372	-0.632657798320	0.386811314628
O	-4.885273636766	5.434782981089	3.338351909792
O	-4.825969455259	3.503073091448	1.866500021803
O	-3.792268509643	4.282467088786	0.383232346769
TV	3.515216102243	-0.000000000000	-0.000000000000
TV	-5.705031082508	7.375798186595	-0.000000000000
TV	-0.900281917016	-0.638826556877	4.026018715618

(v) SiO₂ at 10⁶ atm

EQ'-SiO₂ 0

O	-2.017403679497	2.696753537883	-0.658938800705
O	0.308385753673	-1.022041649257	-0.714801704241
O	2.613230477389	-1.351073025733	-1.247124501559
O	-6.024039289939	8.115818730341	-0.058672387604
O	-3.452419271151	0.876209734755	0.452466641731
O	-1.143788631124	-2.837288506706	0.410522819483
O	1.160435934044	-3.169319807698	-0.122203702328
O	-7.483900688749	6.286630604472	1.051429059275
O	-4.897565966801	-0.947737400707	1.570314374493
O	-2.569550084375	-4.665477712652	1.536950171551
O	-0.279449948784	-4.997340366513	0.976302524878
O	-8.946219514685	4.464555440351	2.180502480651
Si	4.332594752221	-4.027751108311	-0.385768261547
Si	0.316212021314	0.667065194000	-0.954131589178
Si	2.904188863350	-5.862124252339	0.734093158637
Si	-1.141224067388	-1.153748700191	0.166638017828
Si	1.444180632090	-7.670529763967	1.862182057620
Si	-2.590755419793	-2.979020389992	1.287987343629
TV	4.607642826826	-0.000000000001	-0.000000000003
TV	-4.915183313691	7.575917152163	0.000000000002
TV	-4.318891331463	-5.471963315202	3.364684546275

EQ'-SiO₂ 1

O	-1.353014740350	3.470815484831	-0.850431134002
O	-0.694393334570	-0.480145408235	1.271057286347
O	-5.211341383933	-4.957993415686	0.560893327723
O	-5.046101678896	-2.726340083505	1.244112582960
O	-3.059924987918	-3.844956873919	0.534831001307
O	0.577895752058	2.329461375799	-1.534113094549
O	-3.107379384386	6.837245853149	-0.850431808294
O	-2.448754928017	2.886280680753	1.271059603010
O	-6.965702509727	-1.591572629080	0.560896144777
O	-6.800467877005	0.640082017443	1.244115124273
O	-4.814288724819	-0.478527699441	0.534832735676
O	-1.176469068471	5.695883286219	-1.534107668054
Si	-4.173999356482	0.928573201777	-0.143430949274
Si	-2.624965726885	-4.690290165870	1.950824223910
Si	6.902262825825	-1.882563465574	1.952236030013
Si	-4.379324971628	-1.323868707451	1.950821015320
Si	-2.419641433549	-2.437858076343	-0.143435409500
Si	5.147896007694	1.483864402204	1.952239848783
TV	8.240613775669	-0.000000000000	-0.000000000000
TV	-3.508707582052	6.732848833548	-0.000000000000
TV	-1.491154473324	-5.057954123864	2.094521498919

EQ'-SiO₂ 2

O	-2.220334682089	2.657763525042	-0.636622184813
O	0.124899369270	-1.052394645792	-0.669170906924
O	2.405652084225	-1.424741805685	-1.254890858678
O	-6.210613024663	8.020926229232	-0.090045142641
O	-3.641626155302	0.873934063036	0.493653043519
O	-1.302972668960	-2.845736767951	0.462379503225
O	0.973657166209	-3.211564309735	-0.123996808155

O	-7.637804637670	6.232050075825	1.038809057996
O	-5.069257227185	-0.923077624407	1.625567543393
O	-2.732457605630	-4.633418551376	1.589598814983
O	-0.446157665740	-5.006962503456	1.008167164493
O	-9.060705340065	4.445467477017	2.171702792858
Si	4.084205258522	-4.042305452077	-0.380736777347
Si	0.093586031004	0.618934355168	-0.944999154672
Si	2.661693156322	-5.832545817547	0.752028521611
Si	-1.330478373125	-1.175859580162	0.185670541655
Si	1.234600816802	-7.623086181661	1.880741702467
Si	-2.758547054748	-2.964432956641	1.315369509412
TV	4.560709798150	-0.000000000001	-0.000000000003
TV	-4.849078576321	7.526726243151	0.000000000002
TV	-4.276649858863	-5.373132463569	3.394284896779

EQ'-SiO₂ 3

O	-1.395654811958	1.446603358740	-0.756465765975
O	0.074482406444	-0.189093980804	-1.029051910145
O	0.878748990421	1.920012522496	-0.256703656276
O	-0.771885891866	3.643722278663	-0.070599054668
O	-2.829073006363	-0.087744556848	0.701867978748
O	-1.353644926692	-1.720154490963	0.428864358523
O	-0.552258958657	0.389868091713	1.202207522334
O	-2.201179159776	2.111971420465	1.388439793007
O	-4.256887029420	-1.619684601219	2.159711742211
O	-2.781606836998	-3.252282637894	1.890024927632
O	-1.981710545233	-1.144267209664	2.659945228261
O	-3.632181520920	0.579873963948	2.847887813434
Si	0.900995687368	-1.525667099562	-1.623183915682
Si	-1.376712975967	-0.136832189751	-0.163590547484
Si	-0.528448081410	-3.057388564848	-0.164052565876
Si	-2.805415718118	-1.670273650839	1.294537940262
Si	-1.958319181633	-4.589671599722	1.295451431992
Si	-4.234605939639	-3.203013262187	2.753540858266
TV	4.551890288730	0.000000000000	-0.000000000000
TV	-1.694268577412	5.839746200378	0.000000000000
TV	-4.289465121889	-4.596923664961	4.376531713874

EQ'-SiO₂ 4

O	2.984634651327	3.365880869174	-0.631523425862
O	0.494550800552	-0.342047971608	-0.631132611708
O	-8.064607416008	-5.892998929140	2.915758546089
O	-5.626512913606	-4.050951040839	1.513903072255
O	-6.871723265205	-5.891877161556	0.798898576883
O	1.740051983879	1.525787722823	-1.347281840544
O	2.989277355683	7.074437694576	-0.631517718401
O	0.499186219219	3.366513806228	-0.631133269259
O	-8.059969187831	-2.184441268804	2.915764027197
O	-5.621873145665	-0.342393166009	1.513905094565
O	-6.867081437647	-2.183317722244	0.798906479195
O	1.744687915971	5.234340122195	-1.347280095802
Si	-3.165513295826	0.590593698235	0.083914484968
Si	-0.715775194330	0.590115840184	0.083609525535
Si	5.407669383777	-1.264947421228	2.199824911307
Si	-0.711140556321	4.298673767946	0.083615421353
Si	-3.170151480812	-3.117963552860	0.083911892612
Si	5.412309188302	2.443605547278	2.199825790141

TV	7.354649100764	-0.000000000000	-0.000000000000
TV	0.009271484188	7.417110803294	0.000000000000
TV	-3.685820636227	-3.709340125371	2.116069155368

EQ'-SiO₂ 5

O	-0.791277958326	0.932032803018	-0.687321442276
O	-0.785151232425	-1.395318927727	0.194024698463
O	-4.674629673371	-4.512901161865	2.371304155127
O	-4.680580375511	-2.183337058177	1.489472203114
O	-3.059246989132	-3.848667368462	0.607272317261
O	0.784646170652	-0.717832982007	-1.533689080537
O	-2.378346955843	-2.019744556352	1.921568348503
O	-2.372225881416	-4.347098507484	2.802911882749
O	-6.261702299556	-7.464678262713	4.980195794060
O	-6.267658752771	-5.135111509821	4.098355288205
O	-4.646322266480	-6.800444473848	3.216156259439
O	-0.802428299322	-3.669610142903	1.075200210443
Si	-3.520116761057	-5.562999369521	3.016748958189
Si	-0.722260822122	0.179338505723	0.842712984161
Si	2.090232687871	-0.969009288638	1.276620667011
Si	-2.309338070624	-2.772445820469	3.451606829605
Si	-1.933042362051	-2.611223652215	0.407859273807
Si	0.503156281861	-3.920785943732	3.885507549623
TV	5.620349699548	0.000000000000	-0.000000000000
TV	-1.602533824828	3.938380370562	0.000000000000
TV	-3.174150344952	-5.903554962950	5.217776440549

EQ'-SiO₂ 6

O	-3.659466693674	-4.565381121958	-4.159341042341
O	-1.874743822362	-0.796022942956	0.252897141569
O	1.835659518832	3.758919284767	1.917192653234
O	0.043911306698	0.497903933725	-0.011344255999
O	1.870012545814	1.465046010252	1.087972521642
O	-3.698706466446	-2.267831215331	-3.333609358228
O	-3.662028580949	-4.057633008731	-1.671077560383
O	-1.877307126266	-0.288280240932	2.741165059187
O	1.833095926576	4.266665135071	4.405459218194
O	0.041348995801	1.005648424758	2.476923411161
O	1.867447785063	1.972793573214	3.576238167355
O	-3.701268904603	-1.760084343709	-0.845342806368
Si	-0.915879759306	-1.620309044648	3.013039022296
Si	2.787471096639	1.829776565746	-0.281184041658
Si	-2.765169497811	-0.402467865234	-1.123471075905
Si	2.784911344256	2.337521440561	2.207082745255
Si	-0.913317726635	-2.128051952521	0.524770889098
Si	-2.767730534164	0.105275047579	1.364796420882
TV	3.702550567069	0.000000000000	0.000000000000
TV	3.642612002354	6.360191628479	0.000000000001
TV	-0.005123274721	1.015491186747	4.976533525243

EQ'-SiO₂ 7

O	-2.301550296662	-3.532445726693	-3.080989114843
O	-2.638738126395	-1.214961891446	-0.513774134021
O	0.682431714182	2.849837796081	1.174314013577
O	-0.353219702398	0.766683929571	0.738510135311
O	1.992363310466	0.839906546001	0.721341004638
O	-3.615398303099	-1.518056274060	-2.629895700213

O	-3.671898501728	-3.295357388488	-0.950954351071
O	-4.009050804514	-0.977865959267	1.616261968240
O	-0.687912795134	3.086919879010	3.304353544204
O	-1.723550770513	1.003770978972	2.868532985680
O	0.622023373554	1.077009451194	2.851373382982
O	-4.985746593927	-1.280963326797	-0.499861338202
Si	-2.875048722507	-1.858601981099	2.441881803717
Si	3.235415832984	1.650093404950	-0.087668020708
Si	-2.483866252809	-0.460617850737	-2.017338572187
Si	1.865081589658	1.887181732982	2.042366425809
Si	-1.504706307923	-2.095677849725	0.311856144410
Si	-3.854219709729	-0.223525495072	0.112682122501
TV	4.719558643177	-0.000000000000	0.000000000000
TV	3.361946708710	5.840061834830	0.000000000000
TV	-2.740672223381	0.474169731591	4.260065810022

EQ'-SiO₂ 8

O	0.293235270337	6.079329668904	-0.672280574497
O	-1.792591986395	-1.405354823949	-0.015001981349
O	-6.565402331096	-7.799118900777	2.636277390552
O	-5.120578158047	-4.436519597431	0.623367772074
O	-6.173733070031	-7.775186224779	0.224417342158
O	2.925380617646	3.704961521140	-0.250674755365
O	-0.868124005406	10.249450762528	-0.672094628216
O	-2.953990281808	2.764621554073	-0.015188117617
O	-7.726731280332	-3.629190364715	2.636352029185
O	-6.281964113512	-0.266441360523	0.623421241063
O	-7.335191768094	-3.605343281121	0.224657052467
O	1.763628076277	7.874683318470	-0.250476560000
Si	-3.666203991227	1.168234719492	-0.194194713909
Si	-1.500814645346	1.775772384673	0.143658367670
Si	7.090653091692	-2.603137266477	2.490138930427
Si	-2.662245074981	5.945713402694	0.143724980035
Si	-2.504700790702	-3.001842434896	-0.194202546427
Si	5.929070969587	1.566718370179	2.490067632226
TV	8.127171443648	-0.000000000000	-0.000000000000
TV	-2.322917929406	8.339832300799	0.000000000000
TV	-2.886155738776	-5.301397076496	1.771944697864

EQ'-SiO₂ 9

O	-0.621498375589	1.325595126105	-0.890334347500
O	-0.127696630197	-1.077635618632	-1.114467586791
O	1.133935384235	0.165535599157	0.132439004764
O	-0.492422214744	3.514418845320	-0.847687405688
O	-2.258898836641	-0.891748614693	0.697524987803
O	-1.491809423893	-3.052121633126	-0.293872791928
O	-0.233357561556	-1.842352177631	0.971641630967
O	-2.127719930102	1.296405066133	0.725942749460
O	-3.584665772948	-2.851016189760	1.190063210004
O	-3.476779225085	-5.318177930609	1.682973902146
O	-1.620907605468	-3.904243497142	1.987024431680
O	-3.894863182416	-0.834073105920	2.482479684641
Si	1.623717819762	-0.439769847893	-1.299907411078
Si	-0.884143777684	-0.086155481477	0.045113557392
Si	0.505271744326	-2.818416074915	-0.204435788575
Si	-1.989976485390	-2.473104909545	1.148442795161
Si	-0.914991095727	-5.288615475898	1.396934834839

Si	-4.177612544711	-3.928742090546	2.275776436495
TV	5.447358081561	-0.000000000000	0.000000000001
TV	-2.386629410646	5.537741205361	-0.000000000000
TV	-4.727452132462	-6.303812368657	3.828241280251

EQ'-SiO₂ 10

O	-1.404715220905	1.895816170215	-0.907160825890
O	-0.915859733717	-0.456175304075	-1.142221204290
O	0.406921515825	0.719280066422	0.094404955161
O	-1.241007762310	4.104143524725	-0.886250780051
O	-3.084718286707	-0.389621867729	0.652592498897
O	-2.378615740641	-2.571413465326	-0.308705314457
O	-1.032935257617	-1.362059251292	0.896309128403
O	-2.919191701433	1.824089093680	0.694784096017
O	-4.418153182036	-2.351191246681	1.161611579035
O	-4.347383905406	-4.837267353637	1.577456019692
O	-2.449158903284	-3.405839957011	1.995911350612
O	-4.730064222930	-0.328775983948	2.407820730747
Si	0.841385188558	0.142321280265	-1.344661705634
Si	-1.780274483866	0.454675102345	-0.032603715408
Si	-0.162685182389	-2.305226792793	-0.185551175351
Si	-2.800012272026	-1.979401066292	1.121135467199
Si	-1.756964731906	-4.777234033766	1.344280814115
Si	-5.026620615070	-3.462508650171	2.221168981372
TV	5.516603710223	-0.000000000000	-0.000000000000
TV	-2.362089659500	5.552107038975	-0.000000000000
TV	-4.823792092380	-6.404841016010	3.786844689520

EQ'-SiO₂ 11

O	-2.330900077823	0.526932026168	-1.379221864867
O	0.278305166267	-2.604522656202	-1.996612823510
O	2.292755437577	-1.760052451729	-1.046499022249
O	-4.036265238304	13.799530843587	2.120001493184
O	-3.752870148341	-0.913646353938	-0.100294360485
O	-1.147921883700	-4.045773315406	-0.714238808077
O	0.887481838715	-3.187763068542	0.223804408059
O	-6.829937974052	12.390537972923	3.371512767575
O	-5.178510655901	-2.354548314599	1.182147966303
O	-3.898680522812	-5.429777531161	0.517291811968
O	-1.905264886563	-4.596637279594	1.475594920457
O	-8.228485692789	10.961926069582	4.642913292783
Si	3.521842846125	-5.584026354161	-1.045835914828
Si	-0.914412620568	-0.168817740644	-0.760662997870
Si	1.549145966948	-6.124763800431	1.135402066860
Si	-2.564971311172	-1.660379271583	0.564694214515
Si	-0.101534876578	-7.616523065358	2.460788503096
Si	-4.539041028614	-3.892551782500	0.850576613873
TV	4.030271596189	-0.000000000002	-0.000000000003
TV	-2.463136420055	7.647493851953	0.000000000001
TV	-5.598242401678	-4.264988056248	3.792521007237

EQ'-SiO₂ 12

O	-3.223131589020	-2.510518095100	-3.822712922742
O	-1.983393409866	-0.625371034739	1.263913744267
O	2.659123703693	1.281984836023	-0.006776178966
O	0.050247834525	-0.641518840317	-0.009164343914
O	0.643276227455	1.277641418673	-1.279123754849

O	-1.231344127107	-2.494543242212	-2.551208980393
O	-3.221860302371	-2.507625622996	-1.279451596908
O	-1.982104796696	-0.622467402950	3.807153713064
O	2.660378023164	1.284917204284	2.536467843202
O	0.051533337533	-0.638615060438	2.534082353419
O	0.644550561610	1.280536010657	1.264134791054
O	-1.230069332197	-2.491650639045	-0.007938654727
Si	-0.587839174904	-1.561810734391	3.806232859163
Si	-0.173354104643	2.277454134568	-0.007150678842
Si	-2.557456671448	0.285803147336	-0.008534892035
Si	-0.172066700290	2.280354883958	2.536093429684
Si	-0.589121200894	-1.564690958719	1.262988519260
Si	-2.556165454074	0.288699383501	2.534722130113
TV	4.025842192191	-0.000000000000	-0.000000000000
TV	2.475652354821	5.696185981041	0.000000000001
TV	0.002545149373	0.005803202003	5.086513940860

EQ'-SiO₂ 13

O	-2.234216200921	2.786552907750	-1.234164560236
O	-0.782916233589	-0.317359522335	0.600979295432
O	-5.201737818216	-4.883625675132	0.937466628698
O	-5.023883356703	-2.577349959477	0.515058655695
O	-2.962248032034	-3.778877415827	0.846988145557
O	-0.306800111923	1.444418937947	-0.977763238458
O	-2.824635450952	-1.375698785737	0.601708197921
O	-1.373403366633	-4.479594920018	2.436984749311
O	-5.792147224526	-9.045797361958	2.773363788649
O	-5.614292873310	-6.739585544740	2.350946473210
O	-3.552697027843	-7.941055597515	2.682945361556
O	-0.897219687532	-2.717879490205	0.858100887795
Si	-2.826751853362	-6.816916279648	1.565265961828
Si	-3.004935148168	-3.840659932430	2.497646811555
Si	8.161065919108	-1.461903615607	1.726506927772
Si	-3.595340869616	-8.002876329964	4.333542129719
Si	-2.236297535932	-2.654803807954	-0.270836626906
Si	7.570553478886	-5.623967890255	3.562626105887
TV	9.646952393610	-0.000000000000	0.000000000000
TV	-3.137942189856	3.368004426020	-0.000000000000
TV	-1.180580130856	-8.324160197678	3.671989031629

EQ'-SiO₂ 14

O	-1.408866551973	4.537153500795	-0.924345052184
O	-1.218650304973	0.608254930727	-0.900724386428
O	-4.717485396213	-7.084915215283	3.116480453202
O	-4.868284794871	-4.218221043549	1.075471789892
O	-3.399586625105	-6.193285322194	1.150822598205
O	0.058801319047	2.560017419271	-0.853878636183
O	-4.159153271698	8.461939499590	-0.926102312279
O	-3.969070903242	4.530472658942	-0.901465488874
O	-7.468911706467	-3.162780611344	3.116531270416
O	-7.619578661428	-0.295144074798	1.074832312642
O	-6.154866077126	-2.272838707316	1.149431950720
O	-2.693058056625	6.483699014267	-0.854375085460
Si	-5.057990005109	1.099934167134	0.096170101824
Si	-2.502322965703	1.159637994343	0.123053421654
Si	6.619020038240	-3.690372313858	2.103215806267
Si	-5.251409178172	5.080563726390	0.123523177857

Si	-2.306560731695	-2.824208903742	0.100358116671
Si	3.868063080453	0.231682385206	2.102968822557
TV	7.672500081724	-0.000000000000	0.000000000000
TV	-5.500114639351	7.841285365013	-0.000000000000
TV	-1.100122282983	-4.827830718905	1.991082112571

EQ'-SiO₂ 15

O	-1.034943370985	2.603940060628	0.010616603573
O	-0.697264758477	-0.833873463275	0.430602640639
O	-6.746686357963	-5.552458458646	1.573651903749
O	-6.996539817332	-2.187356059812	1.323301320720
O	-3.696615607115	-3.244394601772	0.908007193454
O	0.213747507422	0.778618651195	-1.122972169707
O	-3.698825812334	5.886310462722	0.010610264129
O	-3.361110586649	2.448520781955	0.430621564344
O	-9.410577028392	-2.270102568249	1.573630573196
O	-9.660479611355	1.095016159461	1.323342756166
O	-6.360481139161	0.038006717889	0.908000353554
O	-2.450093982285	4.060995599036	-1.122961918538
Si	-5.212270721509	0.108850091161	-0.401754933743
Si	-2.239540030050	-0.217400097795	0.499234792561
Si	9.080186097383	-1.948063896206	1.742153181901
Si	-4.903412741776	3.064947502412	0.499224132900
Si	-2.548442418589	-3.173493854103	-0.401766166383
Si	6.416331512012	1.334330783258	1.742160063339
TV	10.101693955464	0.000000000000	-0.000000000000
TV	-5.327741611500	6.564724218789	0.000000000002
TV	-1.501021498813	-3.929889154331	1.794093841169

EQ'-SiO₂ 16

O	-2.168289967104	1.969266072436	-1.550658631595
O	-1.173007481988	-0.736428272239	1.262662292306
O	-4.660555872511	-2.893820280997	1.608915257849
O	-6.526490131394	-2.646690020473	0.010561191610
O	-2.511901096191	-3.766182385302	0.961318017618
O	1.954435146074	1.983745243037	-1.358596178702
O	-4.970354844279	5.209356170951	-1.661283953848
O	-3.690663436758	2.384607264782	1.334736498198
O	-7.436010581125	0.165161376738	1.661039501138
O	-9.132359317349	0.649784049849	0.026081745951
O	-5.358201735246	-0.730608133580	0.970664562955
O	-0.725182127445	4.992880344813	-1.200376220250
Si	-5.235427061626	0.176887739942	-0.427830161180
Si	-3.490184200868	-3.627879159713	2.381619508738
Si	7.976763501788	-2.276774018285	1.298182921732
Si	-5.867302651010	-0.544843641920	2.536817817110
Si	-2.888041239559	-2.981438918240	-0.537541949836
Si	5.909010856596	1.429584156587	2.655656640626
TV	9.691833140781	0.000000000000	0.000000000000
TV	-5.524866073551	6.279657370223	0.000000000000
TV	-0.915118729678	-3.595487322271	1.949430332274

EQ'-SiO₂ 17

O	-1.017073034090	3.233522481160	-0.893880496950
O	-0.605054582900	-0.558858824912	1.280683921704
O	-5.535311314170	-4.908581923310	0.551966232881
O	-5.176377474293	-2.721250383872	1.279943598695

O	-3.243994985560	-3.831974234155	0.553291075786
O	0.912151270154	2.126218736586	-1.624572547159
O	-2.574801311985	6.478611607842	-0.894128074508
O	-2.162775214067	2.686146917118	1.280682021921
O	-7.093162698899	-1.663236773892	0.552145114469
O	-6.734096832204	0.524181188325	1.279829129979
O	-4.801874200090	-0.586933173309	0.553424976136
O	-0.645545094600	5.371295641459	-1.624544576875
Si	-4.053724371826	0.784881461742	-0.170830931501
Si	-3.644468401871	-3.008748266340	2.004147444037
Si	7.054359489033	-1.927826492609	2.005227064455
Si	-5.202218945426	0.236552720548	2.004178287673
Si	-2.496111253300	-2.459754910858	-0.170791743467
Si	5.496527929157	1.317348978091	2.005198363181
TV	8.412105943072	0.000000000000	0.000000000000
TV	-3.115563609859	6.490488305491	-0.000000000000
TV	-1.875538032269	-4.874119130720	2.176531901966

EQ'-SiO₂ 18

O	-3.268281973371	3.941674853071	-3.281519020799
O	1.370457637693	0.601649045455	-0.752467252249
O	4.239220123388	2.307849123400	-1.404826185999
O	-4.775010229062	7.335838143119	0.409114237870
O	-5.157492284988	0.180137976755	-1.832790332927
O	-0.518779478722	-3.159994191089	0.696374637871
O	2.350029731728	-1.453795236811	0.044002240916
O	-6.664153437151	3.574322901007	1.857927398844
O	-7.046689721106	-3.581413704811	-0.384031880240
O	-2.407930616684	-6.921579675794	2.145160763680
O	0.460854062412	-5.215332224272	1.492704460157
O	-8.553342412855	-0.187219218744	3.306762909067
Si	0.271533687482	-8.785352491040	0.394822226216
Si	1.849649758927	-0.008536818269	0.713115525700
Si	-1.617664133471	-12.546905923519	1.843658325465
Si	-0.039477351486	-3.770130285121	2.161925129931
Si	-3.506772092922	-16.308398298624	3.292446957042
Si	-1.928663130361	-7.531642307687	3.610775925560
TV	4.353322701652	-0.000000000001	-0.000000000003
TV	-3.709278073198	6.488481747958	0.000000000002
TV	-5.667990114457	-11.284778782613	4.346475928636

EQ'-SiO₂ 19

O	-1.643176311559	1.325013823940	-0.337559862773
O	-1.319818275638	-1.017170313042	0.495891721296
O	-4.604700428081	-4.891662609565	1.929121595126
O	-4.999378748147	-2.715685957557	1.215394105939
O	-3.124655175772	-3.863267048885	0.492213505169
O	0.215078882459	0.182313990030	-1.050915464040
O	-2.799334706418	-2.034856913111	1.926344167664
O	-2.475989002820	-4.377044013799	2.759787554052
O	-5.760865128164	-8.251542516956	4.193023312490
O	-6.155524532264	-6.075550969127	3.479302689586
O	-4.280794494247	-7.223143067090	2.756119622953
O	-0.941069734817	-3.177551524522	1.212980005107
Si	-3.431558637997	-5.833866687195	2.579582132041
Si	-2.510988330885	-0.075592525336	-0.172211090481
Si	6.406427161386	-1.683100623608	2.088219064705

Si	-3.667149910455	-3.435461774178	2.091693292533
Si	-2.275403459649	-2.473990495661	0.315686953839
Si	5.250246992810	-5.042970611440	4.352114299448
TV	7.508567513541	-0.000000000000	0.000000000000
TV	-2.383319035948	3.496648050830	0.000000000000
TV	-2.312310470178	-6.719747771034	4.527802952432

EQ'-SiO₂ 20

O	-1.704690613911	2.265609920128	-1.176172535420
O	-0.449820025916	-0.458922618897	0.673599971418
O	-5.446405556351	-4.891706067447	1.011255591186
O	-5.092623532601	-2.617815571782	0.673572796123
O	-3.124995215375	-3.812273273949	1.011260701885
O	0.262955411480	1.071155301257	-0.838514632861
O	-2.771224580098	-1.538389962392	0.673576502565
O	-1.516332369281	-4.262929622357	2.523329651021
O	-6.512877796925	-8.695668689757	2.860983317744
O	-6.159165345678	-6.421792389799	2.523340297297
O	-4.191503902826	-7.616249702967	2.861002592830
O	-0.803579063890	-2.732800976240	1.011232913260
Si	-3.185107831080	-6.736454129648	1.767704242340
Si	-3.778953821815	-2.418708958929	1.767732447751
Si	8.421898313949	-1.339241781388	1.767723076095
Si	-4.845469293653	-6.222708247162	3.617470746649
Si	-2.118612602848	-2.932457564984	-0.082009645560
Si	7.355416708471	-5.143287655645	3.617480023817
TV	9.879482226201	0.000000000000	-0.000000000000
TV	-2.915225637664	3.238288606387	-0.000000000000
TV	-2.133010794283	-7.607984420588	3.699509914952

EQ'-SiO₂ 21

O	-0.924552062819	2.798940683529	-1.137368459944
O	-0.632861331020	-0.466726045616	0.875447353016
O	-5.375624251585	-5.080948559308	0.903759471381
O	-5.144728018635	-2.768757765405	0.875429033090
O	-3.119687214302	-3.929925701210	0.903770171701
O	1.100483275691	1.637766761089	-1.109041951618
O	-2.741200134548	6.251988308592	-1.137376426870
O	-2.449500984015	2.986341342844	0.875434677288
O	-7.192267872071	-1.627890897031	0.903755122975
O	-6.961357645383	0.684295897141	0.875442536368
O	-4.936336224729	-0.476872557451	0.903758956402
O	-0.716158704499	5.090831842397	-1.109050843148
Si	-4.060455487941	0.586162784366	-0.117209500780
Si	-3.768769138478	-2.679477809143	1.895601580404
Si	7.071617915906	-1.528473288184	1.895607344980
Si	-5.585395447790	0.773565169272	1.895605722852
Si	-2.243817598745	-2.866892944374	-0.117195547040
Si	5.254970029840	1.924588351968	1.895599619357
TV	8.584439022035	-0.000000000000	0.000000000000
TV	-3.633276319451	6.906114212168	-0.000000000000
TV	-1.964234636056	-4.416679533331	2.012809115921

EQ'-SiO₂ 22

O	-3.725908613989	1.552960986500	-0.656925164017
O	1.869178298450	-0.711535755139	-0.656814326288
O	-0.354079424514	2.041996365886	-0.656804796390

O	-2.015250555450	2.928963627894	0.607969844701
O	-5.437089961239	0.175435406270	0.607956740640
O	0.158112934902	-2.089319725477	0.610545984757
O	-2.065117292495	0.664193922133	0.610554290710
O	-3.728429501921	1.548893793324	1.874841816250
O	-7.150271369841	-1.204625851906	1.874868586496
O	-1.555446928510	-3.466935430984	1.876469528872
O	-3.778687986704	-0.713391477457	1.876486371736
O	-5.438150054312	0.172844953097	3.141406356482
Si	3.007189424615	-0.956612291704	-1.922718387492
Si	-0.929349977855	0.421244664021	-0.656809508247
Si	1.293888255563	-2.332267811761	-0.656795712352
Si	-2.640804195784	-0.956562027127	0.609631283393
Si	-0.417560367169	-3.710071692094	0.609629194425
Si	-4.350182382912	-2.336717018625	1.875637592467
TV	5.645095199913	-0.000000000000	-0.000000000000
TV	-4.446477571277	5.507055380528	0.000000000000
TV	-5.134117625806	-4.133640819725	3.798334069892

EQ'-SiO₂ 23

O	-0.752789012980	0.431726737183	-2.139594325030
O	0.520447344434	-1.541513302894	-1.188296222935
O	0.517962909361	0.560756274124	-0.218924817611
O	-3.310827042842	6.718001934947	0.734553412369
O	-2.026893225580	-1.541511408409	-1.188294459128
O	-0.755149903890	-3.530133043567	-0.250058903811
O	-0.755941501655	-1.449263064337	0.734550398457
O	-4.583936994558	4.734289431548	1.673188542216
O	-3.302475114251	-3.530136928590	-0.250064569473
O	-2.027415755671	-5.538161461954	0.707783793636
O	-2.029058342993	-3.432965072097	1.673192029875
O	-5.858884844620	2.758105984611	2.628468276505
Si	1.792810219987	-0.492681587474	-0.693712957249
Si	-0.754528110621	-0.492682070324	-0.693718570823
Si	0.518108791778	-2.489817665323	0.240519451753
Si	-2.029231356692	-2.489814019893	0.240522369304
Si	-0.754760064913	-4.483625613892	1.181833249263
Si	-3.302095200590	-4.483621893532	1.181837779421
TV	5.094673484066	0.000000000000	-0.000000000001
TV	-5.102218810523	8.167257199027	-0.000000000001
TV	-3.821977723534	-5.969890395362	2.847377081349

EQ'-SiO₂ 24

O	-1.269282636266	2.496891893536	-1.481432811110
O	0.412913149801	0.379363990163	-1.479683527651
O	3.730358669472	2.218622158775	-3.138293587021
O	-4.665212483418	7.995756425949	0.177861295101
O	2.038964814930	2.496087436754	-1.483704780999
O	3.744767024692	0.378608104076	-1.478327941887
O	7.063428927651	2.217193057128	-3.137904408988
O	-1.328111906883	7.987756552447	0.180887335153
O	5.396657500478	2.495043241606	-1.479313442627
O	7.072171369574	0.378545242352	-1.478840705208
O	10.395073258158	2.220792918513	-3.155305327949
O	2.005055269535	7.995729756701	0.187755327759
Si	0.499347661242	-8.657279932147	1.841110591490
Si	0.398304612424	0.519634913572	0.182362460952

Si	3.831660984234	-8.660244341828	1.839440115664
Si	3.737458421166	0.519782935263	0.182204114136
Si	7.167389764430	-8.656809899055	1.839667853508
Si	7.070611105197	0.519980092487	0.182883319905
TV	10.004645784288	-0.000000000003	-0.000000000009
TV	-3.398232385834	7.334719150376	0.000000000002
TV	-1.630565040555	-3.671770341237	1.664063756123

EQ'-SiO₂ 25

O	0.110893676807	3.694889203730	-1.359095468143
O	-1.322834942150	-0.743775285098	-0.149700905263
O	-7.590603864642	-5.810163616804	3.305944474775
O	-6.075306926400	-3.254419600105	0.374369873768
O	-6.864976689777	-5.431845886187	0.874673747796
O	3.495556400057	1.731560408447	-0.391219991646
O	-1.463287035664	6.592712654763	-1.358884307562
O	-2.897081557196	2.154087569112	-0.149782481678
O	-9.165046505915	-2.912400525528	3.305863595382
O	-7.649557452929	-0.356352425634	0.374448273608
O	-8.439410033770	-2.533602956930	0.874457187335
O	1.921264314900	4.629654772040	-0.391284644499
Si	-4.892697081556	0.201751827468	0.121160658785
Si	-1.905829474771	0.812822386733	-0.040050467499
Si	9.141573561208	-2.722749967554	2.240625594822
Si	-3.480141063477	3.710401256518	-0.039936336336
Si	-3.318344524600	-2.696508641152	0.121354537538
Si	7.567341400207	0.175329990680	2.240364626416
TV	10.634568777415	0.000000000024	0.000000000003
TV	-3.148606747862	5.795945124683	-0.000000000060
TV	-3.485791101478	-3.700717981460	1.974703020947

EQ'-SiO₂ 26

O	-2.546152938824	3.892624383123	-0.786482923699
O	-0.872896279261	-0.153156103625	1.321383670704
O	-5.575210663711	-4.402600410166	0.316033816300
O	-5.284715710329	-2.265814894328	1.282427229460
O	-3.352899402033	-3.397363292844	0.222280850697
O	-0.737667139178	2.680282758837	-1.726705347239
O	-5.286725298831	7.048631377430	-0.786488101576
O	-3.613448968229	3.002839972184	1.321352936898
O	-8.315782784242	-1.246551994874	0.316046654557
O	-8.025280293611	0.890207438362	1.282420347207
O	-6.093481828924	-0.241346697026	0.222286518515
O	-3.478224677768	5.836302354688	-1.726729120116
Si	-5.488658932242	1.272016513138	-0.204200289937
Si	-0.031774570294	-7.760265246200	2.697867768782
Si	7.840299096976	-1.653777393280	1.863402903865
Si	-2.772331931211	-4.604243075820	2.697880292802
Si	-2.748108373070	-1.883976013698	-0.204200558515
Si	5.099726040649	1.502245179058	1.863392211736
TV	9.350060382690	0.000000000000	-0.000000000000
TV	-5.481133555886	6.312052341614	-0.000000000000
TV	-0.450841600589	-5.015079731405	2.050153003129

EQ'-SiO₂ 27

O	-1.009534910093	-2.380091465481	-3.617747365315
O	-1.671589254808	-1.161896585776	1.622437891999

O	2.709463715275	1.381842050875	1.622444922498
O	-0.974361714833	0.133749308474	-0.098459028412
O	0.479580566714	0.139879148780	-1.896866131976
O	-3.204235217981	-1.108220481201	-3.617744776130
O	-0.970208537720	-2.409995633268	-0.098456068539
O	-1.632241962615	-1.191797490857	5.141730358229
O	2.748803254835	1.351942735672	5.141726588875
O	-0.934996601547	0.103826677172	3.420843780085
O	0.518929140236	0.109973032416	1.622434345921
O	-3.164887064365	-1.138128142554	-0.098457484163
Si	-0.164724794308	-1.197260264858	6.040540090708
Si	-0.247587687138	1.406278616062	-0.998058760721
Si	-2.438111535332	0.134416360083	-0.998051497251
Si	-0.208227092903	1.376369538465	2.521248399786
Si	-0.204068953921	-1.167363737509	2.521245446994
Si	-2.398753538043	0.104506549868	2.521241626360
TV	4.385204123321	0.000000000001	-0.000000000001
TV	2.186359122032	3.815602783786	0.000000000001
TV	0.078694024611	-0.059805743649	7.038591334024

EQ'-SiO₂ 28

O	-2.863538679563	1.999089232767	-0.649918758724
O	1.205194252752	-1.364475815423	-0.653278595303
O	-0.580007551274	2.015703470415	-0.653258895543
O	-1.464216645960	3.686552422914	0.616585491208
O	-4.275810090868	0.306386794649	0.616592506942
O	-0.206532622435	-3.056139760875	0.614797378277
O	-1.991713625740	0.324024580726	0.614795578432
O	-2.873798546392	1.995263302645	1.885247517715
O	-5.685409602565	-1.384919911648	1.885250928900
O	-1.616652240763	-4.747647254252	1.880821173763
O	-3.401841460802	-1.367466117599	1.880802985621
O	-4.280654561614	0.306528975266	3.151725016830
Si	2.364257164023	-1.373552505028	-1.918981165596
Si	-0.832851435901	0.317585841206	-0.651773840129
Si	0.952332268120	-3.062582422818	-0.651788308689
Si	-2.239597586747	-1.375528497464	0.615411908603
Si	-0.454410625511	-4.755693671321	0.615419385458
Si	-3.649690110469	-3.066110865207	1.882664007534
TV	4.596806813989	-0.000000000000	0.000000000000
TV	-3.570383895656	6.760347969918	0.000000000000
TV	-4.228744945043	-5.072737433805	3.801643051250

EQ'-SiO₂ 29

O	-3.225060820312	5.376406478832	-0.107423650144
O	-0.951469079797	-0.258081060926	1.648868956165
O	-5.330088064541	-4.527098025747	0.032522853535
O	-4.945373175716	-2.908845989699	1.648832662003
O	-2.045290415505	-5.171899333030	0.048829703207
O	1.031808340617	1.108934593596	-1.724025202145
O	-5.837448643044	9.331207780877	-0.107384729648
O	-3.563887908221	3.696898364080	1.648820390145
O	-7.942382689551	-0.572445203803	0.032634925149
O	-7.557863770855	1.045955128511	1.648924032179
O	-4.657748310281	-1.216805074945	0.048744743430
O	-1.580633712817	5.063887120693	-1.724089981043
Si	-4.277478105307	0.424299321651	-0.036725242368

Si	-2.052580933009	-5.228831497757	1.736372008597
Si	6.060649439584	0.078838236572	1.738658530544
Si	-4.665073428029	-1.273758516756	1.736308855632
Si	-1.665026552838	-3.530805020891	-0.036651055296
Si	3.448229003105	4.033565151938	1.738751060966
TV	8.634714867159	-0.000000000002	0.000000000000
TV	-5.225016409472	7.909846515440	0.000000000010
TV	-1.047214040547	-4.976560573513	1.774627874861

EQ'-SiO₂ 30

O	-2.517375272842	2.069587035069	-2.418468257133
O	1.736022951064	0.873022663936	-0.623255059866
O	5.065785861692	1.493527345241	-1.518774968077
O	-6.397441764465	6.522527396832	0.266662305784
O	-5.181230940011	-0.814626996471	-1.234904585445
O	-0.927840784004	-2.011194249371	0.560364501149
O	2.402069660408	-1.390637269324	-0.335185575789
O	-9.061312694534	3.638321156599	1.450097323424
O	-7.845081449452	-3.698936202232	-0.051375234629
O	-3.591612129663	-4.895279870524	1.743963045257
O	-0.261769894977	-4.274850290768	0.848357393603
O	-11.725133423586	0.754060002833	2.633677685090
Si	-0.397477780697	-5.798717282417	-0.130209412735
Si	2.518464716806	0.104501676958	0.636721076053
Si	-3.061268739087	-8.682922371036	1.053368994712
Si	-0.145372457413	-2.779783370056	1.820307542407
Si	-5.725102104074	-11.567116661549	2.236962731055
Si	-2.809223574386	-5.663981171898	3.003881652975
TV	5.439380789399	-0.000000000001	-0.000000000003
TV	-4.973545388261	6.229751638537	0.000000000002
TV	-7.991628717165	-8.652704028112	3.550772549538

EQ'-SiO₂ 31

O	3.979385966187	-1.508564117641	-0.159473659604
O	0.747487093497	-1.048366568138	2.217978749744
O	0.517823111073	0.665173480760	0.596440945782
O	2.911457836600	-0.147449692778	1.462429599933
O	2.681075834383	1.566444770961	-0.159465955918
O	-0.550822092804	2.026644733882	2.217980734441
O	-0.780478322096	3.740185308990	0.596448717187
O	1.613146150387	2.927582521970	1.462431254935
O	1.382774592485	4.641450738308	-0.159468279414
O	-1.849119785843	5.101655343582	2.217979310314
O	-2.078781807827	6.815193849190	0.596440514885
O	0.314849053269	6.002564997480	1.462424669806
Si	3.434804110198	0.075131258598	-0.105824366532
Si	-0.007637248058	0.443981000940	2.165045861390
Si	2.136502856809	3.150140304117	-0.105820710054
Si	-1.305942412467	3.518991006790	2.165053624799
Si	0.838202646303	6.225146211565	-0.105824365998
Si	-2.604246454084	6.594000034271	2.165044236533
TV	4.336797548505	-0.000000000000	0.000000000000
TV	-3.894913050326	9.225025222813	-0.000000000000
TV	-1.275442946979	-0.527108744111	3.028270047931

EQ'-SiO₂ 32

O	1.505697914244	1.225318756075	-0.497298904704
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O	0.159178375891	-0.877615114604	-0.819018418942
O	-7.148045654456	-3.043101542021	3.236775026047
O	-5.562030202058	-2.254853532898	1.712330379422
O	-6.509529621576	-4.168702589634	1.028999693888
O	1.766036637365	-0.090514437675	-2.344947273224
O	0.352648814497	3.529030013113	-0.497106862271
O	-0.994329368724	1.426196153850	-0.819081267564
O	-8.301577850060	-0.739189785367	3.236683966218
O	-6.715569673602	0.049127737510	1.712237911767
O	-7.662869653838	-1.864890703544	1.028953324477
O	0.612485932264	2.213428578878	-2.345070830980
Si	-3.898227891898	-0.005543278475	-0.321151599220
Si	-1.216743694289	-0.119988908400	-0.107797579039
Si	6.995838662958	-1.810443446008	3.063030278782
Si	-2.370158079524	2.183876315972	-0.107968863862
Si	-2.744724909982	-2.309318756939	-0.321193188249
Si	5.842142380552	0.493296178495	3.063238033261
TV	8.736347019024	-0.000000000000	0.000000000000
TV	-2.306856336746	4.607691506584	-0.000000000000
TV	-3.201361317660	-1.573503921336	2.948290709601

EQ'-SiO₂ 33

O	-0.658107472474	2.967894209190	-0.342671446690
O	-0.570858336412	-1.050051088771	0.648252621180
O	-6.705207908279	-6.689096654788	1.745434492664
O	-6.719026771795	-2.409255298152	0.977236474046
O	-3.631942662435	-3.934859675318	1.134068504254
O	0.555600095153	1.308161938369	-1.440936147255
O	-2.784348169163	6.617981067090	-0.342635911425
O	-2.697092944978	2.600056408281	0.648283613142
O	-8.831512222962	-3.039097979019	1.745531686520
O	-8.845272346670	1.240878512630	0.977216705400
O	-5.758104914386	-0.284813924824	1.134140368528
O	-1.570628581671	4.958275570529	-1.440926995156
Si	-5.201121785937	0.959003215999	0.152459042427
Si	-2.162129217413	-0.393377082135	0.442327482275
Si	8.033588251423	-2.300614822531	1.669696168380
Si	-4.288375298632	3.256703328316	0.442362293651
Si	-3.074871666378	-2.691074231688	0.152409581268
Si	5.907363863748	1.349478131343	1.669720327283
TV	9.174916647289	-0.000000000000	-0.000000000000
TV	-4.252475963778	7.300215036068	0.000000000000
TV	-2.075430368232	-4.612375150959	1.806449646197

EQ'-SiO₂ 34

O	2.907409020135	-3.102069999244	0.295818861539
O	-0.555325864621	-1.270305033780	1.958897581275
O	0.270283113424	0.876571238810	1.217558767213
O	2.410416422679	0.580676418648	2.282446476231
O	2.192388775848	1.047631315604	0.042878157864
O	-1.175263432382	2.600295636563	1.675865455346
O	-0.414503401958	4.994707278733	0.902422451239
O	1.691860683788	4.553434289996	2.215581532800
O	0.955466402148	3.143825760161	0.578893157131
O	-1.890198025375	6.749923134001	1.422818177939
O	-1.133047273075	8.967500983532	0.835558448742
O	0.523420388253	6.578878800584	2.597532828301

Si	4.191254724932	-2.829750566934	-2.073690654141
Si	-0.458755722681	1.289110375125	2.655355035541
Si	2.925659682540	0.631292029081	-1.399849317567
Si	-1.149125627676	4.160888368986	2.066363079754
Si	2.309782662114	4.414884767297	-1.484707585530
Si	-2.414613745945	7.621796905062	2.740078428576
TV	4.335746934995	0.000000000000	-0.000000000000
TV	-2.571812888251	10.116431532884	0.000000000000
TV	-1.257689067996	1.288280216024	2.760041758404

EQ'-SiO₂ 35

O	-1.637357464601	1.353293727419	-1.347620338854
O	-0.002445056247	-0.577603788269	-0.937031518159
O	-0.011306576514	1.430652828510	0.200308092976
O	-1.639352277567	3.362134989010	-0.218400740059
O	-1.634243714598	0.057173867578	0.923199949745
O	-0.000558736952	-1.873006528313	1.333020378818
O	-0.008838138559	0.135749547887	2.469262838245
O	-1.637310758070	2.066211984564	2.058906172243
O	-1.632089333373	-1.238406667525	3.193809251292
O	0.003135209045	-3.169191650008	3.611405054364
O	-0.006188876067	-1.159007338301	4.740725147207
O	-1.632559184878	0.770228559641	4.329037432276
Si	1.625194831422	-2.108792734725	-1.805508887550
Si	-0.009703562137	-0.432146663847	0.649567408341
Si	1.627693338235	-3.401369229591	0.471149600362
Si	-0.008269667270	-1.732395050223	2.920644538123
Si	1.629964012449	-4.701256084934	2.741831917976
Si	-0.005104374761	-3.024848670000	5.198052920004
TV	3.249294695043	0.000000000001	-0.000000000002
TV	-3.263553196693	5.325799090223	0.000000000001
TV	0.008062574306	-3.886146263975	6.820991897105

EQ'-SiO₂ 36

O	-1.399091551351	1.095973965588	-0.661331854154
O	-0.996071510564	-1.168498033190	0.248346640371
O	-4.356862449327	-4.903715609712	2.522037518652
O	-4.713310917733	-2.567576305249	1.609920983448
O	-2.862734575549	-3.950258515351	0.707568915465
O	0.357317113363	-0.248847529991	-1.432568234699
O	-3.603777972986	4.678148352144	-0.661596011143
O	-3.201044777492	2.413945178261	0.248022656186
O	-6.562049767873	-1.321422332020	2.522157602213
O	-6.917856898304	1.014227774137	1.610561379435
O	-5.067491439691	-0.367898969628	0.707437144069
O	-1.847340743223	3.333517109417	-1.433428118056
Si	-4.132632875371	1.053450206979	0.450678595716
Si	-0.213874453512	0.281116612352	0.190010432666
Si	2.560306060389	-1.176497848943	1.351498070236
Si	-2.418613849667	3.863369575678	0.189624057413
Si	-1.927711584315	-2.528940430000	0.451195988987
Si	0.355310954569	2.405451093238	1.351833093717
TV	6.304622568739	0.000000000000	0.000000000000
TV	-4.409840364217	7.164330858424	0.000000000000
TV	-1.024988542725	-3.079718751091	2.664202748220

EQ'-SiO₂ 37

O	0.144823066592	0.755542926133	-0.558912176236
O	-0.592474857131	-1.381890102942	-0.036782089512
O	-7.257373152526	-4.933487949538	2.355250389579
O	-6.491011262935	-2.725346615332	1.666543885757
O	-5.286068628114	-4.753174428352	1.144352575418
O	1.379548559644	-1.201534769497	-1.246576712401
O	-0.323078001399	4.921031037488	-0.558938881496
O	-1.060442607692	2.783612895615	-0.036783938699
O	-7.725343562932	-0.768000598516	2.355264763280
O	-6.958962579337	1.440152327707	1.666552475950
O	-5.754021919903	-0.587673214223	1.144332790182
O	0.911573417330	2.963938016014	-1.246541950895
Si	-3.406684367116	1.097718713954	0.553922441138
Si	-0.275301885810	0.021003106923	0.907294567971
Si	7.599404083108	2.174083162556	0.200899530534
Si	-0.743189331589	4.186493674080	0.907288691431
Si	-2.938733130109	-3.067773585618	0.553947322984
Si	7.131514777627	6.339550829190	0.200855175595
TV	7.069196256052	-0.000000000006	0.000000000001
TV	-0.935867128116	8.330972147234	0.000000000004
TV	-2.771227930315	-2.470439416099	2.051257527799

EQ'-SiO₂ 38

O	1.035553304762	3.280580709191	-1.214442755815
O	0.938006892764	-0.917418733070	0.038039914641
O	-5.483199157261	-6.175983305640	2.998784575281
O	-3.514334935431	-3.457688656207	2.239870706094
O	-3.604067957525	-5.995439572203	1.927388284732
O	1.356292557524	0.570767107619	-1.789886633146
O	-1.138111263134	6.968824656820	-1.209351101087
O	-1.227762384415	2.784667191009	0.037738910005
O	-7.657683436430	-2.476968843422	2.987385388226
O	-5.675647371423	0.241707994883	2.245771970268
O	-5.768497055352	-2.298453007820	1.929508954979
O	-0.813694731061	4.269829595600	-1.783529288229
Si	-4.337013288533	0.404228899016	-0.301397867522
Si	-1.907167030078	1.921077890282	-1.498989408103
Si	-0.404127610663	-1.071454961233	2.585023830387
Si	-4.076878611356	5.619992593030	-1.501001950495
Si	-2.168966859363	-3.296846141097	-0.303129236754
Si	-2.572084129583	2.627401014385	2.584184567081
TV	6.201909153238	-0.000000000000	-0.000000000000
TV	-4.330372171308	7.397028001931	-0.000000000000
TV	-2.480531075262	-4.107431314997	2.637442809471

EQ'-SiO₂ 39

O	-0.188290261097	3.127975728356	0.270442344469
O	-0.833419122482	-0.974815788038	1.306197600091
O	-8.812882557155	-5.076381407522	-0.117118199001
O	-5.713209429219	-3.521493669995	1.062817427028
O	-3.869222545221	-2.497800484249	0.094042383685
O	1.176775227659	1.935154957660	-1.222676968529
O	-1.789354803227	6.081099629976	0.270404869698
O	-2.434173699419	1.978475502682	1.306295522303
O	-10.413959445870	-2.123269400283	-0.117115164402
O	-7.314330754508	-0.568384442989	1.062763197319
O	-5.470253408659	0.455177572651	0.094047171912

O	-0.424285117702	4.888292216621	-1.222641840190
Si	-4.029695026075	1.120467246391	0.454475037330
Si	-4.205943830699	-2.703133877254	1.730872351280
Si	10.876431708180	-2.498783694483	1.406885929257
Si	-5.807027601304	0.249953938103	1.730887259976
Si	-2.428590241870	-1.832617392330	0.454517312741
Si	9.275340272593	0.454378085656	1.406872625480
TV	11.000128942978	0.000000000000	0.000000000000
TV	-3.202110810515	5.906219428384	-0.000000000000
TV	-2.619998086206	-5.139195630360	1.867436514065

EQ'-SiO₂ 40

O	-1.988265678864	2.603691791068	0.171020482419
O	0.636549379325	-1.039378169406	-0.505646211506
O	1.948355639036	-2.133080929890	-1.967580358098
O	-3.298866780212	8.967999729444	-0.188099486068
O	-3.306052605637	1.438659917896	2.017621043782
O	-0.676237679931	-2.208400341494	1.336994354075
O	0.635252776299	-3.299510578479	-0.125594117257
O	-4.614480793514	7.798955527197	1.652070740725
O	-4.619543505942	0.272990056701	3.858426868000
O	-1.992587873502	-3.373147773521	3.181425995289
O	-0.680396155688	-4.465018856611	1.716603601367
O	-5.928078004779	6.634994187011	3.493732683642
Si	1.948540783968	-4.416840778566	0.024998122403
Si	0.636922508831	0.477531579536	-1.264111436925
Si	0.630370566350	-5.583218288874	1.867886602573
Si	-0.678111121831	-0.690972819014	0.577141337055
Si	-0.682816891581	-6.748031828220	3.711894130454
Si	-1.990663617771	-1.857830925576	2.418846201290
TV	2.624495434396	-0.000000000001	-0.000000000003
TV	-2.624717745861	8.149711423713	0.000000000002
TV	-3.943699614026	-3.497951662490	5.527842012471

EQ'-SiO₂ 41

O	-0.426952011993	3.146105333751	-1.496792718664
O	-1.007233385000	-0.295341713075	1.684612770579
O	-5.302434138204	-3.653615556188	1.217554460559
O	-5.955167972748	-2.369096761458	-0.536259889971
O	-3.241436643452	-4.886697361792	1.129313774726
O	2.727701569359	2.599913684661	-1.443996917416
O	-2.206031562513	6.826905990439	-1.496776852391
O	-2.786302790692	3.385403415778	1.684713609763
O	-7.081437561671	0.027154955374	1.217564969946
O	-7.734243999088	1.311657217846	-0.536255691051
O	-5.020387697514	-1.206105166620	1.129484038601
O	0.948566376856	6.280683606797	-1.443949919995
Si	-4.052776448462	-0.316290408703	0.131850868517
Si	-4.067099016936	-4.110730230990	2.352954504202
Si	6.350468887419	-1.718966812084	1.946597352969
Si	-5.846102390789	-0.430019655325	2.352989027184
Si	-2.273692131775	-3.996987167365	0.131776936245
Si	4.571397164936	1.961813896390	1.946588536643
TV	8.475864978168	-0.000000000000	-0.000000000000
TV	-3.558150354360	7.361542498344	0.000000000000
TV	-2.253874021729	-4.426984593895	1.948043354181

EQ'-SiO₂ 42

O	-0.909920187103	1.369281123283	-0.998347097359
O	0.329916991056	-0.528285736178	-0.988886474874
O	0.398734325732	2.648361561246	0.392100640748
O	0.450042937476	4.837077575528	-0.311318869570
O	1.628984664597	1.367887501844	-0.999319371366
O	2.875025621970	-0.529677986133	-0.986561768750
O	2.936253085951	2.645047554427	0.386855333666
O	2.997175923822	4.835685093397	-0.309773446469
O	4.170023096052	1.369688663671	-1.001554724952
O	5.414046039070	-0.527663302219	-0.988402968635
O	5.484883601102	2.643142094373	0.390594015091
O	5.532120141881	4.831531979386	-0.314134535185
Si	0.263220813594	-2.897120871884	-2.029213824280
Si	-0.966072391687	-0.014391716267	0.038959294064
Si	2.805750009953	-2.893825859609	-2.027661270404
Si	1.575215204025	-0.016852402445	0.038707993509
Si	5.347682050857	-2.902322570215	-2.030704893173
Si	4.119167289691	-0.013609607378	0.040027847270
TV	7.626987938008	0.000000000000	-0.000000000000
TV	0.240564625209	7.509061143378	0.000000000001
TV	-1.350593291621	-0.870845628654	2.067961769187

EQ'-SiO₂ 43

O	-1.301360179814	1.272973530575	-1.187857153902
O	-0.009419676109	-0.594988170377	-0.828059852105
O	-0.067279116426	2.764870131447	-0.059962483772
O	-1.357469518894	4.633920826616	-0.421291153747
O	1.231734244226	1.269818703366	-1.185144683128
O	2.536922117158	-0.591742437290	-0.830160306043
O	2.478494092449	2.761131894853	-0.059544620054
O	1.178837102570	4.625710122198	-0.416591400487
O	3.780469468654	1.274977075379	-1.185808189958
O	5.080038851788	-0.587519558720	-0.829218110622
O	5.025955202818	2.772201255287	-0.062032969342
O	3.718560130381	4.627955715683	-0.414467783928
Si	-0.084335343277	-3.126688210694	-1.333110302480
Si	1.288883932606	0.093297891757	0.085456022589
Si	2.457451597673	-3.138664674848	-1.334754765533
Si	3.831193714258	0.099422455647	0.087087093933
Si	5.000199420834	-3.136288096172	-1.332440313852
Si	6.375269970229	0.101886490619	0.088045144086
TV	7.626670651957	0.000000000003	-0.000000000006
TV	-2.573480404601	7.076026145407	0.000000000001
TV	1.350803508945	-0.479772393398	2.191352174238

EQ'-SiO₂ 44

O	1.046741690546	0.744074122836	-0.389263698267
O	-1.337880146195	-2.996083747875	0.039987566167
O	-5.525993953303	-4.219101125877	1.705467894166
O	-4.771925171309	-1.095492627778	0.693290978945
O	-3.545590009621	-2.916424067863	0.878447000789
O	0.110329058283	-2.270249453316	-1.669922512124
O	-1.685821046510	-2.108222289155	1.945770817141
O	-4.065218154883	-5.844294100635	2.383100525333
O	-8.251344601261	-7.077678665716	4.044916773638
O	-7.503741420955	-3.951479840276	3.032440790927

O	-6.271236958130	-5.769229113633	3.210401022049
O	-2.616829574240	-5.122654536436	0.668586892757
Si	-4.969252319602	-6.599508967453	3.768608233660
Si	0.527358351607	2.649609087302	1.301991548082
Si	2.091558809406	-1.294583031006	1.020478190037
Si	-2.194857234063	-0.206039027879	3.643292141763
Si	-2.243756082452	-3.745684995806	1.432803058545
Si	-0.628013767205	-4.150458847861	3.359309084763
TV	4.914270164033	0.000000000000	0.000000000000
TV	0.719601419687	5.247309056450	0.000000000000
TV	-5.457864957295	-5.706380329581	4.676678958958

EQ'-SiO₂ 45

O	-0.391238608272	2.188504842066	-0.213336097210
O	1.149246849272	1.560894428067	1.511921105803
O	-5.623556378099	-3.145517778582	0.979289453934
O	-8.934330557179	-3.574582493273	0.242108804006
O	-3.698265946601	-4.316922801651	0.520964414972
O	1.786656830868	0.941466592480	-0.749484445181
O	-2.715963309551	5.651691502056	-0.213355018587
O	-1.175873973052	5.023730955699	1.512396740701
O	-7.947780826956	0.317275648780	0.978670528998
O	-11.258764059346	-0.112252968747	0.242519957149
O	-6.023535280877	-0.854176669012	0.520518469452
O	-0.538143025757	4.404952817311	-0.749066980982
Si	-5.690450908613	0.238187563401	-0.630749405118
Si	-4.552142732855	-4.023609367253	1.931168754241
Si	10.952015536687	-1.200976934400	1.394083251177
Si	-6.876975037212	-0.560923995077	1.931073545529
Si	-3.365191514658	-3.224964895995	-0.630681756557
Si	8.627317276361	2.262512297711	1.393927538118
TV	11.274977649234	-0.000000000000	0.000000000000
TV	-4.649953267835	6.925365625537	0.000000000000
TV	-1.547634089980	-3.544457721355	1.548606237834

EQ'-SiO₂ 46

O	-1.703882450492	4.560317421569	1.206038823737
O	-0.389897878454	-2.367015153623	-1.619109575087
O	0.280242683465	-0.201965744203	-0.979739201504
O	-0.568300541471	3.689555694654	-0.612480978150
O	-3.435203464510	3.260296235855	2.485518563928
O	-2.121221698005	-3.667005192285	-0.339651491460
O	-1.451079077343	-1.501955905395	0.299722266701
O	-2.299661664608	2.389525838671	0.667003636023
O	-5.166507961474	1.960300776427	3.764976341329
O	-3.852538979353	-4.967015021328	0.939815301152
O	-3.182405406164	-2.801978006894	1.579187781736
O	-4.030956371011	1.089508099092	1.946473853656
Si	1.948794956789	-0.563154482005	-1.573215261750
Si	-1.386086092887	0.158669506779	-0.392119507310
Si	0.217505296394	-1.863173974857	-0.293728456079
Si	-3.117408349700	-1.141306654645	0.887363010493
Si	-1.513842453975	-3.163169183787	0.985743259563
Si	-4.848741491789	-2.441339481644	2.166845814317
TV	5.496733486257	-0.000000000000	0.000000000000
TV	-2.433912678456	5.627194171435	-0.000000000000
TV	-5.193951702014	-3.900032936364	3.838426375830

EQ'-SiO₂ 47

O	-1.072612595568	4.034746807231	-0.521504054517
O	-1.050419597083	-0.003126870619	-0.679967634266
O	-4.635222079278	-6.038218485561	2.871264340440
O	-4.814152490137	-4.076307928502	1.446457931409
O	-3.588296629364	-6.032339751604	0.839501116021
O	0.073405777503	2.076346685871	-1.400554403155
O	-2.284364231741	-0.027091365870	1.557802435304
O	-2.262425587005	-4.064597650088	1.399356696862
O	-5.847173717490	-10.099510376487	4.950810589601
O	-6.026246499370	-8.137962914054	3.525936309803
O	-4.800305778138	-10.094328487789	2.918925456517
O	-1.138417082634	-1.985248849609	0.678715261137
Si	-3.531221587576	-7.081321404651	2.159064139324
Si	-2.310325439617	-0.690198417009	0.077853084793
Si	6.084953751470	-1.320544511856	2.157909775236
Si	-3.522282833077	-4.751570073734	2.157323033599
Si	-2.319278214741	-3.019524902855	0.079823998587
Si	4.872768144291	-5.382108198994	4.237260831903
TV	7.199391943075	0.000000000000	-0.000000000000
TV	-2.387633961719	4.045084753040	-0.000000000000
TV	-2.424127729238	-8.123399532177	4.158783687083

EQ'-SiO₂ 48

O	0.767160297618	3.171065595293	-0.939809617149
O	1.487249940663	-2.480595567972	-0.506233214183
O	-7.204285662162	-4.680804802783	3.295811303999
O	-4.289603469051	-3.427972005006	0.756465048608
O	-5.041314946025	-5.752844227356	1.243890757378
O	0.587665670852	-0.263971869631	-1.180855810665
O	-1.371625538236	-0.188354269355	1.041575162666
O	-0.661017786590	-5.829945442210	1.470489741933
O	-9.342641401573	-8.050630404921	5.275806456965
O	-6.441703141452	-6.775736367902	2.735972918767
O	-7.188047505454	-9.088149752215	3.228208454411
O	-1.564032065637	-3.610214642929	0.796862472166
Si	-3.721508478467	-6.982902890736	1.135262212972
Si	-3.283055897598	2.144301659404	0.978250704398
Si	4.733931280740	-0.195469192968	2.069108867813
Si	-5.423867839433	-1.219756189758	2.951130033288
Si	-1.587075135679	-3.617291109590	-0.843530440726
Si	2.604107937614	-3.555090967857	4.046518640547
TV	7.562400151488	-0.000000000000	-0.000000000000
TV	-2.112077457179	4.030227079350	-0.000000000000
TV	-4.285618639685	-6.712197833189	3.951812090015

EQ'-SiO₂ 49

O	-1.219699682192	2.303373880707	-1.281533309396
O	-1.370770094607	0.191158913094	1.271257465994
O	-4.501309039466	-3.955339752212	1.102438420437
O	-5.926004095098	-2.371633379560	0.355723652426
O	-2.042745498274	-3.833808983091	0.839812693245
O	1.101321893305	2.339630015845	-1.568678112333
O	-3.939201887942	5.604349280454	-1.281512586281
O	-4.090256384307	3.492156986899	1.271219147626
O	-7.220844544026	-0.654379522957	1.102467276712

O	-8.645517601669	0.929311641180	0.355745765993
O	-4.762290380699	-0.532840359949	0.839755396219
O	-1.618168881982	5.640611934929	-1.568729511092
Si	-5.106529515497	0.354083639825	-0.534504192269
Si	-4.122008233022	-4.108178331953	2.736862725113
Si	6.924013167335	-2.614133872137	2.064612013197
Si	-6.841528152316	-0.807224677246	2.736890193645
Si	-2.387044130560	-2.946878279069	-0.534463529001
Si	4.204472971612	0.686863306169	2.064605350204
TV	9.186592333912	-0.000000000000	-0.000000000000
TV	-5.439043447612	6.601939530693	0.000000000000
TV	-1.162967841815	-3.980322178545	1.973180626551

EQ'-SiO₂ 50

O	-1.092886673892	0.026111793226	-1.581500108965
O	-0.364879999980	-1.447897136750	0.087715614412
O	-3.520309781237	-3.302053341413	2.790231322366
O	-4.426188598519	-1.280290781160	2.224166810317
O	-3.214492833413	-3.198238331553	0.525703963855
O	0.100145171067	-2.006279719211	-2.186332160144
O	-2.032640699380	-1.810618212552	1.753270730340
O	-1.304636004597	-3.284625218829	3.422485329878
O	-4.460067003614	-5.138796831161	6.125011430909
O	-5.365932825947	-3.117026842578	5.558938413669
O	-4.154244187537	-5.034966803580	3.860477555551
O	-0.839618731743	-3.843007432276	1.148438121140
Si	-2.446435074484	-4.457801805441	3.660027056059
Si	-1.218767478969	-0.380993237322	1.506586923166
Si	1.073978010294	-1.506252297466	0.891808936319
Si	-2.158514337022	-2.217730720811	4.841357558983
Si	-1.506680266689	-2.621066204300	0.325257239606
Si	0.134223759870	-3.342982596058	4.226569391793
TV	4.559622004948	0.000000000000	-0.000000000000
TV	-1.981872676611	3.965739390187	-0.000000000000
TV	-1.879509751810	-3.673465797032	6.669539095257

EQ'-SiO₂ 51

O	-2.582950411072	-2.667069878699	-1.852363340321
O	0.773178844117	-0.612774123848	-0.054916019960
O	-0.900093363537	-0.831606844779	-1.733973244984
O	-0.910073586775	-2.402916222244	0.101912451710
O	-0.907260677921	-0.696188635748	1.692957848307
O	-0.899510651634	0.990546774039	-0.197098082392
O	0.763391656874	-2.667066858965	-1.852362694740
O	4.119501517176	-0.612785088955	-0.054906873542
O	2.446231531906	-0.831614165211	-1.733987576374
O	2.436257678154	-2.402915054212	0.101924454201
O	2.439057900059	-0.696192470678	1.692960146534
O	2.446813589583	0.990546236953	-0.197105762680
Si	4.120004149252	-1.066526896887	-1.636251908173
Si	-0.910279198533	-3.994844874842	-0.062909450395
Si	-2.580895089307	-0.724599997390	1.543998786704
Si	2.436040750330	-3.994838307749	-0.062904627830
Si	0.773677501866	-1.066518469687	-1.636254337644
Si	0.765426497144	-0.724601897013	1.543992892832
TV	6.692650400440	0.000000000000	-0.000000000000
TV	-1.661500418790	5.191019647827	-0.000000000000

TV	-1.681054172102	-1.561655419409	3.460242030018
# EQ'-SiO ₂ 52			
O	-2.652701964424	-3.125332417871	-3.136508406669
O	-2.281461337067	-1.544896363051	-1.572895286529
O	1.159926195374	1.922545908145	2.457041792827
O	0.335782937159	0.435544033857	0.752321706053
O	2.750982800760	-0.028248756371	0.016360661900
O	-3.847697450312	-1.219846604076	-3.333411000170
O	-3.406001820386	-3.262292893117	-0.669880295342
O	-3.034759890605	-1.681887006016	0.893751468100
O	0.406630824375	1.785555166775	4.923662284030
O	-0.417529580811	0.298568021303	3.218975688967
O	1.997711633094	-0.165241115831	2.482967236878
O	-4.601000083089	-1.356815750310	-0.866783841695
Si	-2.192051563632	-1.891179436066	2.504169418466
Si	3.369925510601	1.437317563730	0.357425035216
Si	-3.373553279859	-0.371950346028	-0.385510711483
Si	2.616630277308	1.300331427147	2.824060709805
Si	-1.438738377479	-1.754192853775	0.037554649985
Si	-4.126880307342	-0.508871640734	2.081122626973
TV	4.544037256741	-0.000000000000	0.000000000000
TV	3.173190116811	5.378083441813	0.000000000001
TV	-1.506581513721	-0.273969082895	4.933257972366

# EQ'-SiO ₂ 53			
O	-3.098736177363	-2.896988768677	-3.635358795640
O	-3.059347613080	-1.406206181597	0.803142759632
O	1.286964187284	2.334145414068	1.707146779646
O	0.295996222937	0.687524438704	0.589853091153
O	2.486146343972	0.454376750900	0.490999849095
O	-4.190029503217	-1.003070169853	-2.769574797320
O	-3.777491085352	-3.010115927520	-1.280554574113
O	-3.738103875913	-1.519328583703	3.157946011216
O	0.608209581551	2.221025436456	4.061954412524
O	-0.382747340897	0.574407118835	2.944659554446
O	1.807396706729	0.341252967739	2.845806155411
O	-4.868783598978	-1.116193170954	-0.414771934806
Si	-2.146724259197	-2.264356368010	3.014411383152
Si	3.443378368109	1.478944177354	-0.318601358551
Si	-2.596641198300	-0.193294060634	-2.793884049084
Si	2.764627674064	1.365819751417	2.036204264074
Si	-1.467963561527	-2.151233537493	0.659608393101
Si	-3.275395845875	-0.306415933132	-0.439077622626
TV	4.439121337152	0.000000000000	0.000000000000
TV	3.533932288533	5.604861150418	-0.000000000000
TV	-1.357512583378	-0.226246297751	4.709608195365

# EQ'-SiO ₂ 54			
O	-2.950219109598	1.527543695350	-0.527796825158
O	1.641308508658	-0.831481102682	-0.929258863171
O	-0.604937540667	1.658121487743	-0.388903467248
O	-1.711449497869	3.476701868869	0.517591433114
O	-4.306333689314	-0.042041313342	0.920748493021
O	0.285005770780	-2.398940757868	0.511112021067
O	-1.961833028241	0.097957837857	1.054101458090
O	-3.060127576382	1.918628902360	1.959958357553

O	-5.665165371784	-1.610544084422	2.359964765372
O	-1.064199741055	-3.964967015443	1.957151204871
O	-3.317009888479	-1.470264180473	2.495811502902
O	-4.419566285038	0.342177807539	3.408504053925
Si	2.993632548208	-1.141916016804	-2.161465867720
Si	-1.699105783809	0.411959364192	-0.566985154065
Si	1.635946884772	-2.707077297411	-0.719395345873
Si	-3.053155787261	-1.154566531434	0.875804499857
Si	0.286135939917	-4.275562643803	0.724688570693
Si	-4.410374352575	-2.721745706618	2.321175406031
TV	4.692475228585	-0.000000000000	0.000000000000
TV	-4.337765424353	5.869271399330	0.000000000000
TV	-4.064373871510	-4.701477460548	4.331022303296

EQ'-SiO₂ 55

O	5.314219849802	0.125245290417	-1.065252713511
O	0.627380215504	-1.194008285500	2.782814287237
O	-0.407803686106	-0.179981235608	0.931971237413
O	1.877178281971	-0.850899077607	0.703906871191
O	4.603567941298	2.557192891721	-1.062847438113
O	-0.079055955891	1.230822621891	2.782036711229
O	-1.111562353881	2.244781027357	0.934059106584
O	1.171366383526	1.578582149540	0.702706397714
O	3.902355990724	4.980573802642	-1.064503110693
O	-0.784459688565	3.661644973564	2.778355689086
O	-1.815656060925	4.676453212199	0.930183857636
O	0.467075129773	4.004427677825	0.701393980763
Si	2.821993813515	0.727233138263	0.921535345461
Si	0.896063016443	0.201318889569	1.905875000544
Si	2.121502646445	3.156741168753	0.920759059780
Si	0.194259907204	2.626864810995	1.904700054364
Si	1.414363117599	5.583013603445	0.917048043858
Si	-0.509058161028	5.057436716125	1.905078501724
TV	4.629443054446	0.000000000000	-0.000000000000
TV	-2.112863642049	7.283367277204	-0.000000000000
TV	-2.245029333547	-1.945439165746	3.531863373917

EQ'-SiO₂ 56

O	0.502988100057	0.609180842875	-0.322636666757
O	-1.112413919287	-2.335365307765	0.346448228591
O	-6.334364729236	-3.923736258776	1.851098643336
O	-4.984939195763	-1.286240746790	0.745811176953
O	-3.795079755226	-3.547154604176	0.698502386201
O	1.071899859611	-2.277993723049	-1.756184651682
O	0.908851632104	5.184037054453	-0.322631240379
O	-0.706557728061	2.239498126306	0.346440615676
O	-5.928500176092	0.651129973232	1.851093422179
O	-4.579070603572	3.288626584903	0.745825162660
O	-3.389215514416	1.027716130588	0.698512347205
O	1.477763975633	2.296875934198	-1.756196683612
Si	-1.735038597079	1.264893477054	1.254729445682
Si	0.905027852283	1.688908440028	1.099473568076
Si	2.423155716053	-0.703186255416	1.068742236054
Si	1.310899494072	6.263761838003	1.099455311170
Si	-2.140903998151	-3.309970122499	1.254740487422
Si	2.829022778013	3.871675140055	1.068745071745
TV	5.781182786582	0.000000000000	0.000000000000

TV	0.811737366732	9.149732651921	-0.000000000000
TV	-3.137456970567	-2.486856668590	2.256329277468

EQ'-SiO₂ 57

O	-0.405699805955	1.993223715688	-0.337060202579
O	0.010496090791	0.722762217732	-2.291435146571
O	6.053067786813	1.996513186158	-2.290609016729
O	-6.448946188057	5.775320569213	-0.337934775927
O	-2.836281494871	-0.537927073247	1.616406714399
O	-2.420092831546	-1.808416438259	-0.337937110170
O	3.622400092722	-0.534704443894	-0.337064677872
O	-8.879493203886	3.244167459357	1.615606322961
O	-5.266844210064	-3.069132759986	3.569936663986
O	-4.850654032412	-4.339608263348	1.615588475745
O	1.191913207966	-3.065843294168	1.616406056645
O	-11.310050865260	0.712919523105	3.569141086044
Si	0.394731176108	-4.318343379954	0.641449057017
Si	0.394401625281	-1.790447811469	0.641477392575
Si	-2.035824948806	-6.849472491134	2.594989076455
Si	-2.036186066160	-4.321570331748	2.594976803161
Si	-4.466423277193	-9.380717261612	4.548488027885
Si	-4.466745338547	-6.852817275642	4.548513379770
TV	4.027825906918	-0.000000000001	-0.000000000003
TV	-4.028510481976	5.055827611485	0.000000000002
TV	-7.291720352823	-7.593557894325	5.860546438136

EQ'-SiO₂ 58

O	1.999174748414	5.719798103917	-0.178493741418
O	-1.185367459773	-1.176444669868	0.231713375044
O	-7.709838342310	-6.123865026607	1.814079523880
O	-6.794296864645	-4.242439018247	0.699516383070
O	-4.534128811227	-3.651774641840	0.935397807118
O	0.575917983508	1.787139366626	-0.170005867106
O	-0.277059868506	9.468276381196	-0.178493992653
O	-3.461618563770	2.572042581387	0.231744558989
O	-9.986079909908	-2.375419183840	1.814063719620
O	-9.070552220976	-0.493971684188	0.699493371742
O	-6.810406457307	0.096745866578	0.935442429210
O	-1.700304304603	5.535604968758	-0.169974133853
Si	-5.390085629635	0.309382965598	0.029524886302
Si	-2.602845807574	-0.315959000523	-0.214110115079
Si	9.342588584167	-3.835952673418	1.838336887620
Si	-4.879085465110	3.432545315658	-0.214113642704
Si	-3.113825674841	-3.439133858880	0.029459683875
Si	7.066374118542	-0.087522437955	1.838387726876
TV	10.167976366291	0.000000000000	0.000000000000
TV	-4.552501142373	7.496924780959	-0.000000000000
TV	-2.820724344244	-4.770420696316	1.568490099365

EQ'-SiO₂ 59

O	-0.173167561435	1.334287535860	-0.424455082361
O	-0.789076823342	4.491559941384	-1.028294891368
O	-2.424453118958	0.125466265146	-1.242523461835
O	-2.029689869388	2.463503776814	-1.547844777888
O	-0.073898019072	3.391288646027	-0.633417478660
O	-0.565304761778	-0.999473685443	-0.116037019666
O	0.017699490727	-0.158842377115	2.050212929580

O	-0.598253350194	2.998405938951	1.446382244568
O	-2.233624051109	-1.367699247938	1.232167809721
O	-1.838857495796	0.970344853606	0.926861719063
O	0.116929773857	1.898163175015	1.841283558756
O	-0.374480970443	-2.492627230122	2.358642678261
Si	2.475496651972	0.921956584630	2.531243015641
Si	0.481792068995	1.477755592095	-2.069512569477
Si	-3.148418308082	5.465720834569	-1.719567831386
Si	0.672600024521	-0.015390094443	0.405193195733
Si	2.284674563111	2.415109134097	0.056542499567
Si	-2.957585217743	3.972558714686	0.755095210566
TV	3.747466250730	0.000000000000	0.000000000000
TV	-2.019978582912	6.420160626554	-0.000000000001
TV	0.381651944384	-2.986329705599	4.949370267648

EQ'-SiO₂ 60

O	0.921115552380	2.525790707345	-1.302748891147
O	-0.545271643354	-1.995579268181	-0.190752837981
O	-5.948360102360	-5.256964510665	3.379387835118
O	-4.210921448098	-3.992803896039	2.406571164735
O	-2.483849950851	-3.416526737696	0.144272625998
O	0.939992198679	-0.844953862619	-1.122264391046
O	-0.672744768038	-0.391483080157	1.116123628830
O	-2.139126533307	-4.912866500699	2.228131385381
O	-7.542242089058	-8.174230154114	5.798236666937
O	-5.804784706004	-6.910107642941	4.825437107359
O	-4.077715185059	-6.333819700895	2.563133483475
O	-0.653875546507	-3.762248455137	1.296601273575
Si	-3.214897853518	-5.119812706526	3.501690823350
Si	-1.669243678171	0.735900781886	0.022541732390
Si	1.176946252014	-0.733325177434	0.552662349733
Si	-3.263107788048	-2.181385241085	2.441412503190
Si	-1.621029457185	-2.202516334023	1.082821304178
Si	-0.416933813377	-3.650628612971	2.971530508672
TV	5.639487505661	-0.000000000000	0.000000000000
TV	-2.090961243493	4.288968345076	0.000000000000
TV	-3.187725219049	-5.834573786677	4.837738949909

EQ'-SiO₂ 61

O	-1.447502917635	1.037943023225	-1.846736794646
O	-1.942683799432	-0.131966617846	1.820148033269
O	-6.527506965772	-4.450531952462	1.914495980333
O	-3.835357734783	-1.524007099979	1.882633138440
O	-3.114708431190	-2.767001395612	0.099663332140
O	-0.418564843727	-0.049381245492	0.037339819348
O	-2.339615251523	-1.557386575561	0.026795281920
O	-2.834916004746	-2.726540247005	3.693341909065
O	-7.419882669710	-7.045753730419	3.788055477940
O	-4.727216390910	-4.119330499938	3.756329021337
O	-4.007085892942	-5.362242065858	1.973196913940
O	-1.310688901622	-2.644707082991	1.910830868022
Si	-2.877113116507	-6.473149107410	1.178262201433
Si	-3.335682582857	-0.400294630486	0.725954558031
Si	8.839795082119	-1.242720899927	1.081794835116
Si	-4.228023994379	-2.995474483478	2.599499452158
Si	-1.984764484658	-3.877969610707	-0.695297991902
Si	7.947416536535	-3.837849840142	2.955393825819

TV	9.832502917665	0.000000000000	0.000000000000
TV	-2.865100592397	3.329719404390	0.000000000001
TV	-1.784483175723	-5.190533482675	3.747115088221

EQ'-SiO₂ 62

O	-1.114020016637	0.619991709886	3.817247939798
O	-0.756941506819	-1.486201773046	4.608785218263
O	-1.210708606760	-1.119866751399	2.235303924425
O	-1.382696447422	-0.730494363752	0.080692746281
O	-0.779712417127	-3.194651484903	2.924781479276
O	-3.552281792570	-0.079318835569	0.745690564950
O	-3.600917051848	3.532386652263	3.817223339680
O	-3.243837495764	1.426193288114	4.608812878145
O	-3.697570362878	1.792518760646	2.235310607470
O	-3.869554971317	2.181885425621	0.080689723573
O	-3.266554524801	-0.282280090847	2.924728267571
O	-6.039145963104	2.833055784762	0.745720210990
Si	-2.477561434529	1.135841882701	3.158285556428
Si	0.159733914393	-1.839917910912	0.348581086340
Si	-0.641645142360	0.436539762367	1.975111802731
Si	-2.327121013512	1.072458649619	0.348548309708
Si	0.009306544926	-1.776519366329	3.158234736403
Si	-3.128507336745	3.348901829086	1.975155690786
TV	3.991347201631	-0.000000000000	0.000000000000
TV	-4.973739122642	5.824780954937	-0.000000000000
TV	0.104580145855	-2.901925781559	5.121006858226

(vi) GeO₂ at 10⁶ atm

EQ'-GeO₂ 0

O	-3.885538629470	2.474289815930	0.638952035822
O	2.387316434155	1.725987045270	-1.523568400870
O	-2.403308485127	0.764862729870	1.287420079706
O	1.127786467694	-3.325924510114	0.690052932821
O	-6.654253986348	-0.896017291946	2.067272124518
O	-0.393424855662	-1.658747063893	-0.093127230824
O	-5.168844507400	-2.604295249635	2.715724221866
O	-1.637368583156	-6.700396227529	2.112826617475
O	-9.418509544295	-4.271207303445	3.498091203681
O	-3.158692521735	-5.038589224400	1.337787020660
O	-7.946036376538	-5.996754398988	4.132787430101
O	-4.407029797337	-10.066992964208	3.552851916780
Ge	-2.002729964735	-4.810882512998	2.682518686733
Ge	1.301472272787	-11.935418056089	0.718036405834
Ge	-1.466063264742	-15.309732206538	2.148326499820
Ge	3.535510071542	1.939281050211	-0.171004733456
Ge	0.764696366103	-1.438937025730	1.253642029708
Ge	4.075103681736	-8.553758390478	-0.713464277238
TV	5.771193630773	-0.000000000001	0.000000000006
TV	-1.668744460555	5.408800343764	-0.000000000004
TV	-8.311973646671	-10.131433042166	4.284572023817

EQ'-GeO₂ 1

O	-0.528993403499	1.309715655163	0.635535723004
O	-1.872839565729	-0.899648819247	-2.926615500255
O	-0.529620614709	0.416580523421	2.829881058360
O	-1.878322319311	-1.794799574224	-0.735270364144
O	0.863043287824	3.619611998287	0.582816368251
O	-2.758115365693	1.311702337532	-2.940191844664
O	0.352709507829	2.613393663739	2.791712155102
O	-2.759165769276	0.412085776911	-0.718203115677
O	1.746931650207	4.924112303310	2.844786096692
O	-1.363893357974	3.620061977610	-2.888444883299
O	1.751963278975	5.816717434542	5.038244978584
O	-1.873932598244	2.611466534075	-0.683749207957
Ge	0.245556173432	4.278850295664	-2.281752521112
Ge	0.973367751126	1.951861120076	-0.075556570706
Ge	2.472139742737	4.278163791849	-0.024263112344
Ge	-1.200685176042	-0.244240476352	-0.049855041848
Ge	-1.254158464338	1.952172772522	-2.232401177263
Ge	1.026223574779	-0.242059417994	2.158099107142
TV	4.453898820934	0.000000000001	0.000000000000
TV	1.397309406449	6.717868184632	-0.000000000002
TV	0.001119325606	0.000898472069	4.413527048569

EQ'-GeO₂ 2

O	-0.338399414132	-1.061019638863	0.501944056043
O	2.167338556836	0.901863909538	-1.115722222557
O	-1.379676368766	-1.077971390375	2.792023479142
O	-0.350956674617	-3.028564513716	-1.113458057407
O	-0.340818356163	2.885850705917	0.501938596875
O	2.164900076041	4.848754210073	-1.115720303600
O	-1.382105710099	2.868879179458	2.792029571250

O	-0.353364302001	0.918308474744	-1.113457824258
O	-0.343227144661	6.832703688983	0.501937474184
O	2.162493368857	8.795616962373	-1.115716095572
O	-1.384506046217	6.815758625875	2.792031271031
O	-0.355791171424	4.865174826444	-1.113461308081
Ge	3.429456665428	9.787920516663	-0.305275130643
Ge	0.912773100280	-0.078147315766	-0.306141891227
Ge	0.910354378425	3.868734303709	-0.306139877011
Ge	3.434290507769	1.894187130439	-0.305278684705
Ge	3.431868750258	5.841054114320	-0.305278486460
Ge	0.915184802278	-4.025002440242	-0.306138616291
TV	5.044635977727	-0.000000000001	0.000000000006
TV	-0.007251581169	11.840601561076	-0.000000000012
TV	-3.559841565551	-3.952695746310	2.293410256087

EQ'-GeO₂ 3

O	1.059654591462	-0.377603793977	0.503282064593
O	-0.539578475221	-1.488814268788	-2.478732151552
O	0.268468222926	0.754819876327	2.625563100876
O	0.249122851759	-2.620623752450	-0.356319502951
O	-0.524959422091	1.865089717417	0.503089601175
O	-2.124376459481	0.753714259554	-2.478742778912
O	-1.316438287787	2.997263270709	2.625467664931
O	-1.335748113869	-0.378060889569	-0.356248293901
O	-2.110121840321	4.107502811931	0.503321630999
O	-3.709354574830	2.996359553371	-2.478727132018
O	-2.901359505794	5.240020763421	2.625562230150
O	-2.920576472052	1.864586572325	-0.356207370158
Ge	-2.910612417134	3.552397328705	-0.987164690849
Ge	1.069144872174	1.309777518272	1.135021540773
Ge	-0.515758895416	3.552402476169	1.134989364066
Ge	0.259161152955	-0.932823131751	-0.987176148194
Ge	-1.325708255078	1.309743094429	-0.987147628327
Ge	2.653977713764	-0.932855069163	1.134940647216
TV	4.790286993961	0.000000000000	0.000000000000
TV	-4.754721859390	6.727778682812	-0.000000000003
TV	-0.001284206681	0.000608619544	4.244460893149

EQ'-GeO₂ 4

O	-1.159784438290	1.426424433229	-0.093199028067
O	3.053744238724	0.000354665097	-1.438720689518
O	-3.436435553807	1.898015572974	-0.091070795651
O	3.548546446488	7.698223463479	2.508499986394
O	-2.875222631743	0.002698110130	1.254566524809
O	0.697212951593	0.407626360517	1.253023889649
O	-3.577035807271	4.342490791028	-0.093206625185
O	0.636482118301	2.916436787988	-1.438698310429
O	-5.853691183268	4.814116846990	-0.091054354021
O	1.131264972712	10.614300297092	2.508503628001
O	-5.292480786202	2.918808756433	1.254579019066
O	-1.720044503707	3.323703550728	1.253036685399
Ge	-3.507171134353	3.118166912151	-1.409014110670
Ge	-1.088913325862	0.206051215430	1.223234753331
Ge	1.875575188391	0.204065213882	-0.093100696378
Ge	-3.506160006379	3.122115682817	1.223216780664
Ge	-1.089899914406	0.202095386273	-1.409000961937
Ge	-0.541703977950	3.120165773611	-0.093098384173

TV	5.929497262237	-0.000000000000	-0.000000000000
TV	-4.834557494961	5.832171049485	-0.000000000000
TV	-0.658823915375	4.377001015121	3.947760930973

EQ'-GeO₂ 5

O	5.497767148353	0.905389483104	-0.420969674342
O	7.316406604211	-0.829104245410	-1.461237016356
O	-0.472344512051	1.982872699108	0.779330659311
O	4.295628002256	5.299472711562	0.681621828573
O	-10.925485843671	-1.730045494630	1.881766392082
O	-6.620004110255	0.283700182464	-0.316537937797
O	5.984223729101	3.607481273114	-0.420821589094
O	7.802227252190	1.873001410647	-1.461192151337
O	0.013497727704	4.685092017920	0.779324954518
O	4.781492998768	8.001749731121	0.681590390505
O	-10.439925939659	0.972180777387	1.881681098884
O	-6.134151004803	2.985668201228	-0.316632320833
Ge	3.507936131156	6.836967717038	0.137691039885
Ge	-7.474932944577	0.445786654047	1.324400343094
Ge	5.564502687885	2.289490225433	0.730634534694
Ge	-6.989159839649	3.147892818193	1.324172834373
Ge	3.021949929065	4.134922495836	0.137505819596
Ge	6.050340651718	4.991579191908	0.730766740536
TV	7.791135531852	0.000000000000	0.000000000000
TV	0.971671382258	5.404174114314	0.000000000006
TV	-5.150708763029	5.126985462272	3.239781726237

EQ'-GeO₂ 6

O	-0.843922026721	1.383885946169	-0.262274764139
O	2.646709777085	-0.095771368185	-1.185733193652
O	-3.083397229274	1.843798007362	0.055192484225
O	4.786256418913	6.969617585854	2.340107732295
O	-3.315836633829	-0.229537468665	1.099841946648
O	0.205233874732	0.227247222676	1.415547452687
O	-2.569544025447	4.013691302426	-0.262353151557
O	0.921043853477	2.534065634750	-1.185937740555
O	-4.808942572925	4.473594686414	0.055356046274
O	3.060726096720	9.599270513846	2.340263942053
O	-5.041533222763	2.400294597164	1.099739505306
O	-1.520450983821	2.857144604210	1.415637555877
Ge	-3.921224862943	4.092266066310	-1.503917423578
Ge	-1.760162460095	0.811453761418	1.272412861032
Ge	1.120964083242	0.804273680709	-0.116913134023
Ge	-3.485822433765	3.441184447456	1.272413392935
Ge	-2.195572363155	1.462325094860	-1.503961907263
Ge	-0.604669540495	3.434089665683	-0.116924293320
TV	5.759963320280	-0.000000000001	-0.000000000001
TV	-3.451286824677	5.259739708126	-0.000000000000
TV	0.300301816449	3.950887720891	4.163703999264

EQ'-GeO₂ 7

O	-1.681889965355	1.267104278574	1.568850295235
O	-0.123582623338	-1.337361993097	-5.138871826831
O	-0.117155905000	-0.416333093578	1.795566444514
O	-1.654270473708	-2.897181732989	-0.841305182474
O	-1.677495929387	4.076353545396	1.005485222171
O	-0.099222692395	0.938891354804	-4.879955027387

O	-0.088308577142	2.833325206228	2.096153541504
O	-1.661469446866	-0.090094439047	-1.406322211234
O	-1.651832708567	6.351060387699	1.266518702856
O	-0.093799385024	3.743692831280	-5.443436598284
O	-0.116778500157	5.110762018513	2.357455486241
O	-1.688466097971	2.183716594749	-1.147698822374
Ge	-0.104042190053	5.284534745740	0.476929206687
Ge	0.677639909196	-1.655247953130	2.888982165604
Ge	-0.111540257674	1.120719372739	2.888533144721
Ge	-1.673926874781	-0.269547448563	0.475389873926
Ge	-0.889876456438	2.507545776323	0.475103102361
Ge	1.462567082069	-4.432116503719	2.887394630663
TV	3.126065311245	0.000000000008	0.000000000009
TV	-0.004086188677	8.331482424101	-0.000000000001
TV	-0.000061897154	0.004644253786	4.824680467035

EQ'-GeO₂ 8

O	0.181671313612	1.746568192916	-0.423636032419
O	0.931011197957	0.598743898117	-2.612326510561
O	-2.101718110524	1.762812107230	0.442288083549
O	-1.977084536960	1.854729282854	4.862954407876
O	-1.231034005985	0.707821806517	2.670436743105
O	1.049832228684	0.694100435506	1.808511698491
O	-1.454663869646	3.943742907753	-0.423688512678
O	-0.705172332375	2.795855369822	-2.612377099876
O	-3.738192190050	3.960042248830	0.442270119247
O	-3.613290393562	4.051999792686	4.862986249160
O	-2.867379222270	2.905129345566	2.670429117910
O	-0.586453360784	2.891343196687	1.808614490142
Ge	-0.771269435431	4.455052360492	-3.405711360045
Ge	-0.524967976926	1.229521801546	1.124337323151
Ge	1.783706792343	1.230971594932	-1.086763741678
Ge	-2.161311139723	3.426707041650	1.124282635225
Ge	0.865031006246	2.257848788423	-3.405767492975
Ge	0.147387576524	3.428163980855	-1.086782755145
TV	4.603730918247	0.000000000000	0.000000000000
TV	-3.272414962916	4.394453153779	0.000000000000
TV	-3.695652815957	-1.034233863143	6.742326845153

EQ'-GeO₂ 9

O	-0.094693244609	1.960947806986	-0.369528101835
O	2.318588078358	0.270334410314	-2.486312685868
O	-2.438867702440	1.913559296416	0.326568168907
O	0.453826128697	2.411883301826	4.651946401910
O	-1.690034346776	0.716114375695	2.534243427727
O	0.656711969377	0.763761022706	1.837881981410
O	-1.848017948751	4.173295238163	-0.369563243139
O	0.565367370000	2.482723868777	-2.486310056958
O	-4.192181407352	4.125956484492	0.326581338736
O	-1.299482985788	4.624294385288	4.651960370747
O	-3.443323636060	2.928460578553	2.534223216689
O	-1.096574125893	2.976170786953	1.837866960363
Ge	-2.589690049037	3.581435531788	-3.248459540139
Ge	-0.892017800403	1.338523696830	1.082829990738
Ge	1.376218766919	1.325196944956	-1.214894650431
Ge	-2.645311073245	3.550885716080	1.082814301396
Ge	-0.836408741754	1.369049288085	-3.248455058552

Ge	-0.377063344942	3.537568624753	-1.214895510452
TV	4.558838121273	-0.000000000000	0.000000000000
TV	-3.506589678347	4.424733826358	0.000000000000
TV	-2.325930725311	-0.015607935400	6.628799066805

EQ'-GeO₂ 10

O	0.766550803395	2.106021404448	0.031442300334
O	0.700562012308	0.417014890017	-2.004093099326
O	-1.684550959617	2.104309682846	0.013422124039
O	-1.599322067999	2.160964031271	4.067812734500
O	-1.665050564169	0.470433527437	2.031962354850
O	0.788509062420	0.472662550598	2.054156005375
O	-0.761433588501	4.373967235448	0.031417997315
O	-0.827337437909	2.684859244069	-2.004109636189
O	-3.212502723537	4.372197022914	0.013423816912
O	-3.127311531213	4.428831319633	4.067794303208
O	-3.193005286126	2.738374120868	2.031951077846
O	-0.739465946051	2.740574029680	2.054116903669
Ge	-1.135819626097	4.125680876915	-3.095113050812
Ge	-0.447661972762	1.288497859068	1.033737844038
Ge	2.009444181918	1.295523449042	-0.992587673618
Ge	-1.975620379971	3.556441256126	1.033750929186
Ge	0.392146452983	1.857761790706	-3.095138085399
Ge	0.481469406846	3.563414136214	-0.992562482720
TV	4.904368753790	-0.000000000000	0.000000000000
TV	-3.055926357072	4.535837419936	-0.000000000000
TV	-3.298400911916	-0.574942244797	6.152939954187

EQ'-GeO₂ 11

O	5.121127292172	-0.164484905079	-0.965539035547
O	7.416006552128	-0.587785884309	-1.248595017306
O	-1.142455691213	1.026119133129	0.335794683039
O	4.334067793266	5.811945173139	0.748813782803
O	-11.024067815070	-1.455805419356	1.890870221808
O	-6.529555108857	0.596069729886	-0.119587897860
O	5.630154098309	2.640863475877	-0.965560420655
O	7.925014821970	2.217581341394	-1.248542484724
O	-0.633383241614	3.831456965352	0.335780984926
O	4.843073731976	8.617477547106	0.748734369511
O	-10.515078879365	1.349542600232	1.890915136923
O	-6.020554546646	3.401299798211	-0.119576847890
Ge	3.558856346925	7.407034528015	0.270231126527
Ge	-7.465325833325	0.774308468181	1.540101094435
Ge	5.626114146522	2.666778405424	0.884581812530
Ge	-6.956309071769	3.579626216068	1.540082721267
Ge	3.049664637566	4.601759037957	0.270016608029
Ge	6.135155999655	5.472103546588	0.884575108453
TV	7.721393378556	-0.000000000000	-0.000000000000
TV	1.018046848142	5.610669827983	0.000000000006
TV	-5.309295949839	5.371653206486	3.079296780420

EQ'-GeO₂ 12

O	1.500472288413	1.184565920093	-1.165462489829
O	1.986570384767	-1.091525815294	-1.523272623439
O	-0.069283981245	0.747441005607	0.564643465072
O	1.908986459946	9.166315541899	1.892265211855
O	-3.075643124467	-1.409291451270	0.548315606537

O	-1.216051897802	-1.877101387966	1.908534942638
O	4.928670621171	1.153150118525	-1.537830451828
O	4.417172663682	-1.061605476321	-1.151324325366
O	3.360263357624	0.717075999942	0.192871578955
O	4.338810900160	9.198130786646	2.263407034024
O	0.354024436763	-1.438068564498	0.176719692926
O	1.211543611076	-1.849243151406	2.279247553809
Ge	3.256329340826	4.667911122225	-1.539824767605
Ge	-2.880576976866	-0.962709836884	2.282140425048
Ge	1.696850391750	1.631264106350	0.568094313462
Ge	-0.039532976240	-0.517039958467	1.888871990146
Ge	0.415969729037	4.225188672809	-1.149169925937
Ge	4.537951001748	2.076271319335	0.174868715836
TV	5.858496941125	0.000000000000	-0.000000000002
TV	0.092105976534	4.400358560778	0.000000000000
TV	-1.738889254140	5.421599737579	5.145766745700

EQ'-GeO₂ 13

O	1.306149820997	-0.012669172671	-0.181697837670
O	-0.820851544045	-1.770366162935	-2.462678314104
O	-0.391526153494	0.439711628856	2.609551717451
O	0.877213713261	-2.218564581042	0.328910333304
O	-0.506739804106	2.193041690080	-0.181712220588
O	-2.633729527724	0.435346789384	-2.462666852505
O	-2.204728414399	2.645369538771	2.609608131034
O	-0.935639174543	-0.012820049444	0.328928480524
O	-2.319608535341	4.398761460591	-0.181696250096
O	-4.446727534794	2.641137283759	-2.462670297252
O	-4.017280859168	4.851165767596	2.609545292021
O	-2.748518038251	2.192893225814	0.328940903226
Ge	-3.641439368247	3.308499130121	-0.963254987510
Ge	0.414941640332	1.104240889331	1.110769377703
Ge	-1.398066786979	3.309884004740	1.110791256721
Ge	-0.015581724808	-1.102975918088	-0.963307531791
Ge	-1.828459037541	1.102735767851	-0.963312147574
Ge	2.227796527876	-1.101513289762	1.110723095050
TV	4.485212128326	0.000000000000	-0.000000000000
TV	-5.438621887314	6.617162471254	-0.000000000003
TV	0.000662844354	0.003514281435	4.449881170679

EQ'-GeO₂ 14

O	1.378443565428	0.024175829454	0.542984684140
O	-0.785498717146	-1.810470173816	-1.790140629629
O	-0.847704623761	0.006522183992	1.144616096745
O	1.475563686420	-1.759546158265	-1.144127496943
O	-0.468006853285	2.198199419530	0.542990516223
O	-2.631871507817	0.363536234275	-1.790145731602
O	-2.694143118521	2.180527277671	1.144619016088
O	-0.370807823148	0.414466703157	-1.144129560020
O	-2.314452861736	4.372294305828	0.542988152430
O	-4.478291457349	2.537532790690	-1.790141492385
O	-4.540577400133	4.354526687234	1.144624154093
O	-2.217231793481	2.588462275757	-1.144123899067
Ge	-3.608720142088	3.277284145044	-0.231163281435
Ge	0.445600294698	1.101871667975	1.919410654523
Ge	-1.400826313533	3.275877985022	1.919436604819
Ge	0.084091882228	-1.070732595063	-0.231168592004

Ge	-1.762306175734	1.103267759484	-0.231177193930
Ge	2.292010672570	-1.072126026239	1.919420145901
TV	4.400102555931	-0.000000000000	0.000000000000
TV	-5.539221021755	6.522013361292	-0.000000000003
TV	-0.868271885959	-0.747711808337	4.622723999693

EQ'-GeO₂ 15

O	2.987309030310	0.088279885209	3.088100061592
O	1.291595258888	-0.420972393384	1.565009345710
O	0.917748967039	1.967436203964	1.663452762856
O	-0.406875265908	0.961653326575	0.083829690174
O	2.647286191657	2.455062380861	3.307341793647
O	3.026795381405	-1.830232083028	0.894816970393
O	6.576827143879	0.416299529243	3.524066553673
O	4.803120736276	-0.776953982252	1.832170129053
O	4.540248874480	1.722788724506	2.058777239036
O	3.293621028370	0.572850821551	0.452349771554
O	6.199369465331	2.833039583134	3.582338723397
O	5.783891460301	-1.509798656081	-0.072708229075
Ge	7.597452651473	3.793916753613	3.304496572254
Ge	2.569883474735	1.294849322927	1.870613226181
Ge	3.204392608330	0.686082710147	4.792750895940
Ge	5.894552770501	0.545250219042	1.838689411391
Ge	4.392431258901	3.144552381657	3.266636309680
Ge	6.230763650388	1.558831427678	4.833653109093
TV	6.153125111439	-0.000000000002	0.000000000000
TV	-0.098255839153	4.824091652117	-0.000000000000
TV	-1.178916008933	-1.538428378940	4.557933184517

EQ'-GeO₂ 16

O	0.041188171737	2.088775527025	-0.392164698954
O	2.399493554308	0.373060422499	-2.558660739090
O	-2.253730036516	2.033824332067	0.363149367378
O	-0.909368047630	1.313860263674	4.844135547268
O	-1.481862006212	0.843498847836	2.612143100133
O	0.861023099109	0.937576131328	1.965749785175
O	-1.744962710744	4.271502733799	-0.392212409360
O	0.613475375911	2.555767677889	-2.558643485639
O	-4.039835500017	4.216547221846	0.363213047562
O	-2.695442022876	3.496591725877	4.844130846423
O	-3.267985703932	3.026209026267	2.612180705113
O	-0.925039570130	3.120348545617	1.965764747021
Ge	-2.508497301249	3.647588769355	-3.334392542764
Ge	-0.674209179343	1.504009555789	1.112836003984
Ge	1.511556755370	1.469850428412	-1.232836359565
Ge	-2.460264421151	3.686731830888	1.112852951093
Ge	-0.722434171269	1.464842038785	-3.334369965708
Ge	-0.274522497418	3.652582729356	-1.232818537621
TV	4.458501132429	-0.000000000000	-0.000000000000
TV	-3.572107859127	4.365491134885	0.000000000000
TV	-3.748241982591	-1.240162905513	6.844178957437

EQ'-GeO₂ 17

O	-4.237284830938	2.774743554765	0.534571214271
O	1.827558253628	1.060457734514	-1.130623687683
O	-2.043779920967	1.325517599398	1.186251186144
O	1.708693504158	-3.287188151456	0.824434487804

O	-6.549642720224	-0.123680843001	1.837948284870
O	-0.484811782249	-1.837976746961	0.172748137332
O	-4.356146459855	-1.572884499234	2.489620481922
O	-0.603666706206	-6.185610095844	2.127803902447
O	-8.862008589530	-3.022105318226	3.141292612471
O	-2.797153609110	-4.736402309660	1.476117548566
O	-6.668488872557	-4.471313784583	3.792976543474
O	-2.916017620378	-9.084039288759	3.431145913419
Ge	-1.383304395191	-4.603255821488	2.634740394026
Ge	1.864591423920	-10.701919245247	0.679704768330
Ge	-0.447759715302	-13.600331115835	1.983053746860
Ge	3.241419025824	1.193587135418	0.028016241784
Ge	0.929058290674	-1.704820591953	1.331374740230
Ge	4.176953625554	-7.803486425437	-0.623665338413
TV	6.699372315396	-0.000000000001	0.000000000006
TV	-1.564520566172	5.223144511115	-0.000000000004
TV	-6.937078715507	-8.695281740438	3.910083719502

EQ'-GeO₂ 18

O	5.170057817652	-0.193554691712	-0.711883283846
O	7.806680624578	-0.637372948212	-0.715944788531
O	-1.233982156920	1.253888537505	0.112962167799
O	4.845956947709	6.135643889611	0.433059072543
O	-12.277061444486	-2.493078061316	1.383607819426
O	-6.776607868288	0.814760770914	0.109614016314
O	5.951389547522	3.188040896111	-0.711733930239
O	8.588026939383	2.744104022750	-0.716267925961
O	-0.452806547350	4.635177229260	0.112891079569
O	5.627334223640	9.517096396907	0.433095412339
O	-11.495748827392	0.888411528216	1.383347146974
O	-5.995304822414	4.196311073027	0.109824901067
Ge	4.586802504215	7.963959204832	0.863220324907
Ge	-8.194665980519	0.130762328508	0.909085641644
Ge	5.898203503709	2.441637605137	0.952988059583
Ge	-7.413476299343	3.512125948712	0.908858066234
Ge	3.805512881950	4.582538049239	0.863523670864
Ge	6.679487532498	5.823045577122	0.952848495582
TV	8.176688071925	-0.000000000000	0.000000000000
TV	1.562681702248	6.762994275772	0.000000000006
TV	-5.046391259479	6.409749839554	2.421344359495

EQ'-GeO₂ 19

O	6.358273480637	-0.167619493157	-0.694486122899
O	8.646641588473	-1.342745578273	-0.653090080805
O	-2.957751648512	-1.830069747621	0.924878628432
O	6.757701324801	7.558910846661	-0.708673025302
O	-14.053789127595	-0.743028327279	0.912279005474
O	-7.678171310839	0.430940407430	0.868572007881
O	7.779902972410	3.167808130154	-0.694379660572
O	10.068098838012	1.992786698754	-0.652976224148
O	-1.535550639721	1.505054573790	0.925031758016
O	8.179332744288	10.893668027972	-0.708141512230
O	-12.632251331920	2.592313959906	0.912403091753
O	-6.256621229062	3.766498935316	0.868745581207
Ge	5.940159105935	8.903222756087	0.087095593595
Ge	-7.966167586217	-0.399576335056	2.494137459916
Ge	6.237404021772	2.866038917105	0.105430362513

Ge	-6.544687521671	2.936051776469	2.494356006901
Ge	4.518722813878	5.567691631213	0.086912954730
Ge	7.658808122287	6.201950135411	0.105000121801
TV	8.661067490292	0.000000000000	0.000000000000
TV	2.843248450679	6.670801446552	0.000000000004
TV	-4.422084499383	6.090581588285	2.370511784948

EQ'-GeO₂ 20

O	0.263413761667	1.047749200948	0.934778587151
O	3.227241312546	-0.689141571032	-1.439126046063
O	-3.518133418617	1.838860145971	-0.388482298950
O	2.136931709446	9.571666084980	1.642423632181
O	-1.391966431148	-0.756955942248	0.622182683906
O	1.430224183143	-0.479835347013	-0.106802534944
O	-4.093213619381	5.554840343941	0.834237074281
O	-0.439581756753	3.589215576223	-0.903640912468
O	-6.929104959714	5.806776627782	0.112635336978
O	-1.526793448359	13.847987990371	2.184193538234
O	-4.818648194428	3.203292593441	1.121235177449
O	-2.904169263697	3.997465245564	-0.179442464435
Ge	-5.669067832244	4.673364591572	0.532984398224
Ge	0.305889842538	-0.843536615063	1.320316266019
Ge	0.399962583517	2.058682505102	-0.465242114728
Ge	-3.046023330480	2.974923575018	1.213040180815
Ge	-2.668180002039	0.364963758121	0.208369334445
Ge	-2.944620994597	5.887921258677	-0.570563891793
TV	5.691326169268	-0.000000000000	0.000000000002
TV	-7.039451007657	8.126204227393	0.000000000007
TV	1.217678108389	4.253108795502	2.880271654366

EQ'-GeO₂ 21

O	-0.622639276057	1.765658169339	0.497372197166
O	4.605107413035	0.202373898516	0.310732708429
O	-4.404521178253	2.182743600516	-0.403277991351
O	10.898881975603	5.384280395539	2.021119129422
O	-6.626881220846	-1.721891127464	0.352318848983
O	-1.710520660244	-0.178702979550	1.289535146402
O	-0.565014755912	3.387471829695	2.176038894883
O	5.114386461467	1.964183162443	1.735943638045
O	-4.088674805494	3.891370169540	2.459842318301
O	10.958302082670	7.012979397664	3.699788235484
O	-5.661266475137	0.186380987975	2.906046242125
O	-0.743374493785	1.732353192850	3.844462710228
Ge	-2.267986131113	4.456138850530	2.140782055780
Ge	-3.913387983679	0.733799404789	0.774260246234
Ge	2.034552763737	-0.607128243183	0.291648260116
Ge	-4.370734645396	2.204648366252	3.421590622847
Ge	-1.833143545706	2.986170627361	-0.380608280482
Ge	3.295202635318	1.393858735255	2.056458623187
TV	10.221402439922	-0.000000000001	-0.000000000000
TV	-0.911964088125	2.921526504087	0.000000000002
TV	0.825036488245	3.475432773036	4.285779689277

EQ'-GeO₂ 22

O	-0.404042618780	1.972514845851	-0.816722548387
O	3.461447527692	0.630715812193	-0.125931113925
O	-2.509665751948	2.347084742728	1.246147681468

O	0.116005256209	1.586770468570	2.530631372330
O	-1.956490957001	0.520616488435	2.346372959664
O	1.184853597184	1.218555129456	0.682736526074
O	-2.023768618055	4.020835178543	-0.517381030793
O	1.680807738558	2.889726680647	-1.065570276643
O	-4.301174531836	4.606777197691	0.291263499954
O	-2.011322464615	4.577278594457	2.558329675701
O	-4.082379868733	3.494906108339	2.373295865863
O	-0.426556777165	3.246410456282	0.977946982508
Ge	-2.854019653445	3.672387193120	-2.075318953422
Ge	-0.939275415444	1.431053297647	0.861966575283
Ge	1.999073213660	1.165818477767	-0.896195618367
Ge	-2.846274301521	4.062932968705	1.059561655965
Ge	-0.695098632159	1.675839578421	-2.504697614357
Ge	0.096685644208	3.798889198093	-0.697938327638
TV	5.830450101868	0.000000000000	-0.000000000000
TV	-3.802031054861	4.825320311124	0.000000000000
TV	-3.118674284191	-0.126832454064	4.742666672086

EQ'-GeO₂ 23

O	0.576815301236	-0.377704178977	0.934818216535
O	0.329631338758	-0.462281497954	-2.749247877153
O	0.231990347891	-0.494819893533	3.114059345227
O	-0.282833553753	-2.107447446844	-1.019629862228
O	-0.280612881196	2.233307136671	0.934844965387
O	-0.527892092932	2.148689423775	-2.749231098508
O	-0.625490168826	2.116066633101	3.114108037296
O	-1.140327527586	0.503484060177	-1.019571140589
O	-1.138091933086	4.844245442133	0.934859551265
O	-1.385304321110	4.759729732619	-2.749201629692
O	-1.482965030636	4.727161600720	3.114056393161
O	-1.997770594480	3.114521441007	-1.019660299815
Ge	-1.261891521340	4.802460887421	-0.906940430696
Ge	1.312749992955	1.310240360750	1.047421846673
Ge	0.455293935587	3.921235410309	1.047452531166
Ge	0.453068353277	-0.419490024763	-0.906994598614
Ge	-0.404460364953	2.191470713019	-0.906960869863
Ge	2.170180496750	-1.300750834611	1.047421899955
TV	4.391543346370	-0.000000000000	-0.000000000000
TV	-2.572409198830	7.832990564865	-0.000000000003
TV	-0.957298518063	-1.762361138901	3.908870079748

EQ'-GeO₂ 24

O	6.019372363244	0.836754061962	-0.750646710083
O	8.556845725773	-0.063469914164	-0.724690768014
O	-0.992988823023	1.959076280483	0.141998618490
O	5.940910605059	5.230194491590	0.442792976815
O	-14.242567132809	-2.797792558155	1.398934699775
O	-7.333468618025	0.924289039368	0.086085542423
O	7.365931933505	3.853276118246	-0.750645709236
O	9.903411428558	2.953058438401	-0.724688665248
O	0.353559536714	4.975594762582	0.142000835130
O	7.287450132031	8.246716646916	0.442786511511
O	-12.896014928389	0.218725685969	1.398940498925
O	-5.986914425249	3.940812779324	0.086080585488
Ge	5.976250865832	7.017303753921	0.877443335169
Ge	-8.873510954105	0.646004610580	0.906904599773

Ge	6.354466689748	1.430363404492	0.957724527894
Ge	-7.526953185069	3.662530572267	0.906907066038
Ge	4.629704922498	4.000787623871	0.877438534829
Ge	7.701021670356	4.446880473435	0.957729466604
TV	8.968610000461	0.000000000000	-0.000000000000
TV	2.693099485442	6.033039960877	0.000000000006
TV	-4.805013454126	5.387528691916	2.462607030130

EQ'-GeO₂ 25

O	6.288229338250	0.557121884639	0.371168156818
O	6.948952936851	-2.093149500248	-1.414273728693
O	-2.769599412196	4.272466605357	-0.577262848032
O	4.619183999301	5.784244970047	1.008677922088
O	-9.352315513205	-1.059056641575	1.956850715156
O	-6.640796277038	-0.787213911783	-0.077893113734
O	7.166987989424	3.684311758352	0.371153765449
O	7.827816893410	1.034051227680	-1.414282516326
O	-1.890770665468	7.399688938415	-0.577266293988
O	5.497928051135	8.911450004063	1.008655004692
O	-8.473544339520	2.068125622125	1.956843526890
O	-5.762018412686	2.339985123441	-0.077888258850
Ge	3.738476527582	6.812085352696	-0.255171359917
Ge	-7.595751495558	-0.468900952486	1.634655509911
Ge	5.454332226693	3.169416454788	0.689859343005
Ge	-6.716973464404	2.658297151316	1.634621893779
Ge	2.859625841503	3.684881926950	-0.255199595801
Ge	6.333198668339	6.296638286564	0.689847823825
TV	7.383764901369	0.000000000000	0.000000000000
TV	1.757632105176	6.254413268434	0.000000000006
TV	-5.044048039253	6.096757744160	2.872539417392

EQ'-GeO₂ 26

O	-1.050644577483	1.318577996965	0.305412972202
O	2.331215591763	0.045064659326	-0.961819578257
O	-3.001248543046	2.224063198684	-0.375518590687
O	4.554141955260	8.036951930956	2.163857857408
O	-2.426964717160	-0.680912195770	1.581943277704
O	1.067803185346	0.224860032938	0.893941496153
O	-3.063542456675	4.586565741915	0.305472541283
O	0.318277588575	3.313039784683	-0.961834324504
O	-5.014128982436	5.492016322237	-0.375536202569
O	2.541234481653	11.304926877972	2.163843287201
O	-4.439867224252	2.587081773479	1.581953059040
O	-0.945048644660	3.492859523958	0.893922208226
Ge	-3.376657125936	3.763410595231	-1.308622778313
Ge	-0.681308554488	-0.220879791856	1.240001110757
Ge	0.697346745592	1.767971395990	-0.035947117389
Ge	-2.694196410248	3.047119827218	1.240009443926
Ge	-1.363731135576	0.495389593183	-1.308643866528
Ge	-1.315544117774	5.035965766940	-0.035945933189
TV	5.445121793490	-0.000000000001	0.000000000000
TV	-4.025812087945	6.535981509241	0.000000000004
TV	0.738592444344	3.815922630284	3.816732117321

EQ'-GeO₂ 27

O	-1.403385119757	1.472646608692	0.192270372800
O	2.138905821157	0.406859435766	-1.183252879097

O	-3.374635122268	2.334967885120	-0.275709807283
O	4.548219943868	8.200342779670	2.224251345094
O	-2.751790613502	-0.444186999411	1.705752990871
O	0.769034375573	0.493918584208	0.698888906309
O	-3.298309625185	4.682625482308	0.192264162745
O	0.244001918436	3.616886025207	-1.183251996059
O	-5.269540920184	5.544992145767	-0.275698856467
O	2.653306305506	11.410359379572	2.224281670708
O	-4.646717968100	2.765813343520	1.705755016734
O	-1.125876297263	3.703939629539	0.698912771495
Ge	-3.341966153494	3.706996504736	-1.468782614342
Ge	-0.989168361917	0.015250105619	1.198818553695
Ge	2.100761276480	-0.955227639092	0.021971348630
Ge	-2.884092810429	3.225246183180	1.198808656916
Ge	-1.447056751151	0.496997361028	-1.468761486286
Ge	0.205844786686	2.254805647499	0.021979154787
TV	5.411515171559	0.000000000000	-0.000000000000
TV	-3.789851221461	6.420011050222	0.000000000000
TV	0.864972153147	3.723336463111	3.855091127256

EQ'-GeO₂ 28

O	5.133776288146	-0.880184909193	-0.796094259705
O	8.606127582455	-0.238667889293	-1.007698530676
O	-1.118775949932	0.497384438040	0.462950770514
O	4.431199161674	6.092996875753	-0.084707009009
O	-11.473540163905	-1.718582415876	1.238080111129
O	-6.684437354607	1.403492566108	0.711297219840
O	5.791384335336	2.155988038522	-0.796122765272
O	9.263718029274	2.797453675728	-1.007724269080
O	-0.461195268068	3.533597907628	0.462973298837
O	5.088777019649	9.129185027655	-0.084717284525
O	-10.815926497483	1.317580301616	1.238049026393
O	-6.026851925825	4.439656587966	0.711285515401
Ge	3.941811565393	7.778637109590	0.223512769937
Ge	-7.478286809164	-0.031457065911	1.681745511675
Ge	5.479129874187	2.659258079789	0.907489027943
Ge	-6.820676477414	3.004716711140	1.681770646598
Ge	3.284189469965	4.742480597006	0.223499442625
Ge	6.136713671338	5.695414883459	0.907506723675
TV	7.580405590873	-0.000000000000	-0.000000000000
TV	1.315184122735	6.072358617962	0.000000000006
TV	-5.400109907769	5.929042880873	2.907248803630

EQ'-GeO₂ 29

O	1.397081441622	1.957675528657	-0.416790296587
O	2.418096347278	0.537117411806	-2.628745464264
O	-0.747609627349	2.025132540955	0.343331815486
O	-3.335679378886	4.296321961690	5.056170111956
O	-1.944395635221	0.693932395190	1.750515361331
O	0.331599978109	0.725549370934	2.686435922011
O	-2.270266395250	4.124394836729	-0.377009964920
O	0.762145502467	2.910378871145	-2.838536243386
O	-4.409365441250	4.114782314762	0.433519891988
O	-6.197325828296	6.544642598752	5.109745099902
O	-3.185176110777	2.795105906942	1.993677554465
O	-1.042206548569	2.650812207300	2.635757569810
Ge	-2.062463480874	2.111698282060	-3.441617274455

Ge	0.718220664065	1.203458614455	1.046707285222
Ge	2.948189414678	1.143804694515	-1.054614108127
Ge	-1.651124373605	3.405273771421	1.150144686931
Ge	-0.178756443131	-0.001620194970	-3.564388076021
Ge	0.525155747717	3.356998235589	-1.124246508971
TV	4.342112271755	0.000000000003	-0.000000000003
TV	-4.314355132232	4.384932852358	-0.000000000002
TV	-6.455542053342	1.509154616514	6.958653384352

EQ'-GeO₂ 30

O	5.940935192706	1.118325252206	-1.001656849865
O	8.530700847700	0.094918372520	-1.003030586461
O	-1.120423825836	1.995524622541	-0.163163337697
O	5.885013728202	4.709099718233	1.447887281977
O	-13.370227875753	-3.639931838575	2.290213043106
O	-7.388426453357	0.971741181740	-0.163043703549
O	7.050582461030	4.193412418238	-1.001656884469
O	9.640351143654	3.170000243870	-1.003028196066
O	-0.010767700999	5.070610382969	-0.163166598247
O	6.994669724577	7.784187696307	1.447893321717
O	-12.260578389334	-0.564853335395	2.290201689775
O	-6.278776738708	4.046832250851	-0.163045866236
Ge	5.339348925829	7.454577656288	0.643294395813
Ge	-9.427319484520	-0.746621005802	0.642954650535
Ge	6.806458859284	3.348602236910	0.643098888552
Ge	-8.317671838934	2.328468355295	0.642962604337
Ge	4.229694967421	4.379494423583	0.643290682216
Ge	7.916110308620	6.423685760000	0.643091410834
TV	8.855427948850	-0.000000000000	-0.000000000001
TV	2.219302469294	6.150181323390	0.000000000012
TV	-5.224123712214	5.640259518828	2.451632640611

EQ'-GeO₂ 31

O	0.650566964062	2.067961063505	-0.325053122074
O	0.733697032762	-1.458503054624	-2.645906974886
O	-0.844075529036	3.656776506108	0.211894128896
O	1.384955590166	2.904132914117	4.957963864320
O	-0.774235607805	-0.436921376654	2.759922435678
O	0.648934210347	1.160948669646	1.827320452522
O	3.605843795015	2.067956064058	-0.325009696374
O	3.688983448472	-1.458570102796	-2.645908314177
O	2.111174419967	3.656730768562	0.211994732097
O	4.340229823224	2.904050620067	4.957930632737
O	2.181051359399	-0.436950363574	2.759957588495
O	3.604281840824	1.160935819571	1.827323667334
Ge	2.151391633017	1.451086240023	-3.571056883875
Ge	-0.817482774180	2.075196682078	1.065137915505
Ge	0.689110842171	0.469217935265	-1.166052287094
Ge	2.137807978354	2.075170748769	1.065165632616
Ge	-0.803854031990	1.451102637713	-3.571036431021
Ge	3.644361274887	0.469196904202	-1.166090029437
TV	5.910571487463	0.000000000000	0.000000000002
TV	-0.043921322188	3.199966191603	-0.000000000000
TV	-0.737777640747	-0.384346909735	7.045758901539

EQ'-GeO₂ 32

O	-1.648925952347	1.766395287327	0.761522334574
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O	-0.123221122564	-0.806660118909	-2.860518255153
O	1.430627024654	0.196931503195	3.345890278221
O	-0.117797077174	-3.438939524678	-0.717143920887
O	-3.184456005023	5.086683563582	0.865634342709
O	-1.654704528111	1.450830323856	-3.197355035824
O	-0.106245196455	2.458763599034	3.016256010752
O	-1.655780845057	-0.128861652113	-0.622506104522
O	-4.721352810019	7.348555139349	0.536008262368
O	-3.192714872142	4.760897049041	-3.102772029202
O	-1.639157870677	5.683592799762	3.241724095325
O	-3.191587945402	3.110529018450	-0.380264858432
Ge	-3.183749120064	4.685515632300	-1.237851067388
Ge	1.431336173841	-0.204238823581	1.242390804611
Ge	-0.109150277684	2.773872880016	1.314867315664
Ge	-0.118933642419	-1.143328472034	-1.165382309953
Ge	-1.655260799674	1.848085105429	-1.097968316532
Ge	2.959788993418	-3.041665662411	1.382240601530
TV	3.078131755558	-0.000000000002	-0.000000000007
TV	-4.605296293237	8.806953191036	-0.000000000004
TV	1.546700980519	-0.972548961784	4.960457712101

EQ'-GeO₂ 33

O	-0.035698487316	1.218374132398	-0.777379072385
O	-0.347383364253	1.415004694040	-4.061470486037
O	-0.151314892947	2.999144034822	0.486705719808
O	0.115179756156	1.129742242337	6.557482326409
O	0.445832126008	0.942314344431	3.704261873471
O	-0.226496567379	-0.371572495584	2.073088336819
O	2.447618987194	1.448771673845	-0.909865579730
O	2.775512405784	1.256442986532	-3.761922380219
O	3.124598801086	2.754306345151	0.721141543742
O	3.240950052182	0.973531596216	6.859372208042
O	2.926981106474	1.162450693972	3.574374567023
O	3.043379034018	-0.619542529171	2.309961716548
Ge	2.671313988791	3.031327143267	-4.561392369268
Ge	0.046567608558	1.174938341637	1.120677580688
Ge	1.199217988141	0.485556943847	-1.844903690562
Ge	2.849231458949	1.207759242530	1.674685772418
Ge	-0.145006442187	3.002915201092	-4.968413699065
Ge	4.014155315099	0.510749847933	-1.436347005275
TV	5.721395231125	0.000000000000	-0.000000000000
TV	1.511967743291	2.515410090198	0.000000000000
TV	-0.976284292096	-1.127241267707	9.200966127713

EQ'-GeO₂ 34

O	0.659500478241	1.379373100462	-0.926399447865
O	-0.709129499086	-1.165223324072	-4.206352656822
O	0.830359532529	2.961958717208	0.549246099809
O	2.158257797647	2.141164340645	7.034675894300
O	-0.598634819907	0.445088634607	3.780715019939
O	0.781925534448	1.298564313514	2.326368289104
O	3.416776974755	1.392249325549	-0.948511349898
O	2.036023491035	-1.145299928094	-4.177920639904
O	3.624143982988	2.953376327250	0.544606669067
O	4.970401855428	2.124036134418	7.041029580977
O	2.210425598274	0.427106079724	3.764498468001
O	3.549882878100	1.305930569806	2.323883347620

Ge	2.189993569150	2.143508522298	-5.096008647601
Ge	-0.582659574558	2.130076927851	1.456705755196
Ge	-0.765273415934	0.556625821672	-1.784833592884
Ge	2.197018382657	2.129569888630	1.422622697946
Ge	-0.589265155347	2.144354627567	-5.035629792665
Ge	2.010074232175	0.557058597000	-1.840198383055
TV	5.556362406984	0.000000000000	0.000000000002
TV	1.499316188173	2.469123142255	0.000000000000
TV	0.082745827786	-0.065323494571	9.748632582535

EQ'-GeO₂ 35

O	0.380075078180	0.369324955756	0.820221991005
O	0.378564754354	-1.189278586457	-3.915365505520
O	0.384527250602	0.521648214467	4.074656054296
O	0.378211121402	-2.661205228849	-0.661315442233
O	-1.065137412598	2.738685237958	0.820246977046
O	-1.066655648793	1.180039218991	-3.915383224455
O	-1.060751371884	2.890995309604	4.074663616929
O	-1.067018811990	-0.291849549784	-0.661295858403
O	-2.510385722572	5.108018868777	0.820240843797
O	-2.511886934314	3.549383840087	-3.915367680445
O	-2.505971904321	5.260381492350	4.074673155573
O	-2.512264072617	2.077532194448	-0.661318804169
Ge	-2.510181022228	3.665509545371	-1.565369134308
Ge	0.382393474109	1.963058702936	1.688691255789
Ge	-1.062841821493	4.332424508160	1.688749146379
Ge	0.380311120934	-1.073195643846	-1.565298994017
Ge	-1.064923046000	1.296148604727	-1.565361904527
Ge	1.827616533881	-0.406295413988	1.688705655190
TV	2.896064495333	-0.000000000000	0.000000000000
TV	-4.335719942077	7.108063282042	-0.000000000003
TV	0.001181920817	0.001088535401	6.508272587501

EQ'-GeO₂ 36

O	0.717286537883	-0.595375672183	-1.769949770842
O	-0.731075372981	-1.411396141847	-3.554963512336
O	2.169706629634	2.225210987190	6.285304755393
O	0.715198863871	-2.034560105216	1.520548699853
O	-0.725472614387	1.761216799569	-1.769958337353
O	-2.173830005718	0.944996415163	-3.554882978225
O	0.727012178656	4.581683419595	6.285330889438
O	-0.727631227702	0.321862853970	1.520481047708
O	-2.168163831402	4.117677054083	-1.770008046712
O	-3.616583049505	3.301462642601	-3.554967488803
O	-0.715794325327	6.938132647785	6.285337558032
O	-2.170322540278	2.678346247524	1.520570454361
Ge	-2.171200539101	2.530651637236	-2.661245769095
Ge	-0.724531578480	1.907016720795	0.621911230417
Ge	-2.167249112344	4.263473271283	0.621896585042
Ge	0.714339490246	-2.182278556909	-2.661317268031
Ge	-0.728431480094	0.174187643695	-2.661199365588
Ge	0.718242883408	-0.449436222504	0.621883464451
TV	2.892306679302	-0.000000000001	-0.000000000001
TV	-4.328300322184	7.069348517438	-0.000000000000
TV	1.450363059306	1.091492435380	6.564803119618

EQ'-GeO₂ 37

O	2.049254617268	-1.121465423405	0.401347045561
O	-0.848537786948	-1.048090084493	-2.835558134889
O	0.546079983500	-0.208285922650	1.933784682727
O	0.595838017300	-1.929063036518	-1.391015232727
O	4.819727459847	-1.121471976511	0.401340532149
O	1.921936803274	-1.048100235405	-2.835566999076
O	3.316547808329	-0.208291275945	1.933774547759
O	3.366300485667	-1.929066498007	-1.391010574555
O	7.590200181796	-1.121468596223	0.401341378749
O	4.692399771208	-1.048103769646	-2.835565594591
O	6.087022492042	-0.208291611079	1.933774808799
O	6.136772879365	-1.929060730603	-1.391013103023
Ge	6.237294288665	-0.293942432360	-0.485057206024
Ge	4.671731480802	-1.036289595440	2.818093442894
Ge	7.442210686766	-1.036279401086	2.818105668470
Ge	0.696354528946	-0.293939031661	-0.485055115975
Ge	3.466822828897	-0.293939821335	-0.485053412165
Ge	1.901266934514	-1.036287445098	2.818105413915
TV	8.311403901755	-0.000000000000	0.000000000000
TV	1.518455086262	2.461811442337	-0.000000000001
TV	-1.438936014318	-0.814651688925	6.562217399157

EQ'-GeO₂ 38

O	-0.365601999278	1.250577424875	-0.860379335363
O	1.338380336350	0.586997169060	-4.213916353843
O	-1.695507270519	2.143756973834	0.575199185978
O	-1.754840678199	2.101576030626	7.099587601998
O	-0.017335733261	1.459475341065	3.779387070234
O	1.160581627247	0.480199252385	2.289875528988
O	2.501031310533	1.301738513706	-0.945836773516
O	3.963313260975	0.490012413676	-4.108856732512
O	1.178018632415	2.194219275734	0.571168172361
O	1.167852057327	2.190883515040	7.043335736492
O	2.608705078851	1.365154187885	3.850803703556
O	4.023695277034	0.524585528603	2.392814657559
Ge	3.945127097737	2.188280302761	-4.883954900596
Ge	-0.227768723328	1.336516673656	1.372020369398
Ge	1.109206558536	0.447956274079	-1.693090057489
Ge	2.559999082355	1.334645549048	1.542899514877
Ge	1.161403912445	2.186930865884	-5.172070541118
Ge	3.872478394038	0.438152395425	-1.878929484596
TV	5.563628309934	0.000000000000	0.000000000000
TV	-1.525200714228	2.478320019010	0.000000000000
TV	-2.684470053886	0.056432719291	9.720060106688

EQ'-GeO₂ 39

O	0.426611091911	1.432158436234	-0.518324304814
O	0.395277194305	0.542361529170	-2.604868311575
O	-1.163233136768	2.855489436062	0.394113216868
O	-0.972438956924	2.246370034920	4.951203333322
O	-0.998144117705	1.345570346776	2.866233871472
O	0.593466382004	-0.092284761802	1.949828416953
O	0.429408458624	4.382405669130	-0.518249370611
O	0.398082264172	3.492646632109	-2.604796875152
O	-1.160402095852	5.805795240974	0.394104913003
O	-0.969661843470	5.196623810087	4.951303203549
O	-0.995337502667	4.295810513833	2.866295406045

O	0.596280697558	2.858020947095	1.949808438041
Ge	0.399797463759	4.970730081096	-3.567843345801
Ge	-0.285592309452	1.379784348530	1.175359130666
Ge	1.972569062603	0.589900846722	-1.265829328151
Ge	-0.282869428538	4.330027464003	1.175373374778
Ge	0.397013830802	2.020493693341	-3.567832625728
Ge	1.975328848936	3.540123966505	-1.265821780390
TV	3.137341786079	-0.000000000000	-0.000000000000
TV	0.005611991131	5.900500772107	0.000000000000
TV	-2.935595289345	0.176681017250	7.182181760249

EQ'-GeO₂ 40

O	2.757941662835	1.921671820784	-0.207735379981
O	3.836042541206	-0.879359552142	-2.227987664590
O	2.504337120918	6.446020945830	-0.914061218874
O	5.199641471546	5.600767393162	1.711029569482
O	-4.712915255216	-0.751695182705	0.292090880725
O	-9.077008512402	-4.217586279809	1.874009033419
O	7.861365651418	1.568401073681	0.103306500368
O	9.443713374630	0.137715923053	-1.019177777669
O	7.151094152398	5.391572612822	0.130627298373
O	9.334166660066	5.942809424273	1.403994369904
O	-0.989187188760	-2.000761301716	1.386396312522
O	-3.428655350282	-3.871950544039	3.083993117168
Ge	6.379076672119	1.976820029069	-1.151292633919
Ge	-6.213230202768	-1.515606435418	1.229991462016
Ge	3.119942893785	4.908100346980	0.271559156494
Ge	-2.024142419262	-2.710770374526	2.663849312812
Ge	2.526867402375	2.818571686265	-1.922488447392
Ge	9.459658257409	3.796007365778	-0.035007944587
TV	9.239660705364	-0.000000000000	-0.000000000000
TV	1.801910330599	4.126699392525	0.000000000000
TV	-2.210124071884	5.024073939300	3.451943141794

EQ'-GeO₂ 41

O	-1.347705920848	1.081824466320	-0.037316096224
O	1.376551671969	-0.212817017740	-0.974597757107
O	-2.788406126469	2.720055486189	-0.221627610437
O	3.210449327701	10.270692392172	2.069081326558
O	-2.294621804180	-0.785407108661	1.591690628033
O	0.794550209982	0.889671754564	0.908472179571
O	-3.354934709469	5.000963673201	-0.037314158723
O	-0.630680866788	3.706314241307	-0.974591854713
O	-4.795636381629	6.639196026054	-0.221624022129
O	1.203220265533	14.189835186134	2.069084198824
O	-4.301828616624	3.133734609496	1.591691082131
O	-1.212668928168	4.808805228492	0.908463876259
Ge	-2.548953851205	3.977807164622	-1.462572981898
Ge	-0.648289230280	-0.137097308281	1.222032259435
Ge	1.963895172084	-1.596280129116	0.019083953652
Ge	-2.655503349917	3.782043052758	1.222026905678
Ge	-0.541710736470	0.058669564734	-1.462571111292
Ge	-0.043328217547	2.322851621739	0.019086493628
TV	4.531461812749	0.000000000000	-0.000000000000
TV	-4.014463590606	7.838274547845	0.000000000000
TV	0.301121231012	4.789738617851	3.835597243017

EQ'-GeO₂ 42

O	1.444427780280	1.141262679738	3.253575034797
O	-0.203073447117	-0.763480024895	1.898798250222
O	3.071482831832	1.934705763421	1.810273939094
O	-1.851738781117	0.456061472616	0.540401299710
O	4.701015404715	3.839160052773	3.166219361795
O	1.431603446747	-1.871414405454	0.840877811346
O	4.711851956295	1.141265317617	3.253558137672
O	3.064278739627	-0.763155113615	1.899016028444
O	6.338873951964	1.934725902931	1.810314328459
O	1.415515537899	0.456114090289	0.540313211542
O	7.968433496264	3.839024944077	3.166119848185
O	4.698667882858	-1.871343168673	0.840836127350
Ge	9.602805604031	3.321790307025	2.893546718575
Ge	1.431358784031	-0.246036715813	2.169213747648
Ge	3.092317846513	0.939194874367	4.370234986346
Ge	4.698847668693	-0.246095729074	2.169282272304
Ge	6.335362471877	3.321896075966	2.893511602342
Ge	6.359665529122	0.939259832090	4.370291630679
TV	6.534736750775	-0.000000000002	-0.000000000000
TV	3.271082197389	5.689166099880	-0.000000000000
TV	-1.629514670541	-1.197395866071	3.682047864925

EQ'-GeO₂ 43

O	1.917583201334	2.709887193985	-0.838116775098
O	2.071311546815	0.246859307967	-0.620920762828
O	0.370264265287	2.948032684046	0.665423726982
O	9.483608977066	7.805496820555	1.011002996069
O	-8.149080569386	-2.509020027808	-0.711514801771
O	-4.188752624689	-1.930696388928	1.232559081436
O	3.839311508944	6.318031314838	-0.838034012409
O	3.993027311098	3.854944601510	-0.620940702379
O	2.291929823349	6.556184934907	0.665434231852
O	11.405351629711	11.413551115055	1.010910903558
O	-6.227327998966	1.099144303583	-0.711498360249
O	-2.267021767386	1.677439450574	1.232525600990
Ge	2.622386935097	5.071095029551	-0.593240519141
Ge	-5.929726838597	-1.627258308289	1.968569161439
Ge	3.876619339469	3.174985265277	1.222761105206
Ge	-4.007940936420	1.980879237775	1.968618111181
Ge	0.700672817891	1.462947966873	-0.593226667845
Ge	5.798331792569	6.783083608070	1.222783629290
TV	5.184620426055	-0.000000000003	0.000000000001
TV	3.843499604447	7.216213937444	-0.000000000000
TV	-0.391031541904	3.084210625641	3.608123320186

EQ'-GeO₂ 44

O	-1.241994085091	-0.912976312273	-0.124809884002
O	1.770758076174	0.594928685799	-1.569446717511
O	-3.533737789177	0.169644303954	0.135967960273
O	7.606413856263	11.533418735947	4.480179079722
O	-0.729797183532	0.515110002598	2.117986637935
O	-0.028711346343	1.265589120650	0.082755071959
O	-4.144288216007	2.502566703728	-0.124878949963
O	-1.131992294639	4.011025640644	-1.570062177469
O	-6.436067465536	3.585326333717	0.135109425951
O	4.704157153306	14.949106700845	4.480184101136

O	-3.632132833143	3.930638815235	2.117980939452
O	-2.931029595587	4.681246265786	0.082745756115
Ge	-5.598744455670	2.393751610544	-1.744259704212
Ge	-1.785740595676	0.662256031911	0.515624348696
Ge	0.513746309489	-0.311576358884	-0.556602197227
Ge	-4.688039346165	4.077817271019	0.515586801511
Ge	-2.696416346834	-1.021957784690	-1.744334936968
Ge	-2.388540838111	3.104080628433	-0.556629608956
TV	5.802911111471	-0.000000000005	0.000000000008
TV	-5.804589040865	6.831192937051	-0.000000000000
TV	1.169299777214	5.851246743996	3.312386898419

EQ'-GeO₂ 45

O	0.431325182307	-0.785707891249	0.882752578901
O	1.245809641647	-1.784283303725	-0.734639647784
O	3.379343705682	2.367000501308	0.890296450865
O	-0.963077005616	-2.030431916057	-0.721688430740
O	1.194931240082	1.318210228189	0.728630690335
O	1.567207600106	1.067046444215	-0.987098835116
O	4.453564729222	4.893689822024	0.984849907584
O	-0.649544832853	0.655439865486	-0.838195623123
O	2.236453544880	4.488602799225	1.133972066821
O	2.609078454918	4.232130778350	-0.580448033153
O	4.763962071604	7.587201447265	0.866349608101
O	0.424725527272	3.186265564476	-0.742392068093
Ge	-0.236173187230	4.859668431234	-0.953713020760
Ge	4.039939719260	0.693166058196	1.100994488233
Ge	5.265632073064	3.164946245736	1.102467577508
Ge	-2.083027095617	-0.527264631602	-1.145127726139
Ge	-1.457468600698	2.387037344936	-0.955058577769
Ge	3.759829804381	-2.039553619357	1.292820742271
TV	4.550115575151	0.000000000000	0.000000000000
TV	2.123186413211	8.119869114951	-0.000000000003
TV	-0.935801074612	0.080890666806	3.600154727750

EQ'-GeO₂ 46

O	-0.616863020296	1.572890151180	-0.331587671288
O	4.819049212942	0.228265212866	-2.418163515094
O	-3.172937362203	1.834585725638	-0.524769615771
O	4.393354519118	6.279533665163	3.160692949592
O	-2.842195492080	0.129669832861	1.073284401417
O	-0.287608968331	-0.134212292430	1.265677408384
O	-1.933971768262	4.137734003021	-0.695863714670
O	3.485853190496	2.281278490844	-2.418459975043
O	-4.544127356927	3.944633827290	-0.525696039892
O	2.604309151650	9.035038352704	3.158926612858
O	-4.649460982270	2.373015666284	1.437295262889
O	-2.040605067042	2.563720959039	1.265863851028
Ge	-3.252806693593	3.282010875659	-1.623940935958
Ge	-1.562717697527	0.955648415286	2.027134170434
Ge	0.902333215267	0.851170387851	0.371975698821
Ge	-3.329521686254	3.225833440901	2.366642790601
Ge	-1.895675650409	0.746528651230	-1.286443912419
Ge	-0.660001220790	3.254821937568	0.370528180442
TV	5.264479927452	-0.000000000001	0.000000000000
TV	-3.122122770554	4.807129232447	0.000000000004
TV	-0.242969948274	3.256007026493	5.334899581695

EQ'-GeO₂ 47

O	0.406511275870	-0.426745781419	0.383475397069
O	1.242855244806	0.183777982679	-2.072188852695
O	-0.398515169741	-1.237295582663	3.077168460573
O	0.391856741426	-2.436667927970	-1.082153795733
O	-0.828911188130	2.932743798913	0.430894350773
O	0.009182218828	3.495284021498	-2.062111643150
O	-1.650413106567	2.123019068744	3.021933743888
O	-0.852200072538	0.936413213122	-1.076266348856
O	-2.069572221564	6.302654091994	0.396215529168
O	-1.243335656732	6.910858939087	-2.065321811926
O	-2.884730560239	5.492115773683	3.026734145752
O	-2.085961969017	4.248029475901	-1.071473944666
Ge	-0.549741303162	6.817999252770	-0.446021962050
Ge	-0.222458283577	1.291937707144	0.603442743288
Ge	-1.459877050995	4.666303614541	0.588060398270
Ge	1.924012215576	0.097139574308	-0.448244982792
Ge	0.678533152874	3.443649349447	-0.431579892797
Ge	1.030183331909	-2.055531926825	0.587554416652
TV	4.254007505207	-0.000000000000	-0.000000000000
TV	-3.720518370932	10.084776572288	-0.000000000003
TV	-1.701103634508	-3.053345758740	3.294658120851

EQ'-GeO₂ 48

O	-1.110458654126	0.901271792531	0.310976667528
O	2.982821990570	0.521462790249	-1.400822192283
O	-4.864831504235	2.036772760858	-1.386813568680
O	4.140807620195	6.764651494541	3.248196855934
O	-3.060400267548	-0.413092645842	0.810740206485
O	0.900315031678	0.456216202403	1.793192241469
O	-3.114262946134	3.825019337469	0.310975157864
O	0.979011106614	3.445211204808	-1.400818989935
O	-6.868638446363	4.960525390096	-1.386827735070
O	2.137011155957	9.688399696687	3.248203359599
O	-5.064209228148	2.510660299294	0.810748028480
O	-1.103486902923	3.379964880432	1.793202193612
Ge	-2.943450664992	4.205613669595	-1.391184945988
Ge	-0.218027811583	-0.627323683840	0.924603269241
Ge	1.894197433513	1.129962659487	0.205351226890
Ge	-2.221828460075	2.296429055798	0.924606514217
Ge	-0.939643516550	1.281863873981	-1.391182928145
Ge	-0.109609324453	4.053713796046	0.205351950059
TV	5.827102391055	0.000000000001	0.000000000001
TV	-4.007612654297	5.847500672720	0.000000000000
TV	-0.455636530654	3.791395048112	3.910562256960

EQ'-GeO₂ 49

O	3.030487267756	1.421968860931	-0.319580815508
O	3.497210154405	-0.367502528489	-2.005149539271
O	0.929845751130	2.199967534651	-0.006882777175
O	0.166619821183	4.511484831689	2.780142675559
O	-4.062289897069	0.348990866380	1.370698438080
O	-0.122057869115	-1.892723776123	1.976071959137
O	1.481664194802	4.311770415735	-0.319614130772
O	1.948377798680	2.522264556435	-2.005156419694
O	-0.618964615789	5.089718574428	-0.006881095135

O	-1.382242697471	7.401255640560	2.780185993760
O	-5.611127346583	3.238764718473	1.370680280329
O	-1.670920799243	0.997085617257	1.976101891059
Ge	-1.153939195034	6.361708924493	-1.622826463000
Ge	-6.814471578148	-0.627005686154	1.611225398714
Ge	2.897332141771	3.254238068496	-0.447156263202
Ge	-8.363318840510	2.262791199725	1.611230774694
Ge	0.394888831315	3.471919097984	-1.622841445936
Ge	1.348512926127	6.144040605701	-0.447152515309
TV	4.341036099023	0.000000000000	-0.000000000001
TV	-3.097663773348	5.779576873170	-0.000000000000
TV	-3.883855442613	2.663137097232	5.304645354149

EQ'-GeO₂ 50

O	1.361930221224	-2.094471876048	-0.020166235881
O	-0.380375022373	-1.994803609802	-1.582872657472
O	1.145922490614	-0.505942019981	1.536863811088
O	-0.573173245638	-0.393292036245	-0.025505933428
O	0.940691667522	1.252732513536	-0.020093744228
O	-0.801627610267	1.352424886583	-1.582720873717
O	0.724661924872	2.841244935211	1.536838188518
O	-0.994415076485	2.953979457748	-0.025497960795
O	0.519493383610	4.600023734038	-0.020127409922
O	-1.222991411042	4.699559621377	-1.582844972375
O	0.303406625561	6.188490562096	1.536822661338
O	-1.415663988102	6.301202833679	-0.025552244196
Ge	0.248446930366	6.301463909603	-0.951796063368
Ge	-1.148789718781	4.601654001999	0.898856562279
Ge	-1.570104607912	7.948871984827	0.898854920601
Ge	1.090958967315	-0.393000919099	-0.951792175617
Ge	0.669698353932	2.954228617715	-0.951781323013
Ge	-0.727569292424	1.254388951503	0.898876542925
TV	3.409846792790	-0.000000000000	0.000000000000
TV	-1.263775966141	10.041713382368	-0.000000000000
TV	-2.339075624259	-1.034471233909	3.800693098822

EQ'-GeO₂ 51

O	-2.482492228773	2.494044617529	-0.299015848213
O	3.015704312666	0.248745789049	-1.724779798763
O	-4.343028763918	1.409479687477	-0.590214084329
O	5.071975079903	6.465104881521	2.767875508758
O	-2.379928704371	0.526816876688	0.757643115989
O	0.884396724759	0.377108227929	1.510632980242
O	-3.800829336025	4.648959566775	-0.306615195200
O	1.928369333386	3.102780363610	-2.197499942683
O	-5.603992985130	3.489383707336	-0.588924884776
O	3.226424392304	9.563640276253	2.770370016556
O	-4.366558015243	2.832700624731	1.310058202681
O	-0.963028716265	3.484844504025	1.517148073283
Ge	-2.446376428564	3.996984647022	-1.321584784840
Ge	-0.885152187038	-0.408800262067	1.497342664383
Ge	2.013699339490	-0.350206294964	0.198506946289
Ge	-2.489487687495	2.290068624474	1.504809196491
Ge	-1.340583114186	1.144150778445	-1.089983059179
Ge	0.076060772592	1.991487363694	0.512728204616
TV	5.803594942712	-0.000000000000	0.000000000000
TV	-3.090058673358	5.164172479567	-0.000000000000

TV	-0.164603148346	3.448439612959	4.420787123538
# EQ'-GeO ₂ 52			
O	-2.157133407703	1.238488381819	-0.801204250548
O	-0.866210603802	-1.341346919061	2.356046545523
O	-0.851781301201	0.396315297566	-2.250393195844
O	-0.682774992622	1.656127663914	0.900407951481
O	-2.405805450483	0.106658910065	1.277631865211
O	0.626951356521	-1.212554313360	-1.492150055377
O	1.071035104323	1.238474015491	-0.801206091263
O	2.361954678973	-1.341403757493	2.356032850907
O	2.376370837076	0.396351125476	-2.250389268113
O	2.545346208217	1.656126568764	0.900378003932
O	0.822366495280	0.106623135233	1.277620331883
O	3.855136494433	-1.212507218944	-1.492135638945
Ge	1.956710703118	-1.398114762775	0.573506165499
Ge	-1.033131888554	-1.562557052658	-2.436683990797
Ge	-0.441212483895	0.364146133745	-0.399496550383
Ge	2.195028021048	-1.562508795602	-2.436698293192
Ge	-1.271457202268	-1.398104113725	0.573540497503
Ge	2.786969608260	0.364155636849	-0.399477669234
TV	6.456326759737	0.000000000000	-0.000000000000
TV	-1.105801093915	3.915948090503	-0.000000000000
TV	-1.217016127746	-1.953253899135	5.215732220849

# EQ'-GeO ₂ 53			
O	3.038211495283	2.224608561481	-0.848628072259
O	1.588572833804	0.039925389671	-0.789471963194
O	0.767739524826	0.977939299319	-0.086013228780
O	1.549400588984	5.982693486674	2.271281867994
O	-3.364857635154	-0.987685457437	1.098001406625
O	-0.724219345321	-3.166806501008	1.014121498145
O	2.471300900194	5.914387704327	-0.848705038028
O	1.021761687928	3.729695905709	-0.789496174816
O	0.200871537977	4.667695338489	-0.086074701799
O	0.982470162004	9.672523768757	2.271241996848
O	-3.931739338688	2.702079144895	1.097990712029
O	-1.291073284700	0.522946153006	1.014139353156
Ge	-0.844353734079	7.085099074181	-2.084306132473
Ge	-4.327523108624	1.420189304925	2.318149705799
Ge	1.880482038236	2.380221105979	0.443470247944
Ge	-4.894368205650	5.109973469348	2.318240363693
Ge	-0.277523444130	3.395314844240	-2.084327219892
Ge	1.313690435585	6.069890359474	0.443481325304
TV	4.050561788344	-0.000000000000	-0.000000000001
TV	-1.133700451337	7.379543863904	0.000000000000
TV	-3.455678963392	4.108803732598	4.475873482247

# EQ'-GeO ₂ 54			
O	-1.748424474655	-3.174834945184	-2.623330803293
O	-0.320778736914	0.086146617898	0.307748420485
O	0.465704358776	-2.354262947534	-1.886664942927
O	-1.263536286975	-2.052246029598	1.163458127546
O	-2.440951039730	-0.831686542485	-0.291445362203
O	-0.468515513055	-1.569113481596	-1.177729275348
O	-2.902564401366	-0.157099111897	-2.623328768236
O	-1.474922708437	3.103870355968	0.307739706750

O	-0.688416602722	0.663481079497	-1.886668086895
O	-2.417655833343	0.965473413450	1.163458716070
O	-3.595073381288	2.186053122813	-0.291444719384
O	-1.622624310284	1.448606761657	-1.177726715866
Ge	-2.143205650242	-0.648592924267	2.191436563050
Ge	-2.095628354601	-2.439789133040	-0.957135532230
Ge	-3.843504738371	-1.391433484899	1.090839877551
Ge	-3.249748566528	0.577943787816	-0.957125413044
Ge	-0.989063756269	-3.666319805293	2.191431207451
Ge	-4.997627070272	1.626293861389	1.090840278341
TV	4.217835370594	-0.000000000000	-0.000000000000
TV	-2.308273987553	6.035459171785	0.000000000000
TV	-1.858429718249	0.201782512138	5.291767191273

EQ'-GeO₂ 55

O	-1.421741161928	2.292832482133	-0.752827658169
O	3.251388763049	-0.637201086132	-1.860275983809
O	-3.900155089123	1.450706959839	-0.006448779221
O	2.792351515084	6.834145301386	3.058835107175
O	-2.046030428439	1.025450907205	1.038812916982
O	1.999671198521	0.343639674308	1.807451393123
O	-3.858207181108	4.777618817506	-0.752819602810
O	0.814893844502	1.847577827265	-1.860259341086
O	-6.336644280094	3.935524333739	-0.006449946998
O	0.355889569905	9.318963341360	3.058816089546
O	-4.482545002657	3.510229548905	1.038800747842
O	-0.436804934952	2.828448400771	1.807498103019
Ge	-6.578186989880	3.308764191239	-1.617442439838
Ge	-0.397355398569	0.369515850720	0.318772463043
Ge	3.472629750241	-0.578049915076	1.127331053104
Ge	-2.833852634390	2.854302962975	0.318804332043
Ge	-4.141698912935	0.823972416681	-1.617454753222
Ge	1.036133589543	1.906735521246	1.127353610479
TV	6.408923468120	-0.000000000005	0.000000000001
TV	-4.872973075969	4.969600403064	-0.000000000006
TV	0.232277998370	3.351915422370	4.276563064943

EQ'-GeO₂ 56

O	0.542232318249	1.571770841274	0.275945941162
O	-0.687476038015	0.823069786473	-1.496592946226
O	-1.824168983331	1.998127967747	-0.037029943119
O	-0.239426891111	3.237552681934	1.754224055500
O	-1.438731474080	0.215932966104	2.774056903931
O	0.799171225420	0.222171735734	1.985423160324
O	-1.799549230018	4.328047145231	0.385272415710
O	-1.642529446152	3.434441609761	-1.955009484984
O	-3.927215433455	3.965052881936	-0.110937957409
O	-3.122591914955	6.297276285102	2.528113727168
O	-2.598869631125	3.310151195559	3.190864860854
O	-1.043753329849	2.172885627831	2.070468225714
Ge	-0.881120452599	4.781735357467	-2.912747527396
Ge	-0.804235626648	0.592109680770	0.995658772602
Ge	1.420591494765	0.364264739959	-0.992101349532
Ge	-2.778202776792	2.930527141462	1.227771756333
Ge	1.375436560557	2.332496188323	-2.425082764556
Ge	-0.356767100444	2.613255884455	-0.976913482898
TV	4.451755065292	0.000000000000	0.000000000000

TV	-4.208776205826	4.808762438435	-0.000000000000
TV	-3.355738283365	-0.728203471452	6.276703469840

EQ'-GeO₂ 57

O	-0.961992529693	1.050663188643	0.794141059044
O	3.123431109044	0.833385224050	-0.060162903392
O	-4.092824769159	2.995233965186	-0.375042757817
O	4.913021962149	8.163255816226	1.104592364606
O	-2.387595062235	-2.039845397482	1.419997146782
O	1.018522520724	-0.082463355835	0.248691086499
O	0.097027637334	4.684981230160	3.370897362041
O	4.181974607432	4.467687869423	2.516117118667
O	-3.033944314754	6.629623322532	2.201543153775
O	5.971638728858	11.797339598800	3.680846830717
O	-1.328712433621	1.594400411167	3.996516602487
O	2.077147231441	3.551469290722	2.825541323500
Ge	-0.723841378948	4.299055295137	1.811121148980
Ge	-0.825700481096	-0.925384452991	1.301985393046
Ge	0.888165325054	1.883283589881	-0.252440702578
Ge	0.233115529905	2.708735361986	3.878633408247
Ge	-1.782568585757	0.664678279165	-0.765608253449
Ge	1.946768947861	5.517748472064	2.324168590304
TV	6.554246623339	-0.000000000001	0.000000000000
TV	-2.566334467531	4.012465272849	0.000000000003
TV	2.117407909627	7.268430428251	5.153295436162

EQ'-GeO₂ 58

O	3.273257657544	1.643482468934	3.231128330274
O	-2.832307997976	-2.712391975423	-4.996367606625
O	1.614376126516	-1.149036769389	5.099368310033
O	0.118380607185	-1.262169938006	-3.093512725689
O	3.462834358678	4.579125336865	3.207619715847
O	-2.689696345966	0.268724851601	-4.984675476625
O	1.894365488003	1.723469447516	5.146659376922
O	0.310791059059	1.631385849005	-3.073847343026
O	3.653753270341	7.463889513607	3.207440287146
O	-2.431882737771	3.094766206545	-4.953544408794
O	2.003200445369	4.668026410375	5.109107496107
O	0.530945955531	4.537778763616	-3.056948940928
Ge	0.665629948750	4.677683194971	-1.236173065527
Ge	3.410754753718	1.766076331638	1.409460393371
Ge	3.627391597763	4.676061785550	1.381768773058
Ge	0.221396913089	-1.149248428541	-1.265166067212
Ge	0.485486718278	1.766506346004	-1.251858426691
Ge	3.163548706699	-1.145045247915	1.381146357876
TV	2.946662300210	-0.000000000000	0.000000000000
TV	0.601201623215	8.716742839996	-0.000000000000
TV	1.373247032060	-1.429305260506	5.050234209365

EQ'-GeO₂ 59

O	2.598882457412	1.509103925950	-1.542346602314
O	4.740311628946	1.358788851753	-0.610309495146
O	-0.707936078323	1.453419787270	0.834704327402
O	3.547290938641	5.426112015517	2.132835573373
O	-4.572679093557	0.169953155763	-0.053297207651
O	-3.900816440816	-1.105131915848	1.787056063114
O	2.561028387506	4.134496690368	-1.542346540473

O	4.702485405802	3.984135457314	-0.610457692241
O	-0.745807674872	4.078786986771	0.834622718591
O	3.509393447926	8.051515787939	2.132841281880
O	-4.610545614727	2.795339667644	-0.053294700353
O	-3.938697077654	1.520264494763	1.787010082867
Ge	0.682606312060	4.107881896005	-1.277234340004
Ge	-5.223819650215	0.191157230719	1.751963818767
Ge	3.028282909192	2.520958361050	0.313293792256
Ge	-5.261689426093	2.816569330429	1.751990512071
Ge	0.720408288072	1.482483259863	-1.277229247465
Ge	2.990463424663	5.146307877920	0.313293601599
TV	5.679821802692	-0.000000000000	-0.000000000001
TV	-0.075731765973	5.250796450415	0.000000000000
TV	-2.838886611541	2.631466432262	4.553195109263

EQ'-GeO₂ 60

O	2.297740842963	3.305913660835	-0.668369095771
O	2.389940138374	0.622586103929	-0.941359059284
O	-1.415605880553	2.034400051917	0.368596996217
O	9.578277561133	9.684703954139	1.511562639769
O	-4.403003942751	-1.297223169786	1.675105336617
O	-7.482681483590	-5.008218846534	0.155312559564
O	3.492102919117	7.791186191289	-0.668362467786
O	3.584299327107	5.107863734330	-0.941338487944
O	-0.221230129243	6.519693224686	0.368572521601
O	10.772655003177	14.170015015310	1.511526785717
O	-3.208615124932	3.188065246096	1.675102644109
O	-6.288302387574	-0.522909962289	0.155281819526
Ge	2.263116006100	6.354809230180	-0.679269433483
Ge	-6.042268194035	-2.664301994823	1.404607067023
Ge	3.644295788741	3.887962305112	0.510405636321
Ge	-4.847918850230	1.820945984171	1.404598554494
Ge	1.068763951363	1.869531759384	-0.679275056823
Ge	4.838676974953	8.373246953236	0.510396986383
TV	5.261653679189	0.000000000000	-0.000000000001
TV	2.388735700658	8.970546132381	-0.000000000000
TV	-1.936776339747	4.352203911889	2.864232767638

EQ'-GeO₂ 61

O	-1.218017010707	1.408227418997	-0.059601703177
O	7.711638311519	-0.497972394485	-2.027967289677
O	-3.367443245309	1.794882997542	0.408471945055
O	3.739134245284	6.860618772908	2.632650674934
O	-3.173302596225	-0.325792316119	0.021755996434
O	-0.007423707614	0.766942830167	1.810246254923
O	-3.469760913983	4.053726465856	-0.059444865275
O	5.460080920112	2.147472372924	-2.027995296595
O	-5.619230414533	4.440008387760	0.408559763335
O	1.487483458368	9.505853035304	2.632634061150
O	-5.424891531365	2.319463515700	0.021696292491
O	-2.259043195158	3.412347663549	1.810177619626
Ge	-4.874394298561	3.886550995766	-1.191505366202
Ge	-2.016495627864	0.465485634466	1.325978279220
Ge	1.250496958576	0.546374384868	0.416506898752
Ge	-4.268215769053	3.110784575771	1.325939947990
Ge	-2.622789260974	1.241106630224	-1.191487786243
Ge	-1.001197203597	3.191632792621	0.416480519608

TV	6.166861254449	-0.000000000001	0.000000000000
TV	-4.503255874433	5.290631111128	0.000000000004
TV	-1.555934014769	3.422890108244	4.092293306871

EQ'-GeO₂ 62

O	-2.560489445062	-0.007798069631	1.521942160613
O	1.830174923969	3.327318423537	-0.900738168994
O	-4.545179944498	-0.910070171052	1.274409895850
O	-1.963748493283	-1.191621566665	-0.449330440980
O	0.256095659105	-1.039079099906	-0.336083883934
O	1.753023851090	1.262180400596	0.095548531963
O	-4.346148982177	-0.870136529806	3.467927812408
O	0.044711574792	2.465125327177	1.045243594725
O	-6.330647298001	-1.772367627446	3.220242054570
O	-3.749247416266	-2.053766155741	1.496398582593
O	-1.529406955467	-1.901409846898	1.609798897111
O	-0.032064748943	0.400012408087	2.041581626868
Ge	-1.552155546567	1.359821196788	1.069905781014
Ge	-3.255558478464	2.542608562910	0.045806914639
Ge	-0.388464544553	4.180819974499	1.410111991395
Ge	-5.040869317163	1.680728201655	1.991892757119
Ge	0.233189825846	2.221751331888	-0.876189075918
Ge	-2.173817322669	3.318601532317	3.356035043906
TV	6.498365630731	-0.000000000000	-0.000000000000
TV	-0.486142183269	5.422396990063	0.000000000000
TV	-3.570906666631	-1.724391722927	3.891800594372

EQ'-GeO₂ 63

O	0.761471113275	2.457445555838	0.188339247192
O	1.861001876058	-0.144789178294	-2.035243910119
O	-1.345780365562	2.055799763995	0.016696752090
O	0.537428815191	2.514757395589	4.167213037476
O	-5.315999999372	-1.220565992198	2.248345989293
O	2.791682282928	2.374045024330	0.709490360570
O	-1.021813824666	4.678259195490	0.188297368958
O	0.077810668363	2.076059187706	-2.035255933388
O	-3.129164839586	4.277103272186	0.016964877809
O	-1.245957014584	4.735770773844	4.167262556513
O	-7.099603151829	1.000492070326	2.248235939729
O	1.008300697488	4.595306845134	0.709749186906
Ge	-3.145507187892	3.384583098274	-2.859275057202
Ge	-0.249082738785	1.741581564227	1.592915413402
Ge	1.306885882979	1.174804626136	-0.914201074663
Ge	-2.032376590474	3.962479923409	1.592819165660
Ge	-1.362165910026	1.163425809653	-2.859248547250
Ge	-0.476755100651	3.395721277812	-0.914608061704
TV	5.252987527564	-0.000000000014	0.000000000016
TV	-3.566831595453	4.442154491002	0.000000000078
TV	-2.096614246161	0.427908734783	5.870616090892

EQ'-GeO₂ 64

O	1.580394555008	-0.718984087027	0.518504384385
O	0.117825327657	-1.975489584828	-2.270286926513
O	1.714603647228	0.771017849435	3.092553956020
O	-0.483222612538	-4.061952282615	-1.765295382888
O	0.385045164302	2.594671106547	0.518585430094
O	-1.077571227015	1.338149531783	-2.270267107466

O	0.519294064202	4.084628833616	3.092560451277
O	-1.678638456623	-0.748238110911	-1.765343952545
O	-0.810350329302	5.908333883298	0.518541764632
O	-2.272906657365	4.651789532088	-2.270294722028
O	-0.676113423519	7.398299599232	3.092530382628
O	-2.873970682290	2.565376769033	-1.765315257254
Ge	-2.684690500664	5.449615625541	-0.512160287095
Ge	1.050789849090	4.161328915687	1.357207963443
Ge	-0.144568987127	7.474959638480	1.357180781650
Ge	-0.294020782606	-1.177660128864	-0.512162692404
Ge	-1.489398706490	2.135995778245	-0.512124792469
Ge	2.246147475358	0.847667375812	1.357190986080
TV	3.611540919820	-0.000000000000	0.000000000000
TV	-3.586126192165	9.940939067513	-0.000000000003
TV	1.493788056856	0.232088850461	3.725091799518

EQ'-GeO₂ 65

O	1.296779162933	-1.915066719734	0.064064796896
O	-1.155526403514	-2.635924385622	-0.585079533816
O	1.402194450686	0.078668548387	1.210578261886
O	-0.342928270270	-0.493066717913	-0.332767955362
O	4.731819397721	-1.915083989418	0.064108527354
O	2.279519575048	-2.635897942695	-0.585071495053
O	4.837138084865	0.078629036156	1.210524612363
O	3.092022114661	-0.493059942180	-0.332792163052
O	8.166819515699	-1.915077145702	0.064099472393
O	5.714519747611	-2.635904850433	-0.585051062791
O	8.272195964678	0.078657198030	1.210561286235
O	6.527053696993	-0.493062570711	-0.332729214538
Ge	7.996412516840	-0.255510144678	-1.334186807475
Ge	3.164225195799	0.904436857117	0.832870079069
Ge	6.599196759052	0.904412194108	0.832854793568
Ge	1.126453386005	-0.255495697122	-1.334194990818
Ge	4.561370502420	-0.255490790212	-1.334256400611
Ge	-0.270825059355	0.904411793005	0.832828886482
TV	10.305016612416	0.000000000000	0.000000000000
TV	-0.354836958988	4.040204880293	0.000000000000
TV	-2.218113763605	-1.226973370271	3.217403300084

EQ'-GeO₂ 66

O	0.551040109747	1.765612884709	2.130816383250
O	-2.258912582975	-4.597435417623	-4.219180056835
O	3.297214843916	3.400708792556	3.584592757709
O	0.512898595982	-4.164467801959	-0.242342727077
O	3.269237464638	1.765596291924	2.130814616517
O	0.459282515889	-4.597449225654	-4.219172750505
O	6.015416676891	3.400725335525	3.584590036377
O	3.231097961442	-4.164479902242	-0.242367415429
O	5.987434844660	1.765640114632	2.130824310136
O	3.177499813897	-4.597441102636	-4.219173991641
O	8.733633426949	3.400746779623	3.584597509102
O	5.949309659176	-4.164462640097	-0.242368728721
Ge	5.967266676105	-1.471124617058	-1.780580468324
Ge	4.615343945807	-0.639084410042	0.968282931488
Ge	7.333541624211	-0.639086808150	0.968297010248
Ge	0.530874826174	-1.471114927557	-1.780565360235
Ge	3.249066034078	-1.471126212342	-1.780585444289

Ge	1.897153557742	-0.639072217821	0.968293535910
TV	8.154601220911	-0.000000000018	0.000000000036
TV	0.018108539542	3.675097282497	-0.000000000002
TV	1.386243250320	2.204913440502	4.582934773849

EQ'-GeO₂ 67

O	1.787427033867	1.657493770520	-0.083039183348
O	1.776180432773	3.819485332641	-2.940529457854
O	3.228948679238	-0.589670097819	2.176013001033
O	-1.059034486061	-3.880519343202	-0.715017540773
O	4.644018961288	1.656923559154	-0.087792426900
O	4.621883197163	3.816758876876	-2.945802343577
O	6.084834945267	-0.593416664052	2.176668984162
O	1.803148913158	-3.884205659966	-0.724835319073
O	7.500123087758	1.657965237665	-0.079623867178
O	7.481301406424	3.816796421481	-2.938643319093
O	8.943475060935	-0.590376746339	2.179654039073
O	4.661881873545	-3.885028560510	-0.715873754265
Ge	3.229926294401	-4.854378754162	-0.038936769356
Ge	4.650751949154	-1.855435767795	2.044294848256
Ge	7.511586740464	-1.856379921735	2.050409555083
Ge	-2.485766598545	-4.855956291675	-0.033463847557
Ge	0.372912997466	-4.851711929599	-0.042110890505
Ge	1.795787342957	-1.845658542576	2.043400439804
TV	8.575376342539	-0.000000000000	-0.000000000003
TV	1.420617069436	3.929899471317	-0.000000000002
TV	0.010055284019	-2.920094621332	3.985223534811

EQ'-GeO₂ 68

O	1.597169345778	-0.007034719649	0.429413343716
O	-0.333390715462	-2.232180556095	-1.628810904448
O	2.579375042453	2.161228383787	2.501566430926
O	-3.497682015580	-4.523999981285	-0.506644099735
O	1.610026449494	1.256034918441	2.961310798487
O	-0.320625207067	-0.969050245401	0.903072898782
O	2.592146776931	3.424343555783	5.033408595203
O	-3.484884970013	-3.260849071513	2.025230764242
O	1.622761362904	2.519190206808	5.493178023120
O	-0.307861175553	0.294072944526	3.434904144581
O	2.605025614535	4.687500530115	7.565321031584
O	-3.472029368840	-1.997746757303	4.557168740531
Ge	0.267242083147	1.845990313561	4.242526100263
Ge	3.940318498321	2.833743962771	3.750464363588
Ge	3.953020495067	4.096841089102	6.282375545906
Ge	0.241615048816	-0.680168929578	-0.821240443305
Ge	0.254408015765	0.582922915724	1.710641505246
Ge	3.927417818284	1.570621717565	1.218609438965
TV	5.583049531447	0.000000000000	-0.000000000000
TV	1.195941203993	3.194095394172	0.000000000000
TV	0.038429557956	3.789386673692	7.595665352236

EQ'-GeO₂ 69

O	1.246637012964	-0.583991228364	-0.189056249841
O	-0.665151938372	-1.321650693296	-3.380419338120
O	3.625833863862	-1.032420301700	4.798288091945
O	-1.372283701934	-1.473097810840	-0.948065326331
O	0.822775417245	2.104348532365	-0.189053189181

O	-1.088971278758	1.366697611565	-3.380392099828
O	3.201970948049	1.655923575433	4.798277444660
O	-1.796099279989	1.215231324000	-0.948043378854
O	0.398908731837	4.792731982288	-0.189091837233
O	-1.512847378946	4.055005571001	-3.380411230166
O	2.778121474584	4.344286454291	4.798285143894
O	-2.219998837843	3.903575245045	-0.948035930650
Ge	-1.794725555147	5.351565940923	-1.973260687132
Ge	1.727741978085	1.852608236338	2.113037081197
Ge	1.303889053509	4.540966529862	2.113032069695
Ge	-0.947004855073	-0.025117192763	-1.973291993000
Ge	-1.370870734113	2.663224153871	-1.973255730935
Ge	2.151603710565	-0.835727455587	2.113062139356
TV	4.612618573587	-0.000000000005	0.000000000001
TV	-1.271552518801	8.065042632100	0.000000000006
TV	1.049459844977	-1.645863727858	3.710235501772

EQ'-GeO₂ 70

O	-1.587106305753	0.105320012528	-1.144690021994
O	3.099590863695	0.717569678133	-1.975662552858
O	-2.764702755728	-1.129862761737	0.833621189341
O	7.865747913421	8.362314071815	5.234681585677
O	-3.002296486798	1.152471573103	1.874007250577
O	-0.082413340616	2.428181162301	0.005334998958
O	-3.590047893453	3.050043698127	-1.144700953225
O	1.096627631875	3.662307120186	-1.975658234334
O	-4.767644352753	1.814819556539	0.833610321039
O	5.862803470962	11.307027268413	5.234691333276
O	-5.005238600503	4.097164736686	1.873992351978
O	-2.085356763912	5.372901668639	0.005306453437
Ge	-3.658837507982	1.265872257309	-0.571858382755
Ge	-1.820915648453	1.907879833640	0.584178608220
Ge	0.151283956025	0.622547398552	-1.725347950122
Ge	-3.823853100434	4.852590266266	0.584171319658
Ge	-1.655895050985	-1.678851650229	-0.571820880197
Ge	-1.851657248230	3.567251421454	-1.725359125400
TV	5.648291873391	0.000000000000	0.000000000000
TV	-4.005900413083	5.889399267015	-0.000000000000
TV	-0.559607335978	4.963949455681	4.124651927402

EQ'-GeO₂ 71

O	1.191873954682	1.186428743449	0.421478464816
O	1.055615235505	1.039162096444	-3.128076598510
O	1.989051838944	0.533051160000	2.923263368071
O	0.004085997016	-3.727601560042	-1.347440304365
O	4.479727617786	1.186476274992	0.421488480763
O	4.343489799998	1.039160600087	-3.128117881478
O	5.276936131297	0.532997465562	2.923272348513
O	3.292016415730	-3.727614717155	-1.347439448030
O	7.767587755182	1.186445505210	0.421452107899
O	7.631368544108	1.039142599093	-3.128120098754
O	8.564795867484	0.533071102902	2.923298270271
O	6.579847233743	-3.727616279791	-1.347439089019
Ge	4.995661436507	-3.585068402025	-0.172657557054
Ge	4.803065571777	-1.151740253066	1.745086444318
Ge	8.090880117003	-1.151708685936	1.745022223692
Ge	-1.579985728950	-3.585084031983	-0.172680578075

Ge	1.707848744228	-3.585071419760	-0.172679006160
Ge	1.515175063639	-1.151745279062	1.745061001056
TV	9.863600702248	-0.000000000000	0.000000000000
TV	0.737769694968	3.202985799715	-0.000000000001
TV	-0.814606955505	-0.586055371645	4.284721824737

EQ'-GeO₂ 72

O	1.294537586047	-0.641741877647	-0.519727873693
O	3.798555627465	3.150348982412	-1.074879245337
O	-0.394241684830	-0.928429202971	2.617201368254
O	0.067503887502	-2.622682461529	-0.042641289250
O	1.174679930710	3.104349590833	-0.519730640108
O	3.678697892257	6.896436273683	-1.074894307763
O	-0.514063173806	2.817673011902	2.617192238706
O	-0.052340729181	1.123403521120	-0.042640543562
O	1.054849009667	6.850468278446	-0.519725591909
O	3.558848993340	10.642522774400	-1.074894346534
O	-0.633907245992	6.563755014395	2.617208314208
O	-0.172172157311	4.869505311239	-0.042636288299
Ge	2.105895991961	8.253791307899	-1.371644770506
Ge	-3.434269788789	-1.830203027628	0.845069046049
Ge	-3.554119632418	1.915904060707	0.845075443734
Ge	2.345603558741	0.761586863209	-1.371637409198
Ge	2.225740564033	4.507679394299	-1.371645873082
Ge	-3.314414052280	-5.576284531501	0.845067718354
TV	4.908955250355	0.000000000028	0.000000000019
TV	-0.359539160481	11.238289849501	-0.000000000123
TV	-3.697573302631	-3.777497593760	2.500913037704

EQ'-GeO₂ 73

O	0.882382365882	-0.574068161974	-0.046074626751
O	0.067564954416	-2.122925196345	-3.231822566395
O	-0.365623588011	1.323878008338	2.854113914551
O	1.699423723918	-1.764643138521	1.915983134717
O	-0.828013232918	1.635388958861	-0.046070279896
O	-1.642823513306	0.086517258775	-3.231801643841
O	-2.075979095818	3.533297250527	2.854088357629
O	-0.010925937045	0.444847444274	1.916017127190
O	-2.538380494884	3.844834759328	-0.046092182291
O	-3.353176154825	2.295969302700	-3.231830047294
O	-3.786414984110	5.742707553927	2.854102144441
O	-1.721302422870	2.654279836518	1.915977078566
Ge	-3.435389132200	2.836494368210	-1.439018992576
Ge	0.924319243020	1.175775528586	0.388418953609
Ge	-0.786035087309	3.385251515508	0.388393665213
Ge	-0.014639161475	-1.582368467892	-1.439030198504
Ge	-1.725027898739	0.627069392303	-1.439004198669
Ge	2.634695025117	-1.033660624116	0.388422508268
TV	4.555209439606	0.000000000000	0.000000000000
TV	-5.131173897649	6.628344178501	-0.000000000003
TV	-0.517924007004	0.448641144285	4.549990931572

EQ'-GeO₂ 74

O	1.527336969828	-0.157326475329	0.812555856130
O	-1.903937152306	-1.368610060616	-2.197527637209
O	2.804294996045	0.492740796063	2.564193315122
O	-0.904791281388	-2.992312951770	-0.902785727991

O	0.758828352875	3.237147857675	0.821265994611
O	-2.703263511046	2.036083586294	-2.204894917498
O	2.036028631778	3.884537282876	2.570706856653
O	-1.703978190880	0.414297519635	-0.911856795902
O	-0.026774002337	6.633505244140	0.818919013357
O	-3.472738933365	5.429619784843	-2.196563218033
O	1.250679089095	7.287463739557	2.571484929327
O	-2.471999520286	3.805376045242	-0.902277664563
Ge	-1.509844021384	6.594869141315	-0.379335115170
Ge	1.973515658874	1.589425736692	0.512752080151
Ge	1.204027686752	4.989804595143	0.519999370059
Ge	0.044531444390	-0.205217623053	-0.385985954469
Ge	-0.726049422374	3.192194247151	-0.373543477691
Ge	2.770030170453	-1.812125341937	0.524498072642
TV	4.106555649757	0.000000000000	-0.000000000000
TV	-2.353526473413	10.198275889554	-0.000000000003
TV	2.315251197184	-1.056937952472	3.243586603045

EQ'-GeO₂ 75

O	0.086195267911	0.083256880179	0.021829560395
O	1.399728119272	2.796151063355	-1.784340851093
O	0.112547903176	1.295323464603	-0.713689305326
O	-1.190870845244	2.162067000554	1.090415150590
O	2.679791485281	0.083215544773	0.021850843438
O	3.993473054219	2.796140570129	-1.784364027428
O	2.706349353126	1.295245621844	-0.713701064814
O	1.402897315252	2.162080347173	1.090357557046
O	5.273649522412	0.083276432587	0.021852228035
O	6.587261529230	2.796100077499	-1.784408634133
O	5.300072637067	1.295271510263	-0.713695346057
O	3.996675388914	2.162086765877	1.090424311038
Ge	5.295574482455	0.996419689778	1.556452784624
Ge	1.404939784018	3.080760645850	2.835947574274
Ge	3.998746512572	3.080777890433	2.836010278040
Ge	0.108000615327	0.996379832875	1.556483642037
Ge	2.701771435797	0.996396727753	1.556457925335
Ge	-1.188867123181	3.080747349403	2.835990261461
TV	7.781391277789	-0.000000000000	0.000000000000
TV	-2.586129457793	3.578230686708	-0.000000000000
TV	-1.290130261835	-0.882780888327	5.086069211051