

# Role of Fluxionality and Metastable Isomers in the ORR Activity: A Case

## Study for Gas-Phase Pt<sub>13</sub> cluster

### 1. Bare Clusters

13

PRE:0 = -57.78625495

Pt	-2.88463288	0.68951151	-0.82197750
Pt	-0.04411944	0.33584713	-0.76978386
Pt	3.10035147	-1.26321830	-0.48759613
Pt	3.15065319	-3.03859868	-2.31593366
Pt	-1.59856562	1.46955629	-3.01147333
Pt	-0.67416024	0.08816189	3.04253020
Pt	0.15249760	2.79760578	-1.40254316
Pt	-2.47104210	1.31854644	1.61019157
Pt	1.44178554	0.74126581	1.25915607
Pt	-0.34856416	2.61015948	1.17144984
Pt	-1.70530356	-1.11596587	0.93736177
Pt	1.10979285	-2.88381833	-0.75394897
Pt	0.77130734	-1.74905314	1.54256718

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PRE:1 = -57.44097034

Pt	1.99054424	-3.32620150	-1.44341633
Pt	-1.24149377	2.06418162	1.13081681
Pt	0.03752188	0.49788713	-2.74228276
Pt	0.65366254	1.20726219	-0.37852604
Pt	-3.36503571	0.60919375	1.36343171
Pt	1.06644077	2.25811175	2.19733963
Pt	0.60201852	-0.79254692	1.14408695
Pt	-1.23027286	1.05317905	3.56191764
Pt	1.80821187	-0.84715815	-1.52145256
Pt	1.22160354	3.10329586	-2.01603951
Pt	-1.67713913	-1.11439679	2.26005743
Pt	0.32296021	-2.18754593	-3.08319736
Pt	-0.18902211	-2.52526205	-0.47273561

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PRE:2 = -55.52509108

Pt	-1.54941242	-0.78476217	-0.00000000
Pt	-3.93494373	0.14494901	-0.00000000
Pt	1.48887559	5.61966875	0.00000000
Pt	3.10164147	0.58029753	-0.00000000
Pt	-1.82481449	1.82233204	-0.00000000
Pt	-0.73393430	4.25316003	-0.00000000
Pt	3.07356743	-2.01792876	0.00000000
Pt	0.54218906	-2.26728839	-0.00000000
Pt	-1.04713428	-4.31738621	0.00000000
Pt	0.47160909	0.78623308	-0.00000000

Pt	-3.46725843	-2.50252807	-0.00000000
Pt	1.64973003	3.12715256	0.00000000
Pt	2.22988498	-4.44389939	0.00000000

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PRE:3 = -55.31466928

Pt	3.19555674	4.36226000	0.00000000
Pt	4.04867615	-0.08610652	0.00000000
Pt	-1.11884776	2.66247510	0.00000000
Pt	-0.24416763	-5.66650556	0.00000000
Pt	-3.68705833	3.14069866	-0.00000000
Pt	-4.12462787	-1.42845634	-0.00000000
Pt	-2.78601426	0.72601528	-0.00000000
Pt	0.32102153	0.54877972	-0.00000000
Pt	-1.41613550	-1.41143248	-0.00000000
Pt	5.06857564	2.22883409	0.00000000
Pt	0.32824279	-3.16710725	-0.00000000
Pt	2.50046600	1.96655246	0.00000000
Pt	-2.08568750	-3.87600717	0.00000000

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PRE:4 = -55.17306762

Pt	2.83319821	2.36202778	-0.00000000
Pt	0.28754791	2.22879668	0.00000000
Pt	-2.05882271	-2.37823825	-0.00000000
Pt	-3.01773808	1.46772104	0.00000000
Pt	3.51972723	-1.57066254	0.00000000
Pt	3.36516761	-4.09551126	-0.00000000
Pt	-1.00581304	-0.03237205	-0.00000000
Pt	1.22224230	-2.69086711	-0.00000000
Pt	4.86813135	0.54380781	0.00000000
Pt	-5.59835631	1.29654988	0.00000000
Pt	-1.72268388	3.76527238	0.00000000
Pt	-4.15808410	-0.83984693	0.00000000
Pt	1.46548350	-0.05667742	-0.00000000

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PRE:5 = -53.71817940

Pt	-1.82029382	0.41626957	-0.00000000
Pt	4.78207126	-2.48628244	0.00000000
Pt	0.86482573	-5.25704633	0.00000000
Pt	1.90913200	1.75389861	-0.00000000
Pt	-4.15815925	1.40908496	-0.00000000
Pt	-6.16269677	2.99612373	0.00000000
Pt	0.43053962	-0.64715724	-0.00000000
Pt	3.03420402	-0.58262455	0.00000000
Pt	-1.26790679	2.92535507	-0.00000000
Pt	-3.64925195	3.92442662	0.00000000
Pt	4.50330263	1.51898535	0.00000000
Pt	-0.51735184	-2.98570560	0.00000000
Pt	2.05158514	-2.98532774	0.00000000

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PRE:6 = -55.81504941

Pt	-1.07845912	2.36208250	0.00000000
Pt	4.54045075	-1.22548051	-0.00000000
Pt	4.36578052	-3.71425622	0.00000000
Pt	-1.47588836	-2.21693692	0.00000000
Pt	-5.31067413	0.80491574	0.00000000
Pt	4.21483155	1.83705392	0.00000000
Pt	-3.52965512	2.99962272	0.00000000
Pt	-2.78382345	0.44621544	0.00000000
Pt	2.41094215	0.05030973	-0.00000000
Pt	-4.16716287	-1.68266843	0.00000000
Pt	1.75762501	2.49862894	-0.00000000
Pt	1.19901361	-2.18562487	-0.00000000
Pt	-0.14298055	0.02613795	0.00000000

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PRE:7 = -54.14673257

Pt	3.67060671	0.60095338	-1.75122086
Pt	-3.32910180	0.81473271	1.19381957
Pt	-3.31364708	-0.52989359	3.65276291
Pt	-4.18430520	-2.81809260	2.65953710
Pt	0.23384342	-0.52280935	1.53554536
Pt	0.20099460	-1.98695422	-0.80436765
Pt	-2.03211439	-1.70066339	1.91023862
Pt	0.22849597	0.72316479	-0.71889437
Pt	3.35490886	1.35376636	-4.22662429
Pt	-1.95381108	-0.66513495	-0.41665958
Pt	2.46037755	-0.20806070	0.40648919
Pt	1.47265684	1.93156233	-2.61119835
Pt	3.19109560	3.00742922	-0.82942765

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PRE:8 = -58.24128952

Pt	2.20876667	1.14083332	0.35586144
Pt	-2.30718861	-0.79025998	-0.25222349
Pt	-0.15209906	0.35191682	0.59867684
Pt	-1.18015608	0.11563721	-3.18663720
Pt	-0.36396418	-2.17536277	0.91521600
Pt	-2.05953351	2.30188754	-2.05433482
Pt	-2.55685919	1.59912944	0.65276966
Pt	1.07117653	0.45024313	2.90148561
Pt	-1.31516033	-0.67001192	2.78049867
Pt	2.50004518	-1.15708910	-1.37966888
Pt	3.70312930	-0.03008228	2.11516298
Pt	0.83268231	0.61930950	-1.74516019
Pt	-0.38083903	-1.75615091	-1.70164663

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PRE:9 = -54.11824196

Pt	5.62788472	-1.68983375	0.96129036
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Pt	-3.06900440	1.40619960	-1.13466189
Pt	-1.14680109	2.12059270	0.53668301
Pt	-5.21249543	0.72942439	0.17115186
Pt	-0.96792125	-1.47243147	-0.82650610
Pt	0.07462353	-0.09342632	1.04000720
Pt	4.75178656	0.41875293	2.28124297
Pt	1.34308708	-2.09445274	-0.03170520
Pt	2.39473931	1.02420419	0.97537991
Pt	-3.08591197	-0.63210904	0.34500889
Pt	1.29045022	-0.15243235	-1.70584714
Pt	3.58663284	-0.90107534	-0.29937809
Pt	-5.58707012	1.33658720	-2.31266580

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PRE:10 = -55.35824109

Pt	-2.04721173	-1.01678308	-1.26639093
Pt	4.08574320	1.38238112	0.65776132
Pt	1.58469951	0.55946727	-2.24106542
Pt	1.98251820	0.16256878	1.54422356
Pt	-2.48657209	-3.38202083	1.96003948
Pt	1.50211835	2.34565210	0.23409308
Pt	-0.74830566	-1.82427876	0.81402868
Pt	-0.55034554	-4.34175518	0.41401185
Pt	-1.25638309	2.50787918	-0.46965186
Pt	1.06709133	-1.82315043	-1.30527356
Pt	-0.00932641	3.80616561	1.61069174
Pt	-3.14232701	1.34164461	-1.71956923
Pt	0.01830094	0.28222962	-0.23289873

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PRE:11 = -56.00992531

Pt	-1.30758897	1.17196257	-1.82008310
Pt	-1.38337588	-0.21492315	1.66976847
Pt	0.84530708	2.31387300	0.37659131
Pt	-0.92627705	-1.32841385	-2.50684729
Pt	-1.47559893	3.33499189	-0.17001370
Pt	0.26313530	-3.70962471	-2.88995010
Pt	0.50889728	1.35223870	2.74513522
Pt	2.81130344	0.73410169	0.37939531
Pt	-1.25047110	-2.15981455	-0.04913639
Pt	1.33409713	-0.93349096	1.99352174
Pt	2.21518261	3.47655533	2.19222702
Pt	0.31783075	-0.11774611	-0.27655492
Pt	-1.95244166	-3.91970985	-1.64405358

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PRE:12 = -51.70992873

Pt	2.27249192	3.13839764	0.00000000
Pt	4.12102277	5.00161003	0.00000000
Pt	-2.86994580	-4.65474850	-0.00000000
Pt	1.67181370	5.60413888	0.00000000

Pt	-1.36059503	-8.76760723	-0.00000000
Pt	-0.36168353	-3.74951291	-0.00000000
Pt	0.35691467	1.33418505	0.00000000
Pt	-0.87302755	-6.28521177	-0.00000000
Pt	-2.09890954	2.00099990	0.00000000
Pt	-0.27047240	-1.14336034	-0.00000000
Pt	-2.66289670	4.52412151	0.00000000
Pt	2.24820048	-0.84986851	-0.00000000
Pt	-0.17291299	3.84685625	0.00000000

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PRE:13 = -55.11539384

Pt	1.29860180	-0.38661413	0.39821792
Pt	3.24093776	-1.78842230	-0.57538576
Pt	-3.18296762	-1.12379323	1.03016340
Pt	-2.47905027	-3.66842100	-3.02470954
Pt	1.57086413	1.79959920	1.68439062
Pt	-1.74837059	3.01402151	0.29512856
Pt	0.29959044	1.71564143	-0.64487792
Pt	2.88612272	1.66116155	-0.41840895
Pt	1.74590696	-0.01685078	-2.09895673
Pt	-1.92573497	-2.10461686	-1.01803112
Pt	-1.11230033	0.66830442	1.27307510
Pt	-0.62754190	2.80988134	2.59706275
Pt	0.03394189	-2.57989115	0.50233170

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PRE:14 = -56.23742295

Pt	3.35115107	1.92863161	-1.93814829
Pt	1.32024792	2.62718757	2.26013121
Pt	-0.70870728	1.23592067	1.21155298
Pt	2.73644070	-0.57813850	-1.43755990
Pt	-2.86315367	-0.38756814	0.72749543
Pt	-1.40898893	-1.06927149	-2.90975534
Pt	0.75429332	-2.43002665	2.46819373
Pt	0.21913992	-0.60360350	-0.84831293
Pt	-1.80738008	0.90075760	-1.39239162
Pt	-3.99954196	-0.62244570	-1.59676152
Pt	1.74403637	1.12577558	0.21424560
Pt	-1.09187357	-2.20611341	0.65189452
Pt	1.75433620	0.07889436	2.58941613

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PRE:15 = -58.23335602

Pt	0.87455334	-0.24517795	2.15404829
Pt	-3.32110140	-0.45008609	-3.43760833
Pt	2.29093331	-0.81597407	-0.12643946
Pt	1.45841686	0.33784868	-2.20803964
Pt	-0.10455048	-1.63896373	-0.36942912
Pt	-1.17147845	0.00026531	-2.05742177
Pt	3.45795651	-1.36594877	2.14726401

Pt	-1.51193177	2.70810916	1.46478242
Pt	-2.01841035	-0.55590444	0.96887121
Pt	-0.14647677	0.94067801	0.11584635
Pt	-2.26207994	2.09917813	-0.92184659
Pt	0.33532085	-3.01538310	1.74607725
Pt	2.11884830	2.00135886	0.52389539

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PRE:16 = -56.46949707

Pt	0.21983855	2.46493881	0.00678444
Pt	-2.88639612	1.34400016	-2.30472977
Pt	0.34640720	-1.11315202	-0.37924944
Pt	-1.74575452	-0.95598562	2.04172189
Pt	1.93428240	-0.13533191	-2.17696842
Pt	4.08088973	-1.41939165	-2.83645519
Pt	-1.54619519	0.57842050	-0.05613307
Pt	-0.34397697	-0.92110066	4.20521451
Pt	-2.24963938	2.99215235	-0.45106281
Pt	-3.07177127	-1.49882644	-0.03142200
Pt	0.13607017	0.73321839	1.98948120
Pt	2.75627955	-2.09214233	-0.74072757
Pt	2.36996584	0.02320043	0.73354624

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PRE:17 = -55.20775684

Pt	-0.18458736	-1.11116128	-0.00000000
Pt	4.73532646	0.54321581	0.00000000
Pt	-4.80670233	0.12363780	0.00000000
Pt	-0.17880237	-3.65320952	-0.00000000
Pt	-3.26786169	-1.89809367	-0.00000000
Pt	0.09860418	1.46394711	-0.00000000
Pt	-2.19578105	0.39327228	-0.00000000
Pt	2.31727583	-2.97222036	0.00000000
Pt	2.31477262	-0.46648547	0.00000000
Pt	4.77351937	-2.19436673	0.00000000
Pt	-3.68822442	2.48575947	0.00000000
Pt	-1.30514549	3.57076452	-0.00000000
Pt	1.38760627	3.71494003	-0.00000000

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PRE:18 = -57.93997901

Pt	1.48655588	1.21654398	0.73576910
Pt	-2.27345152	0.52749465	1.20124461
Pt	-0.27281715	-0.66463128	0.23357322
Pt	-1.38098851	2.87869074	0.85425741
Pt	-2.41874501	-1.94967637	0.55771885
Pt	3.33390925	0.28217931	-1.38222974
Pt	0.05944683	0.09234283	2.68804833
Pt	-0.03913731	-2.59984609	1.95092254
Pt	-0.76724894	1.52833483	-3.59077747
Pt	2.06136151	-1.22717866	1.04163722

Pt	-1.75962662	1.42007418	-1.18453357
Pt	1.18292003	-2.10142489	-1.35824330
Pt	0.78782156	0.59709678	-1.74738720

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PRE:19 = -56.11988920

Pt	0.44544189	-2.99052589	-0.63987783
Pt	-0.85108695	-0.98636273	3.10023312
Pt	-1.96501151	-2.69688684	0.13730784
Pt	-2.10541632	0.96178789	1.60172901
Pt	0.14207004	4.21930244	-1.14730715
Pt	1.78153484	2.13634775	-0.35097395
Pt	3.63527219	-0.97654760	-2.22541088
Pt	-3.48662985	-1.15388748	1.46927549
Pt	1.97649820	-0.85078919	-0.22164803
Pt	-0.78022298	1.93712803	-0.36993439
Pt	1.25713227	0.46634909	-2.31500445
Pt	-0.50548367	-0.61722644	-0.52030397
Pt	0.45590185	0.55131097	1.48191519

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PRE:20 = -57.38368626

Pt	-1.65945175	2.48186423	2.39782658
Pt	-0.71742059	1.91758447	-1.80907328
Pt	2.58697430	-1.88940973	-1.01114928
Pt	1.24544897	3.47760440	-1.05732987
Pt	0.09350944	1.96468151	0.65873370
Pt	0.58890954	-1.21939454	-2.49198343
Pt	1.53242071	0.64430390	-1.01231882
Pt	-1.83169239	-1.04894819	-1.64086282
Pt	0.10710384	-2.57211982	-0.31042181
Pt	-0.06568009	-0.69587707	1.41345709
Pt	2.57796543	-0.44808055	1.33517388
Pt	-2.00393034	-0.15485397	3.05342431
Pt	-2.45415708	-2.45735464	0.47452373

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PRE:21 = -54.70619541

Pt	2.82922406	-3.33472916	0.00000000
Pt	0.78616145	-1.70446295	0.00000000
Pt	2.16043268	1.39687901	-0.00000000
Pt	3.41669092	-0.79424062	0.00000000
Pt	4.72964006	1.66074379	-0.00000000
Pt	-1.42483495	-0.26746101	-0.00000000
Pt	-1.65898296	-2.75749665	-0.00000000
Pt	-0.35093000	2.05998954	-0.00000000
Pt	5.39611223	-2.39120013	0.00000000
Pt	-2.97391442	3.58844790	0.00000000
Pt	-5.47482125	2.96215645	0.00000000
Pt	-3.87154054	-1.52922964	0.00000000
Pt	-3.56323730	1.11060348	0.00000000

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PRE:22 = -56.53289622

Pt	-3.22514528	-0.88830959	-0.41788889
Pt	-3.47967336	-0.90466982	2.30086429
Pt	2.91687935	-1.16161667	1.71400283
Pt	-3.15774331	1.95900001	-1.22663161
Pt	4.60567563	1.64759316	-0.47200841
Pt	2.31361200	1.61064251	-1.55235583
Pt	-1.32866882	-0.32043824	1.09350437
Pt	1.09645686	-2.39437330	0.07975541
Pt	-2.44062927	1.86679060	1.59949410
Pt	-1.09979209	-1.70537779	-1.50846603
Pt	3.36042799	-0.74827014	-0.78115427
Pt	-0.81677670	0.78169614	-1.13820423
Pt	1.25537702	0.25733313	0.30908829

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PRE:23 = -57.08984967

Pt	0.03436556	2.04346562	0.76198461
Pt	-0.19168915	-3.44190654	-0.55406910
Pt	1.81337994	-0.12278272	3.33922085
Pt	0.47066861	0.95492739	-1.51858081
Pt	-2.92277042	1.13828218	1.95291252
Pt	0.87865419	-1.20399246	0.58198456
Pt	-0.02001519	2.86089831	-3.19158656
Pt	-1.35737756	-0.02822302	0.20452632
Pt	2.31709383	0.97055127	0.84834603
Pt	-1.96743560	1.83638207	-1.66220977
Pt	2.24729582	-2.95025655	-1.44613419
Pt	-0.57647369	-0.70557844	2.65222703
Pt	-0.72569633	-1.35176712	-1.96862151

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PRE:24 = -56.81723668

Pt	-1.38321639	-1.46980915	1.40364288
Pt	-1.12860457	3.39308154	-2.55355275
Pt	1.82235760	-1.02647027	0.57653028
Pt	-0.21032243	0.57312690	0.37534310
Pt	0.35319738	1.34867883	-1.97264934
Pt	2.79674829	-0.17856506	-1.69688444
Pt	1.41611036	3.32127752	-0.79457719
Pt	-1.90389900	0.12638194	-1.48703313
Pt	-0.99723122	3.01157631	-0.05435095
Pt	0.38218324	-3.17016158	0.41584731
Pt	-0.49071846	-3.43067844	2.82606331
Pt	-2.03718173	-3.94970343	0.83127244
Pt	1.38057693	1.45126490	2.13034848

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PRE:25 = -57.06230983

Pt	-2.04990578	-1.47962768	-0.17476372
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Pt	-2.80830239	0.96435037	-0.27907203
Pt	1.53543532	-0.39833258	0.82133181
Pt	-1.34118845	-1.40064627	-4.07976316
Pt	2.20848555	4.13261031	0.81650661
Pt	0.09599501	-3.66798337	0.30087813
Pt	3.12449260	1.78643871	0.06723540
Pt	-0.32617161	0.10584953	-1.08390262
Pt	-1.12905406	0.40846064	1.59801609
Pt	1.05626818	1.63755882	2.26739937
Pt	-0.93998852	-2.20665543	2.02979179
Pt	0.02415093	-2.26302462	-2.07212127
Pt	0.54978322	2.38100158	-0.21153641

13

PRE:26 = -54.17881792

Pt	-3.03360644	-0.05150886	-0.00000000
Pt	3.11361798	-2.94333339	0.00000000
Pt	1.27077668	4.25684140	0.00000000
Pt	-1.10369728	3.14897676	0.00000000
Pt	-3.62139659	2.60428214	0.00000000
Pt	-0.30100584	0.70279342	-0.00000000
Pt	-3.52404958	-2.68351184	-0.00000000
Pt	-1.10308259	-1.76109780	-0.00000000
Pt	2.12379807	1.80167633	-0.00000000
Pt	4.68650486	-0.93047109	-0.00000000
Pt	1.86549074	-0.75471807	-0.00000000
Pt	5.24651469	-4.34968123	0.00000000
Pt	-5.61986470	0.95975221	0.00000000

13

PRE:27 = -58.37999144

Pt	1.16314501	0.60608210	1.11704309
Pt	-1.14444647	0.49030055	-2.88775626
Pt	0.71923748	2.91455885	2.15757141
Pt	1.17011831	-1.93816267	0.32652366
Pt	2.36266332	-1.23472895	-1.84387311
Pt	-0.75928555	-1.60835103	-4.47737729
Pt	0.08890778	1.97445925	-1.18599417
Pt	-1.86208532	0.28083486	1.99844939
Pt	-1.03407299	-2.14171484	-2.00701249
Pt	-0.71755112	-0.30023748	-0.23720744
Pt	2.07509168	2.95923057	-0.03293115
Pt	-0.16825539	-1.55103447	2.70029543
Pt	-1.89346674	-0.45123674	4.37226892

13

PRE:28 = -54.94829948

Pt	2.39682357	-0.77276385	-0.00000000
Pt	-2.58372154	0.34200995	0.00000000
Pt	-0.55994601	2.54536457	-0.00000000
Pt	-5.79016106	2.90747602	0.00000000

Pt	1.91222931	1.77040370	-0.00000000
Pt	4.36740407	0.76739970	-0.00000000
Pt	-5.19273517	0.44908769	0.00000000
Pt	-3.24639601	2.77403670	-0.00000000
Pt	-1.44436908	-2.09328278	0.00000000
Pt	5.04321998	-1.70292785	-0.00000000
Pt	-0.04103441	0.10951411	-0.00000000
Pt	3.93929211	-3.99654059	-0.00000000
Pt	1.19939424	-3.09977736	0.00000000

13

PRE:29 = -58.30573953

Pt	-3.18732912	1.78339841	-1.07079493
Pt	1.26584876	0.01201156	0.06446744
Pt	2.49424829	-1.10268288	2.48873942
Pt	0.58045528	2.02630609	-1.38590732
Pt	1.87890477	-1.20192308	-2.06482678
Pt	0.21354563	0.19285220	2.57870328
Pt	-2.46773857	-1.36943939	-0.13926486
Pt	-1.46281805	0.79592216	0.77970484
Pt	-1.20903284	0.22932363	-1.68251441
Pt	-4.74924576	-0.12512794	-0.57794962
Pt	4.20101785	-0.69148754	-1.01495533
Pt	3.31096305	1.57396565	0.15866967
Pt	-0.86881929	-2.12311888	1.86592858

13

PRE:30 = -51.77269241

Pt	-4.24187207	0.89528839	-0.00000000
Pt	3.96719838	1.77184278	0.00000000
Pt	6.53160889	2.12763075	0.00000000
Pt	-2.39970456	-0.89215441	-0.00000000
Pt	-7.14910991	-2.62211026	-0.00000000
Pt	4.08530052	-0.98181618	0.00000000
Pt	1.71059675	-2.30396347	0.00000000
Pt	1.75862766	0.27407004	0.00000000
Pt	-6.85634965	0.02841238	-0.00000000
Pt	6.59166042	-0.51794953	0.00000000
Pt	-4.85821614	-1.59324218	-0.00000000
Pt	1.49030622	2.84241675	0.00000000
Pt	-0.63004652	0.97157496	-0.00000000

13

PRE:31 = -56.35184633

Pt	-1.30035992	-0.17232141	-0.32579420
Pt	-2.82460555	1.83781788	0.33520763
Pt	-1.37036615	-0.74305578	-4.65513824
Pt	-1.15029634	1.12574451	-2.94740547
Pt	0.83015275	0.42075403	1.02148903
Pt	2.08285762	-0.35694950	3.08934937
Pt	1.51056390	-2.07571263	1.09889044

Pt	-3.42385744	-1.61419650	-0.02129134
Pt	-2.53263559	-1.04521727	-2.41324084
Pt	3.35633203	-0.07548628	0.95684786
Pt	-0.43218025	2.19912711	-0.63154910
Pt	1.54525227	2.82791687	1.59324511
Pt	3.70914268	-2.32842103	2.89938976

13

PRE:32 = -58.35942231

Pt	-2.42328922	1.26097104	1.89170324
Pt	-0.14427169	-1.81940285	-1.75304332
Pt	2.49908897	-1.81516595	-0.06155938
Pt	0.23072781	0.85816730	1.79650604
Pt	1.45288362	2.99063827	-0.24025883
Pt	0.17507225	-1.48214686	0.73411877
Pt	-1.12378326	1.37973723	-1.66790762
Pt	-4.35826228	0.31648172	0.39501036
Pt	-2.00325690	-0.54772747	-0.16938019
Pt	2.93092545	1.18644157	0.96362630
Pt	3.43682527	0.24041918	-1.37922140
Pt	1.03888578	0.51374465	-0.63690865
Pt	-1.71154579	-3.08215782	0.12731466

13

PRE:33 = -53.90836679

Pt	2.12109037	-4.44705297	0.00000000
Pt	1.71163246	1.71905624	-0.00000000
Pt	1.25543678	4.25681663	0.00000000
Pt	4.04703105	-2.76447823	0.00000000
Pt	-2.70825870	-3.78347204	-0.00000000
Pt	-0.25223310	6.47955683	0.00000000
Pt	-2.14697146	-1.18505631	-0.00000000
Pt	-0.25118885	-3.05318987	-0.00000000
Pt	-4.71084595	-2.07912701	-0.00000000
Pt	2.89874358	-0.52515838	0.00000000
Pt	-0.82299858	1.73934235	-0.00000000
Pt	-1.49012881	4.18580898	0.00000000
Pt	0.34869121	-0.54304621	-0.00000000

13

PRE:34 = -57.74325233

Pt	-0.45735826	4.12709709	2.49280154
Pt	2.01701425	0.63512154	-0.60630075
Pt	-2.13208784	0.29380955	1.42378579
Pt	-1.24625367	1.87737780	-0.35163580
Pt	-0.45531126	-2.90628011	-0.02523286
Pt	0.95530075	1.92335654	1.29962501
Pt	1.99605759	-3.16376631	0.44720612
Pt	0.99868043	-3.94007086	-1.89555316
Pt	-2.52623152	2.63183581	2.27546846
Pt	-1.30686956	-0.61034186	-1.09329207

Pt	0.28846979	-0.55318242	0.97193730
Pt	0.96216419	-1.40174914	-2.06889647
Pt	0.90642513	1.08679237	-2.86991313

13

PRE:35 = -52.50930032

Pt	2.83123576	-3.66199824	-0.00000000
Pt	-2.16821039	2.02659859	0.00000000
Pt	-3.52033046	-0.16998303	0.00000000
Pt	-1.05730881	4.34886642	0.00000000
Pt	-0.92065285	-0.17824174	-0.00000000
Pt	-4.72286560	2.14846599	0.00000000
Pt	3.03411829	-0.99254282	-0.00000000
Pt	1.56176126	4.56824247	0.00000000
Pt	-1.83082894	-2.74965969	-0.00000000
Pt	0.71043999	-2.15721827	-0.00000000
Pt	0.10706127	-4.66432266	-0.00000000
Pt	0.38079478	2.31753002	0.00000000
Pt	5.59478570	-0.83573706	0.00000000

13

PRE:36 = -57.11705453

Pt	-1.13492714	-0.36498215	-0.10785525
Pt	0.84392355	1.84472239	-2.62199682
Pt	-0.85718889	2.25361024	-0.19792179
Pt	-3.10932856	-1.19613706	-1.52242539
Pt	1.11084539	-0.62822350	-1.84933040
Pt	1.24125129	0.38699133	0.45801644
Pt	-1.64770653	-0.41793828	2.37563846
Pt	2.11957743	-2.37096785	-0.19278057
Pt	-1.80325078	1.02010356	-2.22180747
Pt	0.95776305	2.51498934	1.70978912
Pt	3.23499506	1.39614238	1.66304151
Pt	0.51589207	-1.64176985	1.83427373
Pt	-1.47184593	-2.79654056	0.67335844

13

PRE:37 = -55.16837294

Pt	-0.26801714	-3.02169478	-0.00000000
Pt	-3.12037170	0.98825641	0.00000000
Pt	-2.24412565	3.36147277	0.00000000
Pt	-0.56190484	0.43837104	-0.00000000
Pt	1.87194590	-1.52645727	-0.00000000
Pt	1.88939188	1.06775430	-0.00000000
Pt	0.46142536	3.22245946	0.00000000
Pt	1.91105446	-4.40140062	-0.00000000
Pt	-4.91006522	-0.91664591	0.00000000
Pt	4.00977153	-2.94294489	-0.00000000
Pt	4.17569164	-0.32248258	-0.00000000
Pt	-0.80816036	5.50338883	0.00000000
Pt	-2.40663586	-1.45007676	0.00000000

13

PRE:38 = -56.67082602

Pt	-2.73820308	1.17305411	-0.77549259
Pt	0.17944217	-1.11806501	1.97806408
Pt	1.21093291	0.90045500	0.01236572
Pt	0.40039985	-3.13026412	-0.97864142
Pt	2.93420383	-1.12816324	-2.19794541
Pt	-4.07025496	1.48387528	1.89408887
Pt	2.02573539	-1.50020678	0.15871122
Pt	2.81030921	1.31749080	1.95525238
Pt	-2.08347399	0.00108815	1.40011939
Pt	2.85243367	-1.15632255	2.59730710
Pt	-0.64578058	-0.63298449	-0.82993024
Pt	-0.35772143	1.58053150	-2.02367663
Pt	-2.51802298	2.20951134	-3.19022247

13

PRE:39 = -54.79428138

Pt	-4.50348813	1.81745035	-0.00000000
Pt	3.31655317	-0.56929607	0.00000000
Pt	1.02875540	-4.94031269	0.00000000
Pt	-1.53605233	1.40286816	-0.00000000
Pt	-3.28465930	-0.44830575	-0.00000000
Pt	-0.87902893	-3.33252500	0.00000000
Pt	1.52269036	-2.45375329	0.00000000
Pt	-0.38685380	-0.81832274	-0.00000000
Pt	2.29330036	4.61393506	0.00000000
Pt	-2.60641215	3.79380611	-0.00000000
Pt	0.00320847	3.49846253	0.00000000
Pt	1.32001009	1.15078379	-0.00000000
Pt	3.71197679	-3.71479049	0.00000000

13

PRE:40 = -55.30985076

Pt	2.10967409	-0.53582053	1.52782544
Pt	-0.87473841	2.73905145	0.77792084
Pt	0.89523828	1.06542906	-0.10130145
Pt	3.30818668	1.71543230	1.99118079
Pt	0.70235715	1.30846826	2.42912634
Pt	0.72429122	0.70537468	-2.59068154
Pt	-1.87901876	0.37995115	2.65867067
Pt	-5.19734139	-2.13262626	0.21172859
Pt	1.82898846	-1.04077578	-1.06043472
Pt	-0.65200452	-1.02369195	-0.23118934
Pt	2.65097939	-0.58165074	-3.77150412
Pt	-2.92840463	-1.25172401	0.91807805
Pt	-0.68820756	-1.34741763	-2.75941955

13

PRE:41 = -54.63199977

Pt	1.51711640	-1.44959365	-0.78789857
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Pt	-0.34233196	-0.30328143	1.25243120
Pt	0.68512932	1.66085796	0.00668207
Pt	1.66662443	-1.83149704	1.70412594
Pt	-1.72611238	2.00420253	0.87711601
Pt	0.83833006	-3.83022972	0.24035865
Pt	3.53054215	0.18316798	-1.06717498
Pt	-2.35128481	4.41600874	1.33077238
Pt	-0.41578530	-0.06443649	-1.46429419
Pt	3.84255976	-2.26539681	-1.43960337
Pt	-3.48534435	3.33967024	-0.86354867
Pt	-2.74953053	0.92944098	-1.34936518
Pt	-1.00991280	-2.78891329	1.56039871

13

PRE:42 = -57.60051143

Pt	-1.38612964	0.45465941	2.12379086
Pt	-0.02886722	-2.52989708	1.73694016
Pt	-2.05378358	1.92579131	-3.54131789
Pt	-2.30223974	1.23730916	-0.09692822
Pt	-0.21980540	1.85941141	-1.74073950
Pt	1.98494681	0.87021154	-0.32044212
Pt	1.06812098	-0.18634935	1.93529430
Pt	-0.32277701	-0.27943803	-0.23250396
Pt	-1.97174861	-0.29074210	-2.19097734
Pt	2.66808788	-0.61823300	3.92468063
Pt	2.80588328	-1.38050334	0.53066669
Pt	2.14750447	0.49323554	-2.85157390
Pt	-2.38919223	-1.55545546	0.72311030

13

PRE:43 = -54.03069221

Pt	2.37615407	-0.69083470	0.60073722
Pt	3.69037012	-2.57249510	-2.26383596
Pt	3.53676808	0.20891309	-2.31630427
Pt	-4.73109327	-1.05953468	1.16879974
Pt	-1.07003459	-1.11738368	-1.60017439
Pt	-0.41238768	0.57004987	0.70466531
Pt	-3.31498106	1.08756556	1.75997770
Pt	1.51130380	-1.28040282	-1.77815578
Pt	1.51201164	1.18952628	-0.92766642
Pt	-3.41415508	-0.97748326	3.41894969
Pt	1.49458179	2.10213416	1.46889693
Pt	-2.25558954	-1.16657638	0.72350543
Pt	1.07705172	3.70652167	-0.95939519

13 (LM5)

PRE:44 = -58.65549475

Pt	-0.61871823	3.20269846	0.72200752
Pt	-1.15448615	0.54913400	0.69246160
Pt	0.33509292	-3.86232551	3.04045389
Pt	-2.95477715	1.01530576	-1.49933833

Pt	-0.43782198	0.93417176	-1.73227357
Pt	2.71090130	-0.81325814	-1.28207881
Pt	0.07437014	-1.38571381	-0.80445336
Pt	1.50847271	-0.11307680	0.87285088
Pt	-3.45503823	-0.54733855	0.51766820
Pt	2.03585111	1.78068047	-2.24609209
Pt	-0.50943959	-1.58707343	1.89064880
Pt	1.34528909	-2.93136951	0.85914441
Pt	1.12030405	3.75816532	-1.03099915

13

PRE:45 = -54.99009773

Pt	-2.29154481	2.70472506	4.07009834
Pt	-3.11135719	1.93615865	1.78514862
Pt	-0.55951864	3.10666431	2.07619868
Pt	-0.93521770	0.62298226	1.38019992
Pt	1.49182956	-3.16842856	-2.20247544
Pt	0.73125622	1.06649456	-1.56651166
Pt	3.79337970	-2.94067632	-0.75873811
Pt	-2.85153677	0.79318828	-0.46665309
Pt	0.59303119	-0.77081491	-3.22929838
Pt	-0.79612973	2.76176310	-0.50622546
Pt	1.18733887	-3.82849856	0.30778832
Pt	0.45942776	-1.37637954	0.35626647
Pt	2.28904153	-0.90717834	-1.24579822

13

PRE:46 = -56.26527492

Pt	0.87657736	-3.88308232	-1.06265326
Pt	1.43901016	0.30483975	2.20939864
Pt	-0.87744948	-2.03009836	-0.42443133
Pt	-0.01033105	0.31037031	0.00520059
Pt	1.43152033	-1.98339996	0.83296581
Pt	1.69645857	1.99815060	-1.57084709
Pt	0.09921351	-0.55352949	4.19152826
Pt	-0.82230658	1.82727245	-1.92589938
Pt	-3.12753717	2.17133949	-0.83411842
Pt	-0.83877315	-0.58090641	-2.78046327
Pt	1.80865964	-1.22873354	-1.56453221
Pt	-0.99878694	0.97144017	2.38726598
Pt	-0.67625520	2.67633731	0.53658566

13

PRE:47 = -56.50016131

Pt	-2.12718177	1.65277934	1.00045266
Pt	-1.67558745	0.29436553	3.29829845
Pt	-1.88387461	-0.15235279	-0.73970536
Pt	2.97542149	-0.16970943	1.58828405
Pt	2.65743428	0.18868723	-2.06376267
Pt	-3.65153046	-0.35286593	1.65311126
Pt	-0.90138710	-1.22723082	1.35631721

Pt	3.22234702	-1.82045631	-0.45781409
Pt	1.04130966	-0.53552408	-0.05321562
Pt	3.90137896	-2.61409206	1.87118667
Pt	-2.68278277	1.09880303	-3.15347461
Pt	-1.03316612	2.91495852	-2.25696919
Pt	0.15761889	0.72263776	-2.04270877

13

PRE:48 = -56.30629941

Pt	-4.60255398	-0.38144758	-1.39155391
Pt	1.53716169	1.19314391	-2.01203361
Pt	1.01108068	2.44561195	2.89206521
Pt	2.20161549	-2.55035994	-1.68649631
Pt	-0.68103771	0.41883054	-0.47895607
Pt	-1.32093290	2.05121426	1.78395005
Pt	3.55725333	-0.29357754	-1.61014026
Pt	-3.11389161	1.14279253	0.09111544
Pt	-2.43677349	-1.46996685	-0.55965144
Pt	2.19177989	-1.38319633	0.57342098
Pt	1.58322915	1.10550094	0.50269368
Pt	-0.01490748	-2.25207403	-0.56389699
Pt	0.08797694	-0.02647186	2.45948322

13

PRE:49 = -55.96790531

Pt	2.81722262	-0.67253432	0.00000000
Pt	4.63569534	1.08471254	0.00000000
Pt	3.10579058	-3.24003000	0.00000000
Pt	-2.35532729	-1.96720241	-0.00000000
Pt	-2.66327717	3.00712065	0.00000000
Pt	0.79887853	0.89401477	-0.00000000
Pt	-5.26700505	3.25463544	0.00000000
Pt	0.45222806	-1.72337939	-0.00000000
Pt	5.39501435	-1.38661588	0.00000000
Pt	-4.29480298	0.83122703	-0.00000000
Pt	-1.83882068	0.57553749	-0.00000000
Pt	-0.74974686	-3.98789098	-0.00000000
Pt	-0.03584945	3.33040505	0.00000000

13

PRE:50 = -57.33015674

Pt	-1.44149577	-0.91198880	1.82416505
Pt	2.31545911	1.13660193	1.75024497
Pt	-1.22150533	0.97351529	-1.83697097
Pt	1.15476106	-1.07003462	2.13400937
Pt	0.53542727	-3.17497827	0.71952223
Pt	-2.31702496	-1.18445467	-1.17457858
Pt	0.70080233	2.06595048	-0.28232471
Pt	0.06876414	-0.77851625	-0.20276068
Pt	-0.92392310	1.49451242	2.31303032
Pt	-0.54202906	-3.37343548	-1.61145116



Pt	1.07192271	1.84097707	-2.77968472
Pt	-1.73851481	2.66567663	0.20408699
Pt	2.33735641	0.31617426	-1.05728810

13

PRE:51 = -58.19703230

Pt	-1.82666842	1.10074664	0.38756185
Pt	2.80713009	-0.68235990	0.88699221
Pt	1.42440047	-1.90783709	-2.58445461
Pt	-0.15279181	-0.15649895	-1.45356536
Pt	2.32500670	0.36193690	3.13352387
Pt	-0.15597858	0.44667756	2.24664785
Pt	-1.60676182	2.79517330	-1.87834466
Pt	1.58943519	1.61975697	0.52388242
Pt	1.89552589	1.16153572	-2.00082442
Pt	-2.12902857	-2.06517878	-0.12931954
Pt	-2.52240474	0.42565536	-2.20665489
Pt	0.18633731	-1.51507824	0.74291643
Pt	-1.83420170	-1.58452949	2.33163887

13

PRE:52 = -56.41371248

Pt	2.05415208	-2.24885812	1.06741382
Pt	-1.00531329	1.33174329	0.20226741
Pt	0.26179892	1.46132434	-2.03264331
Pt	1.21879804	-1.70872507	-1.43468561
Pt	-2.35219570	-0.37250005	1.91207794
Pt	-1.95642236	2.10639229	2.41791583
Pt	-1.47265662	3.55696324	-2.68956920
Pt	1.28350703	1.69803261	1.41185863
Pt	0.94629613	-4.17726540	-0.55234053
Pt	-2.42242614	1.21702085	-1.98574133
Pt	1.64741244	-4.64084789	1.82536933
Pt	-0.18797907	-1.02075749	0.61731147
Pt	1.98502855	2.79747741	-0.75923443

13

PRE:53 = -56.25211460

Pt	1.64000139	2.59134250	-1.46334655
Pt	-2.25700221	0.27107202	-0.70113765
Pt	2.97867329	-0.97733447	-0.46846001
Pt	-2.03539633	1.46044384	1.99001764
Pt	1.03346965	-1.32050063	1.14817789
Pt	0.29660667	-0.08521080	-0.98764760
Pt	2.22350055	0.41852895	-2.59076685
Pt	-0.56315640	2.20981846	-0.16103736
Pt	-0.36031063	1.21146768	-3.14980982
Pt	-0.69051404	-2.33903347	2.77301366
Pt	-0.22402588	-3.25486872	0.23154052
Pt	0.51694674	0.95863673	1.89651560
Pt	-2.55879279	-1.14436210	1.48294053

13

PRE:54 = -57.12568902

Pt	-2.59633397	-1.56176763	-1.17985242
Pt	-0.55510611	1.20048728	2.33974547
Pt	-0.22112440	1.33247234	-0.29668721
Pt	-2.95873612	-2.25082576	1.55066816
Pt	1.88767682	1.93532989	1.51768879
Pt	1.44753532	-0.38521828	2.62892366
Pt	2.96444354	-0.20313917	0.51592689
Pt	0.90608327	-0.11926864	-4.24031851
Pt	2.14952136	-0.31503488	-1.95146851
Pt	0.46694004	-1.10597945	-0.02556858
Pt	-2.08605743	-0.04576728	0.70888005
Pt	-0.24796277	-1.80527365	-2.47396160
Pt	-1.15687955	3.32398522	0.90602380

13

PRE:55 = -56.07714925

Pt	3.51423475	-1.62876482	-0.30020035
Pt	-2.06734300	0.87806797	-0.82407966
Pt	-2.19037993	2.20456848	1.27740490
Pt	0.89243997	-2.76908306	0.02615330
Pt	-1.35295232	-1.47061788	-1.45298026
Pt	2.59606728	-2.39052683	1.92563945
Pt	0.12653759	1.13887352	0.57764887
Pt	-0.13154570	0.30705396	-3.12108534
Pt	1.31359635	-0.42383463	-1.10013958
Pt	4.89968768	-1.54184130	2.54056236
Pt	-2.34957290	-0.30383942	1.55860514
Pt	-4.10856096	2.40485010	-0.49615081
Pt	-1.14220880	3.59509390	-0.61137801

13

PRE:56 = -55.31988456

Pt	-1.67866833	-3.21137346	0.00000000
Pt	-0.76239079	0.57697540	-0.00000000
Pt	0.69879329	2.65928797	0.00000000
Pt	1.94516549	4.81636878	0.00000000
Pt	-3.99686054	-1.79668007	0.00000000
Pt	-0.74120643	5.06326311	0.00000000
Pt	0.86207329	-2.81341811	-0.00000000
Pt	4.15766779	-0.38084531	-0.00000000
Pt	1.57881980	-0.35259603	-0.00000000
Pt	-2.00696617	2.82131973	0.00000000
Pt	3.40134723	-2.84632267	0.00000000
Pt	-3.43294599	0.70757446	0.00000000
Pt	-0.02482866	-5.24355381	-0.00000000

13

PRE:57 = -55.16599832

Pt	2.74108085	1.18938388	-0.00000000
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Pt	2.16404440	3.72565561	-0.00000000
Pt	-0.08245590	5.01390485	0.00000000
Pt	2.57308063	-1.54122806	-0.00000000
Pt	-0.00253800	2.35607536	0.00000000
Pt	-3.82145242	-2.89426937	0.00000000
Pt	4.88804537	-0.14014315	-0.00000000
Pt	1.06987140	-3.60766142	-0.00000000
Pt	-2.50823834	1.68863684	0.00000000
Pt	-1.76882132	-1.39994875	-0.00000000
Pt	-4.14055094	-0.32398296	0.00000000
Pt	-1.56120859	-3.96095211	0.00000000
Pt	0.44914287	-0.10547071	-0.00000000

13

PRE:58 = -58.01563233

Pt	-2.95469308	-1.45793122	1.29783512
Pt	-0.48153671	-0.63300772	-1.36070454
Pt	0.72561417	-1.25152237	0.79109822
Pt	0.33471016	2.30353615	-0.17154935
Pt	1.41846565	-2.80124078	-1.09432857
Pt	-2.20001243	-2.51164559	-1.02295912
Pt	1.84237399	0.32735966	-0.92692955
Pt	-1.70085009	0.63972903	0.50602713
Pt	-2.52290373	3.00585767	-0.01475870
Pt	-1.83777178	1.47170798	-1.90051904
Pt	3.27113249	-1.25035172	1.18223685
Pt	0.38273697	0.94500527	2.08041317
Pt	3.72273438	1.21250366	0.63413836

13

PRE:59 = -57.62605091

Pt	2.88159544	-0.26305793	-0.67567940
Pt	1.88839966	2.75674254	1.40946241
Pt	-0.37673200	-2.20747427	2.36310525
Pt	-2.00804423	2.15817832	-1.07514102
Pt	-1.41897020	-0.21969773	-3.82191247
Pt	-1.38634114	0.00224137	1.32496916
Pt	0.73570041	0.90886492	0.15543829
Pt	0.51534758	-1.68015358	0.01761351
Pt	-0.66856794	-0.12457928	4.11078367
Pt	1.26117626	-0.15920503	2.40539098
Pt	0.04490580	1.15825195	-2.29602456
Pt	-1.69004157	-0.39190717	-1.17312693
Pt	0.22157194	-1.93820409	-2.74487888

13

PRE:60 = -57.65866752

Pt	-2.51089431	0.08326457	-2.41174826
Pt	-0.30903265	-2.57567494	0.91176307
Pt	-1.24913046	-1.97715455	-1.43994505
Pt	-1.46513244	0.23989270	2.48282418

Pt	2.99957584	0.67436916	0.49399265
Pt	0.45762659	-1.12005181	-3.36454911
Pt	0.62590421	2.40132947	1.58689557
Pt	1.26854658	2.00768806	-1.77191409
Pt	0.03516528	-1.75465341	3.33596441
Pt	0.78072425	-0.31876592	1.41019645
Pt	-0.55139845	0.56208039	-0.64429854
Pt	-1.74563545	2.30272105	0.71997870
Pt	1.66368099	-0.52504476	-1.30915999

13

PRE:61 = -56.45592748

Pt	1.41876015	2.79389210	-0.37198692
Pt	1.73663366	-0.72298898	2.17486486
Pt	1.40402549	-2.68920439	0.39943537
Pt	-1.94109821	3.55894925	-1.97975325
Pt	-1.08361943	-3.17421632	0.78673259
Pt	-0.28752741	1.61076198	-1.84360859
Pt	0.53539297	-0.72065663	-1.13515483
Pt	0.18950174	0.88563867	0.87085012
Pt	-2.65034995	0.60578372	-1.78753536
Pt	2.87425070	1.09595853	1.00130003
Pt	-2.20916004	-1.88816389	-1.18108330
Pt	2.00070664	-3.40508014	2.77792813
Pt	-1.98751631	2.04932609	0.28801115

13

PRE:62 = -58.23556266

Pt	-0.44772536	2.41731160	1.21095002
Pt	-0.36386790	-2.09086523	-2.80650984
Pt	0.67827765	2.10347058	-1.80480284
Pt	-0.99704983	-0.23127824	1.83706665
Pt	1.46691823	-0.53931820	-1.98044532
Pt	1.42696464	3.57684986	2.71834381
Pt	-1.05239873	-1.01622889	-0.60978859
Pt	-2.65236257	0.95737543	-1.23929468
Pt	2.12453167	1.05813378	2.42564283
Pt	1.43465613	-1.35777848	1.95010481
Pt	0.83393131	0.50724267	0.23751385
Pt	0.36680742	-3.05032199	0.11419872
Pt	-2.81868268	-2.33459287	-2.05297942

13

PRE:63 = -58.25965427

Pt	0.40568869	-2.83980232	3.02429268
Pt	-0.38789097	2.36032915	-2.32679832
Pt	2.33694659	2.56546370	-1.11257241
Pt	-0.02676226	-0.78848564	-1.42807202
Pt	-2.70234021	2.68663485	0.67587810
Pt	-1.87763458	0.24158988	0.69639380
Pt	2.88990137	-0.11661443	-0.27870046

Pt	1.58135732	0.75171965	-2.71793499
Pt	-2.24551322	-2.13084845	-1.13924008
Pt	1.13252638	-1.67479315	0.69118490
Pt	0.39256011	1.33001691	0.04975303
Pt	-0.11227810	-0.21794902	2.59036257
Pt	-1.38656114	-2.16726114	1.27545322

13

PRE:64 = -55.39704798

Pt	-3.73096036	2.28154579	0.00000000
Pt	2.27711270	-0.67108888	-0.00000000
Pt	-1.28354493	1.72108196	-0.00000000
Pt	0.91193657	4.27329177	0.00000000
Pt	-0.86580757	-4.94949900	-0.00000000
Pt	1.34760374	1.76085934	-0.00000000
Pt	-0.21696970	-0.73654286	-0.00000000
Pt	-2.22400558	-2.68725441	0.00000000
Pt	0.93901649	-3.02318095	-0.00000000
Pt	-1.64310146	4.29130593	0.00000000
Pt	3.42691428	-3.08990813	-0.00000000
Pt	4.15388239	1.08793693	0.00000000
Pt	-3.09207658	-0.25854750	0.00000000

13

PRE:65 = -56.51638655

Pt	1.46507498	1.85634292	0.71378987
Pt	0.30485595	-0.48393627	0.51256756
Pt	-0.21353611	1.75238825	-3.70984424
Pt	0.26613670	-4.90481361	0.40232158
Pt	1.59912251	1.77632975	-1.92636201
Pt	2.73381016	-1.69672049	0.87144026
Pt	-0.81382139	0.69162745	-1.46615070
Pt	-1.08038094	1.03801887	1.96646330
Pt	-0.98951472	3.24671444	-1.79755839
Pt	-1.82275821	-1.43827301	1.91065316
Pt	-1.01172169	-2.73864755	-0.13519719
Pt	0.54896782	-2.63708780	1.92970397
Pt	-0.98623505	3.53805706	0.72817282

13

PRE:66 = -54.15670330

Pt	1.31834173	5.21993021	-0.00000000
Pt	-1.18069485	-4.49233897	0.00000000
Pt	-3.44756588	-3.21899768	0.00000000
Pt	0.99254278	-0.65715212	0.00000000
Pt	3.38363474	-2.12013312	0.00000000
Pt	-1.80615826	6.34327740	0.00000000
Pt	3.14216996	-4.78669987	0.00000000
Pt	1.88328086	2.73279465	-0.00000000
Pt	-0.35712681	1.50394335	-0.00000000
Pt	-0.95039500	3.93114975	-0.00000000

Pt	-1.34709930	-1.78753985	0.00000000
Pt	1.08805492	-3.21013411	0.00000000
Pt	-2.71898488	0.54190036	0.00000000

13

PRE:67 = -56.77856118

Pt	-1.48516460	3.13888367	-1.75706134
Pt	-0.64499064	-1.24670358	1.63080546
Pt	1.54946459	-0.01489950	1.49992705
Pt	1.73762564	-3.44495827	-0.30558287
Pt	0.54510384	1.95478188	3.25198213
Pt	-1.89688251	0.55308724	-1.38487060
Pt	-2.75419201	-1.90328402	-1.60255091
Pt	1.54167079	-2.46041696	2.03339847
Pt	0.52930430	2.49753012	0.76311326
Pt	0.56250962	1.34895025	-1.52686907
Pt	-0.93151580	-3.26320735	-0.35728731
Pt	0.26043950	-1.00660020	-0.75984585
Pt	0.98662727	3.84683672	-1.48515840

13

PRE:68 = -51.80260926

Pt	0.05434665	-2.38546742	-0.00000000
Pt	-0.55099029	2.12945590	-0.00000000
Pt	1.21350283	0.24357100	-0.00000000
Pt	-4.47998836	-4.18344832	0.00000000
Pt	-7.74132250	-1.27141356	0.00000000
Pt	-1.30810769	-0.23323525	-0.00000000
Pt	-5.27503278	-1.74204417	0.00000000
Pt	4.70090846	2.31696323	0.00000000
Pt	3.81080616	-0.15055565	0.00000000
Pt	2.06787395	2.67315562	-0.00000000
Pt	6.29816758	0.19501603	0.00000000
Pt	3.90828862	4.75933064	-0.00000000
Pt	-2.69845262	-2.35132805	0.00000000

13

PRE:69 = -57.60190735

Pt	-0.49236526	0.89865287	-0.36410745
Pt	1.64295052	-1.59023127	-1.96859770
Pt	-1.42713300	2.95657287	1.14408792
Pt	-1.82388398	-1.96060900	1.73335343
Pt	-1.22369141	0.62015081	2.07508928
Pt	-0.20263116	-1.96014569	-0.19180929
Pt	0.24273084	-1.23094448	3.11276426
Pt	-2.28340819	-0.99483231	-1.38180379
Pt	2.12790800	0.52981118	2.85804741
Pt	1.61646990	0.29047265	-3.62471385
Pt	-2.02893959	1.17468777	-2.68927972
Pt	2.25955294	1.55125462	-1.22948053
Pt	1.59244040	-0.28484004	0.52645003

13

PRE:70 = -56.69745060

Pt	-1.76812999	2.68701874	-0.04906072
Pt	-1.93010729	-2.89867008	1.71816054
Pt	0.47947531	-2.31210672	-0.21655634
Pt	2.43097509	-1.68258048	1.55898443
Pt	2.56810297	3.08565867	0.46612174
Pt	-1.32222950	0.33072193	-0.84060661
Pt	0.90415484	0.15500673	0.49566444
Pt	-1.62745453	-2.04650409	-1.75850471
Pt	0.58976896	2.20783480	-1.01289161
Pt	-2.89452043	-0.65664936	0.93374618
Pt	-3.88473850	-0.65581234	-1.42582387
Pt	2.77613173	0.92513149	-1.10814570
Pt	3.67857134	0.86095072	1.23891222

13

PRE:71 = -55.37773125

Pt	3.77861463	0.49024370	-0.07700395
Pt	-1.55274229	-2.77740232	1.32234780
Pt	-1.17342930	-0.28887302	0.68785602
Pt	-3.34811085	-1.01095363	1.80624184
Pt	-0.69914538	-1.20713950	-1.73103688
Pt	-3.35495071	-0.31931405	-0.75397402
Pt	3.07525892	-0.19950409	-2.65368745
Pt	-2.76606126	1.58371299	1.55864928
Pt	1.11731424	-0.71916914	1.91877660
Pt	1.29599850	1.73294894	0.94964153
Pt	2.27842840	2.07942773	-1.32265091
Pt	-0.16661831	1.27899084	-1.09789767
Pt	1.51544343	-0.64296844	-0.60726219

13

PRE:72 = -58.41218232

Pt	-0.01452724	-1.07444092	-2.45179869
Pt	-0.76321143	0.27745098	1.16736522
Pt	-0.77839593	1.17868471	3.54078103
Pt	-2.01217707	0.32054557	-3.26580663
Pt	1.89280563	1.02604373	1.01749371
Pt	-2.35449177	-1.56878737	-0.77579818
Pt	0.32972850	1.31224022	-1.59560406
Pt	0.35023427	-1.07583549	2.97554080
Pt	1.93263870	-0.86152524	-0.79068760
Pt	-0.14904346	-2.10391666	0.30679364
Pt	1.72614071	0.85515689	4.22033656
Pt	1.95578656	0.58854627	-3.47670656
Pt	-2.11548746	1.12583732	-0.87190924

13

PRE:73 = -55.42841408

Pt	3.45157421	-0.49591217	2.66137401
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Pt	-0.85123317	-1.11831781	-1.74391635
Pt	-0.04794962	2.56693122	-0.19095415
Pt	2.60574351	-2.50716534	1.41350704
Pt	3.18467752	-0.17100932	-0.00118719
Pt	0.83688566	-1.16052007	0.20029451
Pt	-1.12379050	-3.61512880	-2.04378805
Pt	-2.44063340	2.26898559	0.71164737
Pt	0.12802762	2.91943099	2.32472966
Pt	-2.05577365	1.20080362	-1.69264046
Pt	-4.39974388	2.24312832	-1.30159704
Pt	1.31422709	-2.75842896	-1.76510632
Pt	-0.60201138	0.62720274	1.42763697

13

PRE:74 = -56.48356899

Pt	-4.40886881	-0.42232504	0.65174696
Pt	-2.69644247	0.28030129	-1.03257853
Pt	2.47374683	1.80976018	-1.11341966
Pt	-3.60508456	-2.10184415	-1.16360562
Pt	3.34406454	1.38012179	1.91446943
Pt	1.15239471	-0.34306335	-0.91291102
Pt	1.01421311	-2.59673195	-2.44636369
Pt	3.08292443	-0.92305324	0.80938369
Pt	-0.69582443	1.63159229	-0.05903228
Pt	-0.82370202	-1.85644057	-0.86899783
Pt	1.69415815	3.01667827	1.11119190
Pt	0.93016182	0.59219153	1.48443410
Pt	-1.46174132	-0.46718705	1.62568254

13

PRE:75 = -54.65755391

Pt	-5.54343951	-1.88573097	-0.00000000
Pt	-1.96943486	1.82012081	-0.00000000
Pt	2.04878761	-4.03286860	0.00000000
Pt	3.17524205	-0.41115716	0.00000000
Pt	-3.86734854	0.08133501	-0.00000000
Pt	0.96878356	-1.67787941	0.00000000
Pt	3.18842335	2.21125616	0.00000000
Pt	-1.33531958	-0.63959321	-0.00000000
Pt	-0.54087327	-3.74253956	0.00000000
Pt	4.32335134	4.46370041	0.00000000
Pt	-2.85842828	-2.69957758	0.00000000
Pt	0.64847130	2.08332049	-0.00000000
Pt	1.76178483	4.42961362	-0.00000000

13

PRE:76 = -53.32702239

Pt	0.00852445	-3.95147768	-0.00000000
Pt	-0.01915157	1.19129597	-0.00000000
Pt	3.27548932	-2.81227092	-0.00000000
Pt	1.77742253	-0.72727824	-0.00000000



Pt	2.45874408	2.02837502	-0.00000000
Pt	-0.73671665	-1.40280355	0.00000000
Pt	4.75944607	-4.97220247	0.00000000
Pt	-4.39066583	2.39057338	0.00000000
Pt	-3.66796026	4.84571406	0.00000000
Pt	-1.91003551	2.95167198	0.00000000
Pt	2.22286021	-5.24041732	-0.00000000
Pt	-1.12663013	5.39586556	0.00000000
Pt	-2.65132671	0.30295419	0.00000000

13

PRE:77 = -57.99968467

Pt	1.97863068	1.65455882	1.65425902
Pt	2.29514165	-3.02814895	0.64216382
Pt	1.59867601	1.26548168	-1.10700286
Pt	0.04020467	-0.09741086	1.35666757
Pt	-2.55396666	1.80185848	-1.83942676
Pt	-2.12559109	0.24195813	2.80208051
Pt	-3.19745745	2.17651947	1.41323794
Pt	1.09251154	-1.22046758	-0.69677995
Pt	-0.18140383	-2.68849689	1.27995474
Pt	-0.42097368	2.22366862	0.36629425
Pt	-2.15684492	0.11854599	0.03472765
Pt	2.73006404	-0.25076998	-2.82588128
Pt	0.90100904	-2.19729694	-3.08029465

13

PRE:78 = -57.50596570

Pt	-0.48677760	-1.65964117	-1.01118646
Pt	-0.61187071	2.62620928	-0.82846289
Pt	2.53731445	-0.77105797	-1.41377674
Pt	-1.77887814	-3.31351898	0.47260246
Pt	-2.46319127	-0.20943313	-0.18542230
Pt	-3.41756560	2.12419700	0.14936063
Pt	3.12236822	1.03853540	0.20283824
Pt	1.61929998	3.28718876	-1.88882972
Pt	-1.27572954	1.62658413	1.48869019
Pt	-1.49852464	-0.92261832	2.05957265
Pt	1.40620308	-3.11893861	-0.19988603
Pt	0.71977660	0.45227594	-0.14716105
Pt	2.12757516	-1.15978233	1.30166102

13

PRE:79 = -56.02865493

Pt	0.95690861	0.76838640	-0.56746523
Pt	-1.50444292	-1.11995621	0.30767247
Pt	3.47473766	-2.37644707	-0.34228050
Pt	1.96139664	0.15410539	-2.99654036
Pt	-3.60380995	1.33234988	1.40129308
Pt	0.40616381	-0.40739392	1.68707005
Pt	-1.58547004	1.29541362	-0.42159129

Pt	0.08228079	-1.58865148	-2.74591301
Pt	2.84124874	-0.17063204	0.94901892
Pt	-2.59073200	1.26401834	3.77626860
Pt	0.95907926	-1.78989995	-0.36213855
Pt	-0.90717606	1.78322001	2.02971436
Pt	-0.49018453	0.85548702	-2.71510855

13

PRE:80 = -55.84653385

Pt	1.08828090	-0.68894746	3.51396255
Pt	-2.37267180	-2.39261454	-3.32266731
Pt	0.05382204	-0.14442289	-0.37764862
Pt	3.09119681	0.06859544	-0.45917676
Pt	-1.01092474	3.42815730	0.76953357
Pt	-2.05627509	1.12657160	0.23480446
Pt	-0.44132453	-2.78546812	-1.63846264
Pt	0.15321775	1.27286333	1.79057808
Pt	0.65291864	3.77103084	-1.24540630
Pt	-2.16221356	-0.96776619	-1.27368735
Pt	-0.21804776	-2.76711440	2.74768191
Pt	1.66668786	-1.37268068	1.13211125
Pt	1.55533346	1.45179576	-1.87162285

13

PRE:81 = -56.67906545

Pt	0.75633781	4.06345248	-0.00000000
Pt	2.03099900	-0.43469021	0.00000000
Pt	2.46418187	2.11093909	-0.00000000
Pt	-2.54826873	0.75975730	-0.00000000
Pt	-0.15618860	1.63195270	-0.00000000
Pt	-0.53569454	-0.87902284	-0.00000000
Pt	-1.90272510	-5.19364410	0.00000000
Pt	-4.57847869	2.39611111	-0.00000000
Pt	-2.05095939	3.39424326	-0.00000000
Pt	4.13336334	-2.19916546	0.00000000
Pt	-2.31286800	-2.70237180	0.00000000
Pt	0.25221931	-3.34158097	0.00000000
Pt	4.44808172	0.39401944	0.00000000

13

PRE:82 = -56.39402585

Pt	-2.64963939	-0.35021190	3.05214143
Pt	-1.14608613	-1.67347523	0.96753581
Pt	1.69832845	-0.89968486	1.26282044
Pt	-3.05225411	0.54705908	-3.06385164
Pt	2.25664383	1.55733886	-0.56933910
Pt	-0.64628876	-0.36267990	-2.97421719
Pt	2.19251679	-0.67363593	-2.17643617
Pt	0.23709926	-0.11636108	-0.58599516
Pt	-0.38154643	0.57588571	2.36634074
Pt	-0.47686678	-1.73496804	3.63933484

Pt	-2.35569219	0.04866825	-0.62700226
Pt	4.38976060	0.88636026	-1.66029289
Pt	-0.06597512	2.19570479	0.36896116

13

PRE:83 = -57.47164657

Pt	1.33948592	-1.50608802	1.95446440
Pt	2.33484889	0.49055687	0.56690447
Pt	3.88763915	-1.48391042	0.86327841
Pt	-1.97086104	-1.76495097	-1.73040096
Pt	2.62419993	-1.22219868	-1.33180681
Pt	0.16199322	-1.35859823	-0.33870047
Pt	-4.83895440	1.46213689	0.44939661
Pt	-2.94160928	2.16362062	-1.09235743
Pt	-0.61524717	0.39867993	2.48233345
Pt	4.79037378	0.04078580	-1.40797057
Pt	-0.37481218	0.37102371	-2.03225683
Pt	-1.75269725	0.17545666	0.17400202
Pt	-2.64435958	2.23348584	1.44311370

13

PRE:84 = -57.85730613

Pt	-3.49403288	-1.00751060	-0.16018186
Pt	2.03998913	-0.22407914	1.73846349
Pt	1.40664219	2.99046254	1.14211695
Pt	0.66018543	-2.50907382	-2.53472727
Pt	-2.22765645	0.89962738	0.90592877
Pt	-0.33976908	0.22505173	-2.27423593
Pt	0.88479057	2.49866656	-1.87537056
Pt	-2.30985686	-2.16271000	1.84452002
Pt	-0.41563038	-0.32259564	2.44361096
Pt	1.58983444	-1.19902563	-0.59000798
Pt	0.34907166	0.90754929	0.09688180
Pt	2.78267800	1.28517124	-0.51453301
Pt	-0.92624578	-1.38153390	-0.22246538

13

PRE:85 = -56.66752062

Pt	-0.77016792	0.30205466	-0.00000000
Pt	1.69846289	-0.08801161	-0.00000000
Pt	3.31687241	1.83604053	0.00000000
Pt	-4.24903633	-0.79221189	-0.00000000
Pt	0.79824636	2.32653411	0.00000000
Pt	-1.50923405	-4.86224445	0.00000000
Pt	-3.75164284	-3.35633401	-0.00000000
Pt	-0.92067567	-2.32651702	-0.00000000
Pt	3.97442165	-1.09814783	-0.00000000
Pt	0.13038658	4.84151550	0.00000000
Pt	1.69484363	-2.59990957	-0.00000000
Pt	2.61506791	4.35087279	0.00000000
Pt	-3.02754461	1.46635878	-0.00000000

13

PRE:86 = -54.80023890

Pt	1.34398560	-0.36479826	-0.00000000
Pt	3.75098456	0.55964130	-0.00000000
Pt	-0.18929821	-4.68253653	-0.00000000
Pt	1.67450903	2.10904611	0.00000000
Pt	-2.83963971	-0.98143881	0.00000000
Pt	3.97158578	3.12103691	0.00000000
Pt	-3.79985365	1.35071559	0.00000000
Pt	6.13805234	1.56458520	-0.00000000
Pt	-0.54055866	3.45567669	0.00000000
Pt	-1.03557443	0.85491392	-0.00000000
Pt	-2.56484878	-3.68455176	0.00000000
Pt	-5.38988175	-1.19223531	0.00000000
Pt	-0.51946211	-2.11005505	-0.00000000

13

PRE:87 = -57.87355073

Pt	0.91581204	2.96509815	-1.15319901
Pt	-2.29553934	2.38249892	-1.05116946
Pt	1.19185588	0.13517154	1.32948383
Pt	-0.93022412	1.14377527	2.43684289
Pt	-0.67511694	2.39802429	-3.09718947
Pt	0.77578000	-1.69418420	3.12888615
Pt	-3.12047077	0.01799999	1.64423178
Pt	0.45200326	-2.24396622	0.46224739
Pt	2.93426530	-1.81676104	0.80813621
Pt	0.19040865	-0.90711618	-1.85441307
Pt	-0.35154741	-3.38149631	-1.65389206
Pt	1.97017636	0.70121104	-0.98504935
Pt	-1.05740291	0.29974475	-0.01491583

13

PRE:88 = -57.38564163

Pt	-0.29858329	1.30076237	-0.47893002
Pt	2.03835934	-1.04031809	-1.61274059
Pt	-2.63405548	0.32802466	-1.04553261
Pt	0.45490337	2.23050488	1.95574692
Pt	-3.50094134	-1.49011101	0.73588514
Pt	1.93275855	0.58875087	0.57340305
Pt	-0.47182822	-0.87012437	-1.84351617
Pt	-1.30766351	-0.24595008	1.34581815
Pt	-2.51737176	2.77575703	-0.32733939
Pt	2.24999721	2.08118687	-1.53857237
Pt	4.03124040	-0.81298004	0.03829034
Pt	-0.55786207	-2.48840616	2.27105634
Pt	0.58104680	-2.35709694	-0.07356880

13

PRE:89 = -56.60586191

Pt	2.11502458	1.41356723	-2.09612695
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Pt	-1.84458816	0.69873229	1.78811027
Pt	-3.07002263	1.64585140	-0.39137170
Pt	-4.32349713	1.84130415	1.87826931
Pt	1.84155295	2.26855361	0.43605204
Pt	1.83028704	-0.91194700	0.69688148
Pt	0.18437130	0.51359375	-0.64630562
Pt	-3.43429068	-0.83501063	-0.64506613
Pt	4.06245275	-0.25680765	1.80109675
Pt	-1.19869839	-1.35353611	0.48729569
Pt	-0.53932597	-1.59886587	-1.96087464
Pt	0.66187197	-3.13094217	-0.39346090
Pt	3.71486238	-0.29449299	-0.95449961

13

PRE:90 = -53.64791326

Pt	-0.69847495	5.63844722	0.00000000
Pt	0.14131300	0.07574075	0.00000000
Pt	0.01483995	-4.47521340	-0.00000000
Pt	2.56608398	-0.73886235	0.00000000
Pt	2.38938271	-3.33217433	-0.00000000
Pt	1.19246553	-6.78000475	-0.00000000
Pt	-2.79647710	3.87030043	0.00000000
Pt	2.10108863	1.75881968	0.00000000
Pt	-2.11968688	1.38404296	0.00000000
Pt	-0.22517047	3.10232785	0.00000000
Pt	2.05328314	4.35294909	0.00000000
Pt	-2.15869575	-1.19911850	0.00000000
Pt	-2.45995177	-3.65725466	-0.00000000

13

PRE:91 = -51.64987794

Pt	1.83726370	-2.77309546	-0.00000000
Pt	-2.70321390	3.14590282	0.00000000
Pt	-0.33616058	2.29103769	0.00000000
Pt	2.00103040	1.28024427	-0.00000000
Pt	-1.99876957	0.38268611	-0.00000000
Pt	-0.90527774	5.00711249	0.00000000
Pt	0.30182487	-0.71940390	-0.00000000
Pt	-3.57058926	-1.71226553	0.00000000
Pt	3.22012472	-5.03817515	0.00000000
Pt	5.68913103	-5.35184892	0.00000000
Pt	-4.55314154	0.83768762	-0.00000000
Pt	-3.49874855	5.53831396	0.00000000
Pt	4.51652643	-2.88819600	0.00000000

13

PRE:92 = -55.63816907

Pt	1.90106799	1.53829469	-0.00000000
Pt	1.93549765	-3.20132630	-0.00000000
Pt	5.08138296	0.68847322	0.00000000
Pt	-0.90070938	-0.28505616	-0.00000000

Pt	-3.01554724	-4.21031516	-0.00000000
Pt	-5.42103460	0.22423643	0.00000000
Pt	-3.23105885	-1.47543129	-0.00000000
Pt	4.06755862	2.97439553	0.00000000
Pt	2.89325630	-0.81775696	0.00000000
Pt	1.09460408	4.10977841	-0.00000000
Pt	-0.81369405	-2.85083155	-0.00000000
Pt	-0.55822941	2.21288672	-0.00000000
Pt	-3.03309405	1.09265241	0.00000000

13

PRE:93 = -56.39153607

Pt	3.71293175	-2.42091956	1.48912068
Pt	0.95430084	-2.25171044	0.39469895
Pt	2.62773198	-0.56116419	-0.76271890
Pt	1.74293086	0.21149210	-3.15469942
Pt	-4.01962267	1.76898890	-0.37419943
Pt	0.57932640	1.90318216	-0.73299561
Pt	2.90152680	0.01590859	1.71344793
Pt	0.43587915	0.11723004	1.28102090
Pt	-3.56077871	-0.76926429	0.09841180
Pt	-0.83029855	1.17785109	3.20668645
Pt	0.14554651	-0.56893857	-1.37398455
Pt	-3.05175741	0.05579279	-2.25331246
Pt	-1.63771695	1.32155139	0.46852364

13

PRE:94 = -56.39299431

Pt	0.70805391	-3.78246029	0.00000000
Pt	-1.58189458	-4.96233790	0.00000000
Pt	-3.77127861	-1.42251532	-0.00000000
Pt	1.89886151	2.35947011	0.00000000
Pt	-1.74959808	0.14830493	-0.00000000
Pt	-0.68987391	2.41351176	-0.00000000
Pt	2.93390845	-2.22337505	0.00000000
Pt	-1.45201318	-2.40350865	-0.00000000
Pt	3.45971631	0.32811772	0.00000000
Pt	4.44520539	2.77852579	0.00000000
Pt	-3.35780917	2.07090575	-0.00000000
Pt	-1.63210546	4.85315333	0.00000000
Pt	0.78882744	-0.15779217	-0.00000000

13

PRE:95 = -57.94733176

Pt	-2.01446887	3.45750781	-1.29659825
Pt	-0.27469581	-1.55570628	-0.97616105
Pt	-0.67856621	1.08816606	-1.20666888
Pt	-0.03599251	-0.37308517	-3.15721244
Pt	2.33447211	-0.60864023	0.43010042
Pt	2.51683214	-2.25339334	-1.49859681
Pt	-1.02462058	-0.59527271	3.48904947

Pt	2.22617497	0.12392099	-2.14893140
Pt	0.57739625	-1.85702227	1.73323845
Pt	0.91443944	1.74031150	0.62521071
Pt	-1.94346143	-2.13193471	1.78401751
Pt	-1.04230185	0.23137997	1.14923808
Pt	-1.55520766	2.73376838	1.07331418

13

PRE:96 = -55.46471282

Pt	-2.57145524	-2.83392015	0.00000000
Pt	-1.62280691	3.35824144	0.00000000
Pt	4.79206936	-2.63836123	-0.00000000
Pt	-0.98542778	0.89336082	-0.00000000
Pt	4.11965357	0.08523001	-0.00000000
Pt	-0.32614868	-1.56304623	-0.00000000
Pt	2.25172049	-1.89679727	-0.00000000
Pt	-0.15600600	5.55869840	0.00000000
Pt	0.93344761	3.19464895	0.00000000
Pt	0.77153413	-4.04444866	-0.00000000
Pt	1.60573984	0.65514391	0.00000000
Pt	-3.54841450	0.57984957	-0.00000000
Pt	-5.26390588	-1.34859956	0.00000000

13

PRE:97 = -55.68910833

Pt	2.85386576	0.17469269	-0.00000000
Pt	0.03985747	-3.67228664	-0.00000000
Pt	0.06218788	1.29701534	-0.00000000
Pt	-4.57649738	-0.80770804	0.00000000
Pt	2.08887226	2.82978373	0.00000000
Pt	4.60834790	2.12551666	0.00000000
Pt	1.04420262	5.15904342	0.00000000
Pt	-1.22111292	3.48779826	0.00000000
Pt	-2.44837487	0.66771679	-0.00000000
Pt	-0.29862803	-1.21822927	-0.00000000
Pt	2.11669724	-2.18927266	-0.00000000
Pt	-1.85714040	-5.27935574	0.00000000
Pt	-2.41227753	-2.57471457	0.00000000

13

PRE:98 = -56.09190995

Pt	0.89485231	-2.82161764	0.20075327
Pt	-1.16835825	-1.33452030	0.10110853
Pt	0.01890612	-1.47238177	-2.18492416
Pt	-0.80659809	0.85204017	-1.07366024
Pt	0.30764330	-1.41473461	-4.75928829
Pt	2.08654695	-0.45713633	-1.05189377
Pt	1.16385503	-0.21060653	4.06417028
Pt	1.17822730	2.13705445	0.36379930
Pt	-1.08339922	1.51854134	1.78701036
Pt	0.83423407	-0.19568123	1.24306480

Pt	-2.72782261	2.19939379	-0.08421373
Pt	-3.26272907	-0.08383006	-1.13262831
Pt	2.56464216	1.28347872	2.52670195

13

PRE:99 = -53.94063921

Pt	1.94595808	-1.40208472	-0.00000000
Pt	4.74826231	-1.42303807	-0.00000000
Pt	4.17877892	1.06822171	-0.00000000
Pt	-0.92252902	2.34603798	0.00000000
Pt	-0.07560599	-2.94910917	-0.00000000
Pt	6.82042190	0.16268072	-0.00000000
Pt	-5.69862129	0.22314383	0.00000000
Pt	-4.34994003	2.38063196	0.00000000
Pt	2.18259201	-4.07062341	-0.00000000
Pt	1.62959882	1.12742312	-0.00000000
Pt	-3.02619965	0.21462592	0.00000000
Pt	-0.55872355	-0.19040632	0.00000000
Pt	-6.87399251	2.51249646	0.00000000

13 (LM2)

PRE:100 = -58.85961753

Pt	2.26335328	0.00612208	2.09629888
Pt	0.64853761	-1.55170771	-0.44729648
Pt	-0.04690103	-1.15083619	2.21463263
Pt	-1.48626501	-2.75723177	-1.05329775
Pt	-3.08066317	-0.12408411	1.44036838
Pt	-0.12817729	2.58446149	-0.71811908
Pt	3.07496651	-1.68091491	0.36227753
Pt	-0.87940957	0.34807215	0.26975471
Pt	-1.06451284	-0.02794967	-2.25102937
Pt	1.63100337	2.17365385	-2.46452054
Pt	0.63023615	2.09222532	1.91321434
Pt	1.61966816	0.75376533	-0.28425344
Pt	-3.18183618	-0.66557585	-1.07802980

13

PRE:101 = -55.25813151

Pt	-1.54142375	-2.19801809	0.00000000
Pt	0.68147217	0.35233099	-0.00000000
Pt	-1.76091013	4.93057193	-0.00000000
Pt	1.22865916	-4.75367051	0.00000000
Pt	-3.51895953	-3.78491670	0.00000000
Pt	-0.61245411	2.61230935	-0.00000000
Pt	-2.03450001	0.35323980	0.00000000
Pt	2.02203439	2.67491795	-0.00000000
Pt	-3.89050242	-1.30105008	0.00000000
Pt	4.36461925	-1.96704686	0.00000000
Pt	0.84481139	4.88129459	-0.00000000
Pt	3.22188795	0.34760403	0.00000000
Pt	0.99526566	-2.14756640	-0.00000000



13

PRE:102 = -56.84755015

Pt	3.83807986	0.47789357	-0.41486204
Pt	-3.61978813	-1.29355871	-2.37294406
Pt	-1.33146161	-1.09520038	-0.66580007
Pt	-0.93826676	-1.39900026	2.05893333
Pt	0.40772534	-2.90945805	-0.47725321
Pt	2.71612399	2.18710702	1.57903081
Pt	0.50340454	-1.09163537	-2.34195631
Pt	1.61954351	2.22877741	-0.79562832
Pt	0.87251100	0.49369340	2.37219110
Pt	-1.66569974	0.18222256	-2.85841529
Pt	1.35466891	-0.20431312	-0.07683760
Pt	-2.81582589	0.21010930	2.07111302
Pt	-0.94101503	2.21336262	1.92242864

13

PRE:103 = -57.90917750

Pt	1.05409385	-0.30366495	-2.60524785
Pt	0.03362738	-1.33440048	1.81706796
Pt	-2.30212080	-0.46887069	0.86134365
Pt	2.72337129	-1.33950465	1.76020034
Pt	-1.26593620	2.61850618	-3.22503335
Pt	2.61073150	0.73028595	0.29067743
Pt	1.41306991	-1.98981147	-0.76731401
Pt	0.87578389	2.18100685	-1.94080579
Pt	-0.62388570	-3.23113316	0.24804998
Pt	-0.17769253	1.37513844	2.07215730
Pt	-2.05029613	0.57351807	-1.48218263
Pt	-2.45327398	1.05363702	3.17692932
Pt	0.16252753	0.13529287	-0.20584236

13

PRE:104 = -57.81438034

Pt	0.54903247	1.54106804	1.58816433
Pt	-2.12404256	0.85772754	0.20040617
Pt	2.57924301	0.72027408	2.91861915
Pt	0.04465218	-0.74554171	2.57454003
Pt	0.02033878	-0.42588000	0.04326309
Pt	-0.82369094	3.05691159	-0.08158272
Pt	1.93575385	-0.79957796	-2.15856028
Pt	-0.82785062	-2.25525187	-1.93856826
Pt	-0.78069058	2.91020588	-2.52820275
Pt	2.37974302	0.35372011	0.24814624
Pt	-0.53333315	-3.33992409	1.77342793
Pt	-0.38367591	0.13631309	-2.87509910
Pt	-2.03547954	-2.01004471	0.23544617

13

PRE:105 = -57.32623240

Pt	0.26860712	0.26298842	-3.68485090
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Pt	-2.17596139	-0.58257738	0.11271796
Pt	-0.90332485	0.33339255	2.22468118
Pt	-1.16856285	-2.22257489	-1.81624532
Pt	0.74958794	-0.88308453	0.78135060
Pt	2.39296771	0.42363767	2.14314023
Pt	-2.51796015	2.21537471	0.86954372
Pt	0.01494436	2.33975924	0.48755235
Pt	0.91873578	0.65221881	-1.23991736
Pt	1.27522539	-1.79550854	-2.14107343
Pt	0.86486448	-0.97739272	3.55859116
Pt	1.36192392	2.46422031	-3.12406928
Pt	-1.08104746	-2.23045363	1.82857910

13

PRE:106 = -56.36514792

Pt	-0.62165912	-1.45392151	-1.58115288
Pt	0.40078308	1.14951903	2.31455658
Pt	-1.06628999	2.86480124	1.07040167
Pt	0.32170457	1.45128890	-0.47750739
Pt	-2.43320598	-3.03046560	0.57265454
Pt	-1.92186316	-0.89626106	1.84975147
Pt	-0.73216802	-4.08326213	-1.27142482
Pt	0.67888600	4.58025359	0.52287013
Pt	0.43196630	-0.84181668	0.68632279
Pt	2.48561491	2.62042153	-0.03748503
Pt	0.06132460	0.68990257	-3.01564869
Pt	2.27108210	0.33094988	-1.71034423
Pt	0.12382469	-3.38140976	1.07700587

13

PRE:107 = -53.28041956

Pt	0.09162232	-0.96956489	0.00000000
Pt	-3.35573024	5.23640497	-0.00000000
Pt	-0.58180294	-3.43131476	0.00000000
Pt	-0.03129939	1.66657116	-0.00000000
Pt	0.71263041	4.08669370	0.00000000
Pt	-4.60810994	1.47482165	-0.00000000
Pt	-2.21815698	0.25855928	-0.00000000
Pt	2.55583635	-0.34161699	0.00000000
Pt	2.63137871	2.13180507	0.00000000
Pt	-2.49526558	2.81770594	-0.00000000
Pt	1.96508095	-2.81887779	0.00000000
Pt	1.35706540	-5.32830438	0.00000000
Pt	3.97675094	-4.78288296	0.00000000

13

PRE:108 = -55.45606351

Pt	-3.51729728	4.24985108	0.00000000
Pt	2.12334005	-0.40022213	-0.00000000
Pt	-0.94500254	4.29942398	0.00000000
Pt	0.11704270	-4.72042235	0.00000000

Pt	-0.16902784	-2.19983378	0.00000000
Pt	4.40380576	-1.79033469	-0.00000000
Pt	2.20887680	-3.14966948	-0.00000000
Pt	-0.30952804	0.30071348	-0.00000000
Pt	-3.78244269	-0.02232212	-0.00000000
Pt	1.31607884	2.23562856	0.00000000
Pt	-2.24797352	1.98647940	-0.00000000
Pt	-2.95983091	-2.42156621	0.00000000
Pt	3.76195866	1.63227423	0.00000000

13

PRE:109 = -57.87237418

Pt	-0.65178796	2.06321905	2.97149083
Pt	1.41579480	0.57845827	2.49204582
Pt	2.46456776	-0.69146508	0.26619141
Pt	0.78533065	-1.94817884	2.32939478
Pt	-2.95430881	-1.61272543	-0.11470274
Pt	-1.11239898	-0.56929558	1.30963391
Pt	-0.82486913	-1.85369844	-1.65061522
Pt	-0.32458491	3.10673242	-1.23970757
Pt	-0.42564987	-0.09414662	-3.41781880
Pt	1.55939412	-2.74713114	-1.56553329
Pt	2.15576003	1.44059104	-1.02403607
Pt	-1.86337134	1.85514743	0.54777533
Pt	-0.22387635	0.47249295	-0.90411838

13

PRE:110 = -56.48917130

Pt	0.09625389	0.06223442	3.94509393
Pt	0.19296857	-2.53813332	4.35309882
Pt	0.05845301	0.04599833	0.00483941
Pt	0.93862855	-0.22309738	-2.33071977
Pt	-2.35218312	0.11108863	0.45657411
Pt	2.54877095	0.46318841	-0.45808071
Pt	0.04055366	1.58903306	-3.88122880
Pt	-1.02856613	2.24006724	1.01912423
Pt	1.56852250	-0.13975734	-5.05864924
Pt	-1.23697995	-2.13452772	-0.64867185
Pt	-1.25421581	1.38655782	-1.68533071
Pt	-1.13349039	-1.53395385	2.27436327
Pt	1.56128426	0.67130171	2.00958729

13

PRE:111 = -55.76690928

Pt	1.58516391	1.66339509	0.00000000
Pt	-0.41060880	-1.59354491	-0.00000000
Pt	-0.39227906	3.37103404	0.00000000
Pt	-2.94219091	-1.05488076	-0.00000000
Pt	2.08386079	-0.85566646	0.00000000
Pt	2.01840007	4.28023183	0.00000000
Pt	4.03560210	-2.44884921	0.00000000

Pt	1.57877785	-3.36575039	-0.00000000
Pt	-1.27229164	0.94951042	0.00000000
Pt	-3.86432160	1.35687914	-0.00000000
Pt	3.93803616	2.58745984	0.00000000
Pt	-5.47866001	-0.71448571	-0.00000000
Pt	-0.87948886	-4.17533293	-0.00000000

13

PRE:112 = -55.79554376

Pt	2.24027849	-4.27463956	0.00000000
Pt	-0.31551373	-3.43998410	0.00000000
Pt	-2.31030097	-1.66807534	0.00000000
Pt	-1.63823974	3.85299222	-0.00000000
Pt	1.48264499	4.95438824	-0.00000000
Pt	-4.13946590	0.12120350	-0.00000000
Pt	-2.81000623	-4.22862733	0.00000000
Pt	3.34133191	2.89270087	-0.00000000
Pt	0.60724101	2.60888348	-0.00000000
Pt	0.11795645	-0.89899518	0.00000000
Pt	-1.67972654	1.27818871	-0.00000000
Pt	2.92807234	-1.78862857	0.00000000
Pt	2.17572793	0.59059306	0.00000000

13

PRE:113 = -57.63755730

Pt	2.63021387	2.12050290	0.38331271
Pt	1.03926394	-3.13128228	0.31228609
Pt	0.09927751	2.16754194	1.02184651
Pt	-1.17645588	-1.78872501	-0.08809763
Pt	3.07726277	-1.76830404	1.09985496
Pt	1.43150533	0.11818158	1.74460034
Pt	1.08406691	3.07373183	-1.40023779
Pt	0.36302319	0.27656445	-0.68938338
Pt	-1.35598872	2.25684267	-1.07501841
Pt	-2.45946232	-0.20860283	-1.62208451
Pt	-1.86126065	0.49530629	0.88782291
Pt	-2.67807298	-2.06126136	1.87827566
Pt	-0.19337297	-1.55049613	-2.45317746

13

PRE:114 = -57.20574168

Pt	3.38302574	-1.37343026	2.84664645
Pt	-1.45762932	-1.90581785	-1.24816777
Pt	0.69318415	0.94269928	-0.38490467
Pt	-4.32269375	-0.04382657	-2.73877783
Pt	2.34676172	-0.93806804	0.49494720
Pt	-0.13766535	-2.33896809	1.10300462
Pt	3.18523732	1.36210275	2.26571860
Pt	0.51334236	0.38156899	2.34452533
Pt	-2.08185748	0.63195750	-1.55308083
Pt	-4.00526785	2.03306476	-0.72647370

Pt	-1.33544625	-0.17373887	0.73770000
Pt	0.04762052	0.07394882	-2.89216734
Pt	3.17138818	1.34850759	-0.24897007

13

PRE:115 = -57.22493393

Pt	3.48422366	0.87819953	-0.27603156
Pt	-0.17250383	-1.85260468	0.98410635
Pt	-1.45214313	-0.28804292	2.70472284
Pt	-1.94181740	0.94193822	0.59542601
Pt	1.23203530	1.16621682	3.58040199
Pt	1.93762951	-0.37830069	1.33247941
Pt	-2.70252002	-1.94991687	0.63297227
Pt	0.46350682	-1.09816877	-3.01147561
Pt	0.71810006	0.11559685	-0.81957036
Pt	0.23994042	1.30065304	-3.88118542
Pt	-1.13589587	-2.31759682	-1.35304063
Pt	0.42738908	1.72553552	1.18970821
Pt	-1.09794461	1.75649079	-1.67851352

13

PRE:116 = -57.86236085

Pt	0.49272487	2.08972091	1.42701907
Pt	0.82672758	-2.20888570	-2.87946680
Pt	1.28613000	0.56949199	3.59820960
Pt	0.74582742	2.36135684	-1.12791618
Pt	1.99910728	-0.65268005	1.46673588
Pt	0.84854509	-0.20072449	-0.76604732
Pt	-0.53611072	-1.15526600	1.15902499
Pt	0.93172930	-2.73627517	-0.15117468
Pt	-1.11363383	-1.76397303	-1.22146516
Pt	-2.57393938	0.09680042	2.23305530
Pt	-1.57541888	2.65754080	-0.20429977
Pt	1.17585445	0.65468204	-3.16068200
Pt	-2.50754317	0.28821144	-0.37299293

13 (LM4)

PRE:117 = -58.69767683

Pt	-0.04157147	-0.91208853	-1.54385649
Pt	-0.00253979	1.61658355	-0.88551463
Pt	1.03493497	-0.97992789	0.89874197
Pt	2.16042541	0.26848512	-1.13150581
Pt	-1.48190256	0.33924372	1.70554208
Pt	-2.18390863	0.34144747	-0.93292816
Pt	-1.32391556	-1.86748977	0.36070926
Pt	2.13120336	2.58560313	-2.19422587
Pt	-2.88884816	-1.78031998	2.41108071
Pt	1.91653130	3.10039615	0.30921099
Pt	1.19028228	-2.97282944	-2.28078214
Pt	-4.13322501	0.48005994	2.36050332
Pt	3.62253386	-0.21916348	0.92302478

### 13 (LM7)

PRE:118 = -58.52594807

Pt	1.92468276	-0.87596294	-0.63838174
Pt	0.88257385	-0.23992049	-3.06365287
Pt	3.02273659	-1.62881171	-3.02838514
Pt	-1.68398080	1.52219278	-0.25376096
Pt	-1.50797142	-0.10925673	3.47629353
Pt	-2.93906037	-1.71379580	-0.32549851
Pt	0.53293000	0.54139173	2.05697962
Pt	1.39105745	2.82575811	0.85312952
Pt	-0.89349589	2.57509198	2.04434779
Pt	0.16297240	-2.02168301	2.32162818
Pt	-1.03130225	-1.72767379	-2.20270920
Pt	-0.54051373	-0.77511780	0.05443953
Pt	0.67937141	1.62778767	-1.29442974

13

PRE:119 = -56.66366739

Pt	-0.80573866	0.66197335	0.23702916
Pt	0.66953370	-1.20502607	1.26653330
Pt	-1.41489383	2.58259943	-1.33213129
Pt	1.48147789	1.33743647	1.97807441
Pt	-2.34233049	1.60374147	-3.46091570
Pt	-2.87421545	0.28695514	-1.14167523
Pt	-1.02037432	2.44654829	2.09156437
Pt	-0.20074866	-0.73353257	-1.76507325
Pt	3.98743694	-2.28928174	0.13528315
Pt	-1.01842250	0.05381033	2.80678880
Pt	2.79659665	-0.08255075	0.30127745
Pt	1.79873115	-2.04971742	-0.98229064
Pt	-1.05705242	-2.61295592	-0.13446453

13

PRE:120 = -54.73770149

Pt	-0.19787948	-0.39847125	-0.00000000
Pt	3.07860824	5.80566382	-0.00000000
Pt	-1.26606441	-5.22693595	0.00000000
Pt	-4.69050134	1.38095567	0.00000000
Pt	3.02563508	3.26020348	-0.00000000
Pt	3.02701130	0.62785299	-0.00000000
Pt	1.04126472	-6.38632059	0.00000000
Pt	0.90071223	-3.76952264	0.00000000
Pt	-3.17766187	-0.69052816	0.00000000
Pt	0.83196453	1.98697131	-0.00000000
Pt	0.78095973	4.52755544	-0.00000000
Pt	-1.95126377	1.52881599	0.00000000
Pt	-1.40278498	-2.64624012	0.00000000

### 13 (LM1)

PRE:121 = -58.99275092

Pt	-0.43675270	2.67398498	-2.36662482
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Pt	0.41806278	2.45604702	1.77221973
Pt	2.15564696	-0.05882736	-2.38000025
Pt	1.59662483	0.26711652	2.53018859
Pt	1.18352830	1.54607379	-0.56819991
Pt	-0.31374317	0.10771496	-2.04030274
Pt	-0.81744556	-2.08857983	-0.78794860
Pt	-0.88456818	-2.01497604	2.25601531
Pt	1.01517953	-3.12740532	0.84004042
Pt	1.93792640	-0.77250473	0.28869604
Pt	-2.54801129	1.27868301	-1.70727344
Pt	-2.83892920	-0.28105436	1.54559164
Pt	-0.46751870	0.01372734	0.61759802

13

PRE:122 = -57.35575336

Pt	0.54386281	0.03134828	3.95686023
Pt	-1.46838420	-0.04959545	2.12124617
Pt	-1.33031001	0.75964915	-0.37538837
Pt	0.43114420	3.25799056	-0.18527454
Pt	-0.84981494	-2.64606746	-2.46152502
Pt	0.53897355	-2.05146389	2.12081285
Pt	1.11483167	0.88792497	-1.04125253
Pt	2.99837415	2.22050011	0.24789078
Pt	0.05770129	-1.39713648	-0.43402101
Pt	-1.50270261	2.65674682	-2.25969621
Pt	0.03079890	-4.01181364	-0.36438906
Pt	1.32386966	0.25863177	1.39555204
Pt	-1.88834448	0.08328524	-2.72081533

13

PRE:123 = -55.66666751

Pt	0.07625645	5.94923075	-0.00000000
Pt	2.13489542	-2.95446776	0.00000000
Pt	3.22215141	-0.36522827	0.00000000
Pt	-1.68454007	4.01905405	-0.00000000
Pt	0.21623484	-4.63857661	0.00000000
Pt	0.78597588	3.54296848	-0.00000000
Pt	-3.94315684	1.21519940	-0.00000000
Pt	1.05750053	0.99231644	-0.00000000
Pt	4.77603509	-2.80552104	0.00000000
Pt	-2.53409336	-3.45311732	0.00000000
Pt	-2.45742936	-0.84041271	0.00000000
Pt	-0.19548644	-2.15863620	0.00000000
Pt	-1.45434356	1.49719077	-0.00000000

13

PRE:124 = -57.95789502

Pt	-1.48817612	1.27483539	1.03953724
Pt	0.95460445	1.59089472	1.52669360
Pt	0.58952448	-2.78094259	1.20477053
Pt	-1.05978805	-0.95892132	2.17239415

Pt	-1.22300545	-0.19208151	-1.72895776
Pt	-3.25035115	-0.29302408	0.04130325
Pt	2.24984662	2.54111916	-0.50799571
Pt	0.77552353	-0.40515648	-0.09399740
Pt	0.97295822	-2.61214112	-1.34745130
Pt	-0.26835376	2.60642033	-0.67309336
Pt	3.28990082	3.12618770	1.81137567
Pt	-1.71361251	-2.47442882	0.09231100
Pt	0.17092891	-1.42276138	-3.53688990

13

PRE:125 = -56.76296338

Pt	-1.16271727	-2.94213900	0.31677775
Pt	-1.03102062	-0.40577430	0.62503568
Pt	3.03836560	-1.22598692	2.67037638
Pt	3.63639139	1.08020736	1.46448778
Pt	2.19594680	1.09592555	-0.67388477
Pt	-0.04521709	1.93548753	-1.46730257
Pt	1.84260372	-1.21059230	0.44317093
Pt	-3.08572491	-1.57451230	1.58814679
Pt	-2.38197265	0.91854016	2.32952598
Pt	-2.79722041	-1.30218475	-0.92932405
Pt	0.08933646	-0.58487700	-1.65400790
Pt	1.98827035	3.33719143	-2.34902504
Pt	-2.28704138	0.87871453	-2.36397695

13

PRE:126 = -57.81651543

Pt	2.19400513	1.05075309	-1.29135139
Pt	-2.12803191	-1.23660908	-1.01346449
Pt	-0.22350476	0.28978046	-0.35566828
Pt	-2.22444638	1.12539834	1.25084977
Pt	0.07640978	2.51548183	-1.56742378
Pt	1.04211595	0.38092715	1.84647285
Pt	-1.88482375	-0.05488725	-3.34660818
Pt	3.42853986	-0.28662975	1.50072516
Pt	-2.83297964	-1.44779538	1.55357913
Pt	-0.05745898	2.59640267	1.14710984
Pt	-0.34502710	-1.75923153	1.55033203
Pt	0.88234172	-0.71038914	-2.56699885
Pt	2.07286008	-2.46320142	1.29244619

13

PRE:127 = -57.13663010

Pt	1.91720060	1.29228907	1.52085011
Pt	-2.94310153	0.59879064	2.13517674
Pt	1.55917238	2.54497455	-0.61815955
Pt	0.25461326	-3.00731072	-2.66405035
Pt	0.90434318	-0.57969999	-1.88971456
Pt	-3.37621507	-0.67786030	-0.05361887
Pt	-1.19872507	0.53853905	-0.48575391



Pt	3.26843049	-1.25981596	0.52069977
Pt	-0.55320089	0.37796204	2.53601750
Pt	3.72579114	1.09208284	-0.74405005
Pt	0.78533305	-0.75043804	0.64763438
Pt	-0.98801640	-2.08515283	-0.63100250
Pt	-3.35562515	1.91563965	-0.27402871

13

PRE:128 = -54.54175884

Pt	2.70623499	-1.71548581	-0.00000000
Pt	-4.53910291	-2.13288250	0.00000000
Pt	-5.04947203	0.60623013	0.00000000
Pt	0.72448450	3.20718991	-0.00000000
Pt	-1.82936977	-3.16783162	0.00000000
Pt	0.16271863	-1.55531571	-0.00000000
Pt	-2.52346591	-0.67511955	0.00000000
Pt	1.34540076	-3.86610637	-0.00000000
Pt	-2.86961180	1.85768113	-0.00000000
Pt	6.37036884	2.71347532	0.00000000
Pt	2.06851347	1.02116652	-0.00000000
Pt	-0.42076677	0.91344740	-0.00000000
Pt	3.85406800	2.79355116	-0.00000000

13

PRE:129 = -56.41795596

Pt	-1.78141780	-0.41026114	-0.39876403
Pt	-1.32980450	2.14557898	-0.60615253
Pt	1.78467836	-1.30291556	2.50535466
Pt	1.05806286	-0.67877387	-3.67075051
Pt	1.37683174	0.74000398	-1.41736329
Pt	2.97256183	0.33634469	0.68202420
Pt	-3.51621615	1.87411405	-2.09436924
Pt	0.39393498	0.09687363	0.89287043
Pt	-1.35365817	-2.43347522	1.47914859
Pt	-0.74642870	0.99254055	-2.86724412
Pt	2.82014225	-2.10476532	-0.04036938
Pt	-1.84612048	0.00125938	2.07914791
Pt	0.16743377	0.74347584	3.45646731

13

PRE:130 = -55.89841619

Pt	-3.40037364	0.49371189	-0.36039922
Pt	0.14247303	2.58446275	2.77133116
Pt	-2.14058320	1.78711203	1.57535002
Pt	-1.65584476	-3.05224629	0.34876651
Pt	2.56765831	-0.27694446	-0.27621205
Pt	0.75688339	-2.03671326	0.18237119
Pt	-1.21721370	-0.73934131	-0.59416694
Pt	4.94514375	-1.15025950	-0.85435064
Pt	0.12414948	1.13637749	0.67698733
Pt	-0.17369047	-0.85325366	2.24437387

Pt	0.77227017	-1.19472925	-2.29654447
Pt	2.87454664	0.26695179	-2.80805713
Pt	-3.59541901	3.03487179	-0.60944965

13

PRE:131 = -54.79915145

Pt	-0.50690230	-0.17209590	-0.00000000
Pt	1.16364735	3.30906600	0.00000000
Pt	-1.09747147	-2.63444883	-0.00000000
Pt	-0.87443107	4.80876953	-0.00000000
Pt	-3.35968445	3.67017909	0.00000000
Pt	1.84393979	0.81671794	0.00000000
Pt	-1.24667532	2.23976844	-0.00000000
Pt	1.45129452	-1.79799007	0.00000000
Pt	-1.82022867	-5.33359885	0.00000000
Pt	3.27801436	-3.63817369	0.00000000
Pt	3.59223773	2.67836134	0.00000000
Pt	0.66953313	-4.43150416	0.00000000
Pt	-3.09327360	0.48494915	-0.00000000

13

PRE:132 = -56.55707297

Pt	1.81116745	0.88815852	-0.29820741
Pt	0.45472622	0.63279021	-3.79016452
Pt	-0.07337972	3.68525399	-1.25158309
Pt	-2.05105441	-0.76332666	-0.95525159
Pt	2.07470469	-0.76816242	1.69835316
Pt	-2.78067443	-0.13711395	2.80103424
Pt	-0.22351810	-1.05794920	0.70813783
Pt	-1.63374201	-1.85882479	4.51720132
Pt	0.17844052	-1.26263430	-2.04735362
Pt	1.24632607	-3.03779480	-0.48963522
Pt	-0.46161781	1.25047466	-1.44545572
Pt	1.71855264	2.49890398	-2.67142454
Pt	-0.25993111	-0.06977524	3.22434916

13

PRE:133 = -56.26366067

Pt	-0.62979360	0.96150697	-2.22394994
Pt	-3.04678215	1.78528305	-2.28963140
Pt	1.99512699	-0.99306734	-0.21285756
Pt	-1.38910373	1.15999923	1.19537846
Pt	0.76668936	1.26966158	-0.17578553
Pt	-2.43837366	-0.75004511	-1.73098276
Pt	2.44435951	-1.69715218	2.44901888
Pt	2.56889977	2.23881405	1.39273254
Pt	0.13195745	-1.53890784	-2.09160228
Pt	3.12477598	1.27839497	-1.11275731
Pt	-1.93944671	-0.80513822	2.90371705
Pt	0.22150547	-0.76542484	1.52156951
Pt	-1.80981470	-2.14392430	0.37515032

13

PRE:134 = -56.55248006

Pt	-1.74058277	-0.06434354	1.02092970
Pt	0.67526349	-0.55205619	2.22953124
Pt	-0.09833874	-2.51864669	-1.16194664
Pt	1.51711806	0.56463812	0.03434843
Pt	-0.41491285	-1.14461621	-3.48623017
Pt	-3.07303139	-0.22966725	-1.17132101
Pt	3.19527658	-0.87925058	1.74680282
Pt	1.63277147	-0.06802576	-2.52477308
Pt	2.00219648	1.58347174	2.67711403
Pt	-1.30482396	-0.12191769	3.80236298
Pt	-0.53859219	-0.05938473	-1.24280928
Pt	-0.21504456	2.14271825	1.17148788
Pt	-1.63729964	1.34708053	-3.09549691

13

PRE:135 = -57.77182631

Pt	0.24328533	-0.41834940	2.24797132
Pt	-2.24727396	-0.94809381	-0.32848758
Pt	0.46830425	1.39350441	0.30379327
Pt	1.51052265	-2.84275138	2.24384349
Pt	-0.48458998	2.83322853	2.26699832
Pt	1.43931287	2.92210077	-1.58879940
Pt	-0.60799440	3.72555381	-0.28986799
Pt	-2.03949864	-1.67471288	2.46050557
Pt	1.52109533	-2.39077903	-0.20087440
Pt	0.03431867	-2.42080986	-2.30217186
Pt	2.50357738	-1.78499630	-2.58462021
Pt	-0.29817896	0.04717110	-1.68264560
Pt	-2.04288053	1.55893403	-0.54564491

13

PRE:136 = -56.80630963

Pt	1.01226209	0.58469241	1.66809977
Pt	-2.96846345	0.74621615	1.39849053
Pt	1.47609844	0.24416726	-0.86249874
Pt	2.18480378	-1.51522800	0.83908186
Pt	-1.01651055	0.69930256	-0.24386085
Pt	1.75299063	2.00286819	-2.83773019
Pt	-0.69812018	1.93878607	-3.46236472
Pt	2.14144530	-2.07401833	-1.76327971
Pt	-1.83448140	-0.51007162	3.62544367
Pt	-0.59250303	-0.44531043	-2.49919807
Pt	1.16741223	2.60098125	-0.08435026
Pt	-0.81620929	-1.23954582	1.37915680
Pt	-1.80872456	-3.03283970	2.84300990

13

PRE:137 = -57.24442896

Pt	0.22461442	2.11098987	-0.91360660
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Pt	-0.46179105	-1.37162511	2.36422302
Pt	0.49048068	1.62221304	3.87570324
Pt	-0.51228759	-2.90934546	-0.35088740
Pt	1.49763459	-2.38218754	1.18685784
Pt	0.60332946	0.79405332	-3.06358276
Pt	-1.78375977	-1.66372365	-2.30884560
Pt	2.69967771	1.95745879	-1.60944453
Pt	-2.33528306	1.65145966	-0.82814405
Pt	2.09449472	-0.17078951	-0.04660684
Pt	0.13782522	0.93250109	1.42128353
Pt	-2.34357189	-0.21378556	0.92326981
Pt	-0.31136344	-0.35721894	-0.65021965

13

PRE:138 = -54.98655623

Pt	2.57409295	-0.40765240	0.64381109
Pt	-0.00399867	-0.31818433	0.94029208
Pt	1.13849496	-2.41306368	1.75592856
Pt	-1.31644715	0.58951137	2.97765362
Pt	-1.06396460	-2.59728801	0.59592072
Pt	-0.24210776	2.63829791	-4.82503252
Pt	3.92701654	1.05167325	2.26942281
Pt	-2.61831414	-0.58814130	1.06391788
Pt	-0.71006819	-0.55271742	-1.52649273
Pt	-0.05272919	-0.37553232	-4.02932390
Pt	1.53939899	-0.21679770	2.99764974
Pt	-1.33196512	1.63800488	-2.76033226
Pt	-1.83940862	1.55188975	-0.10341510

13

PRE:139 = -57.37345001

Pt	-2.27398095	2.53071017	-0.19995389
Pt	1.70225823	-2.31174165	-2.02646684
Pt	0.16920299	0.98914097	0.37957860
Pt	0.60315635	-3.30398015	0.35808185
Pt	-0.12446297	3.34239669	1.89236526
Pt	-2.12860661	0.26131084	1.00487677
Pt	-0.18693787	0.97339102	2.87480723
Pt	-0.67945854	-1.19563151	-0.53369149
Pt	-0.68651185	-1.90531675	-2.98765420
Pt	1.78686353	2.45372855	-1.25694139
Pt	2.22179730	-1.46715929	0.52657929
Pt	-0.28305087	1.19960422	-2.11957695
Pt	-0.12026873	-1.56645311	2.08799576

13

PRE:140 = -57.65303015

Pt	-3.31833847	-0.81777645	-0.86456845
Pt	0.05814528	-0.11839126	-3.27482720
Pt	-0.46231137	-2.31389923	2.14419413
Pt	-1.96599681	-0.50700521	1.21473587

Pt	-0.98907086	0.51382042	-1.05897257
Pt	2.53264750	-1.11953380	-2.18284970
Pt	0.57400662	-0.41262406	0.77188569
Pt	0.22203479	0.11146182	3.27878770
Pt	2.25488799	1.25910679	-3.53742207
Pt	0.04466409	1.99291865	1.41103539
Pt	1.47307154	0.81492708	-1.21106571
Pt	0.59438713	2.59852066	3.95340511
Pt	-1.01812743	-2.00152541	-0.64433819

13

PRE:141 = -55.59374301

Pt	-0.08375590	4.00404839	-0.00000000
Pt	1.76079861	-0.95803116	-0.00000000
Pt	-0.79307977	-0.44367320	-0.00000000
Pt	-3.23559446	-1.05580179	-0.00000000
Pt	3.20994413	-3.31746828	-0.00000000
Pt	-4.45877677	1.18058467	0.00000000
Pt	0.71880177	1.59524498	-0.00000000
Pt	-3.88857660	-3.67389119	0.00000000
Pt	4.45632890	-1.06559608	-0.00000000
Pt	2.52386447	3.66520711	0.00000000
Pt	3.20486715	1.16947877	-0.00000000
Pt	-1.94879040	1.82717592	0.00000000
Pt	-1.46603113	-2.92727814	0.00000000

13

PRE:142 = -54.93120787

Pt	0.62581033	1.79620579	3.10367343
Pt	-0.14360420	-1.38253696	0.20917834
Pt	-1.67986791	3.25429253	2.39745148
Pt	-1.61662307	0.33595684	1.51750831
Pt	-1.20665867	-2.52724152	-1.75043478
Pt	1.26874040	-3.16059569	-2.34487407
Pt	-3.83875298	-0.61503537	2.15959866
Pt	0.80130716	-0.73545225	-2.12101820
Pt	2.65353288	-1.69285268	-0.64261301
Pt	-0.93606722	0.94059772	-0.89094964
Pt	1.01809395	0.79657945	0.80784341
Pt	3.24906492	-0.08970172	-2.75915348
Pt	-0.19497559	3.07978387	0.31378954

13

PRE:143 = -55.39439869

Pt	0.92049725	1.22514964	-0.00000000
Pt	2.55849451	-0.70642624	-0.00000000
Pt	-4.30197801	-0.45577892	0.00000000
Pt	-3.67956970	2.02006165	0.00000000
Pt	-6.19357935	1.21415761	0.00000000
Pt	-2.27594741	-2.17492561	0.00000000
Pt	-0.76822171	3.07350874	-0.00000000

Pt	4.58748326	-2.22289161	-0.00000000
Pt	5.30473301	0.27775791	0.00000000
Pt	0.12421743	-1.45630064	-0.00000000
Pt	2.07851165	-3.25738004	-0.00000000
Pt	-1.74225526	0.31553893	0.00000000
Pt	3.38761434	2.14752857	-0.00000000

13

PRE:144 = -55.79328748

Pt	-1.26011349	2.90299966	0.25726722
Pt	-0.44041874	-1.09972500	-2.18475559
Pt	-0.73887272	-3.31886564	-0.85872511
Pt	2.86301797	-0.49076837	0.87926176
Pt	1.37330511	2.20307428	-2.50983741
Pt	-0.35282339	-2.71939442	1.66456079
Pt	-0.56918284	-0.09190496	1.76692155
Pt	1.00809929	0.48459898	-0.62515864
Pt	-1.17223682	1.29510301	-1.76948358
Pt	0.85116641	1.99872936	1.45668486
Pt	-2.51145715	-1.35966106	2.90320089
Pt	1.84670828	-0.22480494	3.24435041
Pt	-0.89719191	0.42061909	-4.22428715

13 (LM8)

PRE:145 = -58.50636382

Pt	-1.04967444	1.31176355	0.57562265
Pt	-3.26747700	0.20357304	0.58122422
Pt	0.48989395	2.69230058	2.10133040
Pt	-1.73877543	0.74062726	-2.20950409
Pt	-1.07858895	-1.06669791	-0.54089015
Pt	-3.14241062	-2.31039888	0.48490837
Pt	1.18369572	0.36172524	-0.01549932
Pt	0.84950019	-2.53877082	0.33095155
Pt	0.54985577	1.75711192	-2.54480725
Pt	1.91864554	-1.65938059	-1.90745951
Pt	2.96355381	1.81681514	-1.18927243
Pt	-0.01424496	-0.18165563	2.29693780
Pt	2.33602643	-1.12701291	2.03645776

13

PRE:146 = -56.55924791

Pt	0.86325130	-4.33664385	0.00000000
Pt	-1.92065939	-2.14821345	0.00000000
Pt	-0.84368447	0.27519773	-0.00000000
Pt	-1.66957580	-4.89000694	0.00000000
Pt	0.65266381	-1.81981109	0.00000000
Pt	-3.11860863	3.07460824	-0.00000000
Pt	1.47242692	1.35293287	-0.00000000
Pt	3.51635051	-0.21810078	0.00000000
Pt	3.55812078	2.73061388	0.00000000
Pt	-0.45207154	3.02892931	-0.00000000

Pt	-1.72692175	5.28021089	-0.00000000
Pt	-3.33043460	0.52818221	-0.00000000
Pt	2.99914287	-2.85789903	0.00000000

13

PRE:147 = -53.26187392

Pt	1.33967309	-3.03236326	-0.00000000
Pt	-1.48347530	-2.76665571	0.00000000
Pt	2.62147961	-0.79583825	-0.00000000
Pt	-1.31936600	1.38424334	0.00000000
Pt	0.42252259	3.26447375	0.00000000
Pt	-0.50857399	5.68687001	0.00000000
Pt	-2.84116886	-5.21218023	0.00000000
Pt	-2.26677787	3.79826050	0.00000000
Pt	3.03793965	1.70880396	0.00000000
Pt	-3.91504001	1.74564772	0.00000000
Pt	5.05318564	0.09875180	-0.00000000
Pt	-0.24905051	-5.08693492	0.00000000
Pt	0.10865197	-0.79307871	-0.00000000

13

PRE:148 = -57.02296040

Pt	2.36176097	0.39196242	-1.29494162
Pt	-1.47849083	3.30519699	1.30587006
Pt	1.11617015	0.43338035	1.16617770
Pt	0.76758639	-1.01509604	4.45819207
Pt	-1.25145735	-2.33394000	-1.52740211
Pt	-1.57496683	-2.54894150	-4.04249288
Pt	-0.82508864	2.43245854	-2.07170992
Pt	0.97368901	-1.61764152	-0.44190763
Pt	0.72619160	2.64713972	-0.08105765
Pt	-0.89555426	-0.54114613	2.47609060
Pt	1.14855122	-2.05031769	2.07248079
Pt	-1.11471832	0.97214061	0.23555321
Pt	0.04632688	-0.07519575	-2.25485262

13

PRE:149 = -56.98472682

Pt	1.48577767	0.56159237	0.03386019
Pt	1.17684565	-1.56712481	-1.30880385
Pt	0.78462096	3.06202554	-0.89593839
Pt	-1.65751777	-1.32905877	-1.24230849
Pt	-3.56903206	-1.53985280	0.50226449
Pt	-1.04320110	-0.70891493	1.19427013
Pt	2.65387836	2.66576091	0.78132086
Pt	-3.11491206	0.69510856	-0.61196363
Pt	-0.43059308	-3.29431652	1.50649876
Pt	-0.66340945	1.03611833	-1.35746683
Pt	1.25424188	0.50948294	-3.05171724
Pt	1.84047344	1.30917232	2.75864237
Pt	1.28282756	-1.39999315	1.69134164

13

PRE:150 = -55.43971974

Pt	-3.63483897	2.10098984	-1.93427961
Pt	-0.58045969	-2.75455546	1.99199271
Pt	-1.26234916	0.95194640	-2.25060138
Pt	-1.76241066	1.71663212	0.08794934
Pt	0.87865731	3.44555540	-1.40169471
Pt	1.35736125	-1.23094617	3.65358236
Pt	3.31699814	-1.56747815	-0.13436570
Pt	1.68463229	-0.27199815	1.36809548
Pt	-2.75446851	1.37922884	-4.30728253
Pt	1.88766019	-2.86258912	1.75136055
Pt	0.78640652	-1.83614965	-0.40744195
Pt	-0.70384199	-0.12804609	2.17010231
Pt	0.78665327	1.05741019	-0.58741687

13

PRE:151 = -56.78591981

Pt	0.83433140	3.26131729	1.22014918
Pt	-0.13560619	-1.70991197	0.97285529
Pt	1.94582698	-2.40949139	-0.37437839
Pt	1.02746771	0.49027941	1.31139302
Pt	-1.24599904	1.91833316	0.53664209
Pt	-2.40767726	-2.10670420	-0.36589122
Pt	0.32871962	1.68170266	3.54660746
Pt	0.57697249	1.20955802	-1.06909459
Pt	-1.52081788	0.12483513	2.34079286
Pt	-0.58833662	-3.82894700	-0.28636363
Pt	1.35768822	-0.60073833	-2.63666867
Pt	-1.23310482	-0.41034294	-1.96983646
Pt	1.06053539	2.38011017	-3.22620693

13

PRE:152 = -56.15987133

Pt	0.36316621	0.98349627	3.05364661
Pt	-2.80168790	1.70980409	-1.88079192
Pt	0.03994945	-1.99970965	-2.79329684
Pt	0.90881665	-2.02017918	-0.24278901
Pt	2.20519615	0.96913497	-1.03808325
Pt	0.31268773	0.31040335	0.56422693
Pt	-2.18750595	-0.94962537	-2.06480609
Pt	2.11591636	1.99354661	1.35590318
Pt	-1.77673061	-4.23593283	1.67794814
Pt	-1.66802829	-2.71943834	-0.34980660
Pt	0.31838776	2.82051704	-0.28190756
Pt	-0.36184384	0.84605944	-1.87558939
Pt	2.53167629	2.29192358	3.87534579

13

PRE:153 = -54.15415311

Pt -0.95787098 -2.48916506 -0.00000000



Pt	-5.65261938	-0.75650000	0.00000000
Pt	3.45449795	3.28487640	0.00000000
Pt	3.59362889	-3.05899796	0.00000000
Pt	1.40583254	1.59050387	0.00000000
Pt	3.66507049	-0.46080509	-0.00000000
Pt	1.00795416	4.11737119	0.00000000
Pt	-4.78171601	1.60351750	0.00000000
Pt	-1.00554070	2.46698307	0.00000000
Pt	1.48181804	-1.68331005	-0.00000000
Pt	-2.99635618	-0.22670748	-0.00000000
Pt	-0.48493118	-0.05054449	-0.00000000
Pt	1.27023236	-4.33722191	-0.00000000

13

PRE:154 = -57.48350234

Pt	-1.27788103	-0.76628725	-0.23970073
Pt	-2.65862168	-2.81738689	0.53527565
Pt	0.70942325	-0.45316267	-3.40357849
Pt	0.12844087	2.15483723	0.20723930
Pt	0.63464296	1.73919028	2.83538075
Pt	-0.74653227	2.06759409	-2.26548942
Pt	-0.06633305	-2.72109425	0.98428349
Pt	2.15852457	-2.28289868	-0.04832340
Pt	1.07374524	-0.54659776	1.69893016
Pt	2.03763321	3.36377954	1.34678625
Pt	-1.76292642	-0.25020048	-2.69818549
Pt	-1.45667212	0.46071334	1.96532923
Pt	1.22655645	0.05151350	-0.91794731

13

PRE:155 = -57.63119467

Pt	0.12394088	-0.01110531	0.33348715
Pt	1.78601762	-1.79280447	-0.12790428
Pt	-0.50962891	-2.88151319	0.97278250
Pt	-1.20290664	4.31347302	-2.01653751
Pt	-1.61670796	-0.83451137	2.07850888
Pt	3.03244806	-2.55031837	2.09046047
Pt	-1.40674374	2.03599249	-0.86037490
Pt	1.28387601	2.05123314	-0.68983531
Pt	1.07739752	-0.92949745	2.54509530
Pt	0.38223814	-3.14725009	-1.78688422
Pt	-0.01260273	2.26228055	-3.02107666
Pt	-1.07997539	1.98921351	1.69959985
Pt	-1.85735287	-0.50519247	-1.21732127

13

PRE:156 = -55.10621175

Pt	0.74276714	4.00088958	0.00000000
Pt	-3.54272340	-1.24933425	-0.00000000
Pt	3.02859721	-2.49585385	-0.00000000
Pt	-1.70105102	-3.05500979	-0.00000000

Pt	4.80559234	2.22407067	0.00000000
Pt	1.43989877	-0.37373577	-0.00000000
Pt	-3.21045375	1.31296251	-0.00000000
Pt	2.29934509	2.02315240	0.00000000
Pt	-4.07921688	-3.89935190	0.00000000
Pt	-5.95878275	-2.14804287	0.00000000
Pt	3.29584412	4.37010414	0.00000000
Pt	3.98626573	-0.16551722	-0.00000000
Pt	-1.10608259	-0.54433366	-0.00000000

13

PRE:157 = -57.01262091

Pt	1.30901354	0.79273460	0.89984607
Pt	0.81585550	-0.95692377	-0.91591081
Pt	0.09039183	-1.06654093	2.19993229
Pt	-3.56612683	-0.66417670	-0.30178019
Pt	-1.57793137	-2.06101994	-1.13856497
Pt	0.43278877	0.96136465	-2.76582869
Pt	-0.38143253	-1.50536815	-3.33890669
Pt	0.16572530	2.42184721	-0.68560390
Pt	5.43378328	0.70089977	1.76692209
Pt	-2.72822080	-0.40537615	2.16760453
Pt	-1.10345460	0.23316638	0.22066914
Pt	3.61478321	-0.47265439	0.53753454
Pt	-2.50517531	2.02204742	1.35408658

13

PRE:158 = -54.92286069

Pt	-2.66244637	4.00580588	-0.00000000
Pt	-3.11426213	0.08561882	-0.00000000
Pt	-2.52290468	-2.43436763	0.00000000
Pt	-0.11991830	4.09765152	-0.00000000
Pt	1.90874413	-0.51118351	0.00000000
Pt	1.33183732	1.99376338	-0.00000000
Pt	-0.63041855	-0.57446269	-0.00000000
Pt	4.40747154	-0.90005276	0.00000000
Pt	-0.05971159	-3.06912537	0.00000000
Pt	-4.62034052	2.32950890	-0.00000000
Pt	2.54313838	-2.90299498	0.00000000
Pt	-1.32674180	1.87152097	-0.00000000
Pt	4.86555257	-3.99168253	0.00000000

13

PRE:159 = -54.60116779

Pt	-4.30720233	-4.55911696	-0.00000000
Pt	0.15325797	-2.48050816	0.00000000
Pt	1.94764444	3.40645564	0.00000000
Pt	-2.98128799	-2.40055752	-0.00000000
Pt	-4.38830865	-0.06046006	-0.00000000
Pt	-5.54278489	-2.35333499	0.00000000
Pt	-1.47987923	2.32229026	-0.00000000

Pt	3.51397150	1.29995090	0.00000000
Pt	4.64163210	3.66097795	0.00000000
Pt	0.79319222	1.12744293	-0.00000000
Pt	-1.34731922	-0.36234304	-0.00000000
Pt	6.14933782	1.55437753	0.00000000
Pt	2.84774626	-1.15517446	0.00000000

13

PRE:160 = -57.46169534

Pt	0.04839839	0.44251897	1.77844791
Pt	0.75008273	1.02492984	4.38306246
Pt	-0.77844072	-0.73759552	-3.63114863
Pt	-1.13353553	2.12545332	-0.11090846
Pt	-0.50377090	1.97387575	-2.57882037
Pt	0.79954509	2.79846339	1.64500898
Pt	-1.16791770	-0.43640309	-0.72517483
Pt	1.68689484	-0.26361373	-2.94487254
Pt	-0.69231758	-1.13092417	3.92708280
Pt	1.04555573	0.78280578	-0.56718191
Pt	-0.18667219	-2.10815115	1.59833428
Pt	1.10427329	-1.82880472	-0.76443532
Pt	-0.97209545	-2.64255467	-2.00939437

13 (GM)

PRE:161 = -59.24966169

Pt	-2.79722447	1.13877449	1.56489104
Pt	-1.81466734	-0.34455386	-2.87911933
Pt	1.53245427	-2.16516864	-2.98748664
Pt	0.24357809	1.51677118	2.59518047
Pt	-1.52005047	0.63149956	-0.53898583
Pt	0.34156627	-0.48834257	0.92859858
Pt	0.63740785	-0.01308738	-1.71271719
Pt	-1.35932059	-0.87267408	2.76761048
Pt	2.52091321	0.71460149	1.25631669
Pt	3.27112515	2.12714562	-0.78724446
Pt	-2.35676665	-1.61199430	0.45192619
Pt	0.62948109	1.92063927	-0.00879071
Pt	0.67150358	-2.55361077	-0.65017928

13

PRE:162 = -55.95604057

Pt	-2.24826384	-1.40106960	2.37125441
Pt	1.14097774	1.66411680	1.64358564
Pt	4.40947085	0.54480862	0.10478712
Pt	-0.42949662	-1.66244251	-2.31712760
Pt	0.17580626	1.27543628	-1.36609257
Pt	-2.46196324	0.48112560	0.75252315
Pt	0.32463494	-0.48831689	0.45773096
Pt	-3.87051927	0.84450487	2.79183371
Pt	2.30885897	1.96938262	-2.48395208
Pt	2.31620028	-0.45460603	-1.10072583

Pt	-2.51250648	-0.26379022	-2.14384239
Pt	2.62360477	-0.69026554	1.47969800
Pt	-1.77680436	-1.81888398	-0.18967252

13

PRE:163 = -55.12464815

Pt	-5.11305294	1.01405424	0.00000000
Pt	-2.96890717	-0.18610835	0.00000000
Pt	1.79798200	3.05337022	0.00000000
Pt	-0.34013463	1.13825671	-0.00000000
Pt	2.00176946	-2.18574593	-0.00000000
Pt	4.68445735	0.13917725	0.00000000
Pt	2.11812866	0.40235817	-0.00000000
Pt	-5.01649228	-1.59977193	0.00000000
Pt	4.33189953	2.68674926	0.00000000
Pt	-2.62283889	2.30916984	-0.00000000
Pt	-2.72940480	-2.88705865	0.00000000
Pt	4.51843935	-2.52067853	0.00000000
Pt	-0.66184565	-1.36377228	-0.00000000

13

PRE:164 = -58.43725207

Pt	-2.55523638	-1.86105363	1.25396767
Pt	1.36076750	0.74617190	-3.23289611
Pt	-0.10847165	-1.87590670	0.83591172
Pt	-2.41649169	-0.39882906	3.36394148
Pt	-2.42106642	-0.39511974	-0.83266370
Pt	2.21261201	0.28874085	-0.78200267
Pt	-1.35779496	0.69782964	-3.11407195
Pt	-0.49220452	0.40150287	1.75176567
Pt	2.17691845	-1.32857192	2.13515987
Pt	2.11888992	1.19150250	1.57390423
Pt	0.38278770	-1.26895393	-1.94567188
Pt	-0.21374891	0.96206022	-0.87545574
Pt	1.31303895	2.84062701	-0.13188859

13

PRE:165 = -53.92646712

Pt	4.70742547	3.42211295	0.00000000
Pt	-2.39048387	-3.41872864	-0.00000000
Pt	-6.13191182	-0.72025440	-0.00000000
Pt	-2.93403327	3.41822193	0.00000000
Pt	-1.84246256	1.01578146	-0.00000000
Pt	6.23215515	1.25856056	0.00000000
Pt	1.51907829	-0.55514226	-0.00000000
Pt	4.03016707	-1.40801266	-0.00000000
Pt	3.58559549	1.11642711	0.00000000
Pt	-0.87212277	-1.35683340	-0.00000000
Pt	-3.38686331	-0.95712117	-0.00000000
Pt	2.01886267	-3.07409564	-0.00000000
Pt	-4.53540653	1.25908417	0.00000000

13

PRE:166 = -57.43039680

Pt	1.04232801	0.21488138	2.13795927
Pt	0.55397834	2.56354976	0.91693973
Pt	1.89257529	3.49336623	-1.11749369
Pt	-4.21995428	0.17801049	-2.31638736
Pt	-0.82182459	-0.24360260	-0.04782037
Pt	0.94444533	1.13864458	-1.18589399
Pt	-0.34898111	-2.56311246	-1.43089706
Pt	-0.79264081	-2.24773665	1.50965692
Pt	-2.59050837	1.58067311	-0.59322809
Pt	2.93164109	0.56196501	0.41494006
Pt	1.39318518	-1.52300302	0.28286213
Pt	-2.58354923	-1.45173140	-1.40752823
Pt	2.59930516	-1.70190444	2.83689067

13

PRE:167 = -58.36633167

Pt	-0.38964870	0.70204136	0.49169811
Pt	0.39789093	-1.25114151	-1.80457849
Pt	-1.60809043	-2.35419628	-0.04323771
Pt	-0.86336168	1.00428832	-1.94975666
Pt	-2.54082375	1.39527382	1.99338388
Pt	-0.35709628	-4.63433030	0.10881789
Pt	0.61027169	2.81208593	-0.84584284
Pt	0.87491034	-2.45503064	0.49897741
Pt	1.88728700	0.99147388	-2.33970945
Pt	1.98432426	-0.13341254	-0.03114736
Pt	0.22114561	2.38413234	2.26655998
Pt	2.62408980	1.59154590	1.76246545
Pt	-2.84089878	-0.05273029	-0.10763021

13

PRE:168 = -55.96795606

Pt	-4.99585477	-0.01044108	-0.92402595
Pt	-0.91471058	1.05211746	1.24490815
Pt	1.81288354	-1.39368923	-1.02118003
Pt	1.32085407	2.92069170	1.85200652
Pt	1.30416064	0.85386958	0.12396501
Pt	0.02278453	-4.05441227	0.49748647
Pt	1.60667399	3.22416966	-0.71121062
Pt	-0.94310331	-2.33396501	-1.19133376
Pt	0.04790403	-1.23180166	0.80489805
Pt	-2.74344330	1.11071734	-0.50677335
Pt	-3.13195400	-1.52263218	-0.18988305
Pt	3.40072008	0.51209784	-1.63339629
Pt	3.21308508	0.87327787	1.65453885

13

PRE:169 = -57.85378814

Pt	-1.30915862	2.75937215	-1.21540243
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Pt	-0.62994852	-1.24971386	-2.73297057
Pt	-1.78143538	1.01723786	-2.99763405
Pt	2.50265547	1.29666818	-0.88867085
Pt	0.26798908	-3.59228088	-1.46492646
Pt	0.20489639	-1.43412283	1.45163262
Pt	-2.26192960	1.31119710	1.15171705
Pt	1.27357220	-1.28512134	-0.86582834
Pt	3.75817333	-0.90934961	-0.49330180
Pt	0.42887812	1.05883809	1.64484487
Pt	-0.11040456	1.26247348	4.09996774
Pt	-0.80922362	0.16341583	-0.53313372
Pt	-1.53406428	-0.39861416	2.84370596

13

PRE:170 = -56.70118591

Pt	1.13057756	0.84767624	1.17511792
Pt	-1.16025430	-0.43027576	0.97418555
Pt	-2.99604056	-0.07867866	-0.74817839
Pt	1.77557925	2.26264181	-0.81870682
Pt	3.29848481	-0.69032950	0.68722280
Pt	-1.09131485	2.15237421	1.31801780
Pt	-0.10667633	-3.36758697	2.63080444
Pt	-2.43979813	1.40221845	-2.81147023
Pt	-1.67067381	-2.32649162	-0.73812415
Pt	-0.98611783	-0.77688149	-2.87867594
Pt	3.75164526	1.82396316	1.16991471
Pt	0.99805524	-1.73264944	1.13507357
Pt	-0.50346631	0.91401955	-1.09518127

13

PRE:171 = -53.46264420

Pt	0.31796591	2.67500285	-0.00000000
Pt	0.17644064	-3.83340959	0.00000000
Pt	-4.06267156	1.04600690	0.00000000
Pt	5.00140275	-0.40543148	0.00000000
Pt	5.26020411	-3.30436655	0.00000000
Pt	2.74440191	-3.79664927	0.00000000
Pt	-2.42797898	3.24031894	-0.00000000
Pt	-5.12326862	3.41259308	0.00000000
Pt	0.04871670	-1.24362090	-0.00000000
Pt	-1.49206793	0.81018276	-0.00000000
Pt	-0.78831959	5.15729558	-0.00000000
Pt	-2.23867683	-2.46659278	-0.00000000
Pt	2.58385151	-1.29132954	0.00000000

13

PRE:172 = -56.15735186

Pt	-4.01230191	-3.22037716	0.00000000
Pt	-3.91137401	-0.59087832	0.00000000
Pt	2.62474063	4.42854836	0.00000000
Pt	0.02808562	3.85755463	0.00000000

Pt	-1.71753706	-1.99937234	0.00000000
Pt	3.34145132	-0.68851034	0.00000000
Pt	4.80397270	1.30454428	0.00000000
Pt	-0.25702009	1.30908289	0.00000000
Pt	0.80486856	-1.02424572	-0.00000000
Pt	2.18738866	1.92155337	0.00000000
Pt	-2.27167666	2.90613460	0.00000000
Pt	-1.96132984	-4.68862636	-0.00000000
Pt	0.34073207	-3.51540789	-0.00000000

### 13 (LM3)

PRE:173 = -58.80824599

Pt	1.24042846	-1.38687601	1.77549165
Pt	-2.42827178	1.99914779	-0.01317509
Pt	-0.25168159	1.48459426	3.35370316
Pt	2.88624702	0.40038772	0.78288705
Pt	1.18660820	0.42821033	-1.61689825
Pt	-1.95334791	0.22973068	1.85604130
Pt	-2.17772733	-2.76175793	-0.04712014
Pt	-0.19436373	2.99598827	-0.75453805
Pt	1.34993787	-1.31252126	-3.45955192
Pt	0.16671334	-1.86837787	-0.59617916
Pt	-3.56971748	-0.39852373	0.01860726
Pt	3.39434169	-0.63314034	-2.11960513
Pt	0.35083323	0.82313809	0.82033731

13

PRE:174 = -56.27082984

Pt	1.73306830	2.36390391	-1.00600190
Pt	0.61957700	2.09591907	2.20880355
Pt	2.32357981	-0.87390737	1.23388171
Pt	0.45416262	0.55015860	0.14885801
Pt	-0.55528626	0.43067223	-2.63696774
Pt	3.41050491	-1.72872511	-1.09929991
Pt	-3.91203392	-0.06721606	0.64145691
Pt	-1.73986262	-1.66112696	2.74850130
Pt	-1.51862496	-1.67376815	0.09745726
Pt	-2.00645238	1.10882864	-0.60361508
Pt	-1.61401189	0.77359541	1.98936185
Pt	2.17621930	0.15211125	-2.42579793
Pt	0.62916008	-1.47044546	-1.29663804

13

PRE:175 = -55.01734449

Pt	3.82171840	-0.90384506	-0.00000000
Pt	2.22932390	3.93474140	-0.00000000
Pt	-0.96579796	-1.62073150	0.00000000
Pt	-0.11254367	2.91348076	-0.00000000
Pt	0.41212470	5.75839500	-0.00000000
Pt	0.53704807	0.43233025	-0.00000000
Pt	-1.97606719	-6.21359645	0.00000000

Pt	-0.42367350	-4.11548708	0.00000000
Pt	1.46289502	-2.03574115	0.00000000
Pt	-2.90160501	-3.62376158	0.00000000
Pt	-2.02880997	0.78293789	-0.00000000
Pt	-2.94897085	3.23546472	-0.00000000
Pt	2.89435804	1.45581279	-0.00000000

13

PRE:176 = -55.47997526

Pt	-5.37439780	-2.68785904	0.00000000
Pt	-1.97189860	1.13483648	-0.00000000
Pt	2.55695711	-0.50230949	-0.00000000
Pt	0.10094763	-1.22783548	0.00000000
Pt	0.10714813	3.80428692	-0.00000000
Pt	0.60839668	1.24087411	-0.00000000
Pt	0.36298462	-3.91289904	0.00000000
Pt	-3.65725237	-0.78785748	0.00000000
Pt	-4.55219685	1.62159271	0.00000000
Pt	5.66481064	2.18310479	-0.00000000
Pt	4.95410007	-0.13733837	-0.00000000
Pt	3.15389559	2.00272218	-0.00000000
Pt	-1.95349484	-2.73131830	0.00000000

13

PRE:177 = -56.91635747

Pt	2.80988906	2.65485613	3.04261292
Pt	2.01152351	1.03068065	1.31597882
Pt	2.77487412	0.22084171	-0.94827031
Pt	0.84515723	3.35776403	1.47452927
Pt	-2.56763927	-0.83801592	-2.22829410
Pt	1.32897277	2.82214798	-0.99296548
Pt	0.95439219	-1.58422421	0.95983905
Pt	-0.40349827	0.55988243	0.52904522
Pt	-2.26464882	-1.24304425	0.72844358
Pt	-4.07154475	-2.48440210	-1.03633615
Pt	-0.42413589	-1.59571975	-1.22838906
Pt	0.32119962	0.69724668	-1.89518342
Pt	-1.31454151	-3.59801338	0.27898966

13

PRE:178 = -56.31226918

Pt	-0.02155742	1.34091385	-2.05176657
Pt	-0.27226755	1.62664706	0.46704235
Pt	-2.76992750	1.68146478	0.49725014
Pt	0.49170851	-2.77927724	1.16444838
Pt	1.58561500	0.38984493	1.94463499
Pt	0.17778196	-4.00853856	-2.65396654
Pt	-1.23317907	3.38228701	-1.12637788
Pt	0.96512982	-0.67439440	-0.24051044
Pt	0.97554888	-0.86769294	-2.75845200
Pt	-1.46661725	2.56028572	2.55168068



Pt	0.11485660	0.87782821	3.91941114
Pt	-0.92855321	-0.59989315	1.67159680
Pt	2.38146123	-2.92947528	-3.38499104

13

PRE:179 = -57.82934973

Pt	-2.87571781	1.96229334	-0.41799436
Pt	-0.32247490	-2.01138142	-1.60896981
Pt	0.99280344	0.61239688	0.77262688
Pt	3.51579461	-0.14084301	1.12989665
Pt	2.03380447	-3.16437261	1.27888499
Pt	-1.22271668	-0.04534862	-0.24803544
Pt	0.47788844	3.22802761	0.58603965
Pt	1.99860923	-1.29635155	-0.64000736
Pt	-0.11634371	-1.68902677	1.33189462
Pt	-2.57023842	1.25451645	2.03956194
Pt	1.64337332	-3.70904136	-1.17664202
Pt	-1.88498055	0.76815915	-2.57875062
Pt	-1.66980145	4.23097192	-0.46850512

13

PRE:180 = -54.88661586

Pt	-1.50593253	-5.12529892	0.00000000
Pt	-0.99385066	1.27257071	-0.00000000
Pt	0.31660670	-3.43424734	-0.00000000
Pt	0.94829251	-6.03290613	0.00000000
Pt	4.42678401	1.74295719	0.00000000
Pt	1.84430104	1.49950919	-0.00000000
Pt	-3.45079105	1.96469264	-0.00000000
Pt	-4.29985570	4.39889215	0.00000000
Pt	-1.60575384	3.72925592	0.00000000
Pt	2.95471716	-0.75879547	0.00000000
Pt	-1.96885418	-2.26489055	-0.00000000
Pt	0.40649644	-0.81484334	-0.00000000
Pt	2.92784009	3.82310396	0.00000000

13

PRE:181 = -57.26401780

Pt	-0.80039019	1.66709178	-1.24648974
Pt	2.37682135	1.32201065	0.55670817
Pt	-2.36547351	-0.09116128	-0.29661987
Pt	0.95407246	-3.36393511	-0.75124902
Pt	-0.01776519	1.12376209	1.08281582
Pt	1.51555435	-0.63316486	2.07067789
Pt	2.13840513	-1.20086195	-1.43153125
Pt	-2.92690606	1.94850494	-2.65224671
Pt	-0.73216421	-0.23412781	3.16423441
Pt	1.45228486	1.43711939	-2.44853309
Pt	1.52758437	-3.14503755	1.77643412
Pt	-0.10786226	-1.20179938	0.10090462
Pt	-3.01416109	2.37159908	0.07489464

13

PRE:182 = -55.30924676

Pt	-0.56703434	2.15946364	4.39596331
Pt	-1.26472086	-0.54231695	1.79275505
Pt	-0.64410396	-1.37193880	-2.69613722
Pt	1.26296016	0.64112113	-3.73319672
Pt	0.98317741	0.30997107	3.25771362
Pt	1.37306472	-1.84847939	-0.60228208
Pt	-2.08825533	1.29661979	-2.70186985
Pt	0.41143447	-2.71556056	1.56142480
Pt	-3.08619402	-1.04220585	-1.48130623
Pt	0.51701038	2.45304352	2.04026692
Pt	-0.94842011	0.16304174	-0.68550214
Pt	2.76137133	0.02087724	-1.71215450
Pt	1.28971016	0.47636342	0.56432504

13

PRE:183 = -53.97943175

Pt	5.03099804	-2.07921996	0.00000000
Pt	-0.05736007	-3.14075558	0.00000000
Pt	4.37029407	0.45659039	-0.00000000
Pt	-5.09511856	-0.56903717	0.00000000
Pt	4.77268473	3.00099236	-0.00000000
Pt	-5.89694405	1.82606446	0.00000000
Pt	-2.79479329	-1.97210779	-0.00000000
Pt	2.14127680	2.34215529	-0.00000000
Pt	-3.47873561	3.05523491	0.00000000
Pt	2.51474593	-2.73406186	0.00000000
Pt	-2.80176265	0.60377126	0.00000000
Pt	-0.57902080	-0.67591900	-0.00000000
Pt	1.87373545	-0.11370730	-0.00000000

13

PRE:184 = -58.38594276

Pt	-1.26748723	-3.91125436	-0.96343517
Pt	1.44069281	2.05670504	2.21716315
Pt	-3.43311274	-1.83566265	-0.78324531
Pt	1.63011989	0.20812405	-1.23506205
Pt	1.28779078	-1.88286444	1.81340264
Pt	-0.75885810	0.73342774	-2.04047512
Pt	-1.28186387	2.46099971	1.81383007
Pt	-1.59110540	-1.87919336	0.94359613
Pt	-0.12706342	0.23777024	1.33411496
Pt	0.62909974	2.27555903	-0.17205926
Pt	4.02609504	0.11624583	-0.34449699
Pt	0.35010108	-1.92888884	-0.67650475
Pt	-0.90440857	3.34903201	-1.90682831

13

PRE:185 = -58.19735956

Pt	0.06545571	1.76689913	-0.46475172
----	------------	------------	-------------

Pt	0.03217285	-1.74947407	1.38911749
Pt	-0.49419181	3.92189636	-1.64801880
Pt	0.70714060	4.06176397	0.75119498
Pt	1.99769355	-2.61258679	0.07956990
Pt	1.96637174	0.02873912	0.08046379
Pt	-1.91905566	0.26908235	-1.05884508
Pt	0.91376489	0.29294110	-2.34741781
Pt	1.22851284	1.00847386	2.44577494
Pt	-0.51678600	-3.93058451	0.19826976
Pt	-2.62956445	-1.76855314	0.38251959
Pt	-1.08484203	0.50205919	1.41379552
Pt	-0.26667222	-1.79065658	-1.22167257

13

PRE:186 = -52.28418942

Pt	-0.17808851	5.59402260	2.06729659
Pt	-0.81350580	2.53001430	1.29320878
Pt	-1.55294364	-0.53424351	-1.39140687
Pt	-0.47213672	-1.65138574	1.79135123
Pt	-0.11266117	-2.55157476	-0.70812307
Pt	1.58123276	-0.83987911	-1.50600562
Pt	2.65281253	-3.02480029	-0.76645747
Pt	-2.00923452	-2.55082572	-3.12574535
Pt	-0.27384148	4.44352800	-0.30098838
Pt	-1.10254643	-2.86833790	3.99610689
Pt	0.49921094	-2.39036193	-3.28454726
Pt	1.52014449	3.46929249	1.52510995
Pt	0.26155757	0.37455156	0.41020058

13

PRE:187 = -54.47914922

Pt	5.33443064	-1.32272503	0.00000000
Pt	0.07210115	2.97848948	0.00000000
Pt	2.69303197	2.89505984	-0.00000000
Pt	0.92256844	-3.33711092	-0.00000000
Pt	2.73965319	-1.39940703	-0.00000000
Pt	1.00893356	0.52377000	-0.00000000
Pt	-4.09449717	0.04577078	0.00000000
Pt	-0.65314040	-1.33700067	-0.00000000
Pt	4.02720962	-3.59133607	0.00000000
Pt	-2.50517921	3.49470647	0.00000000
Pt	-4.83848242	2.45919356	0.00000000
Pt	-1.75692843	1.00328802	-0.00000000
Pt	-2.94970094	-2.41269843	0.00000000

13

PRE:188 = -57.88024765

Pt	-1.40479697	1.54044130	0.32675786
Pt	2.15288339	-0.24274186	0.79934843
Pt	0.87627642	-0.44985622	2.98770745
Pt	0.35037727	0.20500818	-1.06971510

Pt	-2.96080272	-0.38163566	-0.43412028
Pt	-2.32859611	1.72893302	-2.10531772
Pt	-0.12656722	2.89361747	-1.43103241
Pt	2.44213211	0.32177896	-2.58394205
Pt	-0.34170399	-2.18719040	-0.61632321
Pt	1.72126192	-3.41040762	0.22332713
Pt	-3.78102453	0.88815624	1.54122549
Pt	1.28686496	-2.92088889	2.87822892
Pt	2.11369547	2.01478549	-0.51614451

13

PRE:189 = -54.01522446

Pt	4.12776703	-1.32062043	-0.00000000
Pt	3.32443262	1.09466846	-0.00000000
Pt	-4.20559487	-4.94108004	0.00000000
Pt	-2.15830009	3.13105605	-0.00000000
Pt	-0.25653757	4.89675067	0.00000000
Pt	-0.99702509	-1.61586780	-0.00000000
Pt	1.06370388	2.76056934	0.00000000
Pt	2.16229809	5.73563133	0.00000000
Pt	1.45787422	-0.71912996	-0.00000000
Pt	1.03278249	-3.30691637	-0.00000000
Pt	-0.72919346	0.91068964	-0.00000000
Pt	-1.42659090	-4.09276246	0.00000000
Pt	-3.39561636	-2.53298844	0.00000000

13 (LM9)

PRE:190 = -58.48427702

Pt	0.84682281	-2.50251247	2.25383350
Pt	1.11324765	3.57589300	-1.68226052
Pt	-1.11049170	-2.07785942	-2.06110598
Pt	3.70532225	0.65152371	-0.50363222
Pt	-0.45791053	2.26046498	0.05577766
Pt	1.31002477	1.00727479	-1.19861970
Pt	1.69952817	-1.43982164	-1.95563097
Pt	-1.49212913	-1.99391492	1.47037857
Pt	-3.47149652	-0.75143189	-0.29215046
Pt	-2.62423255	1.37449373	1.32237900
Pt	-0.90201821	-0.21155048	-0.29417826
Pt	-0.32660977	0.59771504	2.10187397
Pt	1.70994277	-0.49027442	0.78333541

13

PRE:191 = -55.73846365

Pt	0.99954521	-3.02474228	0.21010087
Pt	-1.42510894	0.83167128	-2.13080373
Pt	2.81516191	-0.64015734	-2.44797741
Pt	2.72592975	-1.09421642	0.10345125
Pt	-4.48968236	0.09027500	0.62135882
Pt	-0.59893971	1.39544033	3.13454503
Pt	1.15796076	1.72632369	-1.36919868

Pt	0.89465981	0.51615623	0.81335352
Pt	0.27108811	-0.95863757	-1.15754818
Pt	-2.94839860	0.43814624	2.62118050
Pt	1.89799951	0.90535294	3.14893078
Pt	0.52681331	0.05757908	-3.71744580
Pt	-1.82702876	-0.24319116	0.17005302

13

PRE:192 = -56.50169997

Pt	1.67343509	4.66910267	0.00000000
Pt	-0.62827377	-3.90702568	-0.00000000
Pt	2.82388374	-0.45934794	-0.00000000
Pt	-4.22617850	1.13436230	0.00000000
Pt	-0.43723947	3.24332601	0.00000000
Pt	1.33611384	-5.59764817	-0.00000000
Pt	-2.35264962	-1.84976472	-0.00000000
Pt	0.41557512	-1.51884022	-0.00000000
Pt	2.42076818	-3.03863777	-0.00000000
Pt	-3.02589245	3.44038481	0.00000000
Pt	2.98331366	2.26026780	0.00000000
Pt	0.78970285	1.02630800	-0.00000000
Pt	-1.77255869	0.59751290	0.00000000

13

PRE:193 = -58.07514452

Pt	-2.28959239	0.18306178	1.55807854
Pt	1.68393204	-1.70047375	0.05890528
Pt	-3.20944199	-2.25305201	1.54816897
Pt	0.76975164	1.53188408	-2.25847153
Pt	-1.55323356	0.63023996	-0.97988305
Pt	0.24455759	-0.96818195	-1.91224299
Pt	2.08694001	0.77009574	-0.14768989
Pt	0.75363285	2.68718849	0.93616957
Pt	-3.56301318	-0.80068539	-0.46881074
Pt	3.31432843	-0.16030067	-2.30099655
Pt	-1.21079753	-1.69035221	0.07813878
Pt	0.30048739	0.17465407	1.65270034
Pt	2.67244870	1.59592184	2.23593328

13

PRE:194 = -58.95343465

Pt	0.84398488	-1.92257244	-1.84575603
Pt	1.46744434	-0.87766986	1.57875233
Pt	1.70176727	2.65598935	-1.60501058
Pt	-3.05676166	-2.59087478	1.34419834
Pt	0.11046218	0.26835504	3.42905024
Pt	3.15434776	-1.78740945	-0.56890247
Pt	-2.14067739	-0.25884207	1.90607754
Pt	-0.65476098	-1.74753365	0.21945182
Pt	-2.02893538	0.27308357	-0.61207655
Pt	-0.13998294	1.16523063	1.01589893

Pt	-0.73702327	3.49992694	-1.93127861
Pt	-0.19231627	1.02918490	-2.26530034
Pt	1.67245146	0.29313183	-0.66510461

13

PRE:195 = -57.16395350

Pt	1.12182715	-0.82874717	0.35566942
Pt	0.89996787	3.36112930	-2.45539195
Pt	-2.15024561	0.21404717	1.60477171
Pt	0.51194996	1.43793922	1.96409866
Pt	-1.25006206	-0.41236661	-0.72583774
Pt	-1.66087738	1.52103434	-2.34137911
Pt	2.22385049	-1.78610722	2.40327464
Pt	0.68419523	1.39284586	-0.82852843
Pt	-0.08491375	-0.84394229	2.81271697
Pt	-0.79004872	-2.58281945	0.60917672
Pt	0.55553488	3.60837180	0.51889076
Pt	0.91720091	-1.64208428	-2.04313323
Pt	-0.97837898	-3.43930067	-1.87432843

13

PRE:196 = -57.22711674

Pt	0.68399485	-0.39867998	-3.56722774
Pt	-1.02462634	2.13488110	1.44556235
Pt	-2.79546360	-2.66094730	1.24582470
Pt	-2.86380815	2.00769998	-0.24135890
Pt	-0.35989924	1.08553712	-1.62336339
Pt	2.87184790	-1.34492158	0.69300471
Pt	-0.51029100	-1.69603635	1.63550741
Pt	0.81141656	3.83212002	0.43523178
Pt	0.67005466	-0.93415508	-0.44337647
Pt	1.08580472	-3.44451074	0.31387896
Pt	1.29560299	1.37032739	0.43632897
Pt	2.57236075	0.02256203	-1.83335086
Pt	-2.43699412	0.02612339	1.50333847

13

PRE:197 = -57.08547045

Pt	0.41818109	1.61823454	-0.21148344
Pt	0.32957475	-0.22458931	1.50871483
Pt	1.98564295	0.14538306	-1.60226267
Pt	-0.65635883	-0.49226485	3.88778389
Pt	0.50607738	-2.11593456	-1.78791663
Pt	0.69344672	-0.27007415	-3.73679902
Pt	-1.59648845	-1.49568790	-3.12293083
Pt	0.52247415	-2.71637245	0.69295166
Pt	1.41494643	0.97410536	3.48976458
Pt	1.50264581	2.92509022	1.79513294
Pt	-1.31280840	1.23105741	-2.05273818
Pt	-1.55782769	-0.65814024	-0.29546893
Pt	-2.24950591	1.07919287	1.43525179

13

PRE:198 = -57.66403676

Pt	-1.87656175	1.54458263	0.29552893
Pt	0.57553609	-2.40709617	0.46448667
Pt	0.74518397	4.47022934	-1.12090797
Pt	-1.45497426	-3.88296854	-0.56533541
Pt	0.86866493	0.47603069	1.17697551
Pt	-0.13873617	3.40791954	1.06964608
Pt	2.35627555	-0.02525672	-0.89304354
Pt	-0.65198926	-2.24310710	-2.37357831
Pt	0.45959163	1.88869387	-0.93271978
Pt	1.06355180	-4.49216155	-0.93999333
Pt	-2.70219540	-0.75855797	1.41507162
Pt	-0.84376320	-0.60370009	-0.40107389
Pt	1.59941607	2.62539207	2.80494343

13

PRE:199 = -57.68532378

Pt	2.65001656	-0.57406718	-0.22686657
Pt	0.45407095	-1.44738174	0.74268363
Pt	-0.27664969	-0.40986891	-2.82950387
Pt	2.99739050	1.82765885	-0.84371585
Pt	-1.73109424	-2.50625901	0.17009960
Pt	-3.63511938	-0.08734731	1.24900854
Pt	2.23078836	0.50154400	-2.84268113
Pt	-1.02473085	0.42621912	1.68891061
Pt	-1.83549332	-0.10049382	-0.63664124
Pt	-1.21612759	2.37233840	0.10355185
Pt	0.61165872	0.92278546	-0.91836851
Pt	1.56401765	1.04140389	1.47517778
Pt	-0.78872765	-1.96653176	2.86834516

13

PRE:200 = -53.03085364

Pt	5.11681606	3.09245237	0.00000000
Pt	1.08925848	0.12300324	-0.00000000
Pt	-2.34280146	3.97957851	0.00000000
Pt	-1.14678356	-3.81969511	-0.00000000
Pt	-3.37788871	-2.34195607	-0.00000000
Pt	3.02710506	4.54226968	0.00000000
Pt	-3.38524135	-5.12559072	-0.00000000
Pt	1.10142750	-2.47840201	-0.00000000
Pt	3.64418185	-0.57667673	-0.00000000
Pt	-1.28025814	-0.98858204	-0.00000000
Pt	-1.59194649	1.55803619	-0.00000000
Pt	-3.77107489	0.18403741	-0.00000000
Pt	2.91720566	1.85152527	0.00000000

13

PRE:201 = -57.12105373

Pt	-1.49461015	-1.27816383	1.97942528
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Pt	-3.16899314	0.61229139	2.65477276
Pt	-2.36766957	-0.12509544	-0.23281316
Pt	3.11488208	0.30161086	-3.51527744
Pt	-0.77533609	1.12144841	1.28281072
Pt	-0.96314267	-2.50190102	-0.35526591
Pt	0.19588080	3.49627470	2.04278940
Pt	0.43560463	0.91300115	-2.51490464
Pt	2.32196184	-1.53804125	-1.81644734
Pt	-1.18490575	1.99617222	3.67842825
Pt	2.38015886	-1.32570352	1.08513406
Pt	0.93519914	-1.29096851	-3.93230968
Pt	0.57097001	-0.38092515	-0.35634230

13

PRE:202 = -55.19515900

Pt	1.30525603	2.13212331	0.00000000
Pt	-2.08225066	-4.47548387	0.00000000
Pt	1.74472261	-1.38590482	-0.00000000
Pt	3.39609263	0.60102429	-0.00000000
Pt	-0.67620725	-2.40551955	-0.00000000
Pt	-1.72629383	2.28264115	0.00000000
Pt	-0.15721477	4.34471880	0.00000000
Pt	2.36188028	4.62833645	0.00000000
Pt	-0.29064174	0.16252518	-0.00000000
Pt	0.27948986	-6.18423100	0.00000000
Pt	-2.89105722	4.49653820	0.00000000
Pt	-2.78405330	-0.27338213	0.00000000
Pt	1.52027736	-3.92338602	-0.00000000

13

PRE:203 = -54.78550818

Pt	1.26164436	1.21428799	-0.00000000
Pt	2.05739667	5.89724874	-0.00000000
Pt	2.65599807	3.41529945	-0.00000000
Pt	0.14927964	-1.09146651	-0.00000000
Pt	-1.21846682	-3.21843237	0.00000000
Pt	-0.23558331	4.25057378	0.00000000
Pt	-2.47750970	-5.67122324	0.00000000
Pt	0.01967652	-5.43656867	0.00000000
Pt	2.83168702	-0.83716094	-0.00000000
Pt	-2.41535440	-0.96324186	0.00000000
Pt	-2.87963478	3.80507083	0.00000000
Pt	-1.14489999	1.86677388	-0.00000000
Pt	1.39576671	-3.23116107	0.00000000

13

PRE:204 = -54.28525725

Pt	-0.33355720	5.08094761	0.00000000
Pt	0.21064995	0.16904136	-0.00000000
Pt	0.82565021	2.68772466	-0.00000000
Pt	2.26421871	-3.69537514	-0.00000000



Pt	4.55408690	-2.44536357	-0.00000000
Pt	3.14625660	1.58389475	-0.00000000
Pt	-0.28978774	-3.52077552	0.00000000
Pt	2.37558197	-1.05957274	-0.00000000
Pt	-1.73320941	-1.38835366	0.00000000
Pt	-3.70706522	0.13081928	0.00000000
Pt	-2.73178964	4.27692301	0.00000000
Pt	-2.89797611	-3.68722514	0.00000000
Pt	-1.68305903	1.86731510	0.00000000

13

PRE:205 = -57.00401513

Pt	-2.76346529	0.63648477	1.77159805
Pt	2.36529775	0.01162268	0.91136091
Pt	-2.41689732	1.48604289	-0.59594716
Pt	-0.37615258	-0.04749700	2.68122930
Pt	-3.28575749	0.60298002	-3.33235413
Pt	0.16016755	1.21578004	0.37277538
Pt	0.75463874	-0.98148379	-0.98622256
Pt	-1.71060098	-0.67175082	-1.69372919
Pt	1.45539504	1.75485267	2.50299040
Pt	1.59630091	-2.39093790	-2.97716544
Pt	-1.33159968	-1.47378090	0.70237259
Pt	3.11803582	-0.09942133	3.35693417
Pt	2.43463752	-0.04289135	-2.71384232

13

PRE:206 = -55.04435477

Pt	-1.28895273	-1.04322830	-0.00000000
Pt	2.56502516	2.32926156	-0.00000000
Pt	0.98982503	0.14850106	-0.00000000
Pt	-1.37817815	4.80035537	-0.00000000
Pt	1.34329268	-5.09163195	0.00000000
Pt	-0.05162733	2.50922399	-0.00000000
Pt	3.42447064	-0.41522851	-0.00000000
Pt	-3.50794199	3.25282362	0.00000000
Pt	-3.26785716	0.70370495	0.00000000
Pt	1.15451045	4.67791990	-0.00000000
Pt	-0.64771236	-3.53036327	0.00000000
Pt	-1.07844843	-6.01557424	0.00000000
Pt	1.74359420	-2.32576419	-0.00000000

13

PRE:207 = -58.13946535

Pt	-1.87876814	-2.68726609	1.93780621
Pt	-0.12018354	0.25686787	-3.20761226
Pt	0.49065765	2.98193118	1.78576125
Pt	1.08592157	-1.15331156	-1.44518088
Pt	1.25338658	1.04281518	-0.06842132
Pt	0.96627815	0.59535687	2.50731154
Pt	-2.21220856	-2.10052274	-0.48757117

Pt	0.34843256	3.40781969	-0.78294633
Pt	-1.19171724	1.00978617	-0.81293727
Pt	-0.44840462	-0.78441625	0.85241253
Pt	1.56763127	-2.35099444	0.76698727
Pt	3.36658462	0.03599386	0.95291800
Pt	-3.22761031	-0.25405973	-1.99852757

13

PRE:208 = -56.07435763

Pt	0.09363427	-0.66983878	-1.78604117
Pt	-1.40510805	3.29816874	1.41952670
Pt	1.24596403	-5.04985665	-1.11869661
Pt	0.21758773	1.57957384	-0.30031895
Pt	-0.16309414	-0.63339835	0.90434815
Pt	-2.32837817	0.10245094	-0.06638287
Pt	2.15530759	3.00682527	-1.04297802
Pt	-0.45737922	-2.99833892	-2.72074141
Pt	0.24599087	-2.85786897	-0.27486984
Pt	0.92986375	0.23587083	3.04264520
Pt	0.58846743	4.79362076	0.64601291
Pt	-2.17042381	-3.47149947	-0.62739741
Pt	1.04756773	2.66429078	1.92489330

13

PRE:209 = -54.02357923

Pt	2.97072264	1.35688471	-0.00000000
Pt	-4.81061494	0.00508847	0.00000000
Pt	-2.93051478	-1.96485064	0.00000000
Pt	-5.80696258	-2.33594619	0.00000000
Pt	-2.28964325	0.50244531	0.00000000
Pt	-1.49983789	2.95316811	-0.00000000
Pt	0.40285169	1.12713782	-0.00000000
Pt	4.28516301	-0.82996610	0.00000000
Pt	2.00630607	-2.05373304	0.00000000
Pt	0.19725637	-3.83299104	0.00000000
Pt	5.43317986	2.38371494	0.00000000
Pt	-0.40177995	-1.20801113	0.00000000
Pt	2.44387374	3.89705881	-0.00000000

13

PRE:210 = -57.53664896

Pt	-3.69701326	0.02095016	2.16773227
Pt	0.83499325	-1.15622880	2.15848526
Pt	-0.14872561	1.37382387	1.67442087
Pt	2.95427760	0.66187840	0.86633863
Pt	-1.80817564	0.43210033	-0.03529695
Pt	-0.15512931	1.52065171	-1.74305869
Pt	1.97246317	0.08018436	-1.48870521
Pt	2.72562013	-1.82911906	0.58139099
Pt	-0.23288736	-1.14886291	-1.45139696
Pt	1.76257573	2.12681735	-3.32686123

Pt	-1.58866807	-1.41505923	1.61701435
Pt	-2.44927267	2.55917585	-1.49980985
Pt	-0.17005797	-3.22631204	0.47974652

13

PRE:211 = -56.60278469

Pt	-0.30779650	1.49445793	-2.29722111
Pt	0.35040038	-0.53541182	-3.80323331
Pt	-0.01092485	2.57530297	0.01823391
Pt	-2.03255040	-1.10781887	-2.98047434
Pt	0.16113198	1.21789890	2.10492062
Pt	-2.55710237	-2.10112625	-0.58692888
Pt	-1.43916832	-0.39761946	0.95088946
Pt	-0.75678583	-2.35478870	2.54516095
Pt	-0.19017871	-1.09863292	-1.19429480
Pt	0.75550596	3.59328380	2.80449342
Pt	0.97904109	-1.14256081	1.03092681
Pt	2.65001861	1.84565437	2.31270355
Pt	2.39840896	-1.98863913	-0.90517629

13

PRE:212 = -55.40829390

Pt	4.26567804	1.69535337	-0.00000000
Pt	2.21688075	3.63358371	-0.00000000
Pt	-5.46625685	-0.80426676	0.00000000
Pt	-2.96971039	-0.33053039	0.00000000
Pt	-1.28225960	-3.14044773	-0.00000000
Pt	-0.39226815	-0.31225832	-0.00000000
Pt	-4.00251151	-2.99510001	0.00000000
Pt	-4.54875510	1.64373883	0.00000000
Pt	6.05309034	-0.16214285	-0.00000000
Pt	3.46807063	-0.75667273	-0.00000000
Pt	-0.19616360	2.75579049	0.00000000
Pt	1.76186080	1.16521378	-0.00000000
Pt	1.09234465	-2.39226138	-0.00000000

13

PRE:213 = -57.40050099

Pt	1.52636579	0.10530845	-0.41903061
Pt	1.75007314	-1.48593754	3.49120791
Pt	-0.22037043	-0.83839702	-2.60657585
Pt	3.35760354	-1.57539373	-1.59553343
Pt	2.37154517	0.60217494	1.93991507
Pt	-1.02047505	0.64928331	-0.54277348
Pt	-0.81038422	0.24534787	1.98776987
Pt	-2.91316346	1.69203975	1.96690139
Pt	-3.58934901	1.10456394	-0.40601225
Pt	-2.25974710	1.30684536	-2.73349518
Pt	0.52797721	2.52097666	-1.29924465
Pt	0.94707327	-2.50286765	-1.06788893
Pt	0.33285115	-1.82394435	1.28476013

13

PRE:214 = -54.93173792

Pt	3.68797057	-1.77483524	-0.00000000
Pt	-1.02901035	4.45757155	0.00000000
Pt	-4.11421917	-0.01534853	0.00000000
Pt	1.94032808	-3.77990127	-0.00000000
Pt	-1.38208396	-3.58011432	0.00000000
Pt	0.32397556	-1.72300384	-0.00000000
Pt	4.79643213	0.51442733	-0.00000000
Pt	1.42961527	4.17414336	0.00000000
Pt	-1.54617203	-0.06689033	0.00000000
Pt	-2.51963511	2.32031545	0.00000000
Pt	2.01561143	0.14239383	-0.00000000
Pt	0.15107635	1.97191476	0.00000000
Pt	-3.75388876	-2.64067275	0.00000000

13

PRE:215 = -54.74187374

Pt	-2.47034900	-0.88391054	0.00000000
Pt	-1.31795562	2.63244755	-0.00000000
Pt	-0.20960327	0.25668682	-0.00000000
Pt	0.68847583	4.38096003	0.00000000
Pt	2.83319878	-3.80669426	0.00000000
Pt	-5.14552203	-0.53359890	0.00000000
Pt	3.15172475	4.42171149	-0.00000000
Pt	-3.46329641	1.40289121	0.00000000
Pt	1.31379167	-1.81662391	-0.00000000
Pt	1.61961633	1.96909486	-0.00000000
Pt	3.27139318	-0.06458719	-0.00000000
Pt	-0.90692148	-3.01161236	0.00000000
Pt	0.63544726	-4.94676481	0.00000000

13

PRE:216 = -56.71591120

Pt	1.15135710	2.84347237	-1.53811039
Pt	1.54104680	-2.77992729	1.53743751
Pt	-1.23999208	2.09124186	-1.25303548
Pt	-1.37914059	0.09478025	2.85942362
Pt	1.18131982	-2.74891810	-1.97897567
Pt	-2.57329178	2.28722685	1.91525910
Pt	2.96307496	-0.87698715	-1.26603883
Pt	-0.21964911	1.58879485	1.09354000
Pt	-0.95021908	-2.00472952	1.30290699
Pt	0.92017915	-0.58619599	0.27404735
Pt	2.58715446	1.31328110	-0.05575844
Pt	-0.92624853	-1.34477232	-1.32172053
Pt	-3.05559112	0.12273310	-1.56897523

13

PRE:217 = -57.35737429

Pt	-0.90696103	0.45563239	-1.73835939
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Pt	-1.21431593	-2.88183936	2.01372662
Pt	4.10512618	1.78152302	0.83132036
Pt	-1.11882066	3.07190087	-1.32143205
Pt	2.94710062	-1.27702072	0.63493517
Pt	-0.44366407	-3.14339044	-0.48005543
Pt	0.20684752	-0.75829080	1.71570999
Pt	0.87537920	-0.99600049	-0.71138842
Pt	-3.38322436	-0.65359507	-1.06654121
Pt	-2.27570883	1.29204462	0.20007761
Pt	-3.06982852	1.54812056	-2.65788702
Pt	1.74369854	1.21964921	0.00034085
Pt	2.53437135	0.34126621	2.57955291

13

PRE:218 = -57.84502846

Pt	1.07474762	-3.09940794	0.76506343
Pt	1.49513567	-2.71240819	-1.78085713
Pt	-0.51280124	1.18691092	0.59030309
Pt	-2.71911198	0.72282784	-0.65526379
Pt	1.59491206	3.24127515	0.16275661
Pt	0.01459469	-0.96404345	1.91511935
Pt	-0.91704261	-2.37562086	-2.59197808
Pt	-2.36603368	-2.01133177	-0.34266595
Pt	1.93168364	0.86106445	1.60604820
Pt	-1.38490653	3.00431225	-0.98327072
Pt	0.15341481	2.12646033	2.95272665
Pt	1.64152124	0.98873155	-0.96250617
Pt	-0.00611368	-0.96877028	-0.67547550

13

PRE:219 = -55.92012987

Pt	1.26779974	1.92996547	-0.71744605
Pt	0.51390971	1.19416348	1.60859306
Pt	2.47824694	1.14155280	3.26740075
Pt	0.35074027	-3.08915814	0.83034412
Pt	-1.03071739	1.78708979	-1.79169865
Pt	-2.06086813	0.24589621	-0.03536711
Pt	-0.10907320	-3.03765126	-3.25531664
Pt	-0.19546746	4.05592696	-0.87938648
Pt	-1.30676927	-0.68107822	-3.46113485
Pt	-0.73206670	-1.72042869	-1.16575130
Pt	-0.83140916	-0.99301550	1.78517903
Pt	0.16278265	0.10362221	3.89728434
Pt	1.49289199	-0.93688513	-0.08270023

13

PRE:220 = -56.42930785

Pt	-3.67289953	-1.35874499	0.00000000
Pt	-0.82316067	-1.20838987	-0.00000000
Pt	-0.05530718	1.26729602	-0.00000000
Pt	1.74352463	-1.22327755	-0.00000000

Pt	-2.42372368	-3.55214815	0.00000000
Pt	-0.46799574	3.70943714	0.00000000
Pt	4.72866246	3.07083415	-0.00000000
Pt	-4.83643534	0.88859058	0.00000000
Pt	1.99113666	2.86729346	0.00000000
Pt	0.12873099	-3.57445087	0.00000000
Pt	2.66146563	-3.69987601	-0.00000000
Pt	-2.50459893	1.97485448	0.00000000
Pt	3.53060069	0.83858161	-0.00000000

13

PRE:221 = -57.14743038

Pt	0.94195673	-2.69482578	0.25195342
Pt	1.39507868	1.43819520	1.23811880
Pt	-1.12106382	2.90570658	-0.59567971
Pt	-3.03654922	0.02149452	-1.57628248
Pt	-0.74490962	0.31155753	-0.49071276
Pt	2.65337957	1.20213185	-1.08927929
Pt	0.97176424	-1.01140567	-1.77302667
Pt	-1.42720381	-2.16870060	-0.30224131
Pt	-2.78380900	3.33319941	1.27450999
Pt	-2.21397860	0.91610981	1.51004066
Pt	-0.18270101	-0.55541387	1.82723997
Pt	2.59448619	-1.01012626	1.25529030
Pt	2.95354966	-2.68792273	-1.52993091

13

PRE:222 = -54.82098045

Pt	2.74103488	1.18543199	1.87789593
Pt	-0.65522420	-3.70102652	1.72586248
Pt	2.34929088	-0.73762552	0.17988407
Pt	-2.67641372	-1.95457029	-2.02257299
Pt	-0.06889430	-1.44733716	0.30042482
Pt	0.24846649	0.93830721	1.26146119
Pt	-2.84552361	0.77959569	-2.41871203
Pt	2.89171679	3.72104081	1.84584552
Pt	-2.32746930	-1.81947458	1.44374345
Pt	0.69164118	3.28487957	0.26184814
Pt	-1.91971963	0.29644010	-0.07636353
Pt	2.09106719	-0.07473502	-2.34120295
Pt	-0.51997265	-0.47092629	-2.03811410

13

PRE:223 = -58.19187285

Pt	-1.24563167	1.14599422	1.67534495
Pt	2.33900335	-0.89688935	3.06455237
Pt	-3.24479250	1.05270747	0.06891760
Pt	-0.35589927	0.30403719	-2.79151260
Pt	3.65580097	0.67556701	0.32665273
Pt	0.19808159	-1.05943709	1.69770676
Pt	-0.04522628	-3.03831756	0.14286315

Pt	-1.51540354	-0.78339745	-0.12876471
Pt	1.32556026	3.34340410	-0.09100650
Pt	-0.61936253	-2.15420139	-2.27268428
Pt	1.53947124	0.88440329	-1.15755926
Pt	1.36572741	1.16793441	1.35467749
Pt	-3.39732903	-0.64180484	-1.88918769

13

PRE:224 = -57.42505233

Pt	-0.75258734	-0.01839237	3.06671038
Pt	-1.40904933	3.50323730	-2.19627888
Pt	-1.21781056	-1.29520289	-1.92792134
Pt	0.81616650	0.35203208	-2.09909676
Pt	1.24403624	-1.87950092	-0.90915225
Pt	0.02813152	-2.47036455	3.45915705
Pt	1.58955769	-0.77958332	2.18156552
Pt	0.41250623	2.37035614	-3.66016919
Pt	2.15760137	-3.35536911	2.39294439
Pt	0.28102719	0.33609058	0.39152335
Pt	-1.78410166	1.62668151	-0.47568798
Pt	-1.91151597	-1.01647178	0.52204957
Pt	0.54603812	2.62648733	-0.74564387

13

PRE:225 = -54.37321273

Pt	2.70618941	-2.05167524	0.00000000
Pt	1.34757261	3.08180641	-0.00000000
Pt	-0.89154849	-3.77615926	0.00000000
Pt	-2.36811264	-1.72557962	0.00000000
Pt	-0.66898316	4.59826004	0.00000000
Pt	1.70183738	5.71880052	-0.00000000
Pt	1.75506816	-4.35298390	0.00000000
Pt	-4.13247572	0.19836427	0.00000000
Pt	-3.52964769	-4.00034044	0.00000000
Pt	0.15034075	-1.29824918	-0.00000000
Pt	1.77253154	0.56346996	-0.00000000
Pt	3.78777516	2.36967223	-0.00000000
Pt	-1.63054731	0.67461420	0.00000000

13

PRE:226 = -56.41210634

Pt	1.60197279	1.22828328	-0.05056023
Pt	-2.54325145	0.76525701	0.46672816
Pt	-3.39218425	-1.55834184	1.13129636
Pt	0.12615426	-0.12405485	-2.10336749
Pt	3.29820409	2.26358299	1.59150058
Pt	-1.54340694	-1.34136217	-0.64106368
Pt	0.00879434	-0.34547791	1.05849887
Pt	3.80716591	1.58421242	-1.28437525
Pt	2.48824643	-0.87528780	-1.23123521
Pt	2.96210619	-0.28321197	1.60277027

Pt	-3.05926018	-3.44263737	-0.76268725
Pt	-3.91714988	-0.17440979	-1.59430552
Pt	0.16260868	2.30344799	1.81680038

13

PRE:227 = -56.82882265

Pt	-0.69777294	-1.53417085	3.55828086
Pt	-0.47723174	1.08585107	0.31610683
Pt	0.45908186	-1.39893109	-0.33252257
Pt	0.38401878	1.48027059	-2.22915417
Pt	2.06339131	0.82885115	0.17615183
Pt	-0.44190261	-0.93263650	-2.68781071
Pt	-2.03638878	0.85794128	-1.75090916
Pt	2.56664982	2.75046408	-1.47151049
Pt	-1.27410217	-2.38768832	1.07852385
Pt	0.32585289	1.10772640	3.19130145
Pt	0.64789346	-3.19188116	-2.11013164
Pt	-2.76051245	2.21648817	0.26714780
Pt	1.24102257	-0.88228481	1.99452613

13

PRE:228 = -56.91258748

Pt	-0.25951367	3.36777653	2.70546447
Pt	-0.16973856	1.36608333	0.83790547
Pt	1.40493028	-1.31393257	-2.48501053
Pt	-3.51660733	-2.94259227	0.66634654
Pt	-0.83632841	-0.20913087	2.82435243
Pt	-0.15173244	-1.08961126	-0.08316893
Pt	2.05460594	0.03426978	0.42047940
Pt	-1.86504747	2.17097970	-0.87055687
Pt	-2.21525960	-1.99407423	-1.27086056
Pt	-0.32232075	0.59067668	-2.07600508
Pt	1.45410218	1.35590710	2.84196016
Pt	1.97585647	1.07499009	-3.30983608
Pt	2.44705337	-2.41134201	-0.20107042

13

PRE:229 = -57.17186631

Pt	2.42952025	-1.13048882	-0.01413958
Pt	-0.12253841	-0.69377939	0.21793639
Pt	-1.63737731	-2.71812448	0.36710522
Pt	1.17318635	-0.29772060	2.38516606
Pt	-1.83699143	2.51308008	-2.98571457
Pt	-1.93598011	-0.84035160	-1.61240932
Pt	0.42635845	-1.67684921	-2.23775648
Pt	0.07105944	-2.53720198	2.37398584
Pt	-1.27267284	1.57226335	0.40360937
Pt	1.55468536	1.28400951	-0.18867082
Pt	-0.18517094	3.28215188	-1.24527210
Pt	1.03547767	0.20292835	4.91037650
Pt	0.30044352	1.04008292	-2.37421652



13

PRE:230 = -58.39327912

Pt	-1.83848894	-1.02870266	0.47339776
Pt	1.48107987	-2.83266144	1.06860090
Pt	-2.46690297	1.11688564	-1.02883054
Pt	-0.08939022	0.27521265	-1.81854743
Pt	-0.21410637	-1.74195900	2.76338142
Pt	0.10379605	-2.16466066	-1.11736601
Pt	-0.98035357	1.54191794	1.06782069
Pt	-2.66819624	3.42093324	0.43245279
Pt	2.43638942	0.49364060	2.26806618
Pt	2.51028219	0.27489120	-0.76368209
Pt	0.61586079	-0.38905185	0.78871231
Pt	-0.97602228	-1.71120170	-3.39464876
Pt	2.08605227	2.74475602	-0.73935722

13

PRE:231 = -55.84571474

Pt	-3.39068978	3.24778589	-0.00000000
Pt	1.43739803	-2.51086719	0.00000000
Pt	3.42539356	-4.21117155	0.00000000
Pt	-1.49555104	1.46073141	-0.00000000
Pt	0.52880767	-0.13546090	-0.00000000
Pt	1.55261138	4.88006522	0.00000000
Pt	-0.80961496	3.95693081	0.00000000
Pt	3.05718442	0.11537911	0.00000000
Pt	1.45761417	2.26255562	0.00000000
Pt	-0.85504819	-3.41607264	0.00000000
Pt	1.05672858	-5.07694989	0.00000000
Pt	-4.04214813	0.44033603	-0.00000000
Pt	-1.92268571	-1.01326190	-0.00000000

13

PRE:232 = -56.94703473

Pt	-0.43706304	-0.13602665	1.64275560
Pt	0.91017990	-1.38712925	-2.94771644
Pt	-0.68008580	-0.30268929	-1.21517531
Pt	-2.59886624	1.48940539	-1.80823654
Pt	2.13118828	-3.16131475	-1.61722471
Pt	1.80453007	0.47735121	-1.37791524
Pt	0.83860115	-2.01120915	2.58500173
Pt	-0.81030866	3.41170388	2.22700687
Pt	1.18307339	-1.52545106	0.15321872
Pt	0.66608509	1.53930325	3.16996953
Pt	-0.45425246	-3.15212358	-1.61377364
Pt	-0.01749139	2.01709100	0.33292417
Pt	-2.53559030	2.74108901	0.46916525

13

PRE:233 = -56.86631849

Pt	0.64946333	2.26760840	0.67093049
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Pt	1.33806004	0.15001835	2.57851539
Pt	2.43858777	0.44511404	0.25256848
Pt	2.27979018	-1.92194841	-0.65830709
Pt	0.00741587	-0.98873966	-0.12312332
Pt	-1.80078018	-2.72635066	0.64128388
Pt	2.11714042	-2.19115741	1.93255905
Pt	-1.94719556	2.12169069	0.19844318
Pt	-0.04775325	1.96280761	-1.83687499
Pt	-2.14557228	0.28452410	-2.57868238
Pt	-2.56787304	-0.23588374	-0.07107645
Pt	0.31061519	-3.49717210	-0.63554019
Pt	-0.63189849	4.32948879	-0.37069607

13

PRE:234 = -51.98647183

Pt	-1.45113504	-2.27696186	-0.67782927
Pt	0.79574526	-1.18936585	-0.80559295
Pt	-2.90854104	2.34858079	-0.89282005
Pt	-0.43328407	-0.86420025	-2.91445081
Pt	1.99074227	0.98226001	0.29414682
Pt	-1.19140878	0.43606092	-0.84584813
Pt	2.92869580	-2.44813467	0.07014940
Pt	1.72130822	-2.10995403	4.16704397
Pt	2.20117076	0.37037820	2.74245059
Pt	2.16763508	-2.08808797	-2.78180576
Pt	-4.75756480	3.82758983	0.12458953
Pt	1.08307344	-1.74766144	1.73217138
Pt	-2.14643710	4.75949632	-0.21220472

13 (LM6)

PRE:235 = -58.63624244

Pt	-2.81677387	1.34333863	-0.68185985
Pt	1.98291789	1.09368762	0.46539668
Pt	-0.53475947	1.61273908	0.37209481
Pt	1.33818997	2.89267649	-1.21202781
Pt	-0.75341518	-0.91340531	-0.42319274
Pt	2.44518728	-1.90964897	2.04607867
Pt	1.79636978	-1.24253099	-0.50063766
Pt	-3.25569254	-1.29610223	-0.82962526
Pt	0.32054456	-2.33033623	3.60421756
Pt	-2.42138141	-0.89635588	1.53089793
Pt	0.02401297	0.89644154	-2.07057045
Pt	0.34728431	-0.48633584	1.81889777
Pt	1.52751572	1.23583208	-4.11966966

13

PRE:236 = -54.15059910

Pt	3.20711307	1.73059243	0.00000000
Pt	0.95338164	-3.42217464	0.00000000
Pt	5.30096604	-1.18541208	0.00000000
Pt	2.75246298	-0.80234694	-0.00000000

Pt	0.15821085	1.58646235	0.00000000
Pt	-2.36689306	2.16845519	-0.00000000
Pt	0.21662688	-0.98875333	-0.00000000
Pt	-2.30444810	-0.45696973	-0.00000000
Pt	3.84406414	-3.27696610	-0.00000000
Pt	-1.60599217	-3.05582257	-0.00000000
Pt	-4.66853543	0.50590900	-0.00000000
Pt	-4.84960404	3.12119326	-0.00000000
Pt	-0.63735280	4.07583317	0.00000000

13

PRE:237 = -55.60748618

Pt	-0.63983252	0.38371899	-1.73201625
Pt	0.89718075	-1.66243291	1.17928444
Pt	-3.29419783	-0.42564674	2.48185784
Pt	-1.75290140	-0.55459009	0.48532818
Pt	0.50661858	-1.91403868	-2.20424733
Pt	2.47810964	0.03600286	2.23407464
Pt	-0.76338078	2.40912588	1.89755363
Pt	-1.08648255	-2.81586252	2.41956415
Pt	-0.52721663	-0.08659774	2.68420273
Pt	1.49023722	2.88862793	-4.48506046
Pt	0.58703645	0.79021003	0.51266230
Pt	-0.20541758	0.97134463	-4.22533686
Pt	2.31024664	-0.01986164	-1.24786701

13

PRE:238 = -56.95750409

Pt	-1.80480080	1.81217484	-2.08456155
Pt	-0.00945529	2.21744989	0.79452163
Pt	0.58697785	0.69314265	-1.22251424
Pt	1.33360164	-1.89820529	0.93645321
Pt	-1.22724882	-1.59473802	1.52955268
Pt	1.89446629	0.81943655	1.66605496
Pt	-1.71358078	0.22829702	-0.03751454
Pt	0.27108941	-3.49977836	2.59638351
Pt	3.29348271	2.93341765	1.81658001
Pt	-1.16992233	-0.45514398	-3.11730693
Pt	-3.96164722	0.83738860	-1.09707076
Pt	2.81923722	-0.35119508	-0.77843863
Pt	-0.31219987	-1.74224647	-1.00213934

13

PRE:239 = -55.65247790

Pt	3.57938937	-0.58732418	2.44416690
Pt	-3.83058939	0.17910651	-0.90507827
Pt	0.18823000	-0.44046122	-3.31896393
Pt	3.19947328	2.03784185	2.40534670
Pt	-2.25578983	2.25577941	-0.37309469
Pt	1.03722132	0.96246463	1.27399156
Pt	0.26099589	2.47045530	-0.83159355

Pt	-1.26945083	-3.85640243	0.48792965
Pt	3.50810239	0.75383606	0.20824138
Pt	-2.84596891	-2.25338648	-0.81366616
Pt	-1.08383430	-0.34209276	-0.83147894
Pt	-1.85978882	-1.34362044	1.40155311
Pt	1.37200983	0.16380375	-1.14735377

13

PRE:240 = -56.10995674

Pt	0.29321268	-1.08646824	0.00000000
Pt	-2.55713558	-2.79761262	0.00000000
Pt	1.53646678	3.43146679	-0.00000000
Pt	2.56609193	0.05140721	0.00000000
Pt	4.87082881	-0.93348630	0.00000000
Pt	-2.12576391	-0.33710872	-0.00000000
Pt	3.84289551	2.36475308	-0.00000000
Pt	0.07251119	-3.65140239	0.00000000
Pt	-0.15976423	1.47708260	-0.00000000
Pt	-1.96554964	3.27493564	-0.00000000
Pt	-3.94689281	1.56510444	-0.00000000
Pt	-4.91803855	-0.81366425	-0.00000000
Pt	2.49113781	-2.54500724	0.00000000

13

PRE:241 = -55.40143109

Pt	-0.69997368	-3.96163008	2.31623314
Pt	0.85939249	0.73516987	-2.52819265
Pt	-0.62544573	-4.26990101	-0.24292554
Pt	0.14911623	2.72373282	1.30343375
Pt	1.78138570	1.32793388	-0.13696436
Pt	1.25509843	-1.24389627	-0.12767196
Pt	-1.18880318	2.13121657	-1.66364910
Pt	1.69090256	-3.32646010	1.54116648
Pt	-3.08120605	2.77567448	0.15206525
Pt	-1.04375307	-1.82793890	0.58007867
Pt	-0.95644766	0.67005267	0.40048167
Pt	-1.22125249	4.49661856	0.09581295
Pt	3.08098646	-0.23057248	-1.68986831

13

PRE:242 = -57.57503412

Pt	2.40949998	1.16983921	0.20826243
Pt	-1.68214941	-0.55284569	0.97459812
Pt	-1.22355310	-3.33334426	1.15619015
Pt	-1.14021032	-4.10965920	-1.31996500
Pt	-1.89319938	1.58946428	-2.17565661
Pt	0.20431412	1.07664601	1.53285477
Pt	0.52251398	-2.24858929	-0.45101779
Pt	-2.03337305	1.86836129	0.43599070
Pt	0.17962295	0.23109356	-0.92558766
Pt	1.30501666	-1.58305522	1.87216357

Pt	2.85249240	0.29683554	2.51476461
Pt	0.20766746	2.81536890	-0.62680591
Pt	0.29135770	2.77988486	-3.19579137

13

PRE:243 = -54.71899799

Pt	-5.65537953	2.20495331	0.00000000
Pt	5.15999139	-1.32974252	0.00000000
Pt	-1.05533272	-3.32020985	-0.00000000
Pt	0.80680343	3.71031155	-0.00000000
Pt	-3.67023030	0.54722908	-0.00000000
Pt	-1.65807351	2.30127423	-0.00000000
Pt	-3.40733564	-2.12183425	-0.00000000
Pt	0.61321680	1.17684487	-0.00000000
Pt	-1.34030971	-0.54307667	-0.00000000
Pt	2.89836422	-0.05240242	0.00000000
Pt	3.07745332	2.49319451	-0.00000000
Pt	3.20214457	-3.20956952	0.00000000
Pt	1.02868767	-1.85697231	-0.00000000

13

PRE:244 = -55.41597352

Pt	-3.26064393	-0.84664804	-0.00000000
Pt	-0.99226500	3.56161399	0.00000000
Pt	3.69745819	3.53001407	-0.00000000
Pt	2.36519967	-2.05257005	0.00000000
Pt	-0.92136911	-1.96107880	0.00000000
Pt	-2.29964111	-4.09708806	0.00000000
Pt	0.83173345	-4.07619439	0.00000000
Pt	3.27622244	0.68224300	-0.00000000
Pt	-1.58255580	1.08809880	-0.00000000
Pt	1.36457455	4.88679682	0.00000000
Pt	0.76904348	-0.04906315	-0.00000000
Pt	1.37407529	2.37175984	-0.00000000
Pt	-4.62183212	-3.03788403	0.00000000

13

PRE:245 = -58.13525215

Pt	2.35432005	-1.09847319	1.88687244
Pt	-0.14472538	-0.05663672	2.07478960
Pt	1.46304217	-0.23255641	-0.31403103
Pt	-2.63697396	2.55592062	0.01585393
Pt	-0.31313060	1.56666879	0.13749101
Pt	-1.87740623	-1.19765677	0.65217646
Pt	2.04938106	1.46338628	1.54451870
Pt	0.38414266	3.16336817	-1.75805425
Pt	1.61106656	-3.16055849	-2.36292267
Pt	-3.14808956	0.73712697	1.66051381
Pt	-0.39206329	-1.79103880	-1.35091793
Pt	-0.77537769	0.82320797	-2.29432408
Pt	1.42581419	-2.77275842	0.10803402

13

PRE:246 = -56.94740359

Pt	2.24257518	0.91990786	-2.07879457
Pt	-2.71466724	0.25067935	-2.08849979
Pt	-0.47368214	-2.49125752	0.07802443
Pt	1.21930890	2.02556067	0.01369180
Pt	4.30779704	0.44197163	-3.48960917
Pt	-0.78704302	1.85805700	1.55568670
Pt	-2.17400223	-1.17096492	3.89609581
Pt	-0.94249129	0.03358234	-0.30971429
Pt	-0.33213973	-0.70766684	2.07694451
Pt	4.02202090	-0.81958181	-0.88287546
Pt	-3.10225493	1.78070845	0.34446114
Pt	-2.72672287	-1.22214148	1.39145527
Pt	1.46130143	-0.89885473	-0.50686638

13

PRE:247 = -55.06998481

Pt	-1.01376927	-1.66758141	2.68055579
Pt	4.16367938	-4.28475639	-0.42467441
Pt	0.50154269	-1.25894938	0.64937972
Pt	-1.96288454	-0.13067191	0.80756675
Pt	2.11032777	-2.80170102	-0.64935774
Pt	2.17496128	0.03180868	-0.80799659
Pt	-1.34586400	3.44100778	2.31200515
Pt	-0.17070057	1.13804130	2.13059129
Pt	-0.18501589	1.08594596	-0.68026195
Pt	-1.76273097	-0.87264346	-1.59323321
Pt	0.66757271	3.13395709	0.62992890
Pt	-0.41773812	0.77075391	-3.23541635
Pt	-2.75938046	1.41478887	-1.81908735

13

PRE:248 = -57.43054548

Pt	-2.79418637	3.90656862	0.61767940
Pt	1.21843159	-0.09045720	-0.00831367
Pt	-1.00211408	-1.29373484	-0.42744339
Pt	2.21930763	-2.35079873	1.42895439
Pt	2.94446359	-1.83732591	-0.94934298
Pt	-3.02470635	2.41958333	-1.47861810
Pt	-0.80583817	2.95576148	-2.60359695
Pt	-0.28908429	-2.13867174	2.09756001
Pt	-0.29048883	1.43747486	1.86843854
Pt	0.63580273	-0.85635400	-2.44358475
Pt	1.76459346	-0.02421948	2.53169192
Pt	0.30448443	-3.42076110	-0.05335799
Pt	-0.88066535	1.29293471	-0.58006644

13

PRE:249 = -56.45241496

Pt	3.42986870	-0.51552572	-1.11471465
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Pt	-2.57456046	3.05893414	1.05676781
Pt	0.88584953	-0.14915400	-0.71861600
Pt	-1.64681801	-2.19647432	-0.77700515
Pt	-3.51694328	1.44666279	-0.65117082
Pt	2.20725335	-0.72152635	1.30725398
Pt	-0.27246488	-1.24346235	1.26539609
Pt	1.67124524	-3.20047644	0.96152757
Pt	0.10123523	3.71524867	-0.48936441
Pt	-1.42647620	2.13931325	-1.89800556
Pt	0.18124943	-1.70693504	-2.71509928
Pt	1.55009622	-2.13312363	3.26489866
Pt	-0.58953487	1.50651901	0.50813175

## 2. Platinum Oxide Clusters

### 1. GM

#### 1. Pt<sub>13</sub>O<sub>1</sub>

14

PRE:1= -65.68121219

78	5.929951826	9.591867009	10.281256683
78	7.074917692	8.723234598	7.100351592
78	8.789826668	6.962927706	6.426049613
78	8.357423446	10.191108473	10.639758909
78	6.011433829	10.795256541	8.056288269
78	9.166127315	7.939120399	9.820757374
78	9.632443118	9.059399284	7.585471645
78	7.363079932	8.004253368	11.803226145
78	10.857773623	9.447337586	10.914896902
78	10.768749643	10.860317872	8.882919483
78	6.751197640	7.432679868	9.262118889
78	8.258910939	11.720536076	8.493922226
78	8.578247709	5.754724730	8.619508783
8	10.020028162	12.559496941	8.353771539

14

PRE:2= -65.63942832

78	6.579730341	10.216692369	10.761141162
78	7.743967027	9.257586245	7.571727989
78	9.346736532	7.438833481	6.827087334
78	8.974488470	10.780164617	11.305053325
78	6.826129907	11.421014612	8.526267007
78	9.937350555	8.670092530	10.297492004
78	10.281586771	9.594731670	7.773832380
78	8.042679045	8.561928446	12.315325954
78	11.436502442	10.354912405	11.611993038

78	11.775359279	11.172036904	9.272842632
78	7.515914627	8.085594643	9.793121232
78	9.307075672	11.856775278	9.061626814
78	9.323664713	6.426392572	9.133359691
8	11.984745106	10.488983450	7.499615544

14

PRE:3= -65.74174078

78	6.376136721	9.797180209	10.388899745
78	7.343427454	8.950055662	7.104394138
78	9.288367776	7.394107414	6.513160846
78	8.808853137	10.381499251	10.885977938
78	6.254951612	11.001019258	8.184775081
78	9.663540671	8.216213303	9.899990256
78	9.744321459	9.623833607	7.713984639
78	7.777925720	8.138899998	11.874749930
78	11.328398006	9.836155162	10.956612728
78	11.587681911	11.000865722	8.770851514
78	7.246933911	7.681288610	9.322302888
78	9.212952914	11.876800827	8.830581723
78	9.110499895	6.055191243	8.637988658
8	7.450955939	12.475427603	8.365793539

14

PRE:4= -65.85089980

78	6.280931197	9.817911041	10.572910976
78	7.423311734	8.897423099	6.982624996
78	9.345855159	7.249773690	6.499046716
78	8.738767553	10.434235760	10.856414732
78	6.638491567	11.106036506	7.947528116
78	9.612780150	8.256929671	9.906830516
78	9.794935835	9.479858620	7.625974926
78	7.788686196	8.164270314	11.879137588
78	11.267749903	9.904724796	10.908986934
78	11.513300203	11.039317360	8.689854045
78	7.197741044	7.795656439	9.312464832
78	9.014677911	11.684676976	8.603700209
78	9.046495167	6.097963424	8.703624367
8	5.375520495	11.032651431	9.382507985

14

PRE:5= -65.13622997

78	6.581406997	10.078158610	10.154627170
78	7.427991450	8.801541425	6.952296608
78	9.352541090	7.175555654	6.483196644
78	9.036626385	10.664301665	11.276957866
78	6.561665993	11.008741329	7.842672582
78	9.498212088	8.428229107	9.930424652



78	9.773536854	9.461525983	7.580686706
78	7.730501735	8.179557979	11.791422313
78	11.389737113	9.810705004	10.825717381
78	11.451465787	11.039048066	8.650148766
78	7.119526634	7.749894049	9.279490354
78	8.922207005	11.505945487	8.754391530
78	9.139273061	6.171749351	8.759599133
8	7.167883886	11.159962711	11.618993606

14

PRE:6= -65.20230461

78	6.306552626	9.828516830	10.273137754
78	7.459165549	8.903238546	7.017609664
78	9.262594372	7.217418283	6.459720496
78	8.646693310	10.448056518	11.151403440
78	6.433559767	11.005418834	7.997707409
78	9.643711902	8.364679828	9.928413231
78	9.968694689	9.411812416	7.575677001
78	7.728165315	8.110472886	11.813041790
78	11.254284776	10.022988084	10.959503428
78	11.417191036	11.124219546	8.708959657
78	7.265315952	7.762782374	9.269680705
78	8.854122952	11.531946291	8.576031820
78	9.089158976	6.116162022	8.716248746
8	8.909456400	12.203848706	10.377380084

14

PRE:7= -65.23584957

78	6.243333019	9.998816270	10.306374184
78	7.438659264	8.933366102	7.026994708
78	9.262861505	7.207502833	6.503737931
78	8.673331543	10.456517779	10.656196546
78	6.551132703	11.103826201	7.953890411
78	10.070705934	8.084164072	9.939470087
78	9.842784091	9.446728576	7.657887569
78	7.722270171	8.310401348	11.874867914
78	11.181455541	10.169397387	10.925085113
78	11.473808220	11.120292973	8.640519143
78	7.316909291	7.953315196	9.354723959
78	8.979726667	11.636825042	8.480261358
78	8.982005458	6.137559981	8.724390866
8	9.604905272	7.753487586	11.836063180

14

PRE:8= -65.18222701

78	6.078907367	10.103906913	10.241725859
78	7.516367829	9.143153031	7.064383090
78	9.061236078	7.218733485	6.525066733

78	8.576999469	10.232135110	10.612942991
78	6.395405588	11.213290952	8.024808462
78	10.178408806	7.837359708	10.058322065
78	10.090269894	9.228062784	7.714965359
78	8.252144792	7.941600940	11.774026102
78	11.038781340	10.055731489	11.042994535
78	11.363239847	11.158485511	8.807686688
78	7.326168580	8.084997583	9.364911675
78	8.883673360	11.502841993	8.437025203
78	8.762690971	6.123303660	8.768513086
8	11.386691429	8.005535553	8.506645705

14

PRE:9= -65.52084289

78	6.201823265	9.997409468	10.323134169
78	7.457019889	8.894850063	7.046969069
78	9.348623439	7.244814432	6.497990276
78	8.702678654	10.342070133	10.776628449
78	6.581593081	11.058462841	8.084083514
78	9.846174295	8.090167636	9.957068056
78	9.836305862	9.444452383	7.632701994
78	7.860262056	8.136549512	11.872379126
78	11.235698981	9.956395211	10.930448388
78	11.521168056	11.039028240	8.689570875
78	7.277098172	7.870936358	9.347798835
78	9.010248675	11.624351108	8.618813912
78	8.997355357	6.096113540	8.694265699
8	6.110913461	9.063186478	12.055017473

14

PRE:10= -65.12999053

78	6.415438047	9.896727381	10.263510429
78	7.469964178	8.905922692	7.061386963
78	9.295849596	7.218490994	6.477328714
78	8.818522631	10.654034901	10.962009215
78	6.569256914	11.078129537	8.036828960
78	9.631062159	8.262312976	9.940782395
78	9.872821496	9.422534501	7.638002359
78	7.748082525	8.158285556	11.869018286
78	11.295677133	9.917463533	10.895723507
78	11.501871490	11.076802602	8.687124985
78	7.242101178	7.684292341	9.344637381
78	9.000298527	11.587710291	8.631934965
78	9.046666121	6.055271241	8.680217970
8	8.139645729	9.923087615	12.658787572

14

PRE:11= -65.22992333

78	6.275710381	9.904186019	10.340432795
78	7.455579938	8.929255533	7.018465479
78	9.293900668	7.228884048	6.486732705
78	8.727483213	10.290176216	10.772552748
78	6.577525774	11.093995685	8.051530399
78	10.008096141	8.017347470	9.868329923
78	9.845644222	9.420412988	7.688063819
78	7.702914306	8.173459409	11.863196931
78	11.256402286	9.981175433	10.938026963
78	11.485295554	11.091047871	8.710648158
78	7.278852011	7.875932384	9.279605171
78	8.984920887	11.612465689	8.641047434
78	8.913545595	6.051437492	8.654799153
8	9.245010939	7.047115274	11.441874817

14

PRE:12= -65.36143629

78	6.390003071	9.871200852	10.301882296
78	7.465797110	8.912815976	7.061534983
78	9.318436973	7.254904469	6.498319893
78	8.822182459	10.400124405	10.883741445
78	6.565148347	11.057327809	8.055377646
78	9.658413945	8.206999291	9.948610771
78	9.886246390	9.485089002	7.618410169
78	7.735705977	8.212044190	11.872416516
78	11.334320248	9.843249849	10.983598040
78	11.552582479	11.107185196	8.699237583
78	7.253809301	7.736344740	9.310405422
78	9.023971735	11.631716429	8.602517955
78	9.064561590	6.061057207	8.696395475
8	12.751425270	10.936648110	10.240528208

14

PRE:13= -65.42184956

78	6.369013857	9.900252891	10.268565818
78	7.442070578	8.905779646	6.980825812
78	9.297408348	7.204778378	6.465900873
78	8.565580762	10.566054488	11.213371129
78	6.625009575	11.081305318	8.036721008
78	9.752673401	8.228891422	9.964338213
78	9.839704398	9.399569479	7.652423724
78	7.781134350	8.143437275	11.788234645
78	11.273541510	10.082296187	10.801744809
78	11.588911265	10.974561802	8.524713515
78	7.257938046	7.784815408	9.259276945
78	9.023046349	11.490532804	8.768373657
78	9.081952209	6.102526311	8.714620774
8	10.214666634	10.765404542	12.218480075

14

PRE:14= -65.67169646

78	6.422023231	9.907038248	10.320843012
78	7.456276832	8.942053354	7.064659476
78	9.317531262	7.305949262	6.477012253
78	8.911003605	10.258619086	10.746112198
78	6.524024221	11.087173811	8.062271388
78	9.799185417	7.826750251	9.906993623
78	9.838316755	9.498354356	7.731805875
78	7.696722252	8.231531505	11.851537823
78	11.448115054	9.933525887	10.543628716
78	11.446967164	11.407234134	8.553492898
78	7.305450512	7.779757477	9.303934075
78	8.933198670	11.669201605	8.626786123
78	8.826415657	5.911083378	8.526924913
8	11.498661597	8.066650397	10.809225325

2.

**Pt<sub>13</sub>O<sub>2</sub>**

PRE:1= -71.96818298

78	6.414959886	9.743211474	10.522282313
78	7.503674551	8.730695458	7.242396003
78	9.371025793	7.017612906	6.686890588
78	8.872964835	10.268959739	11.103768292
78	6.586781825	10.926332921	8.285159548
78	9.701445882	8.097177905	10.156722321
78	9.899121996	9.283370286	7.829195921
78	7.767009767	8.081175000	12.071176241
78	11.423765087	9.768545432	11.122039058
78	11.505291475	10.935621235	8.956936260
78	7.270285936	7.593610714	9.522054781
78	9.013301892	11.466070264	8.847066740
78	9.090326112	5.938599877	8.879327228
8	9.896070360	6.151824051	5.241249171
8	12.731364393	9.701910939	12.302983461

PRE:2= -70.29405174

78	6.480402889	9.742815880	10.258169466
78	7.516553101	8.794405480	7.183691673
78	9.484606231	7.294732149	6.490101851
78	8.831997625	10.339656288	10.890076111
78	6.682528559	10.992490000	8.076227208
78	9.553208656	8.131798414	9.845144203
78	9.904236856	9.489292271	7.691937369
78	7.870657272	8.136534308	11.888459590
78	11.321552975	9.654384416	10.904179717
78	11.549104771	11.015498460	8.813681034

78	7.054451932	7.394832294	9.460061485
78	9.000755447	11.718091710	8.701276020
78	9.225446010	5.996100411	8.608737591
8	9.664451851	13.317093005	9.147249960
8	6.029687647	6.137559469	8.707176416

PRE:3= -69.98818933

78	6.483499304	9.826459928	10.241761963
78	7.453024268	8.859235595	7.100324784
78	9.328023764	7.201307701	6.493961178
78	8.732923763	10.485992748	11.172345435
78	6.547155998	11.045002617	8.035112777
78	9.656014856	8.171550728	9.921073620
78	9.831593528	9.390963964	7.675687930
78	7.782847086	8.141994443	11.820839386
78	11.256068743	9.828347020	10.889267672
78	11.487326101	11.018552372	8.696892632
78	6.995653412	7.507533321	9.442268128
78	8.963576476	11.525028035	8.665032317
78	9.052840305	6.067533393	8.714040728
8	5.779893218	6.449958091	8.625680345
8	9.089841267	11.981500607	12.062559595

PRE:4= -70.28837405

78	6.470496969	9.842799021	10.317563462
78	7.258592588	8.745857277	7.006797044
78	9.258460152	7.067478438	6.562567548
78	8.742802530	10.466891466	11.262429804
78	6.581999704	10.927509192	8.041574863
78	9.612300391	8.330008536	9.990217514
78	9.743209302	9.299353302	7.616570334
78	7.773758410	8.047162378	11.859358682
78	11.365132729	9.865695739	10.867875260
78	11.460843668	10.892614083	8.591151432
78	7.233412083	7.660754611	9.348854607
78	8.950082555	11.442664128	8.733199792
78	9.186143306	6.063424112	8.854948001
8	9.172204573	11.989831731	12.106728521
8	6.431484101	7.643555984	5.878682408

PRE:5= -72.16908630

78	6.142814221	9.871565527	10.786064026
78	7.299608169	8.957639411	7.168599762
78	9.221992039	7.329998658	6.702692743
78	8.527266947	10.517382171	11.362879157
78	6.475941516	11.148988012	8.103714240
78	9.432153217	8.473657046	10.118729454
78	9.706723832	9.576175065	7.783299553

78	7.630912127	8.145766767	12.055357747
78	11.176404465	9.989161425	11.079804313
78	11.399891387	11.092728830	8.853210780
78	7.068887839	7.897588279	9.499113100
78	8.842691736	11.761108082	8.715308012
78	8.953735964	6.253222899	8.951935434
8	5.277513000	11.106182484	9.592058147
8	8.948763239	12.231991344	10.575542556

PRE:6= -71.19090123

78	5.988736418	10.092604622	10.562106983
78	7.072203171	9.128089363	7.288593166
78	8.968711751	7.422994339	6.741792347
78	8.407334019	10.606936693	11.093617239
78	6.159069467	11.257251838	8.333418698
78	9.318021570	8.395239147	10.145837402
78	9.532807772	9.617216971	7.873677701
78	7.416638770	8.379238469	12.093056332
78	10.968006125	10.068609781	11.132475114
78	11.135908560	11.267412012	8.946295736
78	6.854333973	7.948835726	9.549613004
78	8.588270416	11.811950047	8.847111215
78	8.727285266	6.233387365	8.924676462
8	4.532378954	10.376570374	11.549821397
8	4.832073831	12.298275716	7.809922751

PRE:7= -72.11020431

78	5.677500641	10.024019210	10.968140892
78	6.961296054	8.977981085	7.395777628
78	8.933294842	7.394450758	6.945887839
78	8.325602089	10.591232443	11.287614511
78	6.207760746	11.056355422	8.650979761
78	9.149894958	8.348930099	10.411082973
78	9.288545271	9.642604057	8.063186949
78	7.189948263	8.424371892	12.226564166
78	10.835015923	10.005742203	11.346919906
78	11.059343614	11.132502867	9.102106972
78	6.752863969	7.867752032	9.704202546
78	8.591237089	11.841037074	9.058234096
78	8.638743973	6.203105695	9.148386903
8	4.687981758	11.248676645	9.819886858
8	5.421183160	9.154219005	12.715501832

PRE:8= -71.24126280

78	5.930383497	10.046687707	10.693911731
78	6.858420548	9.117366263	7.514687955
78	8.802782125	7.420491987	7.007448578
78	8.223197996	10.603594461	11.654528510

78	5.996019124	11.293415884	8.442468900
78	8.934296310	8.496981244	10.371630915
78	9.301364324	9.633089326	8.078596250
78	7.168418804	8.354235533	12.368548278
78	10.756548119	9.983332657	11.358963493
78	10.931925430	11.192241748	9.171645266
78	6.533630726	7.686012715	9.953972658
78	8.376101622	11.805101330	9.076239990
78	8.596678585	6.249676930	9.209505252
8	5.870012247	7.587597873	8.123704655
8	8.610053222	12.363279139	10.902595867

PRE:9= -72.09326118

78	5.902712211	9.953308769	10.936680973
78	6.900085025	8.978786485	7.682823199
78	8.747192987	7.442987380	6.854431814
78	8.311186263	10.428083725	11.473465432
78	6.072312303	11.151341044	8.709261800
78	9.188475669	8.185425317	10.602952060
78	9.324934219	9.505682329	8.255048217
78	7.150783601	8.295080845	12.524450295
78	10.767348959	9.836087113	11.744071483
78	10.991879607	11.255902773	9.071099706
78	6.752965386	7.800357806	9.956779228
78	8.494222979	11.699610966	9.255625628
78	8.475086387	5.993623863	9.504996105
8	8.807939734	5.729256091	7.666592076
8	11.894480640	10.931004724	10.703110232

PRE:10= -71.55839267

78	6.040394825	10.013132856	11.039107706
78	6.947367719	8.965451201	7.708727615
78	8.666442398	7.305236287	6.881845146
78	8.424413494	10.428708016	11.890617568
78	6.117515968	11.125876857	8.744599035
78	9.135290276	8.310827141	10.594553434
78	9.430765553	9.384745230	8.211800021
78	7.301603169	8.171016000	12.536929429
78	10.966118791	9.758216558	11.567615093
78	11.071948451	10.931097328	9.351593099
78	6.734590151	7.842834507	10.001821723
78	8.534201288	11.508130182	9.340780622
78	8.435268178	6.026548257	9.625866962
8	8.637385962	5.645568137	7.782109482
8	8.735454616	12.201683264	11.127519338

3.

**Pt<sub>13</sub>O<sub>3</sub>**

PRE:1= -75.98952471

78	6.271363869	9.743904577	10.306612302
78	7.258321912	8.884525099	7.010097998
78	9.131845319	7.229826300	6.497401642
78	8.690516558	10.241042056	10.748376408
78	6.385988493	10.991402340	8.138787188
78	9.743212052	8.034755548	9.887931902
78	9.610326642	9.413799369	7.663099932
78	7.526984772	8.180291657	11.857415260
78	11.193655861	9.945705190	10.954748582
78	11.266910013	11.018232359	8.694724795
78	7.038996761	7.452815786	9.377985199
78	8.797177318	11.637433139	8.593242204
78	8.973557601	5.935552375	8.640086539
8	4.887376184	11.884459911	7.953057436
8	5.851379839	6.340487030	8.577911225
8	10.660146652	6.816910192	10.883209671

PRE:2= -77.38077231

78	6.339167016	9.525143951	10.290694642
78	7.275209404	8.762606977	7.070363551
78	9.148517966	7.085768390	6.532659214
78	8.697325320	10.155159608	10.810121768
78	6.411928351	10.861636707	8.188686153
78	9.526864626	7.899384211	9.861644773
78	9.693656464	9.259728709	7.657597121
78	7.720829418	7.952406975	11.846731446
78	11.191671028	9.698843984	10.928073805
78	11.338631430	10.856600743	8.723528032
78	7.035533410	7.201973666	9.357082913
78	8.826958110	11.476174164	8.618491438
78	9.043605857	5.746384189	8.618466720
8	4.941897874	11.780914318	7.890533217
8	5.739544525	6.204968360	8.590227611
8	9.391883684	4.063255077	8.953542400

PRE:3= -75.73277194

78	5.934078273	9.741503512	10.520607238
78	7.151737527	8.746636543	7.191342289
78	9.009553303	7.070402591	6.597583671
78	8.391689847	10.345262963	11.156476704
78	6.256046304	10.879485157	8.191575566
78	9.370971783	8.034693367	10.014433626
78	9.540390797	9.263538546	7.762421155
78	7.453759586	8.045426325	11.902615902
78	10.882339545	9.749661501	11.009002803
78	11.176854971	10.903983524	8.802770908
78	6.716294112	7.473415306	9.491367811
78	8.660214562	11.407428300	8.731292109



78	8.669267777	5.959187251	8.820133126
8	4.330845414	10.546234471	10.720433305
8	5.270200632	6.541833287	8.955385858
8	8.399202285	11.891174436	12.087638860

PRE:4= -76.17374902

78	6.038678898	9.638328621	10.586090620
78	7.110608783	8.675247503	7.344159741
78	8.974215682	7.010652128	6.737161788
78	8.421464444	10.274664511	11.282208842
78	6.184030581	10.828916575	8.348402346
78	9.253701165	7.983439522	10.216621916
78	9.493841391	9.192629581	7.932624312
78	7.390562820	7.973891455	12.116913996
78	10.923747668	9.679846014	11.153427559
78	11.141374611	10.848718375	8.942683416
78	6.731838584	7.380486446	9.597864764
78	8.620830580	11.344621718	8.891579165
78	8.684383920	5.841283916	8.938896720
8	5.243137893	6.469565766	9.119081705
8	8.369465788	11.808394777	12.245804689
8	7.109708822	7.239515458	13.677387981

PRE:5= -76.29862786

78	5.848847036	9.817931068	10.468946744
78	6.852861332	8.869018338	7.294799948
78	8.709619966	7.177697848	6.749585525
78	8.187071911	10.399334232	11.337223544
78	5.925063227	11.000583397	8.297465203
78	9.100712282	8.114161275	10.142285324
78	9.253710609	9.348654280	7.904812124
78	7.186017489	8.129168454	12.034411297
78	10.680028604	9.810619653	11.145166378
78	10.861539042	10.988819216	8.939769259
78	6.481529726	7.481352407	9.639080069
78	8.347496498	11.515209779	8.830258539
78	8.447802744	5.987019438	8.941112932
8	4.728687599	12.078583438	7.584450856
8	5.020800392	6.611184670	9.050858678
8	8.164928167	11.981131533	12.196683846

PRE:6= -78.44408859

78	5.601913066	9.590924692	11.099556963
78	6.796397705	8.675047485	7.469956205
78	8.732821287	7.192832324	6.684404629
78	8.046887949	10.207198002	11.322244948
78	6.018604485	10.880667161	8.425590892
78	8.989751929	8.028125830	10.411080437

78	9.188640906	9.271720817	8.096870289
78	7.162133895	7.938778578	12.388881991
78	10.528803533	9.685212079	11.593704611
78	10.890251469	10.993768853	8.897537602
78	6.559039549	7.623991103	9.818426248
78	8.385687638	11.472693173	9.094715411
78	8.290322421	5.823280966	9.325107512
8	4.747579785	10.810515545	9.827629667
8	8.679502079	5.489275973	7.512942626
8	11.704552685	10.760616639	10.593177566

PRE:7= -77.99116455

78	5.400742151	9.723196168	11.070322234
78	6.688560471	8.620784493	7.633680919
78	8.778553712	7.218210510	6.791887838
78	7.697702955	10.449365628	11.732841297
78	5.968911218	10.880391989	8.482941126
78	8.878547379	8.123898005	10.379675312
78	9.041442888	9.311321395	8.155950115
78	7.092901307	8.014360470	12.324152388
78	10.285128261	10.129380539	11.196836250
78	10.874156657	10.853382891	8.907480930
78	5.995632131	7.527541157	10.041922388
78	8.303614925	11.429143563	9.263140527
78	7.985584995	6.190753458	8.896173051
8	4.580603946	10.937336584	9.782523182
8	6.456510880	5.631416816	9.873790760
8	9.347885187	10.629147580	12.772793697

PRE:8= -76.28935480

78	5.642067158	9.662587532	10.908120352
78	6.646653053	8.751572577	7.780338644
78	8.418154459	7.000306920	7.190296207
78	7.966440251	10.182875155	11.796862345
78	5.727261815	10.907953120	8.647285576
78	8.890459658	7.914410588	10.717875562
78	9.156260000	9.217137532	8.253912778
78	6.936837445	7.960470809	12.559138748
78	10.481949016	9.741474276	11.658486376
78	10.621644465	10.941024685	9.449445381
78	6.338584202	7.344745517	10.132829392
78	8.096833353	11.347657305	9.286499045
78	8.220766483	5.784994221	9.389426546
8	5.613425427	7.218513592	8.346617673
8	8.322529456	11.967277581	11.113261933
8	10.249233478	7.953937859	9.297890482

PRE:9= -77.29195127

78	5.120568890	9.766993537	11.279786063
78	5.888603189	8.856908450	7.921222530
78	7.958147738	7.067719339	7.513661333
78	7.537041559	10.246892028	11.633900488
78	5.246044440	10.965286801	9.042788295
78	8.723937302	7.975638886	10.794482722
78	8.847496369	9.179237235	8.584153063
78	6.441974878	8.118493730	12.865014798
78	10.082704197	9.786772588	11.927796382
78	10.165459949	10.983775554	9.761120650
78	6.095728193	7.746495568	10.208762784
78	7.521810823	11.751517476	9.565153189
78	7.824322163	5.876615031	9.687435470
8	9.235925754	12.651060569	9.655803721
8	6.282594566	7.430498425	6.685612461
8	8.145833701	7.248404767	12.567329176

PRE:10= -77.92958348

78	4.812424545	9.948180222	11.295570196
78	5.959825432	8.902329666	8.070256398
78	7.837670816	7.235768675	7.493740243
78	7.314016316	10.514147952	11.901719361
78	5.082501136	11.036862923	9.091045095
78	8.151831277	8.208319737	10.921471861
78	8.364186713	9.447636292	8.621608959
78	6.255040576	8.096732703	13.019913086
78	9.835678920	9.879459976	11.869654044
78	10.001046531	11.067786049	9.696290797
78	5.638878058	7.677841607	10.247576215
78	7.484300979	11.591722627	9.631842853
78	7.590878621	6.056832163	9.666215235
8	5.421516597	6.720143431	11.974488300
8	7.194564423	9.635932039	13.681123236
8	4.504843815	9.192990578	12.982286928

#### 4. Pt<sub>13</sub>O<sub>4</sub>

PRE:1= -84.44446857

78	6.302093881	9.780956631	10.607074510
78	7.495640394	8.664230915	7.245109854
78	9.395576616	7.015412595	6.721856422
78	8.841489329	10.288717605	11.157091522
78	6.654893347	10.801454095	8.370760146
78	9.692215187	8.107913991	10.173286446
78	9.892199853	9.263385957	7.833805420
78	7.806899247	8.090304798	12.049113495
78	11.412245590	9.769686364	11.088564188

78	11.526140831	10.904420746	8.896867511
78	7.234312631	7.606601810	9.560248608
78	9.043434502	11.432110231	8.876385929
78	9.127309272	5.949697181	8.943971849
8	4.921262571	9.974521498	11.673379229
8	7.571211827	7.310187480	13.595472788
8	9.870583270	6.259938145	5.225140761
8	12.640747452	9.661271775	12.318863055

PRE:2= -83.95564578

78	6.362349546	9.674314710	10.625218574
78	7.504792273	8.786090091	7.154780124
78	9.396437714	7.149594058	6.646595597
78	8.855231665	10.461022962	11.191171367
78	6.718047658	10.859915426	8.350750718
78	9.571658243	8.117284013	10.228678731
78	9.868459629	9.309333883	7.853422860
78	7.646856513	8.032239353	12.140762547
78	11.345053045	9.698790544	11.098537492
78	11.587755074	10.897221222	8.756880493
78	7.219227554	7.525436932	9.524776198
78	9.100627476	11.503641258	8.845249903
78	9.155443880	5.961148019	8.957702888
8	5.291884950	10.991760258	9.642844464
8	8.521129447	9.571126671	12.918015609
8	9.691851519	5.325164691	7.221778726
8	12.802915393	10.604130553	10.213853700

PRE:3= -84.04164861

78	6.412849400	9.701945333	10.613348855
78	7.421867510	8.794509507	7.270432923
78	9.376343723	7.173471587	6.677496234
78	8.871425125	10.287274098	11.150457819
78	6.592044261	10.935589772	8.369580426
78	9.664959425	8.023347702	10.238070155
78	9.864286809	9.304157842	7.870246236
78	7.753712176	8.082678999	12.036029933
78	11.373559008	9.666225543	11.157944037
78	11.514778044	10.914832221	8.831018240
78	7.253415431	7.520602890	9.523714288
78	9.005158016	11.504001031	8.855787870
78	9.148328488	5.873340529	8.968488381
8	5.098692979	11.886729403	8.443325231
8	7.563806557	7.278058495	13.590719234
8	9.685645215	5.334764011	7.193128129
8	12.793503032	10.613639803	10.251093698

PRE:4= -84.03566749

78	6.402942950	9.726553681	10.448946144
78	7.384523742	8.745841685	7.222089144
78	9.330126946	7.247841898	6.498453084
78	8.697236435	10.333738618	11.461248180
78	6.552785179	10.941254904	8.214923243
78	9.378181124	8.244069464	10.101088486
78	9.795481658	9.386821825	7.767055964
78	7.610792767	8.074697350	12.138856253
78	11.162705372	9.707895790	11.150965637
78	11.427108661	10.997936212	8.827383407
78	7.015035506	7.340626577	9.719712491
78	8.937508632	11.554247980	8.839863382
78	9.081432879	5.900891193	9.166623585
8	9.296183023	5.538233903	7.329795176
8	12.529612267	10.831685311	10.414283059
8	8.807550981	12.098654047	10.688612247
8	6.207628715	7.405116763	7.972030381

PRE:5= -83.84684815

78	6.186004863	9.751387820	10.490196814
78	7.230022577	8.651060290	7.224296240
78	9.220613910	7.188792091	6.572589112
78	8.603690536	10.301258090	11.240791733
78	6.512474270	10.923234453	8.126784999
78	9.471483421	8.003010498	10.166512133
78	9.590554610	9.255558331	7.916191325
78	7.661878160	7.904221560	12.108009664
78	11.078792356	9.646794372	11.262257838
78	11.328395649	10.870577402	8.696808669
78	6.928478827	7.433605958	9.535478494
78	8.867578762	11.489223841	8.892327872
78	8.826156047	5.812962993	9.044843293
8	9.351149539	5.408827278	7.237748890
8	12.386874851	10.640524925	10.252312462
8	6.895798925	11.196836518	11.501133538
8	5.172775972	8.270167944	9.764326916

PRE:6= -85.10530122

78	6.043253971	9.718190010	10.468255412
78	6.942443529	8.663518720	7.051939245
78	8.899131779	7.261796100	6.344206814
78	8.468950598	10.285566282	10.984217678
78	6.155531671	10.943985392	8.177574952
78	9.252129960	8.143581849	9.930617642
78	9.402006717	9.414455290	7.632662483
78	7.399358211	8.065831593	11.962011892
78	10.927769175	9.585155810	11.154447296
78	11.088683098	11.100027525	8.567851742

78	6.866480236	7.547769690	9.424921777
78	8.660216401	11.672192020	8.767931704
78	8.729611109	5.849101013	8.988409601
8	9.088897554	5.559821825	7.164027425
8	12.077895759	10.680480704	10.137509853
8	6.930235730	12.599155522	8.746949601
8	5.262726242	9.662528777	7.087729159

## 5. Pt<sub>13</sub>O<sub>8</sub>

PRE:1= -106.59600869

78	5.927705905	9.799244587	10.430985820
78	7.037120722	8.834615844	7.109997815
78	8.889732542	7.144558192	6.628007491
78	8.366792878	10.459985161	11.030410601
78	6.132698845	10.944184513	8.202074475
78	9.255353690	8.124629876	9.978829416
78	9.504225114	9.347466518	7.675829057
78	7.372753573	8.130351420	11.860808875
78	10.835966454	9.847642707	11.038229294
78	11.043175820	10.977337969	8.823999230
78	6.674751993	7.565436631	9.346451771
78	8.560013212	11.536538198	8.673998883
78	8.555142408	5.951843715	8.795018355
8	4.499878697	10.047117213	11.456439575
8	4.936515655	12.020912842	7.495137216
8	8.992113486	4.254216335	8.929651429
8	9.392564370	6.266602301	5.200650248
8	12.244664860	9.743775934	12.084656210
8	12.498199590	11.849193244	8.395852653
8	5.195219804	6.629069399	8.958604704
8	8.301293250	11.924914391	12.062417723

PRE:2= -109.76525096

78	5.705831250	9.859967214	10.550158963
78	7.066503535	9.324320951	7.286110529
78	8.495092592	7.154951585	6.709095656
78	8.502019080	10.371587858	10.915802285
78	5.730582901	11.143784281	8.306798056
78	9.398172271	7.859641970	10.303149525
78	10.055230415	9.211700725	7.337128265
78	7.331231003	8.255397243	11.723847225
78	11.035043104	10.131863484	11.342534235
78	10.797716535	11.139770964	9.007241568
78	6.885285049	7.573782019	9.303647108
78	8.199965264	11.312848574	8.434443163
78	8.372506998	5.550026782	8.699296496
8	5.614296808	8.929962252	12.294045628
8	4.446972675	11.042556377	9.707852157

8	9.715469155	5.965726904	9.932655272
8	10.139792497	7.768344837	6.042700094
8	11.053122764	8.266169895	11.281479768
8	11.642495080	10.323794057	7.525392941
8	6.564922176	7.266469589	7.306410109
8	9.339658892	12.040098347	10.068832586

PRE:3= -110.10829978

78	5.232792459	10.122433480	10.504433894
78	6.421913941	9.059584770	7.098706977
78	8.802077826	7.594664413	6.827839671
78	7.640726544	10.896388833	11.013279177
78	5.695230068	11.167451259	8.214005945
78	9.430304097	7.910105379	10.026657289
78	8.875722630	9.907799023	8.020511986
78	6.892379175	8.471396110	11.753039698
78	10.598643522	10.028900064	10.927961489
78	10.914437356	11.271108325	8.760722438
78	5.961209030	7.917656305	9.322452225
78	7.908287267	12.142119860	8.774436456
78	8.315069329	6.016357944	8.741063872
8	6.477702615	6.113022704	9.041261113
8	9.325760095	11.015942174	11.872117337
8	9.732798093	12.759627056	8.653695218
8	7.243825475	7.842444453	5.789014305
8	10.157329047	8.297573777	8.163139479
8	4.181103889	11.313526424	9.373533668
8	5.131213783	9.210184986	12.215963294
8	8.566065042	7.598987471	11.746859567

PRE:4= -109.42548663

78	5.097123454	10.331314219	10.280962522
78	5.839200407	9.110238999	6.814004591
78	8.020123842	7.779320270	6.505333453
78	7.509288869	11.309100226	11.295119891
78	5.320580901	11.521833854	8.046092125
78	8.788795618	8.503004143	9.856726912
78	8.907830032	9.744635213	7.676778868
78	6.758289687	8.714089143	11.418401476
78	9.941802734	10.404021157	10.938386213
78	10.134337550	11.573532412	8.758870266
78	5.507095587	7.791466222	9.201501707
78	7.752182388	12.544625313	8.859104454
78	7.784178748	6.589105602	8.669281233
8	6.007420821	5.920753197	8.981034906
8	9.164223680	11.508166131	12.296634945
8	9.491245614	13.393138073	8.728209502
8	6.416475377	7.868670970	5.440196551

8	3.990294857	8.905279653	9.620819727
8	5.640546449	11.812789657	11.365502852
8	5.950772610	13.173714869	8.762244440
8	4.326420391	10.258481954	7.032460645

## 6. Pt<sub>13</sub>O<sub>12</sub>

PRE:1= -128.09205576

78	5.140845644	10.225549478	10.420100438
78	6.144215843	9.393422005	6.838501214
78	7.994559425	7.731300618	6.340149914
78	7.593334710	11.111094329	10.885912619
78	5.359234101	11.422480157	8.141602501
78	8.859560921	8.699633618	9.418760546
78	8.686622916	10.110145271	7.239274458
78	6.957283515	8.657050676	11.356698746
78	10.060300995	10.594251186	10.818035889
78	10.212946295	11.724153686	8.662810010
78	5.876452265	8.062984548	9.089713662
78	7.733947845	12.248535701	8.526109560
78	7.755964842	6.512728861	8.434339854
8	3.578771400	10.663847019	11.082993967
8	4.344985878	7.199408651	8.846654823
8	7.351856562	12.495303924	11.970395178
8	8.209453457	4.831085004	8.626216206
8	11.418594152	10.470316696	11.912699387
8	8.635033159	7.779282284	11.196815464
8	4.165210865	12.465085596	7.398489044
8	7.635929130	13.947200633	8.025047530
8	5.174257288	9.485000950	5.360587526
8	8.513675209	6.798209238	4.940612479
8	11.724606207	12.547610337	8.296503969
8	10.138257619	9.945716974	6.174995499

PRE:2= -136.09157137

78	5.218200278	10.183102917	10.442243958
78	6.383295302	9.525454591	6.274410183
78	8.060197865	7.548882799	6.377812513
78	7.797883031	10.878437221	12.247308267
78	5.549429129	11.537468701	7.778724358
78	8.783694618	8.462138870	9.883227740
78	8.889969714	9.818101663	7.484076836
78	6.889518294	8.602761022	11.528318951
78	10.079472955	10.386133459	11.127399106



78	10.327031005	11.607883440	8.808737180
78	5.624233835	7.026818600	9.969278090
78	8.015936929	12.448003880	8.008973568
78	7.786481040	6.333504948	8.695477046
8	4.453737095	8.486748937	9.926425951
8	6.136529271	11.431983985	11.592546621
8	6.636628645	5.395779580	9.881446112
8	9.558034686	10.531806817	12.953994466
8	6.336034355	13.113620506	8.527055618
8	4.684412891	10.163650405	6.762344602
8	9.792287190	13.021392226	7.638294080
8	7.228565786	8.477286690	4.926998313
8	4.232566872	11.363643848	9.290996639
8	9.229069773	6.454261589	7.442822262
8	10.035872989	8.605656479	8.438821450
8	11.363778067	10.263711471	9.716283843

PRE:3= -135.32519462

78	5.271629399	10.194469859	10.262631731
78	5.883676003	8.766576822	6.701792567
78	8.243352595	7.502796027	6.344906773
78	7.757323187	11.243485716	11.198947455
78	5.732609285	11.288007767	7.982427288
78	9.571011609	7.967859726	9.918359231
78	9.809406556	9.349039827	7.372490572
78	7.349044603	8.668370575	10.856947036
78	10.292358089	10.256607210	10.979219103
78	10.493347738	11.509166188	8.711181589
78	5.729499719	7.631162496	9.063065135
78	8.034225117	12.598884966	8.965513033
78	8.053097375	6.271476197	8.627480360
8	4.252065328	8.743137475	9.595281099
8	5.883840426	11.661001788	11.314470366
8	6.191945866	5.843112935	8.571768976
8	9.447802728	11.611704566	12.016288853
8	6.196819686	12.979249365	8.710950500
8	4.600507021	10.123913774	7.014045081
8	9.820415635	13.200755966	9.226334260
8	6.471784428	7.244771316	5.723128395
8	9.921404990	6.289055345	8.988342405
8	11.301830875	8.736620255	10.412955526
8	11.511425250	10.134642034	7.893690223
8	10.126270745	7.676399028	6.436053572

PRE:4= -132.58975798

78	5.337274319	9.880483839	10.690496855
78	6.173029678	8.801887129	7.022436454
78	8.405825134	7.501425033	6.990597437
78	7.781653211	11.315048082	11.593542866
78	5.491922326	11.362015252	8.083829118
78	8.836390421	8.148157368	10.053217039
78	8.558555727	9.939524768	8.074971323
78	7.031881663	8.278830645	11.889362096
78	10.167008269	10.054594060	11.068773909
78	10.403294417	11.432993554	9.050168494
78	5.580108563	7.437749033	9.287383401
78	8.023835914	12.375899042	9.009196382
78	7.813422970	6.082434999	8.985170507
8	4.179857163	8.558220671	9.875168644
8	5.895666079	11.481102087	11.579629457
8	5.981232138	5.616929425	8.632013748
8	9.651923944	11.510861089	12.187015777
8	6.308590369	13.027455999	8.494449521
8	4.713290699	10.036783091	6.929914396
8	9.818656924	13.238679941	9.024470383
8	6.919720198	7.425120205	5.815852516
8	4.283186153	11.122618249	9.531303775
8	6.157369188	6.767876385	11.118821725
8	7.780593927	9.722955760	12.848271466
8	9.797845761	8.228509999	8.194819664

## 2. LM2

### 1. Pt<sub>13</sub>O<sub>1</sub>

PRE:1= -65.41371876

78	10.771919067	9.371991976	10.927060342
78	9.738941345	7.132264346	8.674061364
78	8.645004780	7.994635136	10.792389064
78	7.748938076	6.811649017	7.148477907
78	6.154493021	8.392652023	11.114465574
78	9.326029470	11.466150088	8.524344153
78	12.047862460	7.529291680	9.651789755
78	7.616156043	10.186284535	9.940720182
78	8.489586804	9.272506144	7.275644024
78	10.297250356	10.711107393	6.327780163
78	9.463152481	11.558906112	11.085042892
78	11.029302740	9.543423414	8.417431772
78	6.388417011	8.374324629	8.598280810
8	10.877629945	11.390975988	4.806572831

PRE:2= -64.91385507

78	10.541385491	9.449201230	10.767487812
78	9.770355465	7.145838465	8.626609250
78	8.470294474	7.967173761	10.680653075
78	7.832680658	6.865743246	6.978888679
78	6.044100036	8.590531951	11.255536740
78	9.499530329	11.321746313	8.693205954
78	11.896436646	7.499274298	9.897127656
78	7.481017653	10.279714688	9.986647476
78	8.522179502	9.248686201	7.474463454
78	10.206627945	10.740252610	6.334266054
78	9.275384174	11.603931893	11.190613485
78	11.367229238	9.341271689	8.155966237
78	6.587257170	8.058497383	8.841517281
8	13.026266754	9.708906074	7.576414327

PRE:3= -65.43910131

78	10.784239979	9.313074436	10.997018579
78	9.678105540	7.120808639	8.634685447
78	8.636656844	8.000737436	10.789693388
78	7.700398219	6.725238768	7.165073656
78	6.139258533	8.332408167	11.068507542
78	9.338003499	11.439617863	8.477390256
78	12.043076201	7.530316537	9.629778928
78	7.571861627	10.178716536	9.950473877
78	8.430919772	9.164421172	7.279675000
78	10.327478574	10.540870016	6.254891981
78	9.465071284	11.515131729	11.037859412
78	10.959269358	9.537141008	8.504354358
78	6.380837516	8.354915938	8.529751141
8	7.441555589	5.273743939	6.194395583

PRE:4= -64.53059064

78	10.773435139	9.343519166	10.982278691
78	9.734977535	7.139584267	8.677491837
78	8.643174449	8.005914330	10.812170246
78	7.765370107	6.823049290	7.164696120
78	6.158896636	8.375166177	11.109049367
78	9.197340413	11.488132901	8.461720462
78	12.018360435	7.556358521	9.681224537
78	7.597672293	10.183762211	9.966645294
78	8.472432656	9.275548714	7.358398529
78	10.351806923	10.547943669	6.217802526
78	9.502928163	11.524124279	11.083829838
78	10.975676708	9.602568396	8.473807763

78	6.368866887	8.347674708	8.598353169
8	8.900308009	13.162131295	7.874776762

PRE:5= -65.03575062

78	10.798329812	9.387725701	10.994012108
78	9.712503762	7.160555929	8.674200774
78	8.684644124	7.978949857	10.853154478
78	7.695183225	6.592412836	7.284182311
78	6.216983906	8.532993539	11.206453320
78	9.442266176	11.498428211	8.520385295
78	12.007392904	7.496104100	9.718931417
78	7.702640671	10.119107599	9.811720280
78	8.097196274	9.092562546	7.012646182
78	10.241621504	10.487384002	6.285283893
78	9.408596403	11.543799492	11.064285696
78	10.967330044	9.493937494	8.492168886
78	6.362866697	8.216644086	8.719148488
8	8.888042652	9.550724406	5.327774590

PRE:6= -65.33126948

78	10.504641675	10.117595350	10.497274302
78	9.340346375	7.689642374	7.754074781
78	8.649841090	8.333538499	10.429029858
78	7.453796156	7.353928993	6.085838438
78	6.154495987	8.678634931	10.773246323
78	9.237043803	11.682928857	8.054835068
78	11.026603621	7.657169759	9.654064246
78	7.440997197	10.413252789	9.426802905
78	8.028263741	9.729740067	6.789659393
78	10.070526265	10.824672929	5.797436592
78	8.952081938	12.113065548	10.542339527
78	11.073149517	9.640650035	7.819422954
78	6.643548114	8.123999466	8.363529323
8	12.029338989	10.344118342	9.334160866

PRE:7= -65.56543150

78	10.411009340	9.606420902	10.539912007
78	9.558654875	7.455532417	7.963907623
78	8.321607635	8.269654861	10.008905341
78	7.550677301	7.168370798	6.433536087
78	5.970305236	9.081238349	10.783799382
78	9.305707551	11.668933510	7.949312181
78	11.610578492	7.631638261	9.453831116
78	7.375421417	10.577284623	9.333061765
78	8.089668359	9.576631050	6.852318100

78	9.888697802	10.791549674	5.581537608
78	9.212621229	11.858788878	10.495546156
78	11.083560389	9.748055347	8.119103709
78	6.337962584	8.278258992	8.382565610
8	11.538797754	10.187082986	6.274366524

PRE:8= -65.12603612

78	10.492568455	9.648360081	10.264360341
78	9.303743213	7.221930154	8.215519917
78	8.325565525	8.371284727	10.236726812
78	7.471936946	7.163250316	6.459924687
78	5.862458285	8.867628810	10.704114689
78	9.196179983	11.708020025	8.051542567
78	11.631884517	7.633960719	9.118404013
78	7.304508269	10.590380030	9.449940419
78	8.283955262	9.509352306	6.954473656
78	9.795544512	11.118575519	5.645029342
78	9.215472126	11.838063765	10.580253204
78	10.879135680	9.860301452	7.588557169
78	6.281970276	8.510671532	8.237103585
8	12.337164112	8.588582331	7.616455204

PRE:9= -65.04751555

78	10.548377345	9.679175170	10.455228770
78	9.487860923	7.392134246	8.160146668
78	8.407119956	8.375015584	10.245883659
78	7.554058544	7.085412816	6.623444709
78	5.929013274	8.756109299	10.661201369
78	9.165033253	11.761695343	8.019778505
78	11.787362541	7.802971327	9.164919139
78	7.318141464	10.527741347	9.390459353
78	8.206945733	9.552360121	6.886909215
78	10.033077651	10.919561553	5.751850855
78	9.269110095	11.864978488	10.559988724
78	10.761896433	9.821594938	7.954337960
78	6.017073207	8.682519510	8.145232004
8	5.745893285	6.954892907	7.214777836

PRE:10= -65.35208210

78	10.457305404	9.608026873	10.470963278
78	9.565464387	7.307896079	8.084067335
78	8.313413075	8.312434062	10.011010268
78	7.606656940	7.021943818	6.545922099
78	5.937727592	9.043823508	10.775941954
78	9.257407679	11.797133044	8.028824871

78	11.760051126	7.781815259	9.247288560
78	7.323128834	10.593603167	9.330289596
78	7.983755163	9.869208090	6.699678230
78	10.042173562	10.974815449	5.762426230
78	9.180552970	11.824485591	10.580027545
78	10.671027004	9.754363942	7.953218970
78	6.335880396	8.321023975	8.376838632
8	7.316345022	8.559559851	5.464642245

PRE:11= -64.96667022

78	10.536179466	9.703113539	10.430706941
78	9.455754056	7.468168373	8.149714555
78	8.429665466	8.304540026	10.304536215
78	7.469266532	7.017634611	6.688461937
78	5.944509483	8.757336405	10.669654039
78	9.173344186	11.810790515	8.114686288
78	11.753491193	7.815921543	9.169450631
78	7.411453812	10.494729049	9.433816645
78	7.971812381	9.510127022	6.533627915
78	10.083008072	11.121347184	5.820343083
78	9.209518506	11.872910233	10.627501404
78	10.715901024	9.800435346	7.917988553
78	6.194679619	8.623875993	8.173407910
8	8.542993769	10.407425575	4.927609444

## 2. Pt<sub>13</sub>O<sub>2</sub>

PRE:1= -70.54167316

78	10.446923107	9.262829243	10.661324540
78	9.776842945	7.098488009	8.417881250
78	8.329415609	7.824463608	10.388051825
78	7.722962626	6.658286155	6.985562919
78	6.007401641	8.449762184	11.194087649
78	9.294848659	11.272538433	8.461806193
78	11.914077478	7.412260168	9.691787868
78	7.358830717	10.176668653	9.837752167
78	8.352651337	9.102110048	7.345653620
78	10.036465296	10.559481227	6.133396251
78	9.213211603	11.458123552	10.984651599
78	11.208247794	9.355652905	8.109855382
78	6.334772726	8.089981828	8.657545197
8	4.686389874	7.844735419	7.985158987
8	12.810477802	10.138474229	7.830268939

PRE:2= -72.18202567

78	10.482021135	9.069956631	10.858699195
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78	9.459910144	6.844600254	8.534558768
78	8.369286602	7.715384807	10.660176295
78	7.480775403	6.531490885	7.065453785
78	5.925672267	8.083500380	10.972270496
78	9.164502222	11.204839439	8.372361052
78	11.770666785	7.257891702	9.549165531
78	7.317316730	9.933695661	9.838605759
78	8.166041283	8.961073106	7.200316021
78	10.042125115	10.311034787	6.134326251
78	9.184782549	11.290299888	10.920972372
78	10.714516698	9.246470714	8.362913705
78	6.154750923	8.044102733	8.521380445
8	4.681214911	7.651726037	12.128471481
8	7.081934164	5.110108728	6.112542004

PRE:3= -71.90146232

78	10.616115621	9.250239603	10.844965473
78	9.558179437	7.027545275	8.517409443
78	8.484232672	7.888717173	10.642195334
78	7.578196638	6.696375328	6.999114548
78	5.994692582	8.293731792	10.939327646
78	9.156604746	11.361380807	8.322163095
78	11.872191779	7.436806267	9.481027940
78	7.479971938	10.109072605	9.814728071
78	8.315008334	9.148525855	7.130739698
78	10.194806011	10.447790282	6.143496482
78	9.392458605	11.446829485	10.869285938
78	10.831642273	9.444260928	8.322951523
78	6.228164880	8.261419289	8.446313569
8	10.847443149	10.845335788	4.565027835
8	9.528579787	12.631866743	12.152392503

PRE:4= -70.42741649

78	10.842075090	9.381122908	11.162676530
78	9.566204149	7.168359637	8.580887550
78	8.632624486	8.254409132	10.689964292
78	7.688998821	6.894582825	6.923642173
78	6.130499865	8.636872107	11.121179846
78	9.156496013	11.660581642	8.369138128
78	11.827911059	7.492615698	9.530586413
78	7.383761398	10.354264469	9.688950472
78	8.337859263	9.318259192	7.373561819
78	10.261968069	10.353536313	6.199424753
78	9.391257305	11.364173599	10.885133099
78	10.855369259	9.623500870	8.540094787

78	6.361453570	8.167592407	8.647117282
8	12.152508246	8.937387556	12.270178812
8	9.157199978	13.193786698	7.508361171

PRE:5= -71.42849031

78	10.624521629	9.398152931	10.598901889
78	9.470201918	7.236323923	8.589470963
78	8.568571366	7.946839933	10.970140347
78	7.714489978	6.813294784	6.786563530
78	6.056994322	8.552269861	10.915312968
78	9.339915248	11.383946376	8.149162730
78	11.857412897	7.443890420	9.421916258
78	7.642470168	10.007448996	9.574144037
78	8.353030182	9.234730462	7.014309800
78	10.247864863	10.432841817	5.928391918
78	9.280172745	11.538706528	10.734959787
78	11.009186922	9.448078955	8.099899657
78	6.367467025	8.088436240	8.463734574
8	8.517771751	6.836899589	12.371350906
8	10.842698984	10.893723781	4.356616466

PRE:6= -71.35672053

78	10.602598554	9.323343235	10.728686077
78	9.638194084	6.994627070	8.611725906
78	8.468631482	7.966093826	10.668745318
78	7.894279569	6.638599324	6.858712419
78	6.012808128	8.460260859	11.107843653
78	9.236596690	11.385185234	8.411200172
78	11.894653215	7.324894076	9.646413596
78	7.380671511	10.122727402	9.755228014
78	8.376247686	9.080129096	7.409493943
78	10.012079326	10.547098562	6.124915509
78	9.227255618	11.438255714	10.944738183
78	11.164115344	9.762221201	8.242958309
78	6.143720064	8.148650221	8.630914782
8	6.043260164	7.116423977	7.029943567
8	12.709397245	8.644027506	8.511405190

PRE:7= -71.29048820

78	10.438708351	9.022358746	10.860433541
78	9.646929309	6.683533970	8.407503298
78	8.351593113	7.734126700	10.263157692
78	7.613399074	6.444695276	6.934633229
78	5.986588369	8.231278043	11.224693275
78	9.304040969	11.224052834	8.416001731



78	11.779070707	7.198759920	9.665452890
78	7.217413884	10.288320549	9.677612662
78	7.962368223	9.324808615	7.225184225
78	10.049188565	10.325559286	6.150137251
78	9.223580285	11.253741700	10.956925366
78	10.700818180	9.157649170	8.360443298
78	6.332669485	7.701296987	8.745050511
8	5.833721291	10.122368244	11.036594193
8	7.451661921	8.016579541	5.887353014

PRE:8= -71.53608694

78	10.942639336	9.085427193	10.946582934
78	9.491765843	7.050009300	8.449379061
78	8.682802742	7.944999038	10.683747344
78	7.521984679	6.678017075	6.936036152
78	6.219459901	8.434196896	11.099162976
78	9.290311474	11.459155293	8.350351952
78	11.824170969	7.271129276	9.397546273
78	7.576161724	10.060389066	9.630229347
78	7.947415709	9.204797527	6.959347680
78	10.239539680	10.402689274	6.177402032
78	9.088813435	11.669951809	10.862833399
78	10.772321747	9.393503933	8.441154982
78	6.303552275	8.072080158	8.631099440
8	8.760711234	9.634315877	5.260561290
8	10.502553729	10.787350080	11.771371424

PRE:9= -71.46432543

78	10.703880422	9.370558978	11.159672260
78	9.511571398	7.259769662	8.661084025
78	8.430752205	8.291034088	10.908991134
78	7.790382238	6.739247586	6.886901360
78	5.904397570	8.601077209	11.124062598
78	8.933026871	11.411162542	8.276391993
78	11.815995339	7.380263901	9.487795328
78	7.306669248	10.421554188	10.023534524
78	8.465645747	9.192691795	7.116430419
78	10.368492049	10.735199728	6.292903823
78	9.485400962	11.509303682	10.913332534
78	10.881695163	9.661132706	8.535842166
78	6.776302894	8.122778380	8.743803861
8	12.238225922	8.191480073	11.172417844
8	7.356998452	12.187656340	9.183447189

PRE:10= -71.56058050

78	10.557937780	9.335047182	10.701930114
78	9.654807163	7.230064493	8.381630145
78	8.235708691	7.663866627	10.600807578
78	7.687643062	6.607619445	6.885954897
78	5.968807581	8.819461320	10.983231267
78	9.396926195	11.519837774	8.354085053
78	11.910621106	7.488297090	9.467786096
78	7.696398685	10.080978721	9.591757795
78	8.142409322	9.082520942	6.922619424
78	10.170137551	10.685899576	6.070565984
78	9.304268533	11.538206766	10.881725875
78	11.016870915	9.515027448	8.213099552
78	6.515866778	7.878518743	8.717325558
8	9.720652309	7.971540014	11.784125326
8	8.696751860	9.806712996	5.230176172

### 3. Pt<sub>13</sub>O<sub>3</sub>

PRE:1= -77.77845815

78	10.714039095	9.483577244	10.813335917
78	9.525381250	7.310383522	8.638744317
78	8.616408639	8.028599354	10.979397623
78	7.692691434	6.887874931	6.926642733
78	6.092056876	8.601250023	10.969816920
78	9.266991919	11.533016210	8.263333669
78	11.887541405	7.569497898	9.491802141
78	7.660355957	10.161467149	9.734844787
78	8.382600681	9.317620862	7.152107108
78	10.263051787	10.561535544	6.086681566
78	9.427078409	11.644848710	10.821492507
78	10.976295993	9.611762615	8.295001411
78	6.335057344	8.261621410	8.505405069
8	8.567074043	7.105354127	12.505238355
8	10.878737620	10.940244383	4.498821513
8	9.457844264	12.835877723	12.103479664

PRE:2= -77.31900461

78	10.630452412	9.486393483	10.546015158
78	9.565076386	7.192233864	8.277307716
78	8.482033272	8.222744270	10.323072744
78	7.573340288	6.884226917	6.818870881
78	6.019460469	8.311947555	10.771005042
78	9.111845820	11.514725805	8.194997775
78	11.865201592	7.600267041	9.275855288
78	7.277986188	10.421353379	9.746935972

78	8.352567253	9.314110675	6.838241338
78	10.181603085	10.842771729	6.016055141
78	9.389065249	11.678802639	10.733088066
78	10.870811612	9.645086478	8.054650792
78	6.345199156	8.456944009	8.269032222
8	10.748286245	11.492260359	4.489828786
8	7.174983229	5.481407735	5.851618528
8	5.996448938	11.669255321	9.968461543

PRE:3= -76.06748660

78	10.624872935	9.466410746	10.825608937
78	9.621273488	7.342077251	8.268233351
78	8.454159713	8.219930861	10.316853962
78	7.586481008	6.997151964	6.837800485
78	6.022658646	8.579738933	10.859240645
78	8.967681565	11.765571203	8.110306479
78	11.863903749	7.747790393	9.302895143
78	7.243231127	10.435583189	9.512019837
78	8.135159097	9.486427049	7.017689228
78	10.115719058	10.670589709	5.908230577
78	9.223111800	11.517106125	10.652535679
78	10.704411969	9.759499422	8.163204650
78	6.059925992	8.496764288	8.265708329
8	8.814241506	13.374322432	7.388531836
8	4.416450562	8.424080566	7.602173073
8	12.059650794	9.040531640	11.811460970

PRE:4= -77.53763271

78	10.704294126	9.772473707	10.522161996
78	9.546961302	7.396934374	8.371418899
78	8.547905569	8.548494647	10.371122956
78	7.344724624	6.841534226	7.265388167
78	6.107265987	8.301521164	10.575876751
78	9.136581538	11.401127259	8.171060472
78	11.863595907	7.840910512	9.361200616
78	7.208540806	10.773490110	9.948704545
78	8.153993226	9.062721666	6.413292325
78	10.012969895	10.855059815	5.830908817
78	9.345593746	11.932619788	10.641345690
78	10.916624854	9.660595715	7.933030415
78	6.319947818	8.999517622	8.111083551
8	8.887925953	9.700614767	4.769796404
8	5.615283744	10.665578889	8.842802577
8	13.164124632	6.741468742	9.714150370

PRE:5= -77.64137890

78	10.482617591	9.745350331	10.512076407
78	9.772271609	7.445247472	8.141213599
78	8.464188056	8.257050971	10.193885681
78	7.782303487	7.241090018	6.624634163
78	5.975903614	8.663617737	10.550028004
78	9.070529303	11.942329647	8.015805077
78	11.908771652	8.018878073	9.305041188
78	7.289645291	10.464991019	9.345860049
78	8.063755481	9.734291412	6.840845667
78	10.023588470	10.870845277	5.742863678
78	9.050468919	11.844488929	10.561783681
78	10.646642485	9.924493859	7.999149668
78	6.079078964	8.591841651	8.023700649
8	9.459117249	6.199903661	6.708105894
8	8.950328559	13.513827852	7.199151465
8	4.811035858	8.544638738	11.850912352

PRE:6= -77.51602669

78	10.687270383	9.231904870	10.816520131
78	9.669798982	7.316421716	8.492480396
78	8.391881658	8.002139400	10.759232942
78	7.469742193	6.741820949	7.250597439
78	5.800913299	8.147871826	10.801423243
78	9.088850368	11.326180007	8.562951712
78	12.093857199	7.663049175	9.387219347
78	7.252579726	10.225213532	10.491465837
78	8.537220639	8.970216863	6.746062079
78	10.076915436	11.039316318	6.245439408
78	9.536131795	11.465813456	11.067603830
78	10.916298054	9.636909709	8.296716720
78	6.668762528	8.800296925	8.493741039
8	8.954808036	6.319272473	9.994795903
8	8.685942648	10.190434538	5.255313345
8	7.679384523	11.821144171	11.503900393

PRE:7= -77.54659261

78	10.532933721	9.429196406	10.702659218
78	9.700324094	7.335336465	8.297565517
78	8.378832132	8.196214401	10.294945432
78	7.895870053	6.918037252	6.651854189
78	5.907046397	8.593788231	10.821035611
78	9.268494343	11.606327412	8.203420631
78	11.926563921	7.691893148	9.440547286
78	7.237614643	10.434109419	9.537743051

78	8.206850626	9.426236813	7.233495787
78	9.921865804	10.750968335	5.844932786
78	9.273776579	11.607716530	10.789171371
78	11.175562381	9.791064688	8.266943007
78	5.995676286	8.466360956	8.338700239
8	11.663139385	10.423184708	6.515755690
8	6.012242550	7.235252479	6.907325478
8	7.374293261	11.888924493	10.860170164

PRE:8= -77.21123696

78	10.577915715	9.641714195	10.451147897
78	9.390784026	7.394930852	8.639073868
78	8.296208863	8.082712741	10.821181234
78	7.468503957	7.066570343	7.135853092
78	5.859075879	8.377947272	10.542504509
78	9.072354043	11.765252537	8.331517060
78	11.808526811	7.700456739	9.322686046
78	7.448514891	10.408079204	9.778953795
78	8.344398647	9.515479903	6.912951912
78	10.145261084	10.915303705	5.726814420
78	9.313504227	11.807544849	10.834475250
78	10.784092219	9.608035132	7.902562897
78	6.092521307	9.037816887	8.135805509
8	9.481309860	12.468398240	6.606409141
8	6.466343313	9.672348317	6.318349787
8	9.766116931	8.594882574	11.897186925

PRE:9= -77.36782562

78	10.523281912	9.584624599	10.817758427
78	9.485942206	7.383225634	8.141730957
78	8.377943346	8.318350796	10.236131971
78	7.533793701	6.845610819	6.658958084
78	5.871889062	8.559265893	10.704308571
78	9.097475205	11.584619344	8.143972155
78	11.834402462	7.567893563	9.093657529
78	7.209602665	10.559818351	9.784283347
78	8.332235016	9.242334516	6.521260997
78	10.140996313	11.016881828	5.879605902
78	9.338524242	11.760428339	10.684050704
78	10.760714817	9.720974951	8.125465013
78	6.529630547	8.647808415	8.224926798
8	8.531892356	10.399422926	4.990241592
8	7.451891108	12.197818797	10.807405748
8	12.031911876	8.385580347	10.832666851

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PRE:10= -78.41804626
78 10.564382585 9.762181077 10.497454200
78 9.722990270 7.361960455 8.226993525
78 8.781548014 8.005362476 10.510462588
78 7.468930848 7.316328509 6.984306087
78 6.016857088 8.556928639 10.304696625
78 9.072258084 11.943447954 7.696146481
78 11.937063281 8.015997591 9.218859378
78 7.474640415 10.345967632 9.257809178
78 7.939760397 9.813136237 6.722649678
78 10.045804848 10.711264914 5.665619994
78 8.965737756 11.740978093 10.775184038
78 10.506540044 9.837912654 8.006537613
78 5.758692549 8.985367073 7.816900894
8 9.074395301 6.220612253 6.822298433
8 8.941377481 12.987462743 9.307070840
8 7.154844218 7.358686373 11.254899742

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#### 4. $\text{Pt}_{13}\text{O}_4$

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PRE:1= -84.89537895
78 10.684308762 9.316057982 11.000108456
78 9.623568911 7.118492590 8.653755877
78 8.557436378 7.962952489 10.788329242
78 7.640942830 6.742859342 7.205577369
78 6.117713595 8.313072759 11.078159359
78 9.271560058 11.468480505 8.461461033
78 11.965023057 7.534773281 9.624241456
78 7.534442611 10.214571889 10.018832850
78 8.406818659 9.175449435 7.260956267
78 10.291491956 10.526809547 6.287066025
78 9.464441949 11.517831448 11.039076234
78 10.905274458 9.527909379 8.473248323
78 6.323437963 8.326733895 8.611283652
8 7.237052966 5.344422905 6.243687435
8 4.859947085 7.876459561 12.214884911
8 10.938974620 10.943385464 4.716089266
8 9.639919317 12.732744151 12.283795870

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PRE:2= -84.14069908
78 10.764585879 9.282062681 10.996215989
78 9.825565151 7.154688665 8.553535153
78 8.602873202 7.973823645 10.607657804
78 7.788197010 6.811653960 7.106768883
78 6.194338403 8.453101211 11.160796339
78 9.343590155 11.495063543 8.375521525

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78	12.061173302	7.573940840	9.615936545
78	7.611691483	10.231812354	9.856320288
78	8.376513912	9.298974519	7.285748694
78	10.307322233	10.514422701	6.235961064
78	9.548773710	11.511587353	10.923664626
78	11.065071450	9.553872458	8.434006889
78	6.321784795	8.291073026	8.615680695
8	4.695854094	8.259408589	7.924093537
8	10.993223939	10.976072242	4.693371495
8	13.444615418	6.533382539	9.790324354
8	9.663853068	12.712133788	12.188120106

PRE:3= -82.14870556

78	10.903786581	9.473298038	11.096022148
78	9.700118949	7.340222139	8.625820351
78	8.751248039	7.958389465	10.948375619
78	7.746868551	6.845048094	7.133063570
78	6.271739766	8.608869947	11.192463617
78	9.509999965	11.673888267	8.559240912
78	11.965235362	7.605611028	9.749612669
78	7.828872660	10.081559564	9.758202209
78	8.111463715	9.411930486	7.126843067
78	10.199312881	10.746646386	6.271896959
78	9.382680066	11.522907764	11.124899203
78	11.017242885	9.535594977	8.371141005
78	6.383553473	8.253562047	8.715481688
8	8.848943936	9.756963934	5.378472881
8	8.838561699	6.595827264	12.113237389
8	11.760310192	9.789582959	12.633367835
8	9.324301921	13.425636891	8.208960999

PRE:4= -84.60636588

78	10.912035081	9.259516720	11.153838684
78	10.343782506	6.928928000	8.659168996
78	8.794235129	8.323443918	10.103819600
78	7.960104731	7.094650210	7.714166415
78	6.239697023	8.435331093	10.657106931
78	9.607143854	11.434210162	8.601977518
78	12.340152113	7.506862753	10.055005425
78	7.466010360	10.824811068	9.938930340
78	7.890537076	9.652352810	7.563866747
78	9.833881772	10.430077485	6.204471430
78	9.552024194	11.433523784	11.155223851
78	11.249466144	9.425724512	8.631817448
78	5.822576185	8.294690916	8.170449126

8	9.417054091	5.896680488	7.310405553
8	6.015750345	10.288202518	11.092429896
8	11.539539617	9.798887690	6.743335397
8	11.130536689	10.936266328	12.168402552

PRE:5= -82.74494517

78	10.340219174	9.629778829	10.694111737
78	9.429803674	7.232068771	8.174229005
78	8.380237234	8.202952367	10.345537683
78	7.577327896	6.995366050	6.416124706
78	6.013871475	8.570738695	11.213886255
78	8.824336391	11.540305475	8.364686039
78	11.502798387	7.658976187	9.491870792
78	7.118225409	10.613978112	10.127810974
78	8.416517909	9.316021823	7.104095738
78	10.308118568	10.843600995	6.077107170
78	9.600342099	12.050630457	10.743345045
78	11.221401267	9.929771649	8.191202196
78	6.449877413	8.482498694	8.701297562
8	11.913516941	10.599344006	9.869013311
8	7.760693286	12.195903834	11.122408028
8	8.331552531	11.257247296	6.441940737
8	5.877124699	7.472083432	7.164125790

PRE:6= -85.08948179

78	10.718039697	10.230853350	10.632561933
78	9.330449769	7.374509752	8.629294459
78	9.433961852	8.099905305	11.062260246
78	7.193342959	8.092789813	7.262463732
78	6.938950243	8.124958455	9.907861927
78	9.367273390	11.779152147	7.851899868
78	11.591739229	7.838780975	9.688950068
78	6.550609413	10.604842210	9.908677060
78	9.390301450	9.394644777	6.995897222
78	10.762783478	11.229297356	5.837562841
78	8.861024463	11.769777960	10.266585770
78	11.525569351	10.335065429	8.138841897
78	5.235425986	9.224257826	8.298185886
8	12.794352984	9.019557004	8.772637652
8	7.690623139	7.502459323	11.597739400
8	9.038116455	7.418015002	6.600696402
8	7.165912465	11.993015700	11.084791836

PRE:7= -83.64102298

78	10.908850047	9.823481274	10.813935951
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78	9.689351013	7.500301780	8.365554015
78	8.701554767	8.701710111	10.463297174
78	7.909851197	7.081763950	6.681684348
78	6.234114909	8.653155454	10.800819252
78	9.412556306	11.738641494	8.052918390
78	12.072413816	7.658772444	9.135980291
78	7.261681298	10.521793059	9.219024557
78	8.025219797	9.692003945	6.871949665
78	10.496310090	10.772673554	5.921694453
78	9.476508255	11.828513092	10.619274085
78	10.968784708	9.790888457	8.195672447
78	6.263327112	8.306546627	8.089092832
8	4.964445225	8.095759843	9.446154877
8	7.568549831	12.073146702	10.373714239
8	8.912907641	10.046042228	5.159290217
8	12.469079292	8.645870564	10.744282379

PRE:8= -83.66521020

78	10.366190242	10.400516207	10.276851839
78	9.712188280	8.122882095	8.628141711
78	8.475694385	8.750616133	10.752376337
78	8.089511756	7.189578464	6.835900135
78	5.874591482	8.451583112	10.271294408
78	9.324058934	11.598514045	8.092763972
78	11.982073991	8.568748009	9.632748180
78	7.309231840	10.603180295	9.354166263
78	8.904898646	9.619040693	6.392822210
78	10.338102380	11.591101270	5.775305719
78	8.774984236	12.359178565	10.490901680
78	11.348817331	9.939033733	7.529580088
78	6.463754844	8.989588983	7.595361173
8	4.873756510	8.629137137	8.663185226
8	13.083578202	10.222039414	7.144619107
8	6.952157496	8.277113375	11.838314953
8	8.520945500	8.093189974	5.204454378

## 5. Pt<sub>13</sub>O<sub>8</sub>

PRE:1= -107.70293311

78	10.826705054	9.243280368	11.000644617
78	9.876533645	6.480817110	8.775458696
78	8.708691993	8.000175685	10.536797896
78	7.799828667	6.568371537	7.292711883
78	6.309669222	8.224237974	11.183042938
78	9.319873974	11.100695768	8.641312032
78	12.025630603	7.489577932	9.636677074
78	7.385243964	10.387249838	10.330077817

78	9.158265421	8.745811570	7.635805243
78	10.508783624	10.496007966	6.427392311
78	9.705666715	11.474122206	11.107571180
78	11.632810497	9.825960057	8.593317113
78	6.792859982	8.368821099	8.719183894
8	5.141224935	7.752683486	12.399214463
8	7.234067384	5.453621324	6.082663937
8	13.381562766	6.439617784	9.984229481
8	9.877362785	12.730978314	12.300437840
8	10.832063549	10.999519967	4.789434940
8	13.330200580	10.296359518	8.342716370
8	6.459588689	11.881531296	10.628027566
8	10.337807071	4.784814317	8.560145916

PRE:2= -106.48223870

78	11.148003989	9.183068217	11.317656661
78	10.069746559	6.703988290	8.745608767
78	8.958642118	7.835922696	10.941639731
78	7.990657259	6.477040488	7.215179860
78	6.386189423	8.091845134	11.095225437
78	9.665544463	11.357745060	8.464410152
78	12.305202854	7.385181726	9.993023046
78	7.666520927	9.942155657	9.864188431
78	8.791841753	8.909783122	7.685865749
78	10.549567926	10.281806493	6.408090982
78	9.670263989	11.224464712	11.070279314
78	11.201316979	9.185330891	8.629508655
78	6.595817617	7.890686907	8.612944450
8	10.410521187	4.948268659	8.817546761
8	7.654155984	5.244433091	6.020477124
8	8.948439058	6.491857410	12.118900355
8	7.769904615	11.336608004	11.256995713
8	12.079161300	9.426924931	12.805161585
8	9.450235999	13.118614114	8.367892707
8	11.255646804	10.586842851	4.840611928
8	13.733297703	6.380638063	9.897038145

PRE:3= -106.60769610

78	11.101991107	8.970886663	11.102879740
78	10.096370279	6.675088555	8.700894478
78	9.008642062	7.626567166	11.285674209
78	8.004482952	6.463525704	7.333308490
78	6.558985603	8.113526091	11.290751011
78	9.832574188	11.306298017	8.595578163
78	12.366839990	7.180031538	9.854911341
78	8.024141768	9.868408666	10.150221052
78	9.040376415	8.853264092	7.725287790
78	10.668894315	10.291626916	6.412374125
78	9.893388055	11.137861605	11.209607630
78	11.563273857	9.300984870	8.569540092
78	6.809863314	8.005996008	8.820802830

8	7.650007336	5.107555156	6.283242815
8	5.251943140	7.710496072	12.371383011
8	11.323614631	10.599133058	4.819231517
8	10.016790937	12.371423530	12.441179730
8	10.642637046	4.963577528	8.920542653
8	9.249091471	6.104947950	12.168817206
8	9.447327972	13.032760848	8.388776001
8	13.275367545	9.920869222	8.641874459

PRE:4= -109.78286123

78	11.350257729	9.265516195	11.180481700
78	10.084289718	6.607980383	8.906547827
78	9.432295016	7.645944370	11.218903741
78	8.102884399	6.438361351	7.452032174
78	6.425239301	7.959103475	11.243249028
78	9.960273339	11.698890676	8.858575016
78	12.473485914	7.360287358	9.597179644
78	7.755810123	9.623229631	9.835140143
78	8.995946696	8.775604323	7.771054467
78	10.541538134	10.403995478	6.334850822
78	9.656440773	11.083403390	11.264453311
78	11.407289993	9.619307281	8.646293042
78	6.221518525	7.751224407	8.697839348
8	6.207077549	6.592060057	7.186387001
8	4.941727479	8.296668063	10.036493833
8	9.755966882	8.797261634	5.858045314
8	7.790247100	10.929101692	11.321765632
8	11.746476154	5.652805866	9.145541647
8	7.912727368	7.435804387	12.327000614
8	10.576027396	12.146372444	7.056001438
8	13.083543087	9.128765332	10.156083497

PRE:5= -107.33320504

78	11.188052346	8.961239527	11.246232653
78	10.254748990	6.731925458	8.815124793
78	9.024863008	7.646578907	11.254514151
78	8.162911131	6.387126391	7.419905128
78	6.589038368	8.005940721	11.414674576
78	9.611319073	11.346329267	8.573156642
78	12.518594416	7.377349824	9.842146105
78	7.952738876	9.829788021	10.197849143
78	8.769343343	8.833481695	7.572969661
78	10.678991607	10.243715630	6.483148967
78	9.888879376	11.105489761	11.275478709
78	11.356681781	9.311022281	8.692411420
78	6.830318809	7.805663671	8.951990557
8	7.734787213	5.029423278	6.409586180
8	5.291570876	7.631525568	12.509299399
8	11.431076164	10.526138614	4.920684582
8	10.062873021	12.337055086	12.512638949
8	9.944048363	13.088443485	8.511689419

8	13.885960858	6.295130973	10.035363863
8	7.831066211	10.606937537	8.160944529
8	9.772004143	6.048785492	10.580552111

PRE:6= -107.11690913

78	11.041052276	9.093238920	11.467560972
78	10.228077509	7.346703754	8.733814043
78	8.847085779	7.873870839	10.805982303
78	8.088185663	6.506780613	7.626635920
78	6.502304407	8.196310990	11.626250494
78	9.534212663	10.969797192	8.916479495
78	12.286746197	7.247376660	10.162713531
78	7.602628741	10.241505341	10.589670023
78	8.600393303	8.971466389	7.498534401
78	10.579742030	10.269316902	6.687122583
78	9.800244377	11.296918024	11.419882011
78	11.655951811	9.501868405	8.853391205
78	6.724443083	8.188570963	9.101136314
8	11.988254880	9.169187848	12.970117459
8	13.358994060	9.998748709	8.937011548
8	11.095741928	10.834517751	5.120363997
8	10.119533834	12.595825397	12.553979312
8	6.593256496	11.710318497	10.732122962
8	5.347206755	7.646960927	12.817805701
8	5.120217284	8.118482573	8.356629107
8	7.719914954	5.180460955	6.549517842

PRE:7= -109.66379316

78	10.753078531	9.090645787	11.203741051
78	10.423529235	6.091777455	8.750832456
78	8.876898238	7.611888489	12.142631853
78	8.155940211	6.886841147	7.638598878
78	6.541265930	8.174590708	11.214814551
78	9.433855039	11.402467151	8.745634506
78	12.290101986	7.432497177	10.008078988
78	7.880574289	10.446441970	10.526225942
78	8.970347288	9.444570483	7.205491144
78	10.828359160	11.031344766	6.614578216
78	9.984090269	11.437551375	11.569396462
78	11.482675026	9.440559725	8.791812920
78	6.798182378	8.894464708	8.678041833
8	7.146034814	6.827698470	12.396833915
8	8.935716076	5.223750426	7.958747352
8	5.942936094	9.799544426	10.212077419
8	7.226230496	8.449092944	6.804625531
8	10.702330269	7.653227045	12.568114235
8	12.141664486	5.641490956	9.419975561
8	12.431450085	10.426289575	7.408121247
8	10.024488236	12.661709501	10.120605109

## 6. Pt<sub>13</sub>O<sub>12</sub>

PRE:1= -127.68826666

78	10.999100267	9.097999611	11.703503963
78	9.984674599	6.679149233	9.196483395
78	8.899966787	7.611042914	11.364150239
78	7.867523013	6.533258374	7.745950639
78	6.412052043	8.114392105	11.588881448
78	9.481566856	11.375685123	8.872375042
78	12.199568759	7.335884207	10.351416638
78	7.636216384	10.045226335	10.372246810
78	8.564651491	9.105640816	7.795345412
78	10.599620304	10.380060224	6.842314957
78	9.699113825	11.229493673	11.448260268
78	10.933188239	9.132948767	9.033906702
78	6.462173557	8.041544136	9.104108835
8	7.528378267	5.081907049	6.823817220
8	4.810308079	7.991292397	8.483784991
8	5.143319736	7.691593732	12.720681811
8	7.642478839	9.301481767	6.246242542
8	10.259974691	4.925057618	9.093037239
8	8.983629979	6.311912974	12.563648087
8	6.709687329	11.361083485	11.220872673
8	9.954220028	12.360010985	12.767896825
8	11.940024185	9.288670286	13.182411906
8	9.348469697	13.132424487	8.695947738
8	13.649340244	6.352863377	10.290999998
8	11.291731797	10.675417166	5.268200506

PRE:2= -134.18033379

78	11.361941184	9.132313549	11.839554588
78	10.188017824	6.628464970	8.904783391
78	8.588561470	7.120406895	12.126349569
78	7.765227822	6.316108871	7.327067284
78	6.568172121	8.691036519	11.772312174
78	9.245231212	11.415881502	9.007495919
78	12.604380274	7.064533497	10.444537337
78	7.154576820	10.690591924	10.220773766
78	8.797303254	9.041212199	7.989298729
78	10.831661668	10.444197376	7.061053173
78	9.380228836	10.843657424	11.425709342
78	11.467587180	8.987062648	9.203376299
78	6.588063989	8.353109553	9.190582310
8	9.240211031	5.274843659	7.763005909
8	6.092218998	7.035084962	7.891032146
8	6.805602824	7.048084862	12.785849531
8	8.310310998	7.926058556	6.489899321
8	11.974557457	5.881358815	9.116191781
8	9.020317045	6.278025105	10.516553855
8	5.603306621	10.293671847	11.323310235
8	11.074242975	10.963429248	12.320460270
8	10.298735989	7.693127416	12.694477047
8	9.608727640	11.905180880	7.140771927

8	13.095080243	8.153824461	11.891854504
8	12.068949009	9.061155302	7.329059453

PRE:3= -130.70874995

78	10.797159487	9.028271529	11.221943953
78	10.131583877	7.244441399	9.434151987
78	8.690977499	6.642352565	12.033383237
78	8.699742393	6.837184095	7.344992150
78	7.025563168	8.223496875	10.749911548
78	9.892778967	11.140254658	9.681646808
78	12.543054954	7.404908662	10.168075065
78	7.060814322	10.874359950	10.092752280
78	8.236657305	9.049993347	8.545138219
78	9.892151977	10.481239855	7.121155105
78	10.101252240	11.451949240	12.222740348
78	11.640535542	9.288617133	8.787712204
78	5.776600958	7.585493970	8.617081013
8	6.902100549	6.348452062	7.804846874
8	4.303116855	8.510989008	8.860275314
8	7.493197235	8.048939210	12.598710643
8	7.113775942	10.675003221	8.204298560
8	9.100010823	5.859743219	10.376957926
8	9.355650807	5.976462915	13.551882447
8	6.647644213	11.505054130	11.676786245
8	9.437164780	13.073150081	12.295069772
8	10.984991978	9.934756140	12.917788166
8	9.659547931	12.853356121	9.189536303
8	13.906995953	6.370428613	10.508686253
8	11.667999809	9.811804877	6.903012243

### 3. LM6

#### 1. $\text{Pt}_{13}\text{O}_1$

PRE:1= -64.45856520

78	7.245050626	9.794973694	9.157613580
78	10.774908993	9.391061138	9.578874765
78	9.076661739	11.246023716	10.224557482
78	10.560496093	11.336269816	7.996981314
78	8.927674323	6.859180821	8.193067473
78	10.593409344	6.862100520	10.225040784
78	11.414350080	7.673061058	7.837074230
78	6.453672232	7.283319049	8.620787101
78	9.339468577	6.847052386	12.499014564
78	7.962122547	7.827007238	10.585962529
78	9.066794072	9.285779505	7.501874065
78	9.613270430	9.301455012	11.868030443
78	11.176028105	9.683750853	6.117180733
8	5.623677671	10.405931342	8.724342258

PRE:2= -65.39186737

78	7.364753799	9.692759295	9.026235167
78	10.769190507	9.366258423	9.592648504
78	9.055982798	11.239727872	10.193426145
78	10.548618820	11.391960767	8.045209842
78	8.890677625	6.858704073	8.192455222
78	10.605204285	6.872127182	10.195370891
78	11.395661779	7.672764866	7.800699733
78	6.430059385	7.307407165	8.653585429
78	9.381742775	6.835958397	12.472959428
78	7.970250176	7.858352770	10.617687121
78	9.187506529	9.229500551	7.348703671
78	9.587325070	9.326774484	11.883279686
78	11.234324044	9.937654449	6.104801847
8	11.826838702	10.246198355	4.500933921

PRE:3= -65.07711047

78	7.309368957	9.722898383	9.089826277
78	10.767253982	9.431726151	9.621416814
78	9.042495329	11.243703225	10.228393079
78	10.571141917	11.322043239	7.920085709
78	8.913216701	6.869763285	8.175119145
78	10.586304022	6.912784246	10.230247392
78	11.398068709	7.687552389	7.855174545
78	6.447650742	7.319707989	8.642898702
78	9.364887900	6.858771213	12.514151081
78	7.952580658	7.829375417	10.632979233
78	9.115412797	9.277585060	7.413518879
78	9.546924099	9.349238341	11.895583442
78	11.213368309	9.704978604	6.062173534
8	8.925947934	13.018458541	10.270765915

PRE:4= -64.89870647

78	7.294789637	9.693460328	9.128253496
78	10.821211456	9.480870004	9.561339819
78	9.045445240	11.246729465	10.182138155
78	10.381257727	11.396572816	7.868451903
78	8.927083138	6.861050392	8.175346626
78	10.554054607	6.918688448	10.222032096
78	11.417575604	7.677246188	7.856407975
78	6.448149518	7.297505226	8.643366377
78	9.369066482	6.834307327	12.522883578
78	7.969330754	7.810729577	10.631117745
78	9.046942367	9.266454385	7.388806111
78	9.616323778	9.304299940	11.833433656
78	11.223192079	9.637981200	6.145867554
8	10.515971834	13.083908639	7.353731469

PRE:5= -65.43791824

78	8.375734304	10.689688442	9.532391770
78	11.729891741	10.213619886	10.013182774
78	10.180337058	12.194415883	10.598556393

78	11.789913904	12.176132305	8.410000637
78	10.032669475	7.802516136	8.488966844
78	11.729730765	7.659315465	10.553470286
78	12.574327785	8.567587941	8.300106645
78	7.636373085	8.327318193	8.956169189
78	10.526665127	7.709804805	12.806892084
78	9.124365312	8.724273411	10.965392647
78	10.163332229	10.260306536	7.787547607
78	10.656480280	10.236283364	12.328851002
78	12.364922502	10.474012235	6.562254128
8	6.113654550	7.607743502	8.420513622

PRE:6= -65.41946789

78	8.420196620	10.620619278	9.570403439
78	11.838094278	10.232367760	10.006730211
78	10.203420822	12.137672836	10.630890839
78	11.685246024	12.181606131	8.426286462
78	10.104615119	7.791052597	8.598013625
78	11.776189238	7.647734962	10.580545019
78	12.573737701	8.593801703	8.268173786
78	7.611459247	8.208859670	9.023416215
78	10.530761377	7.670964195	12.833685584
78	9.113800499	8.689734236	11.040007286
78	10.178735096	10.207226650	7.826624486
78	10.743725651	10.139896459	12.322569891
78	12.379464236	10.526130140	6.564017435
8	10.442095084	6.563621694	14.194033179

PRE:7= -65.60536178

78	6.972760480	9.656635378	8.865011324
78	10.613699487	9.194213378	9.649952063
78	9.238664415	11.428792546	10.162354948
78	10.749595460	11.176392786	8.075320150
78	8.982100454	6.998052003	8.141562087
78	10.635486320	6.687127760	10.136149746
78	11.461183201	7.650532235	7.849213027
78	6.517836539	7.150750654	8.658134634
78	9.422236235	7.041112140	12.382601209
78	8.002979256	8.071903665	10.519824024
78	8.993872326	9.424608809	7.322504639
78	9.534180939	9.532988730	11.912514628
78	11.273533494	9.572688910	6.141599067
8	7.446728246	11.421179085	9.554774959

PRE:8= -65.43990189

78	7.237362550	9.718774772	9.160718219
78	10.683158205	9.445834679	9.482304687
78	8.970923071	11.291294800	10.248777935
78	10.395342504	11.589394361	8.126691053
78	8.957855576	6.989704810	7.977244837
78	10.482982598	6.902673833	10.108374336



78	11.552022968	7.659434223	7.877390837
78	6.525713511	7.271808307	8.634164278
78	9.491407464	6.842702242	12.465060397
78	8.005343381	7.865328904	10.636958587
78	9.062994592	9.453017809	7.441658144
78	9.642639450	9.336871840	11.877081578
78	11.150321657	9.489797101	6.049967471
8	11.332150587	11.360025105	6.427077544

PRE:9= -65.51215728

78	7.278040427	9.740790494	9.096133606
78	10.652651462	9.273961932	9.682445524
78	9.007818872	11.287187001	10.184304742
78	10.584455905	11.257101137	8.078542201
78	8.728084957	6.735405874	8.010472167
78	10.521897659	6.656717712	10.040169427
78	11.374119962	7.710596598	7.693084444
78	6.405738439	7.377100876	8.669192474
78	9.601608688	6.903248086	12.367645996
78	8.027343634	7.889934216	10.590549169
78	9.082815183	9.272076977	7.441739617
78	9.541095019	9.418388038	11.951693458
78	11.310321178	9.708184182	6.178383257
8	10.653641592	5.890431238	8.135791392

PRE:10= -65.25379601

78	7.319821327	9.603117271	9.263532356
78	10.599695935	9.402849979	9.554283562
78	8.992794402	11.269496897	10.243592946
78	10.540155932	11.331770023	7.946520563
78	9.001358509	6.829344588	7.797002241
78	10.166053369	6.889108410	10.066297099
78	11.540203380	7.663368488	7.997043427
78	6.565174276	7.264728796	8.435698469
78	9.747969473	6.865562281	12.575068510
78	7.854053682	7.807701389	11.074820466
78	9.034858977	9.304535017	7.449809738
78	9.679690591	9.348296705	11.934391326
78	11.231835914	9.526576070	6.205206816
8	6.394915440	6.819740653	10.276358669

PRE:11= -65.34745849

78	7.225238083	9.738110315	9.094405754
78	10.579980548	9.360355234	9.647933111
78	8.957030984	11.335817606	10.138812614
78	10.624050361	11.290226967	8.021653314
78	8.917689748	6.941343683	8.138609077
78	10.615883538	6.851493301	10.213155848
78	11.442581748	7.614347342	7.919509557
78	6.480531361	7.274966001	8.801183354
78	9.400915134	6.595959409	12.431530938

78	8.090240267	7.963473561	10.648148200
78	9.049751676	9.352977438	7.402217933
78	9.513515962	9.657009558	11.993026070
78	11.292610297	9.539855769	6.221622641
8	9.650632336	8.253450534	13.337935766

## 2. Pt<sub>13</sub>O<sub>2</sub>

PRE:1= -70.72831198

78	9.653252711	6.745147122	11.565788072
78	9.923308736	12.241046320	7.933063348
78	8.124489756	6.086834954	7.149769306
78	12.538188698	8.507381633	7.894040262
78	8.167005816	10.824693983	8.957343910
78	10.423214661	9.876090743	8.086507175
78	10.349763001	7.257399239	7.464831863
78	7.716709322	6.605381264	9.749426623
78	5.786538981	8.127587570	8.818239794
78	6.345812145	9.874132347	10.525992990
78	8.041240558	8.504453768	7.819337230
78	8.713290384	8.907992301	10.598196405
78	11.026478504	7.983929621	9.871949953
8	7.293068161	4.985253305	10.397490755
8	10.179155747	13.810967065	7.221193296

PRE:2= -71.48498833

78	9.743992713	6.713549513	11.727039440
78	9.783402356	12.245218116	8.040905569
78	8.047650555	6.166849945	7.377757538
78	12.517669732	8.615031071	7.971201029
78	8.104195624	10.827856543	9.290434377
78	10.369783872	9.878926747	8.102744032
78	10.366215689	7.322469872	7.594957878
78	8.113400878	6.836665767	9.828296151
78	6.010362325	7.785373977	8.757251416
78	6.287496911	9.517259169	10.579858196
78	8.066293112	8.754818722	7.740657669
78	8.752503916	9.011165373	10.994595871
78	10.978468695	8.093062213	9.981883210
8	4.919528388	10.123929345	11.496487544
8	14.156580291	8.626042212	7.369340203

PRE:3= -69.52958450

78	9.647061720	6.705318900	11.643986019
78	9.867825730	12.245414633	8.045065409
78	8.196488504	5.998260457	7.366819660
78	12.550067863	8.526724635	7.944030770
78	8.191632442	10.808887906	9.121770866
78	10.389970545	9.830475919	8.209212849
78	10.366647443	7.264898296	7.735415537
78	8.003818369	6.923650286	9.727980046
78	5.830470358	8.043832130	9.072998761

78	6.386472801	9.905103967	10.672733034
78	7.892964384	8.589687550	7.641819949
78	8.796417571	9.027438478	10.919448646
78	11.146554740	8.126727086	10.102231667
8	7.477069517	9.167065923	5.975685502
8	12.455061108	8.067454004	11.333208573

PRE:4= -71.41700812

78	9.548109166	6.829007748	11.617369833
78	9.800996419	12.306449613	7.930277141
78	8.020085255	6.108519407	7.109078066
78	12.390207945	8.566053834	7.869857241
78	8.033712818	10.844613392	8.857466875
78	10.282344029	9.936969512	8.059813422
78	10.195212967	7.339674248	7.422544268
78	8.134927079	7.033927877	9.498808299
78	5.745456213	7.991751898	9.273334070
78	6.332635950	10.024816235	10.559844170
78	7.657358164	8.630738085	7.590449449
78	8.716563957	9.147003319	10.775687613
78	10.879755464	8.033888247	9.847402796
8	4.263666491	7.067351908	9.331993662
8	10.207343891	13.909408276	7.350984641

PRE:5= -70.65848887

78	9.582267552	6.688996949	11.613175536
78	9.901644030	12.110399803	7.861786115
78	8.138526787	6.170365621	7.044355024
78	12.613742489	8.473246596	8.027336768
78	8.109738148	10.859785602	9.037630053
78	10.458363793	9.731582572	7.954761662
78	10.465966432	7.189547877	7.479832031
78	7.826542491	6.480968004	9.660347914
78	5.862527188	7.982433425	8.799271660
78	6.312934312	9.797653811	10.464696699
78	8.113317709	8.571655729	7.825630859
78	8.681526555	8.838522222	10.580332001
78	10.949428231	7.940478330	9.883101809
8	7.509382057	4.738031897	10.005464053
8	14.346512912	8.297072403	7.804903514

PRE:6= -71.23779912

78	9.731244183	6.803087118	11.784063850
78	9.723588363	12.025735710	7.549336657
78	8.043612416	6.167120164	7.218296341
78	12.550865092	8.312008160	7.992095785
78	7.943955113	10.897359093	8.954971313
78	10.441849608	9.757993964	8.137257809
78	10.346570103	7.188990252	7.465606663
78	7.638336772	6.457596866	9.704313185
78	5.825751889	7.936056847	8.708317560

78	6.262409084	9.733840092	10.417880420
78	8.046263574	8.636074266	7.775239857
78	8.703097528	8.875404041	10.432781869
78	11.003692873	7.797494891	9.922569539
8	8.598818855	5.481526838	11.023814811
8	7.971695068	12.630754716	8.090512875

PRE:7= -71.66813893

78	9.769494333	6.934775094	11.881868111
78	9.823915074	12.235206729	8.109831163
78	7.738312898	6.301730134	7.209998162
78	12.449378556	8.080903882	8.193841606
78	8.173004626	10.904517923	9.335494078
78	10.733285733	9.961958531	8.000776962
78	10.135791173	6.979361041	7.796882170
78	8.400590279	6.891475891	9.721536014
78	6.232235931	7.775643655	8.628599581
78	6.207754287	10.101008351	10.607317555
78	8.348879277	8.927106439	7.748558186
78	8.481887274	9.056035098	11.207113250
78	10.735268531	8.516762387	10.121247927
8	5.096113030	8.823061453	9.760891723
8	11.881515491	6.615894337	7.053420764

PRE:8= -70.74473292

78	9.625441756	6.832299788	11.855891353
78	9.946405726	12.163122042	8.071885070
78	8.346944864	6.062993536	7.287276607
78	12.568501753	8.690333340	8.103396235
78	8.159751864	10.886958543	9.187328985
78	10.237221316	9.683149977	8.105030598
78	10.565168890	7.150576849	7.699903962
78	8.167537316	6.863370232	9.730341444
78	6.057738111	8.061978313	9.011794910
78	6.313697923	9.951566503	10.636287800
78	7.799872639	9.040331807	7.436437182
78	8.684063794	9.061738002	10.933338755
78	11.060611968	8.016733456	10.065667116
8	7.606820944	7.498650104	6.267064172
8	11.492006373	7.369524734	11.840887988

PRE:9= -71.39702754

78	9.180521481	7.103617542	11.689368869
78	9.594451581	12.177707359	7.793873313
78	7.809238032	6.514478866	6.836853174
78	12.437455764	8.042504439	8.022737420
78	7.734484133	11.126447726	8.948509664
78	10.614956235	9.752803413	7.690714932
78	10.141164089	7.186891757	7.389397661
78	8.374256208	6.422107991	9.340015639
78	6.036547154	8.002694392	9.453112216

78	6.041067839	10.226440743	10.536766107
78	7.865289166	8.884432542	7.825783944
78	8.493683371	9.255548196	10.522902907
78	10.628544810	8.042691454	9.849429615
8	6.426771986	6.137812423	9.565089599
8	11.250982470	11.481579779	7.188059210

PRE:10= -70.87535600

78	9.674513580	6.664878281	11.643962418
78	9.590514629	12.352160772	7.920506248
78	8.158358812	6.040265820	7.144421673
78	12.643554432	8.249713836	7.936895728
78	8.183111475	10.744025286	9.049222651
78	10.326493752	9.972956154	7.767809925
78	10.344661003	7.249692111	7.388656332
78	7.814201534	6.605355611	9.957318483
78	5.949695360	7.959058981	8.763401197
78	6.325893417	9.760562405	10.484858917
78	8.134281490	8.569809838	7.639228455
78	8.729459532	8.857981518	10.715758291
78	10.981921552	7.850992136	9.879594193
8	7.580017138	5.123753842	8.715313661
8	12.176656224	9.954355445	7.246919455

### 3. Pt<sub>13</sub>O<sub>3</sub>

PRE:1= -77.94288940

78	9.649906643	6.671255700	11.892113443
78	9.859209437	12.152882134	8.122943030
78	8.092092535	6.094676124	7.465304889
78	12.543662125	8.451011141	8.242262729
78	8.147528673	10.811956989	9.381039656
78	10.429634161	9.788295008	8.333297120
78	10.388891184	7.232096838	7.792379969
78	8.178372575	6.741344817	9.922671807
78	6.013244679	7.870134562	9.107945273
78	6.392694237	9.652019420	10.842316423
78	8.091928035	8.652452888	7.952160693
78	8.777554829	8.960512539	11.160736234
78	11.020739641	8.022875856	10.242244179
8	5.348432087	10.491750357	11.958341743
8	9.992710651	5.755021363	13.339030402
8	14.228966093	8.418591811	7.786030603

PRE:2= -76.90518227

78	9.569209930	6.550447776	11.412003893
78	9.666426936	11.974278541	7.589594712
78	8.028742699	5.919940957	7.210247872
78	12.657324692	8.050681369	7.954076136
78	8.139573676	10.618786020	8.933329298
78	10.628456925	9.507720294	7.521166571

78	10.409762908	6.822099315	7.417920502
78	7.806578532	6.784298028	9.610131526
78	5.831694028	8.033967172	8.662361862
78	6.292851186	9.773936914	10.372555978
78	8.135022415	8.476478654	7.561460464
78	8.672494949	8.886512581	10.815134913
78	10.769885601	7.947591504	9.665847519
8	4.281608368	7.443768118	8.067508198
8	11.152691287	11.150380729	6.702334633
8	11.077021506	5.549931922	6.342590746

PRE:3= -76.66752124

78	9.587788008	6.790243958	11.567116633
78	9.761973966	12.319048543	7.736887567
78	8.092285253	6.233136009	7.270756668
78	12.459035007	8.681328351	7.965728665
78	8.109601436	10.949033350	9.008495537
78	10.324219151	10.014676793	8.151647777
78	10.298670643	7.386298800	7.548067682
78	7.953194016	7.066691678	9.704241154
78	5.705046257	8.154899634	9.017295726
78	6.255233026	10.042325972	10.511780029
78	7.859015656	8.749475861	7.736983733
78	8.514208202	9.188310527	11.164122003
78	10.920115627	8.141171566	9.900250809
8	9.357392349	9.293466251	12.739725556
8	4.234087544	7.242412825	8.652582189
8	9.972435234	13.696970946	6.676595577

PRE:4= -78.00491932

78	9.603006737	6.535756718	11.679546165
78	9.797465999	12.105604604	7.922453758
78	8.105398335	6.014771914	7.397598322
78	12.512413493	8.430136168	8.146910172
78	8.124245567	10.699272962	9.114711245
78	10.378877119	9.728575843	7.991147022
78	10.371134916	7.200146991	7.451292568
78	7.929313531	6.646319999	9.791689231
78	5.918921510	7.879550898	8.812775553
78	6.266190524	9.662616900	10.520629861
78	8.036879584	8.558418544	7.625712631
78	8.648727406	8.850263995	10.875828763
78	10.833172816	7.909273927	9.935883905
8	7.601737265	4.727117979	6.318130958
8	5.137394223	10.592377762	11.485876845
8	14.253850917	8.317695069	7.949137361

PRE:5= -76.81606527

78	9.426369732	6.571881523	11.797183723
78	9.704222758	12.067682914	7.995249332
78	8.013949639	5.920216415	7.385622163

78	12.387323705	8.335067341	8.075414873
78	8.031654168	10.656384822	9.116404308
78	10.248637389	9.666527341	8.243186219
78	10.218048541	7.098665850	7.646177774
78	7.827183664	6.661765960	9.874514978
78	5.626991424	7.912788095	9.071289160
78	6.254372143	9.705456079	10.643112595
78	7.797065354	8.415898708	7.886254494
78	8.671721230	8.890774090	11.138845606
78	10.767404931	7.848011516	10.053233878
8	4.037097317	7.393103946	8.561956396
8	9.050370236	10.064347690	12.465779228
8	9.773889236	5.617730419	13.208493489

PRE:6= -77.07959433

78	9.501089683	6.783798062	12.387211330
78	9.608325628	12.509779740	7.946394830
78	7.874375227	6.211846953	7.445559944
78	12.266939626	8.400240238	8.519116585
78	8.394538926	10.957686775	9.420082161
78	10.440410410	10.174799184	7.928910369
78	10.280450072	7.068318077	7.731701064
78	8.174899789	6.835354064	9.880051525
78	6.070021918	7.924094809	8.972825093
78	6.470539567	9.793557173	10.658735751
78	8.335632765	8.710221946	8.027104296
78	8.902702987	9.041483098	11.208396130
78	10.818178884	7.514942471	10.347017107
8	6.928264042	11.658172087	10.558053305
8	8.258432093	5.689526238	11.477398695
8	12.399860725	10.128009524	7.753796094

PRE:7= -78.25612122

78	9.799740424	6.845924170	11.524019800
78	9.604999380	11.818449036	7.843867208
78	7.941276920	6.021029195	7.527605440
78	12.657242503	7.847906924	7.765101008
78	7.770740354	10.770724906	9.084057071
78	10.763860194	9.541399872	7.432445109
78	10.319090602	6.927440132	7.434011941
78	7.808089729	6.675619128	10.003861152
78	6.097110673	7.594190526	8.271063797
78	6.060004942	9.650244533	10.552127793
78	8.292605361	8.724498828	7.753547553
78	8.661645937	8.980273580	10.651539366
78	10.886759500	8.159226256	9.630506739
8	4.964276158	8.427156654	9.586004529
8	11.153491312	11.280486355	6.794088445
8	9.392192155	5.690942608	6.277630580

PRE:8= -77.71590284

78	9.813161808	6.803561831	11.694747911
78	9.568908462	12.252785762	8.051300185
78	7.666666714	6.326002147	7.392984917
78	12.420368447	8.082915537	8.019163652
78	7.923186868	10.885708456	9.181358808
78	10.693984381	9.918277380	7.776179735
78	10.079768833	7.344502604	7.482818423
78	8.311604140	7.394423566	9.642962492
78	5.949051110	7.829779842	8.753084520
78	6.109861786	10.190858048	10.721321935
78	7.932992878	8.928599870	7.575561020
78	8.535938602	9.432376357	11.253336641
78	10.725392679	8.499321601	9.947862777
8	9.030823463	8.213589730	12.699288555
8	4.937696103	8.904799785	9.969227258
8	11.277326917	11.690444027	7.386827348

PRE:9=

78	9.110958221	6.748507691	11.856794796
78	9.591700807	12.192478781	7.864239755
78	8.323806530	6.157237887	6.878208648
78	12.547288763	8.338235150	8.494854804
78	7.982089382	10.848698394	9.119852013
78	10.000343291	9.701563918	7.752532015
78	10.453455148	7.098049544	7.769651949
78	8.447037902	6.435170815	9.402044795
78	6.427575187	7.859898176	9.154365164
78	6.398513919	10.060345513	10.920449144
78	7.601230348	9.075282594	7.271874627
78	8.690998167	8.972506917	10.733346567
78	10.882439633	7.660336110	10.323706003
8	7.535927841	7.636869786	5.982054985
8	5.126154266	8.845290306	10.123389457
8	11.892262214	9.786447671	7.457052478

PRE:10= -76.90929243

78	9.647832435	6.729942663	11.657627906
78	9.960946721	12.035208765	8.038016979
78	7.987801456	5.975967555	7.576781223
78	12.484859624	8.286782679	7.831285979
78	8.282599351	10.691386979	9.226455933
78	10.334316644	9.574613653	8.163673213
78	10.218622734	7.063021700	7.700863564
78	7.748237729	6.801100636	9.988663426
78	5.503678811	7.692129596	9.053191169
78	6.213270424	9.651674145	10.428029727
78	7.961520467	8.607682832	7.586207189
78	8.491608466	8.882172602	11.308730624
78	11.194386916	7.859082879	9.954579710
8	6.040952117	8.477483150	7.420257906
8	7.711000289	10.822138015	11.178403747



8 11.526497773 6.500185523 11.323066724

#### 4. Pt<sub>13</sub>O<sub>4</sub>

PRE:1= -84.10440676

78	9.646433063	6.597820633	11.522168969
78	9.939480357	12.195731685	8.021655138
78	7.991048245	6.100315119	7.225603975
78	12.493964693	8.302927835	8.064985283
78	8.184766431	10.805568543	9.110077590
78	10.444322076	9.829124415	8.054757966
78	10.301880384	7.206346882	7.563870985
78	8.050573617	6.774369466	9.667336975
78	5.922298437	7.945066203	8.779628645
78	6.305697691	9.704566304	10.526238630
78	8.064613435	8.653744327	7.685818866
78	8.638319759	8.928107427	10.999034840
78	10.907151717	8.137625376	10.014166434
8	10.146710968	13.763130033	7.268222260
8	14.182241085	8.171683825	7.649817945
8	5.178414760	10.634616378	11.478135464
8	10.065177542	5.430676518	12.750993189

PRE:2= -84.02994951

78	9.904644672	6.731550577	11.773195481
78	9.779214501	12.151436148	8.276219508
78	7.695319174	6.212754564	7.168835497
78	12.378282793	7.854009768	8.244571707
78	8.088079840	10.751564550	9.324219734
78	10.756422079	9.820903712	7.860395384
78	10.106202595	6.934574881	7.608976475
78	8.473497461	7.056622103	9.637514757
78	6.162900360	7.638605546	8.601709225
78	6.131706861	9.837593366	10.544789089
78	8.268536879	8.830914620	7.641977527
78	8.406069492	9.222481767	11.424449248
78	10.635972728	8.572632666	10.078243677
8	11.453780471	11.572107482	7.505043824
8	11.855952664	6.317786417	7.146962544
8	4.938277710	8.623838110	9.709138342
8	9.035867997	8.073221726	12.821141076

PRE:3= -83.23164123

78	9.841332727	6.427055997	11.686457296
78	9.512269850	12.155324305	8.052799557
78	7.909611567	6.090698675	7.497096682
78	12.605821766	8.153319047	8.206504445
78	7.932798585	10.651033996	9.229156983
78	10.772835527	9.873771036	7.920254694
78	10.426376140	6.997104288	7.466774097
78	8.080055404	6.944803515	9.884045120

78	6.124807291	7.815149557	8.478360370
78	6.134211359	9.391592870	10.480275438
78	8.435685442	8.699992901	7.692290655
78	8.529356895	9.143255340	11.253595230
78	10.567030377	8.148683563	9.811150070
8	11.332806129	11.688875751	7.704251524
8	11.135378034	5.683440826	6.482776050
8	4.828813844	10.148567834	11.347710588
8	9.132912104	7.926376738	12.637195018

PRE:4= -84.32617777

78	9.824725178	6.789451380	11.688566759
78	10.057844931	12.352920619	8.287472893
78	7.930284966	6.312332746	7.251561291
78	12.536616529	8.460787150	8.062726022
78	8.222533207	10.942750767	9.173070620
78	10.515376280	9.969946032	8.153153201
78	10.318515610	7.313255493	7.838011310
78	8.325641749	6.872056712	9.712175476
78	6.131450912	7.875569832	8.853857062
78	6.401543321	9.742261440	10.545084477
78	8.139666191	8.853788508	7.709247633
78	8.773672166	9.055577693	11.004195792
78	11.116577906	8.279153521	10.152560323
8	5.323935863	10.700908693	11.540893503
8	10.204825948	5.700606287	12.997757431
8	10.201385697	13.851581168	7.373452561
8	14.218167648	8.471337792	7.559870005

PRE:5= -82.42105505

78	9.675515848	6.761246038	11.590542808
78	9.903682622	12.392848549	7.941181400
78	8.135519129	6.234449233	7.356405242
78	12.603544045	8.686491128	8.014708532
78	8.231005240	10.956225619	9.035121181
78	10.480051530	10.035302559	8.126143729
78	10.435608157	7.304137504	7.554284687
78	7.924758759	6.972976422	9.819094745
78	5.870840415	8.233761727	8.952009531
78	6.386785403	10.028338157	10.560723636
78	8.075331271	8.757783109	7.780268057
78	8.799221544	9.148036437	11.049704792
78	10.942513447	8.172523776	9.899311189
8	4.259929962	7.696672880	8.501592249
8	8.964402126	10.246040538	12.474230649
8	10.930106670	5.978802459	6.457981288
8	10.246406865	13.985770070	7.313973585

PRE:6= -83.81862511

78	10.023280538	7.124455488	12.023341050
78	9.633018584	12.294755937	7.733740948

78	8.115487824	6.229356768	7.690803161
78	12.642478405	8.293550848	8.158892316
78	8.202380045	10.991455517	9.250860965
78	10.708844886	9.893006104	7.773794988
78	10.474278591	7.311288052	7.235515706
78	8.276643180	6.893034168	10.212117235
78	5.893057053	8.442891796	8.527422148
78	6.425650114	9.779540859	10.585869646
78	8.285359662	8.977628708	7.819808803
78	8.839126497	9.243923737	11.293246045
78	10.563561609	8.065082294	9.696964544
8	6.588721705	6.633584386	8.944413082
8	7.440312816	10.281473921	12.194083922
8	9.606674366	5.648448078	6.676453576
8	11.241083959	11.571410853	7.009160603

PRE:7= -83.78361792

78	9.835390347	6.585339227	11.751064461
78	10.374228422	12.125523298	8.181812241
78	8.261684429	6.107624726	7.631424021
78	12.514238678	8.500584833	8.256528037
78	8.202238586	11.084828978	8.438987480
78	10.305386908	9.669207810	7.818872057
78	10.601172683	7.031677793	7.585979353
78	8.062748158	7.206303907	9.970044896
78	5.629219150	8.510460634	8.893456515
78	6.963307117	10.061284691	10.346591629
78	7.860487991	8.649871991	7.693159157
78	8.853435532	8.903049672	11.852634758
78	10.454654100	8.208587329	9.916522880
8	6.092378629	6.778521976	9.504901159
8	7.842905992	10.531854770	11.987277588
8	9.786037463	5.632663607	6.513445487
8	11.145382132	13.561661722	7.512916696

## 5. Pt<sub>13</sub>O<sub>8</sub>

PRE:1= -106.48112023

78	9.675903353	7.211982282	11.447079852
78	9.860522666	12.630000241	7.946685154
78	8.014767839	6.349014990	7.270232097
78	12.396863834	8.940054007	7.769276051
78	7.960024266	11.338883044	9.040024648
78	10.232962032	10.250288807	7.924573768
78	10.187189804	7.653388403	7.457333528
78	7.842334318	7.224832010	9.590106936
78	5.677944714	8.337038446	8.865032967
78	6.136559540	10.000981357	10.588692554
78	7.839733575	8.998862132	7.530886841
78	8.587195609	9.452938934	10.674464342
78	11.079345668	8.527635899	9.783958756

8	7.562204550	5.032860546	6.203674365
8	14.070545482	8.938278929	7.277774373
8	3.984905835	7.993124501	8.515057427
8	4.930662420	10.949876215	11.464357669
8	11.525823407	7.881485119	11.518875444
8	7.164413615	9.876738628	6.121322073
8	10.276628077	14.120937570	7.115483797
8	7.099291647	12.891117915	9.258529103

PRE:2= -109.78596987

78	9.242867632	7.083354674	11.046244498
78	10.379719512	12.074135915	8.255536253
78	8.583104184	6.673448158	7.905948308
78	12.822366071	9.434516332	8.296809527
78	7.927718347	11.796799914	9.178185084
78	10.029554301	10.052075607	6.820851041
78	11.204376117	7.808972888	7.142546865
78	7.384216163	5.939795571	9.913466807
78	5.689222465	8.303932055	9.382481813
78	5.982992205	10.467642865	10.425543486
78	7.825193218	9.146118068	8.118772538
78	8.667971607	9.524828679	10.546607922
78	11.046971904	8.275809295	9.657838777
8	9.839796480	6.632580537	6.507868528
8	11.799586554	10.873404810	7.482060393
8	5.556991641	6.446974138	9.848786299
8	7.113310492	9.755913980	11.766116805
8	11.048649278	7.640159592	11.477735517
8	8.300663215	9.512791570	6.261762429
8	8.996047111	13.295195727	8.624229247
8	6.037454966	12.173937954	9.662516993

PRE:3= -106.76870808

78	9.687237883	7.179044328	11.777612400
78	9.386044140	12.757379159	7.924512006
78	7.757399015	6.852290537	7.228291373
78	12.447566074	8.832313856	7.801632497
78	8.019398671	11.275328445	9.283527591
78	10.002336757	10.285074580	7.900657785
78	10.440117774	7.377639923	7.464408430
78	8.410980260	7.600586790	9.574839651
78	5.976954063	7.882113252	8.908800590
78	6.044381467	9.955981947	10.668357373
78	7.603109284	9.415546241	7.542691243
78	8.882443972	9.532136179	11.215077596
78	10.935323242	8.298781916	9.853233076
8	9.351966694	6.291614567	6.307105666
8	11.902692130	10.633209791	7.586816353
8	4.397130414	7.163481465	9.201405825
8	7.204252060	9.706524818	12.154401826
8	12.308800622	8.090856562	10.990166918

8	6.897636595	9.965496240	5.995025998
8	9.513439586	14.308444580	7.124636155
8	6.259867215	11.738310661	10.039627737

PRE:4= -107.71546818

78	9.703294943	6.986998266	11.511788590
78	10.116014646	12.786075333	8.491209553
78	8.312006660	6.759641013	7.576329682
78	12.870460553	8.914979480	8.037773926
78	7.785647514	11.673583728	8.881025710
78	10.225306437	10.300412329	7.980325299
78	10.685037521	7.693407767	7.674951312
78	7.583677979	7.338316202	9.985705941
78	5.497404691	8.104711532	8.800390976
78	6.390784654	10.363983946	10.490079566
78	7.817270814	9.165579316	7.967604604
78	8.686427706	9.517210914	11.181153145
78	11.049973737	8.798027779	9.949046458
8	12.155362174	10.535007136	7.411085959
8	8.708712959	13.063747112	9.764588469
8	7.977196676	6.164437996	11.489793165
8	4.797420492	9.559567457	9.834174903
8	6.984169587	10.799492571	7.359567935
8	11.464518775	7.667405884	11.488737685
8	9.153471751	10.539305426	12.562429659
8	9.901602304	6.327585017	6.550143488

## 6. Pt<sub>13</sub>O<sub>12</sub>

PRE:1= -130.10272951

78	9.714944146	7.469096288	11.519448146
78	9.581775821	13.336682127	7.958772987
78	8.139613740	6.923605130	7.227293814
78	12.828664547	9.606987543	7.744083041
78	8.189755938	11.507606837	9.272631368
78	10.391460144	10.752796605	8.029307568
78	10.417447484	8.055286108	7.473251176
78	8.153186864	7.677471280	9.631207978
78	5.950191439	8.728790373	8.864373974
78	6.343697131	10.400832863	10.651898568
78	8.043063885	9.472076587	7.562159281
78	8.842728194	9.812129506	11.125271449
78	11.202717608	8.882356161	9.873950721
8	10.980664017	14.011311565	7.158063640
8	12.126560482	11.294846097	7.331305685
8	14.314774371	8.676638728	7.714009875
8	7.975823281	13.392039527	8.912969254
8	12.501264832	8.629429726	11.083280590
8	9.260379795	10.812930486	12.547970470
8	7.704637869	5.500512633	6.307826274
8	7.494353856	10.338166850	6.099514458
8	5.063757447	11.261222746	11.461915152

8	10.083004400	6.235121079	12.707092199
8	4.268205791	8.300922085	8.602429656
8	11.350416372	6.756662009	6.683768261

PRE:2= -135.02996765

78	9.655238906	7.253546006	11.088593297
78	9.794147468	12.874184729	8.124350427
78	8.043627364	6.924417891	7.104497624
78	12.968750297	8.954240122	7.687791367
78	7.685167469	11.754557053	9.029980239
78	10.852657951	10.559182413	7.476652176
78	10.711280987	7.542803145	7.283601524
78	7.794951420	8.025838728	9.491558856
78	5.518835682	8.327112443	8.398340046
78	6.362100351	10.392190960	10.788443147
78	8.522820883	9.451907485	7.401393563
78	8.961849734	10.016696743	11.074664243
78	11.271374496	9.192466566	9.641832275
8	12.955350384	10.806594837	7.606308006
8	8.680443827	13.313371667	9.598536147
8	7.846861002	6.745570996	11.000785970
8	5.043386421	9.647526438	9.642483340
8	7.124710510	10.778705423	7.498489482
8	11.485302680	7.642404957	10.877866416
8	10.821790447	10.409149063	11.069604780
8	9.666626879	6.076043942	6.624553073
8	12.681623608	7.161154755	7.254947085
8	10.791069670	12.355399904	6.634324737
8	7.579252556	10.786319978	12.195981799
8	6.114257720	6.993756163	7.185582708

PRE:3= -132.29421435

78	9.807382447	7.165942796	11.347750911
78	9.718523873	12.993468215	8.118202365
78	8.364049793	7.298948914	7.165227771
78	13.004996700	9.155584557	7.825017120
78	7.928377815	11.241626680	8.980795599
78	10.314346222	10.565886970	7.690486123
78	10.755828718	7.934118934	7.583867118
78	7.809538455	7.442527052	9.625843118
78	6.044240786	9.017897746	8.800425286
78	5.967879839	10.716079964	10.762303652
78	7.475046614	9.709459589	6.719592239
78	8.869883000	9.633628826	10.842022139
78	11.184486115	9.217698255	9.745300355
8	12.214186280	10.812230138	7.364807770
8	8.964058783	12.709304207	9.809222297
8	8.037629199	6.452500930	11.278799220
8	4.681795517	9.493341644	10.116365412
8	6.730182431	11.334825597	7.379623431
8	11.524734546	7.953223767	11.185582252

8	9.151428590	10.611230839	12.319139696
8	10.067261576	6.436447850	6.580204321
8	14.371864963	8.059585195	7.763563497
8	10.592364529	13.800785258	6.814428273
8	6.336925532	11.982227222	11.913773949
8	8.017772201	8.321567012	5.534820678

PRE:4= -133.62995380

78	9.724995911	7.339285838	11.858200140
78	9.647286957	13.520060990	7.855143136
78	7.941775598	7.002690046	7.471267095
78	12.695061068	9.505927661	8.099896628
78	8.546905056	11.944815976	9.673204242
78	10.633848901	11.271912518	8.161476081
78	10.019681325	8.696704026	8.034797349
78	7.992877054	7.176540515	9.947662835
78	6.568822595	8.841457928	8.665187412
78	6.031665707	10.881401245	10.343366610
78	7.947160310	9.478359654	6.543186877
78	9.083680717	9.527762791	10.599776663
78	11.607895338	8.651990228	10.278820836
8	10.867633471	14.481416979	7.050364102
8	12.146353408	10.929902570	7.011251498
8	13.338342594	8.316356263	9.404085525
8	7.850950932	13.003479980	8.222849514
8	11.422519409	8.087575969	12.152528362
8	9.262029584	11.289474602	11.332564467
8	7.655593318	5.500841753	6.583055132
8	6.724177262	10.641081499	6.079136714
8	6.080707982	12.322206810	11.366367517
8	8.267666951	6.150162232	11.546372030
8	5.068180912	9.406171320	9.711120168
8	9.701262307	8.903865803	6.090936405

#### 4. LM9

##### 1. Pt<sub>13</sub>O<sub>1</sub>

PRE:1= -63.71434922

78	9.557601155	6.502206395	11.468977981
78	9.705368924	12.116901217	7.782057753
78	8.041763655	5.933293705	7.159150396
78	12.434789321	8.350916456	7.850850241
78	8.102909202	10.649978827	8.978753217
78	10.311599492	9.725297208	7.980682413
78	10.261541242	7.130265053	7.430584215
78	7.832179006	6.716563850	9.613810759
78	5.714304821	7.904674043	8.824449759
78	6.210712984	9.773425022	10.428709447
78	7.856558322	8.469805133	7.535118895
78	8.607668433	8.835750189	10.785418185
78	10.833562648	7.924426915	9.825604847

8 7.686335484 8.839331666 5.782743820

PRE:2= -64.90264857

78	9.558593096	6.519930373	11.462219638
78	9.721847124	12.142885112	7.713860044
78	8.031296798	5.942410574	7.160464380
78	12.415416051	8.363084073	7.860015519
78	8.112392089	10.658844366	8.942651008
78	10.320477684	9.789293788	7.969661776
78	10.237327503	7.129261491	7.430937310
78	7.843048268	6.715242835	9.614580069
78	5.721601768	7.910931932	8.814450892
78	6.215969438	9.762084914	10.440053194
78	7.896042036	8.463625182	7.637450728
78	8.592361675	8.854857023	10.773857553
78	10.842856040	7.903283695	9.821711333
8	9.938066970	13.585568077	6.747387945

PRE:3= -65.09059162

78	9.556539218	6.501230832	11.477926404
78	9.703296909	12.106187713	7.806225022
78	8.017621905	5.919975185	7.252859654
78	12.420644224	8.352015962	7.854910716
78	8.092463848	10.645549465	8.961232609
78	10.280489129	9.701456204	7.975803583
78	10.218544770	7.108990428	7.410913254
78	7.855629274	6.656529502	9.615513763
78	5.733102750	7.892399928	8.799429372
78	6.221890728	9.744473533	10.399011110
78	7.870885493	8.458330744	7.536060441
78	8.612323915	8.814054916	10.726511968
78	10.842573039	7.897249050	9.821398304
8	7.606750203	4.580453306	6.178897455

PRE:4= -64.29769320

78	9.596397864	6.483977392	11.579505276
78	9.926697347	12.113269059	7.920499441
78	7.702498942	6.229576083	7.114172637
78	12.365497387	8.255409818	7.817126981
78	8.101991040	10.795320509	9.149914893
78	10.301044561	9.730764601	8.138321583
78	10.084991816	7.155126602	7.450864669
78	8.071991046	6.606128268	9.615855013
78	5.940435446	7.716456937	8.815750078
78	6.241103467	9.553601926	10.549604463
78	7.904786809	8.768989974	7.664493101
78	8.684143743	8.828857810	10.725190410
78	10.914414040	7.725515819	9.848827894
8	7.323756681	12.406455773	9.229155435

PRE:5= -64.26986922



78	9.553107149	6.501645611	11.467665169
78	9.704024254	12.118167745	7.779578554
78	8.038195907	5.940366418	7.159213333
78	12.440796452	8.353755617	7.855342747
78	8.100073595	10.647727504	8.977320665
78	10.304801564	9.720664356	7.981389670
78	10.280468170	7.090816451	7.359749111
78	7.832344710	6.708198972	9.620604477
78	5.718362369	7.906759388	8.821705603
78	6.211903130	9.770540022	10.422761491
78	7.884617935	8.463328488	7.634276428
78	8.608842672	8.833081541	10.785696789
78	10.828039936	7.928693969	9.818466206
8	10.709701288	6.116990824	5.906848645

PRE:6= -64.90310963

78	9.546205951	6.514967232	11.472237936
78	9.704874674	12.112844886	7.784525683
78	8.046493412	5.936943768	7.158423308
78	12.435174482	8.359987130	7.850410913
78	8.100264901	10.644213593	8.976647701
78	10.297620853	9.716472777	7.986582358
78	10.258438445	7.127217774	7.431647444
78	7.807115660	6.719623478	9.585824650
78	5.638754107	7.941299657	8.851206394
78	6.230124162	9.736863737	10.403930100
78	7.830015450	8.445368350	7.631872812
78	8.611708958	8.839894684	10.786798793
78	10.832943486	7.920130591	9.824566885
8	3.978255873	7.470610487	8.468741006

PRE:7= -65.21760756

78	9.339507870	7.201755002	11.554881440
78	9.298632092	12.367896897	7.831072333
78	7.324945177	6.589652036	6.892426755
78	12.115710536	8.154400979	7.669209190
78	7.528650864	11.051289283	8.870280081
78	10.309606580	9.921060310	7.449881418
78	9.770197291	7.349817639	7.318820626
78	8.070918928	7.000659616	9.366479686
78	5.841561516	7.999530400	8.569183549
78	5.738117727	9.936811390	10.230848336
78	7.707201619	9.140785191	7.295167141
78	8.264077962	9.323354468	10.593752235
78	10.504339271	8.483180094	9.667202954
8	10.829922648	11.663998777	6.928297963

PRE:8= -64.69424187

78	9.290185600	6.847333215	11.286805785
78	9.483390715	12.479341912	7.575449396
78	7.734288926	6.284142500	6.999191016

78	12.154887648	8.658770591	7.713402543
78	7.847145715	11.114692543	8.846804947
78	9.973865685	10.085363473	7.729002119
78	9.966061395	7.468220374	7.248462998
78	7.593263288	7.113225640	9.424748867
78	5.423745144	8.209057416	8.657000490
78	5.935215876	10.139371749	10.201342007
78	7.627565519	8.852599848	7.479604977
78	8.301899378	9.163346411	10.701097518
78	10.529518530	8.293511905	9.630850963
8	6.448605599	11.955531924	10.003871066

PRE:9= -63.93977540

78	9.138884744	6.998601412	11.434953545
78	9.437576287	12.425677137	7.603141098
78	7.636020709	6.356051111	7.082509972
78	12.088600257	8.886874939	7.643870717
78	7.692158806	11.121177240	8.763465590
78	9.929687156	10.055648283	8.047385482
78	9.955039937	7.426396354	7.186025464
78	7.492650061	7.072346392	9.550680494
78	5.478906825	8.207215975	8.508015606
78	5.973877161	9.996308130	10.234409908
78	7.648988899	8.900500036	7.427747514
78	8.475181139	9.265048612	10.459702142
78	10.739962002	8.038413034	9.741323189
8	10.794054405	6.432735262	8.637329548

PRE:10= -64.92241512

78	9.201504518	7.149824440	11.549531265
78	9.533601554	12.438786704	7.615235448
78	7.734195013	6.326678595	7.053712191
78	12.080584685	8.735939999	7.719474457
78	7.705756588	11.128400773	8.693971138
78	9.949886991	10.032757455	8.008462955
78	9.938290509	7.467118369	7.252139741
78	7.245862872	6.976158886	9.481914679
78	5.303434818	8.378634347	8.557564716
78	6.002488492	10.099526212	10.252656434
78	7.567762352	8.807488536	7.553638113
78	8.419617922	9.324366521	10.434609132
78	10.588037022	8.085552477	9.700521974
8	7.916235748	5.881872937	10.881621631

PRE:11= -65.07089389

78	9.039995404	7.179042167	11.589105520
78	9.557811174	12.448361906	7.597912397
78	7.610228028	6.458168594	6.814389576
78	12.039320535	8.644887290	7.750551638
78	7.744022220	11.209176310	8.709523580
78	9.918680967	10.023239351	7.846342277

78	9.860921213	7.429509449	7.244853269
78	7.975333186	6.641769050	9.326692856
78	5.556443847	8.256064090	9.157758624
78	5.941750052	10.421032216	10.291466005
78	7.461190893	8.897771394	7.591799894
78	8.249571954	9.266833102	10.343258104
78	10.449109837	8.095434914	9.718026679
8	5.994645207	6.452566542	9.476989656

## 2. Pt<sub>13</sub>O<sub>2</sub>

PRE:1= -71.44850487

78	9.550671394	6.670412189	11.588085919
78	9.765016987	12.195825331	7.797198308
78	8.037674381	6.163103719	7.176964673
78	12.486999950	8.546351635	8.050676470
78	8.090626238	10.838390370	9.067801341
78	10.335518934	9.826985760	7.896638991
78	10.379925845	7.276280683	7.414935580
78	7.981866064	6.831574377	9.635604883
78	5.883083763	7.944618773	8.697193697
78	6.232538747	9.750916168	10.422100326
78	8.007306882	8.714256149	7.618974163
78	8.625441894	9.011424271	10.836862107
78	10.791777431	8.051196239	9.847543361
8	5.097549513	10.692085419	11.377960879
8	14.226383944	8.390823961	7.821766965

PRE:2= -69.18519580

78	9.367170517	6.612766810	11.379482472
78	9.545675407	12.127868898	7.770684675
78	7.854955384	6.002680277	6.881025101
78	12.302390768	8.240135575	7.748507450
78	7.868909010	10.693578245	8.847562121
78	10.161530010	9.702477879	7.431031576
78	10.100032790	7.035519989	7.313337583
78	7.577704530	6.439283906	9.490906775
78	5.571158572	7.909819668	8.674076704
78	6.076900822	9.742302254	10.301174055
78	7.796885432	8.435378499	7.634819856
78	8.462885516	8.792894382	10.432515672
78	10.734954984	7.860514926	9.672369684
8	7.257806403	4.700592589	9.798641480
8	10.636920236	10.062395667	5.723968220

PRE:3= -70.26361011

78	9.784791737	6.897084644	11.662753937
78	10.348130858	11.813622653	8.123902751
78	8.182226574	6.388850785	7.256319743
78	12.518267783	8.789106445	7.975790253
78	8.264290449	10.805301038	8.983877992

78	10.439372072	9.646533494	6.910945757
78	10.630079670	7.117776405	7.315469031
78	8.224713790	7.047173885	9.704713249
78	6.090063359	7.916614876	8.680876020
78	6.316250683	9.848707644	10.264772690
78	7.763424245	8.956379122	7.194103767
78	8.859701116	9.248503680	10.931412542
78	10.763261867	8.072439284	9.629899042
8	8.871222566	9.743441261	5.829232936
8	9.032252493	10.248250755	12.407954032

PRE:4= -70.26361018

78	9.784791737	6.897084649	11.662754009
78	10.348130967	11.813622495	8.123902842
78	8.182226544	6.388850834	7.256319764
78	12.518267722	8.789106542	7.975790278
78	8.264290481	10.805301048	8.983878044
78	10.439372051	9.646533541	6.910945570
78	10.630079658	7.117776442	7.315468935
78	8.224713807	7.047173816	9.704713316
78	6.090063456	7.916614860	8.680875969
78	6.316250660	9.848707600	10.264772703
78	7.763424368	8.956379183	7.194103811
78	8.859701063	9.248503651	10.931412622
78	10.763261773	8.072439258	9.629898983
8	8.871222509	9.743441329	5.829232848
8	9.032252466	10.248250723	12.407954048

PRE:5= -71.39972970

78	9.625919225	6.510458891	11.400745172
78	9.839188432	12.169262622	8.006194686
78	7.856993997	6.139017233	7.182535850
78	12.429645747	8.385503148	7.792963650
78	7.963278801	10.748490984	9.137119456
78	10.375162789	9.825040911	7.691627105
78	10.157240970	7.235696353	7.304186225
78	7.869401637	6.652057128	9.600880809
78	5.881793134	7.870913095	8.611291047
78	6.115553670	9.596712369	10.429563680
78	8.002430394	8.734666310	7.515355453
78	8.586522800	8.808678052	10.677414681
78	10.791209578	7.956125861	9.715772071
8	7.510320208	4.759210264	6.139260765
8	8.595138327	12.576518429	9.375363837

PRE:6= -71.54678710

78	9.896773078	6.697835440	11.555526182
78	9.929631078	12.399125177	7.731155472
78	7.833042341	6.117047606	7.274135719
78	12.301541784	8.172254608	8.219245876
78	8.301156930	10.963067924	8.908986919

78	10.471242113	10.012132250	7.781338604
78	10.162061619	7.092413464	7.384645068
78	8.160848671	6.902123310	9.685892484
78	6.005241944	7.772842887	8.643384950
78	6.420132366	9.774991786	10.192278499
78	8.164418116	8.703064172	7.618750929
78	8.319271727	8.704253687	11.430210308
78	10.414717115	8.541338359	9.911212895
8	6.727479942	11.638256805	9.867198644
8	12.004966372	6.643516706	7.073294621

PRE:7= -70.93246376

78	9.365055525	6.680002593	11.433736285
78	9.376865049	12.174655839	7.630302418
78	7.852427377	5.953968009	6.948324345
78	12.349928039	8.138935920	7.688279888
78	7.777559845	10.691572423	8.818047619
78	10.301946682	9.637343608	7.636088712
78	10.116565077	7.003269620	7.154158064
78	7.537345548	6.557117486	9.707606288
78	5.626050353	7.914480754	8.634187762
78	6.057576338	9.701530387	10.334237145
78	7.854292689	8.447705223	7.546925761
78	8.503226431	8.847609563	10.431367721
78	10.725323287	7.763256701	9.591462123
8	7.277210501	5.044996639	8.521748758
8	10.079260444	11.017175738	6.294841411

PRE:8= -70.844444340

78	9.944129822	6.780601259	11.382763596
78	10.345117509	11.884280733	8.296630550
78	8.210082259	6.277013349	6.942824007
78	12.621744340	8.473748574	7.995548058
78	8.197720919	10.813885507	8.938936978
78	10.476873821	9.638390651	7.260367462
78	10.537517599	7.054255390	7.593344015
78	8.429863415	7.297512516	9.260863590
78	5.971833774	7.869236865	8.987633351
78	6.162711802	10.034876657	10.189906744
78	7.667335234	8.826808912	7.315028277
78	8.529733114	9.292683367	10.937344623
78	10.806588272	8.659840728	9.779319491
8	8.961562989	9.596868489	6.096472957
8	9.019271861	8.082482903	12.398621742

PRE:9= -70.87603623

78	9.616817680	6.847903488	11.373515896
78	10.196976438	12.047144626	7.977770907
78	8.310469698	6.244859956	7.184433902
78	12.648478671	8.718739738	7.926491032
78	8.255815559	10.862399788	8.932524371

78	10.445482873	9.714199792	7.282280610
78	10.626668417	7.140870884	7.576227112
78	8.019627957	7.347388604	9.465623272
78	5.708199846	8.109138722	8.615882759
78	6.455798061	9.684285119	10.380011325
78	7.718726438	8.843503549	7.293012717
78	9.050552613	9.329869491	10.885135690
78	11.038830523	8.194409399	9.822378765
8	9.033432561	9.435574792	6.034082845
8	7.553498931	10.139910447	11.900343177

PRE:10= -71.69741678

78	9.574798452	6.666318360	11.275831493
78	9.709658319	11.930235658	7.701123871
78	8.160223599	6.282551651	7.386831549
78	12.646189039	8.398225296	7.818775106
78	7.749688936	10.965502540	9.162006590
78	10.420356790	9.648317945	7.547318870
78	10.584242535	6.960907690	7.443105406
78	7.540552871	6.648293085	9.778235088
78	5.727239385	7.928474307	8.518602405
78	6.094036548	9.589754758	10.400973834
78	8.016756370	8.800773174	7.807044593
78	8.626679437	8.919703222	10.436184030
78	10.918629818	8.104514304	9.690043234
8	9.613458846	5.819117888	6.192308870
8	8.365151808	12.750859154	8.806298609

### 3. Pt<sub>13</sub>O<sub>3</sub>

PRE:1= -77.80654522

78	9.414173634	6.843956745	11.630469020
78	9.737532196	12.336213832	7.865137112
78	7.977703474	6.154139608	7.253526407
78	12.369175045	8.567199656	7.920910877
78	8.043148821	10.903446027	9.036827502
78	10.283552404	10.012413790	8.076625659
78	10.168948916	7.370097942	7.507312300
78	7.888787862	6.868279614	9.693658762
78	5.713149960	8.118856715	8.888391921
78	6.128348989	9.914621023	10.553433285
78	7.871913860	8.701491060	7.748993858
78	8.483244159	9.096028046	10.899845761
78	10.755617473	8.123997616	9.935681086
8	10.063031325	13.942929453	7.259318509
8	4.885659148	10.730515888	11.484773606
8	9.754618512	5.934770639	13.087316241

PRE:2= -77.19035049

78	9.452414528	6.830157031	11.303253086
78	9.623558434	12.328279105	7.531275061

78	7.848693100	6.269201394	7.023979420
78	12.351218482	8.669634050	7.693300514
78	7.974193681	10.967790250	8.850650894
78	10.240381177	10.031490758	7.845167026
78	10.175836563	7.433286908	7.024745605
78	7.707496681	6.884910083	9.500545471
78	5.699727985	8.098318491	8.487057777
78	6.057832275	9.872857915	10.223650472
78	7.913096893	8.782878545	7.499779115
78	8.442501428	9.099116463	10.570065211
78	10.703368794	8.084543652	9.532194128
8	10.001338672	13.952908951	6.994408333
8	10.603236924	6.468191596	5.584610808
8	4.913954854	10.781630414	11.221475629

PRE:3= -76.08865005

78	9.405688670	6.562657650	11.307394565
78	9.595655051	12.213849118	7.592174764
78	7.920530785	6.078079064	7.035926135
78	12.344298039	8.539165336	7.743176801
78	7.941682015	10.801213634	8.754926145
78	10.165197285	9.829151749	7.889086145
78	10.146409535	7.337680440	7.067058218
78	7.659425525	6.792627664	9.529410346
78	5.574323990	8.050264550	8.654626636
78	6.155471880	9.836769112	10.257143112
78	7.743327072	8.581323419	7.474135552
78	8.573639576	8.967190101	10.761241032
78	10.671668180	7.917983138	9.547913351
8	3.980307039	7.491701065	8.189994250
8	8.997196558	10.124200243	12.077038605
8	10.611294086	6.644976637	5.490282130

PRE:4= -75.85879011

78	9.871980102	6.601068758	11.297679535
78	9.885737499	12.191626162	7.673775752
78	8.014435811	5.942306560	7.165206932
78	12.474288055	8.408205731	7.578003223
78	8.271401438	10.642596516	8.727610611
78	10.414786323	9.783526363	7.554153681
78	10.285544560	7.175363312	7.194927325
78	8.185304956	7.062237361	9.456552063
78	5.958546610	7.963403706	8.671368553
78	6.480753974	9.815389982	10.297689802
78	7.874032073	8.550984382	7.115784123
78	8.970294923	9.051084731	10.899919837
78	10.884030361	8.113291823	9.547525531
8	7.553019183	9.107978785	5.446643026
8	8.648896905	10.070743970	12.347880192
8	14.159901404	8.303749330	7.114182411

PRE:5= -77.86929331

78	9.876032132	6.511156630	11.475908395
78	10.038696135	12.107400325	8.128599275
78	7.979948347	6.200897613	7.204233423
78	12.638794991	8.265619827	7.971418063
78	8.101764870	10.803399336	9.205946467
78	10.598556339	9.755167235	7.780716889
78	10.397718496	7.228845363	7.288507431
78	8.087760900	6.605781215	9.699792574
78	6.151600510	7.743458389	8.523311192
78	6.196459168	9.562397739	10.299710258
78	8.250971627	8.774786255	7.576065149
78	8.682777551	8.823623916	10.736914920
78	10.893848033	8.006272060	9.764886691
8	8.575397558	12.674816188	9.234533855
8	7.582339494	4.895676416	6.113842979
8	14.361685602	8.285046413	7.638385886

PRE:6= -77.31152610

78	9.436036723	6.823183063	11.791336182
78	9.419547720	12.298175753	7.801774536
78	7.890999481	6.223957327	7.239593396
78	12.409267120	8.270465868	8.047139308
78	8.021099963	10.797521626	9.168847726
78	10.527882980	9.919251416	7.838350946
78	10.171549959	7.298248785	7.434228400
78	7.664409555	7.023711000	9.668931375
78	5.595836290	8.188595794	8.566047350
78	6.257224247	9.582962114	10.540238910
78	7.935943637	8.735160705	7.742675903
78	8.821996554	9.241493304	11.162396715
78	10.643039647	7.955152905	9.885169715
8	11.189785672	11.675955102	7.517232266
8	7.265821149	9.974476757	12.135793157
8	7.917438331	5.844212327	11.188569958

PRE:7= -77.90855990

78	9.477254361	6.768265065	11.174033461
78	9.670994064	12.251591651	7.622145618
78	7.927992364	6.333971819	7.061290306
78	12.411068179	8.541445793	7.646414656
78	7.814783922	11.047333708	8.930403342
78	10.208669105	9.875029709	7.614433161
78	10.285326690	7.231116180	7.316945938
78	7.583128643	6.774666025	9.538114448
78	5.608689908	7.865516132	8.412926685
78	6.090494768	10.077430936	10.464399457
78	7.787915701	8.882315456	7.626794991
78	8.454633893	9.070624359	10.432982578
78	10.777169337	8.258704705	9.614703945
8	8.101729217	12.920564552	8.538242271



8	9.534568271	6.071329079	5.963332765
8	4.745312867	8.965954679	9.721015678

PRE:8= -77.71143778

78	9.713207469	6.703625819	11.173814146
78	9.654831923	12.184601374	7.622938377
78	7.673654504	6.246820573	7.205905193
78	12.263823493	8.497498052	7.352068557
78	7.954859891	10.961646484	8.950618161
78	10.177509157	9.800756505	7.970430687
78	10.087986577	7.166164004	7.292228154
78	7.688612333	6.942005404	9.670945875
78	5.714375129	7.667547987	8.186894532
78	6.059756877	9.962515538	10.267875624
78	7.818598314	8.847715443	7.564502662
78	8.365187508	9.209182230	10.887239369
78	11.080872119	7.948188585	9.513149684
8	4.802729113	8.780938728	9.491888376
8	8.967464959	8.029771955	12.306209913
8	9.175662448	6.083075278	5.961585025

PRE:9= -76.96813155

78	9.599656434	6.638631375	11.291734341
78	9.584722591	12.323137037	7.601220186
78	8.301422001	6.146841143	6.921801165
78	12.721678900	8.416313649	7.851794678
78	8.310398586	10.725428489	8.952485418
78	10.286275814	9.925080871	7.492032739
78	10.542607500	7.188951370	7.409989742
78	8.152433302	7.300608942	9.251487047
78	5.846787126	8.155349865	8.370667835
78	6.461486975	9.545259200	10.331715071
78	7.895913115	9.019649291	7.076067539
78	8.961263269	9.108720307	11.016329478
78	10.932930710	8.106395159	9.766790653
8	7.600439471	7.520052084	5.824441746
8	7.535444605	10.095106562	11.899822046
8	12.107598594	9.913935252	6.862158812

PRE:10= -77.11637720

78	9.620253438	6.675922862	11.589452506
78	9.863529806	12.138300596	7.685725240
78	8.110679064	6.085352179	7.038780899
78	12.598117359	8.367887804	7.788024972
78	8.071958922	10.851647923	8.981323768
78	10.521899820	9.797540583	7.728825375
78	10.325636765	7.337904414	7.000376420
78	7.839262848	6.599884437	9.832167217
78	5.956708776	7.953863083	8.666404742
78	6.298268198	9.747636571	10.360059108
78	8.208571147	8.578751806	7.734071760

78	8.799862682	8.900221870	10.519700517
78	11.079173292	7.863593716	9.955059794
8	8.265054651	12.743287393	8.546024595
8	7.611414796	5.124992446	8.608860274
8	12.986222773	7.823819253	9.575286050

#### 4. $\text{Pt}_{13}\text{O}_4$

PRE:1= -83.93827100

78	9.614769879	6.642857521	11.424176325
78	9.716292209	12.174309954	7.746896564
78	8.077555469	5.898992607	7.361759924
78	12.424628776	8.365997074	7.815167080
78	8.051678115	10.775687780	8.931390543
78	10.317041347	9.832624479	7.828390904
78	10.223497205	7.260264412	7.222727523
78	7.874302008	6.814759976	9.628283647
78	5.829178508	7.977382502	8.617463600
78	6.186970659	9.682855108	10.382466092
78	7.969312637	8.545348132	7.406851046
78	8.603318005	8.969884369	10.712824522
78	10.826569920	8.064013252	9.715472999
8	9.889900775	13.824478008	7.188880263
8	14.104435405	8.208365355	7.351137398
8	4.961124729	10.473780965	11.355271382
8	7.645867588	4.323759789	6.717566216

PRE:2= -83.67342305

78	9.712409588	6.705951852	11.211047851
78	9.623075801	12.616005648	7.493070458
78	7.669065418	6.488994872	7.026036001
78	12.297823105	8.367538919	8.039266437
78	8.171444843	11.265942151	8.971732882
78	10.006865638	10.164340850	7.534095134
78	10.043240969	7.302089578	7.483203537
78	7.724628070	7.057282239	9.599466702
78	5.603460805	7.585356599	8.309207669
78	6.034701382	9.847954568	9.535914661
78	7.730006472	8.996746544	7.649029018
78	8.130956498	9.240063655	10.961737804
78	10.341553254	8.645552021	9.664608382
8	9.365849431	5.984044227	6.237176132
8	9.027526326	8.118031171	12.303023522
8	6.459146087	11.715572199	9.827269419
8	11.982975646	10.019288783	7.186590262

PRE:3= -83.05033663

78	9.443280090	6.834246953	11.384318368
78	9.112241244	12.763810690	7.751011103
78	7.853479104	6.404014253	7.067394302
78	12.313495673	8.724590425	7.860182423

78	7.610008641	11.033814708	8.822468334
78	9.966116496	10.405661821	7.550650498
78	10.019749776	7.655262207	7.324977024
78	7.737253173	7.158951170	9.467052241
78	5.668690393	8.168377806	8.387848222
78	5.725641806	9.977754740	10.141580589
78	7.815626948	8.981699851	7.284735669
78	8.130647944	9.355488338	10.760327192
78	10.713486923	8.137424358	9.718209709
8	7.505346746	5.044919777	5.995851384
8	8.499509380	8.177132316	12.321118542
8	11.838606410	10.375320145	7.073964555
8	7.524579152	12.960454828	8.845188957

PRE:4= -83.02256612

78	9.501415435	6.705005236	11.400802729
78	9.418822077	12.699613153	7.959717021
78	7.725325881	6.507358936	7.258064180
78	12.380952318	8.574926175	7.766049000
78	7.928598348	11.068471372	9.020891197
78	10.040680930	10.341489241	7.572365654
78	10.012794704	7.646187249	7.624907628
78	7.685847803	7.226787679	9.685349093
78	5.710452304	8.152796915	8.378024583
78	5.831156387	10.056817179	10.039046534
78	7.848502604	9.057095638	7.378554187
78	8.032572226	9.365988120	11.032586586
78	11.194872582	7.749338001	9.862920812
8	7.338742280	5.126848506	6.269679740
8	8.811709323	8.218396115	12.359900721
8	11.839265229	10.216449461	6.969049299
8	12.404255567	8.121934542	11.133861761

## 5. Pt<sub>13</sub>O<sub>8</sub>

PRE:1= -106.19921517

78	8.765850311	7.237856971	11.512164149
78	8.959156402	12.966256903	7.817544690
78	7.537117675	6.580969268	6.976337298
78	11.870568338	8.991117068	7.718952939
78	7.471146576	11.296075463	8.978403537
78	9.793399486	10.586051566	7.775692140
78	9.609427629	7.789685558	7.664523554
78	7.510465519	7.494505408	9.354498013
78	5.223517813	8.569794235	8.721250918
78	5.873879822	10.108011345	10.533549915
78	7.377585312	9.187427396	7.318210390
78	8.409987419	9.626216252	10.800749041
78	10.536741911	8.350029157	9.990977487
8	7.109936245	5.124373755	6.107162907
8	8.576561734	6.267344152	12.949292080

8	11.602614852	10.781899118	7.106185119
8	12.094962096	8.343235846	10.849622714
8	6.711067529	10.112912111	5.934266036
8	3.629346604	7.997088720	8.331718948
8	7.300114373	13.184140138	8.769929495
8	8.406253244	10.711649517	12.236653694

PRE:2= -109.33789737

78	9.108529044	7.181408682	11.136421537
78	9.287224265	12.926698668	7.765320192
78	7.898170082	6.542980348	7.730207903
78	12.343718788	8.978997173	7.567170315
78	7.707920919	11.302806794	8.923107641
78	9.883846841	10.459488138	7.555763011
78	10.105282875	7.741424903	7.560681789
78	6.628371915	6.953281608	9.927205522
78	5.123990884	8.596182195	8.451938351
78	6.063531224	9.966071458	10.366369122
78	7.680636015	9.109215923	7.509281234
78	8.582483019	9.673923286	10.899980567
78	10.734901225	9.055304733	9.658314697
8	9.415465647	6.266703686	6.495567414
8	7.534479722	6.149591153	11.382091032
8	11.763368359	10.698499487	7.021144211
8	10.917231618	7.833294008	11.162270875
8	5.851121819	9.651428935	7.041052208
8	4.734702652	7.039794907	9.482575281
8	7.561172137	13.192811895	8.584717554
8	7.173572880	10.685143617	11.767877956

PRE:3= -108.30810548

78	9.248150992	7.189636773	11.168214326
78	9.397048436	12.920345894	7.921478617
78	7.964239877	6.606444683	7.498084541
78	12.465518536	8.859640407	7.604503500
78	7.886218905	11.308983847	8.921876778
78	9.956374474	10.523970579	7.579530516
78	10.216986868	7.672352106	7.483094293
78	7.116730154	7.583147723	9.664483660
78	4.776363049	8.255065595	8.641770213
78	6.072706842	9.902656648	10.207077302
78	7.685324297	9.173354616	7.465359710
78	8.562775647	9.786146565	10.935246977
78	10.798830272	9.022054418	9.593269016
8	9.463693263	6.301930317	6.320558061
8	7.462670219	6.470623532	11.213868687
8	11.743341487	10.411637894	6.804266640
8	11.044788504	7.769557501	11.076846989
8	5.759123966	9.009272292	7.210497391
8	3.463195533	7.292026631	9.318716917
8	9.481910545	14.522724809	7.178137617

8 9.028156785 10.693939253 12.396842401

PRE:4= -109.13684983

78	9.450155079	7.384926438	11.386530637
78	8.754714360	12.930425466	7.852378050
78	8.108528123	6.504428562	7.380722124
78	12.294011448	9.391221470	7.759883060
78	7.725301967	11.038252368	8.968400579
78	9.768741174	10.714483719	7.403335666
78	10.104022389	8.004151228	7.548972455
78	7.327353570	7.584888167	9.545380147
78	4.906526929	8.300739312	8.708566843
78	6.005909722	9.620768899	10.539212175
78	7.723972142	9.022511922	7.314813385
78	8.943510734	9.886671476	10.923533437
78	11.048280939	8.625014338	9.826642704
8	7.912847075	4.982048049	6.540918643
8	7.785241417	6.512334116	11.111334892
8	11.566439788	10.826111080	6.753579888
8	11.259146926	8.055089727	11.656540715
8	5.781316240	9.064567457	7.203171141
8	3.530040283	7.384435862	9.289275748
8	8.689994929	14.651508301	7.544368446
8	7.268306985	10.459186730	11.717819518

## 6. Pt<sub>13</sub>O<sub>12</sub>

PRE:1= -129.32486961

78	9.407274824	7.221198009	11.359475679
78	9.866424501	12.845681176	7.571014459
78	7.862628251	6.542200101	7.166344085
78	12.313210528	8.728030979	7.754545514
78	7.949483926	11.500930330	8.847837661
78	10.197889243	10.246287424	8.018993632
78	10.152994736	7.845136286	6.914904378
78	7.612324574	6.929594994	9.643055964
78	5.467917089	8.476779415	8.618464711
78	6.220014075	10.246394846	10.300680206
78	7.861311842	9.095258009	7.529723296
78	8.608018096	9.429066651	10.404601418
78	11.086311141	8.582602683	9.946783515
8	7.239396493	5.335407479	6.062673133
8	6.863641960	5.411896221	10.187554493
8	11.385002703	11.780988968	7.643566995
8	12.361869364	8.417893417	11.175465770
8	5.988455215	9.338179085	7.015617451
8	4.238688367	7.533775842	9.466037122
8	8.941364986	14.289775118	7.236002985
8	5.326346326	11.275263087	11.404991411
8	13.971431478	8.854734944	7.219423487
8	9.689905233	6.333373502	12.840609100

8	7.040098430	13.033981335	8.991440548
8	10.540984396	6.564377869	5.733629365

PRE:2= -135.56347028

78	9.249330618	7.377093061	11.751265463
78	9.696868894	12.379699989	7.851461861
78	7.656917790	7.065202962	6.872473360
78	12.540320854	8.392731564	7.695229125
78	7.542718423	11.731907798	9.191580517
78	10.411972514	9.890937604	7.441630873
78	10.383505391	7.357047340	6.588107212
78	7.322977207	6.335085250	10.073891118
78	5.260703400	7.776453587	9.550181998
78	5.446923525	10.310961353	10.124127285
78	7.892030925	9.649178101	7.655163124
78	8.052737641	9.315397763	10.163080337
78	10.722270889	9.079770371	9.962126992
8	9.006528700	6.238585968	5.876931523
8	8.582036771	5.647832124	11.321162845
8	11.346104815	11.606385463	7.420126659
8	10.932026375	8.213527069	11.705508293
8	6.509789671	8.636601654	6.835200083
8	6.264224275	6.524198936	8.438975505
8	8.146799718	13.341463266	8.192291938
8	4.096714777	8.978473872	10.398211682
8	12.636467947	9.044382633	9.435099128
8	8.170976431	8.894296022	12.075425995
8	5.966575174	12.100715348	10.309914169
8	12.301635055	7.306586522	6.188988457

PRE:3= -132.97025226

78	9.357928464	7.106095836	12.120726572
78	9.465301866	12.329274689	7.086554905
78	7.768366721	6.468263935	6.511743825
78	12.263659313	8.409537213	8.078665857
78	7.548145568	11.457150073	8.603583940
78	10.381024753	10.219090089	8.169967480
78	9.799453190	7.697577990	7.354392106
78	8.100584393	7.264253316	9.339725882
78	4.923162344	8.262226165	9.098087231
78	5.764381202	10.451445754	10.239082814
78	7.314141700	9.044880464	7.720543252
78	8.263157854	9.690574707	10.550515283
78	10.444750751	8.385144618	10.060910493
8	7.989475384	4.754419174	6.227196730
8	8.280988040	6.126742161	10.903504648
8	11.230020066	11.838882687	7.431225557
8	10.870375752	6.562583100	12.890027973
8	6.845249149	8.051380373	6.102243163
8	4.343727267	7.325115196	7.743611463
8	7.668879413	12.801751718	7.040610453

8	5.091321673	8.807098711	10.909780440
8	12.411945238	8.506863725	9.977256881
8	8.343106432	8.705559520	12.269744423
8	6.183128350	12.241558549	9.805589337
8	11.568129496	7.714068493	6.471810521

PRE:4= -133.38883368

78	9.205155150	7.059031001	11.805056470
78	9.886725202	12.756849094	7.398864488
78	8.113847225	6.562645095	6.452411360
78	12.494531191	8.399263349	7.396313556
78	8.124065660	11.286421246	8.706436123
78	10.270739523	10.161280164	7.696723325
78	10.083809134	7.577221415	7.731208546
78	7.103703224	6.881497625	10.131452177
78	5.538656968	8.647328639	9.128485483
78	5.690360060	11.073501547	10.005263024
78	7.713705939	8.867098746	7.846907646
78	8.165013772	9.381074466	10.492993999
78	10.658641959	8.842689411	9.905889678
8	8.484503011	4.871956231	6.197876539
8	8.105329494	5.636721002	11.240137026
8	11.439376473	11.709009146	7.616169051
8	10.926222679	7.810572699	11.547342923
8	7.380405299	8.226126837	6.022758307
8	5.444193173	6.710583625	9.165842245
8	9.044589786	14.217267653	6.950890963
8	4.293178097	10.656839685	10.997938104
8	12.505501602	8.482877471	9.258239295
8	8.457374968	8.742073135	12.331823051
8	6.695613593	12.469113275	9.272486422
8	13.201235987	8.556449321	5.798081969