

Hydroxy-Substituted Aromatic N-Heterocycles as High-Affinity CO₂ Adsorbents: A DFT Study

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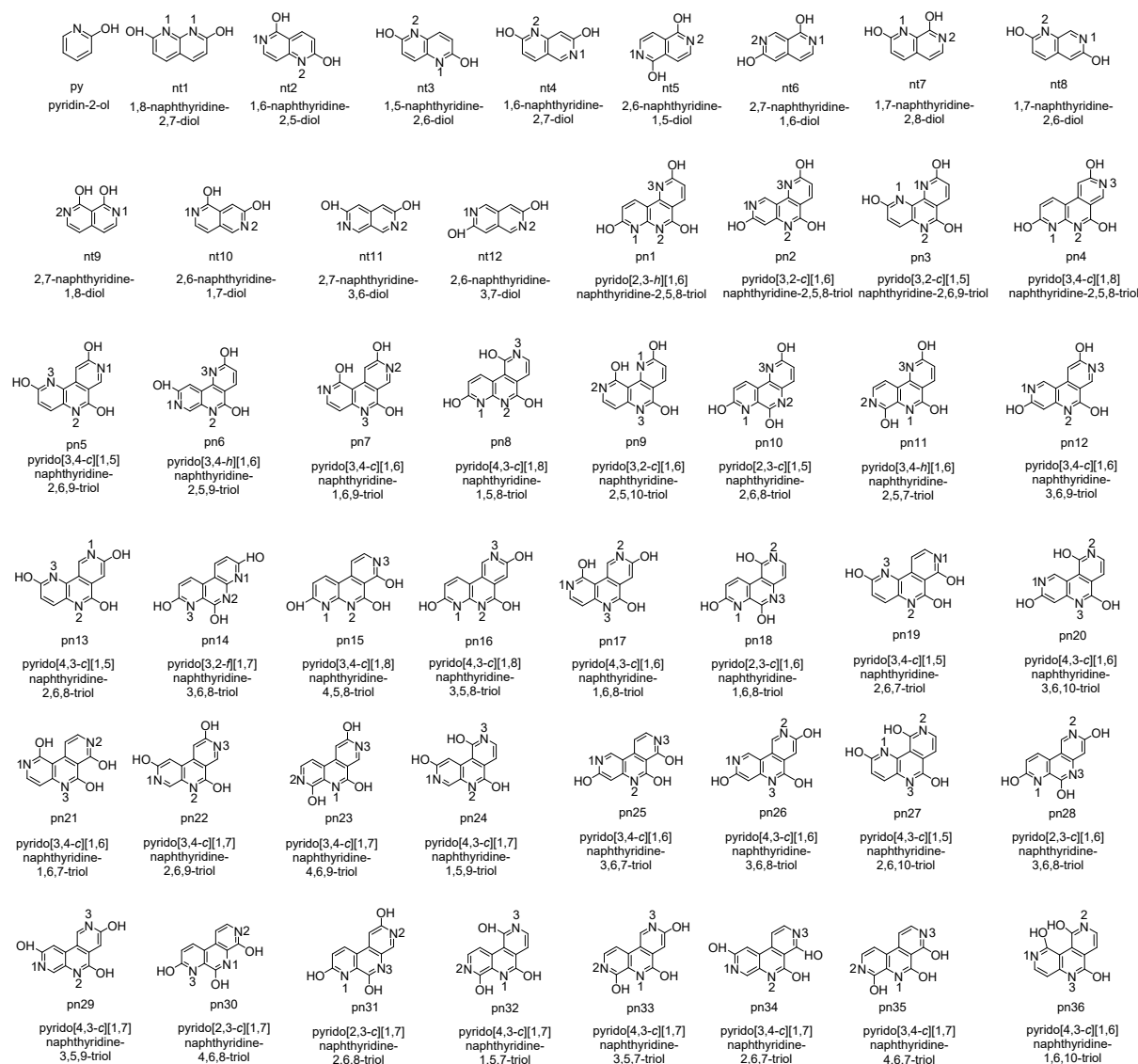


Figure S1. Chemical structures with IUPAC names of hydroxy pyridine (py), 12 dihydroxy naphthyridines (nt), and 36 trihydroxy pyridonaphthyridines (pn).

Table S1. SCF energies, zero-point correction, thermal correction to Gibbs, free energies and BSSE of all the systems under study. All values in au.

I. Neutral system

System	SCF energy	Zero-point correction	TC to Gibbs	e+Gibbs
CO ₂	-188.56728	0.009282 (Hartree/Particle)	-0.00646	-188.57374
py	-323.47756	0.094208 (Hartree/Particle)	0.06542	-323.41215
nt1	-568.38112	0.134262 (Hartree/Particle)	0.10057	-568.28055
nt2	-568.38031	0.134670 (Hartree/Particle)	0.10102	-568.27930
nt3	-568.37866	0.134261 (Hartree/Particle)	0.10060	-568.27805
nt4	-568.37644	0.134187 (Hartree/Particle)	0.10045	-568.27600
nt5	-568.37550	0.134800 (Hartree/Particle)	0.10115	-568.27434

nt6	-568.37467	0.134465 (Hartree/Particle)	0.10072	-568.27395
nt7	-568.37306	0.134312 (Hartree/Particle)	0.10059	-568.27247
nt8	-568.37236	0.133946 (Hartree/Particle)	0.10019	-568.27217
nt9	-568.37133	0.134741 (Hartree/Particle)	0.10096	-568.27037
nt10	-568.37075	0.134181 (Hartree/Particle)	0.10043	-568.27032
nt11	-568.37079	0.133944 (Hartree/Particle)	0.10011	-568.27068
nt12	-568.36469	0.133506 (Hartree/Particle)	0.09965	-568.26504
pn1	-813.28869	0.174728 (Hartree/Particle)	0.13642	-813.15228
pn2	-813.28465	0.174673 (Hartree/Particle)	0.13629	-813.14836
pn3	-813.28119	0.174624 (Hartree/Particle)	0.13631	-813.14488
pn4	-813.28204	0.174471 (Hartree/Particle)	0.13595	-813.14610
pn5	-813.28115	0.174581 (Hartree/Particle)	0.13624	-813.14490
pn6	-813.28075	0.174637 (Hartree/Particle)	0.13633	-813.14442
pn7	-813.28033	0.174852 (Hartree/Particle)	0.13639	-813.14394
pn8	-813.27994	0.174866 (Hartree/Particle)	0.13648	-813.14346
pn9	-813.27957	0.174851 (Hartree/Particle)	0.13639	-813.14319
pn10	-813.28018	0.174369 (Hartree/Particle)	0.13600	-813.14417
pn11	-813.28037	0.174849 (Hartree/Particle)	0.13653	-813.14384
pn12	-813.27877	0.174429 (Hartree/Particle)	0.13584	-813.14293
pn13	-813.27850	0.174282 (Hartree/Particle)	0.13589	-813.14262
pn14	-813.27811	0.174386 (Hartree/Particle)	0.13592	-813.14220
pn15	-813.27686	0.174740 (Hartree/Particle)	0.13613	-813.14073
pn16	-813.27673	0.174275 (Hartree/Particle)	0.13577	-813.14096
pn17	-813.27598	0.174764 (Hartree/Particle)	0.13630	-813.13968
pn18	-813.27767	0.174797 (Hartree/Particle)	0.13634	-813.14133
pn19	-813.27623	0.174788 (Hartree/Particle)	0.13639	-813.13984
pn20	-813.27593	0.174847 (Hartree/Particle)	0.13640	-813.13953
pn21	-813.27443	0.175100 (Hartree/Particle)	0.13648	-813.13795
pn22	-813.27473	0.174493 (Hartree/Particle)	0.13603	-813.13871
pn23	-813.27410	0.174667 (Hartree/Particle)	0.13619	-813.13791
pn24	-813.27374	0.174703 (Hartree/Particle)	0.13631	-813.13743
pn25	-813.27321	0.174597 (Hartree/Particle)	0.13591	-813.13730
pn26	-813.27327	0.174235 (Hartree/Particle)	0.13564	-813.13762
pn27	-813.27347	0.174637 (Hartree/Particle)	0.13622	-813.13726
pn28	-813.27452	0.174376 (Hartree/Particle)	0.13584	-813.13868
pn29	-813.27241	0.174197 (Hartree/Particle)	0.13567	-813.13674
pn30	-813.27234	0.174605 (Hartree/Particle)	0.13616	-813.13619
pn31	-813.27311	0.174285 (Hartree/Particle)	0.13582	-813.13729

pn32	-813.27270	0.175061 (Hartree/Particle)	0.13668	-813.13603
pn33	-813.27135	0.174504 (Hartree/Particle)	0.13602	-813.13534
pn34	-813.26900	0.174634 (Hartree/Particle)	0.13607	-813.13294
pn35	-813.26865	0.174912 (Hartree/Particle)	0.13632	-813.13233
pn36	-813.26399	0.174976 (Hartree/Particle)	0.13689	-813.12710

II. 1CO₂ complex

System	SCF energy	Zero-point correction	TC to Gibbs	e+Gibbs	BSSE
py...CO ₂	-512.06286	0.107309 (Hartree/Particle)	0.07091	-511.99196	0.00077
nt1...CO ₂	-756.96614	0.147510 (Hartree/Particle)	0.10592	-756.86021	0.00093
nt2...CO ₂	-756.96587	0.147701 (Hartree/Particle)	0.10656	-756.85931	0.00089
nt3...CO ₂	-756.96363	0.147359 (Hartree/Particle)	0.10570	-756.85792	0.00089
nt4...CO ₂	-756.96153	0.147264 (Hartree/Particle)	0.10606	-756.85548	0.00075
nt5...CO ₂	-756.96087	0.147915 (Hartree/Particle)	0.10688	-756.85399	0.00082
nt6...CO ₂	-756.96019	0.147528 (Hartree/Particle)	0.10631	-756.85387	0.00076
nt7...CO ₂	-756.95783	0.147576 (Hartree/Particle)	0.10662	-756.85121	0.00118
nt8...CO ₂	-756.95719	0.147114 (Hartree/Particle)	0.10589	-756.85130	0.00072
nt9...CO ₂	-756.95650	0.147689 (Hartree/Particle)	0.10636	-756.85014	0.00076
nt10...CO ₂	-756.95607	0.147259 (Hartree/Particle)	0.10604	-756.85004	0.00075
nt11...CO ₂	-756.95576	0.146955 (Hartree/Particle)	0.10556	-756.85021	0.00073
nt12...CO ₂	-756.94944	0.146677 (Hartree/Particle)	0.10530	-756.84414	0.00075
pn1...CO ₂	-1001.87371	0.187781 (Hartree/Particle)	0.14148	-1001.73224	0.00097
pn2...CO ₂	-1001.86985	0.187714 (Hartree/Particle)	0.14180	-1001.72805	0.00076
pn3...CO ₂	-1001.86822	0.187834 (Hartree/Particle)	0.14190	-1001.72645	0.00119
pn4...CO ₂	-1001.86698	0.187634 (Hartree/Particle)	0.14117	-1001.72581	0.00092
pn5...CO ₂	-1001.86599	0.187568 (Hartree/Particle)	0.14171	-1001.72428	0.00077
pn6...CO ₂	-1001.86568	0.187537 (Hartree/Particle)	0.14167	-1001.72402	0.00074
pn7...CO ₂	-1001.86567	0.187969 (Hartree/Particle)	0.14215	-1001.72352	0.00077
pn8...CO ₂	-1001.86487	0.187948 (Hartree/Particle)	0.14155	-1001.72333	0.00091
pn9...CO ₂	-1001.86484	0.187834 (Hartree/Particle)	0.14190	-1001.72294	0.00075
pn10...CO ₂	-1001.86478	0.187642 (Hartree/Particle)	0.14209	-1001.72269	0.00113
pn11...CO ₂	-1001.86438	0.187832 (Hartree/Particle)	0.14375	-1001.72063	0.00092
pn12...CO ₂	-1001.86395	0.187512 (Hartree/Particle)	0.14134	-1001.72261	0.00076
pn13...CO ₂	-1001.86331	0.187465 (Hartree/Particle)	0.14159	-1001.72172	0.00072
pn14...CO ₂	-1001.86303	0.187339 (Hartree/Particle)	0.14050	-1001.72254	0.00092
pn15...CO ₂	-1001.86187	0.187707 (Hartree/Particle)	0.14104	-1001.72083	0.00093
pn16...CO ₂	-1001.86160	0.187246 (Hartree/Particle)	0.14021	-1001.72139	0.00092
pn17...CO ₂	-1001.86134	0.187867 (Hartree/Particle)	0.14204	-1001.71930	0.00078

pn18...CO ₂	-1001.86131	0.187840 (Hartree/Particle)	0.14358	-1001.71773	0.00090
pn19...CO ₂	-1001.86127	0.187733 (Hartree/Particle)	0.14188	-1001.71940	0.00079
pn20...CO ₂	-1001.86110	0.187814 (Hartree/Particle)	0.14189	-1001.71922	0.00079
pn21...CO ₂	-1001.85975	0.188113 (Hartree/Particle)	0.14207	-1001.71767	0.00074
pn22...CO ₂	-1001.85959	0.187417 (Hartree/Particle)	0.14139	-1001.71820	0.00073
pn23...CO ₂	-1001.85921	0.187896 (Hartree/Particle)	0.14237	-1001.71684	0.00125
pn24...CO ₂	-1001.85864	0.187843 (Hartree/Particle)	0.14201	-1001.71662	0.00069
pn25...CO ₂	-1001.85845	0.187552 (Hartree/Particle)	0.14136	-1001.71710	0.00075
pn26...CO ₂	-1001.85843	0.187335 (Hartree/Particle)	0.14123	-1001.71720	0.00071
pn27...CO ₂	-1001.85839	0.187645 (Hartree/Particle)	0.14176	-1001.71663	0.00077
pn28...CO ₂	-1001.85814	0.187462 (Hartree/Particle)	0.14306	-1001.71507	0.00089
pn29...CO ₂	-1001.85737	0.187459 (Hartree/Particle)	0.14153	-1001.71584	0.00071
pn30...CO ₂	-1001.85725	0.187912 (Hartree/Particle)	0.14237	-1001.71488	0.00125
pn31...CO ₂	-1001.85691	0.187224 (Hartree/Particle)	0.13878	-1001.71813	0.00095
pn32...CO ₂	-1001.85675	0.188057 (Hartree/Particle)	0.14382	-1001.71293	0.00092
pn33...CO ₂	-1001.85631	0.187733 (Hartree/Particle)	0.14212	-1001.71420	0.00123
pn34...CO ₂	-1001.85383	0.187638 (Hartree/Particle)	0.14158	-1001.71224	0.00073
pn35...CO ₂	-1001.85360	0.188070 (Hartree/Particle)	0.14241	-1001.71119	0.00129
pn36...CO ₂	-1001.84930	0.188069 (Hartree/Particle)	0.14265	-1001.70665	0.00076

III. Monocarboxylic acid

System	SCF energy	Zero-point correction	TC to Gibbs	e+Gibbs
py'-COOH	-512.03316	0.109171 (Hartree/Particle)	0.07518	-511.95798
nt1'-COOH	-756.94417	0.148650 (Hartree/Particle)	0.11113	-756.83305
nt2'-COOH	-756.96022	0.149082 (Hartree/Particle)	0.11157	-756.84865
nt3'-COOH	-756.94329	0.148684 (Hartree/Particle)	0.11121	-756.83208
nt4'-COOH	-756.94176	0.147630 (Hartree/Particle)	0.11018	-756.83159
nt5'-COOH	-756.95309	0.149340 (Hartree/Particle)	0.11185	-756.84124
nt6'-COOH	-756.95582	0.149107 (Hartree/Particle)	0.11149	-756.84432
nt7'-COOH	-756.93196	0.149109 (Hartree/Particle)	0.11206	-756.81990
nt8'-COOH	-756.93526	0.147610 (Hartree/Particle)	0.11018	-756.82508
nt9'-COOH	-756.94914	0.149129 (Hartree/Particle)	0.11138	-756.83776
nt10'-COOH	-756.94991	0.148944 (Hartree/Particle)	0.11135	-756.83856
nt11'-COOH	-756.93430	0.147101 (Hartree/Particle)	0.10955	-756.82476
nt12'-COOH	-756.92374	0.146606 (Hartree/Particle)	0.10904	-756.81470
pn1'-COOH	-1001.84993	0.188931 (Hartree/Particle)	0.14691	-1001.70302
pn2'-COOH	-1001.85318	0.188271 (Hartree/Particle)	0.14618	-1001.70700

pn3'-COOH	-1001.83982	0.189263 (Hartree/Particle)	0.14768	-1001.69214
pn4'-COOH	-1001.84183	0.188783 (Hartree/Particle)	0.14660	-1001.69524
pn5'-COOH	-1001.84660	0.188220 (Hartree/Particle)	0.14611	-1001.70049
pn6'-COOH	-1001.84616	0.188227 (Hartree/Particle)	0.14617	-1001.69999
pn7'-COOH	-1001.85782	0.189102 (Hartree/Particle)	0.14672	-1001.71110
pn8'-COOH	-1001.83940	0.189066 (Hartree/Particle)	0.14696	-1001.69243
pn9'-COOH	-1001.85616	0.188980 (Hartree/Particle)	0.14650	-1001.70966
pn10'-COOH	-1001.83598	0.189018 (Hartree/Particle)	0.14741	-1001.68858
pn11'-COOH	-1001.84576	0.189798 (Hartree/Particle)	0.14824	-1001.69751
pn12'-COOH	-1001.84682	0.188170 (Hartree/Particle)	0.14581	-1001.70101
pn13'-COOH	-1001.84300	0.188160 (Hartree/Particle)	0.14612	-1001.69688
pn14'-COOH	-1001.83826	0.188741 (Hartree/Particle)	0.14660	-1001.69166
pn15'-COOH	-1001.83758	0.188980 (Hartree/Particle)	0.14663	-1001.69095
pn16'-COOH	-1001.83566	0.188553 (Hartree/Particle)	0.14637	-1001.68929
pn17'-COOH	-1001.85277	0.189008 (Hartree/Particle)	0.14666	-1001.70611
pn18'-COOH	-1001.83204	0.189467 (Hartree/Particle)	0.14781	-1001.68423
pn19'-COOH	-1001.85113	0.188996 (Hartree/Particle)	0.14662	-1001.70451
pn20'-COOH	-1001.84456	0.188560 (Hartree/Particle)	0.14647	-1001.69809
pn21'-COOH	-1001.85275	0.189244 (Hartree/Particle)	0.14662	-1001.70613
pn22'-COOH	-1001.83993	0.188242 (Hartree/Particle)	0.14598	-1001.69395
pn23'-COOH	-1001.84024	0.189821 (Hartree/Particle)	0.14815	-1001.69209
pn24'-COOH	-1001.83983	0.188580 (Hartree/Particle)	0.14645	-1001.69337
pn25'-COOH	-1001.84090	0.188249 (Hartree/Particle)	0.14586	-1001.69504
pn26'-COOH	-1001.84114	0.188075 (Hartree/Particle)	0.14575	-1001.69539
pn27'-COOH	-1001.83286	0.189333 (Hartree/Particle)	0.14841	-1001.68445
pn28'-COOH	-1001.82871	0.188983 (Hartree/Particle)	0.14723	-1001.68148
pn29'-COOH	-1001.83915	0.188262 (Hartree/Particle)	0.14600	-1001.69316
pn30'-COOH	-1001.83491	0.189676 (Hartree/Particle)	0.14797	-1001.68694
pn31'-COOH	-1001.82696	0.188885 (Hartree/Particle)	0.14715	-1001.67981
pn32'-COOH	-1001.83613	0.190038 (Hartree/Particle)	0.14842	-1001.68771
pn33'-COOH	-1001.83597	0.189692 (Hartree/Particle)	0.14796	-1001.68801
pn34'-COOH	-1001.83336	0.188236 (Hartree/Particle)	0.14585	-1001.68751
pn35'-COOH	-1001.83231	0.189758 (Hartree/Particle)	0.14787	-1001.68444
pn36'-COOH	-1001.84134	0.189615 (Hartree/Particle)	0.14791	-1001.69343

IV. 2CO₂ complex

System	SCF energy	Zero-point correction	TC to Gibbs	e+Gibbs	BSSE
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nt1...2CO ₂	-945.55287	0.160972 (Hartree/Particle)	0.11463	-945.43824	0.00244
nt2...2CO ₂	-945.55083	0.160899 (Hartree/Particle)	0.11244	-945.43840	0.00164
nt3...2CO ₂	-945.54852	0.160539 (Hartree/Particle)	0.11152	-945.43700	0.00173
nt4...2CO ₂	-945.54652	0.160468 (Hartree/Particle)	0.11153	-945.43499	0.00165
nt5...2CO ₂	-945.54609	0.161079 (Hartree/Particle)	0.11256	-945.43353	0.00151
nt6...2CO ₂	-945.54503	0.160541 (Hartree/Particle)	0.11170	-945.43333	0.00151
nt7...2CO ₂	-945.54309	0.160664 (Hartree/Particle)	0.11231	-945.43077	0.00192
nt8...2CO ₂	-945.54180	0.160373 (Hartree/Particle)	0.11123	-945.43057	0.00162
nt9...2CO ₂	-945.54170	0.160766 (Hartree/Particle)	0.11199	-945.42971	0.00157
nt10...2CO ₂	-945.54084	0.160354 (Hartree/Particle)	0.11166	-945.42918	0.00149
nt11...2CO ₂	-945.54071	0.159936 (Hartree/Particle)	0.11092	-945.42979	0.00148
nt12...2CO ₂	-945.53412	0.159673 (Hartree/Particle)	0.11087	-945.42326	0.00148
pn1...2CO ₂	-1190.46075	0.201401 (Hartree/Particle)	0.15081	-1190.30994	0.00250
pn2...2CO ₂	-1190.45503	0.200811 (Hartree/Particle)	0.14734	-1190.30769	0.00170
pn3...2CO ₂	-1190.44754	0.200338 (Hartree/Particle)	0.14569	-1190.30186	0.00198
pn4...2CO ₂	-1190.45400	0.201177 (Hartree/Particle)	0.15027	-1190.30373	0.00255
pn5...2CO ₂	-1190.45119	0.200567 (Hartree/Particle)	0.14689	-1190.30430	0.00169
pn6...2CO ₂	-1190.45054	0.200665 (Hartree/Particle)	0.14712	-1190.30342	0.00166
pn7...2CO ₂	-1190.45049	0.200924 (Hartree/Particle)	0.14752	-1190.30298	0.00153
pn8...2CO ₂	-1190.45172	0.201512 (Hartree/Particle)	0.15075	-1190.30098	0.00253
pn9...2CO ₂	-1190.45191	0.201303 (Hartree/Particle)	0.14971	-1190.30220	0.00249
pn10...2CO ₂	-1190.44859	0.200730 (Hartree/Particle)	0.14910	-1190.29949	0.00178
pn11...2CO ₂	-1190.45078	0.201101 (Hartree/Particle)	0.14823	-1190.30254	0.00200
pn12...2CO ₂	-1190.44910	0.200564 (Hartree/Particle)	0.14688	-1190.30222	0.00176
pn13...2CO ₂	-1190.44828	0.200486 (Hartree/Particle)	0.14693	-1190.30136	0.00163
pn14...2CO ₂	-1190.44966	0.201019 (Hartree/Particle)	0.15013	-1190.29953	0.00249
pn15...2CO ₂	-1190.44840	0.201334 (Hartree/Particle)	0.15036	-1190.29804	0.00258
pn16...2CO ₂	-1190.44846	0.200924 (Hartree/Particle)	0.15002	-1190.29843	0.00253
pn17...2CO ₂	-1190.44611	0.200892 (Hartree/Particle)	0.14751	-1190.29861	0.00156
pn18...2CO ₂	-1190.44770	0.201120 (Hartree/Particle)	0.14828	-1190.29942	0.00191
pn19...2CO ₂	-1190.44590	0.200830 (Hartree/Particle)	0.14713	-1190.29877	0.00172
pn20...2CO ₂	-1190.44604	0.200758 (Hartree/Particle)	0.14727	-1190.29877	0.00156
pn21...2CO ₂	-1190.44471	0.201050 (Hartree/Particle)	0.14741	-1190.29731	0.00152
pn22...2CO ₂	-1190.44443	0.200468 (Hartree/Particle)	0.14659	-1190.29784	0.00172
pn23...2CO ₂	-1190.44433	0.200927 (Hartree/Particle)	0.14791	-1190.29643	0.00197
pn24...2CO ₂	-1190.44320	0.200962 (Hartree/Particle)	0.14700	-1190.29619	0.00168
pn25...2CO ₂	-1190.44300	0.200709 (Hartree/Particle)	0.14673	-1190.29627	0.00171
pn26...2CO ₂	-1190.44334	0.200440 (Hartree/Particle)	0.14689	-1190.29645	0.00165

pn27...2CO ₂	-1190.44550	0.201102 (Hartree/Particle)	0.14962	-1190.29588	0.00251
pn28...2CO ₂	-1190.44340	0.200338 (Hartree/Particle)	0.14855	-1190.29486	0.00165
pn29...2CO ₂	-1190.44200	0.200465 (Hartree/Particle)	0.14651	-1190.29549	0.00169
pn30...2CO ₂	-1190.44262	0.200889 (Hartree/Particle)	0.14788	-1190.29474	0.00209
pn31...2CO ₂	-1190.44187	0.200202 (Hartree/Particle)	0.14492	-1190.29695	0.00170
pn32...2CO ₂	-1190.44295	0.201304 (Hartree/Particle)	0.14841	-1190.29455	0.00197
pn33...2CO ₂	-1190.44156	0.200832 (Hartree/Particle)	0.14782	-1190.29374	0.00198
pn34...2CO ₂	-1190.43807	0.200599 (Hartree/Particle)	0.14614	-1190.29193	0.00173
pn35...2CO ₂	-1190.43881	0.201123 (Hartree/Particle)	0.14802	-1190.29079	0.00208
pn36...2CO ₂	-1190.43429	0.201062 (Hartree/Particle)	0.14826	-1190.28604	0.00162

V. Monocarboxylic acid- CO₂ complex

System	SCF energy	Zero-point correction	TC to Gibbs	e+Gibbs	BSSE
nt1'-COOH...CO ₂	-945.53124	0.162004 (Hartree/Particle)	0.11873	-945.41251	0.00128
nt2'-COOH...CO ₂	-945.54502	0.162243 (Hartree/Particle)	0.11730	-945.42773	0.00091
nt3'-COOH...CO ₂	-945.52767	0.161862 (Hartree/Particle)	0.11680	-945.41087	0.00079
nt4'-COOH...CO ₂	-945.52677	0.160861 (Hartree/Particle)	0.11579	-945.41098	0.00093
nt5'-COOH...CO ₂	-945.53454	0.161989 (Hartree/Particle)	0.11689	-945.41764	0.00068
nt6'-COOH...CO ₂	-945.54055	0.162119 (Hartree/Particle)	0.11702	-945.42353	0.00079
nt7'-COOH...CO ₂	-945.51684	0.162258 (Hartree/Particle)	0.11785	-945.39898	0.00075
nt8'-COOH...CO ₂	-945.52005	0.160750 (Hartree/Particle)	0.11561	-945.40444	0.00099
nt9'-COOH...CO ₂	-945.53396	0.162030 (Hartree/Particle)	0.11672	-945.41724	0.00081
nt10'-COOH...CO ₂	-945.53454	0.161989 (Hartree/Particle)	0.11689	-945.41764	0.00075
nt11'-COOH...CO ₂	-945.51889	0.160140 (Hartree/Particle)	0.11507	-945.40383	0.00075
nt12'-COOH...CO ₂	-945.50799	0.159524 (Hartree/Particle)	0.11437	-945.39363	0.00074
pn1'-COOH...CO ₂	-1190.43736	0.202334 (Hartree/Particle)	0.15460	-1190.28276	0.00137
pn2'-COOH...CO ₂	-1190.43834	0.201325 (Hartree/Particle)	0.15167	-1190.28667	0.00097
pn3'-COOH...CO ₂	-1190.42639	0.202303 (Hartree/Particle)	0.15428	-1190.27212	0.00131
pn4'-COOH...CO ₂	-1190.42767	0.201938 (Hartree/Particle)	0.15239	-1190.27529	0.00118
pn5'-COOH...CO ₂	-1190.43183	0.201223 (Hartree/Particle)	0.15167	-1190.28016	0.00093
pn6'-COOH...CO ₂	-1190.43111	0.201421 (Hartree/Particle)	0.15194	-1190.27918	0.00097
pn7'-COOH...CO ₂	-1190.44250	0.202003 (Hartree/Particle)	0.15199	-1190.29051	0.00077
pn8'-COOH...CO ₂	-1190.42663	0.202425 (Hartree/Particle)	0.15462	-1190.27201	0.00144
pn9'-COOH...CO ₂	-1190.44103	0.201914 (Hartree/Particle)	0.15172	-1190.28932	0.00093
pn10'-COOH...CO ₂	-1190.42082	0.202206 (Hartree/Particle)	0.15329	-1190.26753	0.00097
pn11'-COOH...CO ₂	-1190.43084	0.202833 (Hartree/Particle)	0.15392	-1190.27692	0.00090
pn12'-COOH...CO ₂	-1190.43190	0.201342 (Hartree/Particle)	0.15148	-1190.28042	0.00098

pn13'–COOH...CO ₂	-1190.42793	0.201278 (Hartree/Particle)	0.15172	-1190.27621	0.00092
pn14'–COOH...CO ₂	-1190.42528	0.202108 (Hartree/Particle)	0.15421	-1190.27107	0.00141
pn15'–COOH...CO ₂	-1190.42312	0.202088 (Hartree/Particle)	0.15242	-1190.27071	0.00123
pn16'–COOH...CO ₂	-1190.42153	0.201667 (Hartree/Particle)	0.15186	-1190.26967	0.00119
pn17'–COOH...CO ₂	-1190.43728	0.201924 (Hartree/Particle)	0.15192	-1190.28536	0.00074
pn18'–COOH...CO ₂	-1190.41736	0.202426 (Hartree/Particle)	0.15341	-1190.26396	0.00103
pn19'–COOH...CO ₂	-1190.43559	0.201801 (Hartree/Particle)	0.15118	-1190.28441	0.00083
pn20'–COOH...CO ₂	-1190.42935	0.201523 (Hartree/Particle)	0.15191	-1190.27745	0.00104
pn21'–COOH...CO ₂	-1190.43761	0.202296 (Hartree/Particle)	0.15231	-1190.28530	0.00074
pn22'–COOH...CO ₂	-1190.42484	0.201287 (Hartree/Particle)	0.15141	-1190.27344	0.00103
pn23'–COOH...CO ₂	-1190.42516	0.202850 (Hartree/Particle)	0.15376	-1190.27140	0.00083
pn24'–COOH...CO ₂	-1190.42451	0.201774 (Hartree/Particle)	0.15211	-1190.27240	0.00104
pn25'–COOH...CO ₂	-1190.42553	0.201314 (Hartree/Particle)	0.15116	-1190.27437	0.00104
pn26'–COOH...CO ₂	-1190.42609	0.201207 (Hartree/Particle)	0.15137	-1190.27471	0.00098
pn27'–COOH...CO ₂	-1190.41790	0.202318 (Hartree/Particle)	0.15402	-1190.26388	0.00087
pn28'–COOH...CO ₂	-1190.41383	0.202027 (Hartree/Particle)	0.15290	-1190.26093	0.00076
pn29'–COOH...CO ₂	-1190.42386	0.201249 (Hartree/Particle)	0.15114	-1190.27272	0.00104
pn30'–COOH...CO ₂	-1190.41993	0.202642 (Hartree/Particle)	0.15351	-1190.26642	0.00081
pn31'–COOH...CO ₂	-1190.41170	0.201797 (Hartree/Particle)	0.15257	-1190.25913	0.00075
pn32'–COOH...CO ₂	-1190.42116	0.203053 (Hartree/Particle)	0.15403	-1190.26713	0.00082
pn33'–COOH...CO ₂	-1190.42109	0.202758 (Hartree/Particle)	0.15366	-1190.26743	0.00089
pn34'–COOH...CO ₂	-1190.41772	0.201205 (Hartree/Particle)	0.15072	-1190.26701	0.00105
pn35'–COOH...CO ₂	-1190.41725	0.202878 (Hartree/Particle)	0.15366	-1190.26360	0.00082
pn36'–COOH...CO ₂	-1190.42620	0.202601 (Hartree/Particle)	0.15352	-1190.27268	0.00087

VI. Dicarboxylic acid

System	SCF energy	Zero-point correction	TC to Gibbs	e+Gibbs
nt1''–(COOH) ₂	-945.49734	0.162862 (Hartree/Particle)	0.12273	-945.37461
nt2''–(COOH) ₂	-945.51781	0.162735 (Hartree/Particle)	0.12234	-945.39548
nt3''–(COOH) ₂	-945.49877	0.162957 (Hartree/Particle)	0.12210	-945.37667
nt4''–(COOH) ₂	-945.50936	0.162880 (Hartree/Particle)	0.12143	-945.38793
nt5''–(COOH) ₂	-945.52509	0.163665 (Hartree/Particle)	0.12234	-945.40275
nt6''–(COOH) ₂	-945.52140	0.163083 (Hartree/Particle)	0.12158	-945.39981
nt7''–(COOH) ₂	-945.50333	0.163828 (Hartree/Particle)	0.12301	-945.38032
nt8''–(COOH) ₂	-945.50087	0.162877 (Hartree/Particle)	0.12141	-945.37946
nt9''–(COOH) ₂	-945.52089	0.163040 (Hartree/Particle)	0.12116	-945.39973
nt10''–(COOH) ₂	-945.51236	0.163122 (Hartree/Particle)	0.12168	-945.39068

nt11''-(COOH) ₂	-945.49177	0.159227 (Hartree/Particle)	0.11778	-945.37400
pn1''-(COOH) ₂	-1190.41036	0.203465 (Hartree/Particle)	0.15877	-1190.25159
pn2''-(COOH) ₂	-1190.42291	0.203400 (Hartree/Particle)	0.15747	-1190.26544
pn3''-(COOH) ₂	-1190.39719	0.203490 (Hartree/Particle)	0.15880	-1190.23840
pn4''-(COOH) ₂	-1190.40310	0.203471 (Hartree/Particle)	0.15858	-1190.24451
pn5''-(COOH) ₂	-1190.41736	0.203379 (Hartree/Particle)	0.15762	-1190.25974
pn6''-(COOH) ₂	-1190.41479	0.203481 (Hartree/Particle)	0.15765	-1190.25714
pn7''-(COOH) ₂	-1190.42161	0.202776 (Hartree/Particle)	0.15674	-1190.26487
pn8''-(COOH) ₂	-1190.39802	0.203664 (Hartree/Particle)	0.15881	-1190.23921
pn9''-(COOH) ₂	-1190.41949	0.203439 (Hartree/Particle)	0.15706	-1190.26243
pn10''-(COOH) ₂	-1190.39969	0.203761 (Hartree/Particle)	0.15833	-1190.24135
pn11''-(COOH) ₂	-1190.41799	0.204438 (Hartree/Particle)	0.15917	-1190.25882
pn12''-(COOH) ₂	-1190.41584	0.203504 (Hartree/Particle)	0.15748	-1190.25836
pn13''-(COOH) ₂	-1190.40780	0.202609 (Hartree/Particle)	0.15724	-1190.25056
pn14''-(COOH) ₂	-1190.39596	0.203313 (Hartree/Particle)	0.15843	-1190.23753
pn15''-(COOH) ₂	-1190.39598	0.203491 (Hartree/Particle)	0.15845	-1190.23753
pn16''-(COOH) ₂	-1190.39620	0.203434 (Hartree/Particle)	0.15855	-1190.23765
pn17''-(COOH) ₂	-1190.41489	0.202740 (Hartree/Particle)	0.15663	-1190.25825
pn18''-(COOH) ₂	-1190.40990	0.203717 (Hartree/Particle)	0.15806	-1190.25184
pn19''-(COOH) ₂	-1190.41428	0.203132 (Hartree/Particle)	0.15664	-1190.25764
pn20''-(COOH) ₂	-1190.41469	0.202712 (Hartree/Particle)	0.15658	-1190.25811
pn21''-(COOH) ₂	-1190.42656	0.203552 (Hartree/Particle)	0.15683	-1190.26973
pn22''-(COOH) ₂	-1190.40825	0.203547 (Hartree/Particle)	0.15761	-1190.25064
pn23''-(COOH) ₂	-1190.41127	0.204455 (Hartree/Particle)	0.15903	-1190.25224
pn24''-(COOH) ₂	-1190.40505	0.203828 (Hartree/Particle)	0.15798	-1190.24707
pn25''-(COOH) ₂	-1190.40845	0.203443 (Hartree/Particle)	0.15713	-1190.25132
pn26''-(COOH) ₂	-1190.40874	0.203298 (Hartree/Particle)	0.15722	-1190.25151
pn27''-(COOH) ₂	-1190.40782	0.204019 (Hartree/Particle)	0.15924	-1190.24859
pn28''-(COOH) ₂	-1190.39343	0.202608 (Hartree/Particle)	0.15722	-1190.23620
pn29''-(COOH) ₂	-1190.40512	0.203411 (Hartree/Particle)	0.15742	-1190.24769
pn30''-(COOH) ₂	-1190.40705	0.204252 (Hartree/Particle)	0.15882	-1190.24823
pn31''-(COOH) ₂	-1190.38968	0.202450 (Hartree/Particle)	0.15695	-1190.23273
pn32''-(COOH) ₂	-1190.40817	0.204665 (Hartree/Particle)	0.15933	-1190.24885
pn33''-(COOH) ₂	-1190.40822	0.204385 (Hartree/Particle)	0.15899	-1190.24923
pn34''-(COOH) ₂	-1190.39998	0.203514 (Hartree/Particle)	0.15731	-1190.24267
pn35''-(COOH) ₂	-1190.40360	0.204443 (Hartree/Particle)	0.15882	-1190.24478

pn36''-(COOH)₂ -1190.41446 0.204233 (Hartree/Particle) 0.15872 -1190.25574

VII. 3CO₂ complex

System	SCF energy	Zero-point correction	TC to Gibbs	e+Gibbs	BSSE
pn1...3CO ₂	-1379.04149	0.214239 (Hartree/Particle)	0.15447	-1378.88703	0.00334
pn2...3CO ₂	-1379.03838	0.214045 (Hartree/Particle)	0.15383	-1378.88454	0.00312
pn3...3CO ₂	-1379.03268	0.213527 (Hartree/Particle)	0.15127	-1378.88141	0.00284
pn4...3CO ₂	-1379.03887	0.214173 (Hartree/Particle)	0.15591	-1378.88296	0.00330
pn5...3CO ₂	-1379.03397	0.213733 (Hartree/Particle)	0.15330	-1378.88067	0.00291
pn6...3CO ₂	-1379.03319	0.213882 (Hartree/Particle)	0.15324	-1378.87995	0.00288
pn7...3CO ₂	-1379.03551	0.214020 (Hartree/Particle)	0.15319	-1378.88232	0.00246
pn8...3CO ₂	-1379.03671	0.214440 (Hartree/Particle)	0.15628	-1378.88043	0.00324
pn9...3CO ₂	-1379.03696	0.214411 (Hartree/Particle)	0.15537	-1378.88159	0.00342
pn10...3CO ₂	-1379.03120	0.213564 (Hartree/Particle)	0.15467	-1378.87653	0.00295
pn11...3CO ₂	-1379.03047	0.213795 (Hartree/Particle)	0.15282	-1378.87765	0.00259
pn12...3CO ₂	-1379.03390	0.213619 (Hartree/Particle)	0.15242	-1378.88148	0.00247
pn13...3CO ₂	-1379.03158	0.213842 (Hartree/Particle)	0.15405	-1378.87753	0.00298
pn14...3CO ₂	-1379.03435	0.214124 (Hartree/Particle)	0.15614	-1378.87822	0.00369
pn15...3CO ₂	-1379.03339	0.214186 (Hartree/Particle)	0.15560	-1378.87779	0.00336
pn16...3CO ₂	-1379.03335	0.213941 (Hartree/Particle)	0.15568	-1378.87767	0.00327
pn17...3CO ₂	-1379.03096	0.214024 (Hartree/Particle)	0.15326	-1378.87770	0.00247
pn18...3CO ₂	-1379.03251	0.214322 (Hartree/Particle)	0.15396	-1378.87856	0.00287
pn19...3CO ₂	-1379.02638	0.213427 (Hartree/Particle)	0.15332	-1378.87307	0.00259
pn20...3CO ₂	-1379.03086	0.213817 (Hartree/Particle)	0.15263	-1378.87823	0.00251
pn21...3CO ₂	-1379.02915	0.214123 (Hartree/Particle)	0.15292	-1378.87623	0.00251
pn22...3CO ₂	-1379.02918	0.213450 (Hartree/Particle)	0.15205	-1378.87713	0.00249
pn23...3CO ₂	-1379.02907	0.213887 (Hartree/Particle)	0.15324	-1378.87583	0.00275
pn24...3CO ₂	-1379.02812	0.213915 (Hartree/Particle)	0.15269	-1378.87544	0.00246
pn25...3CO ₂	-1379.02795	0.213608 (Hartree/Particle)	0.15220	-1378.87575	0.00251
pn26...3CO ₂	-1379.02814	0.213306 (Hartree/Particle)	0.15198	-1378.87615	0.00245
pn27...3CO ₂	-1379.02707	0.213837 (Hartree/Particle)	0.15248	-1378.87459	0.00287
pn28...3CO ₂	-1379.02916	0.213602 (Hartree/Particle)	0.15307	-1378.87610	0.00290
pn29...3CO ₂	-1379.02678	0.213339 (Hartree/Particle)	0.15183	-1378.87495	0.00244
pn30...3CO ₂	-1379.02726	0.213995 (Hartree/Particle)	0.15397	-1378.87329	0.00325
pn31...3CO ₂	-1379.02719	0.213420 (Hartree/Particle)	0.15361	-1378.87457	0.00266
pn32...3CO ₂	-1379.02793	0.214236 (Hartree/Particle)	0.15400	-1378.87393	0.00276
pn33...3CO ₂	-1379.02639	0.213798 (Hartree/Particle)	0.15331	-1378.87308	0.00273
pn34...3CO ₂	-1379.02287	0.213508 (Hartree/Particle)	0.15144	-1378.87143	0.00248

pn35...3CO ₂	-1379.02367	0.214066 (Hartree/Particle)	0.15351	-1378.87016	0.00288
pn36...3CO ₂	-1379.01921	0.214215 (Hartree/Particle)	0.15402	-1378.86519	0.00252

VIII. Dicarboxylic acid-CO₂ complex

System	SCF energy	Zero-point correction	TC to Gibbs	e+Gibbs	BSSE
pn1''-(COOH) ₂ ...CO ₂	-1378.99284	0.216392 (Hartree/Particle)	0.16430	-1378.82854	0.00121
pn2''-(COOH) ₂ ...CO ₂	-1379.00676	0.216669 (Hartree/Particle)	0.16393	-1378.84283	0.00136
pn3''-(COOH) ₂ ...CO ₂	-1378.98204	0.216600 (Hartree/Particle)	0.16458	-1378.81746	0.00094
pn4''-(COOH) ₂ ...CO ₂	-1378.98775	0.216584 (Hartree/Particle)	0.16430	-1378.82345	0.00079
pn5''-(COOH) ₂ ...CO ₂	-1378.99976	0.216401 (Hartree/Particle)	0.16330	-1378.83645	0.00134
pn6''-(COOH) ₂ ...CO ₂	-1378.99754	0.216547 (Hartree/Particle)	0.16356	-1378.83398	0.00125
pn7''-(COOH) ₂ ...CO ₂	-1379.00667	0.215921 (Hartree/Particle)	0.16241	-1378.84426	0.00094
pn8''-(COOH) ₂ ...CO ₂	-1378.98283	0.216657 (Hartree/Particle)	0.16441	-1378.81842	0.00080
pn9''-(COOH) ₂ ...CO ₂	-1379.00456	0.216581 (Hartree/Particle)	0.16279	-1378.84178	0.00116
pn10''-(COOH) ₂ ...CO ₂	-1378.97993	0.216564 (Hartree/Particle)	0.16157	-1378.81836	0.00082
pn11''-(COOH) ₂ ...CO ₂	-1379.00019	0.217425 (Hartree/Particle)	0.16481	-1378.83538	0.00106
pn12''-(COOH) ₂ ...CO ₂	-1379.00042	0.216457 (Hartree/Particle)	0.16290	-1378.83752	0.00079
pn13''-(COOH) ₂ ...CO ₂	-1378.99309	0.215969 (Hartree/Particle)	0.16125	-1378.83184	0.00078
pn14''-(COOH) ₂ ...CO ₂	-1378.98070	0.216368 (Hartree/Particle)	0.16439	-1378.81631	0.00125
pn15''-(COOH) ₂ ...CO ₂	-1378.98063	0.216510 (Hartree/Particle)	0.16408	-1378.81654	0.00080
pn16''-(COOH) ₂ ...CO ₂	-1378.98091	0.216363 (Hartree/Particle)	0.16403	-1378.81688	0.00076
pn17''-(COOH) ₂ ...CO ₂	-1378.99967	0.215926 (Hartree/Particle)	0.16264	-1378.83703	0.00086
pn18''-(COOH) ₂ ...CO ₂	-1378.99453	0.216913 (Hartree/Particle)	0.16401	-1378.83052	0.00092
pn19''-(COOH) ₂ ...CO ₂	-1378.99684	0.216155 (Hartree/Particle)	0.16235	-1378.83448	0.00092
pn20''-(COOH) ₂ ...CO ₂	-1378.99957	0.215702 (Hartree/Particle)	0.16200	-1378.83757	0.00095
pn21''-(COOH) ₂ ...CO ₂	-1379.01063	0.216461 (Hartree/Particle)	0.16183	-1378.84880	0.00096
pn22''-(COOH) ₂ ...CO ₂	-1378.99275	0.216593 (Hartree/Particle)	0.16314	-1378.82961	0.00080
pn23''-(COOH) ₂ ...CO ₂	-1378.99582	0.217383 (Hartree/Particle)	0.16438	-1378.83144	0.00080
pn24''-(COOH) ₂ ...CO ₂	-1378.98965	0.216861 (Hartree/Particle)	0.16368	-1378.82597	0.00079
pn25''-(COOH) ₂ ...CO ₂	-1378.99305	0.216402 (Hartree/Particle)	0.16263	-1378.83042	0.00082
pn26''-(COOH) ₂ ...CO ₂	-1378.99315	0.216186 (Hartree/Particle)	0.16250	-1378.83065	0.00078
pn27''-(COOH) ₂ ...CO ₂	-1378.99253	0.217113 (Hartree/Particle)	0.16495	-1378.82758	0.00101
pn28''-(COOH) ₂ ...CO ₂	-1378.97852	0.215820 (Hartree/Particle)	0.16326	-1378.81527	0.00114
pn29''-(COOH) ₂ ...CO ₂	-1378.98966	0.216430 (Hartree/Particle)	0.16288	-1378.82678	0.00079
pn30''-(COOH) ₂ ...CO ₂	-1378.99200	0.217404 (Hartree/Particle)	0.16493	-1378.82707	0.00124
pn31''-(COOH) ₂ ...CO ₂	-1378.97441	0.215655 (Hartree/Particle)	0.16284	-1378.81157	0.00112
pn32''-(COOH) ₂ ...CO ₂	-1378.99291	0.217653 (Hartree/Particle)	0.16500	-1378.82791	0.00081

pn33''-(COOH) ₂ ...CO ₂	-1378.99287	0.217370 (Hartree/Particle)	0.16441	-1378.82847	0.00078
pn34''-(COOH) ₂ ...CO ₂	-1378.98441	0.216456 (Hartree/Particle)	0.16272	-1378.82170	0.00082
pn35''-(COOH) ₂ ...CO ₂	-1378.98808	0.217354 (Hartree/Particle)	0.16426	-1378.82383	0.00081
pn36''-(COOH) ₂ ...CO ₂	-1378.99922	0.217405 (Hartree/Particle)	0.16462	-1378.83460	0.00086

IX. Tricarboxylic acid

System	SCF energy	Zero-point correction	TC to Gibbs	e+Gibbs
pn1'''-(COOH) ₃	-1378.95836	0.217769 (Hartree/Particle)	0.16988	-1378.78848
pn2'''-(COOH) ₃	-1378.96756	0.217538 (Hartree/Particle)	0.16845	-1378.79911
pn3'''-(COOH) ₃	-1378.95569	0.217654 (Hartree/Particle)	0.16911	-1378.78658
pn4'''-(COOH) ₃	-1378.96833	0.217591 (Hartree/Particle)	0.16892	-1378.79941
pn5'''-(COOH) ₃	-1378.96060	0.217924 (Hartree/Particle)	0.16908	-1378.79152
pn6'''-(COOH) ₃	-1378.95912	0.217792 (Hartree/Particle)	0.16879	-1378.79033
pn7'''-(COOH) ₃	-1378.98709	0.218136 (Hartree/Particle)	0.16850	-1378.81859
pn8'''-(COOH) ₃	-1378.96811	0.217854 (Hartree/Particle)	0.16907	-1378.79903
pn9'''-(COOH) ₃	-1378.97859	0.218368 (Hartree/Particle)	0.17001	-1378.80858
pn10'''-(COOH) ₃	-1378.94528	0.218151 (Hartree/Particle)	0.16983	-1378.77544
pn11'''-(COOH) ₃	-1378.96413	0.218648 (Hartree/Particle)	0.17008	-1378.79405
pn12'''-(COOH) ₃	-1378.98083	0.217623 (Hartree/Particle)	0.16777	-1378.81305
pn13'''-(COOH) ₃	-1378.95379	0.217692 (Hartree/Particle)	0.16883	-1378.78496
pn14'''-(COOH) ₃	-1378.94652	0.217972 (Hartree/Particle)	0.16967	-1378.77685
pn15'''-(COOH) ₃	-1378.96567	0.217454 (Hartree/Particle)	0.16838	-1378.79729
pn16'''-(COOH) ₃	-1378.95882	0.217619 (Hartree/Particle)	0.16896	-1378.78987
pn17'''-(COOH) ₃	-1378.97944	0.218041 (Hartree/Particle)	0.16838	-1378.81105
pn18'''-(COOH) ₃	-1378.96765	0.218301 (Hartree/Particle)	0.16890	-1378.79875
pn19'''-(COOH) ₃	-1378.96012	0.217990 (Hartree/Particle)	0.16881	-1378.79132
pn20'''-(COOH) ₃	-1378.97982	0.218003 (Hartree/Particle)	0.16815	-1378.81168
pn21'''-(COOH) ₃	-1378.98377	0.218169 (Hartree/Particle)	0.16803	-1378.81574
pn22'''-(COOH) ₃	-1378.97223	0.217758 (Hartree/Particle)	0.16803	-1378.80420
pn23'''-(COOH) ₃	-1378.97573	0.218539 (Hartree/Particle)	0.16925	-1378.80648
pn24'''-(COOH) ₃	-1378.97245	0.217997 (Hartree/Particle)	0.16824	-1378.80422
pn25'''-(COOH) ₃	-1378.97676	0.217465 (Hartree/Particle)	0.16703	-1378.80974
pn26'''-(COOH) ₃	-1378.97030	0.217515 (Hartree/Particle)	0.16765	-1378.80265
pn27'''-(COOH) ₃	-1378.96611	0.218576 (Hartree/Particle)	0.17029	-1378.79583
pn28'''-(COOH) ₃	-1378.95976	0.217943 (Hartree/Particle)	0.16847	-1378.79129
pn29'''-(COOH) ₃	-1378.96763	0.217606 (Hartree/Particle)	0.16787	-1378.79975
pn30'''-(COOH) ₃	-1378.95725	0.218691 (Hartree/Particle)	0.16983	-1378.78742

pn31'''-(COOH) ₃	-1378.95483	0.217953 (Hartree/Particle)	0.16867	-1378.78616
pn32'''-(COOH) ₃	-1378.97679	0.218939 (Hartree/Particle)	0.16972	-1378.80707
pn33'''-(COOH) ₃	-1378.97145	0.218581 (Hartree/Particle)	0.16945	-1378.80201
pn34'''-(COOH) ₃	-1378.96583	0.217578 (Hartree/Particle)	0.16742	-1378.79841
pn35'''-(COOH) ₃	-1378.97037	0.218377 (Hartree/Particle)	0.16870	-1378.80167
pn36'''-(COOH) ₃	-1378.97666	0.218787 (Hartree/Particle)	0.16970	-1378.80697

X. Anionic system

System	SCF energy	Zero-point correction	TC to Gibbs	e+Gibbs	BSSE
py ⁻	-322.91198	0.07966(Hartree/Particle)	0.05078	-322.86120	
(py-CO ₂ ⁻) _O	-511.50616	0.09488(Hartree/Particle)	0.06074	-511.44542	0.00190
(py-CO ₂ ⁻) _N	-511.50805	0.09480(Hartree/Particle)	0.06114	-511.44691	0.00233
(py-CO ₂ ⁻) _O ...CO ₂	-700.09584	0.10829(Hartree/Particle)	0.06692	-700.02892	0.00064
(py-CO ₂ ⁻) _N ...CO ₂	-700.09715	0.10813(Hartree/Particle)	0.06703	-700.03012	0.00060
(py...(CO ₂ ⁻) ₂) _{N&O}	-700.09100	0.10582(Hartree/Particle)	0.05996	-700.03103	0.00152
nt5 ⁻	-567.82996	0.12059(Hartree/Particle)	0.08679	-567.74317	
(nt5...CO ₂) _O	-756.41730	0.13365(Hartree/Particle)	0.09101	-756.32629	0.00084
(nt5-CO ₂ ⁻) _N	-756.42122	0.13541(Hartree/Particle)	0.09695	-756.32427	0.00230
(nt5-CO ₂ ⁻) _N ...CO ₂	-945.00976	0.14866(Hartree/Particle)	0.10281	-944.90694	0.00063
((CO ₂)...nt5-(CO ₂ ⁻)) _{N&O}	-945.01245	0.14877(Hartree/Particle)	0.10393	-944.90853	0.00113
nt5 ²⁻	-567.15475	0.10663(Hartree/Particle)	0.07294	-567.08181	
(nt5 ⁻ -CO ₂ ⁻) _O	-755.76696	0.12159(Hartree/Particle)	0.08143	-755.68535	0.00206
(nt5 ⁻ -CO ₂ ⁻) _N	-755.77629	0.12210(Hartree/Particle)	0.08391	-755.69238	0.00247
(nt5-(CO ₂ ⁻) ₂) _{O&O}	-944.36691	0.13547(Hartree/Particle)	0.08958	-944.27733	0.00174
(nt5-(CO ₂ ⁻) ₂) _{N&N}	-944.38628	0.13699(Hartree/Particle)	0.09426	-944.29202	0.00241
(nt5-(CO ₂ ⁻) ₂) _{O&N}	-944.37712	0.13630(Hartree/Particle)	0.09198	-944.28515	0.00243
(nt5-CO ₂ ⁻) _N ...(CO ₂) _O	-944.37220	0.13540(Hartree/Particle)	0.09051	-944.28170	0.00290
(nt5-(CO ₂ ⁻) ₂) _{N&N} ...(CO ₂) _O	-1132.98029	0.15020(Hartree/Particle)	0.10042	-1132.87989	0.00100
(nt5-(CO ₂ ⁻) ₂) _{N&N} ...CO ₂	-1132.97818	0.13540(Hartree/Particle)	0.09051	-1132.87811	0.00061
(nt5-(CO ₂ ⁻) ₂) _{O&O} ...CO ₂	-1132.95822	0.14889(Hartree/Particle)	0.09643	-1132.86182	0.00066
(nt5-(CO ₂ ⁻) ₂) _{N&O} -(CO ₂) _O	-1132.97127	0.14952(Hartree/Particle)	0.09865	-1132.87261	0.00283
pn36 ⁻	-812.71656	0.16072(Hartree/Particle)	0.12261	-812.59395	
(pn36...CO ₂ ⁻) _O	-1001.30789	0.17378(Hartree/Particle)	0.12849	-1001.17940	0.00077
(pn36...CO ₂ ⁻) _O	-1001.31035	0.17397(Hartree/Particle)	0.12910	-1001.18126	0.00111
(pn36...CO ₂ ⁻) _O	-1001.31953	0.17419(Hartree/Particle)	0.12772	-1001.19181	0.00085
(pn36-CO ₂ ⁻) _N	-1001.30738	0.17546(Hartree/Particle)	0.13284	-1001.17453	0.00226

$(\text{pn}36\text{-CO}_2^-)_\text{N}$	-1001.30993	0.17550(Hartree/Particle)	0.13288	-1001.17706	0.00226
$(\text{pn}36\text{-CO}_2^-)_\text{N}$	-1001.31614	0.17538(Hartree/Particle)	0.13208	-1001.18406	0.00250
$(\text{pn}36\text{-CO}_2^-)_\text{N}\dots(\text{CO}_2)_\text{O}$	-1189.89437	0.18813(Hartree/Particle)	0.13869	-1189.75569	0.00131
$(\text{pn}36\text{-CO}_2^-)_\text{N}\dots\text{CO}_2$	-1189.89977	0.18884(Hartree/Particle)	0.14115	-1189.75862	0.00177
$\text{pn}36^{2-}$	-812.05154	0.14636(Hartree/Particle)	0.10814	-811.94341	
$(\text{pn}36\text{-CO}_2^-)_\text{O}$	-1000.6505	0.16080(Hartree/Particle)	0.11738	-1000.53311	0.00184
$(\text{pn}36\text{-CO}_2^-)_\text{N}$	-1000.665	0.16161(Hartree/Particle)	0.11892	-1000.54607	0.00241
$(\text{pn}36\text{-CO}_2^-)_\text{O}\dots(\text{CO}_2)_\text{O}$	-1189.2471	0.17415(Hartree/Particle)	0.12462	-1189.12248	0.00233
$(\text{pn}36\text{-CO}_2^-)_\text{O}\text{-CO}_2^-$	-1189.2392	0.17557(Hartree/Particle)	0.12659	-1189.11265	0.00161
$((\text{pn}36\text{-CO}_2)_2^-)_{\text{N}\&\text{N}}$	-1189.2683	0.17641(Hartree/Particle)	0.12920	-1189.13907	0.00245
$(\text{pn}36\text{-CO}_2^-)_\text{N}\dots\text{CO}_2$	-1189.2568	0.17469(Hartree/Particle)	0.12490	-1189.13191	0.00069
$(\text{pn}36\text{-CO}_2^-)_\text{N}\dots(\text{CO}_2)_\text{O}$	-1189.2585	0.17487(Hartree/Particle)	0.12543	-1189.13304	0.00123
$(\text{pn}36\text{-CO}_2^-)_\text{N}\dots(\text{CO}_2)_\text{O}$	-1189.259	0.17470(Hartree/Particle)	0.12514	-1189.13384	0.00090
$((\text{pn}36\text{-CO}_2)_2^-)_{\text{N}\&\text{N}}\dots(\text{CO}_2)_\text{O}$	-1377.8627	0.18978(Hartree/Particle)	0.13739	-1377.72533	0.00153
$((\text{pn}36\text{-CO}_2)_2^-)_{\text{N}\&\text{N}}\dots\text{CO}_2$	-1377.8599	0.18965(Hartree/Particle)	0.13533	-1377.72458	0.00069
$((\text{pn}36\text{-CO}_2)_2^-)_{\text{N}\&\text{N}}\text{-(CO}_2)_\text{N}$	-1377.8513	0.18948(Hartree/Particle)	0.13853	-1377.71277	0.00271
$\text{pn}36^{3-}$	-811.27775	0.13264(Hartree/Particle)	0.09458	-811.18317	
$(\text{pn}36^{2-}\text{-CO}_2^-)_\text{O}$	-999.90785	0.14770(Hartree/Particle)	0.10439	-999.80346	0.00209
$(\text{pn}36^{2-}\text{-CO}_2^-)_\text{O}$	-999.90536	0.14758(Hartree/Particle)	0.10441	-999.80095	0.00202
$(\text{pn}36^{2-}\text{-CO}_2^-)_\text{O}$	-999.90964	0.14754(Hartree/Particle)	0.10402	-999.80562	0.00227
$(\text{pn}36^{2-}\text{-CO}_2^-)_\text{N}$	-999.92095	0.14826(Hartree/Particle)	0.10575	-999.81520	0.00253
$(\text{pn}36^{2-}\text{-CO}_2^-)_\text{N}$	-999.91814	0.14811(Hartree/Particle)	0.10556	-999.81258	0.00255
$(\text{pn}36^{2-}\text{-CO}_2^-)_\text{N}$	-999.91392	0.14780(Hartree/Particle)	0.10525	-999.80867	0.00253
$(\text{pn}36\text{-CO}_2)_2^-)_{\text{O}\&\text{O}}$	-1188.5252	0.16213(Hartree/Particle)	0.11350	-1188.41172	0.00222
$(\text{pn}36\text{-CO}_2)_2^-)_{\text{O}\&\text{O}}$	-1188.5211	0.16226(Hartree/Particle)	0.11406	-1188.40703	0.00215
$((\text{pn}36\text{-CO}_2)_2^-)_{\text{N}\&\text{N}}$	-1188.5517	0.16353(Hartree/Particle)	0.11649	-1188.43518	0.00257
$((\text{pn}36\text{-CO}_2)_2^-)_{\text{N}\&\text{N}}$	-1188.5446	0.16308(Hartree/Particle)	0.11604	-1188.42853	0.00251
$((\text{pn}36\text{-CO}_2)_2^-)_{\text{N}\&\text{N}}$	-1188.5443	0.16303(Hartree/Particle)	0.11595	-1188.42833	0.00250
$((\text{pn}36\text{-CO}_2)_2^-)_{\text{O}\&\text{N}}$	-1188.5406	0.16272(Hartree/Particle)	0.11428	-1188.42635	0.00190
$((\text{pn}36\text{-CO}_2)_2^-)_{\text{O}\&\text{N}}$	-1188.5389	0.16266(Hartree/Particle)	0.11458	-1188.42434	0.00220
$((\text{pn}36\text{-CO}_2)_2^-)_{\text{O}\&\text{N}}$	-1188.5362	0.16288(Hartree/Particle)	0.11536	-1188.42089	0.00208
$((\text{pn}36\text{-CO}_2)_2^-)_{\text{O}\&\text{N}}$	-1188.5354	0.16291(Hartree/Particle)	0.11530	-1188.42013	0.00209
$((\text{pn}36\text{-CO}_2)_2^-)_{\text{O}\&\text{N}}$	-1188.5325	0.16253(Hartree/Particle)	0.11472	-1188.41782	0.00199
$((\text{pn}36\text{-CO}_2)_2^-)_{\text{N}\&\text{N}}$	-1188.5308	0.16248(Hartree/Particle)	0.11476	-1188.41602	0.00199
$(\text{pn}36^{2-}\text{-CO}_2^-)_\text{N}\dots(\text{CO}_2)_\text{O}$	-1188.5158	0.16129(Hartree/Particle)	0.11188	-1188.40395	0.00129
$((\text{pn}36\text{-CO}_2)_2^-)_{\text{O}\&\text{N}}$	-1188.5145	0.16223(Hartree/Particle)	0.11588	-1188.39860	0.00256
$((\text{pn}36\text{-CO}_2)_2^-)_{\text{O}\&\text{N}}$	-1188.5091	0.16149(Hartree/Particle)	0.11431	-1188.39484	0.00223

$(\text{pn36}-(\text{CO}_2)_3)^{3-}_{\text{N\&N\&N}}$	-1377.1654	0.17806(Hartree/Particle)	0.12639	-1377.03901	0.00243
$(\text{pn36}-(\text{CO}_2)_3)^{3-}_{\text{O\&O\&N}}$	-1377.1359	0.17664(Hartree/Particle)	0.12365	-1377.01222	0.00251
$(\text{pn36}-(\text{CO}_2)_3)^{3-}_{\text{O\&O\&O}}$	-1377.1295	0.17619(Hartree/Particle)	0.12261	-1377.00691	0.00186
$((\text{pn36}-(\text{CO}_2)_2)^{-}_{\text{O\&O}}-\text{CO}_2^{-})$	-1377.1264	0.17727(Hartree/Particle)	0.12408	-1377.00227	0.00184
$(\text{pn36}-(\text{CO}_2)_3)^{3-}_{\text{N\&N\&N}\cdots(\text{CO}_2)_\text{O}}$	-1565.7622	0.19136(Hartree/Particle)	0.13449	-1565.62771	0.00151
$(\text{pn36}-(\text{CO}_2)_3)^{3-}_{\text{N\&N\&N}^-(\text{CO}_2)_\text{O}}$	-1565.7616	0.19208(Hartree/Particle)	0.13467	-1565.62689	0.00193
$(\text{pn36}-(\text{CO}_2)_3)^{3-}_{\text{N\&N\&N}^-\text{CO}_2}$	-1565.761	0.19202(Hartree/Particle)	0.13460	-1565.62644	0.00193
$(\text{pn36}-(\text{CO}_2)_3)^{3-}_{\text{N\&N\&N}\cdots(\text{CO}_2)_\text{O}}$	-1565.7592	0.19123(Hartree/Particle)	0.13282	-1565.62642	0.00119
$(\text{pn36}-(\text{CO}_2)_3)^{3-}_{\text{N\&N\&N}\cdots(\text{CO}_2)_\text{O}}$	-1565.7591	0.19128(Hartree/Particle)	0.13341	-1565.62565	0.00108
$(\text{pn36}-(\text{CO}_2)_3)^{3-}_{\text{N\&N\&N}^-\text{CO}_2}$	-1565.7581	0.19174(Hartree/Particle)	0.13410	-1565.62402	0.00154
$(\text{pn36}-(\text{CO}_2)_3)^{3-}_{\text{N\&N\&N}^-\text{CO}_2}$	-1565.7574	0.19170(Hartree/Particle)	0.13418	-1565.62324	0.00152
$(\text{pn36}-(\text{CO}_2)_3)^{3-}_{\text{N\&N\&N}^-\text{CO}_2}$	-1565.7568	0.191967 (Hartree/Particle)	0.13511	-1565.62167	0.00180
$(\text{pn36}-(\text{CO}_2)_3)^{3-}_{\text{O\&O\&N}\cdots(\text{CO}_2)_\text{O}}$	-1565.7423	0.19014(Hartree/Particle)	0.13132	-1565.61098	0.00278
$(\text{pn36}-(\text{CO}_2)_3)^{3-}_{\text{O\&O\&N}\cdots(\text{CO}_2)_\text{O}}$	-1565.7411	0.19011(Hartree/Particle)	0.13128	-1565.60984	0.00269
$(\text{pn36}-(\text{CO}_2)_3)^{3-}_{\text{O\&O\&N}\cdots(\text{CO}_2)_\text{O}}$	-1565.7303	0.18986(Hartree/Particle)	0.13075	-1565.59952	0.00311
$(\text{pn36}-(\text{CO}_2)_3)^{2-}_{\text{O\&O\&O}}-\text{CO}_2^{-}$	-1565.7262	0.19071(Hartree/Particle)	0.13202	-1565.59419	0.00178
$(\text{pn36}-(\text{CO}_2)_3)^{2-}_{\text{O\&O\&O}}-\text{CO}_2^{-}$	-1565.7254	0.19044(Hartree/Particle)	0.13097	-1565.59440	0.00190
$(\text{pn36}-(\text{CO}_2)_3)^{2-}_{\text{O\&O\&O}}-\text{CO}_2^{-}$	-1565.7242	0.19020(Hartree/Particle)	0.13131	-1565.59288	0.00172
$(\text{pn36}-(\text{CO}_2)_3)^{2-}_{\text{O\&O\&O}}-\text{CO}_2^{-}$	-1565.724	0.19020(Hartree/Particle)	0.13120	-1565.59283	0.00171
$(\text{pn36}-(\text{CO}_2)_3)^{2-}_{\text{O\&O\&O}}-\text{CO}_2^{-}$	-1565.7239	0.19041(Hartree/Particle)	0.13080	-1565.59307	0.00190
$(\text{pn36}-(\text{CO}_2)_3)^{2-}_{\text{N\&N\&N}^-\text{CO}_2^{-}}$	-1754.354	0.20521(Hartree/Particle)	0.14084	-1754.21317	0.00067
$\cdots\text{CO}_2$					
$(\text{pn36}-(\text{CO}_2)_3)^{2-}_{\text{N\&N\&N}^-\text{CO}_2^{-}}$	-1754.3537	0.20510(Hartree/Particle)	0.14042	-1754.21333	0.00066
$\cdots\text{CO}_2$					
$(\text{pn36}-(\text{CO}_2)_3)^{-}_{\text{N\&N\&N}}(\text{CO}_2)_2^{2-}$	-1754.353	0.20564(Hartree/Particle)	0.14194	-1754.21107	0.00184
$(\text{pn36}-(\text{CO}_2)_3)^{-}_{\text{O\&O\&O}}(\text{CO}_2)_2^{2-}$	-1754.3175	0.20498(Hartree/Particle)	0.14080	-1754.17672	0.00184
$(\text{pn36}-(\text{CO}_2)_3)^{3-}_{\text{N\&N\&N}}$	-1942.9493	0.21786(Hartree/Particle)	0.14913	-1942.80022	0.00108
$\cdots((\text{CO}_2)_3)_{\text{O\&O\&O}}$					
$(\text{pn36}-(\text{CO}_2)_3)^{-}_{\text{N\&N\&N}}(\text{CO}_2)_2^{2-}\cdots$	-1942.9447	0.21876(Hartree/Particle)	0.14823	-1942.79645	0.00073
CO_2					
$(\text{pn36}-(\text{CO}_2)_3)^{-}_{\text{O\&O\&O}}(\text{CO}_2)_2^{2-}$	-1942.9081	0.21827(Hartree/Particle)	0.14671	-1942.76140	0.00067
$\cdots\text{CO}_2$					

XI. CO_2 complexes of Li^+ -incorporated anionic systems

System	SCF energy	Zero-point correction	TC to Gibbs	e+Gibbs	BSSE
HCl	-460.79648	0.006797 (Hartree/Particle)	-0.01109	-460.80757	
LiCl	-467.79485	0.001471 (Hartree/Particle)	-0.01922	-467.81406	
py-Li complex	-519.06571	0.099446 (Hartree/Particle)	0.06444	-519.00127	0.00267

nt5-2Li complex	-959.55859	0.144836 (Hartree/Particle)	0.09913	-959.45946	0.00515
pn36-3Li complex	-1400.02910	0.189946 (Hartree/Particle)	0.13586	-1399.89324	0.00842

XII. CO₂ complexes of anionic systems in presence of trimethyl phosphonium cation

System	SCF energy	Zero-point correction	TC to Gibbs	e+Gibbs	BSSE
(CH ₃) ₄ P ⁺ (OH) ⁻	-576.72200	0.16341(Hartree/Particle)	0.12903	-576.59297	
H ₂ O	-76.42091	0.02162(Hartree/Particle)	0.00398	-76.41693	
py-(CO ₂) ⁻ ... ⁺ P(CH ₃) ₄	-1012.40703	0.251004(Hartree/Particle)	0.20590	-1012.20112	0.00204
nt-(CO ₂) ⁻ ... ⁺ P(CH ₃) ₄	-1257.31263	0.29135(Hartree/Particle)	0.24130	-1257.07134	0.00244
pn-(CO ₂) ⁻ ... ⁺ P(CH ₃) ₄	-1502.20159	0.33167(Hartree/Particle)	0.27802	-1501.92357	0.00293
(nt-(CO ₂) ₂) ⁻ ... ⁺ (P(CH ₃) ₄) ₂	-1946.24562	0.44797(Hartree/Particle)	0.38136	-1945.86426	0.00481
(pn-(CO ₂) ₂) ⁻ ... ⁺ (P(CH ₃) ₄) ₂	-2191.13266	0.48847(Hartree/Particle)	0.41837	-2190.71428	0.00615
(pn-(CO ₂) ₃) ⁻ ... ⁺ (P(CH ₃) ₄) ₃	-2880.06340	0.64573(Hartree/Particle)	0.55984	-2879.50356	0.00802

XIII. Anionic systems in presence of trimethyl phosphonium cation

System	SCF energy	Zero-point correction	TC to Gibbs	e+Gibbs	BSSE
py ⁻ ... ⁺ P(CH ₃) ₄	-823.82062	0.23683 (Hartree/Particle)	0.19603	-823.62459	0.00226
nt ⁻ ... ⁺ P(CH ₃) ₄	-1068.718	0.27669 (Hartree/Particle)	0.22962	-1068.4884	0.00229
pn ⁻ ... ⁺ P(CH ₃) ₄	-1313.6061	0.31633 (Hartree/Particle)	0.26556	-1313.3406	0.00235
nt ²⁻ ... ⁺ (P(CH ₃) ₄) ₂	-1569.0507	0.41909 (Hartree/Particle)	0.36181	-1568.6888	0.00471
pn ²⁻ ... ⁺ (P(CH ₃) ₄) ₂	-1813.9618	0.45796 (Hartree/Particle)	0.39860	-1813.5632	0.00615
pn ³⁻ ... ⁺ (P(CH ₃) ₄) ₃	-2314.2947	0.59960 (Hartree/Particle)	0.52808	-2313.7666	0.01165

Table S2. $V_{\min}$ values of trihydroxy pyridonaphthyridines at M06-2X/ 6-311++G(d,p) level of theory. All values in kcal/mol.

Molecules	$V_{\min}$		
	N1	N2	N3
pn1	-53.1	-51.8	-31.3
pn2	-46.9	-42.4	-31.8
pn3	-55.1	-55.1	-42.3
pn4	-50.5	-49.7	-40.5
pn5	-42.0	-41.3	-35.5
pn6	-46.5	-41.8	-31.9
pn7	-43.3	-41.7	-40.1
pn8	-52.3	-48.9	-39.4
pn9	-56.4	-47.9	-41.9
pn10	-49.4	-42.6	-34.4

pn11	-51.9	-48.8	-32.1
pn12	-43.4	-40.5	-39.9
pn13	-41.5	-39.3	-34.9
pn14	-52.2	-51.6	-48.5
pn15	-51.3	-50.8	-41.5
pn16	-50.4	-48.5	-38.6
pn17	-44.1	-42.0	-38.3
pn18	-48.2	-44.4	-41.3
pn19	-43.3	-41.1	-33.9
pn20	-47.0	-38.9	-38.8
pn21	-43.0	-42.7	-40.4
pn22	-43.4	-40.7	-38.8
pn23	-50.4	-45.7	-38.5
pn24	-46.2	-38.8	-38.0
pn25	-42.6	-41.0	-40.8
pn26	-44.0	-38.7	-38.4
pn27	-57.5	-42.7	-39.6
pn28	-46.4	-44.0	-41.8
pn29	-44.8	-38.6	-37.2
pn30	-51.8	-47.5	-47.2
pn31	-46.6	-45.2	-41.4
pn32	-49.7	-48.2	-37.7
pn33	-49.0	-46.2	-37.0
pn34	-43.1	-41.0	-39.4
pn35	-50.7	-45.6	-40.0
pn36	-47.0	-42.2	-38.9

Table S3. N-C bond distance, H-O hydrogen bond in Å and OCO angle θ in $^{\circ}$.

System	1CO ₂			2CO ₂			3CO ₂		
	d _{N...C}	d _{H...O}	θ_{oco}	d _{N...C}	d _{H...O}	θ_{oco}	d _{N...C}	d _{H...O}	θ_{oco}
py	2.70	2.12	176.5						
nt1	2.84	2.04	176.8	2.84	2.04	176.8			
nt2	2.70	2.09	176.5	2.87	2.00	177.2			
nt3	2.88	2.02	177.2	2.88	2.02	177.2			
nt4	2.70	2.15	176.7	2.86	2.00	177.2			
nt5	2.71	2.10	176.7	2.71	2.10	176.7			
nt6	2.71	2.09	176.6	2.72	2.12	176.9			
nt7	2.80	2.20	177.0	2.71	2.11	176.5			

nt8	2.72	2.12	176.8	2.87	2.00	177.4			
nt9	2.70	2.11	176.6	2.70	2.11	176.7			
nt10	2.71	2.09	176.7	2.72	2.13	177.0			
nt11	2.71	2.13	176.9	2.71	2.13	176.9			
nt12	2.72	2.13	177.0	2.72	2.13	177.0			
pn1	2.84	2.05	176.8	2.84	2.02	176.7	3.53	1.99	179.3
pn2	2.68	2.27	176.6	2.86	1.98	177.2	2.90	2.17	178.6
pn3	2.87	3.12	176.5	2.87	3.12	178.2	2.87	2.00	177.2
pn4	2.86	2.04	177.0	2.84	2.02	176.8	2.72	2.10	177.0
pn5	2.72	2.11	177.0	2.87	2.00	177.2	2.84	2.26	178.3
pn6	2.71	2.12	176.7	2.88	1.99	177.3	2.85	2.22	178.5
pn7	2.71	2.09	176.7	2.72	2.11	176.9	2.90	1.98	177.4
pn8	2.86	2.05	176.9	2.86	2.01	176.9	2.72	2.09	176.9
pn9	2.78	2.22	176.7	2.70	2.10	176.6	2.90	1.98	177.3
pn10	3.30	2.00	177.4	2.88	2.01	177.2	2.83	2.26	178.2
pn11	3.27	1.98	177.2	2.71	2.13	176.4	3.54	1.98	179.2
pn12	2.70	2.13	176.7	2.88	1.98	177.3	2.72	2.10	177.0
pn13	2.70	2.22	177.0	2.88	2.00	177.3	2.88	2.19	178.4
pn14	2.85	2.04	176.9	2.85	2.02	176.9	2.81	2.20	177.2
pn15	2.85	2.03	176.9	2.86	2.03	177.0	2.71	2.12	176.8
pn16	2.85	2.05	176.9	2.86	2.01	176.9	2.71	2.14	177.0
pn17	2.71	2.09	176.6	2.73	2.10	176.9	2.91	1.98	177.5
pn18	2.81	2.19	177.1	2.71	2.08	176.6	2.91	1.98	177.4
pn19	2.71	2.11	176.7	2.91	2.00	177.3	3.57	2.00	179.3
pn20	2.71	2.12	176.6	2.73	2.09	177.0	2.90	1.97	177.5
pn21	2.71	2.08	176.7	2.71	2.11	176.8	2.93	1.98	177.5
pn22	2.72	2.11	176.8	2.89	1.99	177.4	2.73	2.10	177.1
pn23	2.79	2.17	177.0	2.71	2.11	176.7	2.73	2.10	177.2
pn24	2.71	2.13	176.7	2.91	1.98	177.6	2.72	2.08	177.0
pn25	2.70	2.15	176.7	2.90	1.98	177.5	2.71	2.11	176.9
pn26	2.70	2.14	176.7	2.89	1.97	177.5	2.72	2.13	177.1
pn27	3.79	1.98	178.0	2.72	2.12	177.0	2.90	1.99	177.4
pn28	2.81	2.19	177.2	2.70	2.16	176.6	2.89	1.98	177.4
pn29	2.72	2.12	176.8	2.90	1.98	177.6	2.72	2.12	177.1
pn30	2.79	2.19	177.1	2.71	2.11	176.6	2.81	2.20	177.3
pn31	2.81	2.18	177.1	2.72	2.11	176.8	2.90	1.99	177.5
pn32	2.80	2.17	177.0	2.71	2.11	176.6	2.72	2.08	177.1
pn33	2.80	2.17	177.1	2.71	2.11	176.6	2.72	2.12	177.1

pn34	2.72	2.11	176.9	2.91	1.99	177.6	2.72	2.12	177.0
pn35	2.78	2.23	177.1	2.71	2.11	176.7	2.72	2.11	177.0
pn36	2.70	2.11	176.5	2.72	2.11	176.8	2.90	1.98	177.4

Table S4. ΔE_{ad} values of all possibilities of selected anions at M06-2X/6-311++G(d,p) level of theory. All values in kcal/mol.

Molecule	ΔE_{ad1_O}	ΔE_{ad1_N}	ΔE_{ad2_OO}	ΔE_{ad2_NN}	ΔE_{ad2_ON}	ΔE_{ad3}	ΔE_{ad4}	ΔE_{ad5}	ΔE_{ad6}
py ⁻	-16.9	-18.1	-30.9	-31.8	-27.9				
nt5 ⁻	-12.6	-15.0	--	-28.4	-30.0				
nt5 ²⁻	-28.2	-34.0	-48.7	-60.8	-55.1	-77.6			
					-52.0	-76.3			
						-72.0			
						-63.8			
pn36 ⁻	-15.1	-14.8		-30.5	-27.1				
	-13.9	-13.7							
	-11.8	-9.6							
pn36 ²⁻	-19.9	-29.0	-38.3	-51.6	-45.7	-68.6			
					-45.4	-66.8			
					-44.4	-61.4			
					-33.3				
pn36 ³⁻	-40.5	-47.6	-70.8	-87.4	-80.5	-116.6	-135.1	-150.5	-168.1
	-39.4	-45.9	-68.3	-83.0	-79.4	-98.1	-134.7	-150.3	-165.2
	-37.9	-43.2		-82.8	-77.8	-94.1	-134.4	-149.9	-142.2
					-77.3	-92.1	-133.3	-127.6	
					-75.4		-133.1		
					-74.3		-132.6		
					-65.0		-132.1		
					-64.1		-131.7		
					-60.8		-131.7		
							-122.6		
							-121.9		
							-121.9		
							-115.1		
							-112.5		
							-112.0		
							-111.3		
							-111.2		

-111.1

Table S5. ΔG_{ad} values of all possibilities of selected anions at M06-2X/6-311++G(d,p) level of theory. All values in kcal/mol.

Molecule	ΔG_{ad1_O}	ΔG_{ad1_N}	ΔG_{ad2_OO}	ΔG_{ad2_NN}	ΔG_{ad2_ON}	ΔG_{ad3}	ΔG_{ad4}	ΔG_{ad5}	ΔG_{ad6}
py ⁻	-6.6	-7.5	-12.7	-13.5	-14.0				
nt5 ⁻	-5.9	-4.6	--	-10.2	-11.2				
nt5 ²⁻	-18.7	-23.1	-30.2	-39.4	-35.1	-48.2			
					-32.9	-47.1			
						-43.7			
						-36.9			
pn36 ⁻	-7.4	-4.3		-10.8	-8.9				
	-6.0	-3.3							
	-4.9	-0.0							
pn36 ²⁻	-10.0	-18.2	-19.8	-30.2	-27.0	-38.1			
					-26.5	-37.6			
					-25.7	-30.2			
					-13.7				
pn36 ³⁻	-30.6	-36.6	-50.9	-65.6	-60.1	-84.5	-93.9	-101.2	-109.6
	-29.2	-34.9	-47.9	-61.4	-58.8	-67.7	-93.4	-101.3	-107.2
	-27.6	-32.5		-61.3	-56.6	-64.3	-93.1	-99.9	-85.2
					-56.2	-61.4	-93.1	-78.4	
					-54.7		-92.6		
					-53.6		-91.6		
					-46.0		-91.1		
					-42.6		-90.1		
					-40.3		-90.0		
							-83.4		
							-82.7		
							-82.6		
							-76.2		
							-72.8		
							-73.0		
							-72.0		
							-72.0		
							-72.1		

Table S6. ΔG_{ad} values of covalently bonded CO_2 complexes of selected anions at M06-2X/6-311++G(d,p) level of theory. All values in kcal/mol.

Molecule	ΔG_{ad1}	ΔG_{ad2}	ΔG_{ad3}	ΔG_{ad4}	ΔG_{ad5}
py ⁻	-6.6				
nt5 ⁻	-4.6				
nt5 ²⁻	-23.1	-39.4			
pn36 ⁻	-4.3				
pn36 ²⁻	-18.2	-30.2			
pn36 ³⁻	-36.6	-65.6	-84.5	-93.4	-99.9

Table S7. Relative interaction energies of all complexes (X=py, nt, pn). All values in kcal/mol.

System	Neutral	1CO ₂	X'-COOH	2CO ₂	X'-COOH...CO ₂	X''-(COOH) ₂	3CO ₂	X''-(COOH) ₂ ...CO ₂	X'''-(COOH) ₃
nt1	0.0	-10.5	2.7	-21.8	-9.0	11.5			
nt2	0.0	-10.9	-7.9	-21.5	-18.3	-1.8			
nt3	0.0	-10.5	1.7	-21.1	-8.6	9.1			
nt4	0.0	-10.7	1.2	-21.3	-9.3	1.0			
nt5	0.0	-10.8	-6.5	-21.7	-17.1	-9.4			
nt6	0.0	-11.0	-8.7	-21.5	-19.2	-7.6			
nt7	0.0	-10.2	5.3	-21.0	-5.3	2.7			
nt8	0.0	-10.6	2.8	-20.9	-7.6	3.8			
nt9	0.0	-10.8	-6.6	-21.5	-17.1	-9.4			
nt10	0.0	-10.8	-7.5	-21.4	-17.9	-4.4			
nt11	0.0	-10.6	2.4	-21.3	-8.0	8.5			
nt12	0.0	-10.5	5.2	-21.0	-5.0	--			
pn1	0.0	-10.5	3.8	-22.0	-8.0	8.1	-29.9	-0.7	20.2
pn2	0.0	-10.8	-0.8	-21.4	-11.4	-2.3	-30.6	-11.9	11.9
pn3	0.0	-11.6	5.4	-18.7	-5.9	11.6	-29.4	1.2	17.2
pn4	0.0	-10.5	4.7	-21.9	-6.2	8.5	-32.4	-1.9	9.8
pn5	0.0	-10.5	1.1	-21.2	-9.5	-1.0	-30.2	-9.7	14.0
pn6	0.0	-10.6	1.2	-21.1	-9.3	0.3	-29.9	-8.6	14.7
pn7	0.0	-10.8	-6.4	-21.4	-16.8	-4.2	-31.9	-14.8	-3.1
pn8	0.0	-10.5	4.9	-21.8	-6.7	10.3	-32.4	-0.2	8.6
pn9	0.0	-10.8	-5.8	-22.1	-16.3	-3.4	-32.7	-13.8	1.8
pn10	0.0	-10.2	7.2	-20.1	-3.2	9.4	-29.0	1.8	23.1

pn11	0.0	-9.9	1.2	-21.2	-9.4	-1.9	-28.7	-10.6	11.4
pn12	0.0	-10.8	-0.5	-21.3	-11.0	-1.6	-31.9	-11.9	-0.1
pn13	0.0	-10.5	1.7	-21.1	-8.8	3.3	-30.3	-7.5	16.7
pn14	0.0	-10.5	4.5	-21.6	-7.0	10.5	-31.8	0.3	21.0
pn15	0.0	-10.5	4.1	-21.6	-6.6	9.7	-32.2	-0.7	8.2
pn16	0.0	-10.5	5.2	-21.7	-5.7	9.5	-32.3	-1.0	12.4
pn17	0.0	-10.9	-6.0	-21.3	-16.3	-2.7	-31.8	-13.2	-1.0
pn18	0.0	-9.7	8.1	-21.1	-2.6	1.5	-31.5	-8.8	7.4
pn19	0.0	-10.6	-4.8	-20.9	-15.0	-2.2	-28.7	-11.2	11.3
pn20	0.0	-10.7	-0.8	-21.3	-11.2	-2.6	-31.7	-13.1	-1.3
pn21	0.0	-10.9	-6.9	-21.5	-17.5	-11.0	-31.6	-21.0	-4.7
pn22	0.0	-10.6	1.3	-21.0	-9.1	0.7	-31.4	-9.6	2.7
pn23	0.0	-10.4	0.7	-21.1	-9.8	-1.6	-31.6	-12.0	0.1
pn24	0.0	-10.6	0.8	-20.8	-9.5	2.0	-31.4	-8.3	2.0
pn25	0.0	-10.8	-0.3	-21.0	-10.5	-0.4	-31.6	-10.8	-1.1
pn26	0.0	-10.8	-0.4	-21.3	-10.8	-0.6	-31.7	-10.8	3.0
pn27	0.0	-10.6	5.0	-21.9	-5.6	0.1	-30.7	-10.2	5.8
pn28	0.0	-9.7	8.2	-20.5	-2.5	9.8	-31.3	-0.6	10.4
pn29	0.0	-10.6	0.3	-20.9	-9.9	1.2	-31.4	-9.2	4.2
pn30	0.0	-10.3	3.0	-21.1	-7.7	-0.1	-31.3	-10.4	10.6
pn31	0.0	-9.8	8.4	-20.4	-2.1	11.3	-31.1	1.0	12.6
pn32	0.0	-9.9	2.4	-21.2	-8.2	-0.6	-31.8	-11.0	-1.4
pn33	0.0	-10.3	1.7	-21.1	-9.0	-1.4	-31.7	-11.9	1.1
pn34	0.0	-10.5	1.8	-20.6	-8.2	2.2	-31.1	-8.0	3.2
pn35	0.0	-10.3	2.3	-21.0	-8.3	-0.2	-31.6	-10.5	0.1
pn36	0.0	-10.8	-6.3	-21.4	-16.8	-10.0	-31.9	-20.4	-6.8

Table S8. Relative free energies of all complexes. All values in kcal/mol.

System	Neutral	1CO ₂	X'-COOH	2CO ₂	X'-COOH...CO ₂	X''-(COOH) ₂	3CO ₂	X''-(COOH) ₂ ...CO ₂	X'''-(COOH) ₃
nt1	0.0	-3.7	13.3	-6.4	9.7	33.5			
nt2	0.0	-3.9	2.8	-7.3	-0.6	19.6			
nt3	0.0	-3.8	12.4	-7.2	9.2	30.7			
nt4	0.0	-3.6	11.4	-7.2	7.8	22.3			
nt5	0.0	-3.7	4.3	-7.4	0.8	12.0			

nt6	0.0	-3.9	2.1	-7.5	-1.3	13.6			
nt7	0.0	-3.1	16.5	-6.8	13.2	24.9			
nt8	0.0	-3.4	13.1	-6.9	9.5	25.2			
nt9	0.0	-3.8	4.0	-7.4	0.4	11.4			
nt10	0.0	-3.7	3.5	-7.1	0.1	17.0			
nt11	0.0	-3.6	12.3	-7.3	9.0	27.7			
nt12	0.0	-3.4	15.1	-6.7	11.9	--			
pn1	0.0	-3.9	14.4	-6.4	10.7	30.2	-8.5	28.2	53.3
pn2	0.0	-3.7	9.5	-7.4	5.8	19.1	-9.4	16.8	44.2
pn3	0.0	-4.9	16.6	-6.0	12.7	33.9	-9.6	30.5	49.9
pn4	0.0	-3.8	15.4	-6.4	11.5	30.8	-9.8	27.5	42.6
pn5	0.0	-3.5	11.4	-7.5	7.7	20.5	-9.1	18.6	46.8
pn6	0.0	-3.7	11.4	-7.2	8.0	21.8	-9.0	19.9	47.3
pn7	0.0	-3.7	4.1	-7.3	0.6	16.7	-10.8	13.1	29.2
pn8	0.0	-3.8	15.5	-6.3	11.9	32.5	-9.9	29.0	41.2
pn9	0.0	-3.8	4.6	-7.2	0.8	17.7	-10.8	14.2	35.0
pn10	0.0	-3.0	18.4	-4.9	15.1	31.6	-7.0	29.5	56.4
pn11	0.0	-1.9	12.6	-7.0	9.0	20.4	-7.9	18.6	44.6
pn12	0.0	-3.7	9.8	-7.4	6.3	20.1	-10.9	16.7	32.1
pn13	0.0	-3.4	12.2	-7.1	8.7	24.8	-8.6	20.1	49.5
pn14	0.0	-4.1	15.2	-6.2	11.7	32.7	-9.3	29.6	54.3
pn15	0.0	-4.0	14.8	-6.2	11.0	31.8	-9.9	28.5	40.6
pn16	0.0	-4.2	15.9	-6.3	11.8	31.9	-9.7	28.4	45.4
pn17	0.0	-3.7	4.6	-7.2	1.1	18.1	-10.5	15.0	31.3
pn18	0.0	-1.7	19.3	-6.7	15.6	23.2	-10.1	20.1	40.0
pn19	0.0	-3.6	5.7	-7.2	1.8	18.6	-7.5	16.7	43.8
pn20	0.0	-3.7	9.5	-7.4	6.0	18.1	-11.0	14.5	30.8
pn21	0.0	-3.8	3.5	-7.5	0.1	9.8	-10.7	6.5	27.2
pn22	0.0	-3.6	11.6	-7.3	8.0	22.3	-10.8	19.0	35.0
pn23	0.0	-3.3	12.3	-6.9	8.8	20.8	-10.5	17.4	33.0
pn24	0.0	-3.4	11.2	-7.1	7.8	23.7	-10.5	20.5	34.2
pn25	0.0	-3.8	10.0	-7.2	6.5	21.0	-10.8	17.6	30.6
pn26	0.0	-3.7	10.0	-7.1	6.5	21.1	-10.9	17.7	35.3
pn27	0.0	-3.5	16.7	-7.0	13.1	22.7	-10.1	19.4	39.3
pn28	0.0	-1.7	19.4	-5.5	15.8	31.3	-10.2	28.0	43.0
pn29	0.0	-3.4	10.9	-7.1	7.2	22.9	-10.7	19.6	36.5
pn30	0.0	-3.1	14.4	-7.0	10.8	22.2	-10.0	19.0	43.9
pn31	0.0	-4.5	19.6	-7.6	16.1	32.7	-8.9	29.4	45.4

pn32	0.0	-2.0	13.8	-6.9	10.3	21.7	-10.5	18.4	31.5
pn33	0.0	-3.2	13.2	-6.9	9.7	21.1	-10.4	17.6	34.2
pn34	0.0	-3.5	12.0	-7.2	8.4	23.7	-10.8	20.4	35.0
pn35	0.0	-3.2	13.6	-6.9	10.2	22.0	-10.4	18.6	32.5
pn36	0.0	-3.6	4.6	-7.2	1.2	11.8	-10.6	8.6	25.9

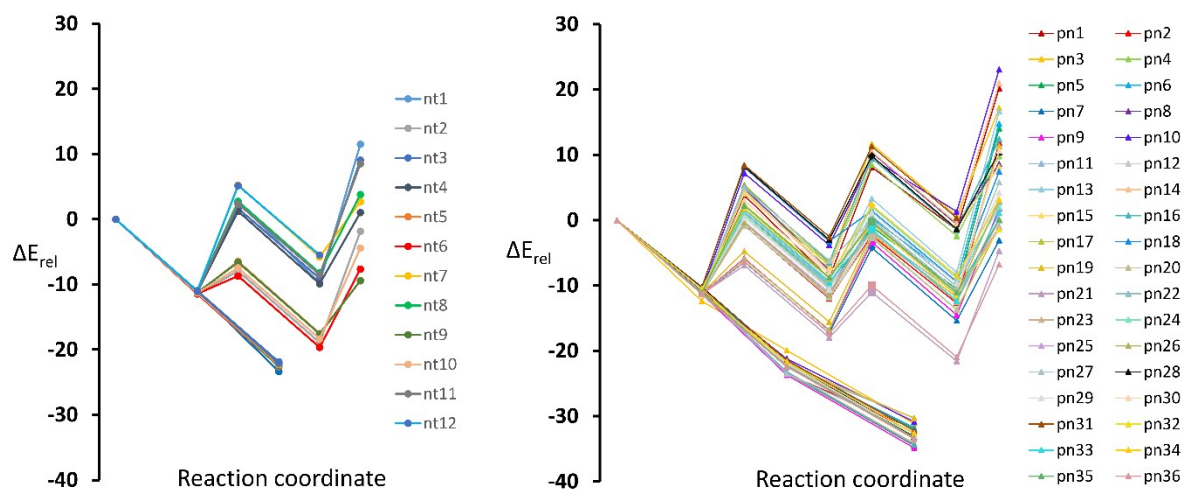


Figure S2. Relative adsorption energy of the CO₂ complexes of nt and pn molecules. All values in kcal/mol.

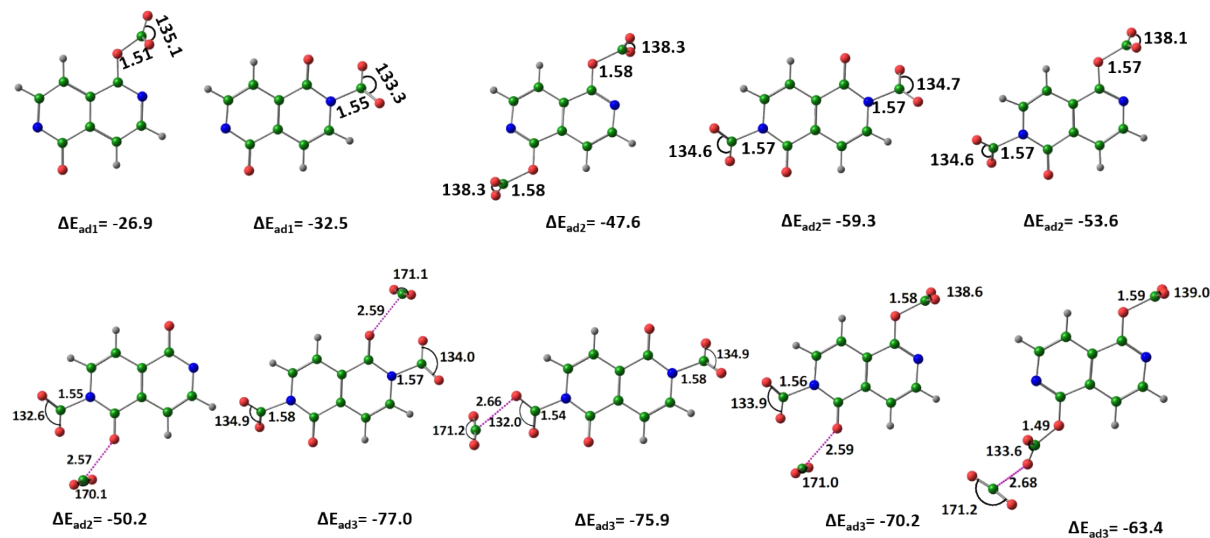


Figure S3. Optimized structures of the CO₂-adsorbed nt5²⁻ at all the possible positions along with its interaction energy in kcal/mol at M06-2X/6-311++G(d,p) level of theory. Distances in Å and angles in degrees.

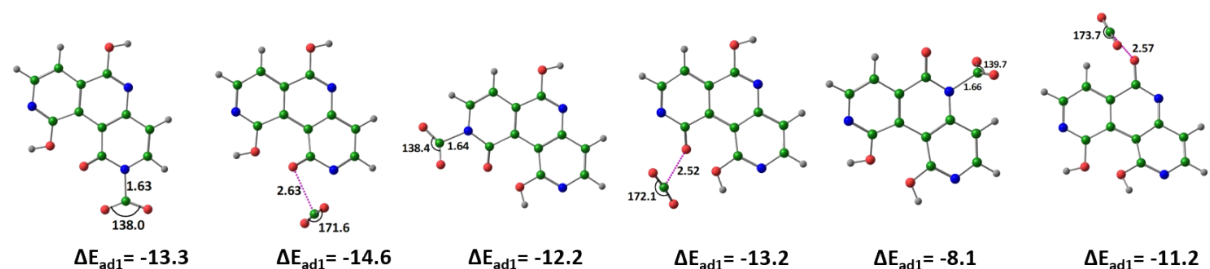


Figure S4. Optimized structures of the CO₂-adsorbed pn36⁻ at all the possible positions along with its interaction energy in kcal/mol at M06-2X/6-311++G(d,p) level of theory. Distances in Å and angles in degrees.

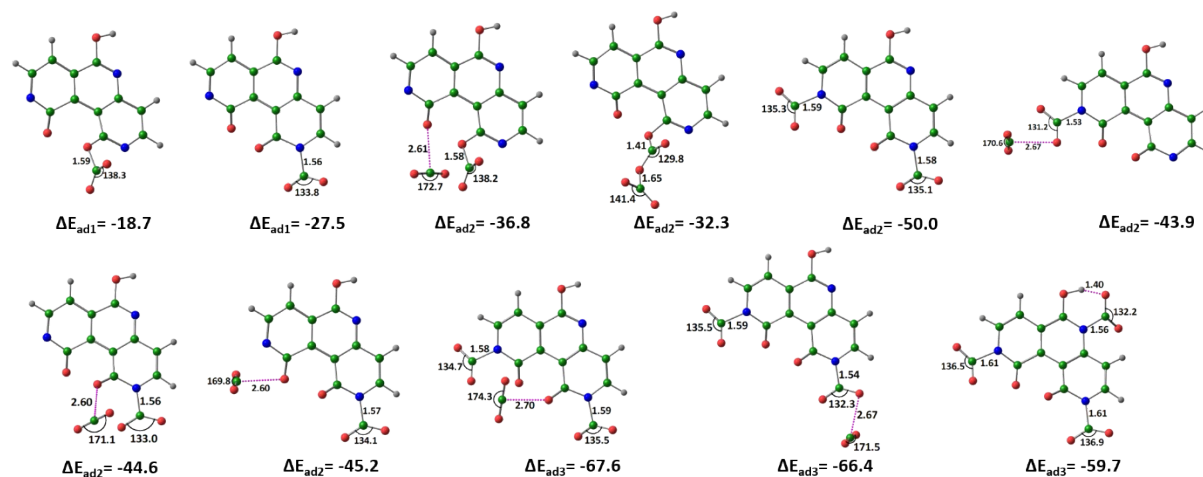


Figure S5. Optimized structures of the CO₂-adsorbed pn36²⁻ at all the possible positions along with its interaction energy in kcal/mol at M06-2X/6-311++G(d,p) level of theory. Distances in Å and angles in degrees.

Table S9. CO₂ wt% uptake for anionic N-heterocycles.

System	Formula	CO ₂ Molecules Adsorbed	CO ₂ wt%
Anion of Hydroxypyridine	C ₅ H ₄ NO ⁻	1	31.4%
		2	47.8%
Anion of Dihydroxy Naphthyridine	C ₈ H ₅ N ₂ O ₂ ⁻	1	21.5%
		2	35.3%
Dianion of Dihydroxy Naphthyridine	C ₈ H ₄ N ₂ O ₂ ²⁻	1	21.6%
		2	35.5%
		3	45.2%
Anion of Trihydroxy Pyridonaphthyridine	C ₁₁ H ₆ N ₃ O ₃ ⁻	1	16.2%
		2	27.8%
		3	36.7%
Dianion of Trihydroxy Pyridonaphthyridine	C ₁₁ H ₅ N ₃ O ₃ ²⁻	1	16.2%
		2	27.9%
		3	36.8%
Trianion of Trihydroxy Pyridonaphthyridine	C ₁₁ H ₄ N ₃ O ₃ ³⁻	1	16.3%
		2	28.0%
		3	36.9%
		4	43.8%
		5	49.3%

Table S10. BSSE corrected ΔE_{ad} values of hydroxy pyridine, dihydroxy naphthyridine and trihydroxy pyridonaphthyridines in solvent phase at M06-2X/6-311++G(d,p) level of theory. All values in kcal/mol.

Molecules	ΔE_{ad1}	ΔE_{ad2}	ΔE_{ad3}
py	-7.6		
nt1	-6.5	-9.0	
nt2	-7.5	-7.0	
nt3	-7.4	-6.8	
nt4	-7.7	-6.9	
nt5	-7.5	-7.0	
nt6	-7.5	-7.0	
nt7	-7.6	-6.8	
nt8	-7.6	-5.1	
nt9	-7.7	-7.0	
nt10	-7.6	-7.1	
nt11	-7.8	-6.9	
nt12	-7.5	-7.2	
pn1	-6.4	-9.0	-5.0
pn2	-7.7	-7.0	-7.5
pn3	-6.7	-8.0	-6.2
pn4	-6.3	-9.1	-6.0
pn5	-7.5	-7.1	-7.0
pn6	-7.5	-6.9	-7.1
pn7	-7.6	-7.1	-6.4
pn8	-6.4	-9.0	-6.0
pn9	-7.7	-9.4	-5.8
pn10	-7.5	-5.5	-7.1
pn11	-6.4	-8.2	-4.0
pn12	-7.6	-7.0	-6.4
pn13	-7.6	-6.9	-7.6
pn14	-6.5	-9.0	-6.1
pn15	-6.4	-9.0	-5.9
pn16	-6.5	-9.0	-5.9
pn17	-7.7	-7.0	-6.4
pn18	-6.4	-8.4	-6.2
pn19	-7.5	-6.9	-5.4

pn20	-7.7	-7.0	-6.4
pn21	-7.6	-7.2	-6.4
pn22	-7.5	-7.0	-6.4
pn23	-7.7	-6.7	-6.3
pn24	-7.5	-6.9	-6.5
pn25	-7.4	-7.0	-6.5
pn26	-7.7	-6.9	-6.5
pn27	-7.5	-9.3	-3.8
pn28	-6.5	-6.9	-7.7
pn29	-7.5	-6.9	-6.5
pn30	-7.8	-6.8	-6.4
pn31	-6.3	-7.0	-6.3
pn32	-6.4	-8.2	-6.4
pn33	-7.7	-6.8	-6.3
pn34	-7.6	-6.8	-6.4
pn35	-7.9	-6.8	-6.2
pn36	-7.7	-7.0	-6.4

Table S11. BSSE corrected ΔE_{ad} values of anionic systems in solvent phase at M06-2X/6-311++G(d,p) level of theory. All values in kcal/mol.

Molecule	ΔE_{ad1}	ΔE_{ad2}	ΔE_{ad3}	ΔE_{ad4}	ΔE_{ad5}
py ⁻	-15.6				
nt5 ⁻	-14.5				
nt5 ²⁻	-19.4	-59.3			
pn36 ⁻	-10.4				
pn36 ²⁻	-19.0	-50.0			
pn36 ³⁻	-23.0	-43.6	-58.4	-58.8	-57.8

Table S12. ΔE_{ad} values of selected anions in the presence of lithium counter cation, and with and without CO₂ in the presence of a phosphonium counter cation in solvent phase at M06-2X/6-311++G(d,p) level of theory. All values in kcal/mol.

Reaction								ΔE_{ad}	ΔG_{ad}	
py	+	LiCl	+	CO ₂	→	py ⁻ -Li ⁺ -CO ₂	+	HCl	-2.3	6.3
nt5	+	2LiCl	+	2CO ₂	→	nt5 ²⁻ -(Li) ₂ ⁺ -(CO ₂) ₂	+	2HCl	-8.4	8.7
pn36	+	3LiCl	+	3CO ₂	→	pn36 ³⁻ -(Li) ₃ ⁺ -(CO ₂) ₃	+	3HCl	-8.9	17.9
py	+	(CH ₃) ₄ P ⁺ (OH) ⁻			→	py ⁻ ... ⁺ P(CH ₃) ₄	+	H ₂ O	-11.9	-8.4
nt5	+	(CH ₃) ₄ P ⁺ (OH) ⁻			→	nt5 ⁻ ... ⁺ P(CH ₃) ₄	+	H ₂ O	-20.5	-18.3

pn36	+	$(\text{CH}_3)_4\text{P}^+(\text{OH})^-$	$\rightarrow$	$\text{pn36}^{--}\dots^+\text{P}(\text{CH}_3)_4$	+	H_2O	-22.9	-20.6		
nt5	+	$2(\text{CH}_3)_4\text{P}^+(\text{OH})^-$	$\rightarrow$	$\text{nt5}^{2-}\dots^+\text{P}(\text{CH}_3)_4)_2$	+	$2\text{H}_2\text{O}$	-36.7	-30.1		
pn36	+	$2(\text{CH}_3)_4\text{P}^+(\text{OH})^-$	$\rightarrow$	$\text{pn36}^{2-}\dots^+\text{P}(\text{CH}_3)_4)_2$	+	$2\text{H}_2\text{O}$	-53.5	-46.2		
pn36	+	$3(\text{CH}_3)_4\text{P}^+(\text{OH})^-$	$\rightarrow$	$\text{pn36}^{3-}\dots^+\text{P}(\text{CH}_3)_4)_3$	+	$3\text{H}_2\text{O}$	-70.3	-60.2		
py	+	$(\text{CH}_3)_4\text{P}^+(\text{OH})^-$	+	CO_2	$\rightarrow$	$\text{py}-(\text{CO}_2)^-\dots^+\text{P}(\text{CH}_3)_4$	+	H_2O	-40.6	-26.8
nt5	+	$(\text{CH}_3)_4\text{P}^+(\text{OH})^-$	+	CO_2	$\rightarrow$	$\text{nt5}-(\text{CO}_2)^-\dots^+\text{P}(\text{CH}_3)_4$	+	H_2O	-44.6	-31.0
pn36	+	$(\text{CH}_3)_4\text{P}^+(\text{OH})^-$	+	CO_2	$\rightarrow$	$\text{pn36}-(\text{CO}_2)^-\dots^+\text{P}(\text{CH}_3)_4$	+	H_2O	-44.3	-30.2
nt5	+	$2(\text{CH}_3)_4\text{P}^+(\text{OH})^-$	+	2CO_2	$\rightarrow$	$(\text{nt5}-(\text{CO}_2)_2)^{2-}\dots^+\text{P}(\text{CH}_3)_4)_2$	+	$2\text{H}_2\text{O}$	-87.2	-60.2
pn36	+	$2(\text{CH}_3)_4\text{P}^+(\text{OH})^-$	+	2CO_2	$\rightarrow$	$(\text{pn36}-(\text{CO}_2)_2)^{2-}\dots^+\text{P}(\text{CH}_3)_4)_2$	+	$2\text{H}_2\text{O}$	-83.9	-56.1
pn36	+	$3(\text{CH}_3)_4\text{P}^+(\text{OH})^-$	+	3CO_2	$\rightarrow$	$(\text{pn36}-(\text{CO}_2)_3)^{3-}\dots^+\text{P}(\text{CH}_3)_4)_3$	+	$3\text{H}_2\text{O}$	-123.4	-81.2

Table S13. ΔG_{ad} values of hydroxy pyridine, dihydroxy naphthyridine and trihydroxy pyridonaphthyridines in solvent phase at M06-2X/6-311++G(d,p) level of theory. All values in kcal/mol.

Molecules	ΔG_{ad1}	ΔG_{ad2}	ΔG_{ad3}
py	-0.1		
nt1	0.9	0.5	
nt2	0.1	0.8	
nt3	-0.2	0.9	
nt4	-0.1	0.6	
nt5	0.1	0.6	
nt6	0.0	0.4	
nt7	0.2	0.8	
nt8	0.1	2.3	
nt9	-0.3	0.6	
nt10	0.0	0.5	
nt11	-0.3	0.5	
nt12	0.1	0.4	
pn1	0.8	0.9	1.4
pn2	-0.1	0.5	0.6
pn3	0.9	-1.6	1.4
pn4	1.0	0.7	1.6
pn5	0.0	0.2	1.1
pn6	-0.1	0.6	0.8
pn7	0.0	0.3	1.2
pn8	0.8	0.8	1.5

pn9	-0.2	-0.4	1.8
pn10	0.3	3.0	0.5
pn11	2.2	-1.3	2.9
pn12	-0.1	0.6	1.1
pn13	0.0	0.5	0.9
pn14	0.4	1.1	1.7
pn15	0.7	0.9	1.4
pn16	0.3	1.2	1.7
pn17	0.0	0.5	1.3
pn18	2.2	-1.4	1.5
pn19	0.0	0.4	2.5
pn20	-0.2	0.4	1.0
pn21	0.0	0.2	1.1
pn22	0.0	0.3	1.1
pn23	0.3	0.8	1.1
pn24	0.1	0.3	1.2
pn25	0.0	0.4	1.0
pn26	-0.1	0.7	0.8
pn27	0.0	-0.3	2.1
pn28	2.1	0.6	-0.8
pn29	0.2	0.3	0.9
pn30	0.2	0.7	1.5
pn31	-0.4	0.9	3.2
pn32	2.1	-1.2	1.2
pn33	0.2	0.8	1.2
pn34	0.0	0.1	1.0
pn35	0.0	0.8	1.3
pn36	0.0	0.5	1.3

Table S14. ΔG_{ad} values of anionic systems in solvent phase at M06-2X/6-311++G(d,p) level of theory. All values in kcal/mol.

Molecules	ΔG_{ad}
$(\text{py}-\text{CO}_2^-)_\text{O}$	-3.5
$(\text{py}-\text{CO}_2^-)_\text{N}$	-5.1

$(py-CO_2^-)_O \dots CO_2$	-0.1
$(py-CO_2^-)_N \dots CO_2$	-6.9
$(py \dots (CO_2^-)_2)_{N\&O}$	-8.5
$(nt5^- \dots CO_2)_O$	-2.0
$(nt5-CO_2^-)_N$	-4.1
$(nt5-CO_2^-)_N \dots CO_2$	-7.8
$((CO_2) \dots nt5 - (CO_2^-))_{N\&O}$	-7.5
$(pn36 \dots CO_2^-)_O$	-0.2
$(pn36-CO_2^-)_N$	0.1
$(pn36-CO_2^-)_N \dots CO_2$	-8.7
$(pn36-CO_2^-)_N \dots (CO_2)_O$	-7.1

Table S15. ΔG_{ad} values of dianionic systems in solvent phase at M06-2X/6-311++G(d,p) level of theory. All values in kcal/mol.

Molecules	ΔG_{ad}
$(nt5^- - CO_2^-)_O$	-4.2
$(nt5^- - CO_2^-)_N$	-8.5
$(nt5(CO_2^-)_2)_{O\&O}$	-4.4
$(nt5-(CO_2^-)_2)_{N\&N}$	-14.9
$(nt5-(CO_2^-)_2)_{O\&N}$	-10.0
$(nt5^- - CO_2^-)_N \dots (CO_2)_O$	-9.1
$(nt5-(CO_2^-)_2)_{N\&N} \dots (CO_2)_O$	-17.0
$(nt5-(CO_2^-)_2)_{N\&N} \dots CO_2$	-23.4
$(nt5-(CO_2^-)_2)_{N\&O} - (CO_2)_O$	-10.6
$(nt5-(CO_2^-)_2)_{O\&O} \dots CO_2$	-6.7
$(pn36^- - CO_2^-)_O$	-1.8
$(pn36^- - CO_2^-)_N$	-8.1
$(pn36^- - CO_2^-)_O \dots (CO_2)_O$	-5.3
$((pn36-CO_2)^{2-})_{N\&N}$	-14.3
$(pn36^- - CO_2^-)_N \dots (CO_2)_O$	-10.4
$(pn36^- - CO_2^-)_N \dots (CO_2)_O$	-9.6
$(pn36^- - CO_2^-)_N \dots CO_2$	-9.3
$((pn36-CO_2)^{2-})_{N\&N} \dots (CO_2)_O$	-18.5
$((pn36-CO_2)^{2-})_{N\&N} \dots CO_2$	-16.9

Table S16. ΔG_{ad} values of trianionic systems in solvent phase at M06-2X/6-311++G(d,p) level of theory. All values in kcal/mol.

Molecules	ΔG_{ad}
$(pn36-CO_2)^{3-}_N$	-12.1
$((pn36-CO_2)^{3-})_{N\&N}$	-21.8
$(pn36-(CO_2)_3)^{3-}_{N\&N\&N}$	-26.3
$(pn36-(CO_2)_3)^{3-}_{N\&N\&N}-(CO_2)_O$	-17.5
$(pn36-(CO_2)_3)^{3-}_{N\&N\&N}-(CO_2)_2^{2-}$	-7.8
$(pn36-(CO_2)_3)^{3-}_{N\&N\&N} (CO_2)_2^{2-} \dots CO_2$	-9.8

Table S10. Cartesian coordinates for all the systems (Given in the order Atomic number, x, y, z coordinates, respectively).

I. Neutral system

CO ₂				py			
6	0.000012000	-0.000054000	-0.000094000	6	-1.188368000	-1.156244000	0.000000000
8	0.416888000	-1.095491000	0.250825000	6	0.044036000	-1.812563000	0.000000000
8	-0.416897000	1.095531000	-0.250755000	6	1.191049000	-1.037054000	0.000000000
				7	1.177328000	0.300274000	0.000000000
				6	0.000000000	0.899740000	0.000000000
				6	-1.224893000	0.224266000	0.000000000
				1	-2.112562000	-1.722235000	0.000000000
				1	0.111034000	-2.892030000	0.000000000
				1	2.173412000	-1.497737000	0.000000000
				1	-2.148593000	0.786676000	0.000000000
				8	-0.012910000	2.247244000	0.000000000
				1	0.907739000	2.536593000	0.000000000
nt1				nt2			
6	-5.000003000	1.720875000	0.093953000	6	-4.960557000	1.634347000	0.008664000
6	-5.065976000	0.359807000	0.090694000	6	-5.001113000	0.272809000	0.003123000
6	-3.874223000	-0.402342000	0.024548000	6	-3.782634000	-0.449060000	-0.001620000
6	-2.640121000	0.293816000	-0.036209000	6	-2.567002000	0.267408000	-0.000470000
7	-2.584633000	1.648082000	-0.032784000	7	-2.538386000	1.627259000	0.005077000
6	-3.707855000	2.306819000	0.028885000	6	-3.680775000	2.255919000	0.009353000
8	-3.653634000	3.649802000	0.032936000	8	-3.666723000	3.598196000	0.014904000
6	-3.841108000	-1.818058000	0.015415000	6	-3.699629000	-1.868280000	-0.007536000
6	-2.644682000	-2.467001000	-0.050434000	7	-2.585387000	-2.542643000	-0.011901000
6	-1.474601000	-1.664009000	-0.107476000	6	-1.425045000	-1.834738000	-0.010727000
7	-1.454955000	-0.360543000	-0.101777000	6	-1.356647000	-0.469624000	-0.005263000
8	-0.299697000	-2.313655000	-0.172143000	8	-4.862836000	-2.546616000	-0.008494000
1	-5.871803000	2.358125000	0.142889000	1	-5.847438000	2.252727000	0.012500000
1	-6.021893000	-0.151084000	0.138200000	1	-5.940177000	-0.266924000	0.002272000
1	-2.720141000	3.893471000	-0.014691000	1	-2.740880000	3.873183000	0.014685000
1	-4.772818000	-2.372014000	0.061158000	1	-0.521277000	-2.433486000	-0.014482000
1	-2.552445000	-3.543988000	-0.061013000	1	-0.411814000	0.056355000	-0.004492000
1	0.392233000	-1.640423000	-0.204192000	1	-4.639224000	-3.485918000	-0.012581000
nt3				nt4			
6	-4.947271000	1.744369000	-0.094877000	6	-4.950236000	1.533567000	0.015348000

6	-4.980817000	0.395524000	0.092137000	6	-4.985354000	0.175322000	0.010018000
6	-3.762488000	-0.331006000	0.151470000	6	-3.765871000	-0.553673000	0.000885000
6	-2.563412000	0.397095000	0.011049000	6	-2.546194000	0.172547000	-0.002296000
7	-2.537023000	1.745693000	-0.175635000	7	-2.522887000	1.537828000	0.003029000
6	-3.676947000	2.370391000	-0.223626000	6	-3.665893000	2.158257000	0.011277000
8	-3.676053000	3.705482000	-0.407624000	8	-3.662244000	3.500125000	0.016863000
7	-3.788883000	-1.679590000	0.338165000	6	-3.694290000	-1.958508000	-0.005135000
6	-2.648959000	-2.304304000	0.386099000	7	-2.565640000	-2.632093000	-0.013646000
6	-1.378643000	-1.678286000	0.257378000	6	-1.419685000	-1.926766000	-0.016559000
6	-1.345091000	-0.329428000	0.070438000	6	-1.344270000	-0.550254000	-0.011340000
8	-2.649882000	-3.639398000	0.570064000	8	-0.282447000	-2.646531000	-0.025426000
1	-5.840674000	2.351909000	-0.148662000	1	-5.836387000	2.152689000	0.022399000
1	-5.912425000	-0.147284000	0.198105000	1	-5.928987000	-0.360109000	0.012620000
1	-2.753889000	3.981666000	-0.476640000	1	-2.738111000	3.781572000	0.013334000
1	-0.485232000	-2.285807000	0.311254000	1	-4.611995000	-2.542068000	-0.002983000
1	-0.413474000	0.213376000	-0.035470000	1	-0.391042000	-0.040678000	-0.014158000
1	-3.572058000	-3.915581000	0.638875000	1	-0.537897000	-3.576877000	-0.027820000
nt5				nt6			
6	-6.148510000	0.697565000	-0.000458000	6	-1.769707000	1.571683000	0.000312000
6	-6.117716000	-0.705412000	-0.005434000	6	-1.803037000	0.167548000	-0.002448000
6	-4.876228000	-1.384668000	-0.009926000	6	-0.566266000	-0.520387000	-0.001359000
6	-3.737070000	-0.629659000	-0.009142000	6	0.625876000	0.228099000	0.002376000
7	-3.734761000	0.730759000	-0.004368000	7	0.644871000	1.541893000	0.004944000
6	-4.877418000	1.350357000	-0.000331000	6	-0.536688000	2.187852000	0.003880000
8	-4.887640000	2.695226000	0.004543000	8	-0.473485000	3.530602000	0.006673000
6	-7.390054000	1.376823000	0.004115000	6	-2.992307000	-0.615298000	-0.006252000
6	-8.529186000	0.621857000	0.003487000	6	-2.879408000	-1.974270000	-0.008597000
7	-8.531495000	-0.738630000	-0.001296000	7	-1.695337000	-2.651598000	-0.007504000
6	-7.388880000	-1.358194000	-0.005508000	6	-0.603657000	-1.946911000	-0.004023000
8	-7.378577000	-2.703071000	-0.010323000	8	0.577345000	-2.587057000	-0.002896000
1	-4.842002000	-2.465104000	-0.013797000	1	-2.674415000	2.164692000	-0.000283000
1	-2.757730000	-1.093365000	-0.012393000	1	1.582689000	-0.283502000	0.003259000
1	-3.966559000	2.984935000	0.004101000	1	0.461431000	3.770047000	0.009185000
1	-7.424238000	2.457262000	0.007923000	1	-3.963995000	-0.138853000	-0.007318000
1	-9.508546000	1.085508000	0.006844000	1	-3.763741000	-2.601423000	-0.011566000
1	-8.299639000	-2.992844000	-0.009631000	1	0.385363000	-3.533700000	-0.006103000
nt7				nt8			
6	-4.960207000	1.399177000	0.007703000	6	-4.959586000	1.755391000	0.012362000
6	-5.004984000	0.039411000	0.002808000	6	-5.038299000	0.400741000	0.006857000
6	-3.792543000	-0.705870000	-0.001724000	6	-3.836535000	-0.371528000	-0.000473000
6	-2.594745000	0.032266000	-0.000832000	6	-2.616557000	0.341443000	-0.001578000
7	-2.548154000	1.388292000	0.004027000	7	-2.545289000	1.706718000	0.004072000
6	-3.681143000	2.024865000	0.008053000	6	-3.662998000	2.359983000	0.010647000
8	-3.667498000	3.370056000	0.013008000	8	-3.637270000	3.706679000	0.015864000
6	-3.728558000	-2.122166000	-0.006909000	6	-3.800612000	-1.775633000	-0.006771000
6	-2.499403000	-2.716995000	-0.010878000	6	-2.566929000	-2.387823000	-0.013641000
7	-1.331531000	-2.023777000	-0.010147000	7	-1.398782000	-1.726034000	-0.014654000
6	-1.376404000	-0.721775000	-0.005403000	6	-1.423384000	-0.412021000	-0.008915000
8	-0.225447000	-0.036455000	-0.004796000	8	-2.493875000	-3.735698000	-0.019768000
1	-5.848515000	2.016605000	0.011302000	1	-5.832638000	2.394261000	0.018058000
1	-5.953565000	-0.486161000	0.002301000	1	-5.998370000	-0.103350000	0.008166000
1	-2.741362000	3.643986000	0.012628000	1	-2.709844000	3.974771000	0.014044000
1	-4.636048000	-2.713074000	-0.007704000	1	-4.706109000	-2.368636000	-0.006250000
1	-2.398572000	-3.796056000	-0.014888000	1	-0.474043000	0.114759000	-0.009623000
1	0.483537000	-0.691905000	-0.008246000	1	-1.557316000	-3.966486000	-0.024612000
nt9				nt10			

6	-6.132532000	0.441308000	0.003107000	6	-0.663842000	1.541905000	0.000979000
6	-6.148532000	-0.973252000	-0.002985000	6	-0.681000000	0.140767000	-0.002488000
6	-4.909948000	-1.661714000	-0.005522000	6	0.529169000	-0.582276000	0.000247000
6	-3.756349000	-0.930854000	-0.001947000	6	1.719936000	0.178699000	0.006454000
7	-3.719669000	0.422636000	0.003845000	7	1.741342000	1.491250000	0.009741000
6	-4.852199000	1.076097000	0.006202000	6	0.571410000	2.153837000	0.007060000
8	-4.790026000	2.411299000	0.011832000	8	0.646605000	3.498735000	0.010716000
6	-7.398246000	1.104893000	0.005637000	6	-1.884550000	-0.643098000	-0.008865000
7	-8.545232000	0.477274000	0.002539000	7	-1.913569000	-1.937423000	-0.012083000
6	-8.539181000	-0.876766000	-0.003334000	6	-0.727137000	-2.616942000	-0.009307000
6	-7.402441000	-1.633502000	-0.006234000	6	0.488687000	-2.003991000	-0.003330000
8	-7.430079000	2.441172000	0.011460000	8	-3.042378000	0.040794000	-0.011475000
1	-4.886338000	-2.743633000	-0.010192000	1	-1.576064000	2.121381000	-0.001022000
1	-2.787907000	-1.419132000	-0.003660000	1	2.681752000	-0.327574000	0.008757000
1	-3.850258000	2.636613000	0.013097000	1	1.582806000	3.731266000	0.014677000
1	-9.518438000	-1.342962000	-0.005677000	1	-0.814876000	-3.696542000	-0.012218000
1	-7.450482000	-2.714613000	-0.010896000	1	1.405648000	-2.579860000	-0.001293000
1	-8.364482000	2.687792000	0.012334000	1	-3.756980000	-0.608610000	-0.015350000
nt11				nt12			
6	-1.536873000	1.693453000	0.002930000	6	-1.742986000	1.763447000	0.006822000
6	-1.611243000	0.285218000	0.000159000	6	-1.757101000	0.353431000	-0.000169000
6	-0.388524000	-0.437899000	-0.001948000	6	-0.532799000	-0.353997000	-0.001426000
6	0.822581000	0.288082000	-0.001197000	6	0.655634000	0.424418000	0.004567000
7	0.880942000	1.595528000	0.001372000	7	0.660097000	1.732126000	0.011010000
6	-0.290992000	2.273305000	0.003396000	6	-0.521498000	2.387667000	0.012172000
8	-0.185578000	3.613267000	0.006046000	8	-0.452312000	3.734895000	0.018968000
6	-2.809483000	-0.458374000	-0.000680000	6	-2.945470000	-0.424931000	-0.006137000
6	-2.717433000	-1.829474000	-0.003482000	7	-2.949921000	-1.732719000	-0.012510000
7	-1.558886000	-2.529944000	-0.005475000	6	-1.768410000	-2.388191000	-0.013422000
6	-0.441286000	-1.848964000	-0.004701000	6	-0.546857000	-1.763940000	-0.008328000
8	-3.840849000	-2.567402000	-0.004424000	8	-1.837415000	-3.735438000	-0.019966000
1	-2.424231000	2.312054000	0.004656000	1	-2.657228000	2.342605000	0.008074000
1	1.769799000	-0.246815000	-0.002809000	1	1.622596000	-0.072256000	0.003708000
1	0.756200000	3.823537000	0.005915000	1	0.482570000	3.971524000	0.021653000
1	-3.779041000	0.021242000	0.000798000	1	-3.912465000	0.071666000	-0.005734000
1	0.483782000	-2.421320000	-0.006336000	1	0.367361000	-2.343139000	-0.009525000
1	-3.571377000	-3.493977000	-0.006406000	1	-2.772256000	-3.972214000	-0.023506000
pn1				pn2			
6	-8.652906000	1.876415000	0.399284000	6	-6.163363000	1.347526000	0.013502000
6	-8.662928000	0.512003000	0.319981000	6	-6.209057000	-0.053639000	0.000608000
6	-7.443211000	-0.171304000	0.135172000	6	-4.957034000	-0.768629000	-0.001690000
6	-6.258051000	0.572005000	0.038702000	6	-3.753545000	-0.024777000	0.009141000
7	-6.251833000	1.921502000	0.117417000	7	-3.732147000	1.354573000	0.021879000
6	-7.400644000	2.527251000	0.289258000	6	-4.863762000	1.971939000	0.023823000
8	-7.401531000	3.866563000	0.368175000	8	-4.868571000	3.314351000	0.035378000
6	-7.333020000	-1.600292000	0.037872000	6	-4.868162000	-2.165593000	-0.014082000
7	-6.235641000	-2.257741000	-0.130730000	7	-3.723184000	-2.824671000	-0.016139000
6	-5.064740000	-1.548278000	-0.227490000	6	-2.594868000	-2.104800000	-0.005651000
6	-5.022982000	-0.140380000	-0.149687000	6	-2.543922000	-0.722207000	0.007018000
8	-8.486649000	-2.283276000	0.133848000	8	-1.441717000	-2.798215000	-0.007977000
7	-3.948162000	-2.283283000	-0.403147000	6	-7.374515000	2.067179000	0.015928000
6	-2.804535000	-1.654357000	-0.501633000	6	-8.556283000	1.378174000	0.005995000
6	-2.642919000	-0.252002000	-0.438402000	6	-8.486590000	-0.033976000	-0.006249000
6	-3.772039000	0.498359000	-0.260487000	7	-7.375450000	-0.731061000	-0.009191000
8	-1.696253000	-2.394803000	-0.676478000	8	-9.648261000	-0.703268000	-0.016426000
1	-9.547217000	2.467087000	0.540109000	1	-3.945398000	3.599639000	0.040915000

1	-9.584321000	-0.052076000	0.395837000	1	-5.778855000	-2.754401000	-0.022574000
1	-6.486474000	4.160906000	0.277320000	1	-1.600202000	-0.195434000	0.015046000
1	-8.264036000	-3.220023000	0.052110000	1	-1.677600000	-3.733943000	-0.017127000
1	-1.655176000	0.177488000	-0.530365000	1	-7.352450000	3.149904000	0.025810000
1	-3.731647000	1.579001000	-0.201771000	1	-9.522765000	1.862349000	0.007184000
1	-1.976312000	-3.318812000	-0.696987000	1	-9.438654000	-1.645885000	-0.023342000
pn3				pn4			
6	-6.154056000	1.492300000	-0.147066000	6	1.649985000	-1.474232000	-0.000004000
6	-6.204371000	0.096006000	-0.015615000	6	0.752438000	-0.402624000	0.000032000
6	-4.949242000	-0.618204000	0.101668000	6	1.295301000	0.899278000	0.000078000
6	-3.766860000	0.139757000	0.075715000	6	2.686696000	1.059860000	-0.000014000
7	-3.738330000	1.511096000	-0.054026000	7	3.528382000	0.043485000	-0.000070000
6	-4.864219000	2.127409000	-0.157066000	6	3.005038000	-1.188709000	-0.000050000
8	-4.870672000	3.469081000	-0.285530000	8	3.877583000	-2.209669000	-0.000098000
7	-4.953180000	-1.962396000	0.229805000	6	-0.687495000	-0.526648000	0.000014000
6	-3.804054000	-2.571346000	0.333030000	6	-1.463278000	0.653840000	-0.000510000
6	-2.548911000	-1.918690000	0.320087000	7	-0.906240000	1.911476000	-0.000280000
6	-2.543251000	-0.558640000	0.190483000	6	0.378155000	2.008671000	0.000022000
8	-3.801055000	-3.913603000	0.461192000	8	0.933104000	3.230076000	0.000412000
6	-7.367008000	2.205327000	-0.262765000	6	-1.372869000	-1.757162000	0.000249000
6	-8.545988000	1.515833000	-0.243111000	6	-2.741185000	-1.784838000	0.000190000
6	-8.476277000	0.108251000	-0.106011000	6	-3.406652000	-0.541321000	0.000086000
7	-7.369432000	-0.580752000	0.003152000	7	-2.809313000	0.624079000	-0.000228000
8	-9.638601000	-0.562387000	-0.087739000	8	-4.749682000	-0.557082000	0.000101000
1	-3.949020000	3.756497000	-0.277106000	1	1.334587000	-2.507824000	-0.000065000
1	-1.643379000	-2.503161000	0.411522000	1	3.114565000	2.056511000	0.000049000
1	-1.622011000	0.011132000	0.172324000	1	4.763601000	-1.826380000	-0.000131000
1	-4.723622000	-4.197347000	0.452163000	1	0.206754000	3.867706000	0.000263000
1	-7.343288000	3.283112000	-0.364751000	1	-0.818416000	-2.687868000	0.000579000
1	-9.511365000	1.995569000	-0.326740000	1	-3.313106000	-2.701972000	0.000287000
1	-9.422315000	-1.498809000	0.010519000	1	-5.042643000	0.363274000	-0.000811000
pn5				pn6			
6	-5.955430000	1.573996000	-0.150740000	6	-6.163945000	1.488229000	0.008529000
6	-5.973499000	0.174875000	0.011191000	6	-6.244331000	0.091275000	-0.003073000
6	-4.699110000	-0.504165000	0.130478000	6	-5.005688000	-0.663140000	-0.002085000
6	-3.535716000	0.275663000	0.076985000	6	-3.802280000	0.069166000	0.010535000
7	-3.539325000	1.648422000	-0.082345000	7	-3.741715000	1.449466000	0.021855000
6	-4.677296000	2.239613000	-0.187149000	6	-4.852182000	2.094023000	0.020806000
8	-4.713295000	3.575189000	-0.343642000	8	-4.838940000	3.441570000	0.031160000
7	-4.679090000	-1.845806000	0.286762000	6	-4.957655000	-2.057829000	-0.012899000
6	-3.516568000	-2.433885000	0.391904000	6	-3.710109000	-2.655186000	-0.010617000
6	-2.277813000	-1.754841000	0.352550000	7	-2.556756000	-1.981029000	0.001274000
6	-2.299210000	-0.396491000	0.194319000	6	-2.603937000	-0.661677000	0.011497000
8	-3.484369000	-3.771749000	0.548086000	8	-3.626665000	-4.002215000	-0.020920000
6	-7.178686000	2.247947000	-0.267895000	6	-7.362204000	2.231918000	0.007722000
7	-8.343950000	1.628893000	-0.233008000	6	-8.556660000	1.566213000	-0.004157000
6	-8.342741000	0.298669000	-0.078344000	6	-8.519381000	0.152537000	-0.014904000
6	-7.203147000	-0.479084000	0.048124000	7	-7.421815000	-0.564258000	-0.014759000
8	-9.544498000	-0.300561000	-0.046955000	8	-9.695648000	-0.491342000	-0.027409000
1	-3.798239000	3.883653000	-0.350814000	1	-3.912786000	3.714650000	0.038554000
1	-1.360036000	-2.319272000	0.447299000	1	-5.862063000	-2.649611000	-0.022768000
1	-1.388157000	0.188478000	0.155487000	1	-1.662083000	-0.122347000	0.021118000
1	-4.398185000	-4.081350000	0.554973000	1	-2.688240000	-4.225328000	-0.017376000
1	-7.193999000	3.325104000	-0.393607000	1	-7.318541000	3.313883000	0.016578000
1	-7.267317000	-1.550758000	0.170487000	1	-9.512670000	2.071326000	-0.005546000
1	-10.209797000	0.391403000	-0.148415000	1	-9.507164000	-1.438456000	-0.032487000

pn7				pn8		
6	-5.988161000	1.492910000	0.002278000	6	1.570321000	0.777271000
6	-6.037719000	0.077815000	-0.007714000	6	0.888491000	-0.447839000
6	-4.764266000	-0.619172000	-0.003749000	6	-0.557448000	-0.446612000
6	-3.578140000	0.146560000	0.009363000	6	-1.209137000	0.810276000
7	-3.567328000	1.524659000	0.018668000	7	-0.523012000	2.001214000
6	-4.700959000	2.135938000	0.015459000	6	0.761044000	1.974469000
8	-4.710384000	3.476335000	0.024148000	8	1.437495000	3.134157000
6	-4.589646000	-2.026497000	-0.011682000	6	2.975822000	0.832423000
7	-3.429977000	-2.638766000	-0.007882000	6	3.660446000	-0.354430000
6	-2.316434000	-1.883205000	0.004532000	7	3.041674000	-1.552240000
6	-2.334512000	-0.512271000	0.013358000	6	1.735769000	-1.595704000
8	-5.681193000	-2.816560000	-0.024533000	8	1.173552000	-2.821554000
6	-7.180489000	2.224544000	-0.001426000	6	-1.386903000	-1.593635000
7	-8.373601000	1.659338000	-0.013329000	6	-2.749194000	-1.457290000
6	-8.413560000	0.323862000	-0.021976000	6	-3.275791000	-0.151564000
6	-7.305099000	-0.511774000	-0.020439000	7	-2.549161000	0.936285000
8	-9.632952000	-0.238049000	-0.034891000	8	-4.613334000	-0.015082000
1	-3.788372000	3.765255000	0.032119000	1	0.780480000	3.842739000
1	-1.379321000	-2.428888000	0.007303000	1	3.485252000	1.785424000
1	-1.427121000	0.075465000	0.023352000	1	4.743668000	-0.383615000
1	-5.354840000	-3.725989000	-0.028096000	1	1.904057000	-3.454114000
1	-7.146882000	3.308428000	0.005849000	1	-0.944468000	-2.577399000
1	-7.447780000	-1.579237000	-0.029125000	1	-3.418083000	-2.306624000
1	-10.277212000	0.480745000	-0.034523000	1	-4.799635000	0.932419000
pn9				pn10		
6	-6.177142000	1.423161000	0.010300000	6	-8.547536000	2.733580000
6	-6.253012000	0.017532000	-0.001136000	6	-8.592585000	1.372188000
6	-5.009888000	-0.722105000	-0.000927000	6	-7.389219000	0.633139000
6	-3.802799000	0.011419000	0.010535000	6	-6.200720000	1.350535000
7	-3.757946000	1.386424000	0.021607000	7	-6.149906000	2.695636000
6	-4.876039000	2.028358000	0.021432000	6	-7.280658000	3.345282000
8	-4.850833000	3.370892000	0.031702000	8	-7.252963000	4.685668000
6	-4.883906000	-2.139892000	-0.011345000	6	-7.331739000	-0.803909000
7	-3.734348000	-2.775192000	-0.010874000	6	-6.069950000	-1.409742000
6	-2.599853000	-2.050459000	0.000188000	7	-4.905356000	-0.695582000
6	-2.576279000	-0.680894000	0.011006000	6	-4.967235000	0.589603000
8	-5.984554000	-2.905949000	-0.022722000	8	-3.840593000	1.295686000
6	-7.368527000	2.175865000	0.010526000	7	-8.474206000	-1.509727000
6	-8.569807000	1.523887000	-0.000153000	6	-8.382302000	-2.811912000
6	-8.533219000	0.111401000	-0.010868000	6	-7.168955000	-3.532288000
7	-7.442493000	-0.613950000	-0.011616000	6	-6.014320000	-2.817791000
8	-9.707956000	-0.535160000	-0.021752000	8	-9.514204000	-3.525507000
1	-3.921526000	3.634835000	0.038143000	1	-9.431545000	3.354883000
1	-1.679025000	-2.623498000	0.000141000	1	-9.526122000	0.839611000
1	-1.652718000	-0.119111000	0.019827000	1	-6.329169000	4.944140000
1	-5.661886000	-3.817006000	-0.028146000	1	-3.117219000	0.657039000
1	-7.312373000	3.257267000	0.019266000	1	-7.186880000	-4.611165000
1	-9.521892000	2.035986000	-0.000679000	1	-5.047378000	-3.301693000
1	-9.507659000	-1.480629000	-0.027598000	1	-10.245416000	-2.897240000
pn11				pn12		
6	-6.171296000	1.244650000	0.007912000	6	-5.968728000	1.404047000
6	-6.223232000	-0.155114000	-0.002770000	6	-5.997494000	-0.006516000
6	-4.975604000	-0.886936000	-0.001753000	6	-4.722386000	-0.694583000
6	-3.794767000	-0.134360000	0.009728000	6	-3.535483000	0.079964000
7	-3.751809000	1.237444000	0.020156000	7	-3.540295000	1.461914000

6	-4.873717000	1.868200000	0.019253000	6	-4.680970000	2.058148000	0.016843000
8	-4.871615000	3.214159000	0.029175000	8	-4.710717000	3.398046000	0.027452000
6	-4.903846000	-2.294670000	-0.011662000	6	-4.582451000	-2.085853000	-0.016781000
6	-3.663942000	-2.877581000	-0.009642000	7	-3.419269000	-2.714817000	-0.016380000
7	-2.509151000	-2.173864000	0.001260000	6	-2.313771000	-1.965028000	-0.005098000
6	-2.572582000	-0.868620000	0.010445000	6	-2.307549000	-0.580282000	0.006186000
8	-1.426414000	-0.171945000	0.021225000	8	-1.139885000	-2.620136000	-0.005017000
6	-7.383468000	1.967483000	0.006849000	6	-7.175889000	2.110909000	0.004868000
6	-8.564307000	1.280295000	-0.004253000	7	-8.357201000	1.519223000	-0.005953000
6	-8.499978000	-0.133795000	-0.014072000	6	-8.374524000	0.182718000	-0.016854000
7	-7.391514000	-0.831490000	-0.013575000	6	-7.247609000	-0.625957000	-0.018060000
8	-9.665700000	-0.796913000	-0.024974000	8	-9.582294000	-0.402445000	-0.028586000
1	-3.946692000	3.493153000	0.035725000	1	-3.793262000	3.701746000	0.034317000
1	-5.811109000	-2.882319000	-0.020542000	1	-5.460334000	-2.724037000	-0.026073000
1	-3.552715000	-3.955811000	-0.016884000	1	-1.381222000	-0.023507000	0.015190000
1	-0.712714000	-0.822002000	0.020343000	1	-1.342668000	-3.563659000	-0.013454000
1	-7.358634000	3.050126000	0.014899000	1	-7.167084000	3.195347000	0.013846000
1	-9.529940000	1.766814000	-0.005815000	1	-7.374833000	-1.698972000	-0.027881000
1	-9.461490000	-1.740661000	-0.031126000	1	-10.241179000	0.303228000	-0.024932000
pn13				pn14			
6	-5.141665000	1.394778000	-0.113863000	6	-8.549984000	2.754979000	0.055720000
6	-5.156861000	-0.000346000	0.052596000	6	-8.668973000	1.394859000	0.032175000
6	-3.901362000	-0.709848000	0.135737000	6	-7.507091000	0.583835000	0.005238000
6	-2.722773000	0.045025000	0.044331000	6	-6.280407000	1.256775000	0.004807000
7	-2.718268000	1.418114000	-0.119451000	7	-6.152803000	2.600221000	0.027910000
6	-3.841457000	2.034774000	-0.191731000	6	-7.246973000	3.309093000	0.052177000
8	-3.861694000	3.370038000	-0.351367000	8	-7.146483000	4.649685000	0.075482000
7	-3.899062000	-2.050463000	0.295665000	6	-7.510765000	-0.858390000	-0.020977000
6	-2.741149000	-2.657690000	0.366821000	6	-6.267379000	-1.524945000	-0.045497000
6	-1.492665000	-2.004193000	0.287448000	7	-5.074449000	-0.849080000	-0.045638000
6	-1.496414000	-0.644387000	0.125205000	6	-5.082177000	0.440618000	-0.022396000
8	-2.731817000	-3.995225000	0.526404000	8	-3.918273000	1.095703000	-0.022967000
6	-6.341286000	2.100013000	-0.196577000	6	-8.673732000	-1.655636000	-0.023837000
6	-7.510569000	1.362543000	-0.107179000	6	-8.573093000	-3.020191000	-0.049556000
7	-7.552082000	0.035290000	0.051135000	6	-7.274065000	-3.571100000	-0.072592000
6	-6.411152000	-0.625223000	0.128664000	7	-6.170846000	-2.870035000	-0.070997000
8	-8.692243000	2.000152000	-0.181876000	8	-7.170426000	-4.912356000	-0.097946000
1	-2.943801000	3.667379000	-0.388990000	1	-9.406942000	3.414788000	0.076767000
1	-0.583093000	-2.584945000	0.355726000	1	-9.653766000	0.944727000	0.034329000
1	-0.577117000	-0.075156000	0.056269000	1	-6.205032000	4.865011000	0.069694000
1	-3.651350000	-4.285332000	0.561589000	1	-3.225026000	0.422676000	-0.042285000
1	-6.365803000	3.172803000	-0.324670000	1	-9.654113000	-1.195028000	-0.005827000
1	-6.465378000	-1.700318000	0.256707000	1	-9.434420000	-3.673356000	-0.052821000
1	-9.382003000	1.329960000	-0.101402000	1	-6.227671000	-5.120924000	-0.110518000
pn15				pn16			
6	1.456443000	0.263227000	0.000125000	6	-2.720182000	0.644535000	0.000041000
6	0.600057000	-0.855234000	0.000107000	6	-1.326605000	0.617958000	0.000048000
6	-0.823153000	-0.626976000	0.000224000	6	-0.631673000	-0.604161000	0.000135000
6	-1.288477000	0.705379000	-0.000100000	6	-1.421803000	-1.765967000	0.000453000
7	-0.439412000	1.775563000	-0.000161000	7	-2.742490000	-1.753602000	0.000328000
6	0.837652000	1.568225000	0.000064000	6	-3.372426000	-0.576255000	0.000122000
8	1.635617000	2.638421000	0.000409000	8	-4.718096000	-0.603246000	-0.000425000
6	2.858344000	0.017826000	-0.000049000	6	-0.520875000	1.824265000	0.000070000
7	3.384793000	-1.184858000	-0.000225000	7	0.762420000	1.856681000	0.000075000
6	2.551323000	-2.241000000	-0.000230000	6	1.460810000	0.667586000	0.000033000
6	1.184018000	-2.139708000	-0.000051000	6	0.815015000	-0.584983000	0.000006000

8	3.708046000	1.048664000	-0.000099000	8	-1.207423000	2.976281000	-0.000172000
6	-1.790690000	-1.654130000	0.000442000	7	2.801028000	0.791311000	0.000137000
6	-3.122506000	-1.345367000	0.000273000	6	3.524607000	-0.299292000	-0.000017000
6	-3.464838000	0.024989000	-0.000090000	6	2.996893000	-1.606026000	-0.000427000
7	-2.603031000	1.008360000	-0.000254000	6	1.632859000	-1.732075000	-0.000389000
8	-4.771681000	0.334048000	-0.000280000	8	4.863509000	-0.168435000	0.000242000
1	1.050305000	3.408194000	0.000310000	1	-3.271999000	1.573813000	-0.000056000
1	3.032058000	-3.213411000	-0.000396000	1	-0.963143000	-2.748995000	0.000656000
1	0.581891000	-3.036478000	-0.000151000	1	-4.985210000	-1.530364000	-0.000039000
1	4.595093000	0.665175000	-0.000290000	1	-0.559345000	3.693193000	-0.000332000
1	-1.485474000	-2.693011000	0.000796000	1	3.664751000	-2.456046000	-0.000853000
1	-3.901751000	-2.094392000	0.000382000	1	1.190307000	-2.720740000	-0.000723000
1	-4.833458000	1.298016000	-0.000692000	1	5.054288000	0.778102000	-0.000041000
pn17				pn18			
6	-5.175625000	1.305427000	0.012137000	6	-7.437535000	2.617373000	-0.008890000
6	-5.233282000	-0.103146000	0.002675000	6	-7.562415000	1.255918000	-0.007376000
6	-3.979702000	-0.833882000	-0.009750000	6	-6.399016000	0.440047000	-0.002132000
6	-2.778321000	-0.098891000	-0.011702000	6	-5.172427000	1.121570000	0.001321000
7	-2.747579000	1.282522000	-0.002352000	7	-5.045172000	2.462510000	-0.000201000
6	-3.860531000	1.920727000	0.008657000	6	-6.140014000	3.173685000	-0.005109000
8	-3.849370000	3.260442000	0.017836000	8	-6.034323000	4.513484000	-0.007045000
6	-3.830533000	-2.243770000	-0.020309000	6	-6.371446000	-1.007163000	0.000011000
7	-2.683607000	-2.877212000	-0.031228000	6	-5.117559000	-1.651181000	0.005448000
6	-1.552441000	-2.147908000	-0.032781000	7	-3.928371000	-0.962211000	0.008953000
6	-1.545931000	-0.776815000	-0.023495000	6	-3.957701000	0.326611000	0.007025000
8	-4.940595000	-3.012605000	-0.019085000	8	-2.807244000	1.001813000	0.010141000
6	-6.336865000	2.073303000	0.024291000	6	-7.500679000	-1.867508000	-0.003106000
6	-7.540604000	1.389979000	0.026580000	7	-7.446925000	-3.174966000	-0.001432000
7	-7.634391000	0.061266000	0.017890000	6	-6.234150000	-3.763862000	0.003812000
6	-6.528024000	-0.664109000	0.006315000	6	-5.060121000	-3.059447000	0.007414000
8	-8.691817000	2.085756000	0.038488000	8	-8.736902000	-1.320162000	-0.008648000
1	-2.924248000	3.538973000	0.014305000	1	-8.296742000	3.274827000	-0.012830000
1	-0.627416000	-2.713230000	-0.041950000	1	-8.540103000	0.800063000	-0.010159000
1	-0.628588000	-0.204439000	-0.024916000	1	-5.092184000	4.725346000	-0.003882000
1	-4.633608000	-3.928555000	-0.026948000	1	-2.100503000	0.343010000	0.013804000
1	-6.304821000	3.153422000	0.031607000	1	-6.238314000	-4.847950000	0.005050000
1	-6.660959000	-1.735436000	-0.000383000	1	-4.094963000	-3.546896000	0.011624000
1	-9.411492000	1.442706000	0.038147000	1	-9.355716000	-2.062091000	-0.010242000
pn19				pn20			
6	-6.166233000	1.388241000	-0.078771000	6	-6.207141000	1.365376000	0.007524000
6	-6.199154000	-0.009463000	0.072404000	6	-6.222916000	-0.035492000	0.000467000
6	-4.944088000	-0.720332000	0.152597000	6	-4.960754000	-0.747754000	-0.007813000
6	-3.763653000	0.027530000	0.074827000	6	-3.771593000	0.027091000	-0.008306000
7	-3.746315000	1.392390000	-0.072846000	7	-3.776459000	1.408969000	-0.001308000
6	-4.869989000	2.026493000	-0.144483000	6	-4.907970000	2.013063000	0.006019000
8	-4.833338000	3.356995000	-0.289139000	8	-4.934103000	3.353690000	0.012771000
7	-4.953707000	-2.066234000	0.298108000	6	-4.800326000	-2.146000000	-0.015439000
6	-3.804726000	-2.681618000	0.367699000	7	-3.623296000	-2.751339000	-0.022808000
6	-2.548251000	-2.033129000	0.300847000	6	-2.523753000	-1.996899000	-0.023032000
6	-2.538387000	-0.675265000	0.154089000	6	-2.534189000	-0.614655000	-0.016098000
8	-3.798451000	-4.021501000	0.512352000	8	-1.343582000	-2.643572000	-0.030666000
6	-7.423021000	2.053711000	-0.153967000	6	-7.398407000	2.109356000	0.015693000
7	-8.576053000	1.430777000	-0.089562000	6	-8.583132000	1.416851000	0.016559000
6	-8.578405000	0.091488000	0.055372000	7	-8.639499000	0.072247000	0.009935000
6	-7.439936000	-0.668212000	0.140533000	6	-7.524755000	-0.612990000	0.002324000
8	-7.458524000	3.382823000	-0.297855000	8	-7.639144000	-1.955021000	-0.004098000

1	-3.898606000	3.600082000	-0.313418000	1	-4.016268000	3.655657000	0.010850000
1	-1.643752000	-2.622567000	0.366966000	1	-5.664773000	-2.793274000	-0.015548000
1	-1.614996000	-0.111779000	0.095638000	1	-1.618020000	-0.041186000	-0.016623000
1	-4.718532000	-4.310474000	0.540755000	1	-1.542221000	-3.587966000	-0.034743000
1	-9.559454000	-0.368579000	0.102617000	1	-7.369759000	3.189622000	0.021068000
1	-7.474599000	-1.741614000	0.256650000	1	-9.537908000	1.929618000	0.022700000
1	-8.393701000	3.624267000	-0.326443000	1	-8.585525000	-2.149676000	-0.001629000
pn21				pn22			
6	-6.216082000	1.310676000	0.008054000	6	-5.974507000	1.556132000	0.002233000
6	-6.289799000	-0.102151000	0.000684000	6	-6.034906000	0.148636000	-0.009226000
6	-5.041645000	-0.838592000	-0.003866000	6	-4.772147000	-0.578258000	-0.006092000
6	-3.834160000	-0.108620000	-0.000792000	6	-3.587045000	0.184830000	0.008180000
7	-3.793706000	1.259919000	0.006262000	7	-3.554477000	1.568926000	0.019328000
6	-4.906148000	1.919249000	0.010388000	6	-4.675063000	2.192181000	0.016444000
8	-4.832089000	3.250543000	0.017193000	8	-4.687130000	3.537522000	0.026705000
6	-4.902323000	-2.253425000	-0.011217000	6	-4.671885000	-1.970480000	-0.016401000
7	-3.758270000	-2.892195000	-0.015175000	6	-3.406206000	-2.532700000	-0.012046000
6	-2.622893000	-2.167083000	-0.012113000	7	-2.275826000	-1.826370000	0.001423000
6	-2.604970000	-0.798359000	-0.005069000	6	-2.367898000	-0.508287000	0.011219000
8	-6.007184000	-3.026286000	-0.014535000	8	-3.290532000	-3.876380000	-0.021970000
6	-7.436560000	2.039426000	0.012593000	6	-7.171786000	2.281130000	-0.000541000
7	-8.621020000	1.472438000	0.010262000	7	-8.361865000	1.706226000	-0.013415000
6	-8.673880000	0.131311000	0.003218000	6	-8.406266000	0.371830000	-0.023864000
6	-7.572490000	-0.689823000	-0.001703000	6	-7.290567000	-0.453844000	-0.022636000
8	-7.411840000	3.376503000	0.019684000	8	-9.623589000	-0.193240000	-0.038112000
1	-3.889969000	3.467762000	0.017744000	1	-3.766456000	3.829022000	0.035585000
1	-1.701366000	-2.738735000	-0.015600000	1	-5.537554000	-2.618272000	-0.027584000
1	-1.683693000	-0.232531000	-0.002682000	1	-1.444652000	0.062012000	0.022157000
1	-5.691098000	-3.939485000	-0.019383000	1	-2.347300000	-4.078775000	-0.016785000
1	-9.671332000	-0.295537000	0.001491000	1	-7.147360000	3.365149000	0.008150000
1	-7.696088000	-1.758635000	-0.007254000	1	-7.427698000	-1.525846000	-0.032113000
1	-8.335910000	3.659043000	0.021789000	1	-10.271657000	0.522346000	-0.035145000
pn23				pn24			
6	-5.974388000	1.299943000	0.000275000	6	-6.204712000	1.523721000	0.006399000
6	-5.999753000	-0.109167000	-0.010106000	6	-6.256808000	0.122138000	-0.000794000
6	-4.725372000	-0.807723000	-0.006259000	6	-5.010536000	-0.626544000	-0.008220000
6	-3.567454000	-0.019975000	0.007247000	6	-3.817230000	0.135588000	-0.007595000
7	-3.557940000	1.355322000	0.017339000	7	-3.782790000	1.516289000	-0.000452000
6	-4.692370000	1.959655000	0.014115000	6	-4.894347000	2.149695000	0.006000000
8	-4.721459000	3.302791000	0.023593000	8	-4.898190000	3.496087000	0.013002000
6	-4.595338000	-2.211894000	-0.015353000	6	-4.888243000	-2.021416000	-0.015880000
6	-3.335753000	-2.753950000	-0.010638000	6	-3.614281000	-2.566996000	-0.022281000
7	-2.208109000	-2.013275000	0.002235000	7	-2.484742000	-1.859200000	-0.021809000
6	-2.320352000	-0.710134000	0.010714000	6	-2.592269000	-0.543112000	-0.014638000
8	-1.200999000	0.026539000	0.023581000	8	-3.490214000	-3.910423000	-0.029663000
6	-7.189037000	1.998803000	-0.003607000	6	-7.381153000	2.289268000	0.013731000
7	-8.364015000	1.397726000	-0.016035000	6	-8.580008000	1.619008000	0.013633000
6	-8.376982000	0.060560000	-0.025445000	7	-8.669767000	0.277821000	0.006875000
6	-7.244708000	-0.739050000	-0.023368000	6	-7.567189000	-0.431033000	0.000026000
8	-9.582684000	-0.529732000	-0.038147000	8	-7.710654000	-1.767705000	-0.006559000
1	-3.803325000	3.603935000	0.032055000	1	-3.976121000	3.782527000	0.011927000
1	-5.462145000	-2.858268000	-0.025798000	1	-5.743590000	-2.676257000	-0.016957000
1	-3.191323000	-3.828212000	-0.017282000	1	-1.677020000	0.040252000	-0.014206000
1	-0.463473000	-0.596807000	0.023623000	1	-2.545441000	-4.104988000	-0.033532000
1	-7.187779000	3.083265000	0.004278000	1	-7.332022000	3.368704000	0.019237000
1	-7.359140000	-1.813479000	-0.032181000	1	-9.522967000	2.153923000	0.019114000

1	-10.244947000	0.172724000	-0.037020000	1	-8.661103000	-1.942022000	-0.004759000
pn25				pn26			
6	-6.194515000	1.218767000	0.009314000	6	-5.164246000	1.223783000	0.012815000
6	-6.238285000	-0.189478000	0.001584000	6	-5.196014000	-0.181403000	0.004196000
6	-4.983306000	-0.906208000	-0.004604000	6	-3.937284000	-0.902019000	-0.009203000
6	-3.780044000	-0.162477000	-0.002947000	6	-2.738923000	-0.150401000	-0.013039000
7	-3.762782000	1.210402000	0.004376000	7	-2.729276000	1.235195000	-0.004547000
6	-4.887862000	1.846780000	0.010134000	6	-3.851914000	1.855505000	0.007361000
8	-4.844484000	3.179288000	0.017666000	8	-3.864318000	3.194753000	0.015970000
6	-4.874034000	-2.303827000	-0.012046000	6	-3.813920000	-2.294845000	-0.018621000
7	-3.727077000	-2.956670000	-0.017727000	7	-2.655661000	-2.936603000	-0.030843000
6	-2.601350000	-2.231467000	-0.016262000	6	-1.540275000	-2.206078000	-0.034327000
6	-2.563615000	-0.850233000	-0.009034000	6	-1.517748000	-0.821327000	-0.025899000
8	-1.445604000	-2.917989000	-0.022189000	8	-0.372806000	-2.876737000	-0.046626000
6	-7.434959000	1.913176000	0.015431000	6	-6.344158000	1.962025000	0.025867000
7	-8.603644000	1.311601000	0.014143000	6	-7.532684000	1.248466000	0.029892000
6	-8.624512000	-0.031279000	0.006586000	7	-7.596588000	-0.082867000	0.021801000
6	-7.498976000	-0.817421000	0.000215000	6	-6.468113000	-0.772875000	0.009357000
8	-7.446396000	3.248731000	0.023111000	8	-8.698864000	1.919378000	0.042283000
1	-3.907846000	3.419951000	0.017149000	1	-2.944173000	3.490144000	0.011266000
1	-5.764168000	-2.924209000	-0.013384000	1	-4.696189000	-2.926662000	-0.016240000
1	-1.626271000	-0.312106000	-0.007964000	1	-0.585881000	-0.273679000	-0.029111000
1	-1.674091000	-3.855549000	-0.026581000	1	-0.588083000	-3.817265000	-0.050972000
1	-9.611118000	-0.482619000	0.005738000	1	-6.341568000	3.042754000	0.032568000
1	-7.597826000	-1.893020000	-0.005751000	1	-6.579098000	-1.851713000	0.003301000
1	-8.376863000	3.510014000	0.026143000	1	-9.406403000	1.263257000	0.043115000
pn27				pn28			
6	-6.203163000	1.521451000	-0.144718000	6	-8.549985000	2.718563000	-0.003504000
6	-6.208497000	0.124008000	-0.014996000	6	-8.643181000	1.354956000	-0.004852000
6	-4.939410000	-0.564756000	0.089248000	6	-7.466528000	0.567755000	-0.002169000
6	-3.772257000	0.223048000	0.052972000	6	-6.253942000	1.263367000	0.001691000
7	-3.783463000	1.594425000	-0.074770000	7	-6.150912000	2.606937000	0.003001000
6	-4.918632000	2.186822000	-0.165702000	6	-7.259210000	3.296700000	0.000444000
8	-4.958166000	3.526710000	-0.292544000	8	-7.182368000	4.638786000	0.002114000
7	-4.886174000	-1.906929000	0.215653000	6	-7.433290000	-0.877917000	-0.003054000
6	-3.715947000	-2.480714000	0.306086000	6	-6.171163000	-1.517674000	0.000045000
6	-2.483231000	-1.793514000	0.281139000	7	-4.985530000	-0.814883000	0.003691000
6	-2.527651000	-0.432713000	0.153277000	6	-5.029914000	0.472846000	0.004404000
8	-3.678924000	-3.821653000	0.431680000	8	-3.888652000	1.162571000	0.008165000
6	-7.405507000	2.241975000	-0.249728000	6	-8.566613000	-1.700289000	-0.006591000
6	-8.576824000	1.529119000	-0.220433000	7	-8.523295000	-3.021348000	-0.007075000
7	-8.621091000	0.189753000	-0.097315000	6	-7.320505000	-3.603488000	-0.004087000
6	-7.499782000	-0.485270000	0.000832000	6	-6.122616000	-2.913323000	-0.000480000
8	-7.608692000	-1.813857000	0.120247000	8	-7.300285000	-4.950213000	-0.004348000
1	-4.044244000	3.837892000	-0.292684000	1	-9.419519000	3.361986000	-0.005330000
1	-1.558039000	-2.347571000	0.361812000	1	-9.618806000	0.885419000	-0.007918000
1	-1.627856000	0.169940000	0.125719000	1	-6.245294000	4.872148000	0.005295000
1	-4.595177000	-4.126450000	0.430941000	1	-3.172253000	0.513958000	0.009865000
1	-7.393546000	3.317700000	-0.349395000	1	-9.561468000	-1.266059000	-0.008988000
1	-9.537929000	2.024979000	-0.296766000	1	-5.173967000	-3.431369000	0.001949000
1	-8.557147000	-1.999984000	0.107390000	1	-8.218669000	-5.245750000	-0.006877000
pn29				pn30			
6	-5.115762000	1.388181000	0.012822000	6	-8.557796000	2.562477000	-0.010157000
6	-5.194784000	-0.016872000	0.004270000	6	-8.643683000	1.199326000	-0.008385000
6	-3.963739000	-0.787325000	-0.009509000	6	-7.463676000	0.417678000	-0.003543000
6	-2.754350000	-0.061000000	-0.013287000	6	-6.249097000	1.115248000	-0.000888000

7	-2.691920000	1.323134000	-0.004653000	7	-6.154636000	2.459588000	-0.002645000
6	-3.786960000	1.984250000	0.007314000	6	-7.267390000	3.143570000	-0.007144000
8	-3.762790000	3.328886000	0.016191000	8	-7.194670000	4.483857000	-0.008612000
6	-3.895171000	-2.181919000	-0.019161000	6	-7.442672000	-1.027936000	-0.001234000
6	-2.642485000	-2.774129000	-0.031880000	6	-6.183109000	-1.642159000	0.003500000
7	-1.492170000	-2.101028000	-0.035618000	7	-4.996271000	-0.956370000	0.005987000
6	-1.553475000	-0.780141000	-0.026536000	6	-5.027006000	0.330322000	0.003926000
8	-2.563634000	-4.120213000	-0.041336000	8	-3.879000000	1.016897000	0.006670000
6	-6.275049000	2.156538000	0.025995000	6	-8.593688000	-1.846527000	-0.003272000
6	-7.483937000	1.475428000	0.030041000	6	-8.430747000	-3.207725000	-0.000575000
7	-7.590309000	0.145846000	0.022334000	7	-7.226463000	-3.817151000	0.003917000
6	-6.480661000	-0.573400000	0.009825000	6	-6.154919000	-3.066530000	0.005798000
8	-8.627814000	2.179364000	0.043027000	8	-4.957159000	-3.667077000	0.010182000
1	-2.835568000	3.598736000	0.011334000	1	-9.429103000	3.203372000	-0.013752000
1	-4.772520000	-2.813643000	-0.017132000	1	-9.615288000	0.721592000	-0.010668000
1	-0.616963000	-0.231683000	-0.029521000	1	-6.257947000	4.719776000	-0.005842000
1	-1.626005000	-4.347465000	-0.049397000	1	-3.167758000	0.362934000	0.009871000
1	-6.243395000	3.236761000	0.032866000	1	-9.589797000	-1.425671000	-0.006877000
1	-6.616650000	-1.649575000	0.003914000	1	-9.289896000	-3.869001000	-0.001936000
1	-9.355271000	1.544967000	0.043879000	1	-5.128310000	-4.617230000	0.011175000
pn31				pn32			
6	-8.336665000	2.686466000	-0.009832000	6	-6.206906000	1.263829000	0.005146000
6	-8.446747000	1.324053000	-0.009265000	6	-6.221204000	-0.139441000	-0.001524000
6	-7.281923000	0.523313000	-0.003972000	6	-4.959654000	-0.857198000	-0.007061000
6	-6.054566000	1.195893000	0.000461000	6	-3.794916000	-0.068244000	-0.005357000
7	-5.935952000	2.536896000	-0.000052000	7	-3.788347000	1.304583000	0.001225000
6	-7.036749000	3.242558000	-0.004905000	6	-4.914889000	1.915972000	0.006124000
8	-6.936441000	4.580920000	-0.005855000	8	-4.939740000	3.260503000	0.012603000
6	-7.283650000	-0.925350000	-0.002848000	6	-4.804439000	-2.263541000	-0.013907000
6	-6.028712000	-1.568041000	0.002667000	6	-3.535234000	-2.785329000	-0.018502000
7	-4.825677000	-0.893164000	0.006967000	7	-2.410881000	-2.041264000	-0.017027000
6	-4.839417000	0.391137000	0.005981000	6	-2.540966000	-0.740082000	-0.010792000
8	-3.684845000	1.069563000	0.009938000	8	-1.429549000	0.011263000	-0.009149000
6	-8.434985000	-1.719687000	-0.006846000	6	-7.402450000	2.002090000	0.010651000
6	-8.278805000	-3.094063000	-0.005131000	6	-8.583131000	1.303728000	0.009297000
7	-7.098186000	-3.716914000	0.000010000	7	-8.638380000	-0.040934000	0.002973000
6	-6.008874000	-2.970738000	0.003815000	6	-7.520978000	-0.723569000	-0.002166000
8	-9.379879000	-3.874192000	-0.009133000	8	-7.637359000	-2.063722000	-0.008367000
1	-9.196014000	3.343187000	-0.013856000	1	-4.020965000	3.559001000	0.012448000
1	-9.426407000	0.862640000	-0.012904000	1	-5.658961000	-2.918993000	-0.015523000
1	-5.995064000	4.797588000	-0.002014000	1	-3.384651000	-3.859065000	-0.023731000
1	-2.977779000	0.411804000	0.013348000	1	-0.686586000	-0.605035000	-0.013491000
1	-9.433993000	-1.306199000	-0.011227000	1	-7.378211000	3.082420000	0.015749000
1	-5.049081000	-3.477493000	0.007964000	1	-9.539666000	1.813839000	0.013334000
1	-9.075298000	-4.789554000	-0.007276000	1	-8.584758000	-2.254135000	-0.007741000
pn33				pn34			
6	-5.162441000	1.129666000	0.011479000	6	-6.195264000	1.376519000	0.008477000
6	-5.198146000	-0.277188000	0.002550000	6	-6.276964000	-0.027422000	0.000748000
6	-3.949492000	-1.013238000	-0.009142000	6	-5.038229000	-0.787634000	-0.004787000
6	-2.770770000	-0.256233000	-0.010736000	6	-3.834650000	-0.059590000	-0.002005000
7	-2.740314000	1.120910000	-0.001808000	7	-3.774156000	1.314618000	0.005602000
6	-3.852829000	1.756803000	0.008454000	6	-4.875065000	1.982097000	0.010527000
8	-3.854223000	3.100084000	0.017431000	8	-4.806600000	3.319166000	0.017721000
6	-3.845888000	-2.420131000	-0.018915000	6	-4.972907000	-2.185099000	-0.012645000
6	-2.595687000	-2.986098000	-0.029502000	6	-3.724100000	-2.778426000	-0.017252000
7	-1.451575000	-2.273434000	-0.031248000	7	-2.572988000	-2.101393000	-0.014706000

6	-1.539289000	-0.966728000	-0.022343000	6	-2.630048000	-0.783839000	-0.007314000
8	-0.404608000	-0.253596000	-0.023555000	8	-3.640613000	-4.125063000	-0.024919000
6	-6.344828000	1.865202000	0.022656000	6	-7.423584000	2.095328000	0.013708000
6	-7.531647000	1.150009000	0.024402000	7	-8.602991000	1.515726000	0.011689000
7	-7.598222000	-0.183895000	0.016280000	6	-8.656949000	0.174178000	0.004301000
6	-6.470088000	-0.870640000	0.005703000	6	-7.545933000	-0.632871000	-0.001310000
8	-8.697556000	1.817608000	0.035302000	8	-7.409463000	3.431038000	0.021102000
1	-2.931074000	3.385301000	0.014192000	1	-3.866181000	3.540891000	0.018030000
1	-4.721709000	-3.054109000	-0.018186000	1	-5.851825000	-2.814062000	-0.015269000
1	-2.476088000	-4.063650000	-0.037184000	1	-1.693157000	-0.235992000	-0.005247000
1	0.319151000	-0.892512000	-0.032013000	1	-2.702480000	-4.349675000	-0.027146000
1	-6.343350000	2.945930000	0.029738000	1	-9.653467000	-0.254008000	0.002911000
1	-6.575888000	-1.950043000	-0.000605000	1	-7.658543000	-1.707218000	-0.007169000
1	-9.404539000	1.160644000	0.034806000	1	-8.334604000	3.710101000	0.023386000
pn35				pn36			
6	-6.195567000	1.123722000	0.007125000	6	-6.220078000	1.453231000	0.109631000
6	-6.244872000	-0.282804000	-0.000108000	6	-6.254877000	0.056288000	-0.012393000
6	-4.995191000	-1.017045000	-0.004143000	6	-4.998089000	-0.662183000	0.002511000
6	-3.815887000	-0.264994000	-0.000643000	6	-3.813401000	0.091329000	-0.136614000
7	-3.776736000	1.100802000	0.006339000	7	-3.804935000	1.470851000	-0.131030000
6	-4.891706000	1.751360000	0.010070000	6	-4.917167000	2.085402000	0.057077000
8	-4.838125000	3.087163000	0.016665000	8	-4.916927000	3.422005000	0.159600000
6	-4.901639000	-2.426957000	-0.011346000	6	-4.803696000	-2.047242000	0.265233000
6	-3.658322000	-3.001614000	-0.014606000	7	-3.650276000	-2.664179000	0.150872000
7	-2.508062000	-2.292233000	-0.011313000	6	-2.559135000	-1.936947000	-0.148350000
6	-2.584605000	-0.988456000	-0.004684000	6	-2.576981000	-0.569888000	-0.252904000
8	-1.448105000	-0.279369000	-0.001344000	8	-5.826714000	-2.767063000	0.744765000
6	-7.439167000	1.818234000	0.010906000	6	-7.400999000	2.208804000	0.197747000
7	-8.605508000	1.215669000	0.007908000	6	-8.592234000	1.531952000	0.115864000
6	-8.630226000	-0.128392000	0.000982000	7	-8.662297000	0.216611000	-0.153088000
6	-7.504438000	-0.912592000	-0.003154000	6	-7.555201000	-0.478466000	-0.265007000
8	-7.448572000	3.153659000	0.017681000	8	-7.667143000	-1.727677000	-0.727275000
1	-3.899199000	3.317599000	0.017573000	1	-3.998956000	3.712643000	0.079636000
1	-5.782271000	-3.053582000	-0.014327000	1	-1.636604000	-2.495910000	-0.258802000
1	-3.543255000	-4.079364000	-0.020136000	1	-1.678188000	0.011394000	-0.404175000
1	-0.725656000	-0.919805000	-0.005064000	1	-5.489559000	-3.662385000	0.876310000
1	-9.617780000	-0.576910000	-0.001245000	1	-7.358928000	3.281526000	0.319551000
1	-7.597402000	-1.988589000	-0.008694000	1	-9.541811000	2.044492000	0.218465000
1	-8.378376000	3.416836000	0.018956000	1	-8.610140000	-1.888177000	-0.860453000

II. 1CO₂ complex

py...CO₂				nt1...CO₂			
6	-2.794598000	-0.292283000	-0.000301000	6	3.192650000	-0.154188000	-0.000099000
6	-2.054776000	-1.477865000	-0.000041000	6	2.703843000	1.118396000	-0.000015000
6	-0.675428000	-1.378829000	0.000300000	6	1.304896000	1.335824000	0.000034000
7	-0.022177000	-0.209804000	0.000366000	6	0.455530000	0.201334000	-0.000041000
6	-0.739185000	0.902774000	0.000092000	7	0.949676000	-1.058888000	-0.000081000
6	-2.139042000	0.922203000	-0.000225000	6	2.244868000	-1.211229000	-0.000061000
1	-3.877950000	-0.321907000	-0.000556000	8	2.731929000	-2.463196000	0.000067000
1	-2.536212000	-2.446186000	-0.000081000	6	0.701960000	2.617652000	0.000208000
1	-0.047461000	-2.264167000	0.000483000	6	-0.655340000	2.726121000	0.000201000
1	-2.659414000	1.870203000	-0.000407000	6	-1.410436000	1.521069000	-0.000096000
8	-0.085936000	2.076741000	0.000266000	7	-0.897168000	0.318158000	-0.000135000
1	0.863807000	1.893303000	0.000865000	8	-2.742100000	1.654409000	-0.000314000
6	2.679433000	-0.271837000	-0.000145000	1	4.248722000	-0.384909000	-0.000165000
8	2.695961000	-1.424033000	-0.000043000	1	3.374180000	1.971441000	-0.000035000

8	2.734231000	0.886344000	-0.000342000	1	1.971741000	-3.059719000	-0.000070000
				1	1.331007000	3.501613000	0.000378000
				1	-1.175746000	3.673631000	0.000415000
				1	-3.136308000	0.769429000	0.000058000
				6	-2.622603000	-1.974068000	0.000090000
				8	-3.490524000	-1.202210000	0.000099000
				8	-1.808475000	-2.785481000	0.000100000
nt2...CO ₂				nt3...CO ₂			
6	2.973046000	1.304336000	-0.000028000	6	-2.058069000	-1.702865000	-0.000271000
6	1.636868000	1.568385000	0.000024000	6	-0.727557000	-1.407928000	-0.000317000
6	0.724282000	0.485016000	0.000037000	6	-0.313822000	-0.049552000	-0.000141000
6	1.230763000	-0.831617000	-0.000010000	6	-1.323632000	0.934189000	0.000081000
7	2.567010000	-1.083671000	-0.000045000	7	-2.650724000	0.632236000	0.000134000
6	3.375521000	-0.060164000	-0.000043000	6	-2.983979000	-0.625306000	-0.000038000
8	4.696638000	-0.295315000	-0.000084000	8	-4.292295000	-0.948132000	0.000009000
6	-0.689210000	0.642801000	0.000105000	7	1.017296000	0.257406000	-0.000194000
7	-1.533903000	-0.353136000	0.000107000	6	1.346192000	1.520250000	-0.000059000
6	-1.028472000	-1.615963000	0.000054000	6	0.411037000	2.593532000	0.000171000
6	0.306016000	-1.906493000	0.000005000	6	-0.916189000	2.294448000	0.000244000
8	-1.161004000	1.899120000	0.000229000	8	2.643025000	1.868957000	-0.000090000
1	3.728948000	2.077359000	-0.000049000	1	-2.431664000	-2.718034000	-0.000401000
1	1.258442000	2.583137000	0.000040000	1	0.027362000	-2.183904000	-0.000476000
1	4.815496000	-1.253873000	-0.000099000	1	-4.789077000	-0.120699000	0.000176000
1	-1.772790000	-2.404753000	0.000055000	1	0.785005000	3.608538000	0.000273000
1	0.670931000	-2.924280000	-0.000023000	1	-1.679961000	3.062875000	0.000411000
1	-2.128557000	1.857973000	0.000122000	1	3.180637000	1.065187000	-0.000456000
6	-4.213655000	-0.016954000	-0.000132000	6	3.115485000	-1.699699000	0.000176000
8	-4.408315000	-1.152118000	0.000116000	8	2.404158000	-2.605840000	0.000732000
8	-4.089215000	1.136563000	-0.000329000	8	3.875724000	-0.825470000	-0.000423000
nt4...CO ₂				nt5...CO ₂			
6	3.097704000	-1.425512000	0.000099000	6	-1.369271000	-0.589367000	-0.000077000
6	1.780780000	-1.758163000	0.000291000	6	-0.792617000	0.689485000	-0.000127000
6	0.801722000	-0.727775000	0.000260000	6	-1.619627000	1.837664000	0.000040000
6	1.242261000	0.622493000	0.000014000	6	-2.973045000	1.647602000	0.000236000
7	2.569234000	0.944303000	-0.000169000	7	-3.561353000	0.421107000	0.000284000
6	3.425175000	-0.034892000	-0.000119000	6	-2.797563000	-0.630656000	0.000136000
8	4.733006000	0.262655000	-0.000312000	8	-3.367426000	-1.848755000	0.000173000
6	-0.582840000	-0.965677000	0.000450000	6	-0.543000000	-1.739436000	-0.000233000
7	-1.485461000	-0.008193000	0.000412000	6	0.809345000	-1.550779000	-0.000416000
6	-1.054042000	1.268703000	0.000164000	7	1.396349000	-0.322043000	-0.000461000
6	0.275190000	1.637628000	-0.000013000	6	0.636869000	0.736384000	-0.000344000
8	-1.998736000	2.222355000	0.000141000	8	1.200997000	1.952107000	-0.000324000
1	3.896278000	-2.154145000	0.000108000	1	-1.183985000	2.826938000	0.000000000
1	1.465338000	-2.796154000	0.000465000	1	-3.656938000	2.488020000	0.000364000
1	4.805600000	1.226043000	-0.000460000	1	-4.323629000	-1.714140000	0.000321000
1	-0.959673000	-1.986253000	0.000647000	1	-0.979044000	-2.728468000	-0.000211000
1	0.564935000	2.678939000	-0.000170000	1	1.498386000	-2.387574000	-0.000553000
1	-2.864723000	1.791900000	0.000330000	1	2.162783000	1.839695000	-0.000487000
8	-4.433536000	0.340392000	-0.000009000	6	4.105846000	-0.197592000	0.000329000
6	-4.079767000	-0.763332000	-0.000357000	8	4.071420000	0.961896000	0.000310000
8	-3.792142000	-1.879645000	-0.000740000	8	4.206988000	-1.344966000	0.000409000
nt6...CO ₂				nt7...CO ₂			
6	2.593900000	1.126986000	0.000012000	6	-0.007434000	2.660361000	-0.130606000
6	1.204674000	0.925970000	-0.000014000	6	-1.295604000	2.275909000	-0.338900000
6	0.732068000	-0.407832000	-0.000016000	6	-1.661094000	0.909512000	-0.172823000
6	1.668136000	-1.458714000	-0.000038000	6	-0.637347000	0.023884000	0.204046000

7	2.967219000	-1.258874000	0.000076000	7	0.651247000	0.402977000	0.397989000
6	3.407362000	0.013459000	0.000112000	6	0.939961000	1.662556000	0.241008000
8	4.741182000	0.175448000	-0.000075000	8	2.204300000	2.070043000	0.431056000
6	0.235764000	1.970810000	0.000040000	6	-2.971302000	0.401995000	-0.360737000
6	-1.084541000	1.634908000	0.000077000	6	-3.186417000	-0.932094000	-0.160826000
7	-1.553481000	0.352545000	0.000039000	7	-2.213584000	-1.800232000	0.220199000
6	-0.680437000	-0.614615000	-0.000031000	6	-1.006465000	-1.345324000	0.396764000
8	-1.109623000	-1.882537000	-0.000245000	8	-0.044059000	-2.192114000	0.792036000
1	3.027777000	2.117948000	-0.000023000	1	0.324788000	3.684226000	-0.238696000
1	1.323539000	-2.487480000	0.000133000	1	-2.051213000	2.997946000	-0.628085000
1	5.133686000	-0.706322000	-0.000114000	1	2.733486000	1.296717000	0.676101000
1	0.545461000	3.007649000	0.000082000	1	-3.778794000	1.060243000	-0.656042000
1	-1.855413000	2.397897000	0.000208000	1	-4.169499000	-1.367556000	-0.295837000
1	-2.078306000	-1.873434000	0.000283000	1	-0.453231000	-3.064463000	0.855873000
6	-4.225808000	-0.065519000	-0.000030000	6	2.708167000	-1.260268000	-0.529750000
8	-4.454067000	1.063428000	-0.000222000	8	3.417456000	-0.722002000	0.213132000
8	-4.064945000	-1.214422000	0.000287000	8	2.051807000	-1.806616000	-1.302436000
nt8...CO ₂				nt9...CO ₂			
6	-3.518992000	0.627369000	-0.000079000	6	1.004104000	-0.135017000	0.000098000
6	-2.505191000	1.528774000	0.000007000	6	1.333758000	1.240484000	-0.000017000
6	-1.153605000	1.063932000	0.000118000	6	0.280006000	2.189499000	0.000075000
6	-0.957567000	-0.335913000	0.000124000	6	-1.006468000	1.735529000	0.000265000
7	-1.985380000	-1.238144000	0.000038000	7	-1.340972000	0.422011000	0.000364000
6	-3.190455000	-0.765651000	-0.000053000	6	-0.385297000	-0.474459000	0.000283000
8	-4.231649000	-1.619193000	-0.000151000	8	-0.736737000	-1.759659000	0.000454000
6	-0.031437000	1.907401000	0.000226000	6	2.091200000	-1.063020000	0.000000000
6	1.218011000	1.325117000	0.000344000	7	3.348913000	-0.704672000	-0.000188000
7	1.416990000	-0.005029000	0.000324000	6	3.643159000	0.616494000	-0.000284000
6	0.371465000	-0.804568000	0.000215000	6	2.702257000	1.606562000	-0.000205000
8	2.313343000	2.107329000	0.000395000	8	1.827639000	-2.373004000	0.000054000
1	-4.561477000	0.916793000	-0.000168000	1	0.499326000	3.249054000	0.000005000
1	-2.704297000	2.594579000	-0.000008000	1	-1.846998000	2.421548000	0.000356000
1	-3.868054000	-2.513557000	-0.000148000	1	-1.704909000	-1.798317000	0.000438000
1	-0.129014000	2.985399000	0.000206000	1	4.701333000	0.854047000	-0.000418000
1	0.555775000	-1.874892000	0.000203000	1	2.988294000	2.650144000	-0.000285000
1	3.093028000	1.535654000	0.000537000	1	2.684912000	-2.819247000	-0.000056000
6	3.865899000	-1.179786000	-0.000465000	6	-3.979830000	-0.165206000	-0.000295000
8	3.403880000	-2.235344000	-0.000277000	8	-3.755138000	-1.302802000	-0.000604000
8	4.389925000	-0.145518000	-0.000689000	8	-4.270125000	0.949990000	-0.000003000
nt10...CO ₂				nt11...CO ₂			
6	1.858451000	-1.113500000	-0.000371000	6	2.604727000	0.989446000	0.000090000
6	0.820493000	-0.172986000	-0.000922000	6	1.220047000	0.721595000	0.000004000
6	1.114602000	1.205693000	-0.000193000	6	0.814746000	-0.640746000	-0.000103000
6	2.481503000	1.560513000	0.001085000	6	1.812252000	-1.640951000	-0.000071000
7	3.458519000	0.682611000	0.001604000	7	3.094390000	-1.380989000	-0.000031000
6	3.148172000	-0.625075000	0.000885000	6	3.468530000	-0.079210000	0.000043000
8	4.183502000	-1.486093000	0.001452000	8	4.793661000	0.142235000	0.000154000
6	-0.572117000	-0.528450000	-0.002221000	6	0.210228000	1.705116000	0.000041000
7	-1.537769000	0.338879000	-0.002735000	6	-1.100785000	1.290590000	-0.000097000
6	-1.230389000	1.672662000	-0.002008000	7	-1.494495000	-0.007235000	-0.000196000
6	0.045169000	2.145282000	-0.000781000	6	-0.565234000	-0.930876000	-0.000209000
8	-0.853030000	-1.838559000	-0.002857000	8	-2.081874000	2.204218000	-0.000171000
1	1.662693000	-2.176434000	-0.000910000	1	2.990867000	1.999872000	0.000186000
1	2.765800000	2.609466000	0.001688000	1	1.522377000	-2.689354000	-0.000192000
1	4.991737000	-0.959436000	0.002345000	1	5.225627000	-0.720699000	0.000134000
1	-2.085819000	2.337877000	-0.002446000	1	0.442603000	2.761584000	0.000171000

1	0.247698000	3.208866000	-0.000231000	1	-0.905548000	-1.964521000	-0.000205000
1	-1.815826000	-1.943315000	-0.003952000	1	-2.930755000	1.740501000	0.000338000
6	-4.151930000	-0.376402000	0.002228000	6	-4.069270000	-0.843803000	0.000123000
8	-4.503645000	0.720416000	0.002403000	8	-3.746107000	-1.950229000	0.000122000
8	-3.863733000	-1.499998000	0.002152000	8	-4.455164000	0.249179000	0.000173000
nt12...CO₂							
6	-2.028702000	-1.271174000	0.000213000				
6	-0.921415000	-0.397862000	0.000193000				
6	-1.138570000	1.000238000	-0.000055000				
6	-2.490593000	1.437442000	-0.000299000				
7	-3.511301000	0.620238000	-0.000275000				
6	-3.280739000	-0.711167000	-0.000023000				
8	-4.373166000	-1.502247000	-0.000029000				
6	0.428488000	-0.834241000	0.000399000				
7	1.448059000	-0.012492000	0.000401000				
6	1.222852000	1.321204000	0.000193000				
6	-0.033587000	1.874671000	-0.000082000				
8	2.308208000	2.116774000	0.000237000				
1	-1.906921000	-2.346637000	0.000406000				
1	-2.711046000	2.501833000	-0.000488000				
1	-5.143966000	-0.922657000	-0.000197000				
1	0.657958000	-1.897196000	0.000553000				
1	-0.157463000	2.949948000	-0.000313000				
1	3.096337000	1.557045000	-0.000043000				
6	3.914384000	-1.153212000	-0.000280000				
8	3.460084000	-2.212465000	-0.000285000				
8	4.426761000	-0.113556000	-0.000217000				
pn1...CO₂				pn2...CO₂			
6	-4.153193000	0.848505000	-0.000020000	6	2.474084000	-0.500021000	0.000922000
6	-3.055392000	1.662353000	-0.000090000	6	1.364614000	0.356616000	-0.000825000
6	-1.771376000	1.078919000	-0.000099000	6	0.052326000	-0.241188000	-0.001555000
6	-1.662361000	-0.319562000	-0.000008000	6	-0.048873000	-1.653501000	-0.000426000
7	-2.750747000	-1.121522000	0.000064000	7	1.057686000	-2.476831000	0.001297000
6	-3.929233000	-0.549434000	0.000057000	6	2.220488000	-1.919502000	0.001881000
8	-5.013585000	-1.339241000	0.000123000	8	3.311880000	-2.700196000	0.003497000
6	-0.549152000	1.832969000	-0.000195000	6	-1.131088000	0.502970000	-0.003177000
7	0.639514000	1.330131000	-0.000135000	7	-2.335235000	-0.044155000	-0.003920000
6	0.766422000	-0.034562000	-0.000015000	6	-2.417641000	-1.382633000	-0.002930000
6	-0.346570000	-0.899199000	0.000011000	6	-1.320995000	-2.227793000	-0.001072000
8	-0.682752000	3.169622000	-0.000162000	8	-3.648388000	-1.917022000	-0.003673000
7	2.033972000	-0.501351000	-0.000050000	6	3.765974000	0.061820000	0.001641000
6	2.215118000	-1.801888000	-0.000035000	6	3.897660000	1.423541000	0.000637000
6	1.171281000	-2.757151000	0.000057000	6	2.711438000	2.192978000	-0.001077000
6	-0.112266000	-2.288965000	0.000062000	7	1.496109000	1.698495000	-0.001796000
8	3.468223000	-2.273024000	0.000034000	8	2.846985000	3.526315000	-0.002037000
1	-5.167035000	1.223502000	-0.000022000	1	3.003907000	-3.616136000	0.004011000
1	-3.151169000	2.741140000	-0.000163000	1	-1.083988000	1.586979000	-0.003880000
1	-4.703898000	-2.253758000	0.000176000	1	-1.444632000	-3.301507000	-0.000234000
1	0.210594000	3.539072000	-0.000175000	1	-4.290611000	-1.193707000	-0.004520000
1	1.417401000	-3.809767000	0.000100000	1	4.631830000	-0.588648000	0.002967000
1	-0.961596000	-2.960994000	0.000098000	1	4.855739000	1.924071000	0.001106000
1	4.076965000	-1.519731000	0.000039000	1	1.959557000	3.907427000	-0.003175000
6	4.304734000	1.263717000	0.000131000	6	-4.462698000	1.626767000	0.003897000
8	3.733822000	2.261582000	0.000876000	8	-3.783786000	2.558025000	0.004044000
8	4.938228000	0.290503000	-0.000664000	8	-5.200875000	0.732708000	0.004064000
pn3...CO₂				pn4...CO₂			

6	-2.097379000	0.522682000	0.000362000	6	2.820415000	-1.163928000	-0.000048000
6	-0.698881000	0.411322000	-0.002805000	6	1.643061000	-0.410294000	-0.000012000
6	-0.125771000	-0.918570000	-0.002209000	6	1.771396000	0.994810000	0.000011000
6	-1.013125000	-2.006682000	0.001101000	6	3.051036000	1.564539000	0.000007000
7	-2.384416000	-1.877342000	0.003934000	7	4.158182000	0.846744000	-0.000030000
6	-2.874404000	-0.686220000	0.003632000	6	4.027719000	-0.485698000	-0.000060000
8	-4.212764000	-0.525637000	0.006348000	8	5.165753000	-1.198574000	-0.000083000
7	1.217724000	-1.065630000	-0.004690000	6	0.307099000	-0.960595000	0.000007000
6	1.700434000	-2.280011000	-0.004143000	6	-0.785500000	-0.067298000	0.000079000
6	0.906256000	-3.452670000	-0.000987000	7	-0.631364000	1.297677000	0.000103000
6	-0.450983000	-3.304093000	0.001649000	6	0.564097000	1.778053000	0.000057000
8	3.034739000	-2.445694000	-0.006636000	8	0.722848000	3.109425000	0.000094000
6	-2.672580000	1.812475000	0.000223000	6	0.020152000	-2.340070000	-0.000039000
6	-1.851656000	2.903171000	-0.002935000	6	-1.276741000	-2.773661000	-0.000001000
6	-0.452772000	2.673985000	-0.006129000	6	-2.289963000	-1.789912000	0.000095000
7	0.109620000	1.490000000	-0.006211000	7	-2.064465000	-0.495631000	0.000125000
8	0.338165000	3.753141000	-0.009148000	8	-3.556883000	-2.218644000	0.000138000
1	-4.601596000	-1.409317000	0.008183000	1	2.828807000	-2.244546000	-0.000060000
1	1.390746000	-4.419770000	-0.000743000	1	3.160986000	2.643593000	0.000027000
1	-1.121045000	-4.155407000	0.004149000	1	5.896692000	-0.567946000	-0.000079000
1	3.437512000	-1.567013000	-0.008802000	1	-0.163080000	3.496890000	0.000148000
1	-3.750620000	1.914750000	0.002672000	1	0.827096000	-3.062990000	-0.000111000
1	-2.221136000	3.919373000	-0.003117000	1	-1.549430000	-3.819555000	-0.000044000
1	1.255745000	3.445109000	-0.010616000	1	-4.140329000	-1.445481000	0.000173000
6	3.501828000	1.450822000	0.009211000	6	-4.290456000	1.347619000	-0.000142000
8	3.062525000	2.518936000	0.017239000	8	-3.693407000	2.329987000	-0.000046000
8	4.000347000	0.409979000	0.001600000	8	-4.947199000	0.389945000	-0.000249000
pn5...CO₂				pn6...CO₂			
6	0.353440000	0.947342000	-0.000004000	6	2.336057000	0.921102000	0.000033000
6	-0.367113000	-0.263763000	-0.000003000	6	1.661771000	-0.304782000	-0.000036000
6	-1.814090000	-0.183180000	-0.000002000	6	0.211045000	-0.285058000	-0.000286000
6	-2.397797000	1.091037000	-0.000002000	6	-0.418277000	0.976502000	-0.000360000
7	-1.672419000	2.267570000	-0.000006000	7	0.264598000	2.177570000	-0.000274000
6	-0.388698000	2.183514000	-0.000010000	6	1.547744000	2.132361000	-0.000095000
8	0.346057000	3.309625000	0.000002000	8	2.253895000	3.279570000	-0.000050000
7	-2.537087000	-1.324184000	0.000001000	6	-0.569456000	-1.440910000	-0.000371000
6	-3.840310000	-1.224463000	0.000004000	6	-1.945669000	-1.290209000	-0.000700000
6	-4.541699000	0.002544000	0.000003000	7	-2.559380000	-0.101223000	-0.000641000
6	-3.808589000	1.157082000	0.000001000	6	-1.820137000	0.994629000	-0.000426000
8	-4.572275000	-2.355300000	0.000006000	8	-2.724354000	-2.387896000	-0.001170000
6	1.752135000	0.889892000	0.000001000	6	3.746209000	0.914043000	0.000275000
7	2.420024000	-0.250186000	0.000001000	6	4.403938000	-0.285057000	0.000423000
6	1.722895000	-1.396755000	-0.000006000	6	3.620986000	-1.462612000	0.000314000
6	0.338034000	-1.464510000	-0.000003000	7	2.310028000	-1.485974000	0.000097000
8	2.426769000	-2.536269000	-0.000002000	8	4.274801000	-2.633028000	0.000466000
1	-0.271776000	4.051829000	0.000007000	1	1.615958000	4.004553000	-0.000172000
1	-5.623267000	-0.004469000	0.000005000	1	-0.117377000	-2.422694000	-0.000169000
1	-4.279426000	2.132780000	0.000000000	1	-2.338668000	1.948564000	-0.000262000
1	-3.955004000	-3.096924000	0.000004000	1	-3.648068000	-2.102372000	0.000493000
1	2.338568000	1.802911000	0.000006000	1	4.284536000	1.853580000	0.000344000
1	-0.172479000	-2.416846000	-0.000001000	1	5.482193000	-0.365274000	0.000613000
1	3.368820000	-2.314522000	0.000010000	1	3.612315000	-3.335699000	0.000348000
6	5.134800000	-0.124598000	0.000003000	6	-5.251557000	0.226915000	0.000801000
8	5.124229000	1.027356000	0.000016000	8	-5.418271000	-0.920501000	0.001341000
8	5.208080000	-1.281913000	-0.000009000	8	-5.152762000	1.375003000	0.000302000
pn7...CO₂				pn8...CO₂			

6	-2.347876000	0.538079000	-0.000107000	6	1.889272000	1.102214000	-0.000098000
6	-1.204531000	-0.297790000	0.000020000	6	1.775222000	-0.295538000	-0.000006000
6	0.087623000	0.365078000	0.000064000	6	0.459360000	-0.894064000	-0.000056000
6	0.118996000	1.776588000	0.000078000	6	-0.652876000	-0.020381000	-0.000186000
7	-1.014705000	2.558952000	0.000015000	7	-0.521763000	1.345808000	-0.000316000
6	-2.157605000	1.963899000	-0.000106000	6	0.657031000	1.856270000	-0.000274000
8	-3.271318000	2.708830000	-0.000181000	8	0.787233000	3.191773000	-0.000295000
6	1.349200000	-0.284748000	0.000070000	6	3.146165000	1.733841000	-0.000027000
7	2.505532000	0.340494000	0.000232000	6	4.260390000	0.936574000	0.000127000
6	2.506524000	1.687278000	0.000248000	7	4.192516000	-0.410143000	0.000209000
6	1.361615000	2.439234000	0.000170000	6	3.021789000	-0.989902000	0.000141000
8	1.385418000	-1.627276000	0.000163000	8	3.016161000	-2.338482000	0.000231000
6	-3.623073000	-0.036994000	-0.000153000	6	0.177630000	-2.281863000	0.000021000
7	-3.825916000	-1.341532000	-0.000092000	6	-1.118639000	-2.718819000	-0.000023000
6	-2.743405000	-2.124802000	0.000035000	6	-2.144337000	-1.751622000	-0.000131000
6	-1.429013000	-1.677386000	0.000112000	7	-1.928798000	-0.457197000	-0.000208000
8	-2.963289000	-3.448922000	0.000093000	8	-3.408565000	-2.192844000	-0.000193000
1	-2.992613000	3.634099000	-0.000148000	1	-0.106438000	3.560610000	-0.000352000
1	3.487081000	2.151406000	0.000357000	1	3.215557000	2.812284000	-0.000102000
1	1.382387000	3.520001000	0.000189000	1	5.258727000	1.357912000	0.000185000
1	2.316082000	-1.897279000	0.000126000	1	3.942572000	-2.613285000	0.000331000
1	-4.500747000	0.599844000	-0.000237000	1	0.987086000	-2.995028000	0.000110000
1	-0.626712000	-2.395637000	0.000225000	1	-1.378006000	-3.768389000	0.000013000
1	-3.919816000	-3.578963000	0.000077000	1	-3.998655000	-1.425200000	-0.000393000
6	4.910394000	-0.899001000	-0.000217000	6	-4.164211000	1.371476000	0.000339000
8	4.399675000	-1.940488000	-0.000228000	8	-3.572149000	2.357168000	0.000681000
8	5.477872000	0.103420000	-0.000217000	8	-4.817095000	0.411472000	0.000007000
pn9...CO₂				pn10...CO₂			
6	-2.403952000	-0.503862000	-0.000075000	6	1.069551000	2.658303000	-0.062414000
6	-1.249467000	0.301891000	0.000048000	6	-0.206373000	2.181829000	0.029689000
6	0.034802000	-0.364629000	0.000138000	6	-0.440581000	0.793373000	-0.111603000
6	0.046866000	-1.777107000	0.000098000	6	0.667877000	-0.025418000	-0.339643000
7	-1.097108000	-2.539757000	-0.000032000	7	1.933087000	0.437933000	-0.416473000
6	-2.232728000	-1.928048000	-0.000098000	6	2.115516000	1.726837000	-0.287133000
8	-3.359377000	-2.657563000	-0.000225000	8	3.363258000	2.210393000	-0.365766000
6	1.305413000	0.279470000	0.000258000	6	-1.746272000	0.190534000	-0.033087000
7	2.449467000	-0.371470000	0.000283000	6	-1.830374000	-1.200492000	-0.198409000
6	2.432805000	-1.719067000	0.000212000	7	-0.733232000	-1.995501000	-0.440628000
6	1.281045000	-2.457841000	0.000137000	6	0.429602000	-1.445288000	-0.509541000
8	1.371200000	1.614595000	0.000364000	8	1.507530000	-2.202072000	-0.764372000
6	-3.672076000	0.111348000	-0.000164000	7	-2.828675000	0.969187000	0.195089000
6	-3.751757000	1.475611000	-0.000125000	6	-3.996825000	0.385746000	0.264129000
6	-2.532222000	2.189634000	0.000014000	6	-4.204780000	-1.004468000	0.115872000
7	-1.340680000	1.645478000	0.000106000	6	-3.110195000	-1.790836000	-0.116447000
8	-2.602746000	3.528294000	0.000054000	8	-5.082509000	1.150938000	0.491513000
1	-3.093825000	-3.586498000	-0.000238000	1	1.311752000	3.708300000	0.032385000
1	3.408185000	-2.194279000	0.000239000	1	-1.048870000	2.838743000	0.205844000
1	1.288052000	-3.538721000	0.000098000	1	3.964213000	1.466925000	-0.521688000
1	2.310857000	1.850013000	0.000079000	1	1.196623000	-3.113450000	-0.836861000
1	-4.561208000	-0.506692000	-0.000252000	1	-5.208075000	-1.401346000	0.188438000
1	-4.689159000	2.014056000	-0.000181000	1	-3.193378000	-2.863791000	-0.241662000
1	-1.693948000	3.857502000	0.000159000	1	-4.778468000	2.063219000	0.568811000
6	4.892059000	0.779028000	-0.000289000	6	3.999054000	-1.029860000	0.798364000
8	4.429196000	1.842206000	-0.000461000	8	3.309519000	-1.588906000	1.532240000
8	5.417298000	-0.246745000	-0.000145000	8	4.737293000	-0.473037000	0.098904000
pn11...CO₂				pn12...CO₂			

6	-1.222095000	-1.121444000	-0.002965000	6	2.420511000	-0.541107000	-0.000007000
6	-1.644952000	0.213300000	0.001027000	6	1.332711000	0.357238000	-0.000044000
6	-0.636192000	1.249198000	-0.001281000	6	0.001716000	-0.215756000	-0.000104000
6	0.700451000	0.834649000	-0.006593000	6	-0.128573000	-1.628099000	-0.000009000
7	1.110884000	-0.475843000	-0.009231000	7	0.958020000	-2.481388000	0.000093000
6	0.195176000	-1.385881000	-0.008266000	6	2.133861000	-1.956835000	0.000064000
8	0.541938000	-2.680128000	-0.012320000	8	3.202195000	-2.765191000	0.000080000
6	-0.936317000	2.626743000	0.001220000	6	-1.174440000	0.537237000	-0.000261000
6	0.106128000	3.515975000	-0.002022000	7	-2.389088000	0.011120000	-0.000334000
7	1.406030000	3.141095000	-0.007795000	6	-2.494075000	-1.322943000	-0.000217000
6	1.684333000	1.865108000	-0.010093000	6	-1.407452000	-2.182588000	-0.000015000
8	2.971326000	1.483999000	-0.016168000	8	-3.731067000	-1.840161000	-0.000282000
6	-2.199112000	-2.140056000	-0.001372000	6	3.723909000	-0.033195000	0.000060000
6	-3.520353000	-1.791320000	0.004171000	7	3.992758000	1.260424000	0.000077000
6	-3.834163000	-0.411160000	0.007994000	6	2.955648000	2.103607000	0.000055000
7	-2.950649000	0.555895000	0.006473000	6	1.621895000	1.721732000	0.000018000
8	-5.134051000	-0.080801000	0.013485000	8	3.245920000	3.413429000	0.000067000
1	1.509876000	-2.729380000	-0.018571000	1	2.870763000	-3.673092000	0.000154000
1	-1.966089000	2.955473000	0.005507000	1	-1.138740000	1.622520000	-0.000392000
1	-0.070652000	4.585319000	-0.000175000	1	-1.543909000	-3.254740000	0.000096000
1	3.502750000	2.289933000	-0.015972000	1	-4.365096000	-1.109426000	0.000321000
1	-1.886963000	-3.176921000	-0.004551000	1	4.569143000	-0.712695000	0.000111000
1	-4.321814000	-2.517063000	0.005730000	1	0.859001000	2.487161000	0.000053000
1	-5.186927000	0.883370000	0.015442000	1	4.208136000	3.492877000	0.000161000
6	4.180377000	-1.591042000	0.014343000	6	-4.481635000	1.719107000	0.000199000
8	4.923749000	-0.715424000	0.059729000	8	-5.238317000	0.840995000	0.000979000
8	3.474073000	-2.510544000	-0.031040000	8	-3.780679000	2.634166000	-0.000568000
pn13...CO₂				pn14...CO₂			
6	0.050428000	1.582578000	0.000000000	6	3.914160000	-1.230015000	-0.000015000
6	-0.164779000	0.193432000	0.000027000	6	2.629594000	-1.692723000	-0.000014000
6	-1.519913000	-0.306812000	0.000015000	6	1.548010000	-0.776592000	-0.000003000
6	-2.558572000	0.635658000	-0.000018000	6	1.885402000	0.581784000	-0.000004000
7	-2.337094000	2.000755000	-0.000045000	7	3.151955000	1.048349000	-0.000002000
6	-1.128027000	2.430621000	-0.000041000	6	4.116901000	0.171577000	-0.000003000
8	-0.888653000	3.753844000	-0.000051000	8	5.387657000	0.610606000	0.000005000
7	-1.741428000	-1.638247000	0.000033000	6	0.155044000	-1.149622000	0.000011000
6	-2.983533000	-2.053128000	0.000019000	6	-0.806435000	-0.118650000	-0.000005000
6	-4.107994000	-1.200078000	-0.000012000	7	-0.458811000	1.205588000	-0.000031000
6	-3.881488000	0.150469000	-0.000031000	6	0.789758000	1.530928000	-0.000017000
8	-3.211941000	-3.380238000	0.000035000	8	1.120420000	2.824246000	-0.000031000
6	1.348727000	2.088551000	0.000016000	6	-0.319898000	-2.477760000	0.000032000
6	2.386649000	1.169232000	0.000075000	6	-1.664319000	-2.726745000	0.000031000
7	2.202747000	-0.157852000	0.000076000	6	-2.535487000	-1.614189000	0.000013000
6	0.968666000	-0.631511000	0.000057000	7	-2.135105000	-0.365669000	0.000013000
8	3.651468000	1.614840000	0.000067000	8	-3.850749000	-1.869861000	0.000027000
1	-1.745199000	4.199630000	-0.000059000	1	4.771319000	-1.889894000	-0.000030000
1	-5.100722000	-1.628670000	-0.000020000	1	2.446283000	-2.759875000	-0.000030000
1	-4.695397000	0.865630000	-0.000056000	1	5.355985000	1.575868000	0.000008000
1	-2.352413000	-3.818804000	0.000062000	1	0.289730000	3.318967000	0.000040000
1	1.547835000	3.150749000	-0.000015000	1	0.375135000	-3.308813000	0.000058000
1	0.852602000	-1.709897000	0.000071000	1	-2.077529000	-3.725646000	0.000042000
1	4.244748000	0.850496000	0.000053000	1	-4.323617000	-1.024899000	-0.000104000
6	4.231647000	-1.969038000	-0.000072000	6	-4.083020000	1.764479000	0.000003000
8	5.018552000	-1.117426000	-0.000027000	8	-4.869340000	0.909966000	-0.000178000
8	3.496589000	-2.856214000	-0.000113000	8	-3.353217000	2.652740000	0.000174000
pn15...CO₂				pn16...CO₂			

6	-1.996046000	0.425037000	0.001885000	6	-3.184129000	-1.101935000	0.000036000
6	-1.602735000	-0.927911000	-0.001705000	6	-1.860455000	-0.665245000	0.000029000
6	-0.193940000	-1.231501000	0.000436000	6	-1.557031000	0.707860000	-0.000032000
6	0.721030000	-0.158700000	0.005740000	6	-2.655135000	1.584659000	-0.000088000
7	0.318195000	1.144743000	0.009597000	7	-3.913083000	1.182856000	-0.000081000
6	-0.946949000	1.416937000	0.007659000	6	-4.167554000	-0.128068000	-0.000013000
8	-1.298536000	2.704023000	0.011303000	8	-5.461130000	-0.499492000	0.000008000
6	-3.391691000	0.704230000	-0.000345000	6	-0.734247000	-1.578982000	0.000097000
7	-4.318068000	-0.225773000	-0.005585000	7	0.500726000	-1.227775000	0.000115000
6	-3.923648000	-1.512265000	-0.009035000	6	0.816073000	0.112794000	0.000048000
6	-2.612661000	-1.913416000	-0.007344000	6	-0.169774000	1.117795000	-0.000026000
8	-3.808979000	1.973135000	0.003020000	8	-1.044809000	-2.882911000	0.000109000
6	0.338041000	-2.538948000	-0.002348000	7	2.136400000	0.387256000	0.000081000
6	1.690606000	-2.730613000	-0.000052000	6	2.510155000	1.645831000	0.000077000
6	2.512231000	-1.579343000	0.004821000	6	1.613556000	2.735523000	-0.000042000
7	2.059029000	-0.348306000	0.007427000	6	0.273885000	2.455306000	-0.000087000
8	3.834867000	-1.776882000	0.006900000	8	3.819584000	1.929285000	0.000127000
1	-0.471847000	3.206697000	0.014286000	1	-3.436995000	-2.152734000	0.000081000
1	-4.724128000	-2.244312000	-0.013407000	1	-2.507081000	2.659281000	-0.000148000
1	-2.376255000	-2.967415000	-0.010442000	1	-5.990461000	0.307177000	-0.000042000
1	-4.774771000	1.938567000	0.000774000	1	-0.211112000	-3.372615000	0.000115000
1	-0.321475000	-3.397806000	-0.006143000	1	2.002248000	3.744259000	-0.000091000
1	2.147512000	-3.710171000	-0.001809000	1	-0.440106000	3.269947000	-0.000170000
1	4.272651000	-0.912580000	0.010252000	1	4.311616000	1.095373000	0.000173000
6	3.909569000	1.858410000	-0.010747000	6	4.133256000	-1.699046000	-0.000119000
8	3.143745000	2.715520000	-0.023181000	8	4.898683000	-0.826020000	0.000068000
8	4.730325000	1.036814000	0.001035000	8	3.424171000	-2.604112000	-0.000312000
pn17...CO₂				pn18...CO₂			
6	-2.254385000	0.452949000	0.000159000	6	-0.670140000	2.748459000	-0.000736000
6	-1.105034000	-0.363887000	-0.000155000	6	0.583255000	2.204485000	-0.003012000
6	0.191411000	0.289309000	-0.000259000	6	0.738515000	0.791486000	0.001230000
6	0.229378000	1.696974000	-0.000223000	6	-0.449537000	0.047471000	0.007522000
7	-0.911364000	2.475754000	-0.000089000	7	-1.688786000	0.577774000	0.009424000
6	-2.053542000	1.890392000	0.000201000	6	-1.787843000	1.882407000	0.005627000
8	-3.169924000	2.630128000	0.000413000	8	-3.004520000	2.440914000	0.007816000
6	1.453906000	-0.358187000	-0.000229000	6	1.991269000	0.066278000	-0.000510000
7	2.608729000	0.267267000	-0.000212000	6	1.948797000	-1.342975000	0.004144000
6	2.615102000	1.614276000	-0.000266000	7	0.770345000	-2.051216000	0.010625000
6	1.468732000	2.364120000	-0.000275000	6	-0.340587000	-1.398555000	0.012342000
8	1.488340000	-1.703499000	-0.000331000	8	-1.494718000	-2.069564000	0.018911000
6	-3.531631000	-0.100567000	0.000294000	6	3.290600000	0.638578000	-0.006613000
6	-3.616117000	-1.482208000	0.000082000	7	4.408877000	-0.040652000	-0.008226000
7	-2.553819000	-2.285888000	-0.000314000	6	4.337949000	-1.387134000	-0.003797000
6	-1.341633000	-1.755007000	-0.000427000	6	3.153766000	-2.074220000	0.002334000
8	-4.827411000	-2.066516000	0.000251000	8	3.408542000	1.985285000	-0.011213000
1	-2.899016000	3.557638000	0.000311000	1	-0.833217000	3.817970000	-0.003655000
1	3.596189000	2.076577000	-0.000267000	1	1.452762000	2.842812000	-0.007884000
1	1.486311000	3.445037000	-0.000322000	1	-3.660980000	1.728941000	0.013227000
1	2.418444000	-1.974789000	-0.000336000	1	-1.278569000	-3.011343000	0.020075000
1	-4.419065000	0.515928000	0.000528000	1	5.289004000	-1.907332000	-0.005386000
1	-0.516936000	-2.451389000	-0.000765000	1	3.113836000	-3.154672000	0.005896000
1	-4.682296000	-3.020693000	-0.000023000	1	4.357108000	2.168914000	-0.014979000
6	5.013124000	-0.972881000	0.000408000	6	-4.568136000	-1.081814000	-0.014642000
8	5.580123000	0.029774000	0.000211000	8	-4.414049000	-2.221858000	-0.034243000
8	4.503333000	-2.014877000	0.000623000	8	-4.775310000	0.058547000	0.004555000
pn19...CO₂				pn20...CO₂			

6	-0.394509000	0.759933000	-0.000376000	6	-2.617167000	-0.230393000	-0.000035000
6	0.383137000	-0.411729000	-0.000367000	6	-1.447905000	0.540783000	0.000018000
6	1.821520000	-0.280612000	-0.000075000	6	-0.165607000	-0.135299000	0.000053000
6	2.359459000	1.011495000	0.000245000	6	-0.172930000	-1.555596000	0.000029000
7	1.588660000	2.146831000	0.000313000	7	-1.337980000	-2.298595000	-0.000022000
6	0.301569000	2.027975000	0.000020000	6	-2.458425000	-1.673673000	-0.000056000
8	-0.432520000	3.146994000	0.000110000	8	-3.599528000	-2.376678000	-0.000087000
7	2.587767000	-1.396878000	-0.000113000	6	1.095074000	0.485837000	0.000104000
6	3.884191000	-1.247550000	0.000147000	7	2.240818000	-0.180181000	0.000143000
6	4.542117000	0.006234000	0.000464000	6	2.207770000	-1.515701000	0.000115000
6	3.769426000	1.132204000	0.000513000	6	1.035160000	-2.249667000	0.000052000
8	4.660858000	-2.348589000	0.000110000	8	3.383315000	-2.162906000	0.000137000
6	-1.810266000	0.593891000	-0.000691000	6	-3.887049000	0.369505000	-0.000068000
7	-2.391610000	-0.585376000	-0.000765000	6	-3.944488000	1.740783000	-0.000047000
6	-1.623301000	-1.693593000	-0.000681000	7	-2.844218000	2.515457000	-0.000002000
6	-0.253599000	-1.666883000	-0.000567000	6	-1.664913000	1.948010000	0.000026000
8	-2.597745000	1.669361000	-0.001007000	8	-0.596574000	2.767057000	0.000065000
1	0.195040000	3.881639000	0.000460000	1	-3.357320000	-3.312194000	-0.000083000
1	5.623326000	0.036599000	0.000653000	1	1.179199000	1.563109000	0.000138000
1	4.202753000	2.125093000	0.000750000	1	1.047875000	-3.330360000	0.000033000
1	4.073362000	-3.113900000	-0.000099000	1	4.091286000	-1.503554000	0.000102000
1	-2.168611000	-2.631655000	-0.000728000	1	-4.780539000	-0.238176000	-0.000112000
1	0.337371000	-2.571006000	-0.000564000	1	-4.892073000	2.266628000	-0.000065000
1	-3.515303000	1.358858000	-0.000232000	1	-0.939985000	3.670215000	0.000081000
6	-5.074348000	-0.970566000	0.000837000	6	4.516302000	1.282273000	-0.000136000
8	-4.949461000	-2.116114000	0.000760000	8	3.930442000	2.274390000	0.000125000
8	-5.265385000	0.173041000	0.000889000	8	5.165632000	0.321437000	-0.000397000
pn21...CO₂				pn22...CO₂			
6	2.285577000	0.063152000	-0.000020000	6	-2.306674000	0.890790000	0.000033000
6	1.055145000	-0.635268000	0.000073000	6	-1.635355000	-0.347765000	-0.000010000
6	-0.162205000	0.151819000	0.000119000	6	-0.178164000	-0.322367000	-0.000107000
6	-0.048868000	1.558073000	0.000041000	6	0.445784000	0.942776000	-0.000168000
7	1.156120000	2.206566000	-0.000074000	7	-0.237718000	2.146631000	-0.000131000
6	2.244144000	1.506429000	-0.000092000	6	-1.519338000	2.104789000	-0.000029000
8	3.400598000	2.169232000	-0.000218000	8	-2.221687000	3.251796000	0.000007000
6	-1.489606000	-0.360465000	0.000255000	6	0.621662000	-1.465438000	-0.000140000
7	-2.570242000	0.385432000	0.000292000	6	1.998363000	-1.304129000	-0.000293000
6	-2.430658000	1.726801000	0.000193000	7	2.600370000	-0.112386000	-0.000331000
6	-1.214704000	2.352149000	0.000087000	6	1.846302000	0.974484000	-0.000249000
8	-1.680324000	-1.690689000	0.000315000	8	2.780154000	-2.398324000	-0.000432000
6	3.484146000	-0.701477000	-0.000048000	6	-3.706219000	0.897583000	0.000126000
7	3.507996000	-2.014246000	-0.000014000	7	-4.431863000	-0.207247000	0.000177000
6	2.332319000	-2.662120000	0.000065000	6	-3.784383000	-1.374817000	0.000131000
6	1.104719000	-2.045547000	0.000121000	6	-2.402729000	-1.509837000	0.000034000
8	4.668122000	-0.079792000	-0.000132000	8	-4.537801000	-2.485180000	0.000169000
1	3.172374000	3.108857000	-0.000264000	1	-1.582673000	3.976037000	-0.000054000
1	-3.357773000	2.290001000	0.000243000	1	0.210804000	-2.465601000	-0.000041000
1	-1.118099000	3.428746000	0.000031000	1	2.352865000	1.934694000	-0.000264000
1	-2.636623000	-1.847208000	0.000410000	1	3.703684000	-2.111117000	-0.000057000
1	2.397618000	-3.744964000	0.000089000	1	-4.242118000	1.840197000	0.000164000
1	0.205006000	-2.635261000	0.000191000	1	-1.969730000	-2.500089000	-0.000010000
1	5.335189000	-0.779014000	-0.000143000	1	-5.461688000	-2.204944000	0.000259000
6	-5.101485000	-0.569024000	-0.000289000	6	5.295927000	0.221810000	0.000345000
8	-4.716732000	-1.663369000	-0.000659000	8	5.459632000	-0.926171000	0.000628000
8	-5.547408000	0.493051000	0.000067000	8	5.197489000	1.369699000	0.000123000
pn23...CO₂				pn24...CO₂			

6	-1.256528000	-0.948146000	0.221299000	6	2.505394000	0.782808000	0.000006000
6	-1.479912000	0.427334000	0.005861000	6	1.772530000	-0.413097000	0.000001000
6	-0.328036000	1.313580000	0.039637000	6	0.319584000	-0.346337000	-0.000015000
6	0.918217000	0.724645000	0.280906000	6	-0.251177000	0.950478000	-0.000012000
7	1.123970000	-0.622560000	0.465683000	7	0.485247000	2.119097000	-0.000004000
6	0.096209000	-1.398589000	0.441542000	6	1.761440000	2.030277000	0.000001000
8	0.258121000	-2.716306000	0.622147000	8	2.511152000	3.148082000	-0.000004000
6	-0.394355000	2.709328000	-0.147744000	6	-0.552985000	-1.440424000	-0.000044000
6	0.766983000	3.436620000	-0.079662000	6	-1.918345000	-1.195655000	-0.000066000
7	1.974499000	2.888855000	0.170304000	7	-2.461848000	0.023814000	-0.000049000
6	2.042808000	1.595213000	0.346780000	6	-1.645306000	1.063785000	-0.000028000
8	3.237447000	1.046443000	0.616407000	8	-2.757961000	-2.246782000	-0.000012000
6	-2.351275000	-1.822457000	0.201404000	6	3.908599000	0.768968000	0.000018000
7	-3.590155000	-1.418645000	-0.010376000	6	4.535645000	-0.453415000	0.000027000
6	-3.790690000	-0.112505000	-0.214131000	7	3.867865000	-1.619574000	0.000026000
6	-2.790643000	0.847995000	-0.217830000	6	2.556828000	-1.599252000	0.000012000
8	-5.057004000	0.276609000	-0.427983000	8	1.936402000	-2.791465000	0.000006000
1	1.203898000	-2.884985000	0.751925000	1	1.903118000	3.898252000	-0.000005000
1	-1.333805000	3.208398000	-0.341854000	1	-0.202470000	-2.459016000	-0.000054000
1	0.760043000	4.511022000	-0.222412000	1	-2.091928000	2.053312000	-0.000052000
1	3.880443000	1.766672000	0.604771000	1	-3.664188000	-1.909468000	-0.000100000
1	-2.197444000	-2.883399000	0.364932000	1	4.465554000	1.694822000	0.000023000
1	-3.053776000	1.881611000	-0.391109000	1	5.616994000	-0.530304000	0.000038000
1	-5.609902000	-0.513995000	-0.390955000	1	2.630902000	-3.463503000	0.000025000
6	3.340096000	-1.824479000	-0.738152000	6	-5.128440000	0.511311000	0.000043000
8	3.480323000	-1.004678000	-1.534434000	8	-4.963863000	1.651803000	-0.000001000
8	3.225502000	-2.690831000	0.024607000	8	-5.360660000	-0.624655000	0.000092000
pn25...CO₂				pn26...CO₂			
6	2.365394000	-0.024997000	0.000602000	6	2.337173000	0.428961000	0.000699000
6	1.172003000	0.722204000	-0.003009000	6	1.233748000	-0.441532000	-0.001324000
6	-0.079965000	-0.001083000	-0.004057000	6	-0.098921000	0.131087000	-0.001958000
6	-0.044697000	-1.416591000	-0.001152000	6	-0.220009000	1.541549000	-0.000406000
7	1.133185000	-2.122458000	0.002351000	7	0.881428000	2.381911000	0.001632000
6	2.249534000	-1.470759000	0.003090000	6	2.052272000	1.857655000	0.002096000
8	3.378780000	-2.178889000	0.006553000	8	3.129290000	2.652889000	0.004082000
6	-1.339508000	0.608349000	-0.007629000	6	-1.284329000	-0.607033000	-0.003906000
7	-2.481088000	-0.058119000	-0.008321000	7	-2.493288000	-0.063231000	-0.004484000
6	-2.428375000	-1.397576000	-0.005425000	6	-2.587088000	1.269075000	-0.003012000
6	-1.249832000	-2.121483000	-0.001929000	6	-1.489348000	2.115106000	-0.000929000
8	-3.597785000	-2.053710000	-0.005639000	8	-3.819529000	1.801860000	-0.003479000
6	3.590201000	0.696314000	0.001605000	6	3.636454000	-0.069797000	0.001335000
7	3.658833000	2.009215000	-0.000649000	6	3.780736000	-1.448727000	-0.000111000
6	2.509489000	2.703698000	-0.004045000	7	2.755433000	-2.300249000	-0.002021000
6	1.263258000	2.127134000	-0.005338000	6	1.525402000	-1.813758000	-0.002610000
8	4.750106000	0.034051000	0.004977000	8	5.017884000	-1.976912000	0.000419000
1	3.114822000	-3.109243000	0.007919000	1	2.812207000	3.565863000	0.004880000
1	-1.436629000	1.689396000	-0.009861000	1	-1.267201000	-1.692547000	-0.005000000
1	-1.256962000	-3.202233000	0.000171000	1	-1.610811000	3.189161000	0.000254000
1	-4.311555000	-1.400771000	-0.010418000	1	-4.461243000	1.078293000	-0.005241000
1	2.616782000	3.783184000	-0.005752000	1	4.498555000	0.581956000	0.002873000
1	0.383391000	2.753700000	-0.008063000	1	0.729813000	-2.550919000	-0.004199000
1	5.443808000	0.707003000	0.005069000	1	4.919489000	-2.936873000	-0.000744000
6	-4.752105000	1.398534000	0.008234000	6	-4.596042000	-1.757427000	0.004166000
8	-4.159082000	2.387217000	0.007421000	8	-5.348604000	-0.875889000	0.004816000
8	-5.404838000	0.440836000	0.009386000	8	-3.899806000	-2.676311000	0.003794000
pn27...CO₂				pn28...CO₂			

6	-0.050998000	1.704667000	0.000034000	6	1.188214000	2.820578000	0.003616000
6	0.068355000	0.306397000	0.000082000	6	-0.125234000	2.445348000	0.005249000
6	1.394866000	-0.273520000	0.000025000	6	-0.463793000	1.070326000	0.000307000
6	2.487850000	0.615191000	-0.000051000	6	0.603966000	0.170268000	-0.005772000
7	2.354334000	1.985625000	-0.000082000	7	1.904375000	0.527671000	-0.007042000
6	1.169983000	2.480844000	-0.000050000	6	2.177838000	1.807303000	-0.002866000
8	1.010775000	3.817751000	-0.000090000	8	3.457772000	2.200238000	-0.004442000
7	1.568851000	-1.611532000	0.000037000	6	-1.810168000	0.542319000	0.001237000
6	2.786626000	-2.084351000	-0.000021000	6	-1.978498000	-0.863110000	-0.004013000
6	3.953981000	-1.290256000	-0.000087000	7	-0.911047000	-1.736170000	-0.010291000
6	3.787481000	0.066774000	-0.000101000	6	0.281034000	-1.248966000	-0.011218000
8	2.944123000	-3.422081000	-0.000009000	8	1.328019000	-2.076605000	-0.017437000
6	-1.313545000	2.324796000	0.000075000	6	-2.971156000	1.324561000	0.007002000
6	-2.417848000	1.513684000	0.000167000	7	-4.197503000	0.830325000	0.007858000
7	-2.340904000	0.168631000	0.000233000	6	-4.331809000	-0.498804000	0.002893000
6	-1.164188000	-0.418143000	0.000196000	6	-3.272406000	-1.387505000	-0.003076000
8	-1.149206000	-1.752035000	0.000277000	8	-5.589746000	-0.980204000	0.003878000
1	1.893793000	4.208085000	-0.000132000	1	1.496880000	3.857385000	0.007072000
1	4.925919000	-1.764423000	-0.000122000	1	-0.898749000	3.202941000	0.010248000
1	4.630210000	0.747551000	-0.000154000	1	4.015499000	1.408490000	-0.010041000
1	2.058415000	-3.806857000	0.000027000	1	0.980488000	-2.978380000	-0.019089000
1	-1.395703000	3.401982000	0.000035000	1	-2.905366000	2.407990000	0.011161000
1	-3.422790000	1.921746000	0.000205000	1	-3.434354000	-2.456177000	-0.007051000
1	-2.071877000	-2.047126000	0.000310000	1	-6.182299000	-0.218894000	0.007937000
6	-4.724079000	-1.135864000	-0.000193000	6	4.526716000	-1.489343000	0.011298000
8	-5.306790000	-0.141631000	-0.000170000	8	4.210413000	-2.595115000	0.033091000
8	-4.194506000	-2.167171000	-0.000251000	8	4.894654000	-0.390061000	-0.010321000
pn29...CO₂				pn30...CO₂			
6	-2.299667000	0.646806000	0.000016000	6	3.721616000	0.969913000	0.337857000
6	-1.543407000	-0.540066000	0.000012000	6	2.522452000	1.623240000	0.314857000
6	-0.093849000	-0.446705000	0.000104000	6	1.331988000	0.904172000	0.051525000
6	0.463281000	0.850447000	0.000158000	6	1.466847000	-0.471891000	-0.174409000
7	-0.294460000	2.010380000	0.000161000	7	2.645680000	-1.124353000	-0.153857000
6	-1.569390000	1.907122000	0.000104000	6	3.720365000	-0.423921000	0.091978000
8	-2.335251000	3.012084000	0.000112000	8	4.904200000	-1.055237000	0.116106000
6	0.774564000	-1.539322000	0.000135000	6	0.015614000	1.500332000	-0.002586000
6	2.139635000	-1.295305000	0.000227000	6	-1.053861000	0.640430000	-0.278900000
7	2.675586000	-0.072452000	0.000263000	7	-0.920478000	-0.708436000	-0.480123000
6	1.856501000	0.967636000	0.000211000	6	0.256601000	-1.232838000	-0.436456000
8	2.982004000	-2.343297000	0.000367000	8	0.404723000	-2.544446000	-0.632279000
6	-3.689231000	0.593567000	-0.000071000	6	-0.259496000	2.871115000	0.198437000
6	-4.272935000	-0.665555000	-0.000164000	6	-1.558833000	3.300142000	0.108425000
7	-3.582929000	-1.806945000	-0.000173000	7	-2.599243000	2.486690000	-0.173071000
6	-2.262024000	-1.742675000	-0.000087000	6	-2.352410000	1.216859000	-0.361251000
8	-5.612276000	-0.761599000	-0.000242000	8	-3.376137000	0.401621000	-0.659469000
1	-1.740887000	3.773270000	0.000164000	1	4.658416000	1.473697000	0.534124000
1	0.429818000	-2.563997000	0.000101000	1	2.486892000	2.689685000	0.498062000
1	2.304174000	1.956766000	0.000251000	1	4.735300000	-1.988442000	-0.068071000
1	3.887583000	-2.003531000	0.000287000	1	-0.476173000	-2.914498000	-0.793594000
1	-4.294677000	1.488739000	-0.000070000	1	0.525288000	3.581352000	0.419887000
1	-1.744199000	-2.695821000	-0.000106000	1	-1.809372000	4.343843000	0.260132000
1	-5.833126000	-1.701244000	-0.000296000	1	-4.171961000	0.948429000	-0.657163000
6	5.344324000	0.414743000	-0.000343000	6	-2.820271000	-2.368860000	0.704409000
8	5.574051000	-0.721878000	-0.000331000	8	-2.549926000	-3.178876000	-0.079673000
8	5.181111000	1.555288000	-0.000393000	8	-3.104584000	-1.608502000	1.521898000
pn31...CO₂				pn32...CO₂			

6	0.875638000	2.806951000	0.002244000	6	1.220299000	-1.313332000	0.000095000
6	-0.389072000	2.290140000	0.004721000	6	1.751891000	-0.014754000	-0.000559000
6	-0.575656000	0.888607000	-0.001874000	6	0.843782000	1.117081000	0.000538000
6	0.580315000	0.101832000	-0.010527000	6	-0.527981000	0.809859000	0.001491000
7	1.831720000	0.599308000	-0.012576000	7	-1.044630000	-0.462347000	0.001482000
6	1.965420000	1.903119000	-0.006769000	6	-0.222687000	-1.450050000	0.001339000
8	3.196163000	2.424820000	-0.009215000	8	-0.685621000	-2.706299000	0.002045000
6	-1.865458000	0.229591000	0.000081000	6	1.212503000	2.483370000	0.000905000
6	-1.866934000	-1.180964000	-0.007003000	6	0.222300000	3.433606000	0.002275000
7	-0.718104000	-1.945655000	-0.015949000	7	-1.097213000	3.152523000	0.003371000
6	0.416263000	-1.344941000	-0.017717000	6	-1.447415000	1.893828000	0.002987000
8	1.553167000	-2.054702000	-0.026723000	8	-2.755601000	1.589260000	0.004024000
6	-3.096773000	0.893056000	0.008582000	6	2.060392000	-2.439630000	-0.000721000
6	-4.249534000	0.128442000	0.009608000	6	3.415325000	-2.225529000	-0.002256000
7	-4.267065000	-1.206223000	0.003024000	7	3.962755000	-0.995852000	-0.003028000
6	-3.106797000	-1.836698000	-0.005040000	6	3.175111000	0.049988000	-0.002225000
8	-5.445137000	0.753853000	0.017747000	8	3.775461000	1.254063000	-0.003062000
1	1.072427000	3.870502000	0.006886000	1	-1.653945000	-2.664481000	0.003995000
1	-1.243521000	2.955469000	0.011579000	1	2.247447000	2.781241000	0.000175000
1	3.831768000	1.693586000	-0.016734000	1	0.475090000	4.487805000	0.002637000
1	1.307712000	-2.988749000	-0.028578000	1	-3.237101000	2.426042000	0.004358000
1	-3.182795000	1.970843000	0.014322000	1	1.639284000	-3.434674000	-0.000159000
1	-3.121666000	-2.921964000	-0.010432000	1	4.116409000	-3.052249000	-0.002967000
1	-6.121634000	0.066078000	0.017146000	1	4.726689000	1.083604000	-0.004251000
6	4.661397000	-1.138278000	0.021245000	6	-4.256571000	-1.287661000	-0.002933000
8	4.896996000	-0.003200000	-0.003654000	8	-4.948413000	-0.369437000	-0.022874000
8	4.478687000	-2.273636000	0.046722000	8	-3.603571000	-2.246115000	0.017095000
pn33...CO₂				pn34...CO₂			
6	1.428403000	-0.563824000	-0.182805000	6	-2.393441000	0.313738000	-0.000018000
6	1.357898000	0.824015000	0.042541000	6	-1.545332000	-0.808085000	-0.000010000
6	0.066130000	1.481262000	-0.001822000	6	-0.108818000	-0.583499000	0.000065000
6	-1.043017000	0.669699000	-0.267220000	6	0.334660000	0.752403000	0.000143000
7	-0.972004000	-0.691716000	-0.464461000	7	-0.510620000	1.837614000	0.000143000
6	0.177902000	-1.261673000	-0.430519000	6	-1.781383000	1.631373000	0.000063000
8	0.278564000	-2.583430000	-0.623434000	8	-2.596571000	2.693051000	0.000050000
6	-0.146246000	2.861512000	0.195566000	6	0.845334000	-1.605413000	0.000069000
6	-1.427692000	3.347527000	0.111905000	6	2.183867000	-1.253950000	0.000200000
7	-2.503234000	2.581987000	-0.160833000	7	2.615837000	0.011934000	0.000247000
6	-2.313064000	1.300125000	-0.346162000	6	1.719694000	0.981721000	0.000205000
8	-3.374152000	0.531735000	-0.637810000	8	3.112472000	-2.227443000	0.000277000
6	2.655187000	-1.221159000	-0.155149000	6	-3.794511000	0.064450000	-0.000092000
6	3.777972000	-0.449740000	0.100914000	7	-4.316401000	-1.141974000	-0.000153000
7	3.743281000	0.867146000	0.319191000	6	-3.487609000	-2.197962000	-0.000135000
6	2.573379000	1.479900000	0.290216000	6	-2.118251000	-2.091674000	-0.000065000
8	4.983133000	-1.041586000	0.136906000	8	-4.649950000	1.090071000	-0.000112000
1	-0.612937000	-2.932975000	-0.773834000	1	-2.025029000	3.472247000	0.000107000
1	0.670451000	3.537141000	0.409032000	1	0.582818000	-2.653780000	-0.000043000
1	-1.629746000	4.402018000	0.262030000	1	2.085778000	2.003840000	0.000239000
1	-4.144744000	1.113503000	-0.631898000	1	3.986320000	-1.813132000	0.000026000
1	2.734819000	-2.285582000	-0.324535000	1	-3.968227000	-3.170264000	-0.000180000
1	2.596862000	2.548856000	0.472202000	1	-1.507464000	-2.982620000	-0.000042000
1	5.634664000	-0.355306000	0.326802000	1	-5.535411000	0.702974000	-0.000163000
6	-2.943171000	-2.317824000	0.681853000	6	5.240611000	0.716080000	-0.000269000
8	-3.245656000	-1.554394000	1.488940000	8	5.561142000	-0.398349000	-0.000368000
8	-2.655358000	-3.130886000	-0.093727000	8	4.984229000	1.839248000	-0.000165000
pn35...CO₂				pn36...CO₂			

6	1.585083000	-0.375668000	-0.125503000	6	2.513149000	0.237435000	-0.170378000
6	1.406567000	1.005608000	0.082539000	6	1.320503000	-0.470060000	0.040433000
6	0.065673000	1.550797000	-0.003445000	6	0.082624000	0.278359000	0.088736000
6	-0.965330000	0.652393000	-0.290127000	6	0.170914000	1.681673000	0.198072000
7	-0.786073000	-0.689938000	-0.469963000	7	1.367921000	2.360113000	0.105124000
6	0.409560000	-1.176559000	-0.395787000	6	2.432959000	1.684057000	-0.139780000
8	0.567406000	-2.489455000	-0.571215000	8	3.590133000	2.332749000	-0.328897000
6	-0.257354000	2.914248000	0.176723000	6	-1.233102000	-0.235602000	-0.089511000
6	-1.566953000	3.299666000	0.057092000	7	-2.324165000	0.479178000	0.083577000
7	-2.573798000	2.446646000	-0.235517000	6	-2.205694000	1.792434000	0.356353000
6	-2.283463000	1.185375000	-0.404203000	6	-1.000111000	2.442845000	0.376112000
8	-3.271273000	0.330833000	-0.712378000	8	-1.382289000	-1.483382000	-0.541146000
6	2.915505000	-0.878191000	-0.047137000	6	3.740331000	-0.428821000	-0.323596000
7	3.960327000	-0.125620000	0.210652000	6	3.734244000	-1.797132000	-0.215306000
6	3.767041000	1.189356000	0.409761000	7	2.639307000	-2.492416000	0.138142000
6	2.537712000	1.797091000	0.357475000	6	1.502315000	-1.861138000	0.310650000
8	3.141036000	-2.179266000	-0.243446000	8	0.498459000	-2.555432000	0.855067000
1	-0.311697000	-2.860796000	-0.742340000	1	3.402343000	3.277531000	-0.253087000
1	0.499584000	3.651155000	0.405395000	1	-3.139083000	2.322098000	0.514207000
1	-1.856115000	4.335463000	0.191657000	1	-0.921351000	3.513057000	0.506066000
1	-4.086691000	0.847635000	-0.732989000	1	-2.331346000	-1.662240000	-0.607248000
1	4.661312000	1.766115000	0.619625000	1	4.647300000	0.126742000	-0.513599000
1	2.454338000	2.860852000	0.524640000	1	4.635973000	-2.379780000	-0.364792000
1	4.094205000	-2.306464000	-0.147035000	1	0.823778000	-3.455639000	0.983995000
6	-2.669661000	-2.345766000	0.744606000	6	-4.835778000	-0.464345000	-0.224140000
8	-2.955471000	-1.572096000	1.549433000	8	-4.439799000	-1.507187000	-0.540894000
8	-2.397251000	-3.167726000	-0.025785000	8	-5.295652000	0.547235000	0.080956000

III. Monocarboxylic acid

py'-COOH				nt1'-COOH			
6	-2.543185000	-0.125288000	0.000021000	6	3.029792000	0.643581000	-0.023038000
6	-1.876066000	-1.382679000	-0.000039000	6	2.145087000	1.682004000	-0.153886000
6	-0.524412000	-1.399269000	0.000032000	6	0.759154000	1.443010000	-0.134110000
7	0.210842000	-0.235242000	0.000160000	6	0.341279000	0.110095000	0.008800000
6	-0.397574000	1.028037000	-0.000029000	7	1.189069000	-0.896463000	0.188777000
6	-1.835315000	1.031716000	0.000089000	6	2.478883000	-0.637684000	0.162738000
1	-3.626659000	-0.093836000	0.000027000	8	3.318003000	-1.664428000	0.338418000
1	-2.423957000	-2.313369000	-0.000141000	6	-0.223206000	2.483868000	-0.183867000
1	0.074008000	-2.298855000	0.000068000	6	-1.530342000	2.203001000	-0.034569000
1	-2.300561000	2.007767000	0.000132000	6	-1.992156000	0.838327000	0.133608000
8	0.286734000	2.060139000	-0.000264000	7	-1.031566000	-0.180731000	0.024627000
1	1.668130000	1.495006000	-0.000015000	8	-3.175376000	0.572042000	0.334328000
6	1.681122000	-0.396603000	0.000025000	1	4.102472000	0.773243000	-0.037506000
8	2.142128000	-1.495227000	-0.000204000	1	2.500941000	2.699917000	-0.269701000
8	2.334354000	0.724400000	0.000244000	1	2.783460000	-2.466265000	0.413621000
				1	0.111206000	3.508191000	-0.311384000
				1	-2.304785000	2.957116000	-0.024285000
				6	-1.472718000	-1.571118000	-0.226810000
				8	-0.811896000	-2.310805000	-0.875390000
				8	-2.631310000	-1.858395000	0.316569000
				1	-3.105827000	-1.009673000	0.530825000
nt2'-COOH				nt3'-COOH			
6	2.838151000	-1.280836000	0.000143000	6	2.275387000	-1.422248000	0.260082000
6	1.501844000	-1.571063000	0.000033000	6	0.904325000	-1.426715000	0.268271000
6	0.571495000	-0.513724000	-0.000143000	6	0.209682000	-0.218069000	0.044874000
6	1.047295000	0.804009000	-0.000111000	6	0.981529000	0.939016000	-0.103332000

7	2.363321000	1.091258000	-0.000022000	7	2.330710000	0.934497000	-0.121335000
6	3.207539000	0.083938000	0.000080000	6	2.947696000	-0.207686000	0.035322000
8	4.515091000	0.364558000	0.000221000	8	4.291083000	-0.226259000	0.000080000
6	-0.850587000	-0.805137000	-0.000293000	7	-1.203492000	-0.112265000	0.053847000
7	-1.705361000	0.298239000	-0.000499000	6	-1.832315000	1.136485000	0.098092000
6	-1.217283000	1.601399000	-0.000241000	6	-1.001644000	2.313768000	-0.066695000
6	0.095887000	1.880398000	-0.000169000	6	0.330564000	2.219314000	-0.189764000
8	-1.291341000	-1.957740000	-0.000044000	8	-3.053909000	1.241310000	0.237113000
1	3.607738000	-2.039943000	0.000275000	1	2.845229000	-2.325767000	0.428669000
1	1.137219000	-2.591107000	0.000033000	1	0.374728000	-2.348744000	0.439759000
1	4.606473000	1.326330000	0.000210000	1	4.591007000	0.678715000	-0.149600000
1	-1.992479000	2.353187000	-0.000158000	1	-1.538463000	3.252195000	-0.090566000
1	0.447078000	2.901987000	0.000002000	1	0.961733000	3.089848000	-0.323643000
6	-3.167639000	0.162487000	0.000141000	6	-2.016667000	-1.323694000	-0.146221000
8	-3.846107000	1.142008000	0.000586000	8	-1.512989000	-2.329505000	-0.542043000
8	-3.597570000	-1.067755000	0.000060000	8	-3.279340000	-1.180644000	0.138877000
1	-2.812535000	-1.694327000	0.000051000	1	-3.474873000	-0.202109000	0.291810000
nt4'-COOH				nt5'-COOH			
6	-3.010712000	1.309540000	-0.000177000	6	-1.197481000	-0.567024000	0.000022000
6	-1.728173000	1.727365000	-0.000291000	6	-0.635240000	0.706823000	0.000074000
6	-0.676399000	0.752530000	-0.000192000	6	-1.456163000	1.845371000	0.000036000
6	-1.027432000	-0.643907000	0.000069000	6	-2.816981000	1.649553000	-0.000053000
7	-2.341490000	-1.038644000	0.000195000	7	-3.390866000	0.428308000	-0.000098000
6	-3.247880000	-0.113286000	0.000050000	6	-2.615474000	-0.624036000	-0.000054000
8	-4.532212000	-0.475078000	0.000204000	8	-3.178192000	-1.844115000	-0.000110000
6	0.648721000	1.095341000	-0.000201000	6	-0.358554000	-1.730232000	0.000056000
7	1.625755000	0.160609000	-0.000226000	6	0.973597000	-1.571360000	0.000131000
6	1.341028000	-1.229695000	-0.000183000	7	1.569997000	-0.307962000	0.000178000
6	-0.025046000	-1.589540000	0.000182000	6	0.823337000	0.865610000	0.000175000
8	2.289679000	-2.039068000	-0.000157000	8	1.356047000	1.974494000	0.000172000
1	-3.858639000	1.979787000	-0.000253000	1	-1.016508000	2.832917000	0.000079000
1	-1.476034000	2.781968000	-0.000476000	1	-3.502645000	2.488670000	-0.000088000
1	-4.562080000	-1.441704000	0.000359000	1	-4.135869000	-1.720057000	-0.000173000
1	0.998546000	2.120073000	-0.000152000	1	-0.793969000	-2.718486000	0.000014000
1	-0.260269000	-2.644226000	0.000454000	1	1.682629000	-2.385030000	0.000176000
6	3.027863000	0.674632000	0.000091000	6	3.040922000	-0.301215000	0.000205000
8	3.196897000	1.854628000	0.000668000	8	3.629613000	-1.336348000	-0.000097000
8	3.913071000	-0.261299000	-0.000141000	8	3.580535000	0.885519000	-0.000450000
1	3.417311000	-1.181002000	-0.000396000	1	2.860629000	1.582230000	-0.000245000
nt6'-COOH				nt7'-COOH			
6	-2.384245000	1.146960000	-0.000182000	6	-0.892649000	2.426052000	0.069319000
6	-1.014706000	0.899896000	-0.000150000	6	0.419788000	2.438379000	-0.206627000
6	-0.580922000	-0.440896000	0.000044000	6	1.188691000	1.212782000	-0.180407000
6	-1.539802000	-1.458855000	0.000176000	6	0.508328000	0.018564000	0.036406000
7	-2.840208000	-1.224502000	0.000173000	7	-0.895160000	-0.006163000	0.093611000
6	-3.239348000	0.051566000	-0.000012000	6	-1.623514000	1.175406000	0.267037000
8	-4.559677000	0.268870000	-0.000069000	8	-2.825487000	1.155669000	0.501163000
6	-0.014253000	1.935718000	-0.000147000	6	2.590085000	1.194851000	-0.277904000
6	1.285212000	1.603284000	-0.000060000	6	3.239300000	-0.006447000	-0.113046000
7	1.727327000	0.281355000	-0.000142000	7	2.599557000	-1.138139000	0.219767000
6	0.830672000	-0.791268000	0.000244000	6	1.291616000	-1.123322000	0.331173000
8	1.228320000	-1.956077000	0.000295000	8	0.681192000	-2.210290000	0.814030000
1	-2.787786000	2.150609000	-0.000316000	1	-1.496975000	3.322026000	0.117729000
1	-1.218836000	-2.494993000	0.000400000	1	0.939017000	3.370978000	-0.398770000
1	-4.993797000	-0.594028000	0.000077000	1	3.138095000	2.109408000	-0.464087000
1	-0.301985000	2.977821000	-0.000183000	1	4.316717000	-0.080725000	-0.203738000

1	2.088395000	2.325355000	0.000096000	1	1.353881000	-2.892801000	0.931303000
6	3.181715000	0.096281000	0.000026000	6	-1.582421000	-1.185690000	-0.447838000
8	3.894181000	1.051520000	0.000762000	8	-1.021400000	-1.903655000	-1.208437000
8	3.572883000	-1.147958000	-0.000908000	8	-2.821318000	-1.321452000	-0.036449000
1	2.772579000	-1.749684000	-0.000557000	1	-3.120762000	-0.484392000	0.392779000
nt8'–COOH				nt9'–COOH			
6	3.283795000	0.865694000	0.000300000	6	-0.851253000	-0.139602000	0.000012000
6	2.198362000	1.663771000	0.000433000	6	-1.110220000	1.242972000	-0.000009000
6	0.884339000	1.067883000	0.000166000	6	-0.000954000	2.155808000	-0.000008000
6	0.828972000	-0.363222000	-0.000175000	6	1.253371000	1.681722000	0.000005000
7	1.954898000	-1.162231000	-0.000309000	7	1.532355000	0.322956000	0.000001000
6	3.094581000	-0.569536000	-0.000085000	6	0.516906000	-0.649061000	0.000028000
8	4.226490000	-1.291002000	-0.000254000	8	0.803338000	-1.841852000	0.000022000
6	-0.279496000	1.802218000	0.000205000	6	-1.974596000	-1.009429000	0.000011000
6	-1.553314000	1.180310000	-0.000185000	7	-3.221618000	-0.580270000	-0.000003000
7	-1.548362000	-0.228150000	-0.000258000	6	-3.442597000	0.741389000	-0.000019000
6	-0.405253000	-0.960240000	-0.000245000	6	-2.441511000	1.685830000	-0.000022000
8	-2.638352000	1.798161000	-0.000310000	8	-1.794517000	-2.328117000	0.000026000
1	4.295323000	1.250322000	0.000485000	1	-0.174716000	3.222631000	-0.000018000
1	2.290002000	2.743626000	0.000735000	1	2.133793000	2.307385000	0.000024000
1	3.978405000	-2.224669000	-0.000510000	1	-4.485545000	1.040414000	-0.000031000
1	-0.273825000	2.884297000	0.000516000	1	-2.670717000	2.743114000	-0.000036000
1	-0.530719000	-2.034041000	-0.000248000	1	-2.677396000	-2.722457000	0.000022000
6	-2.824794000	-1.010942000	0.000148000	6	2.959568000	-0.028198000	0.000016000
8	-2.759025000	-2.199558000	0.000933000	8	3.773644000	0.842792000	0.000062000
8	-3.877924000	-0.266772000	-0.000370000	8	3.206562000	-1.306531000	-0.000113000
1	-3.577598000	0.730875000	-0.000372000	1	2.334922000	-1.808817000	-0.000013000
nt10'–COOH				nt11'–COOH			
6	1.751870000	-1.073307000	-0.000007000	6	-2.371907000	1.087790000	0.000295000
6	0.678907000	-0.192017000	0.000009000	6	-0.996198000	0.741451000	0.000030000
6	0.896155000	1.193709000	0.000013000	6	-0.687744000	-0.661465000	-0.000383000
6	2.230294000	1.622691000	0.000010000	6	-1.760457000	-1.605083000	-0.000474000
7	3.261728000	0.794981000	-0.000002000	7	-3.009197000	-1.261322000	-0.000204000
6	3.025312000	-0.516820000	-0.000010000	6	-3.295813000	0.080212000	0.000154000
8	4.090432000	-1.334493000	-0.000020000	8	-4.600454000	0.371934000	0.000443000
6	-0.691081000	-0.731967000	0.000020000	6	0.050303000	1.650438000	0.000071000
7	-1.718552000	0.201516000	0.000011000	6	1.395154000	1.237624000	-0.000206000
6	-1.474978000	1.582474000	0.000017000	7	1.630042000	-0.170993000	-0.000147000
6	-0.233698000	2.084666000	0.000021000	6	0.625566000	-1.062924000	-0.000428000
8	-0.907170000	-1.941648000	-0.000029000	8	2.382822000	2.001132000	-0.000502000
1	1.602982000	-2.144257000	-0.000011000	1	-2.695193000	2.119630000	0.000604000
1	2.459130000	2.684459000	0.000011000	1	-1.533119000	-2.669073000	-0.000808000
1	4.880996000	-0.780863000	-0.000022000	1	-5.085135000	-0.463125000	0.000267000
1	-2.373863000	2.179126000	0.000023000	1	-0.122233000	2.718019000	0.000221000
1	-0.088030000	3.156389000	0.000025000	1	0.932904000	-2.102260000	-0.000688000
6	-3.133658000	-0.189424000	0.000003000	6	3.018981000	-0.737690000	0.000306000
8	-3.974083000	0.654592000	-0.000092000	8	3.138712000	-1.923239000	0.000626000
8	-3.347150000	-1.476861000	0.000048000	8	3.932241000	0.166893000	0.000284000
1	-2.474410000	-1.963074000	0.000205000	1	3.462992000	1.107129000	-0.000123000
nt12'–COOH							
6	-1.999835000	-1.199438000	0.000277000				
6	-0.796226000	-0.432501000	0.000061000				
6	-0.877603000	0.993891000	-0.000227000				
6	-2.204243000	1.557253000	-0.000375000				
7	-3.280967000	0.840995000	-0.000156000				
6	-3.180063000	-0.525646000	0.000147000				

8	-4.351936000	-1.187834000	0.000372000			
6	0.463041000	-0.993656000	0.000063000			
7	1.577428000	-0.229560000	0.000019000			
6	1.548947000	1.180084000	-0.000088000			
6	0.263962000	1.767941000	-0.000347000			
8	2.625398000	1.819877000	0.000277000			
1	-1.980446000	-2.281026000	0.000516000			
1	-2.319551000	2.638325000	-0.000617000			
1	-5.057473000	-0.530421000	0.000254000			
1	0.641226000	-2.061026000	-0.000031000			
1	0.224806000	2.849499000	-0.000519000			
6	2.885985000	-0.979165000	-0.000155000			
8	2.846324000	-2.168698000	-0.000997000			
8	3.908348000	-0.201401000	0.000955000			
1	3.567348000	0.796481000	0.000366000			
pn1'–COOH				pn2'–COOH		
6	4.107344000	0.511482000	-0.009858000	6	2.307789000	-0.676492000
6	3.118161000	1.444968000	0.084373000	6	1.311953000	0.303556000
6	1.771164000	1.015650000	0.083962000	6	-0.069701000	-0.141535000
6	1.495092000	-0.359036000	-0.012740000	6	-0.346152000	-1.552839000
7	2.482217000	-1.281768000	-0.098831000	7	0.668783000	-2.488567000
6	3.717820000	-0.850982000	-0.098243000	6	1.885030000	-2.062931000
8	4.702736000	-1.753278000	-0.187283000	8	2.879399000	-2.955434000
6	0.653772000	1.891082000	0.206522000	6	-1.113991000	0.734187000
7	-0.589392000	1.510639000	0.198721000	7	-2.402590000	0.308779000
6	-0.852789000	0.199708000	0.044646000	6	-2.738654000	-1.067091000
6	0.129038000	-0.784516000	-0.023589000	6	-1.652244000	-1.977876000
8	0.916554000	3.193802000	0.354841000	8	-3.936812000	-1.402375000
7	-2.199850000	-0.174937000	0.020719000	6	3.654477000	-0.270371000
6	-2.590624000	-1.519913000	0.157194000	6	3.943975000	1.068705000
6	-1.547186000	-2.515310000	0.061386000	6	2.858296000	1.970927000
6	-0.251156000	-2.160022000	-0.045410000	7	1.590824000	1.616019000
8	-3.774091000	-1.815446000	0.323465000	8	3.142982000	3.277124000
1	5.158845000	0.761947000	-0.017674000	1	2.476987000	-3.834793000
1	3.340633000	2.502263000	0.159059000	1	-0.974732000	1.806693000
1	4.295056000	-2.627077000	-0.241589000	1	-1.891343000	-3.031664000
1	0.068157000	3.656982000	0.387777000	1	4.439622000	-1.016145000
1	-1.880878000	-3.543033000	0.091595000	1	4.954147000	1.453283000
1	0.534181000	-2.902653000	-0.115213000	1	2.307310000	3.761936000
6	-3.224142000	0.843303000	-0.310438000	6	-3.443534000	1.371746000
8	-2.955778000	1.775795000	-0.991553000	8	-3.096168000	2.511662000
8	-4.400824000	0.581970000	0.203091000	8	-4.650475000	0.910311000
1	-4.434572000	-0.387193000	0.444458000	1	-4.605969000	-0.123146000
pn3'–COOH				pn4'–COOH		
6	-1.948311000	0.666037000	0.064774000	6	2.556240000	-1.320185000
6	-0.808523000	-0.148452000	-0.056573000	6	1.469969000	-0.440941000
6	0.471368000	0.491540000	0.029725000	6	1.761076000	0.938190000
6	0.507380000	1.872546000	0.006861000	6	3.100557000	1.360276000
7	-0.604009000	2.660362000	0.104368000	7	4.113686000	0.526459000
6	-1.757484000	2.075623000	0.179317000	6	3.830479000	-0.782839000
8	-2.863510000	2.825045000	0.326658000	8	4.878957000	-1.612710000
7	1.660680000	-0.246082000	-0.016101000	6	0.087905000	-0.838316000
6	2.867392000	0.345856000	-0.406670000	6	-0.871960000	0.168395000
6	2.881177000	1.800324000	-0.463535000	7	-0.587197000	1.477799000

6	1.775276000	2.522327000	-0.211420000	6	0.659114000	1.837742000	-0.217434000
8	3.867312000	-0.333824000	-0.623003000	8	0.943927000	3.131628000	-0.375858000
6	-3.223135000	0.054698000	-0.008404000	6	-0.344595000	-2.198591000	0.043779000
6	-3.302313000	-1.288067000	-0.225044000	6	-1.650347000	-2.519689000	-0.061614000
6	-2.084610000	-2.000606000	-0.397032000	6	-2.664068000	-1.496359000	-0.155338000
7	-0.894707000	-1.468410000	-0.325257000	7	-2.227177000	-0.166468000	-0.016415000
8	-2.180883000	-3.307893000	-0.661283000	8	-3.856000000	-1.752277000	-0.321351000
1	-2.583117000	3.748349000	0.360598000	1	2.444815000	-2.391485000	0.190036000
1	3.841466000	2.246169000	-0.684642000	1	3.331770000	2.417359000	-0.164111000
1	1.785192000	3.606051000	-0.217951000	1	5.677700000	-1.070453000	0.173723000
1	-4.110634000	0.665055000	0.102360000	1	0.104342000	3.610760000	-0.413323000
1	-4.240459000	-1.821730000	-0.288520000	1	0.393174000	-2.988805000	0.113021000
1	-1.283263000	-3.663825000	-0.704722000	1	-2.009231000	-3.538804000	-0.090378000
6	1.715964000	-1.511576000	0.727865000	6	-3.219817000	0.883243000	0.322175000
8	0.980304000	-1.705211000	1.639974000	8	-2.924887000	1.792346000	1.022638000
8	2.646861000	-2.334533000	0.306035000	8	-4.399030000	0.671539000	-0.207729000
1	3.291311000	-1.831337000	-0.254420000	1	-4.468811000	-0.292861000	-0.454811000
pn5'-COOH				pn6'-COOH			
6	-0.494135000	0.962095000	0.000034000	6	-2.220072000	0.893127000	-0.000035000
6	0.226960000	-0.273633000	0.000002000	6	-1.525049000	-0.316105000	-0.000014000
6	1.680818000	-0.183545000	-0.000003000	6	-0.063485000	-0.269476000	-0.000068000
6	2.261159000	1.089329000	0.000039000	6	0.543120000	1.028445000	-0.000082000
7	1.536724000	2.276509000	0.000067000	7	-0.179685000	2.214334000	-0.000095000
6	0.258448000	2.202850000	0.000016000	6	-1.455512000	2.131562000	-0.000084000
8	-0.480292000	3.321721000	0.000171000	8	-2.199936000	3.250637000	-0.000070000
7	2.400403000	-1.322742000	-0.000036000	6	0.712219000	-1.396172000	-0.000090000
6	3.705845000	-1.225588000	-0.000038000	6	2.133812000	-1.321502000	-0.000132000
6	4.404443000	0.001172000	-0.000007000	7	2.680223000	-0.026752000	-0.000079000
6	3.669461000	1.156304000	0.000036000	6	1.907187000	1.096393000	-0.000056000
8	4.435505000	-2.355374000	-0.000074000	8	2.882877000	-2.317078000	-0.000251000
6	-1.858791000	0.937457000	0.000022000	6	-3.627326000	0.856437000	0.000023000
7	-2.538227000	-0.236221000	0.000084000	6	-4.259775000	-0.358553000	0.000079000
6	-1.881313000	-1.492089000	-0.000102000	6	-3.454801000	-1.518232000	0.000052000
6	-0.458742000	-1.457587000	-0.000028000	7	-2.140522000	-1.509008000	0.000025000
8	-2.555080000	-2.534195000	-0.000130000	8	-4.079312000	-2.701968000	0.000193000
1	0.128511000	4.071843000	0.000141000	1	-1.591814000	4.001324000	-0.000072000
1	5.486029000	-0.003621000	-0.000016000	1	0.271578000	-2.383099000	-0.000067000
1	4.140123000	2.131974000	0.000063000	1	2.441619000	2.035664000	-0.000012000
1	3.820925000	-3.099369000	-0.000085000	1	-4.186570000	1.783537000	0.000019000
1	-2.469635000	1.830434000	-0.000057000	1	-5.336270000	-0.460300000	0.000137000
1	0.056875000	-2.407267000	-0.000086000	1	-3.403930000	-3.392393000	0.000212000
6	-4.027394000	-0.127591000	-0.000082000	6	4.153585000	0.197930000	0.000153000
8	-4.517576000	0.956719000	-0.000726000	8	4.560012000	1.317375000	0.000417000
8	-4.627351000	-1.271921000	0.000703000	8	4.840862000	-0.896583000	0.000026000
1	-3.917325000	-2.017466000	0.000355000	1	4.185830000	-1.696928000	-0.000172000
pn7'-COOH				pn8'-COOH			
6	-2.185550000	0.669411000	-0.000005000	6	1.924899000	0.966784000	-0.085565000
6	-1.118846000	-0.266030000	0.000023000	6	1.600880000	-0.396831000	0.010596000
6	0.221523000	0.280397000	-0.000038000	6	0.218138000	-0.797175000	0.009381000
6	0.374027000	1.669997000	-0.000072000	6	-0.727866000	0.225612000	-0.056330000
7	-0.667924000	2.551795000	-0.000138000	7	-0.419060000	1.528040000	-0.217322000
6	-1.870516000	2.064626000	-0.000139000	6	0.825523000	1.877818000	-0.222425000
8	-2.899036000	2.915120000	-0.000052000	8	1.128763000	3.168675000	-0.381848000
6	1.391772000	-0.572781000	-0.000055000	6	3.263707000	1.407257000	-0.074716000
7	2.641430000	0.061495000	-0.000309000	6	4.243240000	0.459878000	0.035516000
6	2.761778000	1.436583000	-0.000049000	7	3.972632000	-0.860838000	0.132149000

6	1.685071000	2.240392000	-0.000042000	6	2.734011000	-1.264719000	0.119930000
8	1.335429000	-1.809938000	-0.000071000	8	2.527141000	-2.592443000	0.226975000
6	-3.509977000	0.209457000	0.000058000	6	-0.259295000	-2.151526000	0.008532000
7	-3.826022000	-1.068658000	0.000110000	6	-1.574195000	-2.426480000	-0.114255000
6	-2.814652000	-1.947504000	0.000134000	6	-2.565104000	-1.382646000	-0.191629000
6	-1.465855000	-1.621621000	0.000112000	7	-2.093922000	-0.070988000	-0.030787000
8	-3.154218000	-3.243080000	0.000203000	8	-3.764587000	-1.607833000	-0.358297000
1	-2.533566000	3.810101000	-0.000070000	1	0.296521000	3.659627000	-0.423794000
1	3.781954000	1.790894000	0.000127000	1	3.491657000	2.460825000	-0.151794000
1	1.789608000	3.315243000	0.000058000	1	5.292993000	0.726921000	0.050976000
1	-4.327215000	0.922489000	0.000024000	1	3.400605000	-3.000148000	0.298644000
1	-0.728402000	-2.406146000	0.000147000	1	0.453226000	-2.959121000	0.072250000
1	-4.118631000	-3.288672000	0.000238000	1	-1.955980000	-3.436849000	-0.161281000
6	3.913039000	-0.687153000	0.000104000	6	-3.053527000	0.997613000	0.338390000
8	4.939752000	-0.082508000	0.001189000	8	-2.723317000	1.894191000	1.040600000
8	3.780205000	-1.980230000	-0.000967000	8	-4.248036000	0.815705000	-0.165694000
1	2.795919000	-2.205905000	-0.000769000	1	-4.338745000	-0.144622000	-0.431720000
pn9'-COOH				pn10'-COOH			
6	-2.244198000	-0.636910000	-0.000011000	6	1.299729000	2.518072000	0.221472000
6	-1.158684000	0.265367000	0.000008000	6	0.033437000	2.103612000	0.046539000
6	0.172090000	-0.290746000	0.000008000	6	-0.273627000	0.695653000	0.041905000
6	0.298460000	-1.684534000	0.000000000	6	0.762373000	-0.210150000	0.117159000
7	-0.759841000	-2.542147000	-0.000019000	7	2.090652000	0.225149000	0.080542000
6	-1.954635000	-2.032762000	-0.000021000	6	2.410111000	1.576662000	0.282500000
8	-3.001467000	-2.865164000	-0.000065000	8	3.572075000	1.934356000	0.435141000
6	1.361338000	0.549839000	0.000000000	6	-1.619589000	0.208540000	0.019724000
7	2.598678000	-0.122044000	0.000003000	6	-1.809385000	-1.178862000	0.129884000
6	2.689701000	-1.500089000	0.000056000	7	-0.777970000	-2.042533000	0.350856000
6	1.598578000	-2.282194000	0.000025000	6	0.432795000	-1.585538000	0.380086000
8	1.341842000	1.781079000	-0.000123000	8	1.429681000	-2.393120000	0.759643000
6	-3.563256000	-0.131494000	-0.000006000	7	-2.645582000	1.084977000	-0.116113000
6	-3.757985000	1.218257000	0.000019000	6	-3.854346000	0.596575000	-0.170446000
6	-2.600280000	2.034886000	0.000047000	6	-4.167585000	-0.785031000	-0.087824000
7	-1.367189000	1.596427000	0.000042000	6	-3.138315000	-1.665891000	0.068329000
8	-2.787777000	3.358984000	0.000073000	8	-4.887406000	1.445784000	-0.314090000
1	-2.652287000	-3.766361000	-0.000077000	1	1.577105000	3.561614000	0.287648000
1	3.702296000	-1.875538000	0.000137000	1	-0.789529000	2.801888000	-0.039800000
1	1.680791000	-3.358903000	0.000030000	1	1.058460000	-3.274954000	0.888166000
1	-4.395768000	-0.823930000	-0.000022000	1	-5.202308000	-1.094505000	-0.143754000
1	-4.737147000	1.676380000	0.000025000	1	-3.302766000	-2.733466000	0.150422000
1	-1.912035000	3.769524000	0.000081000	1	-4.525461000	2.339124000	-0.358381000
6	3.885105000	0.596115000	0.000053000	6	3.078569000	-0.637198000	-0.587204000
8	4.899768000	-0.030593000	0.000146000	8	2.717935000	-1.455380000	-1.367880000
8	3.780224000	1.891549000	-0.000219000	8	4.320937000	-0.379753000	-0.258760000
1	2.794491000	2.131937000	0.000083000	1	4.364025000	0.493393000	0.203539000
pn11'-COOH				pn12'-COOH			
6	1.229569000	-0.988939000	-0.230306000	6	2.256223000	0.696309000	0.000258000
6	1.346129000	0.369867000	0.054909000	6	1.280708000	-0.319814000	-0.000183000
6	0.134916000	1.190359000	0.070127000	6	-0.113936000	0.105104000	-0.000328000
6	-1.090048000	0.552121000	-0.074636000	6	-0.411132000	1.517258000	-0.000206000
7	-1.195880000	-0.855265000	-0.085124000	7	0.585086000	2.473898000	0.000179000
6	-0.076924000	-1.650470000	-0.326727000	6	1.809229000	2.075911000	0.000493000
8	-0.178703000	-2.852798000	-0.533363000	8	2.781983000	2.989580000	0.000645000
6	0.177547000	2.590448000	0.121209000	6	-1.157497000	-0.769709000	-0.000246000
6	-1.005633000	3.280703000	-0.011805000	7	-2.452800000	-0.357124000	-0.000454000
7	-2.176160000	2.679755000	-0.272756000	6	-2.801740000	1.013109000	-0.000627000

6	-2.212826000	1.369508000	-0.341696000	6	-1.719243000	1.930293000	-0.000395000
8	-3.345560000	0.783213000	-0.747014000	8	-4.000570000	1.339562000	-0.000925000
6	2.400535000	-1.757485000	-0.343273000	6	3.606333000	0.341592000	0.000346000
6	3.616232000	-1.152372000	-0.161433000	7	4.021078000	-0.915410000	0.000129000
6	3.616094000	0.224999000	0.137969000	6	3.089192000	-1.868941000	-0.000281000
7	2.532305000	0.967545000	0.236293000	6	1.716045000	-1.638757000	-0.000508000
8	4.799666000	0.816688000	0.330995000	8	3.517322000	-3.136720000	-0.000551000
1	1.124721000	3.094853000	0.247229000	1	2.360427000	3.860039000	0.000606000
1	-1.032655000	4.362666000	0.046871000	1	-1.041851000	-1.844964000	-0.000011000
1	-4.010627000	1.475956000	-0.845161000	1	-1.964080000	2.982796000	-0.000234000
1	2.314390000	-2.814411000	-0.564393000	1	4.369492000	1.111865000	0.000687000
1	4.555606000	-1.682728000	-0.231855000	1	1.045733000	-2.487079000	-0.000951000
1	4.634906000	1.747958000	0.526818000	1	4.482976000	-3.117005000	-0.000402000
6	-2.361227000	-1.449942000	0.574135000	6	-3.480139000	-1.430635000	0.000574000
8	-2.985551000	-0.821440000	1.364327000	8	-3.119281000	-2.566807000	0.001292000
8	-2.604361000	-2.693889000	0.226859000	8	-4.692839000	-0.984634000	0.000558000
1	-1.838305000	-3.055513000	-0.273668000	1	-4.663420000	0.046630000	-0.000189000
pn13'-COOH				pn14'-COOH			
6	0.374382000	1.458375000	0.000133000	6	-3.652921000	-1.492983000	-0.159781000
6	-0.048839000	0.095888000	0.000255000	6	-2.327325000	-1.808002000	-0.158876000
6	-1.471486000	-0.202697000	0.000136000	6	-1.355726000	-0.776812000	-0.043988000
6	-2.357780000	0.879242000	-0.000078000	6	-1.850994000	0.530272000	0.070081000
7	-1.937020000	2.205625000	-0.000065000	7	-3.164999000	0.849220000	0.072404000
6	-0.686387000	2.466540000	0.000082000	6	-4.019129000	-0.125914000	-0.040488000
8	-0.256784000	3.737828000	-0.000046000	8	-5.331377000	0.156309000	-0.046250000
7	-1.877029000	-1.483674000	0.000181000	6	0.063092000	-0.992036000	-0.049013000
6	-3.169537000	-1.718702000	-0.000012000	6	0.877607000	0.131984000	0.041493000
6	-4.155509000	-0.712681000	-0.000250000	7	0.406306000	1.379135000	0.216635000
6	-3.734031000	0.592867000	-0.000279000	6	-0.877360000	1.578095000	0.222044000
8	-3.582251000	-2.997566000	0.000012000	8	-1.329738000	2.816009000	0.395039000
6	1.702007000	1.783235000	0.000107000	6	0.679067000	-2.281506000	-0.075412000
6	2.704602000	0.768101000	0.000157000	6	2.015212000	-2.419047000	0.044179000
7	2.235363000	-0.562191000	0.000315000	6	2.881448000	-1.267538000	0.154307000
6	0.912057000	-0.874443000	0.000324000	7	2.271144000	-0.011737000	0.024049000
8	3.924719000	0.997876000	-0.000062000	8	4.097144000	-1.367753000	0.323929000
1	-1.036229000	4.308368000	-0.000215000	1	-4.428582000	-2.241736000	-0.249210000
1	-5.200204000	-0.991173000	-0.000396000	1	-2.025620000	-2.843351000	-0.252189000
1	-4.436025000	1.418081000	-0.000443000	1	-5.421534000	1.114241000	0.039668000
1	-2.796571000	-3.558121000	0.000139000	1	-0.557257000	3.395836000	0.444986000
1	2.042998000	2.808820000	-0.000029000	1	0.062983000	-3.168591000	-0.158939000
1	0.677777000	-1.930029000	0.000482000	1	2.510164000	-3.379701000	0.068973000
6	3.176657000	-1.723315000	-0.000064000	6	3.109764000	1.165704000	-0.301736000
8	2.722458000	-2.822836000	0.000041000	8	2.690061000	2.040584000	-0.982495000
8	4.421945000	-1.377550000	-0.000618000	8	4.312307000	1.104647000	0.215255000
1	4.481528000	-0.350731000	-0.000241000	1	4.509115000	0.155302000	0.454407000
pn15'-COOH				pn16'-COOH			
6	-1.956578000	-0.320797000	-0.050840000	6	3.197871000	0.902151000	-0.071871000
6	-1.380341000	0.964517000	0.049919000	6	1.830964000	0.616883000	-0.077824000
6	0.048688000	1.080285000	0.041341000	6	1.370121000	-0.708410000	0.033931000
6	0.788409000	-0.097810000	-0.038303000	6	2.364414000	-1.701128000	0.146668000
7	0.240101000	-1.310573000	-0.199180000	7	3.655246000	-1.440690000	0.156247000
6	-1.058371000	-1.426402000	-0.199783000	6	4.061320000	-0.169295000	0.050262000
8	-1.556525000	-2.645979000	-0.367160000	8	5.387323000	0.049298000	0.064203000
6	-3.379363000	-0.413687000	-0.019588000	6	0.819842000	1.632480000	-0.226848000
7	-4.169788000	0.625001000	0.090292000	7	-0.451207000	1.403849000	-0.222059000
6	-3.603396000	1.844986000	0.178932000	6	-0.890081000	0.135714000	-0.044763000

6	-2.252703000	2.071161000	0.163548000	6	-0.047479000	-0.962875000	0.039926000
8	-3.953168000	-1.614575000	-0.102446000	8	1.252083000	2.883112000	-0.399587000
6	0.747613000	2.326599000	0.060406000	7	-2.277930000	-0.040007000	-0.025216000
6	2.089796000	2.377098000	-0.057095000	6	-2.858102000	-1.310853000	-0.152899000
6	2.877888000	1.170909000	-0.160240000	6	-1.962617000	-2.439088000	-0.045003000
7	2.184947000	-0.044324000	-0.019393000	6	-0.629651000	-2.267915000	0.070734000
8	4.095000000	1.185534000	-0.335645000	8	-4.071784000	-1.439958000	-0.318361000
1	-0.801865000	-3.250069000	-0.416051000	1	3.567769000	1.913943000	-0.159182000
1	-4.297916000	2.673172000	0.268893000	1	2.097567000	-2.748420000	0.238235000
1	-1.881999000	3.082021000	0.246800000	1	5.821186000	-0.807718000	0.155652000
1	-4.907325000	-1.465160000	-0.060177000	1	0.475113000	3.456943000	-0.451447000
1	0.189168000	3.251036000	0.137013000	1	-2.432563000	-3.412341000	-0.066416000
1	2.646336000	3.303143000	-0.088815000	1	0.009371000	-3.138520000	0.153487000
6	2.946842000	-1.275198000	0.302883000	6	-3.144540000	1.116275000	0.306643000
8	2.479287000	-2.113562000	0.997440000	8	-2.741276000	2.001062000	0.984796000
8	4.141985000	-1.301802000	-0.234309000	8	-4.347843000	1.024116000	-0.201774000
1	4.403258000	-0.371762000	-0.479830000	1	-4.521607000	0.069364000	-0.441090000
pn17'-COOH				pn18'-COOH			
6	2.110255000	0.539188000	-0.000058000	6	-1.299074000	2.448882000	-0.278844000
6	1.019244000	-0.355895000	-0.000130000	6	-0.013290000	2.100344000	-0.096535000
6	-0.314209000	0.205389000	-0.000169000	6	0.375976000	0.703698000	-0.055641000
6	-0.449407000	1.591601000	-0.000031000	6	-0.638009000	-0.230295000	-0.122485000
7	0.617871000	2.451971000	0.000012000	7	-1.984902000	0.142799000	-0.081020000
6	1.807728000	1.952915000	-0.000074000	6	-2.371547000	1.468494000	-0.304544000
8	2.856909000	2.777065000	0.000143000	8	-3.551188000	1.772993000	-0.443440000
6	-1.501686000	-0.626524000	-0.000436000	6	1.732943000	0.224663000	-0.019432000
7	-2.736889000	0.028015000	0.000093000	6	1.949839000	-1.166526000	-0.130231000
6	-2.838849000	1.406174000	0.000102000	7	0.932489000	-2.039979000	-0.377760000
6	-1.747126000	2.189165000	0.000028000	6	-0.281276000	-1.595339000	-0.407501000
8	-1.462917000	-1.866105000	-0.000725000	8	-1.259423000	-2.404307000	-0.814265000
6	3.425293000	0.077385000	0.000045000	6	2.903618000	1.015692000	0.164662000
6	3.605811000	-1.293238000	0.000083000	7	4.115330000	0.539796000	0.245603000
7	2.599617000	-2.169860000	0.000041000	6	4.292653000	-0.796940000	0.144521000
6	1.353915000	-1.731673000	-0.000069000	6	3.264264000	-1.676272000	-0.042700000
8	4.852288000	-1.793400000	0.000174000	8	2.773774000	2.355059000	0.284230000
1	2.517628000	3.682229000	0.000226000	1	-1.613607000	3.480117000	-0.369086000
1	-3.853241000	1.775583000	0.000191000	1	0.751302000	2.858652000	-0.032060000
1	-1.830595000	3.265935000	0.000038000	1	-0.874931000	-3.278472000	-0.960204000
1	4.266825000	0.755168000	0.000095000	1	5.318348000	-1.138901000	0.219141000
1	0.578471000	-2.482116000	-0.000109000	1	3.422556000	-2.742112000	-0.129715000
1	4.774539000	-2.755623000	0.000206000	1	3.666422000	2.699399000	0.421402000
6	-4.021017000	-0.702304000	0.000162000	6	-2.922159000	-0.759373000	0.609404000
8	-5.037852000	-0.081603000	-0.000221000	8	-2.509469000	-1.562718000	1.380167000
8	-3.907408000	-1.996960000	0.000799000	8	-4.179613000	-0.550639000	0.310496000
1	-2.925682000	-2.237140000	0.000253000	1	-4.266804000	0.317735000	-0.158804000
pn19'-COOH				pn20'-COOH			
6	0.540416000	0.735725000	-0.000186000	6	-2.479019000	-0.394101000	0.000010000
6	-0.267547000	-0.399587000	-0.000160000	6	-1.397484000	0.490222000	-0.000088000
6	-1.690906000	-0.235571000	-0.000061000	6	-0.048144000	-0.057237000	-0.000126000
6	-2.194008000	1.073705000	0.000037000	6	0.095769000	-1.492886000	-0.000023000
7	-1.397382000	2.178231000	0.000079000	7	-0.999637000	-2.339397000	0.000085000
6	-0.106879000	2.022168000	-0.000002000	6	-2.172413000	-1.823190000	0.000044000
8	0.649892000	3.121493000	0.000052000	8	-3.238747000	-2.625758000	0.000311000
7	-2.488031000	-1.335592000	-0.000051000	6	1.099733000	0.688662000	-0.000135000
6	-3.776315000	-1.149692000	0.000051000	7	2.335351000	0.116846000	-0.000181000
6	-4.401830000	0.127247000	0.000146000	6	2.525820000	-1.279791000	-0.000018000

6	-3.605434000	1.231695000	0.000143000	6	1.343014000	-2.061229000	0.000029000
8	-4.589567000	-2.220742000	0.000067000	8	3.677501000	-1.749726000	-0.000352000
6	1.994841000	0.610002000	-0.000402000	6	-3.798659000	0.073178000	0.000077000
7	2.494195000	-0.703096000	0.000089000	6	-3.992075000	1.436508000	-0.000004000
6	1.664714000	-1.809800000	-0.000046000	7	-2.978157000	2.314481000	-0.000148000
6	0.325484000	-1.699482000	-0.000187000	6	-1.745973000	1.864794000	-0.000198000
8	2.768544000	1.563717000	-0.000541000	8	-0.758995000	2.777239000	-0.000330000
1	0.039380000	3.870761000	0.000226000	1	-2.915429000	-3.537215000	0.000400000
1	-5.482178000	0.183069000	0.000223000	1	1.109774000	1.766908000	-0.000114000
1	-4.012611000	2.235426000	0.000223000	1	1.456929000	-3.135741000	0.000103000
1	-4.033244000	-3.009295000	-0.000004000	1	-4.628572000	-0.618709000	0.000154000
1	2.192784000	-2.752084000	0.000007000	1	-4.988208000	1.863468000	0.000031000
1	-0.304512000	-2.575438000	-0.000274000	1	-1.173952000	3.649999000	-0.000287000
6	3.939618000	-0.995080000	0.000144000	6	3.485267000	1.062407000	0.000291000
8	4.301272000	-2.130635000	-0.000111000	8	3.265729000	2.233197000	0.001034000
8	4.704911000	0.056234000	0.000726000	8	4.636656000	0.473901000	-0.000318000
1	4.125564000	0.882249000	0.000374000	1	4.484378000	-0.547069000	-0.000502000
pn21'-COOH				pn22'-COOH			
6	-2.163294000	0.121423000	0.000018000	6	-2.188164000	0.867571000	-0.000055000
6	-0.966675000	-0.639879000	-0.000031000	6	-1.497933000	-0.358417000	0.000000000
6	0.283008000	0.085174000	-0.000052000	6	-0.030809000	-0.310528000	0.000000000
6	0.237821000	1.482527000	-0.000014000	6	0.574132000	0.990859000	-0.000030000
7	-0.916043000	2.195094000	0.000029000	7	-0.146268000	2.179846000	-0.000074000
6	-2.049604000	1.552194000	0.000060000	6	-1.421657000	2.104629000	-0.000094000
8	-3.158183000	2.282684000	0.000107000	8	-2.157584000	3.227448000	-0.000125000
6	1.568044000	-0.589551000	-0.000003000	6	0.762647000	-1.425032000	0.000051000
7	2.711781000	0.220666000	-0.000422000	6	2.186913000	-1.342106000	0.000061000
6	2.632897000	1.600175000	-0.000242000	7	2.723049000	-0.046712000	-0.000023000
6	1.452498000	2.238994000	-0.000064000	6	1.936817000	1.068474000	0.000007000
8	1.699352000	-1.820992000	0.000480000	8	2.935388000	-2.335517000	0.000176000
6	-3.402144000	-0.580877000	0.000016000	6	-3.584002000	0.849764000	-0.000061000
7	-3.492708000	-1.888483000	-0.000072000	7	-4.291107000	-0.271125000	-0.000019000
6	-2.349604000	-2.595681000	-0.000170000	6	-3.626362000	-1.423742000	0.000035000
6	-1.090804000	-2.047019000	-0.000158000	6	-2.237315000	-1.532452000	0.000045000
8	-4.547716000	0.106071000	0.000109000	8	-4.350688000	-2.550241000	0.000147000
1	-2.877952000	3.208570000	0.000122000	1	-1.544702000	3.974357000	-0.000130000
1	3.591541000	2.097219000	-0.000365000	1	0.363569000	-2.429621000	0.000119000
1	1.398393000	3.317528000	0.000125000	1	2.461051000	2.013469000	0.000076000
1	-2.471327000	-3.673545000	-0.000268000	1	-4.138109000	1.781459000	-0.000128000
1	-0.221374000	-2.680325000	-0.000217000	1	-1.787564000	-2.515227000	0.000081000
1	-5.255786000	-0.552041000	0.000091000	1	-5.282665000	-2.296973000	0.000042000
6	4.079695000	-0.332720000	0.000016000	6	4.192930000	0.191176000	0.000074000
8	5.006302000	0.416428000	0.000247000	8	4.589878000	1.313224000	0.000764000
8	4.140686000	-1.631453000	-0.000027000	8	4.892176000	-0.897457000	-0.000770000
1	3.200726000	-1.998807000	0.000196000	1	4.252156000	-1.702362000	-0.001000000
pn23'-COOH				pn24'-COOH			
6	-1.262818000	-0.875960000	0.253524000	6	-2.397733000	0.724248000	-0.000045000
6	-1.312054000	0.491777000	-0.067694000	6	-1.626223000	-0.446360000	-0.000007000
6	-0.052584000	1.243725000	-0.075358000	6	-0.168796000	-0.331933000	-0.000018000
6	1.131877000	0.532504000	0.072872000	6	0.359759000	1.008876000	-0.000045000
7	1.160209000	-0.879066000	0.084471000	7	-0.430246000	2.150772000	-0.000081000
6	0.003765000	-1.609983000	0.358682000	6	-1.696065000	2.008459000	-0.000088000
8	0.048521000	-2.810035000	0.587828000	8	-2.497002000	3.086525000	-0.000137000
6	0.005645000	2.645210000	-0.117124000	6	0.713915000	-1.384037000	0.000014000
6	1.230903000	3.258201000	0.018721000	6	2.127492000	-1.191111000	0.000016000
7	2.359431000	2.583745000	0.275805000	7	2.576924000	0.137067000	-0.000030000

6	2.306284000	1.273569000	0.342393000	6	1.711050000	1.188840000	0.000001000
8	3.395634000	0.610795000	0.744453000	8	2.947665000	-2.127477000	0.000158000
6	-2.457950000	-1.585850000	0.363529000	6	-3.793370000	0.664967000	-0.000025000
7	-3.648398000	-1.034218000	0.176399000	6	-4.380656000	-0.583195000	0.000035000
6	-3.681121000	0.257049000	-0.142321000	7	-3.678083000	-1.721491000	0.000076000
6	-2.554708000	1.068703000	-0.277784000	6	-2.363633000	-1.656745000	0.000057000
8	-4.883802000	0.808017000	-0.340579000	8	-1.707396000	-2.826320000	0.000100000
1	-0.888845000	3.240552000	-0.232683000	1	-1.929556000	3.868363000	-0.000156000
1	1.324221000	4.336743000	-0.034650000	1	0.392495000	-2.412041000	0.000079000
1	4.108046000	1.254712000	0.843621000	1	2.160690000	2.171517000	0.000077000
1	-2.429702000	-2.642698000	0.604885000	1	-4.382897000	1.570280000	-0.000053000
1	-2.686787000	2.110020000	-0.533934000	1	-5.459329000	-0.693701000	0.000053000
1	-5.545008000	0.115421000	-0.212355000	1	-2.377032000	-3.523607000	0.000140000
6	2.277241000	-1.535007000	-0.595070000	6	4.023907000	0.477424000	0.000122000
8	2.923787000	-0.939297000	-1.393525000	8	4.341293000	1.625416000	0.000711000
8	2.456135000	-2.792320000	-0.256944000	8	4.796606000	-0.559914000	-0.000696000
1	1.690295000	-3.108889000	0.272308000	1	4.208263000	-1.407686000	-0.001070000
pn25'-COOH				pn26'-COOH			
6	-2.252798000	-0.116630000	0.000152000	6	2.197091000	0.525998000	0.000216000
6	-1.128923000	0.726452000	-0.000295000	6	1.182702000	-0.443671000	-0.000185000
6	0.185161000	0.099611000	-0.000429000	6	-0.203900000	0.008850000	-0.000304000
6	0.271487000	-1.337175000	-0.000178000	6	-0.460292000	1.426627000	-0.000148000
7	-0.856009000	-2.122273000	0.000217000	7	0.570515000	2.353498000	0.000249000
6	-2.016318000	-1.554983000	0.000514000	6	1.780443000	1.930301000	0.000524000
8	-3.086602000	-2.340465000	0.000368000	8	2.781975000	2.810088000	0.000591000
6	1.348742000	0.810557000	-0.000456000	6	-1.277451000	-0.828121000	-0.000318000
7	2.566048000	0.209564000	-0.000582000	7	-2.561361000	-0.367340000	-0.000518000
6	2.708648000	-1.198440000	-0.000617000	6	-2.864982000	1.008319000	-0.000594000
6	1.504494000	-1.943457000	-0.000311000	6	-1.750059000	1.888556000	-0.000345000
8	3.848914000	-1.695479000	-0.000700000	8	-4.051504000	1.380736000	-0.000805000
6	-3.531158000	0.497708000	0.000151000	6	3.533923000	0.155267000	0.000271000
7	-3.706140000	1.804043000	-0.000092000	6	3.808738000	-1.208463000	-0.000076000
6	-2.621788000	2.588154000	-0.000481000	7	2.869968000	-2.149235000	-0.000518000
6	-1.328548000	2.113754000	-0.000651000	6	1.596980000	-1.778690000	-0.000586000
8	-4.632780000	-0.254161000	0.000546000	8	5.089644000	-1.609919000	0.000022000
1	-2.760292000	-3.251605000	0.000346000	1	2.393432000	3.695824000	0.000573000
1	1.398420000	1.890363000	-0.000425000	1	-1.205004000	-1.906584000	-0.000226000
1	1.587869000	-3.020778000	-0.000042000	1	-1.956544000	2.949291000	-0.000167000
1	-2.814896000	3.655611000	-0.000749000	1	4.331555000	0.884509000	0.000572000
1	-0.503783000	2.811878000	-0.001109000	1	0.875009000	-2.588608000	-0.001032000
1	-5.380336000	0.358761000	0.000528000	1	5.091248000	-2.575276000	-0.000216000
6	3.743414000	1.118657000	0.000513000	6	-3.624230000	-1.404222000	0.000498000
8	3.554550000	2.296139000	0.001026000	8	-3.303610000	-2.552756000	0.001019000
8	4.873953000	0.495768000	0.000883000	8	-4.821517000	-0.917495000	0.000710000
1	4.686970000	-0.523231000	0.000194000	1	-4.757240000	0.112636000	-0.000018000
pn27'-COOH				pn28'-COOH			
6	-2.129150000	0.208854000	0.066023000	6	-1.725241000	2.471350000	0.179098000
6	-0.863541000	-0.374253000	-0.114171000	6	-0.411152000	2.246068000	0.012505000
6	0.289222000	0.471505000	-0.026444000	6	0.112864000	0.899542000	0.025830000
6	0.082116000	1.839675000	-0.037962000	6	-0.787698000	-0.134955000	0.115564000
7	-1.154038000	2.411711000	0.083983000	7	-2.167529000	0.093484000	0.069803000
6	-2.180454000	1.638637000	0.203518000	6	-2.688182000	1.379658000	0.246493000
8	-3.393205000	2.175547000	0.410834000	8	-3.891594000	1.568752000	0.380146000
7	1.600221000	-0.023746000	0.008649000	6	1.516206000	0.589739000	0.009541000
6	2.693921000	0.783124000	-0.336329000	6	1.901746000	-0.766994000	0.146157000
6	2.438718000	2.207440000	-0.446106000	7	0.987352000	-1.750610000	0.409969000

6	1.207419000	2.710235000	-0.241076000	6	-0.268067000	-1.446775000	0.430392000
8	3.817355000	0.300392000	-0.468521000	8	-1.148945000	-2.351532000	0.856364000
6	-3.291184000	-0.588277000	0.044097000	6	2.540246000	1.533465000	-0.174006000
6	-3.142371000	-1.925035000	-0.210479000	7	3.818839000	1.223192000	-0.243580000
7	-1.953812000	-2.488918000	-0.521143000	6	4.160008000	-0.067983000	-0.126246000
6	-0.880223000	-1.751799000	-0.502345000	6	3.259146000	-1.094870000	0.071751000
8	0.262453000	-2.294137000	-0.948262000	8	5.471580000	-0.351699000	-0.203639000
1	-3.282970000	3.133832000	0.453315000	1	-2.149950000	3.465160000	0.227425000
1	3.304766000	2.822355000	-0.648860000	1	0.267569000	3.084351000	-0.079020000
1	1.013009000	3.776169000	-0.266335000	1	-0.666433000	-3.170914000	1.028195000
1	-4.260658000	-0.143964000	0.218033000	1	2.310110000	2.588346000	-0.283329000
1	-3.993285000	-2.595978000	-0.212439000	1	3.586290000	-2.119744000	0.175183000
1	0.084794000	-3.225126000	-1.137207000	1	5.936658000	0.483096000	-0.337422000
6	1.843806000	-1.236354000	0.805852000	6	-3.007588000	-0.923558000	-0.584848000
8	1.036236000	-1.592038000	1.604543000	8	-2.515668000	-1.701637000	-1.334091000
8	2.992523000	-1.810339000	0.569715000	8	-4.279079000	-0.842083000	-0.281026000
1	3.555160000	-1.198543000	0.019126000	1	-4.458968000	0.024710000	0.160205000
pn29'-COOH				pn30'-COOH			
6	-2.179959000	0.617844000	-0.000072000	6	3.497271000	1.329843000	-0.329238000
6	-1.398068000	-0.552424000	-0.000012000	6	2.212744000	1.798787000	-0.414327000
6	0.055040000	-0.428900000	-0.000105000	6	1.130283000	0.934812000	-0.151442000
6	0.583329000	0.906909000	-0.000178000	6	1.445309000	-0.382720000	0.169617000
7	-0.213267000	2.047109000	-0.000235000	7	2.694274000	-0.851077000	0.269652000
6	-1.480066000	1.905301000	-0.000206000	6	3.680748000	-0.019175000	0.035322000
8	-2.282820000	2.980010000	-0.000291000	8	4.936154000	-0.474726000	0.139742000
6	0.925073000	-1.488446000	-0.000145000	6	-0.265548000	1.366578000	-0.112485000
6	2.337773000	-1.311710000	-0.000271000	6	-1.245262000	0.398049000	0.067162000
7	2.793967000	0.016906000	-0.000172000	7	-0.925545000	-0.976528000	0.078577000
6	1.936274000	1.076507000	-0.000124000	6	0.374783000	-1.411504000	0.326759000
8	3.151853000	-2.252856000	-0.000408000	8	0.629053000	-2.577514000	0.558172000
6	-3.562572000	0.534724000	0.000022000	6	-0.662182000	2.713850000	-0.150397000
6	-4.120091000	-0.742116000	0.000182000	6	-1.994184000	3.015898000	0.022758000
7	-3.406763000	-1.865190000	0.000263000	7	-2.922931000	2.094655000	0.310932000
6	-2.085289000	-1.769186000	0.000169000	6	-2.553498000	0.835576000	0.372034000
8	-5.453667000	-0.860216000	0.000267000	8	-3.441305000	-0.067714000	0.802420000
1	-1.719748000	3.765129000	-0.000340000	1	4.359502000	1.952046000	-0.527344000
1	0.598396000	-2.518693000	-0.000086000	1	2.035966000	2.830887000	-0.688762000
1	2.395866000	2.054752000	-0.000032000	1	4.887405000	-1.408617000	0.382982000
1	-4.189452000	1.415023000	-0.000022000	1	0.055780000	3.509263000	-0.290864000
1	-1.547176000	-2.710792000	0.000243000	1	-2.342604000	4.041284000	-0.025778000
1	-5.663120000	-1.802968000	0.000393000	1	-4.284162000	0.387886000	0.920502000
6	4.243225000	0.348906000	0.000333000	6	-1.873225000	-1.893734000	-0.558339000
8	4.567576000	1.494730000	0.001009000	8	-2.665861000	-1.483002000	-1.341201000
8	5.011671000	-0.691968000	-0.000126000	8	-1.735222000	-3.151224000	-0.202968000
1	4.422755000	-1.536283000	-0.000324000	1	-0.898476000	-3.266229000	0.301263000
pn31'-COOH				pn32'-COOH			
6	1.413840000	2.526222000	-0.223025000	6	-1.299941000	-1.086270000	-0.259184000
6	0.132763000	2.152447000	-0.059375000	6	-1.461927000	0.268216000	0.039513000
6	-0.233384000	0.758173000	-0.051833000	6	-0.288032000	1.146455000	0.033271000
6	0.776735000	-0.175071000	-0.119367000	6	0.961870000	0.541369000	-0.092729000
7	2.116392000	0.212469000	-0.070913000	7	1.117482000	-0.863001000	-0.061014000
6	2.491065000	1.549035000	-0.272737000	6	0.051285000	-1.697730000	-0.343688000
8	3.666345000	1.861711000	-0.416817000	8	0.197244000	-2.892377000	-0.550141000
6	-1.598547000	0.298691000	-0.026720000	6	-0.334314000	2.552891000	0.031510000
6	-1.807530000	-1.091343000	-0.146728000	6	0.841114000	3.253301000	-0.133055000
7	-0.793975000	-1.981060000	-0.377286000	7	2.022724000	2.671900000	-0.371804000

6	0.419590000	-1.549573000	-0.394208000	6	2.071423000	1.360032000	-0.388286000
8	1.409895000	-2.363282000	-0.778719000	8	3.214244000	0.769083000	-0.762378000
6	-2.718237000	1.128303000	0.130434000	6	-2.396937000	-1.940400000	-0.375822000
6	-3.963355000	0.533772000	0.176221000	6	-3.650502000	-1.401529000	-0.176688000
7	-4.175791000	-0.784686000	0.070963000	7	-3.843978000	-0.115749000	0.137795000
6	-3.131033000	-1.567783000	-0.089876000	6	-2.802252000	0.680281000	0.245598000
8	-5.051426000	1.311071000	0.338036000	8	-3.057584000	1.956832000	0.579476000
1	1.722702000	3.560840000	-0.287982000	1	-1.268039000	3.077004000	0.144700000
1	-0.641770000	2.905334000	0.015245000	1	0.842070000	4.337220000	-0.114810000
1	1.030600000	-3.239759000	-0.920802000	1	3.874139000	1.464012000	-0.877630000
1	-2.648617000	2.201915000	0.234148000	1	-2.246539000	-2.986547000	-0.602174000
1	-3.304712000	-2.635102000	-0.183613000	1	-4.544078000	-2.009786000	-0.258077000
1	-5.819019000	0.726611000	0.350829000	1	-4.015673000	2.028664000	0.684394000
6	3.068957000	-0.688624000	0.604264000	6	2.290726000	-1.402627000	0.633096000
8	2.670951000	-1.482082000	1.391274000	8	2.863883000	-0.742382000	1.434830000
8	4.320046000	-0.486703000	0.273860000	8	2.596647000	-2.637841000	0.303045000
1	4.402777000	0.381877000	-0.190549000	1	1.873981000	-3.033064000	-0.231116000
pn33'-COOH				pn34'-COOH			
6	1.411869000	-0.476528000	-0.190579000	6	-2.273412000	0.262613000	-0.000015000
6	1.158033000	0.863678000	0.136324000	6	-1.387822000	-0.826216000	0.000015000
6	-0.218729000	1.354363000	0.110790000	6	0.052015000	-0.548259000	0.000038000
6	-1.236472000	0.424368000	-0.065680000	6	0.444684000	0.827453000	0.000025000
7	-0.974350000	-0.967272000	-0.080524000	7	-0.456367000	1.876573000	-0.000002000
6	0.299686000	-1.451731000	-0.338358000	6	-1.710391000	1.613208000	-0.000025000
8	0.511576000	-2.629343000	-0.575185000	8	-2.578625000	2.628788000	-0.000031000
6	-0.564414000	2.715067000	0.153047000	6	1.014077000	-1.524295000	0.000081000
6	-1.885517000	3.066707000	-0.012363000	6	2.404819000	-1.216631000	0.000146000
7	-2.849771000	2.182420000	-0.298540000	7	2.730330000	0.147194000	0.000043000
6	-2.527717000	0.910492000	-0.363974000	6	1.779588000	1.122809000	0.000033000
8	-3.451181000	0.041105000	-0.790516000	8	3.303358000	-2.079070000	0.000192000
6	2.708814000	-0.948238000	-0.277271000	6	-3.661256000	-0.036809000	-0.000035000
6	3.732643000	-0.037648000	-0.019670000	7	-4.136178000	-1.266660000	-0.000030000
7	3.523649000	1.230380000	0.313910000	6	-3.272761000	-2.287455000	-0.000004000
6	2.272169000	1.666823000	0.386167000	6	-1.904195000	-2.127615000	0.000018000
8	5.002518000	-0.457755000	-0.101038000	8	-4.557614000	0.950759000	-0.000065000
1	0.184102000	3.482252000	0.290775000	1	-2.052736000	3.439927000	-0.000024000
1	-2.194542000	4.104463000	0.040236000	1	0.784125000	-2.579926000	0.000103000
1	-4.276804000	0.528153000	-0.905031000	1	2.146560000	2.139308000	0.000022000
1	2.918046000	-1.981243000	-0.518848000	1	-3.714391000	-3.278092000	-0.000001000
1	2.154758000	2.708819000	0.661703000	1	-1.261173000	-2.995345000	0.000037000
1	5.572039000	0.291535000	0.114494000	1	-5.427791000	0.530047000	-0.000072000
6	-1.957877000	-1.845034000	0.559320000	6	4.146696000	0.613565000	0.000041000
8	-2.720667000	-1.404599000	1.354305000	8	4.360969000	1.784324000	0.000286000
8	-1.885230000	-3.105188000	0.191317000	8	5.005981000	-0.352397000	-0.000560000
1	-1.065358000	-3.260357000	-0.324821000	1	4.496120000	-1.249118000	-0.000638000
pn35'-COOH				pn36'-COOH			
6	-1.556618000	-0.179592000	0.141072000	6	2.391947000	0.320337000	-0.120790000
6	-1.123915000	1.118843000	-0.165453000	6	1.223815000	-0.442319000	0.033212000
6	0.311362000	1.414491000	-0.098057000	6	-0.040580000	0.244065000	0.044552000
6	1.190238000	0.355516000	0.071633000	6	-0.028624000	1.633687000	0.145894000
7	0.744297000	-0.977917000	0.048504000	7	1.119936000	2.375224000	0.093427000
6	-0.600330000	-1.292819000	0.291109000	6	2.237479000	1.754640000	-0.100900000
8	-0.933014000	-2.441477000	0.519643000	8	3.356054000	2.468646000	-0.248072000
6	0.828222000	2.720971000	-0.095105000	6	-1.303145000	-0.423850000	-0.238098000
6	2.179212000	2.894771000	0.100712000	7	-2.466755000	0.319283000	0.017507000
7	3.015166000	1.882624000	0.371624000	6	-2.421771000	1.675112000	0.285385000

6	2.533238000	0.662462000	0.396470000	6	-1.258611000	2.347608000	0.309192000
8	3.327642000	-0.330813000	0.808020000	8	-1.381697000	-1.547981000	-0.729937000
6	-2.954998000	-0.405387000	0.188784000	6	3.653705000	-0.292557000	-0.227676000
7	-3.849064000	0.533799000	-0.071670000	6	3.699643000	-1.659730000	-0.135491000
6	-3.412665000	1.751781000	-0.394138000	7	2.619761000	-2.407745000	0.163388000
6	-2.077029000	2.100185000	-0.448272000	6	1.451658000	-1.831834000	0.295040000
8	-3.429484000	-1.607082000	0.505003000	8	0.454605000	-2.566022000	0.792985000
1	0.187123000	3.581424000	-0.219760000	1	3.114699000	3.402706000	-0.187927000
1	2.621622000	3.884146000	0.086173000	1	-3.390171000	2.128569000	0.435905000
1	4.207659000	0.039719000	0.950102000	1	-1.231311000	3.416161000	0.463436000
1	-4.181990000	2.485036000	-0.612615000	1	4.543592000	0.302335000	-0.374617000
1	-1.794166000	3.109339000	-0.708523000	1	4.630339000	-2.202513000	-0.252675000
1	-4.393116000	-1.539744000	0.463267000	1	0.800321000	-3.458466000	0.924566000
6	1.601214000	-1.957762000	-0.616717000	6	-3.808766000	-0.270997000	-0.074264000
8	2.432417000	-1.597219000	-1.385764000	8	-4.757159000	0.391136000	0.214776000
8	1.347584000	-3.207682000	-0.302486000	8	-3.830428000	-1.510621000	-0.472491000
1	0.511330000	-3.256039000	0.214599000	1	-2.889570000	-1.802349000	-0.683367000

IV. 2CO₂ complex

nt1...2CO ₂				nt2...2CO ₂			
6	-2.230860000	-2.401056000	0.273950000	6	-1.640485000	-2.554414000	-0.001407000
6	-2.963895000	-1.260455000	0.145771000	6	-0.288207000	-2.405005000	0.000154000
6	-2.306888000	-0.014455000	0.000793000	6	0.255297000	-1.096732000	0.001610000
6	-0.890619000	-0.005598000	-0.001099000	6	-0.622527000	0.007171000	0.001407000
7	-0.167438000	-1.148714000	0.103062000	7	-1.976730000	-0.153652000	-0.000168000
6	-0.815346000	-2.277128000	0.239799000	6	-2.441856000	-1.377216000	-0.001491000
8	-0.116297000	-3.412797000	0.353331000	8	-3.764630000	-1.570719000	-0.003028000
6	-2.979827000	1.223223000	-0.142467000	6	1.651289000	-0.826477000	0.003274000
6	-2.261546000	2.372913000	-0.272828000	7	2.161739000	0.375498000	0.004660000
6	-0.844531000	2.266691000	-0.242526000	6	1.301808000	1.428389000	0.004415000
7	-0.182183000	1.146523000	-0.107388000	6	-0.059288000	1.308509000	0.002878000
8	-0.159858000	3.410857000	-0.358292000	8	2.475546000	-1.885544000	0.003371000
1	-2.671805000	-3.380997000	0.391616000	1	-2.130061000	-3.518404000	-0.002572000
1	-4.048328000	-1.291645000	0.155197000	1	0.378526000	-3.258492000	0.000311000
1	0.826368000	-3.197979000	0.296207000	1	-4.205613000	-0.708971000	-0.002879000
1	-4.064585000	1.240838000	-0.148967000	1	1.775405000	2.404056000	0.005496000
1	-2.715173000	3.347181000	-0.389391000	1	-0.705205000	2.174726000	0.002732000
1	0.785356000	3.207342000	-0.302765000	1	3.386705000	-1.557638000	0.005153000
6	2.432052000	1.344206000	0.977423000	6	4.821237000	0.855062000	-0.004093000
8	2.468821000	2.415617000	0.537317000	8	4.668067000	1.996596000	-0.004105000
8	2.450248000	0.292259000	1.447474000	8	5.046349000	-0.283086000	-0.004417000
6	2.450824000	-1.313536000	-0.974840000	6	-3.850054000	2.024652000	-0.000721000
8	2.457783000	-0.259845000	-1.441259000	8	-4.695857000	1.231930000	-0.002227000
8	2.499220000	-2.385870000	-0.538004000	8	-3.049238000	2.851845000	0.000926000
nt3...2CO ₂				nt4...2CO ₂			
6	-0.559362000	-2.412753000	-0.000007000	6	-1.780582000	-2.678618000	-0.000078000
6	0.626398000	-1.744507000	-0.000074000	6	-0.425253000	-2.615111000	-0.000204000
6	0.625835000	-0.324296000	0.000053000	6	0.211589000	-1.344452000	-0.000081000
6	-0.625807000	0.324275000	0.000260000	6	-0.600781000	-0.179292000	0.000158000
7	-1.811927000	-0.352344000	0.000324000	7	-1.967883000	-0.255885000	0.000270000
6	-1.763882000	-1.656664000	0.000192000	6	-2.504780000	-1.445552000	0.000164000
8	-2.905727000	-2.363106000	0.000277000	8	-3.835912000	-1.560630000	0.000294000
7	1.811951000	0.352334000	-0.000043000	6	1.605505000	-1.175150000	-0.000181000
6	1.763892000	1.656652000	0.000067000	7	2.196244000	0.000840000	-0.000064000
6	0.559374000	2.412741000	0.000315000	6	1.414901000	1.098088000	0.000167000
6	-0.626384000	1.744484000	0.000406000	6	0.034772000	1.070456000	0.000290000

8	2.905737000	2.363101000	-0.000013000	8	2.044323000	2.283434000	0.000280000
1	-0.622748000	-3.492604000	-0.000093000	1	-2.334512000	-3.606933000	-0.000153000
1	1.575060000	-2.266121000	-0.000229000	1	0.178781000	-3.516312000	-0.000388000
1	-3.650903000	-1.747089000	0.000392000	1	-4.224431000	-0.673648000	0.000469000
1	0.622760000	3.492591000	0.000417000	1	2.258346000	-2.045407000	-0.000361000
1	-1.575052000	2.266088000	0.000589000	1	-0.536059000	1.987887000	0.000469000
1	3.650907000	1.747080000	-0.000157000	1	2.997429000	2.120169000	0.000188000
6	-4.392512000	0.919904000	-0.000383000	6	4.899552000	0.016967000	-0.000062000
8	-3.972705000	1.992709000	-0.000586000	8	4.924683000	1.175659000	0.000095000
8	-4.867166000	-0.136901000	-0.000145000	8	4.940681000	-1.135157000	-0.000224000
6	4.392480000	-0.919875000	-0.000164000	6	-3.696055000	2.028853000	-0.000280000
8	3.972460000	-1.992593000	-0.000335000	8	-2.843049000	2.801654000	-0.000496000
8	4.867353000	0.136835000	-0.000057000	8	-4.592136000	1.292844000	-0.000077000
nt5...2CO₂				nt6...2CO₂			
6	0.271474000	0.645949000	-0.005997000	6	1.249660000	2.158022000	-0.000019000
6	-0.271268000	-0.647332000	-0.005377000	6	-0.026693000	1.575094000	-0.000229000
6	0.584136000	-1.775415000	-0.007458000	6	-0.107782000	0.161614000	0.002217000
6	1.931282000	-1.551746000	-0.009967000	6	1.083518000	-0.584432000	0.004554000
7	2.485879000	-0.308338000	-0.010705000	7	2.274484000	-0.025257000	0.004805000
6	1.699253000	0.730233000	-0.008809000	6	2.347286000	1.321680000	0.002604000
8	2.230903000	1.960338000	-0.009340000	8	3.576332000	1.855487000	0.002923000
6	-0.583920000	1.774012000	-0.003941000	6	-1.249580000	2.306606000	-0.002709000
6	-1.931086000	1.550358000	-0.001354000	6	-2.422922000	1.614316000	-0.002675000
7	-2.485682000	0.306974000	-0.000681000	7	-2.514654000	0.251837000	-0.000418000
6	-1.699019000	-0.731555000	-0.002587000	6	-1.406255000	-0.432643000	0.001915000
8	-2.230739000	-1.961688000	-0.001959000	8	-1.462650000	-1.769357000	0.004182000
1	0.173192000	-2.775096000	-0.006932000	1	1.387417000	3.231011000	-0.001853000
1	2.641804000	-2.370349000	-0.011404000	1	1.048086000	-1.669429000	0.006188000
1	3.195523000	1.874462000	-0.012086000	1	4.221884000	1.134775000	0.004775000
1	-0.173004000	2.773705000	-0.004409000	1	-1.242602000	3.388667000	-0.004618000
1	-2.641579000	2.368991000	0.000340000	1	-3.376650000	2.130838000	-0.004572000
1	-3.195313000	-1.875721000	-0.000034000	1	-2.394921000	-2.032835000	0.003639000
6	-5.192508000	0.104991000	0.008354000	6	-4.964519000	-0.898330000	-0.001395000
8	-5.123305000	-1.052954000	0.007847000	8	-4.487520000	-1.955816000	0.001098000
8	-5.327356000	1.248853000	0.009108000	8	-5.499649000	0.121559000	-0.003888000
6	5.192143000	-0.102461000	0.012993000	6	4.435406000	-1.675790000	-0.004181000
8	5.329128000	-1.246031000	0.013802000	8	5.156414000	-0.767634000	-0.005736000
8	5.120751000	1.055401000	0.012927000	8	3.768233000	-2.614977000	-0.002926000
nt7...2CO₂				nt8...2CO₂			
6	-2.836934000	1.984559000	-0.021951000	6	2.691855000	-2.228148000	0.000016000
6	-1.688864000	2.668295000	0.233320000	6	1.458035000	-2.787872000	-0.000093000
6	-0.435603000	1.995133000	0.167644000	6	0.305581000	-1.942101000	-0.000047000
6	-0.469316000	0.630588000	-0.165191000	6	0.531559000	-0.546839000	0.000126000
7	-1.614238000	-0.056199000	-0.405614000	7	1.784610000	0.012150000	0.000228000
6	-2.737153000	0.598838000	-0.339427000	6	2.798592000	-0.799152000	0.000160000
8	-3.885862000	-0.052398000	-0.576588000	8	4.049420000	-0.315097000	0.000288000
6	0.817622000	2.612348000	0.412175000	6	-1.013575000	-2.420031000	-0.000163000
6	1.946689000	1.852247000	0.308684000	6	-2.037917000	-1.497317000	-0.000101000
7	1.933136000	0.535282000	-0.028475000	7	-1.836733000	-0.168875000	0.000084000
6	0.788659000	-0.047987000	-0.258641000	6	-0.602099000	0.290658000	0.000192000
8	0.765645000	-1.337271000	-0.611295000	8	-3.314077000	-1.924395000	-0.000196000
1	-3.814815000	2.446181000	0.010068000	1	3.602368000	-2.812524000	-0.000006000
1	-1.714272000	3.722839000	0.484602000	1	1.330993000	-3.864685000	-0.000217000
1	-3.669740000	-0.975275000	-0.776233000	1	4.009483000	0.651780000	0.000292000
1	0.872415000	3.661241000	0.675065000	1	-1.235036000	-3.479534000	-0.000296000
1	2.930501000	2.270439000	0.488924000	1	-0.470579000	1.367942000	0.000338000

1	1.678482000	-1.660137000	-0.616759000	1	-3.892365000	-1.149485000	-0.000166000
6	4.308534000	-0.753036000	-0.168365000	6	-3.836252000	1.672259000	0.000084000
8	3.782321000	-1.741987000	-0.468271000	8	-4.639382000	0.835661000	-0.000032000
8	4.892235000	0.196013000	0.125257000	8	-3.086186000	2.546656000	0.000204000
6	-1.856991000	-2.647723000	0.625891000	6	2.318058000	2.836198000	-0.000244000
8	-1.062101000	-2.497697000	1.445823000	8	1.209942000	3.147926000	-0.000020000
8	-2.684078000	-2.838965000	-0.163909000	8	3.447405000	2.573954000	-0.000457000
nt9...2CO₂				nt10...2CO₂			
6	-0.000037000	0.289649000	0.000028000	6	-0.620899000	1.501045000	-0.000396000
6	-0.000033000	1.704092000	0.000076000	6	0.273542000	0.423970000	-0.000475000
6	1.244899000	2.382006000	0.000107000	6	-0.209606000	-0.900935000	-0.000811000
6	2.390759000	1.641148000	0.000078000	6	-1.611173000	-1.061131000	-0.001074000
7	2.410631000	0.286480000	0.000043000	7	-2.453633000	-0.051563000	-0.001016000
6	1.272541000	-0.363819000	0.000044000	6	-1.968820000	1.204258000	-0.000673000
8	1.316899000	-1.694965000	0.000046000	8	-2.866564000	2.203049000	-0.000576000
6	-1.272574000	-0.363824000	-0.000049000	6	1.702921000	0.581145000	-0.000249000
7	-2.410708000	0.286512000	-0.000034000	7	2.537376000	-0.412653000	-0.000261000
6	-2.390805000	1.641127000	0.000033000	6	2.046837000	-1.690809000	-0.000527000
6	-1.244927000	2.382010000	0.000080000	6	0.718120000	-1.981012000	-0.000833000
8	-1.316956000	-1.694942000	-0.000110000	8	2.163520000	1.838941000	0.000043000
1	1.277742000	3.463483000	0.000148000	1	-0.276733000	2.525619000	-0.000132000
1	3.367670000	2.113147000	0.000087000	1	-2.047152000	-2.057123000	-0.001315000
1	2.249853000	-1.956751000	0.000014000	1	-3.753094000	1.816846000	-0.001111000
1	-3.367676000	2.113228000	0.000038000	1	2.800953000	-2.468914000	-0.000478000
1	-1.277755000	3.463486000	0.000121000	1	0.368727000	-3.005722000	-0.001064000
1	-2.249892000	-1.956799000	-0.000154000	1	3.131701000	1.809522000	0.000554000
6	-4.842871000	-0.896032000	-0.000035000	6	5.226361000	-0.064220000	0.000920000
8	-4.359405000	-1.949924000	0.000062000	8	5.424830000	-1.198743000	0.000487000
8	-5.383717000	0.121516000	-0.000142000	8	5.093382000	1.088141000	0.001239000
6	4.842938000	-0.895973000	-0.000049000	6	-5.099491000	-0.674355000	0.000892000
8	4.359689000	-1.949968000	0.000373000	8	-4.869044000	-1.803685000	0.001412000
8	5.383647000	0.121653000	-0.000503000	8	-5.390794000	0.447490000	0.001374000
nt11...2CO₂				nt12...2CO₂			
6	-1.249049000	-2.031972000	0.000232000	6	-0.757852000	1.701808000	-0.000026000
6	0.000101000	-1.378369000	0.000003000	6	0.208584000	0.675902000	0.000014000
6	0.000149000	0.043619000	-0.000074000	6	-0.208506000	-0.676583000	0.000031000
6	-1.239790000	0.716435000	0.000096000	6	-1.608231000	-0.912138000	-0.000002000
7	-2.393525000	0.096763000	0.000323000	7	-2.497023000	0.048835000	-0.000034000
6	-2.386844000	-1.260017000	0.000381000	6	-2.081053000	1.336405000	-0.000039000
8	-3.587734000	-1.854820000	0.000585000	8	-3.039579000	2.280392000	-0.000058000
6	1.249229000	-2.032040000	-0.000161000	6	1.608330000	0.911467000	0.000049000
6	2.387055000	-1.260152000	-0.000423000	7	2.497120000	-0.049483000	0.000078000
7	2.393829000	0.096630000	-0.000521000	6	2.081132000	-1.337055000	0.000078000
6	1.240132000	0.716365000	-0.000343000	6	0.757954000	-1.702482000	0.000069000
8	3.587915000	-1.855045000	-0.000604000	8	3.039715000	-2.280965000	0.000069000
1	-1.328530000	-3.110744000	0.000311000	1	-0.479104000	2.747647000	-0.000045000
1	-1.269859000	1.804239000	0.000019000	1	-1.989641000	-1.930504000	-0.000006000
1	-4.269357000	-1.168295000	0.000753000	1	-3.900881000	1.841402000	-0.000126000
1	1.328666000	-3.110816000	-0.000096000	1	1.989739000	1.929831000	0.000053000
1	1.270270000	1.804168000	-0.000389000	1	0.479216000	-2.748325000	0.000091000
1	4.269610000	-1.168599000	-0.000738000	1	3.900912000	-1.841805000	0.000222000
6	4.626611000	1.630112000	0.000443000	6	5.104606000	0.719499000	-0.000084000
8	4.003481000	2.599704000	0.000490000	8	4.810022000	1.833785000	-0.000134000
8	5.305002000	0.690235000	0.000414000	8	5.458658000	-0.384142000	0.000007000
6	-4.627077000	1.629748000	-0.000295000	6	-5.104747000	-0.718289000	0.000017000
8	-4.004358000	2.599596000	-0.000513000	8	-4.811172000	-1.832832000	-0.000421000

8	-5.305060000	0.689569000	-0.000076000	8	-5.457922000	0.385647000	0.000394000
pn1...2CO₂				pn2...2CO₂			
6	-4.361963000	-1.162587000	0.202093000	6	-2.085456000	-1.094339000	0.000199000
6	-3.149700000	-1.793369000	0.214787000	6	-0.735989000	-1.468542000	0.000166000
6	-1.974808000	-1.020018000	0.109447000	6	0.252423000	-0.418954000	0.000390000
6	-2.089521000	0.372180000	-0.005441000	6	-0.185726000	0.927402000	0.000614000
7	-3.289757000	0.993407000	-0.019521000	7	-1.524344000	1.274007000	0.000607000
6	-4.362490000	0.247794000	0.080318000	6	-2.394518000	0.315564000	0.000431000
8	-5.557140000	0.857217000	0.067496000	8	-3.698811000	0.606451000	0.000488000
6	-0.651335000	-1.581013000	0.101199000	6	1.628250000	-0.665378000	0.000300000
7	0.445590000	-0.898086000	0.007818000	7	2.540146000	0.292396000	0.000605000
6	0.353009000	0.469533000	-0.076185000	6	2.113261000	1.563083000	0.000952000
6	-0.882167000	1.146599000	-0.103956000	6	0.779332000	1.936179000	0.000841000
8	-0.589716000	-2.914124000	0.194350000	8	3.052506000	2.521069000	0.001240000
7	1.529381000	1.130009000	-0.132192000	6	-3.069420000	-2.102788000	-0.000012000
6	1.501298000	2.438127000	-0.247047000	6	-2.677145000	-3.413361000	-0.000256000
6	0.319852000	3.213515000	-0.302864000	6	-1.288188000	-3.677608000	-0.000287000
6	-0.872126000	2.550545000	-0.222555000	7	-0.349911000	-2.760285000	-0.000080000
8	2.663977000	3.098733000	-0.313617000	8	-0.909519000	-4.963001000	-0.000516000
1	-5.303015000	-1.688841000	0.279346000	1	-3.801067000	1.569924000	0.000710000
1	-3.072873000	-2.869867000	0.303835000	1	1.989661000	-1.688390000	0.000056000
1	-5.396386000	1.805381000	-0.018755000	1	0.498424000	2.979422000	0.000918000
1	0.342290000	-3.177614000	0.161228000	1	3.920250000	2.093550000	0.000267000
1	0.394811000	4.287614000	-0.398863000	1	-4.116568000	-1.827063000	0.000021000
1	-1.817800000	3.077709000	-0.249266000	1	-3.375184000	-4.238699000	-0.000425000
1	3.383571000	2.455307000	-0.241407000	1	0.056155000	-4.980292000	-0.000499000
6	3.852881000	0.034267000	1.089175000	6	5.137432000	-0.455074000	-0.000738000
8	3.329998000	-0.892160000	1.532895000	8	5.484371000	0.651212000	-0.001269000
8	4.430802000	0.950184000	0.677710000	8	4.859524000	-1.573515000	-0.000231000
6	2.728169000	-2.291190000	-0.950696000	6	-2.487993000	3.975220000	-0.000986000
8	2.222915000	-3.258430000	-0.558965000	8	-3.562511000	3.538123000	-0.000516000
8	3.274952000	-1.368081000	-1.369680000	8	-1.444372000	4.459699000	-0.001528000
pn3...2CO₂				pn4...2CO₂			
6	2.712774000	0.865630000	-0.093650000	6	3.348677000	1.060987000	-0.022643000
6	1.607093000	0.015698000	-0.229228000	6	2.074090000	0.487530000	-0.014688000
6	0.287258000	0.599971000	-0.137914000	6	1.992468000	-0.914979000	0.105011000
6	0.200314000	1.983357000	0.078933000	6	3.173349000	-1.661572000	0.208909000
7	1.298078000	2.803959000	0.212423000	7	4.373861000	-1.114046000	0.201384000
6	2.465491000	2.264754000	0.129830000	6	4.442002000	0.218093000	0.087169000
8	3.558921000	3.040375000	0.256033000	8	5.671913000	0.756422000	0.081545000
7	-0.801200000	-0.189867000	-0.268205000	6	0.834107000	1.222528000	-0.111405000
6	-1.975994000	0.369169000	-0.194020000	6	-0.377878000	0.501283000	-0.075134000
6	-2.194962000	1.749499000	0.022015000	7	-0.428748000	-0.871509000	0.010395000
6	-1.093885000	2.547960000	0.159781000	6	0.685816000	-1.521107000	0.101708000
8	-3.064510000	-0.423284000	-0.331255000	8	0.664098000	-2.852964000	0.195335000
6	4.007212000	0.308082000	-0.186188000	6	0.755211000	2.623533000	-0.235053000
6	4.138684000	-1.033421000	-0.409193000	6	-0.462359000	3.241551000	-0.309936000
6	2.951288000	-1.796036000	-0.531361000	6	-1.609528000	2.421644000	-0.242145000
7	1.740096000	-1.308647000	-0.443065000	7	-1.578373000	1.113300000	-0.123775000
8	3.084568000	-3.112038000	-0.752036000	8	-2.798999000	3.030910000	-0.300617000
1	3.249681000	3.943418000	0.401882000	1	3.516451000	2.125075000	-0.108014000
1	-3.207295000	2.127537000	0.072016000	1	3.122269000	-2.740921000	0.300785000
1	-1.180418000	3.614593000	0.328370000	1	6.301446000	0.029457000	0.166862000
1	-2.752021000	-1.319989000	-0.512953000	1	-0.259610000	-3.144930000	0.162062000
1	4.872288000	0.951045000	-0.081862000	1	1.660743000	3.217004000	-0.273499000
1	5.097574000	-1.525678000	-0.494151000	1	-0.576419000	4.311761000	-0.409201000

1	2.195726000	-3.480699000	-0.847446000	1	-3.490821000	2.358581000	-0.218356000
6	-0.242288000	-2.590180000	1.141891000	6	-2.663595000	-2.333289000	-0.968936000
8	-0.611911000	-3.303755000	0.309270000	8	-3.239647000	-1.424506000	-1.380162000
8	0.110774000	-1.927758000	2.019195000	8	-2.126493000	-3.285928000	-0.584245000
6	-5.702009000	0.027069000	-0.268000000	6	-3.860948000	-0.082969000	1.103660000
8	-5.540102000	1.155108000	-0.073567000	8	-3.306500000	-0.998544000	1.530934000
8	-5.900268000	-1.093357000	-0.461553000	8	-4.468085000	0.820907000	0.707739000
pn5...2CO₂				pn6...2CO₂			
6	0.614288000	-0.497261000	-0.000560000	6	2.414068000	0.580120000	0.000255000
6	0.306561000	0.876910000	-0.000128000	6	1.899288000	-0.719460000	0.000052000
6	-1.093718000	1.249052000	-0.000203000	6	0.457619000	-0.880316000	0.000039000
6	-2.045711000	0.220637000	-0.000647000	6	-0.326228000	0.291581000	0.000240000
7	-1.722313000	-1.127379000	-0.000993000	7	0.201600000	1.572770000	0.000485000
6	-0.471545000	-1.448131000	-0.000978000	6	1.484983000	1.689175000	0.000492000
8	-0.105345000	-2.736466000	-0.001368000	8	2.057397000	2.902497000	0.000753000
7	-1.422281000	2.558946000	0.000134000	6	-0.167572000	-2.126541000	-0.000186000
6	-2.690786000	2.874052000	0.000024000	6	-1.551595000	-2.154329000	-0.000182000
6	-3.739732000	1.928329000	-0.000419000	7	-2.311308000	-1.053933000	0.000022000
6	-3.406129000	0.601515000	-0.000750000	6	-1.719254000	0.128995000	0.000245000
8	-3.030256000	4.177522000	0.000353000	8	-2.182597000	-3.342829000	-0.000424000
6	1.961821000	-0.877128000	-0.000551000	6	3.814211000	0.749245000	0.000215000
7	2.950927000	-0.001049000	-0.000130000	6	4.616723000	-0.358175000	-0.000002000
6	2.644516000	1.305212000	0.000298000	6	3.987132000	-1.624205000	-0.000199000
6	1.349087000	1.799796000	0.000303000	7	2.689143000	-1.810770000	-0.000177000
8	3.667287000	2.169647000	0.000684000	8	4.781274000	-2.704103000	-0.000341000
1	-0.901817000	-3.286479000	-0.001750000	1	1.359054000	3.572948000	0.000030000
1	-4.765223000	2.272116000	-0.000479000	1	0.407800000	-3.041493000	-0.000336000
1	-4.163633000	-0.171880000	-0.001066000	1	-2.359958000	1.004535000	0.000465000
1	-2.211315000	4.687793000	0.000655000	1	-3.135405000	-3.178462000	-0.000646000
1	2.235230000	-1.927084000	-0.000882000	1	4.230398000	1.748784000	0.000346000
1	1.159343000	2.863481000	0.000630000	1	5.696538000	-0.302804000	-0.000031000
1	4.493760000	1.666081000	0.000633000	1	4.211135000	-3.483576000	-0.000407000
6	5.492795000	-0.964670000	0.000292000	6	-5.026358000	-1.078649000	0.000324000
8	5.921977000	0.112663000	0.000590000	8	-5.041131000	-2.238257000	0.000295000
8	5.124607000	-2.056225000	0.000042000	8	-5.078614000	0.072263000	0.000326000
6	-3.654824000	-3.248739000	0.001198000	6	-1.359466000	3.991281000	-0.000642000
8	-4.571173000	-2.551209000	0.001588000	8	-2.378557000	3.456869000	-0.000866000
8	-2.768399000	-3.995320000	0.000850000	8	-0.358636000	4.577469000	-0.000450000
pn7...2CO₂				pn8...2CO₂			
6	1.300230000	1.103825000	0.000082000	6	-2.038722000	-1.123393000	0.120882000
6	0.329178000	0.071632000	0.000093000	6	-2.192736000	0.265028000	0.011281000
6	-1.062254000	0.487406000	0.000058000	6	-1.014150000	1.095574000	-0.092796000
6	-1.351771000	1.869452000	0.000008000	6	0.243087000	0.448837000	-0.071584000
7	-0.380430000	2.846577000	-0.000005000	7	0.375334000	-0.918214000	0.003249000
6	0.852024000	2.471243000	0.000035000	6	-0.687814000	-1.640921000	0.099606000
8	1.811334000	3.405849000	0.000023000	8	-0.581906000	-2.970213000	0.182570000
6	-2.183252000	-0.382540000	0.000074000	6	-3.151797000	-1.975743000	0.234066000
7	-3.434732000	0.019879000	0.000041000	6	-4.396446000	-1.402879000	0.234891000
6	-3.682382000	1.343526000	-0.000011000	7	-4.585808000	-0.072045000	0.130753000
6	-2.694601000	2.292888000	-0.000030000	6	-3.547232000	0.713486000	0.025033000
8	-1.973374000	-1.708716000	0.000125000	8	-3.797865000	2.034759000	-0.075927000
6	2.657538000	0.772206000	0.000102000	6	-1.002186000	2.506021000	-0.211796000
7	3.092802000	-0.475530000	0.000147000	6	0.186179000	3.178900000	-0.291911000
6	2.174764000	-1.449840000	0.000172000	6	1.376425000	2.426860000	-0.236477000
6	0.800683000	-1.243523000	0.000127000	7	1.411530000	1.119250000	-0.125349000
8	2.625750000	-2.709915000	0.000224000	8	2.533512000	3.098104000	-0.299994000

1	1.370406000	4.265752000	-0.000014000	1	0.357602000	-3.204054000	0.137701000
1	-4.731352000	1.620243000	-0.000038000	1	-3.014760000	-3.044358000	0.316857000
1	-2.913408000	3.351465000	-0.000071000	1	-5.295695000	-2.001478000	0.319727000
1	-2.839458000	-2.143115000	0.000134000	1	-4.758883000	2.131366000	-0.045946000
1	3.409642000	1.554177000	0.000082000	1	-1.932760000	3.050703000	-0.241064000
1	0.142583000	-2.095881000	0.000119000	1	0.239951000	4.254426000	-0.387540000
1	3.593285000	-2.688627000	0.000241000	1	3.258911000	2.462010000	-0.223703000
6	-5.578237000	-1.637620000	-0.000152000	6	3.750809000	0.043538000	1.110138000
8	-4.887806000	-2.569683000	-0.000041000	8	4.312396000	0.979703000	0.723120000
8	-6.316321000	-0.753203000	-0.000278000	8	3.242929000	-0.903241000	1.527921000
6	5.777365000	-0.907471000	-0.000323000	6	2.708805000	-2.243116000	-0.989834000
8	5.611367000	-2.055118000	-0.000232000	8	2.220046000	-3.224881000	-0.613792000
8	6.002691000	0.222336000	-0.000215000	8	3.237504000	-1.302318000	-1.392097000
pn9...2CO₂				pn10...2CO₂			
6	2.447466000	-0.886060000	-0.129567000	6	-1.247563000	-3.317097000	0.005770000
6	1.279158000	-0.110688000	-0.233997000	6	0.055732000	-2.913133000	0.003745000
6	0.006728000	-0.788153000	-0.116847000	6	0.349071000	-1.529124000	0.001258000
6	0.020863000	-2.175851000	0.147895000	6	-0.729439000	-0.642852000	0.000938000
7	1.178653000	-2.905572000	0.275773000	7	-2.021257000	-1.033803000	0.003014000
6	2.302877000	-2.289257000	0.131694000	6	-2.258882000	-2.321363000	0.005366000
8	3.442484000	-2.989551000	0.236685000	8	-3.528431000	-2.744246000	0.007547000
6	-1.275058000	-0.188107000	-0.269312000	6	1.687447000	-0.996581000	-0.001095000
7	-2.406371000	-0.845799000	-0.147952000	6	1.835481000	0.398767000	-0.003513000
6	-2.366124000	-2.164140000	0.131430000	7	0.763066000	1.268833000	-0.003704000
6	-1.201008000	-2.865463000	0.281680000	6	-0.433174000	0.778980000	-0.001812000
8	-1.369265000	1.116401000	-0.572564000	8	-1.498027000	1.584404000	-0.002319000
6	3.702640000	-0.258295000	-0.268387000	7	2.739147000	-1.846945000	-0.000948000
6	3.755500000	1.088114000	-0.494502000	6	3.941643000	-1.333256000	-0.003196000
6	2.524317000	1.781425000	-0.554987000	6	4.214625000	0.052289000	-0.005815000
7	1.344364000	1.220529000	-0.431786000	6	3.150607000	0.912667000	-0.005964000
8	2.571975000	3.104818000	-0.741381000	8	4.996384000	-2.172428000	-0.003026000
1	3.195754000	-3.906342000	0.415987000	1	-1.538488000	-4.359025000	0.007732000
1	-3.332565000	-2.648008000	0.225244000	1	0.873910000	-3.622162000	0.003983000
1	-1.188512000	-3.925470000	0.492935000	1	-4.104707000	-1.965536000	0.007354000
1	-2.313176000	1.311948000	-0.675680000	1	-1.193318000	2.502743000	-0.004675000
1	4.603972000	-0.853731000	-0.192926000	1	5.241294000	0.391859000	-0.007631000
1	4.682013000	1.632711000	-0.611376000	1	3.290704000	1.986193000	-0.007896000
1	1.663014000	3.440413000	-0.724912000	1	4.646214000	-3.071309000	-0.001154000
6	-0.223108000	2.725780000	1.304477000	6	-4.684005000	0.909925000	-0.007139000
8	-0.098831000	3.645540000	0.611176000	8	-4.393984000	2.022816000	-0.009414000
8	-0.347329000	1.851200000	2.046031000	8	-5.028395000	-0.197518000	-0.005003000
6	-4.867356000	0.242802000	-0.406530000	6	1.035720000	4.137735000	0.008106000
8	-4.415490000	1.283863000	-0.645716000	8	-0.120961000	4.202845000	0.004510000
8	-5.379593000	-0.763304000	-0.176707000	8	2.187678000	4.128992000	0.011938000
pn11...2CO₂				pn12...2CO₂			
6	-2.373370000	0.503038000	-0.235932000	6	2.156176000	-0.857661000	-0.000608000
6	-1.892261000	-0.793619000	-0.011963000	6	0.853603000	-1.396422000	-0.000067000
6	-0.460837000	-1.004822000	-0.014508000	6	-0.248781000	-0.456448000	-0.000305000
6	0.345432000	0.115385000	-0.241917000	6	0.040751000	0.932369000	-0.001092000
7	-0.132539000	1.385950000	-0.439101000	7	1.333055000	1.430760000	-0.001574000
6	-1.411322000	1.555545000	-0.438547000	6	2.306457000	0.580165000	-0.001394000
8	-1.915878000	2.783717000	-0.632037000	8	3.566559000	1.018563000	-0.001937000
6	0.140428000	-2.263613000	0.191544000	6	-1.592852000	-0.834251000	0.000166000
6	1.507320000	-2.339212000	0.154004000	7	-2.602423000	0.021585000	-0.000087000
7	2.305492000	-1.271669000	-0.082628000	6	-2.312774000	1.327566000	-0.000859000
6	1.754321000	-0.100467000	-0.276909000	6	-1.022447000	1.834283000	-0.001400000

8	2.536409000	0.955463000	-0.532749000	8	-3.344358000	2.183550000	-0.001205000
6	-3.768798000	0.715448000	-0.243590000	6	3.252751000	-1.726715000	-0.000425000
6	-4.601517000	-0.346846000	-0.032650000	7	3.129372000	-3.042197000	0.000248000
6	-4.007230000	-1.613244000	0.184956000	6	1.890069000	-3.543013000	0.000744000
7	-2.717090000	-1.841003000	0.197159000	6	0.727788000	-2.785494000	0.000614000
8	-4.834709000	-2.647222000	0.392141000	8	1.782199000	-4.880088000	0.001389000
1	-1.172687000	3.394067000	-0.752853000	1	3.557516000	1.987498000	-0.002396000
1	-0.474131000	-3.134106000	0.372613000	1	-1.873531000	-1.883145000	0.000808000
1	2.026224000	-3.278416000	0.309832000	1	-0.848465000	2.900581000	-0.002025000
1	3.456442000	0.655635000	-0.505081000	1	-4.164425000	1.670189000	-0.000883000
1	-4.154892000	1.712424000	-0.415741000	1	4.260106000	-1.325468000	-0.000842000
1	-5.679131000	-0.258939000	-0.025035000	1	-0.226440000	-3.292659000	0.001034000
1	-4.289449000	-3.433343000	0.523528000	1	2.678481000	-5.239134000	0.001327000
6	1.195628000	3.529886000	0.766393000	6	-5.100228000	-1.004111000	0.000404000
8	1.703559000	2.891173000	1.578591000	8	-5.568080000	0.056436000	-0.000199000
8	0.685509000	4.222217000	-0.012201000	8	-4.696203000	-2.083684000	0.000976000
6	4.979955000	-1.678855000	-0.107678000	6	1.989797000	4.233772000	0.002062000
8	4.857264000	-2.802180000	0.117420000	8	0.898607000	4.598938000	0.003824000
8	5.174108000	-0.558421000	-0.335475000	8	3.105636000	3.917143000	0.000380000
pn13...2CO₂				pn14...2CO₂			
6	-0.209456000	-1.211357000	-0.000093000	6	-4.373768000	1.076252000	0.035023000
6	-0.538223000	0.154038000	-0.000039000	6	-3.160345000	1.695836000	-0.054116000
6	0.526036000	1.130491000	-0.000059000	6	-1.970538000	0.925808000	-0.032919000
6	1.845489000	0.654862000	-0.000143000	6	-2.128711000	-0.459040000	0.080589000
7	2.161536000	-0.695942000	-0.000206000	7	-3.323522000	-1.079985000	0.169412000
6	1.203031000	-1.555693000	-0.000177000	6	-4.393399000	-0.335247000	0.147402000
8	1.463547000	-2.869428000	-0.000232000	8	-5.595634000	-0.930216000	0.235487000
7	0.221273000	2.445017000	0.000003000	6	-0.637591000	1.470369000	-0.110474000
6	1.209346000	3.304440000	-0.000015000	6	0.448882000	0.573984000	-0.064954000
6	2.573235000	2.945281000	-0.000092000	7	0.276766000	-0.784987000	0.015259000
6	2.881654000	1.610497000	-0.000156000	6	-0.922581000	-1.267116000	0.090715000
8	0.911731000	4.617719000	0.000044000	8	-1.100733000	-2.581555000	0.178128000
6	-1.217794000	-2.172622000	-0.000073000	6	-0.339950000	2.843780000	-0.226993000
6	-2.527406000	-1.716797000	0.000001000	6	0.960069000	3.263394000	-0.285721000
7	-2.861619000	-0.419591000	0.000044000	6	1.967926000	2.276665000	-0.210808000
6	-1.899792000	0.487310000	0.000027000	7	1.733317000	0.991092000	-0.098838000
8	-3.527521000	-2.610008000	0.000025000	8	3.238581000	2.699698000	-0.255811000
1	2.422929000	-2.996350000	-0.000292000	1	-5.308428000	1.620751000	0.023533000
1	3.327877000	3.719709000	-0.000095000	1	-3.116221000	2.774309000	-0.139335000
1	3.908758000	1.267910000	-0.000221000	1	-5.439130000	-1.880717000	0.305384000
1	-0.050211000	4.693674000	0.000101000	1	-0.228122000	-3.002037000	0.156446000
1	-0.997936000	-3.230615000	-0.000112000	1	-1.137708000	3.575266000	-0.273210000
1	-2.201763000	1.528946000	0.000065000	1	1.239133000	4.303558000	-0.378860000
1	-4.367038000	-2.128999000	0.000057000	1	3.818657000	1.929242000	-0.173777000
6	-5.427501000	0.484551000	0.000100000	6	3.803262000	-0.558784000	1.105014000
8	-5.831641000	-0.602258000	0.000090000	8	4.545272000	0.245957000	0.725228000
8	-5.084628000	1.584467000	0.000110000	8	3.112541000	-1.384735000	1.516028000
6	4.862660000	-1.708406000	0.000249000	6	2.272297000	-2.556795000	-0.996968000
8	5.359377000	-0.669476000	0.000324000	8	2.972404000	-1.738729000	-1.407277000
8	4.411809000	-2.776046000	0.000194000	8	1.604141000	-3.422649000	-0.613752000
pn15...2CO₂				pn16...2CO₂			
6	2.227819000	-0.353215000	-0.083486000	6	3.354982000	-1.144462000	-0.171195000
6	2.036044000	1.037361000	0.029120000	6	2.100924000	-0.543538000	-0.079469000
6	0.686587000	1.537078000	0.107023000	6	1.980674000	0.852076000	0.032250000
6	-0.374854000	0.610855000	0.059477000	6	3.182683000	1.579340000	0.044668000
7	-0.167012000	-0.738621000	-0.013924000	7	4.376655000	1.021468000	-0.041989000

6	1.048828000	-1.189597000	-0.086998000	6	4.457120000	-0.307027000	-0.147707000
8	1.228070000	-2.503875000	-0.163561000	8	5.689751000	-0.839971000	-0.234193000
6	3.567816000	-0.826005000	-0.174475000	6	0.868252000	-1.311635000	-0.080441000
7	4.618055000	-0.037729000	-0.153709000	7	-0.313184000	-0.803651000	-0.000476000
6	4.414533000	1.286911000	-0.041638000	6	-0.449091000	0.567524000	0.077671000
6	3.175978000	1.868027000	0.050108000	6	0.659203000	1.434056000	0.116343000
8	3.801089000	-2.135641000	-0.290188000	8	1.022831000	-2.634671000	-0.165186000
6	0.352914000	2.903433000	0.221065000	7	-1.721164000	1.012092000	0.116113000
6	-0.956230000	3.289700000	0.274650000	6	-1.926366000	2.304553000	0.225486000
6	-1.937118000	2.274839000	0.195214000	6	-0.895213000	3.264632000	0.293496000
7	-1.669900000	0.994638000	0.086038000	6	0.395419000	2.813286000	0.230438000
8	-3.216121000	2.663625000	0.232646000	8	-3.187233000	2.755486000	0.274453000
1	0.353689000	-2.921580000	-0.136359000	1	3.467779000	-2.215876000	-0.256461000
1	5.311732000	1.896531000	-0.028578000	1	3.176396000	2.660891000	0.127366000
1	3.094433000	2.941793000	0.133812000	1	6.320004000	-0.110172000	-0.201057000
1	4.761450000	-2.233671000	-0.336899000	1	0.146628000	-3.048194000	-0.134759000
1	1.131788000	3.654066000	0.269369000	1	-1.147298000	4.311843000	0.384970000
1	-1.263897000	4.321815000	0.365924000	1	1.210713000	3.525317000	0.271129000
1	-3.776732000	1.878669000	0.147803000	1	-3.785443000	1.998840000	0.195384000
6	-3.703923000	-0.616730000	-1.099085000	6	-2.353950000	-2.541352000	0.979092000
8	-2.996922000	-1.437196000	-1.492461000	8	-3.049005000	-1.713541000	1.376930000
8	-4.461403000	0.181581000	-0.736159000	8	-1.690226000	-3.416084000	0.607194000
6	-2.131905000	-2.535109000	1.037842000	6	-3.814630000	-0.481406000	-1.120533000
8	-1.450482000	-3.393447000	0.661550000	8	-4.541908000	0.332953000	-0.733442000
8	-2.844156000	-1.723914000	1.441071000	8	-3.137332000	-1.315207000	-1.538593000
pn17...2CO₂				pn18...2CO₂			
6	1.365827000	1.723806000	0.000296000	6	1.616703000	2.620778000	-0.193402000
6	0.575401000	0.555302000	-0.000105000	6	0.388416000	2.024359000	-0.131741000
6	-0.867746000	0.711848000	-0.000576000	6	0.283125000	0.608668000	-0.221181000
6	-1.397704000	2.016260000	-0.000535000	6	1.492008000	-0.084094000	-0.372086000
7	-0.602620000	3.146220000	-0.000093000	7	2.705917000	0.499168000	-0.417924000
6	0.672132000	2.999763000	0.000306000	6	2.760487000	1.802725000	-0.334665000
8	1.457963000	4.083953000	0.000757000	8	3.958039000	2.403636000	-0.381419000
6	-1.821304000	-0.338433000	-0.001100000	6	-0.937833000	-0.166929000	-0.170943000
7	-3.122434000	-0.159118000	-0.001472000	6	-0.843521000	-1.569088000	-0.285420000
6	-3.601667000	1.099594000	-0.001487000	7	0.353016000	-2.223067000	-0.455260000
6	-2.792206000	2.205055000	-0.000986000	6	1.437016000	-1.527377000	-0.498077000
8	-1.379051000	-1.608791000	-0.001130000	8	2.604360000	-2.150004000	-0.681439000
6	2.755318000	1.655506000	0.000698000	6	-2.250429000	0.351675000	-0.008171000
6	3.326539000	0.393196000	0.000659000	7	-3.336137000	-0.381990000	0.040820000
7	2.607731000	-0.731066000	0.000253000	6	-3.217696000	-1.721864000	-0.069755000
6	1.284697000	-0.662781000	-0.000050000	6	-2.014884000	-2.352669000	-0.232214000
8	4.662601000	0.279456000	0.001004000	8	-2.409760000	1.684454000	0.106472000
1	0.879233000	4.857749000	0.000719000	1	1.738851000	3.693991000	-0.132798000
1	-4.682638000	1.187654000	-0.001924000	1	-0.500843000	2.624111000	-0.017987000
1	-3.189169000	3.210586000	-0.000927000	1	4.635140000	1.717993000	-0.477641000
1	-2.153037000	-2.191485000	-0.001507000	1	2.410214000	-3.095166000	-0.735083000
1	3.369075000	2.544849000	0.001031000	1	-4.148170000	-2.276835000	-0.021607000
1	0.762858000	-1.608433000	-0.000268000	1	-1.934032000	-3.427065000	-0.320663000
1	4.888392000	-0.661419000	0.000931000	1	-3.357270000	1.856898000	0.212103000
6	-4.941108000	-2.161568000	0.001489000	6	4.822194000	-0.700721000	0.987336000
8	-5.822373000	-1.419678000	0.002135000	8	4.140108000	-1.283832000	1.709810000
8	-4.099479000	-2.959721000	0.001038000	8	5.549040000	-0.114060000	0.300980000
6	3.717105000	-3.222610000	-0.000449000	6	-5.834868000	0.606559000	0.363565000
8	4.784229000	-2.768204000	-0.000331000	8	-5.427021000	1.691782000	0.407425000
8	2.682964000	-3.729689000	-0.000702000	8	-6.303237000	-0.445080000	0.328266000

pn19...2CO ₂				pn20...2CO ₂		
6	-0.697792000	-0.325686000	-0.005102000	6	-1.481633000	1.850118000
6	-0.299967000	1.021863000	-0.000701000	6	-0.810751000	0.620883000
6	1.113671000	1.318648000	-0.002269000	6	0.638844000	0.616446000
6	2.010235000	0.243854000	-0.007764000	6	1.298355000	1.874636000
7	1.608087000	-1.072927000	-0.011537000	7	0.617756000	3.077148000
6	0.338166000	-1.337698000	-0.010599000	6	-0.664766000	3.050703000
8	-0.053461000	-2.611740000	-0.014806000	8	-1.343577000	4.206284000
7	1.512223000	2.612197000	0.001426000	6	1.462103000	-0.523237000
6	2.793972000	2.857561000	-0.000347000	7	2.786170000	-0.471145000
6	3.793566000	1.856577000	-0.005898000	6	3.382792000	0.724222000
6	3.392209000	0.550750000	-0.009564000	6	2.690806000	1.921988000
8	3.205974000	4.140347000	0.003241000	8	4.724308000	0.744969000
6	-2.100686000	-0.582719000	-0.003855000	6	-2.885117000	1.918768000
7	-3.002046000	0.375343000	0.001194000	6	-3.580370000	0.736796000
6	-2.592966000	1.659617000	0.005413000	7	-2.970059000	-0.463881000
6	-1.275476000	2.035663000	0.004716000	6	-1.660022000	-0.523851000
8	-2.542685000	-1.839735000	-0.007890000	8	-1.098117000	-1.742194000
1	0.738880000	-3.167251000	-0.019131000	1	-0.691727000	4.919704000
1	4.835391000	2.147303000	-0.007046000	1	1.032183000	-1.514401000
1	4.107336000	-0.261861000	-0.013626000	1	3.208200000	2.870848000
1	2.416802000	4.695361000	0.006725000	1	5.040120000	-0.169454000
1	-3.389437000	2.396512000	0.009513000	1	-3.387393000	2.875384000
1	-0.975162000	3.073108000	0.008129000	1	-4.664262000	0.711254000
1	-3.510827000	-1.806803000	-0.006256000	1	-1.809169000	-2.400408000
6	-5.682428000	-0.036418000	0.005998000	6	4.114040000	-2.831104000
8	-5.533074000	-1.186181000	0.001076000	8	3.131445000	-3.432688000
8	-5.895119000	1.096136000	0.010987000	8	5.137521000	-2.285675000
6	3.478551000	-3.294060000	0.014552000	6	-4.589599000	-2.654719000
8	4.420575000	-2.630885000	0.025061000	8	-3.668352000	-3.359201000
8	2.563147000	-4.003738000	0.004411000	8	-5.539867000	-2.003704000
pn21...2CO ₂				pn22...2CO ₂		
6	-1.315231000	0.905151000	0.000154000	6	-2.396619000	0.529838000
6	-0.301032000	-0.081175000	0.000216000	6	-1.875342000	-0.777630000
6	1.075553000	0.372140000	0.000119000	6	-0.425300000	-0.921025000
6	1.321525000	1.761546000	-0.000029000	6	0.343568000	0.261806000
7	0.319893000	2.693232000	-0.000061000	7	-0.195331000	1.541365000
6	-0.910201000	2.291477000	0.000026000	6	-1.477881000	1.649529000
8	-1.860239000	3.225753000	0.000021000	8	-2.056911000	2.857470000
6	2.230670000	-0.459229000	0.000143000	6	0.231378000	-2.151422000
7	3.464499000	-0.010296000	0.000025000	6	1.617311000	-2.157040000
6	3.668481000	1.322882000	-0.000122000	7	2.356232000	-1.045920000
6	2.650196000	2.235269000	-0.000153000	6	1.738256000	0.124668000
8	2.079416000	-1.794331000	0.000293000	8	2.261912000	-3.336980000
6	-2.670668000	0.471859000	0.000225000	6	-3.786118000	0.699785000
7	-3.018608000	-0.797037000	0.000361000	7	-4.635717000	-0.312870000
6	-2.044969000	-1.722961000	0.000435000	6	-4.128713000	-1.547928000
6	-0.703214000	-1.434771000	0.000363000	6	-2.772195000	-1.842869000
8	-3.652503000	1.373350000	0.000137000	8	-5.006208000	-2.562815000
1	-1.401145000	4.076815000	-0.000060000	1	-1.362996000	3.532690000
1	4.707881000	1.633348000	-0.000209000	1	-0.297137000	-3.094652000
1	2.828743000	3.301323000	-0.000266000	1	2.360556000	1.013228000
1	2.965083000	-2.187793000	0.000280000	1	3.213401000	-3.163075000
1	-2.387302000	-2.752798000	0.000565000	1	-4.208212000	1.698374000
1	0.019501000	-2.231443000	0.000425000	1	-2.457601000	-2.876784000
1	-4.491263000	0.888510000	0.000202000	1	-5.891225000	-2.176923000

6	5.670370000	-1.577259000	-0.000183000	6	1.348498000	3.979540000	0.004894000
8	5.018982000	-2.537169000	0.000010000	8	2.372502000	3.454332000	0.008204000
8	6.372089000	-0.663849000	-0.000514000	8	0.341712000	4.555140000	0.001734000
6	-5.581254000	-1.689086000	-0.000433000	6	5.074878000	-1.043734000	-0.002916000
8	-5.984194000	-0.601789000	-0.000577000	8	5.118961000	0.107287000	-0.004884000
8	-5.241469000	-2.790003000	-0.000343000	8	5.095109000	-2.203432000	-0.001003000
pn23...2CO ₂				pn24...2CO ₂			
6	-2.352843000	0.454847000	-0.237986000	6	-2.567286000	0.379052000	0.000051000
6	-1.867568000	-0.847843000	-0.002118000	6	-1.952898000	-0.880468000	0.000003000
6	-0.427020000	-1.044548000	-0.004353000	6	-0.500251000	-0.951053000	0.000103000
6	0.366132000	0.083170000	-0.241614000	6	0.193382000	0.284714000	0.000338000
7	-0.120891000	1.352128000	-0.447509000	7	-0.429022000	1.522649000	0.000395000
6	-1.398523000	1.515803000	-0.448417000	6	-1.712154000	1.556151000	0.000233000
8	-1.907687000	2.738607000	-0.648075000	8	-2.367018000	2.725599000	0.000262000
6	0.203250000	-2.288335000	0.209390000	6	0.259505000	-2.125651000	-0.000006000
6	1.572282000	-2.344563000	0.169885000	6	1.642348000	-2.017578000	0.000124000
7	2.351731000	-1.269464000	-0.076249000	7	2.301867000	-0.857986000	0.000418000
6	1.777840000	-0.109217000	-0.278422000	6	1.592242000	0.258872000	0.000524000
8	2.540958000	0.956670000	-0.544230000	8	2.373760000	-3.146488000	-0.000086000
6	-3.737539000	0.669266000	-0.248658000	6	-3.965333000	0.499243000	-0.000054000
7	-4.615763000	-0.295328000	-0.047063000	6	-4.706473000	-0.657578000	-0.000215000
6	-4.144995000	-1.526645000	0.176623000	7	-4.153317000	-1.882025000	-0.000236000
6	-2.800073000	-1.862739000	0.210881000	6	-2.846302000	-1.986928000	-0.000117000
8	-5.054436000	-2.491987000	0.379429000	8	-2.343151000	-3.233313000	-0.000178000
1	-1.167393000	3.352490000	-0.770271000	1	-1.718487000	3.444450000	0.000263000
1	-0.369043000	-3.185300000	0.401734000	1	-0.190573000	-3.104269000	-0.000178000
1	2.103012000	-3.275920000	0.332751000	1	2.139996000	1.195249000	0.000761000
1	3.466411000	0.673626000	-0.516248000	1	3.308857000	-2.900148000	0.000355000
1	-4.127924000	1.664899000	-0.428528000	1	-4.430926000	1.474045000	-0.000016000
1	-2.518624000	-2.889051000	0.398180000	1	-5.790219000	-0.630647000	-0.000309000
1	-5.926348000	-2.081425000	0.321311000	1	-3.099072000	-3.835405000	-0.000274000
6	1.187164000	3.492867000	0.776566000	6	5.005934000	-0.638570000	-0.000204000
8	1.686995000	2.850217000	1.590951000	8	5.123119000	-1.792331000	-0.000112000
8	0.684723000	4.187905000	-0.004315000	8	4.956040000	0.512442000	-0.000343000
6	5.037189000	-1.629304000	-0.109092000	6	0.956758000	4.074373000	-0.000257000
8	4.935190000	-2.752387000	0.127161000	8	-0.090003000	4.573820000	-0.000441000
8	5.207080000	-0.507428000	-0.348332000	8	2.015615000	3.624120000	-0.000074000
pn25...2CO ₂				pn26...2CO ₂			
6	-2.010479000	-1.097319000	0.001181000	6	-2.161197000	-0.642803000	-0.000105000
6	-0.688733000	-1.580297000	-0.002863000	6	-0.933354000	-1.324114000	-0.000016000
6	0.384423000	-0.611600000	-0.002692000	6	0.288750000	-0.543282000	-0.000088000
6	0.057714000	0.766400000	0.001448000	6	0.182491000	0.868565000	-0.000224000
7	-1.243912000	1.215324000	0.004951000	7	-1.042338000	1.523602000	-0.000227000
6	-2.203682000	0.341781000	0.005003000	6	-2.117662000	0.815235000	-0.000190000
8	-3.457003000	0.777952000	0.008491000	8	-3.312146000	1.407036000	-0.000248000
6	1.741521000	-0.950915000	-0.006069000	6	1.575698000	-1.084621000	-0.000078000
7	2.723996000	-0.066799000	-0.005658000	7	2.683966000	-0.357542000	-0.000201000
6	2.397096000	1.232668000	-0.001596000	6	2.564145000	0.972099000	-0.000344000
6	1.095117000	1.701348000	0.002100000	6	1.346261000	1.634695000	-0.000344000
8	3.406621000	2.114898000	-0.000910000	8	3.695944000	1.694491000	-0.000489000
6	-3.058767000	-2.058608000	0.001184000	6	-3.363208000	-1.344023000	-0.000076000
7	-2.850875000	-3.357258000	-0.002387000	6	-3.284100000	-2.728264000	0.000059000
6	-1.582587000	-3.796825000	-0.006221000	7	-2.135253000	-3.403749000	0.000170000
6	-0.484062000	-2.972978000	-0.006633000	6	-0.999614000	-2.725406000	0.000134000
8	-4.332432000	-1.657767000	0.004983000	8	-4.420348000	-3.448243000	0.000091000
1	-3.438196000	1.746855000	0.010652000	1	-3.185392000	2.367830000	-0.000398000

1	2.055982000	-1.989627000	-0.009068000	1	1.729353000	-2.159270000	0.000015000
1	0.889650000	2.761839000	0.005307000	1	1.303630000	2.714372000	-0.000442000
1	4.239332000	1.622587000	-0.004588000	1	4.445044000	1.082737000	-0.000298000
1	-1.462296000	-4.874982000	-0.009080000	1	-4.318660000	-0.839160000	-0.000147000
1	0.506935000	-3.402384000	-0.009806000	1	-0.096002000	-3.325156000	0.000228000
1	-4.866226000	-2.463535000	0.004216000	1	-4.169278000	-4.379987000	0.000177000
6	5.244727000	-1.028188000	0.005109000	6	5.026801000	-1.696852000	0.000267000
8	4.867163000	-2.117521000	0.003608000	8	5.630140000	-0.707286000	0.000192000
8	5.687209000	0.042984000	0.007587000	8	4.485156000	-2.714571000	0.000367000
6	-1.948394000	4.033411000	-0.004354000	6	-1.340388000	4.397989000	0.000426000
8	-3.057351000	3.695290000	0.002808000	8	-2.486605000	4.220292000	0.000151000
8	-0.863335000	4.417553000	-0.011511000	8	-0.212272000	4.624173000	0.000702000
pn27...2CO₂				pn28...2CO₂			
6	-0.120368000	2.105606000	0.096537000	6	-1.566116000	2.788346000	-0.004226000
6	0.031833000	0.731858000	-0.147313000	6	-0.340125000	2.185959000	-0.000932000
6	1.372379000	0.196365000	-0.250570000	6	-0.251978000	0.772692000	-0.011949000
6	2.442142000	1.104972000	-0.154258000	6	-1.462073000	0.076631000	-0.025117000
7	2.276570000	2.453135000	0.069615000	7	-2.678283000	0.659074000	-0.026822000
6	1.081599000	2.904972000	0.198009000	6	-2.720101000	1.967019000	-0.017788000
8	0.890393000	4.216184000	0.433471000	8	-3.909601000	2.581053000	-0.021525000
7	1.578601000	-1.126128000	-0.428368000	6	0.979221000	0.013555000	-0.010388000
6	2.806574000	-1.564172000	-0.539839000	6	0.896111000	-1.400528000	-0.022253000
6	3.951667000	-0.737946000	-0.488884000	7	-0.309537000	-2.069361000	-0.036367000
6	3.753235000	0.599266000	-0.287372000	6	-1.396061000	-1.377639000	-0.038046000
8	2.999145000	-2.883990000	-0.703948000	8	-2.572994000	-2.005504000	-0.052563000
6	-1.396970000	2.682795000	0.217512000	6	2.258859000	0.576605000	0.002493000
6	-2.482175000	1.858202000	0.076619000	7	3.376784000	-0.131949000	0.004138000
7	-2.372624000	0.540492000	-0.182675000	6	3.279370000	-1.466428000	-0.007058000
6	-1.183318000	-0.004535000	-0.294619000	6	2.075076000	-2.147532000	-0.020271000
8	-1.140756000	-1.312742000	-0.580075000	8	4.426147000	-2.166118000	-0.005075000
1	1.762825000	4.627883000	0.472643000	1	-1.685834000	3.863473000	0.003084000
1	4.933704000	-1.178004000	-0.595961000	1	0.555792000	2.793994000	0.009598000
1	4.579357000	1.297121000	-0.222060000	1	-4.599684000	1.901544000	-0.035874000
1	2.131981000	-3.313184000	-0.679073000	1	-2.392078000	-2.954899000	-0.055215000
1	-1.504503000	3.740161000	0.411364000	1	2.395167000	1.653874000	0.012081000
1	-3.496323000	2.233045000	0.160925000	1	2.043261000	-3.227919000	-0.029137000
1	-2.057561000	-1.611708000	-0.680189000	1	5.162129000	-1.539017000	0.004341000
6	0.178802000	-2.711475000	1.363024000	6	5.688111000	1.255013000	0.034234000
8	-0.041655000	-1.817761000	2.059012000	8	6.315252000	0.280564000	0.030989000
8	0.397629000	-3.647457000	0.717450000	8	5.123128000	2.260226000	0.038260000
6	-4.717268000	-0.818059000	-0.416174000	6	-5.612936000	-0.853718000	0.059185000
8	-4.152096000	-1.805148000	-0.641918000	8	-5.494325000	-1.994900000	0.141862000
8	-5.332175000	0.131551000	-0.198204000	8	-5.783311000	0.290273000	-0.022301000
pn29...2CO₂				pn30...2CO₂			
6	-2.399924000	0.190975000	-0.006668000	6	-3.890074000	-2.148260000	-0.303084000
6	-1.735881000	-1.048386000	0.001576000	6	-2.531505000	-2.287099000	-0.311453000
6	-0.283742000	-1.062719000	0.001094000	6	-1.705907000	-1.165314000	-0.058820000
6	0.370935000	0.188197000	-0.007155000	6	-2.357123000	0.050046000	0.189641000
7	-0.298359000	1.406097000	-0.014359000	7	-3.696510000	0.196059000	0.199785000
6	-1.581923000	1.399011000	-0.014556000	6	-4.422229000	-0.863936000	-0.037009000
8	-2.276971000	2.543185000	-0.021978000	8	-5.758003000	-0.739620000	-0.030736000
6	0.496027000	-2.219782000	0.007811000	6	-0.260619000	-1.206438000	-0.037344000
6	1.875910000	-2.084122000	0.005894000	6	0.399085000	-0.002191000	0.233659000
7	2.504366000	-0.907224000	-0.002259000	7	-0.240524000	1.188419000	0.456471000
6	1.769576000	0.195024000	-0.008573000	6	-1.529462000	1.218083000	0.440217000
8	2.633505000	-3.194699000	0.012369000	8	-2.167928000	2.369569000	0.655105000

6	-3.789521000	0.241995000	-0.006932000	6	0.516760000	-2.364563000	-0.264997000
6	-4.466240000	-0.969696000	0.001302000	6	1.881551000	-2.260426000	-0.204618000
7	-3.863968000	-2.159553000	0.009293000	7	2.531319000	-1.108175000	0.072076000
6	-2.541997000	-2.194240000	0.009347000	6	1.822390000	-0.027538000	0.286271000
8	-5.809005000	-0.964741000	0.001340000	8	2.452209000	1.115588000	0.579839000
1	-1.655900000	3.286081000	-0.026902000	1	-4.563363000	-2.973908000	-0.489857000
1	0.071391000	-3.213919000	0.014132000	1	-2.090934000	-3.255740000	-0.510860000
1	2.298402000	1.142281000	-0.015052000	1	-5.959509000	0.185003000	0.163804000
1	3.562778000	-2.926369000	0.009335000	1	-1.494981000	3.051009000	0.803095000
1	-4.325581000	1.180221000	-0.013289000	1	0.061592000	-3.320604000	-0.483815000
1	-2.097265000	-3.183487000	0.015935000	1	2.517929000	-3.121494000	-0.376711000
1	-6.099930000	-1.885073000	0.007739000	1	3.404452000	0.941890000	0.561020000
6	5.205131000	-0.631786000	-0.010917000	6	0.843489000	3.450760000	-0.753758000
8	5.132094000	0.517797000	-0.019106000	8	1.375860000	2.857309000	-1.585532000
8	5.344514000	-1.783210000	-0.002963000	8	0.303018000	4.094588000	0.044489000
6	1.002801000	3.993420000	0.021121000	6	5.234806000	-1.155884000	0.128518000
8	2.074218000	3.573862000	0.035607000	8	5.265585000	-2.278578000	-0.129189000
8	-0.057739000	4.462517000	0.007144000	8	5.273989000	-0.026819000	0.389981000
pn31...2CO₂				pn32...2CO₂			
6	-2.332014000	2.784583000	0.001604000	6	2.513307000	0.357889000	0.222838000
6	-0.992449000	2.515610000	0.001838000	6	1.955670000	-0.911467000	0.002036000
6	-0.544787000	1.174478000	-0.000683000	6	0.511430000	-1.060237000	0.008867000
6	-1.531610000	0.183878000	-0.003249000	6	-0.229888000	0.110694000	0.240163000
7	-2.854075000	0.436191000	-0.003354000	7	0.321091000	1.352387000	0.432183000
6	-3.231842000	1.691461000	-0.001127000	6	1.600419000	1.463358000	0.428480000
8	-4.538658000	1.971492000	-0.001350000	8	2.166235000	2.664023000	0.617575000
6	0.846459000	0.770366000	-0.000763000	6	-0.204673000	-2.265278000	-0.188921000
6	1.112876000	-0.615828000	-0.003360000	6	-1.574891000	-2.231622000	-0.138394000
7	0.128655000	-1.583303000	-0.005889000	7	-2.295015000	-1.115442000	0.101542000
6	-1.098268000	-1.206694000	-0.005890000	6	-1.648088000	0.007677000	0.287653000
8	-2.081483000	-2.116921000	-0.008344000	8	-2.342853000	1.122983000	0.546954000
6	1.929492000	1.654546000	0.001516000	6	3.905284000	0.546716000	0.234170000
6	3.209376000	1.126699000	0.001245000	6	4.699635000	-0.551561000	0.021792000
7	3.471974000	-0.184393000	-0.001219000	7	4.203250000	-1.783383000	-0.195118000
6	2.452425000	-1.025840000	-0.003499000	6	2.905026000	-1.953602000	-0.204835000
8	4.258476000	1.969091000	0.003610000	8	2.464862000	-3.204835000	-0.426711000
1	-2.725754000	3.791987000	0.003344000	1	1.455380000	3.311391000	0.740934000
1	-0.279115000	3.330438000	0.003902000	1	0.306560000	-3.194295000	-0.376132000
1	-5.026092000	1.133959000	-0.004405000	1	-2.156943000	-3.134100000	-0.289597000
1	-1.665638000	-2.988630000	-0.009262000	1	-3.283332000	0.894303000	0.528015000
1	1.809564000	2.729083000	0.003411000	1	4.322119000	1.528774000	0.405496000
1	2.679245000	-2.087690000	-0.005578000	1	5.780721000	-0.472963000	0.018777000
1	5.069226000	1.441779000	0.002035000	1	3.251549000	-3.754626000	-0.540291000
6	5.973757000	-1.232288000	0.002438000	6	-0.899867000	3.557171000	-0.781887000
8	5.569060000	-2.311007000	0.000018000	8	-1.415307000	2.944868000	-1.609698000
8	6.443345000	-0.171916000	0.004898000	8	-0.376888000	4.220898000	0.012667000
6	-5.301624000	-1.800026000	0.006704000	6	-4.994907000	-1.308199000	0.145377000
8	-4.911247000	-2.881954000	0.015118000	8	-5.095006000	-0.175618000	0.374084000
8	-5.744250000	-0.728292000	-0.001557000	8	-4.965053000	-2.437651000	-0.080058000
pn33...2CO₂				pn34...2CO₂			
6	-2.353182000	0.139359000	-0.196063000	6	-2.458761000	-0.215405000	0.000002000
6	-1.733482000	-1.100692000	0.049864000	6	-1.654821000	-1.368064000	-0.000039000
6	-0.285832000	-1.181082000	0.037488000	6	-0.210978000	-1.196822000	-0.000014000
6	0.406861000	0.006984000	-0.221024000	6	0.285673000	0.120425000	0.000021000
7	-0.202880000	1.222218000	-0.438605000	7	-0.518834000	1.241767000	0.000026000
6	-1.485343000	1.280818000	-0.431939000	6	-1.800947000	1.082265000	0.000006000

8	-2.105280000	2.448767000	-0.644384000	8	-2.589960000	2.156341000	0.000021000
6	0.459404000	-2.358767000	0.259581000	6	0.698731000	-2.257978000	-0.000016000
6	1.828311000	-2.288499000	0.205656000	6	2.050883000	-1.964148000	0.000020000
7	2.507975000	-1.153718000	-0.060511000	7	2.534108000	-0.718093000	0.000052000
6	1.826237000	-0.052674000	-0.270082000	6	1.679761000	0.290057000	0.000052000
8	2.487411000	1.074798000	-0.555130000	8	2.937516000	-2.975869000	0.000057000
6	-3.741048000	0.245687000	-0.199147000	6	-3.868898000	-0.412214000	0.000017000
6	-4.462386000	-0.911818000	0.048297000	7	-4.434476000	-1.599557000	-0.000041000
7	-3.903981000	-2.101409000	0.285828000	6	-3.646204000	-2.685196000	-0.000108000
6	-2.586125000	-2.190067000	0.285874000	6	-2.273738000	-2.629721000	-0.000098000
8	-5.804033000	-0.856399000	0.054891000	8	-4.689864000	0.640652000	0.000157000
1	-1.426865000	3.127251000	-0.782689000	1	-2.025006000	2.942645000	-0.000003000
1	-0.020846000	-3.304359000	0.469252000	1	0.391504000	-3.294028000	-0.000032000
1	2.440832000	-3.167443000	0.374429000	1	2.094603000	1.292321000	0.000070000
1	3.434671000	0.875610000	-0.535065000	1	3.827850000	-2.598147000	0.000037000
1	-4.239621000	1.186430000	-0.384830000	1	-4.162551000	-3.639058000	-0.000175000
1	-2.180521000	-3.176532000	0.482638000	1	-1.696636000	-3.542706000	-0.000140000
1	-6.128108000	-1.746105000	0.241905000	1	-5.587016000	0.281279000	0.000134000
6	5.210505000	-1.270792000	-0.125196000	6	5.188729000	-0.125481000	-0.000007000
8	5.276997000	-0.140982000	-0.377968000	8	5.460738000	-1.252998000	0.000113000
8	5.212971000	-2.395792000	0.123736000	8	4.980824000	1.007452000	-0.000143000
6	0.924198000	3.503373000	0.722983000	6	0.513955000	3.966313000	-0.000037000
8	1.482080000	2.927577000	1.549471000	8	-0.588635000	4.323953000	-0.000004000
8	0.357849000	4.130098000	-0.071914000	8	1.623298000	3.658556000	-0.000069000
pn35...2CO₂				pn36...2CO₂			
6	-2.417904000	-0.202534000	0.149619000	6	1.416271000	1.823084000	-0.209254000
6	-1.677430000	-1.376302000	-0.088707000	6	0.697507000	0.631381000	-0.039310000
6	-0.229707000	-1.301231000	-0.049663000	6	-0.743121000	0.711954000	0.069313000
6	0.331413000	-0.052167000	0.226885000	6	-1.312283000	1.985423000	0.277595000
7	-0.393968000	1.085680000	0.436704000	7	-0.571618000	3.147342000	0.223561000
6	-1.684942000	1.020059000	0.402679000	6	0.674778000	3.061241000	-0.077023000
8	-2.378072000	2.141286000	0.604886000	8	1.390338000	4.183793000	-0.229531000
6	0.633558000	-2.399292000	-0.266305000	6	-1.675627000	-0.344600000	-0.136616000
6	1.985389000	-2.194885000	-0.190810000	7	-2.965443000	-0.232207000	0.097013000
7	2.542803000	-0.995174000	0.092082000	6	-3.459337000	0.965754000	0.463361000
6	1.755291000	0.029013000	0.296296000	6	-2.694457000	2.100926000	0.519272000
8	2.291387000	1.217311000	0.595239000	8	-1.246682000	-1.486526000	-0.679455000
6	-3.837736000	-0.311581000	0.116876000	6	2.806136000	1.816830000	-0.419009000
7	-4.472582000	-1.434980000	-0.126530000	6	3.440754000	0.601130000	-0.404842000
6	-3.746638000	-2.542523000	-0.355249000	7	2.805830000	-0.543123000	-0.090182000
6	-2.374525000	-2.571470000	-0.347634000	6	1.511286000	-0.531225000	0.137055000
8	-4.586529000	0.769913000	0.343625000	8	0.961657000	-1.635388000	0.640458000
1	-1.734177000	2.849960000	0.757790000	1	0.789436000	4.926679000	-0.085673000
1	0.252232000	-3.385740000	-0.488846000	1	-4.524464000	0.988513000	0.667384000
1	2.687147000	-3.005047000	-0.353989000	1	-3.116846000	3.074481000	0.724716000
1	3.254557000	1.118200000	0.589814000	1	-2.004311000	-2.085422000	-0.747819000
1	-4.318346000	-3.443074000	-0.551570000	1	3.342269000	2.741190000	-0.577945000
1	-1.853934000	-3.498672000	-0.536630000	1	4.503364000	0.508296000	-0.599876000
1	-5.506603000	0.482055000	0.275383000	1	1.652508000	-2.310711000	0.705908000
6	0.571745000	3.383823000	-0.806803000	6	-4.757608000	-2.220432000	-0.252566000
8	1.128512000	2.804072000	-1.632663000	8	-3.935417000	-2.935059000	-0.650125000
8	0.004543000	4.012217000	-0.015216000	8	-5.622232000	-1.562450000	0.131332000
6	5.246380000	-0.829351000	0.171240000	6	4.382546000	-2.733268000	0.224355000
8	5.368528000	-1.945711000	-0.086370000	8	5.314498000	-2.163974000	-0.143431000
8	5.191128000	0.298949000	0.433215000	8	3.482287000	-3.357431000	0.604074000

V. Monocarboxylic acid- CO₂ complex

nt1'–COOH...CO ₂				nt2'–COOH...CO ₂			
6	-1.401202000	2.874296000	0.053020000	6	1.411750000	2.598035000	-0.000073000
6	-0.050644000	3.074929000	-0.047976000	6	0.061110000	2.395406000	-0.000253000
6	0.835001000	1.981771000	-0.035669000	6	-0.432336000	1.076031000	-0.000147000
6	0.273699000	0.701716000	0.093648000	6	0.479298000	0.012488000	0.000172000
7	-1.039158000	0.493306000	0.121189000	7	1.815349000	0.210703000	0.000285000
6	-1.843272000	1.539311000	0.123154000	6	2.248487000	1.456619000	0.000174000
8	-3.157497000	1.320950000	0.179783000	8	3.562334000	1.677948000	0.000324000
6	2.249467000	2.116572000	-0.208390000	6	-1.865647000	0.847955000	-0.000252000
6	3.035719000	1.029655000	-0.302570000	7	-2.277488000	-0.484917000	0.000139000
6	2.488898000	-0.306411000	-0.174310000	6	-1.360898000	-1.530737000	0.000419000
7	1.122986000	-0.419269000	0.145102000	6	-0.033039000	-1.330044000	0.000435000
8	3.194054000	-1.305377000	-0.304785000	8	-2.683859000	1.771982000	-0.000108000
1	-2.121887000	3.679449000	0.060981000	1	1.862495000	3.580546000	-0.000166000
1	0.354463000	4.076848000	-0.138851000	1	-0.642495000	3.219056000	-0.000467000
1	-3.311626000	0.368439000	0.277367000	1	4.026304000	0.828003000	0.000955000
1	2.669680000	3.113104000	-0.295390000	1	-1.819732000	-2.508307000	0.000643000
1	4.101999000	1.076673000	-0.473529000	1	0.650389000	-2.166046000	0.000696000
6	0.610463000	-1.687749000	0.706408000	6	-3.694044000	-0.872959000	0.000242000
8	-0.339533000	-1.698383000	1.421601000	8	-3.983747000	-2.028686000	0.000552000
8	1.300168000	-2.739359000	0.355176000	8	-4.529306000	0.127309000	-0.000654000
1	2.163246000	-2.446588000	-0.056504000	1	-4.014865000	0.990300000	-0.001188000
6	-2.241307000	-1.946665000	-0.700161000	6	3.774973000	-1.914386000	-0.000349000
8	-3.187688000	-1.634825000	-0.108656000	8	4.589063000	-1.089490000	0.000326000
8	-1.332454000	-2.274350000	-1.328249000	8	2.999884000	-2.765877000	-0.001146000
nt3'–COOH...CO ₂				nt4'–COOH...CO ₂			
6	0.661001000	2.463535000	-0.276457000	6	1.632558000	2.684402000	-0.001014000
6	-0.599256000	1.930247000	-0.241787000	6	0.285761000	2.634979000	-0.002721000
6	-0.751306000	0.535392000	-0.081404000	6	-0.364791000	1.357141000	-0.000801000
6	0.416478000	-0.232185000	-0.039980000	6	0.445512000	0.166242000	0.002849000
7	1.660257000	0.302454000	-0.059873000	7	1.818447000	0.248122000	0.004200000
6	1.771105000	1.606122000	-0.153869000	6	2.352937000	1.433311000	0.002493000
8	2.986022000	2.169899000	-0.156502000	8	3.676276000	1.554646000	0.003771000
7	-2.011473000	-0.111084000	-0.052978000	6	-1.726606000	1.226154000	-0.002127000
6	-2.112100000	-1.500854000	-0.173310000	7	-2.325776000	0.013766000	-0.000117000
6	-0.882486000	-2.266093000	-0.120874000	6	-1.581456000	-1.193717000	0.003647000
6	0.314992000	-1.668184000	-0.027905000	6	-0.173442000	-1.064852000	0.005142000
8	-3.204653000	-2.063524000	-0.283529000	8	-2.194044000	-2.279144000	0.005483000
1	0.824360000	3.525399000	-0.399845000	1	2.198468000	3.605254000	-0.002234000
1	-1.456489000	2.575980000	-0.334297000	1	-0.315009000	3.537705000	-0.005451000
1	3.655922000	1.477603000	-0.074442000	1	4.074605000	0.670289000	0.005711000
1	-1.009895000	-3.339563000	-0.150652000	1	-2.405287000	2.069862000	-0.004780000
1	1.234657000	-2.237389000	0.025250000	1	0.403428000	-1.978424000	0.008077000
6	-3.214174000	0.673940000	0.271650000	6	-3.818115000	0.017014000	-0.001868000
8	-3.113397000	1.768083000	0.735093000	8	-4.381389000	1.067693000	-0.005017000
8	-4.339111000	0.070750000	0.012991000	8	-4.330407000	-1.165433000	0.000387000
1	-4.151745000	-0.895343000	-0.212155000	1	-3.551637000	-1.859230000	0.003127000
6	4.125674000	-1.233176000	0.205000000	6	3.561609000	-2.028378000	-0.004646000
8	3.598327000	-2.255915000	0.263631000	8	2.714863000	-2.807166000	-0.009031000
8	4.695579000	-0.226638000	0.149529000	8	4.447567000	-1.279654000	-0.000439000
nt5'–COOH...CO ₂				nt6'–COOH...CO ₂			
6	0.127831000	0.613058000	-0.000373000	6	0.989170000	2.129112000	0.000027000
6	-0.399520000	-0.674716000	-0.000279000	6	-0.236853000	1.472007000	0.000032000
6	0.449565000	-1.793403000	-0.000468000	6	-0.238387000	0.062007000	-0.000046000
6	1.803720000	-1.563365000	-0.000717000	6	0.985739000	-0.611052000	-0.000115000
7	2.343615000	-0.325119000	-0.000808000	7	2.150686000	0.015154000	-0.000129000

6	1.545107000	0.713166000	-0.000636000	6	2.144633000	1.355081000	-0.000054000
8	2.069240000	1.945435000	-0.000776000	8	3.327257000	1.972237000	-0.000070000
6	-0.741909000	1.753163000	-0.000158000	6	-1.507542000	2.149803000	0.000106000
6	-2.069596000	1.558269000	0.000087000	6	-2.641847000	1.433799000	0.000108000
7	-2.631199000	0.279450000	0.000144000	7	-2.656627000	0.039980000	0.000027000
6	-1.853486000	-0.872448000	0.000021000	6	-1.474199000	-0.705334000	-0.000068000
8	-2.354876000	-1.996231000	-0.000002000	8	-1.494201000	-1.935607000	-0.000159000
1	0.034801000	-2.791636000	-0.000432000	1	1.063056000	3.208337000	0.000100000
1	2.516410000	-2.380235000	-0.000908000	1	1.005690000	-1.696218000	-0.000175000
1	3.035035000	1.869681000	-0.000658000	1	4.027263000	1.302316000	-0.000063000
1	-0.333004000	2.752670000	-0.000201000	1	-1.554097000	3.229878000	0.000172000
1	-2.800472000	2.352361000	0.000255000	1	-3.628371000	1.873632000	0.000186000
6	-4.102143000	0.232934000	0.000368000	6	-3.984241000	-0.582682000	0.000079000
8	-4.717843000	1.252016000	0.000654000	8	-4.955166000	0.108143000	-0.000050000
8	-4.608977000	-0.968122000	0.000280000	8	-3.975048000	-1.886885000	0.000008000
1	-3.870435000	-1.644448000	0.000051000	1	-3.029474000	-2.215024000	0.000221000
6	5.060082000	-0.073752000	0.000841000	6	4.445748000	-1.463543000	0.000093000
8	5.215693000	-1.214657000	0.001024000	8	3.863782000	-2.456971000	0.000222000
8	4.960869000	1.082041000	0.000624000	8	5.078899000	-0.491425000	-0.000038000
nt7'-COOH...CO₂				nt8'-COOH...CO₂			
6	2.920985000	1.727061000	-0.266828000	6	2.194007000	-2.515152000	-0.000420000
6	1.831428000	2.436643000	0.061586000	6	0.894780000	-2.867600000	-0.004932000
6	0.539631000	1.792963000	0.170302000	6	-0.115170000	-1.837083000	-0.002763000
6	0.484495000	0.410679000	0.026448000	6	0.347753000	-0.481871000	0.003986000
7	1.662292000	-0.346086000	-0.084697000	7	1.689552000	-0.142324000	0.008429000
6	2.880876000	0.270221000	-0.387525000	6	2.542239000	-1.108619000	0.006481000
8	3.876111000	-0.385752000	-0.667399000	8	3.856210000	-0.861753000	0.010695000
6	-0.655861000	2.515684000	0.327532000	6	-1.464174000	-2.105921000	-0.006802000
6	-1.843222000	1.824853000	0.290449000	6	-2.431344000	-1.069557000	-0.004599000
7	-1.907644000	0.509584000	0.025439000	7	-1.921134000	0.242991000	0.002208000
6	-0.795818000	-0.172588000	-0.143414000	6	-0.591058000	0.517850000	0.006155000
8	-0.870196000	-1.436099000	-0.560536000	8	-3.665095000	-1.258798000	-0.007605000
1	3.895783000	2.171991000	-0.415897000	1	2.999372000	-3.237971000	-0.001700000
1	1.886798000	3.511411000	0.195848000	1	0.589913000	-3.907583000	-0.010097000
1	-0.633836000	3.589522000	0.460078000	1	3.996304000	0.096836000	0.015483000
1	-2.796035000	2.322751000	0.431320000	1	-1.845923000	-3.118459000	-0.011805000
1	-1.802074000	-1.697353000	-0.595584000	1	-0.326254000	1.566337000	0.010753000
6	1.678542000	-1.680417000	0.529557000	6	-2.831270000	1.431924000	0.005434000
8	0.889076000	-1.956497000	1.371656000	8	-2.344014000	2.517664000	0.010625000
8	2.630586000	-2.465699000	0.083415000	8	-4.082304000	1.115983000	0.002227000
1	3.285036000	-1.934559000	-0.429486000	1	-4.161748000	0.079383000	-0.002328000
6	-4.371213000	-0.620987000	-0.209938000	6	2.671480000	2.528658000	-0.009841000
8	-4.896981000	0.361972000	0.081457000	8	3.746170000	2.092811000	-0.006158000
8	-3.895755000	-1.634541000	-0.511153000	8	1.622277000	3.001721000	-0.013655000
nt9'-COOH...CO₂				nt10'-COOH...CO₂			
6	-0.134933000	0.211780000	-0.000176000	6	-0.500081000	1.508847000	0.000035000
6	-0.211987000	1.616021000	-0.000073000	6	0.398867000	0.451623000	0.000019000
6	-1.505769000	2.239661000	0.000032000	6	-0.058271000	-0.875231000	-0.000038000
6	-2.612055000	1.481447000	0.000049000	6	-1.445748000	-1.062184000	-0.000059000
7	-2.560663000	0.095907000	-0.000075000	7	-2.312964000	-0.062008000	-0.000070000
6	-1.343610000	-0.607804000	-0.000216000	6	-1.854577000	1.191875000	-0.000026000
8	-1.339942000	-1.834234000	-0.000169000	8	-2.752074000	2.185434000	-0.000091000
6	1.162512000	-0.370366000	-0.000207000	6	1.843496000	0.742071000	0.000093000
7	2.269842000	0.350916000	-0.000210000	7	2.690398000	-0.357382000	-0.000007000
6	2.172039000	1.688661000	-0.000128000	6	2.207742000	-1.674279000	-0.000078000
6	0.975267000	2.365508000	-0.000032000	6	0.897746000	-1.950886000	-0.000077000

8	1.296752000	-1.690339000	-0.000280000	8	2.268019000	1.894945000	0.000035000
1	-1.589796000	3.317254000	0.000108000	1	-0.163110000	2.536266000	0.000093000
1	-3.615898000	1.880258000	0.000138000	1	-1.865685000	-2.064394000	-0.000103000
1	3.117537000	2.221794000	-0.000075000	1	-3.640152000	1.800679000	0.000147000
1	0.944474000	3.446809000	0.000064000	1	2.988102000	-2.419313000	-0.000131000
1	2.245598000	-1.888969000	-0.000389000	1	0.565995000	-2.980288000	-0.000131000
6	-3.864534000	-0.583970000	-0.000022000	6	4.152453000	-0.221836000	-0.000059000
8	-4.861562000	0.069655000	0.000848000	8	4.830654000	-1.200826000	-0.000133000
8	-3.801237000	-1.884160000	-0.000275000	8	4.589768000	1.007780000	0.000203000
1	-2.835459000	-2.165257000	-0.000929000	1	3.817472000	1.640586000	0.000344000
6	4.781653000	-0.692924000	0.000232000	6	-4.965990000	-0.695203000	0.000154000
8	5.256598000	0.356990000	-0.000167000	8	-5.250334000	0.428531000	-0.000300000
8	4.356616000	-1.771380000	0.000832000	8	-4.735842000	-1.824187000	0.000353000
nt11'–COOH...CO₂				nt12'–COOH...CO₂			
6	0.981857000	-2.024289000	-0.000127000	6	0.689537000	1.754333000	-0.000269000
6	-0.231026000	-1.289119000	-0.000079000	6	-0.334253000	0.760872000	-0.000149000
6	-0.115702000	0.143256000	0.000014000	6	0.029684000	-0.620629000	-0.000108000
6	1.184420000	0.730873000	0.000028000	6	1.441174000	-0.906673000	-0.000165000
7	2.276764000	0.032698000	0.000063000	7	2.350341000	0.014642000	-0.000329000
6	2.164518000	-1.336927000	-0.000038000	6	1.983842000	1.337061000	-0.000448000
8	3.320923000	-2.001085000	-0.000152000	8	2.993202000	2.222945000	-0.000852000
6	-1.498337000	-1.850854000	-0.000150000	6	-1.681105000	1.058657000	0.000007000
6	-2.663250000	-1.062004000	0.000046000	7	-2.619505000	0.087374000	0.000053000
7	-2.475039000	0.354432000	0.000073000	6	-2.310025000	-1.289260000	0.000047000
6	-1.253984000	0.912608000	-0.000053000	6	-0.933822000	-1.607979000	0.000015000
8	-3.831036000	-1.501879000	-0.000116000	8	-3.236996000	-2.130438000	0.000129000
1	0.987071000	-3.105587000	-0.000197000	1	0.451661000	2.809644000	-0.000304000
1	1.286944000	1.814584000	0.000055000	1	1.778882000	-1.940637000	-0.000132000
1	4.048468000	-1.362334000	-0.000213000	1	3.830895000	1.740354000	-0.000205000
1	-1.646342000	-2.922103000	-0.000328000	1	-2.070084000	2.068611000	0.000156000
1	-1.242668000	1.996466000	-0.000299000	1	-0.678400000	-2.659684000	0.000106000
6	-3.637253000	1.303619000	-0.000226000	6	-4.052495000	0.560159000	0.000303000
8	-3.404097000	2.471954000	-0.001440000	8	-4.250968000	1.733700000	0.001009000
8	-4.775500000	0.706323000	0.001472000	8	-4.898479000	-0.406350000	-0.000642000
1	-4.603084000	-0.329553000	0.000925000	1	-4.365632000	-1.316113000	-0.000307000
6	4.641466000	1.385674000	0.000244000	6	4.941101000	-0.862633000	0.000473000
8	5.232507000	0.388579000	-0.000238000	8	4.596923000	-1.962553000	-0.000447000
8	4.097364000	2.401308000	0.000619000	8	5.333192000	0.227728000	0.001351000
pn1'–COOH...CO₂				pn2'–COOH...CO₂			
6	4.305392000	-1.072630000	0.052498000	6	-2.202427000	-0.561645000	-0.000062000
6	3.125207000	-1.751647000	0.121979000	6	-1.011263000	-1.289843000	-0.000033000
6	1.914583000	-1.021853000	0.095569000	6	0.232540000	-0.542473000	-0.000059000
6	1.966631000	0.378208000	0.001349000	6	0.182846000	0.894930000	-0.000094000
7	3.141244000	1.046959000	-0.075316000	7	-1.019960000	1.578513000	-0.000169000
6	4.243654000	0.342119000	-0.048571000	6	-2.113085000	0.886501000	-0.000157000
8	5.411905000	0.991467000	-0.120713000	8	-3.287383000	1.511958000	-0.000210000
6	0.622406000	-1.623256000	0.127504000	6	1.446440000	-1.161649000	-0.000018000
7	-0.499379000	-0.958481000	0.107614000	7	2.607121000	-0.458894000	-0.000005000
6	-0.446949000	0.387345000	0.101557000	6	2.624537000	0.956464000	0.000021000
6	0.737280000	1.111258000	-0.000996000	6	1.361099000	1.601329000	-0.000056000
8	0.581268000	-2.954678000	0.163273000	8	3.716299000	1.552746000	0.000075000
7	-1.668714000	1.075272000	0.144136000	6	-3.421767000	-1.263412000	-0.000033000
6	-1.739459000	2.451127000	-0.154580000	6	-3.399671000	-2.633188000	0.000037000
6	-0.490602000	3.168698000	-0.253914000	6	-2.137443000	-3.265201000	0.000106000
6	0.691068000	2.528874000	-0.154014000	7	-0.983878000	-2.631302000	0.000048000
8	-2.828300000	3.010802000	-0.291344000	8	-2.117509000	-4.601827000	0.000090000

1	5.270423000	-1.559403000	0.068271000	1	-3.133556000	2.469874000	-0.000367000
1	3.094174000	-2.831607000	0.196150000	1	1.550352000	-2.238121000	0.000000000
1	5.218988000	1.935700000	-0.182894000	1	1.364058000	2.681646000	-0.000034000
1	-0.344965000	-3.234989000	0.240384000	1	-4.355363000	-0.714950000	-0.000074000
1	-0.579152000	4.234285000	-0.412187000	1	-4.296172000	-3.237031000	0.000044000
1	1.630904000	3.062814000	-0.221797000	1	-1.193444000	-4.883771000	0.000086000
6	-2.866380000	0.392269000	0.683695000	6	3.859850000	-1.260932000	0.000017000
8	-2.759063000	-0.553086000	1.398073000	8	3.777211000	-2.449731000	0.000011000
8	-3.992610000	0.936644000	0.314925000	8	4.932381000	-0.540235000	0.000030000
1	-3.805218000	1.841980000	-0.077913000	1	4.656732000	0.456712000	0.000079000
6	-2.767991000	-2.475136000	-0.713369000	6	-1.244268000	4.441883000	0.000144000
8	-2.320276000	-3.368549000	-0.125186000	8	-2.395022000	4.292819000	0.000559000
8	-3.226205000	-1.623510000	-1.338692000	8	-0.110966000	4.638126000	-0.000271000
pn3'–COOH...CO₂				pn4'–COOH...CO₂			
6	-2.088980000	-1.308301000	0.121203000	6	-3.335475000	0.819879000	0.309338000
6	-0.874341000	-0.643609000	-0.123099000	6	-2.029250000	0.384061000	0.053630000
6	-0.867132000	0.783978000	0.011804000	6	-1.851709000	-0.983713000	-0.252840000
6	-2.078808000	1.428608000	0.167875000	6	-2.970464000	-1.831955000	-0.282713000
7	-3.258002000	0.777459000	0.392325000	7	-4.193471000	-1.413668000	-0.037320000
6	-3.241074000	-0.518386000	0.411375000	6	-4.355364000	-0.112330000	0.250558000
8	-4.379048000	-1.183145000	0.674266000	8	-5.609977000	0.290619000	0.497124000
7	0.306181000	1.528972000	-0.171578000	6	-0.861613000	1.223924000	0.087552000
6	0.261875000	2.883075000	-0.525900000	6	0.368434000	0.621903000	-0.168357000
6	-1.027156000	3.540756000	-0.380378000	7	0.525079000	-0.669057000	-0.515775000
6	-2.122085000	2.859614000	0.001755000	6	-0.525993000	-1.433465000	-0.544421000
8	1.277022000	3.480016000	-0.876282000	8	-0.372741000	-2.711024000	-0.875919000
6	-2.118239000	-2.718487000	-0.007516000	6	-0.904843000	2.631749000	0.312261000
6	-0.983370000	-3.372759000	-0.380675000	6	0.207168000	3.390696000	0.221117000
6	0.176775000	-2.592836000	-0.648526000	6	1.489362000	2.799612000	-0.070405000
7	0.230625000	-1.290777000	-0.543452000	7	1.535480000	1.394082000	-0.133066000
8	1.270728000	-3.246533000	-1.036626000	8	2.509025000	3.470415000	-0.235824000
1	-5.070515000	-0.524869000	0.818514000	1	-3.580737000	1.842930000	0.555221000
1	-1.028890000	4.605310000	-0.571233000	1	-2.841416000	-2.883251000	-0.517157000
1	-3.079658000	3.348090000	0.139870000	1	-6.181811000	-0.483026000	0.414242000
1	-3.041248000	-3.249414000	0.189191000	1	0.579602000	-2.884120000	-0.961767000
1	-0.931743000	-4.447252000	-0.490224000	1	-1.854702000	3.105853000	0.528157000
1	2.003517000	-2.611479000	-1.069866000	1	0.203206000	4.464539000	0.343261000
6	1.557784000	0.994067000	0.352941000	6	2.846301000	0.716127000	-0.043660000
8	1.564168000	0.217577000	1.255329000	8	2.949676000	-0.350642000	0.470537000
8	2.633516000	1.469353000	-0.233524000	8	3.828961000	1.409791000	-0.553702000
1	2.391778000	2.295815000	-0.730954000	1	3.541265000	2.368633000	-0.619505000
6	4.045417000	-0.917247000	0.538176000	6	3.189262000	-3.020909000	0.520993000
8	3.515556000	-1.466494000	-0.335240000	8	2.470951000	-3.160297000	-0.379408000
8	4.613198000	-0.400350000	1.394506000	8	3.907865000	-2.941928000	1.414987000
pn5'–COOH...CO₂				pn6'–COOH...CO₂			
6	-0.686822000	-0.595841000	-0.008742000	6	2.270972000	0.663683000	0.000503000
6	-0.482560000	0.818921000	-0.001328000	6	1.807656000	-0.650890000	0.000182000
6	0.898947000	1.279193000	-0.004153000	6	0.362279000	-0.870074000	0.000255000
6	1.915485000	0.317982000	-0.013179000	6	-0.471779000	0.294695000	0.000594000
7	1.689520000	-1.058223000	-0.019349000	7	0.024352000	1.595509000	0.001066000
6	0.472393000	-1.470676000	-0.017670000	6	1.298243000	1.748374000	0.001037000
8	0.189930000	-2.776075000	-0.023975000	8	1.839590000	2.972559000	0.001552000
7	1.135567000	2.605562000	0.001707000	6	-0.191869000	-2.120378000	-0.000044000
6	2.380675000	3.009194000	-0.001322000	6	-1.602497000	-2.310242000	-0.000073000
6	3.489042000	2.136223000	-0.010312000	7	-2.377181000	-1.138399000	0.000202000
6	3.245123000	0.788706000	-0.016209000	6	-1.825476000	0.109021000	0.000573000

8	2.629046000	4.330915000	0.004428000	8	-2.154027000	-3.427132000	-0.000349000
6	-1.961350000	-1.084857000	-0.007264000	6	3.661779000	0.882561000	0.000218000
7	-3.031277000	-0.252135000	0.001167000	6	4.504155000	-0.197400000	-0.000290000
6	-2.893157000	1.158195000	0.008954000	6	3.922995000	-1.483801000	-0.000462000
6	-1.561682000	1.659843000	0.007340000	7	2.628663000	-1.712755000	-0.000274000
8	-3.908577000	1.871758000	0.016539000	8	4.751221000	-2.534929000	-0.000869000
1	1.018474000	-3.277861000	-0.031740000	1	1.127106000	3.629425000	0.000278000
1	4.489536000	2.547151000	-0.012274000	1	0.424353000	-3.008267000	-0.000275000
1	4.053189000	0.068166000	-0.022843000	1	-2.527501000	0.930838000	0.000888000
1	1.778699000	4.787140000	0.010442000	1	4.043255000	1.895746000	0.000381000
1	-2.192087000	-2.141812000	-0.012675000	1	5.581214000	-0.101849000	-0.000563000
1	-1.439646000	2.733484000	0.013008000	1	4.211630000	-3.335985000	-0.000989000
6	-4.371461000	-0.911536000	0.001876000	6	-3.867136000	-1.188506000	0.000108000
8	-4.419039000	-2.100462000	-0.004427000	8	-4.472918000	-0.163595000	0.000425000
8	-5.356008000	-0.075189000	0.009366000	8	-4.341563000	-2.391275000	-0.000266000
1	-4.975866000	0.882469000	0.013956000	1	-3.551770000	-3.057204000	-0.000375000
6	3.760302000	-3.043647000	0.023053000	6	-1.604735000	3.935120000	-0.001156000
8	4.625659000	-2.284249000	0.034576000	8	-2.595769000	3.350801000	-0.000511000
8	2.924167000	-3.846119000	0.012392000	8	-0.629864000	4.564050000	-0.001857000
pn7'-COOH...CO₂				pn8'-COOH...CO₂			
6	-1.150465000	1.102002000	0.003867000	6	-1.990177000	-1.105913000	0.078059000
6	-0.241729000	0.011480000	0.003326000	6	-2.073732000	0.292746000	-0.008432000
6	1.167249000	0.344563000	0.001199000	6	-0.863538000	1.073337000	-0.017485000
6	1.532586000	1.693972000	-0.000230000	6	0.337158000	0.370837000	0.085897000
7	0.639748000	2.726911000	0.000348000	7	0.420928000	-0.975824000	0.072963000
6	-0.623503000	2.432110000	0.002280000	6	-0.671748000	-1.673699000	0.092335000
8	-1.508769000	3.430144000	0.002811000	8	-0.597488000	-3.002172000	0.107442000
6	2.191817000	-0.679059000	0.000396000	6	-3.145845000	-1.911365000	0.115943000
7	3.524301000	-0.245296000	-0.001941000	6	-4.359444000	-1.283578000	0.066211000
6	3.855624000	1.094502000	-0.003282000	7	-4.482040000	0.059570000	-0.017523000
6	2.915837000	2.055107000	-0.002474000	6	-3.411200000	0.801103000	-0.053455000
8	1.945300000	-1.892600000	0.001387000	8	-3.599493000	2.133882000	-0.130124000
6	-2.528570000	0.853485000	0.005926000	6	-0.798018000	2.497745000	-0.180973000
7	-3.036231000	-0.362622000	0.007289000	6	0.387169000	3.132528000	-0.281393000
6	-2.176887000	-1.393826000	0.006708000	6	1.637224000	2.428763000	-0.160073000
6	-0.793278000	-1.273955000	0.004940000	7	1.558016000	1.059255000	0.145648000
8	-2.706260000	-2.620058000	0.007624000	8	2.727471000	2.991232000	-0.280569000
1	-1.011098000	4.258975000	0.001559000	1	0.335105000	-3.262258000	0.179160000
1	4.918343000	1.286874000	-0.005013000	1	-3.058368000	-2.986393000	0.181615000
1	3.184879000	3.100963000	-0.003554000	1	-5.288702000	-1.839781000	0.091976000
1	-3.231154000	1.680507000	0.006377000	1	-4.555842000	2.274082000	-0.139505000
1	-0.185257000	-2.162504000	0.004817000	1	-1.715365000	3.059791000	-0.259480000
1	-3.671212000	-2.540928000	0.009838000	1	0.466771000	4.197697000	-0.447892000
6	4.665513000	-1.181520000	-0.003094000	6	2.743092000	0.381856000	0.723041000
8	5.772944000	-0.742046000	-0.005108000	8	2.618722000	-0.562035000	1.436985000
8	4.334713000	-2.438455000	-0.001875000	8	3.875470000	0.932668000	0.387879000
1	3.327489000	-2.509742000	-0.000272000	1	3.694101000	1.834536000	-0.020425000
6	-5.744029000	-0.640200000	-0.009302000	6	2.755567000	-2.451783000	-0.710824000
8	-5.638927000	-1.794839000	-0.008575000	8	2.305189000	-3.358307000	-0.144999000
8	-5.904963000	0.500470000	-0.010662000	8	3.215742000	-1.584537000	-1.312385000
pn9'-COOH...CO₂				pn10'-COOH...CO₂			
6	-1.617097000	1.442692000	-0.008575000	6	2.258060000	-2.642399000	-0.406920000
6	-0.207085000	1.461607000	-0.001848000	6	0.931077000	-2.606618000	-0.198297000
6	0.476173000	0.191157000	-0.005484000	6	0.252794000	-1.341388000	-0.070214000
6	-0.301763000	-0.971856000	-0.015190000	6	0.999681000	-0.185235000	-0.066961000
7	-1.667637000	-0.974546000	-0.020950000	7	2.396514000	-0.241334000	-0.064551000

6	-2.277958000	0.177723000	-0.018243000	6	3.068409000	-1.431304000	-0.381766000
8	-3.609730000	0.210058000	-0.024148000	8	4.280582000	-1.443465000	-0.560007000
6	1.929799000	0.100104000	0.000686000	6	-1.174134000	-1.242396000	-0.004761000
7	2.472715000	-1.197677000	-0.004719000	6	-1.737856000	0.044120000	0.008632000
6	1.678686000	-2.326742000	-0.014410000	7	-0.984635000	1.175550000	-0.142472000
6	0.337936000	-2.252362000	-0.019668000	6	0.307171000	1.068715000	-0.217396000
8	2.686666000	1.071844000	0.008916000	8	1.051811000	2.127486000	-0.535952000
6	-2.324297000	2.665492000	-0.005739000	7	-1.915840000	-2.375543000	0.057353000
6	-1.626742000	3.837402000	0.003466000	6	-3.210328000	-2.246530000	0.160244000
6	-0.213463000	3.743756000	0.009665000	6	-3.890244000	-1.003069000	0.203795000
7	0.468846000	2.626738000	0.007238000	6	-3.147219000	0.138229000	0.122190000
8	0.474547000	4.890412000	0.018718000	8	-3.965755000	-3.357102000	0.231056000
1	-3.946533000	-0.698541000	-0.031858000	1	2.807859000	-3.560745000	-0.564045000
1	2.231003000	-3.254773000	-0.017356000	1	0.331443000	-3.507788000	-0.175054000
1	-0.266347000	-3.146448000	-0.026818000	1	0.486105000	2.911483000	-0.582129000
1	-3.406883000	2.650558000	-0.011021000	1	-4.967931000	-0.994434000	0.293801000
1	-2.099870000	4.809395000	0.006107000	1	-3.605438000	1.119088000	0.140137000
1	1.413390000	4.657913000	0.022082000	1	-3.371123000	-4.116105000	0.195166000
6	3.925457000	-1.445150000	-0.000355000	6	3.124272000	0.798108000	0.681399000
8	4.322420000	-2.569710000	-0.004392000	8	2.569978000	1.413675000	1.531545000
8	4.655736000	-0.370185000	0.008967000	8	4.382238000	0.921447000	0.335599000
1	4.038096000	0.434688000	0.010576000	1	4.653563000	0.137078000	-0.201915000
6	-3.341017000	-3.363202000	0.025604000	6	-2.089229000	3.832820000	-0.227653000
8	-2.468691000	-4.113750000	0.038834000	8	-1.028508000	4.215566000	-0.492651000
8	-4.249960000	-2.643434000	0.012836000	8	-3.160529000	3.497692000	0.031405000
pn11'-COOH...CO ₂				pn12'-COOH...CO ₂			
6	-2.346799000	0.453881000	-0.284784000	6	-2.230428000	-0.203813000	0.002223000
6	-1.794823000	-0.775427000	0.069022000	6	-1.178270000	-1.138883000	0.000206000
6	-0.339514000	-0.887867000	0.172748000	6	0.177230000	-0.603505000	0.001337000
6	0.416956000	0.268224000	0.037472000	6	0.362245000	0.827800000	0.004346000
7	-0.183769000	1.542177000	-0.045054000	7	-0.708333000	1.705297000	0.006054000
6	-1.533121000	1.672615000	-0.368632000	6	-1.902143000	1.210175000	0.005146000
8	-2.025278000	2.761364000	-0.634298000	8	-2.951149000	2.026025000	0.006923000
6	0.309559000	-2.124746000	0.300024000	6	1.285032000	-1.395213000	-0.000333000
6	1.683474000	-2.143352000	0.247268000	7	2.544815000	-0.885068000	0.000813000
7	2.416975000	-1.047561000	-0.006094000	6	2.785505000	0.507555000	0.003836000
6	1.811659000	0.111286000	-0.148005000	6	1.635406000	1.339405000	0.005638000
8	2.521749000	1.168392000	-0.545729000	8	3.955084000	0.926259000	0.004756000
6	-3.735723000	0.538343000	-0.480703000	6	-3.548276000	-0.665362000	0.001432000
6	-4.503080000	-0.583840000	-0.310720000	7	-3.861610000	-1.951276000	-0.001204000
6	-3.841274000	-1.771486000	0.061426000	6	-2.856736000	-2.827601000	-0.003104000
7	-2.540010000	-1.876696000	0.238913000	6	-1.506558000	-2.488598000	-0.002509000
8	-4.588187000	-2.865671000	0.242262000	8	-3.182668000	-4.125345000	-0.005738000
1	-0.272255000	-3.027030000	0.420892000	1	-2.636759000	2.943906000	0.008813000
1	2.242995000	-3.064614000	0.365904000	1	1.251690000	-2.476098000	-0.002607000
1	3.455894000	0.916704000	-0.586611000	1	1.804745000	2.406352000	0.007777000
1	-4.169262000	1.492517000	-0.754620000	1	-4.370145000	0.041660000	0.002985000
1	-5.576000000	-0.590410000	-0.443049000	1	-0.770729000	-3.280718000	-0.004187000
1	-3.997633000	-3.587609000	0.492958000	1	-4.146855000	-4.182294000	-0.005732000
6	0.496311000	2.652890000	0.626982000	6	3.651889000	-1.875740000	-0.001165000
8	1.299308000	2.435891000	1.473872000	8	3.380071000	-3.036479000	-0.003638000
8	0.116275000	3.844450000	0.223968000	8	4.826371000	-1.337060000	0.000091000
1	-0.696607000	3.767239000	-0.324553000	1	4.716602000	-0.311099000	0.002224000
6	5.106339000	-1.338862000	-0.273340000	6	-0.448664000	4.575010000	-0.007676000
8	5.055555000	-2.459057000	-0.008659000	8	-1.608062000	4.618325000	-0.003801000
8	5.218170000	-0.218143000	-0.548645000	8	0.701597000	4.579305000	-0.011739000

pn13'–COOH...CO ₂				pn14'–COOH...CO ₂			
6	0.391670000	-1.161495000	0.000006000	6	4.202892000	-1.264607000	-0.091426000
6	0.643547000	0.241725000	0.000009000	6	2.951905000	-1.803693000	-0.119233000
6	-0.482176000	1.160621000	-0.000001000	6	1.814657000	-0.955273000	-0.032873000
6	-1.767806000	0.609847000	-0.000006000	6	2.073335000	0.418158000	0.069041000
7	-2.007373000	-0.765010000	-0.000031000	7	3.311751000	0.959641000	0.096349000
6	-1.014396000	-1.575668000	-0.000032000	6	4.324385000	0.145834000	0.021841000
8	-1.199362000	-2.899199000	-0.000106000	8	5.567636000	0.650396000	0.050928000
7	-0.248802000	2.483779000	-0.000001000	6	0.455115000	-1.416264000	-0.025972000
6	-1.284966000	3.291141000	-0.000001000	6	-0.545044000	-0.456595000	0.094130000
6	-2.623360000	2.854563000	-0.000005000	7	-0.301258000	0.867005000	0.103094000
6	-2.854875000	1.501977000	-0.000003000	6	0.930181000	1.292079000	0.115038000
8	-1.057987000	4.615664000	-0.000017000	8	1.165223000	2.595112000	0.151549000
6	1.420393000	-2.061062000	0.000020000	6	0.078251000	-2.784019000	-0.193196000
6	2.778217000	-1.621562000	0.000022000	6	-1.217491000	-3.142824000	-0.286480000
7	2.974145000	-0.224905000	0.000011000	6	-2.275472000	-2.168961000	-0.159263000
6	1.942918000	0.661402000	-0.000002000	7	-1.892358000	-0.853213000	0.150386000
8	3.755129000	-2.387604000	-0.000019000	8	-3.462815000	-2.475879000	-0.280931000
1	-2.150130000	-3.084166000	-0.000054000	1	5.098129000	-1.869118000	-0.149762000
1	-3.421800000	3.583582000	-0.000015000	1	2.836657000	-2.876800000	-0.200712000
1	-3.861086000	1.101934000	-0.000021000	1	5.488626000	1.609854000	0.131330000
1	-0.101970000	4.748113000	-0.000015000	1	0.315756000	3.057164000	0.232900000
1	1.250483000	-3.128322000	0.000022000	1	0.844107000	-3.544821000	-0.281356000
1	2.220730000	1.706295000	-0.000011000	1	-1.539615000	-4.161020000	-0.453226000
6	4.344275000	0.372369000	-0.000006000	6	-2.896578000	0.073374000	0.722224000
8	4.447302000	1.557548000	0.000011000	8	-2.566351000	0.964664000	1.437333000
8	5.290553000	-0.507865000	0.000039000	8	-4.123813000	-0.205629000	0.379927000
1	4.870780000	-1.446850000	0.000018000	1	-4.151577000	-1.122634000	-0.028043000
6	-4.653043000	-1.926172000	0.000050000	6	-2.214332000	2.814690000	-0.727563000
8	-4.136882000	-2.963963000	0.000041000	8	-2.835326000	2.061146000	-1.339065000
8	-5.208152000	-0.917549000	0.000040000	8	-1.595786000	3.607935000	-0.151934000
pn15'–COOH...CO ₂				pn16'–COOH...CO ₂			
6	-2.132171000	-0.374371000	-0.130285000	6	-3.234378000	-1.215330000	-0.213456000
6	-1.981286000	0.998671000	0.162819000	6	-2.003932000	-0.556140000	-0.198673000
6	-0.663650000	1.565116000	0.147729000	6	-1.924325000	0.814204000	0.112651000
6	0.398394000	0.708231000	-0.135057000	6	-3.146044000	1.455842000	0.397730000
7	0.249780000	-0.579258000	-0.465970000	7	-4.310978000	0.841116000	0.388202000
6	-0.944706000	-1.108003000	-0.459330000	6	-4.353030000	-0.463143000	0.090043000
8	-1.044055000	-2.385221000	-0.787939000	8	-5.562664000	-1.049218000	0.091786000
6	-3.450418000	-0.917471000	-0.095139000	6	-0.761240000	-1.215462000	-0.519308000
7	-4.516922000	-0.211312000	0.189365000	7	0.393140000	-0.631495000	-0.506118000
6	-4.354755000	1.098127000	0.462942000	6	0.470175000	0.668216000	-0.146851000
6	-3.145634000	1.741792000	0.463335000	6	-0.635528000	1.458558000	0.131659000
8	-3.627390000	-2.211834000	-0.361884000	8	-0.835873000	-2.497852000	-0.859877000
6	-0.390631000	2.952026000	0.349294000	7	1.754978000	1.229321000	-0.135876000
6	0.856414000	3.447370000	0.211870000	6	1.947068000	2.618462000	-0.068990000
6	1.970713000	2.587678000	-0.105480000	6	0.785135000	3.413974000	0.244508000
7	1.708309000	1.206035000	-0.144996000	6	-0.437666000	2.854559000	0.358862000
8	3.105015000	3.019947000	-0.310239000	8	3.062414000	3.113516000	-0.244972000
1	-0.140927000	-2.722507000	-0.911752000	1	-3.311907000	-2.266566000	-0.452451000
1	-5.265441000	1.640139000	0.693829000	1	-3.175997000	2.510722000	0.648436000
1	-3.104111000	2.794711000	0.699672000	1	-6.210951000	-0.373685000	0.325069000
1	-4.576540000	-2.378795000	-0.285925000	1	0.069709000	-2.833047000	-0.968228000
1	-1.203339000	3.627734000	0.584420000	1	0.963715000	4.472733000	0.369023000
1	1.090843000	4.497383000	0.314927000	1	-1.286205000	3.485289000	0.594252000
6	2.839267000	0.258156000	-0.080872000	6	2.930609000	0.338465000	-0.059466000

8	2.720922000	-0.801289000	0.444786000	8	2.851110000	-0.738218000	0.439218000
8	3.936529000	0.713825000	-0.626003000	8	4.016474000	0.862865000	-0.561403000
1	3.865162000	1.709884000	-0.703513000	1	3.891667000	1.857596000	-0.623131000
6	2.391044000	-3.456604000	0.499691000	6	2.645785000	-3.409623000	0.465896000
8	3.100355000	-3.541277000	1.401036000	8	1.898697000	-3.414386000	-0.421801000
8	1.669964000	-3.429290000	-0.408452000	8	3.382869000	-3.464349000	1.346544000
pn17'-COOH...CO ₂				pn18'-COOH...CO ₂			
6	1.085500000	1.781061000	0.000036000	6	1.756234000	-2.507465000	-0.364342000
6	0.438948000	0.526033000	0.000101000	6	0.545551000	-1.940678000	-0.220359000
6	-1.007846000	0.511892000	0.000055000	6	0.408867000	-0.498488000	-0.139579000
6	-1.682298000	1.730005000	-0.000094000	6	1.574688000	0.240267000	-0.129786000
7	-1.044179000	2.943922000	-0.000172000	7	2.830594000	-0.368862000	-0.048933000
6	0.245613000	2.958808000	-0.000096000	6	2.985804000	-1.734831000	-0.308208000
8	0.881679000	4.131350000	-0.000141000	8	4.097714000	-2.241128000	-0.410781000
6	-1.766448000	-0.723588000	0.000222000	6	-0.841545000	0.215207000	-0.137737000
7	-3.159946000	-0.613819000	0.000028000	6	-0.802073000	1.625492000	-0.203248000
6	-3.801190000	0.610220000	-0.000148000	7	0.364166000	2.309318000	-0.377040000
6	-3.110533000	1.762837000	-0.000194000	6	1.479808000	1.655096000	-0.376544000
8	-1.237462000	-1.844843000	0.000338000	8	2.603124000	2.287443000	-0.714002000
6	2.474633000	1.881395000	0.000093000	6	-2.140301000	-0.363036000	-0.029609000
6	3.191977000	0.698006000	0.000208000	7	-3.249267000	0.327673000	0.021765000
7	2.610661000	-0.505961000	0.000201000	6	-3.182471000	1.678220000	-0.034130000
6	1.292015000	-0.602107000	0.000166000	6	-2.006756000	2.362220000	-0.147027000
8	4.530236000	0.742934000	0.000284000	8	-2.250235000	-1.702759000	0.042320000
1	0.211561000	4.828092000	-0.000240000	1	1.886549000	-3.574974000	-0.482564000
1	-4.878863000	0.545880000	-0.000252000	1	-0.343522000	-2.551537000	-0.216823000
1	-3.614939000	2.717802000	-0.000332000	1	2.388124000	3.221010000	-0.838960000
1	2.976358000	2.838424000	0.000034000	1	-4.136238000	2.191671000	0.014015000
1	0.884608000	-1.602265000	0.000162000	1	-1.967320000	3.441194000	-0.199041000
1	4.868204000	-0.164106000	0.000250000	1	-3.192014000	-1.914574000	0.130898000
6	-4.048030000	-1.794552000	0.000025000	6	3.879928000	0.329382000	0.712816000
8	-5.227730000	-1.628941000	-0.000030000	8	3.580948000	1.170434000	1.495836000
8	-3.429481000	-2.937478000	0.000083000	8	5.092721000	-0.092505000	0.457915000
1	-2.433372000	-2.769284000	0.000186000	1	5.045905000	-0.947792000	-0.040403000
6	4.037782000	-2.844021000	-0.000302000	6	-5.718841000	-0.782125000	0.259731000
8	5.033767000	-2.249080000	-0.000118000	8	-6.232553000	0.248342000	0.248392000
8	3.078985000	-3.481375000	-0.000497000	8	-5.258379000	-1.847012000	0.276628000
pn19'-COOH...CO ₂				pn20'-COOH...CO ₂			
6	0.792301000	-0.374373000	-0.000654000	6	-1.223865000	1.897396000	0.000117000
6	0.434903000	0.971207000	0.000066000	6	-0.703908000	0.601047000	0.000104000
6	-0.955918000	1.316935000	-0.000307000	6	0.742124000	0.428795000	0.000043000
6	-1.888791000	0.269879000	-0.001401000	6	1.561336000	1.616538000	-0.000026000
7	-1.531639000	-1.048804000	-0.001993000	7	1.010818000	2.886794000	-0.000034000
6	-0.264044000	-1.356424000	-0.001641000	6	-0.265195000	3.001088000	0.000035000
8	0.077071000	-2.641185000	-0.002200000	8	-0.811998000	4.218541000	0.000036000
7	-1.310320000	2.627931000	0.000336000	6	1.387963000	-0.778605000	0.000073000
6	-2.580445000	2.912882000	-0.000106000	7	2.746014000	-0.873642000	-0.000003000
6	-3.616348000	1.940756000	-0.001214000	6	3.586997000	0.257608000	-0.000107000
6	-3.264355000	0.624766000	-0.001861000	6	2.927954000	1.512784000	-0.000102000
8	-2.959494000	4.203139000	0.000508000	8	4.822377000	0.113574000	-0.000281000
6	2.199779000	-0.765530000	-0.000493000	6	-2.605252000	2.128545000	0.000203000
7	3.126965000	0.290979000	0.000434000	6	-3.434092000	1.030350000	0.000205000
6	2.737490000	1.617357000	0.001208000	7	-2.968445000	-0.228680000	0.000126000
6	1.444125000	1.982182000	0.001064000	6	-1.670821000	-0.438345000	0.000142000
8	2.594341000	-1.928165000	-0.001124000	8	-1.244890000	-1.708633000	0.000183000
1	-0.735940000	-3.166950000	-0.003336000	1	-0.089118000	4.861012000	-0.000016000

1	-4.646923000	2.269675000	-0.001513000	1	0.876607000	-1.727813000	0.000177000
1	-4.006103000	-0.163464000	-0.002673000	1	3.546055000	2.399050000	-0.000173000
1	-2.159391000	4.742672000	0.001241000	1	-2.996006000	3.135820000	0.000248000
1	3.561792000	2.315471000	0.001909000	1	-4.513496000	1.132771000	0.000271000
1	1.159625000	3.022871000	0.001663000	1	-2.017780000	-2.293890000	0.000511000
6	4.583786000	0.059647000	0.000649000	6	3.297044000	-2.257408000	0.000088000
8	5.318944000	0.997663000	0.001475000	8	2.539484000	-3.176375000	-0.000049000
8	4.933716000	-1.192444000	-0.000090000	8	4.589509000	-2.297446000	-0.000135000
1	4.101496000	-1.763606000	-0.000687000	1	4.949038000	-1.329960000	0.000130000
6	-3.478470000	-3.215043000	0.002352000	6	-4.808887000	-2.250059000	-0.000231000
8	-2.582617000	-3.948945000	0.001228000	8	-3.958046000	-3.038120000	0.000901000
8	-4.398672000	-2.521672000	0.003451000	8	-5.689236000	-1.507378000	-0.001284000
pn21'–COOH...CO₂				pn22'–COOH...CO₂			
6	1.178406000	0.897244000	0.000286000	6	-2.258915000	0.601838000	-0.012124000
6	0.216455000	-0.144925000	0.000371000	6	-1.782424000	-0.720832000	-0.000200000
6	-1.176988000	0.235317000	0.000163000	6	-0.328142000	-0.916138000	-0.001385000
6	-1.491536000	1.597906000	-0.000128000	6	0.486156000	0.265523000	-0.015124000
7	-0.559067000	2.581904000	-0.000175000	7	-0.027634000	1.560986000	-0.026006000
6	0.701834000	2.251442000	0.000041000	6	-1.302363000	1.700268000	-0.024774000
8	1.584716000	3.242313000	0.000020000	8	-1.854294000	2.917975000	-0.035448000
6	-2.246426000	-0.746270000	0.000200000	6	0.265823000	-2.148318000	0.009225000
7	-3.559518000	-0.256028000	-0.000102000	6	1.682847000	-2.307754000	0.006748000
6	-3.836598000	1.097580000	-0.000380000	7	2.428805000	-1.121633000	-0.007526000
6	-2.859477000	2.017721000	-0.000398000	6	1.843083000	0.110861000	-0.017741000
8	-2.057953000	-1.970039000	0.000459000	8	2.252338000	-3.413649000	0.016130000
6	2.558180000	0.539583000	0.000457000	6	-3.638964000	0.815496000	-0.011602000
7	2.973996000	-0.706490000	0.000649000	7	-4.521950000	-0.172370000	-0.000249000
6	2.050591000	-1.684760000	0.000678000	6	-4.057421000	-1.419354000	0.010926000
6	0.694824000	-1.475086000	0.000619000	6	-2.705827000	-1.756571000	0.011462000
8	3.483183000	1.497054000	0.000456000	8	-4.958472000	-2.409891000	0.022238000
1	1.075461000	4.064856000	-0.000167000	1	-1.147702000	3.581126000	-0.043813000
1	-4.890606000	1.332493000	-0.000578000	1	-0.297355000	-3.070907000	0.019853000
1	-3.083632000	3.074084000	-0.000614000	1	2.523114000	0.950930000	-0.027289000
1	2.449646000	-2.693948000	0.000872000	1	-4.030665000	1.826086000	-0.020709000
1	0.015342000	-2.308845000	0.000736000	1	-2.425156000	-2.800172000	0.020958000
1	4.351082000	1.065288000	0.000242000	1	-5.835582000	-2.005616000	0.019993000
6	-4.740398000	-1.141128000	-0.000112000	6	3.918586000	-1.134370000	-0.012744000
8	-5.827676000	-0.653857000	-0.000499000	8	4.498669000	-0.095542000	-0.026110000
8	-4.467289000	-2.412329000	-0.000101000	8	4.424528000	-2.325442000	-0.001711000
1	-3.465061000	-2.527533000	0.000155000	1	3.658764000	-3.010827000	0.007702000
6	5.594039000	-1.435190000	-0.000398000	6	1.574561000	3.926327000	0.036144000
8	5.920056000	-0.322172000	-0.000678000	8	2.571354000	3.351886000	0.054672000
8	5.327769000	-2.555808000	-0.001113000	8	0.593133000	4.544491000	0.018592000
pn23'–COOH...CO₂				pn24'–COOH...CO₂			
6	-2.316159000	0.417266000	-0.303607000	6	2.445062000	0.401471000	-0.008471000
6	-1.770752000	-0.817955000	0.087632000	6	1.839792000	-0.861833000	0.000484000
6	-0.310696000	-0.927620000	0.182564000	6	0.380536000	-0.944290000	-0.000598000
6	0.439514000	0.232682000	0.041502000	6	-0.326165000	0.312034000	-0.011001000
7	-0.161582000	1.506956000	-0.042102000	7	0.303174000	1.553748000	-0.018931000
6	-1.504421000	1.636599000	-0.397809000	6	1.580917000	1.585030000	-0.018033000
8	-1.984511000	2.723050000	-0.686281000	8	2.240683000	2.748187000	-0.025976000
6	0.361451000	-2.154754000	0.302801000	6	-0.348616000	-2.107757000	0.006974000
6	1.735811000	-2.160323000	0.246332000	6	-1.774683000	-2.112412000	0.004690000
7	2.457568000	-1.058852000	-0.006207000	7	-2.401865000	-0.859467000	-0.006697000
6	1.835842000	0.091646000	-0.147615000	6	-1.690048000	0.302563000	-0.013818000
8	2.530160000	1.157407000	-0.545618000	8	-2.456883000	-3.153769000	0.011298000

6	-3.693652000	0.514867000	-0.496342000	6	3.836116000	0.531365000	-0.008351000
7	-4.523275000	-0.504534000	-0.325753000	6	4.586995000	-0.625440000	0.000827000
6	-3.997011000	-1.664125000	0.059236000	7	4.044813000	-1.848470000	0.009478000
6	-2.636836000	-1.882830000	0.279619000	6	2.733990000	-1.961931000	0.009325000
8	-4.838298000	-2.687916000	0.240711000	8	2.242021000	-3.209744000	0.018226000
1	-0.180364000	-3.082598000	0.417637000	1	1.597120000	3.472689000	-0.032668000
1	2.301830000	-3.078128000	0.360910000	1	0.111867000	-3.081371000	0.014866000
1	3.468226000	0.920236000	-0.587734000	1	-2.275438000	1.211070000	-0.021431000
1	-4.124448000	1.465078000	-0.792093000	1	4.297019000	1.508266000	-0.015278000
1	-2.306911000	-2.865302000	0.585081000	1	5.670671000	-0.589047000	0.001352000
1	-5.729818000	-2.368946000	0.048832000	1	3.000168000	-3.809544000	0.022893000
6	0.506060000	2.610382000	0.648861000	6	-3.882539000	-0.721088000	-0.011611000
8	1.301020000	2.386373000	1.502267000	8	-4.354988000	0.371912000	-0.021350000
8	0.127253000	3.805850000	0.256411000	8	-4.505216000	-1.855108000	-0.004473000
1	-0.665696000	3.733960000	-0.320229000	1	-3.806284000	-2.613424000	0.003362000
6	5.153774000	-1.308943000	-0.280371000	6	-1.079918000	4.074774000	0.027717000
8	5.244906000	-0.185571000	-0.552342000	8	-2.128064000	3.600966000	0.044500000
8	5.120801000	-2.430522000	-0.018998000	8	-0.040879000	4.590777000	0.011670000
pn25'-COOH...CO ₂				pn26'-COOH...CO ₂			
6	2.021641000	-0.918800000	-0.000530000	6	-2.157939000	-0.299035000	-0.000379000
6	0.772359000	-1.559924000	0.000395000	6	-1.093912000	-1.212546000	0.000068000
6	-0.416051000	-0.719468000	-0.000211000	6	0.265474000	-0.685397000	-0.000114000
6	-0.260432000	0.711706000	-0.001701000	6	0.446842000	0.744023000	-0.000729000
7	0.985449000	1.298651000	-0.002237000	7	-0.633596000	1.617482000	-0.001195000
6	2.037610000	0.540609000	-0.001660000	6	-1.824161000	1.129316000	-0.001009000
8	3.228487000	1.113765000	-0.002431000	8	-2.877291000	1.936999000	-0.001380000
6	-1.681019000	-1.227938000	0.000482000	6	1.380153000	-1.466549000	0.000156000
7	-2.782788000	-0.435108000	-0.000312000	7	2.639055000	-0.942079000	0.000026000
6	-2.688837000	0.976518000	-0.002041000	6	2.870615000	0.446798000	-0.000358000
6	-1.377380000	1.512408000	-0.002611000	6	1.712177000	1.270048000	-0.000822000
8	-3.730027000	1.656199000	-0.002401000	8	4.036174000	0.879902000	-0.000544000
6	3.177861000	-1.741986000	-0.000238000	6	-3.472827000	-0.741744000	-0.000287000
7	3.127272000	-3.059446000	0.000986000	6	-3.673828000	-2.118234000	0.000281000
6	1.926082000	-3.648125000	0.001962000	7	-2.685908000	-3.007156000	0.000760000
6	0.732505000	-2.960874000	0.001701000	6	-1.435030000	-2.568280000	0.000657000
8	4.393020000	-1.193111000	-0.001220000	8	-4.931366000	-2.588060000	0.000353000
1	3.105264000	2.076291000	-0.003160000	1	-2.571310000	2.857931000	-0.002278000
1	-1.907728000	-2.284736000	0.001670000	1	1.361857000	-2.547237000	0.000480000
1	-1.288464000	2.588872000	-0.003682000	1	1.870850000	2.338719000	-0.001318000
1	1.935123000	-4.732924000	0.002957000	1	-4.308330000	-0.056403000	-0.000639000
1	-0.198780000	-3.508739000	0.002496000	1	-0.670276000	-3.337852000	0.001072000
1	5.021424000	-1.927789000	-0.000806000	1	-4.881029000	-3.552086000	0.000784000
6	-4.093401000	-1.136415000	0.000717000	6	3.753410000	-1.922977000	0.000208000
8	-4.102683000	-2.328973000	0.002139000	8	3.492099000	-3.086477000	0.000311000
8	-5.105668000	-0.335045000	-0.000124000	8	4.924076000	-1.375279000	0.000237000
1	-4.752627000	0.638186000	-0.001169000	1	4.806433000	-0.349586000	-0.000196000
6	1.375390000	4.177929000	0.003026000	6	-0.388263000	4.501156000	0.001209000
8	2.513947000	3.957188000	0.000829000	8	-1.548141000	4.532301000	0.001209000
8	0.255211000	4.441017000	0.005317000	8	0.761785000	4.514278000	0.001274000
pn27'-COOH...CO ₂				pn28'-COOH...CO ₂			
6	-0.289868000	2.064245000	0.143706000	6	1.915160000	2.561140000	-0.322645000
6	-0.070552000	0.683272000	0.010370000	6	0.690856000	2.027159000	-0.176593000
6	1.282036000	0.213910000	-0.027970000	6	0.515388000	0.593979000	-0.121009000
6	2.281393000	1.155134000	-0.204061000	6	1.644678000	-0.188883000	-0.123445000
7	2.062795000	2.502823000	-0.131182000	7	2.923105000	0.375533000	-0.056560000
6	0.864095000	2.919850000	0.103297000	6	3.118620000	1.739482000	-0.298524000

8	0.639496000	4.233251000	0.265581000	8	4.243033000	2.212798000	-0.412752000
7	1.623357000	-1.143479000	0.046222000	6	-0.768489000	-0.052540000	-0.120700000
6	2.863756000	-1.609275000	-0.411952000	6	-0.804723000	-1.468552000	-0.183371000
6	3.870686000	-0.602557000	-0.692750000	7	0.333108000	-2.207523000	-0.363434000
6	3.607096000	0.707131000	-0.531975000	6	1.475217000	-1.603688000	-0.371041000
8	3.091585000	-2.814567000	-0.500899000	8	2.567023000	-2.283093000	-0.719064000
6	-1.600609000	2.573824000	0.248059000	6	-1.997224000	0.616590000	-0.020431000
6	-2.637209000	1.685996000	0.158674000	7	-3.161458000	-0.000395000	0.036583000
7	-2.458635000	0.371586000	-0.107840000	6	-3.177507000	-1.342247000	-0.008880000
6	-1.247407000	-0.104203000	-0.207744000	6	-2.040870000	-2.118758000	-0.122082000
8	-1.089950000	-1.369088000	-0.610012000	8	-4.376404000	-1.939242000	0.053806000
1	1.489334000	4.685116000	0.188792000	1	2.084519000	3.625130000	-0.420741000
1	4.840805000	-0.981438000	-0.983623000	1	-0.176219000	2.674965000	-0.154198000
1	4.364789000	1.466781000	-0.685218000	1	2.308247000	-3.204526000	-0.852627000
1	-1.764694000	3.632559000	0.387781000	1	-2.046119000	1.700018000	0.030045000
1	-3.668979000	2.002980000	0.259814000	1	-2.100457000	-3.196823000	-0.170274000
1	-1.964312000	-1.781801000	-0.684114000	1	-5.055358000	-1.254190000	0.127357000
6	0.856660000	-1.983481000	0.980809000	6	3.960008000	-0.366075000	0.680920000
8	0.194860000	-1.473084000	1.828542000	8	3.643880000	-1.201357000	1.462668000
8	1.013981000	-3.266280000	0.799613000	8	5.183712000	0.011645000	0.406706000
1	1.772273000	-3.416433000	0.169698000	1	5.163203000	0.870817000	-0.082898000
6	-4.672806000	-1.187097000	-0.403681000	6	-5.349428000	1.571077000	0.225920000
8	-5.378130000	-0.317680000	-0.132705000	8	-6.050177000	0.648639000	0.246608000
8	-4.010024000	-2.095648000	-0.686648000	8	-4.702469000	2.525511000	0.209342000
pn29''-COOH...CO₂				pn30''-COOH...CO₂			
6	2.279668000	0.202880000	-0.005610000	6	3.760187000	-2.198539000	0.258229000
6	1.618449000	-1.038224000	0.001358000	6	2.402194000	-2.239349000	0.435109000
6	0.160669000	-1.058581000	0.000306000	6	1.626796000	-1.087779000	0.190591000
6	-0.499356000	0.217535000	-0.007589000	6	2.313404000	0.055582000	-0.209296000
7	0.181364000	1.434577000	-0.013799000	7	3.636357000	0.106542000	-0.398902000
6	1.460369000	1.420260000	-0.013104000	6	4.328997000	-0.985489000	-0.179206000
8	2.163829000	2.555729000	-0.019506000	8	5.653707000	-0.948821000	-0.372897000
6	-0.596598000	-2.201131000	0.006112000	6	0.166483000	-1.062484000	0.246690000
6	-2.019822000	-2.170322000	0.004541000	6	-0.473209000	0.158026000	0.073952000
7	-2.607686000	-0.895421000	-0.003843000	7	0.255286000	1.362535000	-0.017998000
6	-1.863112000	0.247264000	-0.009413000	6	1.607226000	1.362970000	-0.356149000
8	-2.732841000	-3.190099000	0.009327000	8	2.194583000	2.384423000	-0.654202000
6	3.663798000	0.256972000	-0.005171000	6	-0.624444000	-2.218339000	0.370267000
6	4.345239000	-0.958090000	0.002462000	6	-1.991465000	-2.094957000	0.281982000
7	3.746711000	-2.146384000	0.009172000	7	-2.603232000	-0.936008000	-0.001479000
6	2.422355000	-2.181450000	0.008565000	6	-1.870522000	0.147971000	-0.143596000
8	5.683958000	-0.943478000	0.003154000	8	-2.453046000	1.269438000	-0.569055000
1	1.550570000	3.306248000	-0.024474000	1	4.397709000	-3.053429000	0.438633000
1	-0.166026000	-3.192376000	0.012027000	1	1.932464000	-3.156239000	0.767446000
1	-2.424380000	1.171037000	-0.014992000	1	5.881776000	-0.054190000	-0.658119000
1	4.199602000	1.195380000	-0.010502000	1	-0.180292000	-3.193241000	0.511489000
1	1.980078000	-3.171625000	0.014091000	1	-2.642583000	-2.954649000	0.396421000
1	5.985824000	-1.860795000	0.008933000	1	-3.407765000	1.119439000	-0.630173000
6	-4.083406000	-0.712024000	-0.007055000	6	-0.316786000	2.545213000	0.630054000
8	-4.522562000	0.394492000	-0.013771000	8	-1.142074000	2.420923000	1.474562000
8	-4.742469000	-1.825960000	-0.002159000	8	0.179470000	3.687595000	0.212059000
1	-4.071927000	-2.605667000	0.003324000	1	0.973114000	3.524029000	-0.344964000
6	-1.107382000	3.999687000	0.018136000	6	-5.296682000	-0.946479000	-0.353078000
8	-2.171049000	3.561539000	0.028341000	8	-5.372318000	-2.063349000	-0.080220000
8	-0.051578000	4.480244000	0.008322000	8	-5.281119000	0.177129000	-0.638417000
pn31''-COOH...CO₂				pn32''-COOH...CO₂			

6	2.707008000	2.416194000	-0.213696000	6	2.467212000	0.289332000	-0.337823000
6	1.382958000	2.235566000	-0.065725000	6	1.851731000	-0.906290000	0.039234000
6	0.815030000	0.910692000	-0.065572000	6	0.390237000	-0.954755000	0.145394000
6	1.676802000	-0.161424000	-0.123524000	6	-0.297791000	0.252883000	0.039667000
7	3.057886000	0.023875000	-0.058921000	7	0.375840000	1.493671000	-0.011133000
6	3.628548000	1.290728000	-0.253020000	6	1.702582000	1.561757000	-0.395997000
8	4.838618000	1.425907000	-0.383130000	8	2.247268000	2.619673000	-0.669450000
6	-0.603643000	0.657806000	-0.055522000	6	-0.371468000	-2.135770000	0.234127000
6	-1.013815000	-0.687135000	-0.179336000	6	-1.743767000	-2.042892000	0.170651000
7	-0.140063000	-1.716734000	-0.401008000	7	-2.396597000	-0.894469000	-0.052033000
6	1.123639000	-1.468762000	-0.404761000	6	-1.695485000	0.213864000	-0.153830000
8	1.987333000	-2.418837000	-0.780645000	8	-2.315652000	1.340778000	-0.513766000
6	-1.588284000	1.644402000	0.091961000	6	3.842272000	0.358745000	-0.562591000
6	-2.911118000	1.246905000	0.125592000	6	4.577196000	-0.795276000	-0.389528000
7	-3.309602000	-0.029706000	0.015683000	7	4.027975000	-1.951949000	-0.002688000
6	-2.392123000	-0.962312000	-0.136337000	6	2.730256000	-2.005888000	0.206289000
8	-3.866215000	2.179099000	0.276980000	8	2.238588000	-3.190026000	0.608731000
1	3.166007000	3.393894000	-0.272548000	1	0.104403000	-3.095873000	0.338474000
1	0.727388000	3.094662000	0.000981000	1	-2.365678000	-2.926905000	0.259363000
1	1.485315000	-3.230671000	-0.926592000	1	-3.267559000	1.169227000	-0.558721000
1	-1.360346000	2.695653000	0.197469000	1	4.297176000	1.296631000	-0.848504000
1	-2.728527000	-1.990248000	-0.232734000	1	5.648691000	-0.809914000	-0.553201000
1	-4.726519000	1.736681000	0.283993000	1	2.989757000	-3.795128000	0.670074000
6	3.859410000	-1.009241000	0.624211000	6	-0.226178000	2.623409000	0.704731000
8	3.339613000	-1.735124000	1.405262000	8	-1.007776000	2.427123000	1.575158000
8	5.129789000	-0.994878000	0.306846000	8	0.198669000	3.803630000	0.312066000
1	5.345770000	-0.147274000	-0.153391000	1	0.974000000	3.703160000	-0.281350000
6	-5.919676000	-0.806991000	0.069609000	6	-5.099610000	-0.949443000	-0.326611000
8	-5.636983000	-1.914871000	-0.070237000	8	-5.114276000	0.186429000	-0.559365000
8	-6.261538000	0.292040000	0.211081000	8	-5.146128000	-2.078862000	-0.104303000
pn33"-COOH...CO ₂				pn34"-COOH...CO ₂			
6	-2.307278000	0.142883000	-0.230091000	6	-2.333731000	-0.266563000	-0.005127000
6	-1.651289000	-1.029345000	0.174302000	6	-1.496029000	-1.391508000	0.004044000
6	-0.191083000	-1.041299000	0.240739000	6	-0.046163000	-1.174270000	0.001744000
6	0.476075000	0.165364000	0.069956000	6	0.407732000	0.182564000	-0.010048000
7	-0.223525000	1.392553000	-0.024069000	7	-0.449074000	1.273019000	-0.017843000
6	-1.567151000	1.424973000	-0.367308000	6	-1.717803000	1.062567000	-0.015831000
8	-2.136214000	2.460773000	-0.668305000	8	-2.553369000	2.097673000	-0.023543000
6	0.575179000	-2.212778000	0.367264000	6	0.869536000	-2.193782000	0.009598000
6	1.945149000	-2.117091000	0.284016000	6	2.272792000	-1.952265000	0.005902000
7	2.582329000	-0.972160000	0.000699000	7	2.659639000	-0.605421000	-0.006555000
6	1.871985000	0.126517000	-0.144792000	6	1.755857000	0.414266000	-0.013880000
8	2.478818000	1.236223000	-0.568687000	8	3.129864000	-2.855922000	0.013105000
6	-3.678630000	0.159234000	-0.405384000	6	-3.733827000	-0.507925000	-0.003465000
6	-4.363331000	-1.029574000	-0.156207000	7	-4.258819000	-1.717682000	0.006329000
7	-3.773720000	-2.147837000	0.249796000	6	-3.439097000	-2.773483000	0.015034000
6	-2.455699000	-2.146316000	0.406723000	6	-2.065251000	-2.670521000	0.014281000
8	-5.692411000	-1.053191000	-0.323494000	8	-4.591708000	0.512723000	-0.012077000
1	0.109869000	-3.177965000	0.506934000	1	-2.027103000	2.911360000	-0.031092000
1	2.577546000	-2.990202000	0.401937000	1	0.590375000	-3.237344000	0.018748000
1	3.430666000	1.066960000	-0.625867000	1	2.175170000	1.410424000	-0.022157000
1	-4.197673000	1.058514000	-0.707321000	1	-3.921727000	-3.744799000	0.022841000
1	-2.022678000	-3.083097000	0.738938000	1	-1.458944000	-3.564132000	0.021497000
1	-5.998910000	-1.941211000	-0.100333000	1	-5.476689000	0.123976000	-0.009331000
6	0.378124000	2.560720000	0.625466000	6	4.096394000	-0.204332000	-0.012648000
8	1.189481000	2.414418000	1.478718000	8	4.364369000	0.954842000	-0.024508000

8	-0.077086000	3.717322000	0.197507000	8	4.910504000	-1.209190000	-0.003997000
1	-0.867445000	3.582196000	-0.367759000	1	4.360878000	-2.080869000	0.004869000
6	5.277290000	-1.031555000	-0.338510000	6	0.480343000	4.001441000	0.026693000
8	5.332573000	-2.149136000	-0.064093000	8	1.594065000	3.711295000	0.044667000
8	5.281962000	0.091905000	-0.625215000	8	-0.629812000	4.335434000	0.009268000
pn35''-COOH...CO₂				pn36''-COOH...CO₂			
6	-2.361376000	-0.195615000	-0.193806000	6	-1.125168000	1.916712000	0.158567000
6	-1.591908000	-1.302526000	0.193141000	6	-0.550329000	0.642005000	0.045778000
6	-0.132004000	-1.162180000	0.234906000	6	0.882871000	0.544959000	-0.026979000
6	0.407151000	0.105683000	0.082750000	6	1.607369000	1.718133000	-0.227243000
7	-0.410018000	1.247906000	0.023545000	7	1.033127000	2.959924000	-0.214994000
6	-1.765637000	1.147963000	-0.320648000	6	-0.232473000	3.043624000	0.035736000
8	-2.402236000	2.143420000	-0.613408000	8	-0.791853000	4.250915000	0.145496000
6	0.743122000	-2.258951000	0.321754000	6	1.608335000	-0.677048000	0.292197000
6	2.095641000	-2.030482000	0.226972000	7	2.975075000	-0.686000000	-0.030032000
7	2.614164000	-0.819953000	-0.029314000	6	3.645472000	0.467012000	-0.395079000
6	1.802521000	0.208342000	-0.140588000	6	3.019219000	1.654465000	-0.454720000
8	2.293113000	1.381375000	-0.539646000	8	1.100670000	-1.637694000	0.866929000
6	-3.756234000	-0.394377000	-0.347142000	6	-2.513355000	2.080505000	0.324844000
7	-4.352702000	-1.551008000	-0.110592000	6	-3.283956000	0.947852000	0.330419000
6	-3.604696000	-2.579322000	0.290187000	7	-2.780374000	-0.276207000	0.071493000
6	-2.233764000	-2.516454000	0.449211000	6	-1.491390000	-0.427173000	-0.117765000
8	-4.536074000	0.606798000	-0.744919000	8	-1.057146000	-1.598521000	-0.574715000
1	0.374177000	-3.267364000	0.438512000	1	-0.093944000	4.907711000	0.019394000
1	2.811704000	-2.840203000	0.312923000	1	4.698217000	0.323900000	-0.588393000
1	3.256195000	1.308416000	-0.610198000	1	3.557489000	2.561833000	-0.685558000
1	-4.139523000	-3.502992000	0.485195000	1	-2.941260000	3.065719000	0.440939000
1	-1.688329000	-3.392251000	0.767982000	1	-4.354721000	0.986356000	0.496361000
1	-5.437944000	0.258859000	-0.766561000	1	-1.812839000	-2.201793000	-0.635975000
6	0.069177000	2.446666000	0.710536000	6	3.800543000	-1.894966000	0.091678000
8	0.907558000	2.357355000	1.547968000	8	4.940869000	-1.858599000	-0.254132000
8	-0.514597000	3.561492000	0.334885000	8	3.179107000	-2.930183000	0.579545000
1	-1.285099000	3.354685000	-0.241280000	1	2.238966000	-2.663583000	0.821232000
6	5.303420000	-0.607588000	-0.381679000	6	-4.581467000	-2.294751000	-0.227754000
8	5.468348000	-1.721183000	-0.136307000	8	-5.455553000	-1.618088000	0.097138000
8	5.195916000	0.517654000	-0.639274000	8	-3.741187000	-3.019347000	-0.564178000

VI. Dicarboxylic acid

nt1''-(COOH)₂				nt2''-(COOH)₂			
6	-2.406366000	1.954942000	0.246976000	6	1.766022000	2.289326000	-0.000014000
6	-1.248136000	2.628099000	0.100771000	6	0.426349000	2.188597000	-0.000098000
6	0.000044000	1.941713000	-0.000360000	6	-0.190389000	0.904569000	-0.000076000
6	0.000066000	0.559252000	-0.000213000	6	0.566753000	-0.262949000	-0.000039000
7	-1.196257000	-0.131761000	-0.072551000	7	1.967342000	-0.158055000	-0.000070000
6	-2.427035000	0.513929000	0.198817000	6	2.596165000	1.115483000	0.000049000
8	-3.454351000	-0.145680000	0.327761000	8	3.824752000	1.222015000	0.000209000
6	1.248249000	2.627972000	-0.101218000	6	-1.639867000	0.891360000	-0.000060000
6	2.406584000	1.954774000	-0.246875000	7	-2.250554000	-0.356722000	0.000072000
6	2.427286000	0.513897000	-0.198314000	6	-1.494701000	-1.502812000	0.000207000
7	1.196181000	-0.131798000	0.072162000	6	-0.144628000	-1.509818000	0.000158000
8	3.454535000	-0.145959000	-0.326622000	8	-2.308882000	1.929827000	-0.000079000
1	-3.364788000	2.436536000	0.378868000	1	2.297830000	3.230213000	0.000025000
1	-1.237196000	3.712773000	0.099292000	1	-0.215895000	3.060541000	-0.000140000
1	1.237446000	3.712651000	-0.100109000	1	-2.075792000	-2.413977000	0.000348000
1	3.364982000	2.436481000	-0.378522000	1	0.357343000	-2.456565000	0.000254000
6	1.218888000	-1.475499000	0.715659000	6	-3.717988000	-0.531645000	0.000115000

8	0.321199000	-1.791158000	1.428964000	8	-4.166415000	-1.632939000	0.000485000
8	2.278878000	-2.171195000	0.448974000	8	-4.387055000	0.583250000	-0.000096000
1	2.950284000	-1.591934000	-0.017183000	1	-3.747191000	1.358629000	-0.000383000
6	-1.219108000	-1.475431000	-0.715834000	6	2.824976000	-1.388257000	-0.000328000
8	-0.321196000	-1.791612000	-1.428678000	8	2.332743000	-2.471490000	-0.000937000
8	-2.279403000	-2.170867000	-0.449553000	8	4.097889000	-1.154338000	0.000401000
1	-2.950323000	-1.591705000	0.017166000	1	4.265778000	-0.149135000	0.000535000
nt3''-(COOH)₂				nt4''-(COOH)₂			
6	-1.089889000	-2.238672000	-0.404318000	6	2.002753000	2.343561000	-0.004733000
6	0.191449000	-1.851086000	-0.269895000	6	0.672728000	2.392081000	0.128960000
6	0.510253000	-0.460594000	-0.084988000	6	-0.102917000	1.181976000	0.094127000
6	-0.510304000	0.460613000	-0.084897000	6	0.545093000	-0.100880000	-0.024771000
7	-1.849677000	0.028013000	-0.076840000	7	1.957623000	-0.121166000	-0.026765000
6	-2.187923000	-1.308713000	-0.310357000	6	2.702556000	1.073908000	-0.134348000
8	-3.362633000	-1.669149000	-0.412892000	8	3.914849000	1.049915000	-0.302553000
7	1.849659000	-0.027999000	-0.076894000	6	-1.463310000	1.238348000	0.110938000
6	2.187905000	1.308719000	-0.310311000	7	-2.237968000	0.130661000	0.002948000
6	1.089892000	2.238678000	-0.404309000	6	-1.662061000	-1.143775000	-0.167578000
6	-0.191443000	1.851108000	-0.269807000	6	-0.233474000	-1.214711000	-0.172604000
8	3.362599000	1.669128000	-0.412886000	8	-2.390614000	-2.133275000	-0.301846000
1	-1.364648000	-3.268944000	-0.583617000	1	2.638418000	3.217430000	-0.023388000
1	0.982585000	-2.579680000	-0.343033000	1	0.152440000	3.337507000	0.236985000
1	1.364553000	3.268957000	-0.583705000	1	-2.008740000	2.169024000	0.200645000
1	-0.982575000	2.579706000	-0.342947000	1	0.163713000	-2.209446000	-0.274465000
6	2.890020000	-0.963812000	0.401700000	6	-3.707059000	0.344317000	0.041738000
8	2.575071000	-1.960935000	0.973495000	8	-4.116511000	1.452764000	0.187606000
8	4.105409000	-0.583665000	0.146039000	8	-4.392822000	-0.743889000	-0.093940000
1	4.092464000	0.373713000	-0.181837000	1	-3.749485000	-1.529404000	-0.206116000
6	-2.889972000	0.963790000	0.401650000	6	2.657886000	-1.400149000	0.202712000
8	-2.575005000	1.960936000	0.973389000	8	2.076366000	-2.329915000	0.662803000
8	-4.105410000	0.583649000	0.146117000	8	3.918367000	-1.403719000	-0.136039000
1	-4.092427000	-0.373748000	-0.181630000	1	4.215813000	-0.474683000	-0.341854000
nt5''-(COOH)₂				nt6''-(COOH)₂			
6	-0.249142000	-0.640576000	-0.000005000	6	1.261338000	1.976525000	0.000050000
6	0.248917000	0.639964000	-0.000005000	6	0.013765000	1.414857000	0.000104000
6	-0.622214000	1.769361000	-0.000049000	6	-0.107010000	-0.012197000	0.000057000
6	-1.951643000	1.559247000	-0.000086000	6	1.019176000	-0.781627000	-0.000062000
7	-2.489794000	0.278834000	-0.000091000	7	2.253677000	-0.226081000	-0.000110000
6	-1.695560000	-0.862350000	-0.000050000	6	2.445698000	1.181760000	-0.000050000
8	-2.177965000	-1.994901000	-0.000025000	8	3.591998000	1.642158000	-0.000121000
6	0.622387000	-1.769729000	0.000036000	6	-1.212701000	2.173024000	0.000200000
6	1.951770000	-1.559365000	0.000074000	6	-2.393343000	1.538710000	0.000208000
7	2.489765000	-0.278882000	0.000076000	7	-2.523637000	0.146699000	0.000160000
6	1.695366000	0.862023000	0.000040000	6	-1.405350000	-0.688358000	0.000142000
8	2.177587000	1.994845000	-0.000005000	8	-1.510536000	-1.908331000	-0.000053000
1	-0.213487000	2.768956000	-0.000044000	1	1.409902000	3.047978000	0.000080000
1	-2.691705000	2.345360000	-0.000117000	1	0.986817000	-1.864129000	-0.000108000
1	0.213971000	-2.769457000	0.000030000	1	-1.186202000	3.253611000	0.000234000
1	2.692099000	-2.345208000	0.000108000	1	-3.342999000	2.053898000	0.000245000
6	3.967319000	-0.206901000	0.000126000	6	-3.897746000	-0.361931000	0.000133000
8	4.594307000	-1.217260000	0.000040000	8	-4.805803000	0.408046000	0.000154000
8	4.449064000	1.002030000	0.000079000	8	-4.004745000	-1.663535000	0.000081000
1	3.699660000	1.666926000	0.000173000	1	-3.104239000	-2.081673000	0.000102000
6	-3.967069000	0.207231000	-0.000140000	6	3.399810000	-1.183146000	-0.000227000
8	-4.593822000	1.217743000	-0.000026000	8	3.165882000	-2.348208000	-0.000198000
8	-4.449300000	-1.001562000	-0.000015000	8	4.557752000	-0.605669000	-0.000344000

1	-3.700096000	-1.666822000	-0.000082000	1	4.428240000	0.404609000	-0.000385000
nt7''-(COOH)₂				nt8''-(COOH)₂			
6	2.653387000	1.906514000	-0.190033000	6	2.527473000	2.063478000	-0.133750000
6	1.488933000	2.514942000	0.087167000	6	1.292079000	2.522471000	0.071639000
6	0.262848000	1.753139000	0.147907000	6	0.172040000	1.601638000	0.116161000
6	0.340068000	0.390437000	0.022516000	6	0.424952000	0.196487000	0.011687000
7	1.569809000	-0.259568000	-0.067737000	7	1.774908000	-0.269618000	-0.037178000
6	2.746511000	0.454241000	-0.319684000	6	2.823314000	0.629175000	-0.218492000
8	3.798567000	-0.118062000	-0.568634000	8	3.979098000	0.261511000	-0.395456000
6	-1.017106000	2.377960000	0.282243000	6	-1.107988000	2.072786000	0.183960000
6	-2.130639000	1.624400000	0.239667000	6	-2.239263000	1.204640000	0.129876000
7	-2.068246000	0.266541000	-0.014241000	7	-1.934039000	-0.148530000	-0.053013000
6	-0.862028000	-0.396802000	-0.241636000	6	-0.652969000	-0.630134000	-0.106239000
8	-0.826498000	-1.539540000	-0.687309000	8	-3.412941000	1.593833000	0.210969000
1	3.588672000	2.439909000	-0.296668000	1	3.395515000	2.703467000	-0.219588000
1	1.439997000	3.590241000	0.218204000	1	1.091249000	3.583346000	0.167698000
1	-1.089437000	3.445867000	0.432669000	1	-1.318426000	3.131557000	0.256782000
1	-3.132573000	2.005777000	0.367553000	1	-0.591910000	-1.697708000	-0.235681000
6	1.668312000	-1.613370000	0.512869000	6	-3.005610000	-1.176016000	-0.215709000
8	0.893151000	-1.951887000	1.343953000	8	-2.691605000	-2.303191000	-0.420850000
8	2.671817000	-2.318873000	0.054684000	8	-4.203949000	-0.694523000	-0.113392000
1	3.302353000	-1.731194000	-0.423397000	1	-4.150804000	0.310715000	0.045709000
6	-3.369373000	-0.426334000	-0.117235000	6	2.052912000	-1.676496000	0.273701000
8	-4.363823000	0.180657000	0.125048000	8	1.197998000	-2.373335000	0.722584000
8	-3.293944000	-1.675646000	-0.470417000	8	3.273260000	-2.067056000	0.020486000
1	-2.339579000	-1.923364000	-0.645800000	1	3.831763000	-1.290425000	-0.255305000
nt9''-(COOH)₂				nt10''-(COOH)₂			
6	-0.000067000	0.143134000	0.000018000	6	-0.672126000	-1.446187000	-0.000036000
6	-0.000002000	1.535321000	0.000017000	6	0.230305000	-0.429489000	0.000029000
6	-1.239206000	2.241772000	0.000019000	6	-0.184578000	0.936127000	0.000112000
6	-2.395747000	1.550145000	0.000016000	6	-1.524749000	1.187422000	0.000112000
7	-2.426871000	0.176789000	0.000018000	7	-2.445520000	0.177585000	0.000099000
6	-1.249938000	-0.604524000	0.000031000	6	-2.082801000	-1.179871000	0.000082000
8	-1.331697000	-1.826917000	-0.000003000	8	-2.946258000	-2.065188000	-0.000043000
6	1.249781000	-0.604625000	0.000007000	6	1.680830000	-0.768564000	0.000005000
7	2.426877000	0.176794000	0.000001000	7	2.561156000	0.298052000	0.000004000
6	2.395706000	1.550033000	0.000002000	6	2.119049000	1.638458000	0.000051000
6	1.239168000	2.241740000	0.000010000	6	0.825968000	1.969375000	0.000117000
8	1.331674000	-1.826993000	0.000005000	8	2.051188000	-1.934034000	-0.000312000
1	-1.253515000	3.322209000	0.000016000	1	-0.363058000	-2.482712000	-0.000152000
1	-3.372597000	2.013182000	0.000011000	1	-1.947163000	2.183174000	0.000128000
1	3.372466000	2.013236000	-0.000003000	1	2.926599000	2.353647000	0.000042000
1	1.253590000	3.322177000	0.000009000	1	0.539620000	3.012043000	0.000157000
6	-3.777436000	-0.427811000	0.000005000	6	4.016715000	0.120091000	-0.000070000
8	-4.727636000	0.289985000	-0.000047000	8	4.722611000	1.078098000	-0.000453000
8	-3.786678000	-1.725915000	-0.000040000	8	4.425830000	-1.121664000	0.000448000
1	-2.835883000	-2.062630000	-0.000015000	1	3.651979000	-1.739944000	0.000931000
6	3.777517000	-0.427765000	-0.000006000	6	-3.873994000	0.606425000	-0.000041000
8	4.727670000	0.290081000	-0.000038000	8	-4.117674000	1.770616000	-0.000037000
8	3.786822000	-1.725877000	0.000011000	8	-4.713835000	-0.377854000	-0.000086000
1	2.835993000	-2.062690000	0.000045000	1	-4.200043000	-1.258177000	-0.000131000
nt11''-(COOH)₂				nt12''-(COOH)₂			

6	-1.240022000	-1.879420000	-0.000160000	6	0.757235000	-1.702175000	0.002188000
6	-0.000030000	-1.237656000	-0.000098000	6	-0.208939000	-0.675983000	0.001874000
6	0.000020000	0.207898000	0.000063000	6	0.208606000	0.676364000	0.002214000
6	-1.202354000	0.905153000	0.000161000	6	1.608443000	0.911473000	0.002810000
7	-2.363007000	0.269600000	0.000074000	7	2.496933000	-0.049724000	0.003099000
6	-2.447720000	-1.178133000	-0.000105000	6	2.080491000	-1.337175000	0.002833000
8	-3.590802000	-1.675258000	-0.000147000	8	3.038748000	-2.281398000	0.003391000
6	1.239824000	-1.879579000	-0.000175000	6	-1.608727000	-0.911086000	0.001220000
6	2.447584000	-1.178234000	-0.000129000	7	-2.497188000	0.050207000	0.000969000
7	2.363099000	0.269512000	0.000110000	6	-2.080779000	1.337572000	0.001306000
6	1.202435000	0.905095000	0.000166000	6	-0.757469000	1.702594000	0.001890000
8	3.590588000	-1.675533000	-0.000230000	8	-3.039030000	2.281855000	0.000994000
1	-1.314403000	-2.957935000	-0.000263000	1	0.478202000	-2.747940000	0.001950000
1	-1.260005000	1.989079000	0.000307000	1	1.990130000	1.929742000	0.002968000
1	1.314369000	-2.958053000	-0.000317000	1	-1.990547000	-1.929296000	0.000871000
1	1.259899000	1.989027000	0.000326000	1	-0.478409000	2.748348000	0.002100000
6	3.603183000	1.140791000	0.000304000	6	-5.103861000	-0.719694000	-0.003423000
8	3.442210000	2.319240000	-0.000004000	8	-4.808276000	-1.833732000	-0.005550000
8	4.686012000	0.457443000	-0.000207000	8	-5.459107000	0.383519000	-0.001187000
1	4.432006000	-0.568047000	-0.000040000	1	-3.900290000	1.842923000	0.000590000
6	-3.603340000	1.140859000	0.000194000	6	5.104457000	0.718936000	-0.004258000
8	-3.442096000	2.319370000	0.000360000	8	4.809658000	1.833176000	-0.002906000
8	-4.685785000	0.457294000	-0.000072000	8	5.458737000	-0.384607000	-0.006318000
1	-4.431025000	-0.568956000	-0.000225000	1	3.900118000	-1.842621000	0.003731000
pn1''-(COOH)₂				pn2''-(COOH)₂			
6	-4.299314000	0.634438000	0.227165000	6	2.244764000	-0.273719000	-0.129399000
6	-3.207290000	1.457036000	0.284520000	6	1.100608000	-1.041155000	0.044077000
6	-1.923872000	0.899183000	0.145091000	6	-0.187312000	-0.364811000	0.046539000
6	-1.802192000	-0.477409000	-0.038442000	6	-0.265573000	1.069045000	-0.036303000
7	-2.871283000	-1.289443000	-0.098605000	7	0.940418000	1.812219000	-0.029102000
6	-4.063009000	-0.742827000	0.025913000	6	2.184716000	1.183068000	-0.211506000
8	-5.129036000	-1.545093000	-0.039777000	8	3.202951000	1.837749000	-0.396553000
6	-0.754709000	1.761536000	0.130665000	6	-1.337614000	-1.089551000	0.054580000
7	0.484001000	1.145465000	-0.124651000	7	-2.562075000	-0.510782000	-0.028690000
6	0.620912000	-0.240786000	-0.038634000	6	-2.699591000	0.882609000	-0.168512000
6	-0.479222000	-1.063173000	-0.088839000	6	-1.494586000	1.652140000	-0.163515000
8	-0.832555000	2.976139000	0.268266000	8	-3.823973000	1.384191000	-0.286236000
7	1.886203000	-0.786625000	0.098240000	6	3.491334000	-0.922350000	-0.198341000
6	2.116906000	-2.160347000	-0.150229000	6	3.539881000	-2.285202000	-0.079472000
6	0.952910000	-3.002021000	-0.247166000	6	2.316107000	-2.963191000	0.105487000
6	-0.285087000	-2.474424000	-0.166307000	7	1.137763000	-2.375052000	0.161490000
8	3.266249000	-2.591491000	-0.219933000	8	2.358658000	-4.290387000	0.229406000
1	-5.314731000	0.991737000	0.324306000	1	-1.330941000	-2.168820000	0.116975000
1	-3.301957000	2.526439000	0.428894000	1	-1.642605000	2.715510000	-0.238845000
1	-4.814130000	-2.447469000	-0.178517000	1	4.386562000	-0.329371000	-0.338949000
1	1.143406000	-4.059760000	-0.361301000	1	4.461068000	-2.849082000	-0.119422000
1	-1.169192000	-3.098345000	-0.202114000	1	1.454510000	-4.610250000	0.347709000
6	2.952709000	0.007539000	0.768351000	6	-3.729669000	-1.427600000	-0.002080000
8	2.646788000	0.933983000	1.450000000	8	-3.536261000	-2.596021000	0.117025000
8	4.150719000	-0.437197000	0.558880000	8	-4.867674000	-0.821126000	-0.116993000
1	4.097531000	-1.335159000	0.109226000	1	-4.700875000	0.182047000	-0.208788000
6	1.564005000	1.928996000	-0.765045000	6	0.890947000	3.249534000	0.299860000
8	2.355530000	1.374809000	-1.458736000	8	-0.056118000	3.707515000	0.853380000
8	1.520648000	3.206067000	-0.524328000	8	1.943631000	3.934015000	-0.062890000
1	0.683416000	3.432587000	-0.042607000	1	2.665753000	3.314884000	-0.350166000
pn3''-(COOH)₂				pn4''-(COOH)₂			

6	-1.816174000	1.208115000	0.065797000	6	2.931750000	-1.348843000	-0.132015000
6	-0.792112000	0.262557000	-0.058471000	6	1.775665000	-0.580174000	-0.051424000
6	0.550497000	0.737746000	0.042737000	6	1.926553000	0.800999000	0.162847000
6	0.733428000	2.115556000	-0.109622000	6	3.208939000	1.336560000	0.298503000
7	-0.264132000	3.022835000	-0.111754000	7	4.307974000	0.604422000	0.232744000
6	-1.476900000	2.579093000	0.056202000	6	4.156465000	-0.703134000	0.017445000
8	-2.480138000	3.463485000	0.179512000	8	5.269742000	-1.439145000	-0.055822000
7	1.692666000	-0.060951000	0.253003000	6	0.429750000	-1.124718000	-0.091572000
6	2.966926000	0.374200000	-0.125483000	6	-0.643051000	-0.263729000	-0.039139000
6	3.112375000	1.791411000	-0.426148000	7	-0.466048000	1.118478000	-0.131394000
6	2.065521000	2.622571000	-0.346579000	6	0.783670000	1.700060000	0.154800000
8	3.933000000	-0.381704000	-0.119542000	8	0.887126000	2.907807000	0.312146000
6	-3.179714000	0.784883000	0.223631000	6	0.165713000	-2.526508000	-0.149827000
6	-3.478261000	-0.521139000	0.296062000	6	-1.091892000	-3.006670000	-0.223236000
6	-2.457764000	-1.529202000	0.075793000	6	-2.220550000	-2.118655000	-0.135369000
7	-1.171273000	-1.068312000	-0.266233000	7	-1.928176000	-0.757249000	0.107976000
8	-2.710336000	-2.727114000	0.108645000	8	-3.385954000	-2.501695000	-0.205962000
1	-2.096107000	4.347722000	0.127224000	1	2.928934000	-2.416018000	-0.298575000
1	4.118474000	2.116148000	-0.653741000	1	3.326170000	2.402610000	0.460223000
1	2.160089000	3.690443000	-0.502799000	1	6.020853000	-0.844046000	0.067665000
1	-3.941033000	1.547488000	0.329130000	1	0.999579000	-3.216497000	-0.173039000
1	-4.475581000	-0.898781000	0.473496000	1	-1.321573000	-4.058165000	-0.321120000
6	1.552120000	-1.255589000	1.079127000	6	-2.964383000	0.088445000	0.768168000
8	0.558549000	-1.412213000	1.724107000	8	-2.621691000	1.001227000	1.449618000
8	2.564733000	-2.075072000	1.050120000	8	-4.179608000	-0.301656000	0.549493000
1	3.301301000	-1.677364000	0.505771000	1	-4.166555000	-1.202420000	0.105344000
6	-0.276024000	-1.939625000	-1.031466000	6	-1.512858000	1.926078000	-0.789808000
8	0.581210000	-1.453436000	-1.704040000	8	-2.314790000	1.389664000	-1.486299000
8	-0.514587000	-3.215174000	-0.920983000	8	-1.435624000	3.204444000	-0.561888000
1	-1.350918000	-3.354307000	-0.396231000	1	-0.611889000	3.411552000	-0.052317000
pn5''-(COOH) ₂				pn6''-(COOH) ₂			
6	0.685921000	-0.623025000	-0.124610000	6	-2.282274000	0.465414000	-0.193464000
6	0.270346000	0.726056000	0.074503000	6	-1.629245000	-0.731805000	0.057287000
6	-1.166501000	0.994700000	0.027905000	6	-0.162644000	-0.729699000	0.113764000
6	-2.063220000	-0.063660000	-0.094110000	6	0.529599000	0.518052000	0.011292000
7	-1.614029000	-1.420324000	-0.069354000	7	-0.201077000	1.747888000	-0.017799000
6	-0.264877000	-1.733631000	-0.224634000	6	-1.571361000	1.750109000	-0.250814000
8	0.120193000	-2.885620000	-0.383369000	8	-2.197184000	2.787534000	-0.441912000
7	-1.547248000	2.283664000	0.026688000	6	0.529689000	-1.901596000	0.172143000
6	-2.817641000	2.562886000	-0.124327000	6	1.955343000	-1.941321000	0.109464000
6	-3.797867000	1.579479000	-0.340553000	7	2.575310000	-0.701671000	-0.082332000
6	-3.413997000	0.263520000	-0.328516000	6	1.883945000	0.479254000	-0.124817000
8	-3.205277000	3.846993000	-0.098645000	8	2.620827000	-2.984198000	0.186818000
6	2.016842000	-0.913552000	-0.161438000	6	-3.682459000	0.452744000	-0.329580000
7	2.954285000	0.054044000	-0.009406000	6	-4.352281000	-0.734411000	-0.200961000
6	2.604483000	1.412158000	0.200854000	6	-3.586851000	-1.888212000	0.069027000
6	1.204648000	1.705053000	0.228399000	7	-2.274640000	-1.897017000	0.188552000
8	3.490239000	2.260162000	0.340220000	8	-4.239103000	-3.043630000	0.208418000
1	-4.823629000	1.872403000	-0.517180000	1	0.012624000	-2.847797000	0.239578000
1	-4.148077000	-0.509216000	-0.491871000	1	2.507754000	1.347375000	-0.259126000
1	-2.420716000	4.391315000	0.041195000	1	-4.200276000	1.383115000	-0.526717000
1	2.391975000	-1.918791000	-0.305831000	1	-5.426367000	-0.817423000	-0.291995000
1	0.923446000	2.739190000	0.365225000	1	-3.589818000	-3.736264000	0.387631000
6	4.374907000	-0.399940000	-0.068696000	6	4.050089000	-0.583913000	-0.265770000
8	4.595487000	-1.553248000	-0.250389000	8	4.517482000	0.487024000	-0.483480000
8	5.232927000	0.555930000	0.092410000	8	4.675534000	-1.714265000	-0.166585000

1	4.736113000	1.433262000	0.224961000	1	3.998207000	-2.457880000	0.005319000
6	-2.563909000	-2.460568000	0.328271000	6	0.482988000	2.980706000	0.385859000
8	-3.598004000	-2.167824000	0.843008000	8	1.554773000	2.932930000	0.902195000
8	-2.183675000	-3.685806000	0.072538000	8	-0.170892000	4.084594000	0.134116000
1	-1.240094000	-3.691410000	-0.236448000	1	-1.078014000	3.872623000	-0.210760000
pn7''-(COOH)₂				pn8''-(COOH)₂			
6	-1.295822000	1.065551000	0.000105000	6	-2.036881000	-0.878337000	0.201186000
6	-0.359889000	-0.029749000	0.000071000	6	-1.893984000	0.493389000	-0.008573000
6	1.044427000	0.344555000	0.000020000	6	-0.558722000	1.073776000	-0.054019000
6	1.378866000	1.700094000	0.000035000	6	0.524033000	0.222271000	-0.029320000
7	0.463682000	2.725840000	0.000116000	7	0.357723000	-1.161203000	-0.150174000
6	-0.788485000	2.414679000	0.000137000	6	-0.860921000	-1.761592000	0.164810000
8	-1.697833000	3.385222000	0.000210000	8	-0.956860000	-2.969924000	0.310245000
6	2.089949000	-0.655606000	-0.000083000	6	-3.292972000	-1.473598000	0.353702000
7	3.413733000	-0.190658000	-0.000131000	6	-4.397139000	-0.656883000	0.281054000
6	3.712130000	1.151921000	-0.000120000	7	-4.302795000	0.662095000	0.056065000
6	2.748703000	2.092911000	-0.000036000	6	-3.120286000	1.209181000	-0.085938000
8	1.871467000	-1.873298000	-0.000229000	8	-3.097943000	2.535197000	-0.323918000
6	-2.640471000	0.826957000	0.000075000	6	-0.285672000	2.481359000	-0.084018000
7	-3.128432000	-0.431840000	0.000066000	6	0.976114000	2.954492000	-0.154627000
6	-2.271695000	-1.561338000	0.000151000	6	2.105452000	2.072212000	-0.089374000
6	-0.868859000	-1.306814000	0.000104000	7	1.812394000	0.708408000	0.122371000
8	-2.768168000	-2.695787000	0.000343000	8	3.273363000	2.457493000	-0.150141000
1	-1.228754000	4.231120000	0.000169000	1	-3.369810000	-2.540088000	0.511690000
1	4.770069000	1.371066000	-0.000178000	1	-5.400833000	-1.049129000	0.393948000
1	2.994106000	3.144442000	-0.000027000	1	-4.019277000	2.826657000	-0.347884000
1	-3.381297000	1.615904000	0.000057000	1	-1.115943000	3.169589000	-0.093864000
1	-0.238955000	-2.180302000	0.000089000	1	1.201785000	4.008585000	-0.233610000
6	4.579594000	-1.102142000	-0.000216000	6	2.848927000	-0.151272000	0.760915000
8	5.674138000	-0.633985000	-0.000243000	8	2.509775000	-1.092289000	1.407183000
8	4.277671000	-2.365378000	0.000369000	8	4.060705000	0.256823000	0.564810000
1	3.274413000	-2.463533000	0.000568000	1	4.037601000	1.176024000	0.147083000
6	-4.616341000	-0.561853000	-0.000214000	6	1.404865000	-1.946393000	-0.842031000
8	-5.270507000	0.431791000	-0.000449000	8	2.176852000	-1.387668000	-1.552492000
8	-5.024201000	-1.787139000	-0.000171000	8	1.354499000	-3.228567000	-0.626422000
1	-4.205647000	-2.408501000	0.000135000	1	0.555197000	-3.456885000	-0.091909000
pn9''-(COOH)₂				pn10''-(COOH)₂			
6	2.092587000	0.535585000	-0.189527000	6	1.863015000	-2.710838000	-0.644953000
6	0.823196000	1.080510000	0.040446000	6	0.544799000	-2.507095000	-0.476452000
6	-0.322403000	0.177803000	0.028855000	6	0.053581000	-1.179124000	-0.211514000
6	-0.110300000	-1.192110000	-0.029937000	6	0.947148000	-0.169801000	-0.038793000
7	1.192351000	-1.715256000	-0.049022000	7	2.314808000	-0.411419000	-0.023834000
6	2.303666000	-0.892330000	-0.295372000	6	2.834777000	-1.640771000	-0.452729000
8	3.405783000	-1.376521000	-0.537097000	8	4.039246000	-1.802681000	-0.595577000
6	-1.680013000	0.708682000	0.015406000	6	-1.363210000	-0.891149000	-0.079689000
7	-2.717289000	-0.231192000	-0.084300000	6	-1.785789000	0.427261000	0.086246000
6	-2.466508000	-1.573199000	-0.191212000	7	-0.851037000	1.483338000	-0.080190000
6	-1.219563000	-2.080290000	-0.165786000	6	0.514783000	1.235647000	-0.147204000
8	-1.955976000	1.906562000	0.076998000	8	1.331968000	2.112639000	-0.399747000
6	3.206621000	1.391217000	-0.266790000	7	-2.196071000	-1.945440000	-0.010073000
6	3.031293000	2.736327000	-0.093923000	6	-3.457138000	-1.724197000	0.272047000
6	1.717041000	3.176689000	0.165668000	6	-3.968862000	-0.448599000	0.559205000
7	0.659706000	2.395876000	0.225928000	6	-3.126448000	0.630419000	0.466474000
8	1.527789000	4.482329000	0.366228000	8	-4.299621000	-2.768547000	0.316951000
1	-3.349388000	-2.186330000	-0.299957000	1	2.283430000	-3.675812000	-0.895354000
1	-1.088792000	-3.143992000	-0.249715000	1	-0.177030000	-3.306794000	-0.579641000

1	4.182479000	0.960447000	-0.453978000	1	-5.004697000	-0.338886000	0.848702000
1	3.841591000	3.450375000	-0.137315000	1	-3.497265000	1.619079000	0.681246000
1	0.582096000	4.616299000	0.518933000	1	-3.793725000	-3.566126000	0.120464000
6	-4.146117000	0.159251000	-0.116596000	6	3.152278000	0.470245000	0.815225000
8	-4.970915000	-0.693501000	-0.215664000	8	2.654241000	1.072162000	1.707910000
8	-4.352263000	1.437370000	-0.030412000	8	4.420382000	0.461138000	0.495330000
1	-3.454563000	1.904520000	0.031328000	1	4.607634000	-0.302984000	-0.101781000
6	1.414142000	-3.119291000	0.353752000	6	-1.365230000	2.816404000	-0.450398000
8	0.607756000	-3.684339000	1.020902000	8	-2.516945000	2.959737000	-0.716769000
8	2.533299000	-3.633674000	-0.075321000	8	-0.478378000	3.772125000	-0.442963000
1	3.117572000	-2.906195000	-0.432496000	1	0.438371000	3.383172000	-0.380814000
pn11''-(COOH)₂				pn12''-(COOH)₂			
6	-2.223775000	0.573295000	-0.240152000	6	-2.216477000	-0.121070000	-0.180566000
6	-1.721417000	-0.690796000	0.060029000	6	-1.139451000	-0.986458000	0.056484000
6	-0.273272000	-0.869541000	0.130025000	6	0.199626000	-0.405830000	0.053624000
6	0.522583000	0.236416000	0.022662000	6	0.378614000	1.023196000	-0.028974000
7	-0.002939000	1.534387000	-0.043390000	7	-0.766726000	1.854762000	-0.030157000
6	-1.352137000	1.749656000	-0.323112000	6	-2.046184000	1.326265000	-0.277502000
8	-1.785763000	2.868786000	-0.556404000	8	-2.995820000	2.060580000	-0.512471000
6	0.318647000	-2.164561000	0.237078000	6	1.308013000	-1.192686000	0.043788000
6	1.658139000	-2.282117000	0.186626000	7	2.568767000	-0.692819000	-0.036335000
7	2.468035000	-1.186504000	-0.048928000	6	2.797230000	0.688536000	-0.158360000
6	1.950547000	0.092837000	-0.244024000	6	1.640825000	1.528386000	-0.151138000
8	2.645206000	1.015825000	-0.662598000	8	3.950772000	1.118705000	-0.267423000
6	-3.612365000	0.726200000	-0.395082000	6	-3.507911000	-0.646926000	-0.256876000
6	-4.423353000	-0.366391000	-0.238980000	7	-3.773751000	-1.933860000	-0.106289000
6	-3.807880000	-1.596573000	0.074515000	6	-2.744114000	-2.744473000	0.137057000
7	-2.508395000	-1.765658000	0.212529000	6	-1.414744000	-2.334759000	0.231731000
8	-4.600831000	-2.658739000	0.237231000	8	-3.014787000	-4.041204000	0.299713000
1	-0.311922000	-3.030136000	0.370249000	1	1.268564000	-2.271990000	0.084055000
1	2.193786000	-3.213492000	0.292798000	1	1.850939000	2.581775000	-0.225226000
1	-4.009440000	1.706801000	-0.628035000	1	-4.345060000	0.017348000	-0.440229000
1	-5.498684000	-0.321515000	-0.341690000	1	-0.657701000	-3.078826000	0.435465000
1	-4.043199000	-3.419274000	0.445852000	1	-3.969958000	-4.155439000	0.208207000
6	0.772866000	2.601187000	0.606899000	6	3.672739000	-1.685049000	-0.026948000
8	1.566152000	2.325395000	1.444929000	8	3.400679000	-2.839831000	0.074884000
8	0.473519000	3.811562000	0.199808000	8	4.847856000	-1.154532000	-0.134853000
1	-0.357439000	3.793704000	-0.323882000	1	4.749528000	-0.141438000	-0.210653000
6	3.913352000	-1.467462000	-0.165071000	6	-0.618922000	3.272388000	0.345337000
8	4.303463000	-2.571826000	0.046504000	8	0.338820000	3.637635000	0.947642000
8	4.641314000	-0.441292000	-0.494756000	8	-1.602375000	4.046824000	-0.030750000
1	4.053916000	0.357732000	-0.642980000	1	-2.350957000	3.497446000	-0.382024000
pn13''-(COOH)₂				pn14''-(COOH)₂			
6	-0.382585000	-1.204301000	-0.000676000	6	-3.966473000	1.562025000	-0.096892000
6	-0.484707000	0.205520000	0.000138000	6	-2.658856000	1.948547000	-0.211177000
6	0.731454000	1.006090000	0.000104000	6	-1.628036000	0.988077000	-0.095844000
6	1.988749000	0.390988000	-0.000194000	6	-2.031118000	-0.326855000	0.112960000
7	2.088539000	-1.057889000	0.000109000	7	-3.307186000	-0.718739000	0.235079000
6	0.953641000	-1.856235000	-0.000792000	6	-4.236964000	0.196751000	0.140733000
8	0.993739000	-3.081848000	-0.001332000	8	-5.518939000	-0.171533000	0.268084000
7	0.556774000	2.335542000	-0.000060000	6	-0.211102000	1.308072000	-0.104927000
6	1.608772000	3.118888000	-0.000793000	6	0.705516000	0.286394000	-0.048146000
6	2.915007000	2.622281000	-0.001776000	7	0.293946000	-1.043609000	-0.148357000
6	3.100959000	1.260098000	-0.001530000	6	-1.032640000	-1.416707000	0.128091000
8	1.421001000	4.446796000	-0.000789000	8	-1.338884000	-2.583291000	0.281092000
6	-1.488217000	-1.996857000	-0.001081000	6	0.284278000	2.646802000	-0.150082000

6	-2.802781000	-1.421930000	-0.000758000	6	1.605668000	2.911013000	-0.208502000
7	-2.852090000	-0.015502000	0.000197000	6	2.572029000	1.849205000	-0.113118000
6	-1.730187000	0.759118000	0.000521000	7	2.056360000	0.556715000	0.115445000
8	-3.842373000	-2.090191000	-0.001032000	8	3.786599000	2.039143000	-0.162703000
1	3.754905000	3.302934000	-0.002709000	1	-4.787457000	2.261258000	-0.181540000
1	4.103893000	0.877089000	-0.002276000	1	-2.429523000	2.990248000	-0.393829000
1	0.470252000	4.612792000	-0.000146000	1	-5.536027000	-1.125843000	0.418270000
1	-1.419309000	-3.075589000	-0.001659000	1	-0.418554000	3.469858000	-0.175390000
1	-1.896545000	1.826665000	0.001080000	1	2.006693000	3.910847000	-0.295425000
6	-4.148660000	0.724549000	0.000753000	6	2.924981000	-0.449332000	0.787002000
8	-4.125624000	1.912950000	0.000429000	8	2.424670000	-1.301819000	1.449775000
8	-5.188337000	-0.046807000	0.000246000	8	4.192319000	-0.258863000	0.599290000
1	-4.886378000	-1.018823000	0.000137000	1	4.333579000	0.635658000	0.162043000
6	3.421484000	-1.705711000	0.002254000	6	1.199435000	-2.017276000	-0.796233000
8	4.420824000	-1.058642000	0.007104000	8	2.082968000	-1.621171000	-1.487514000
8	3.414009000	-3.009762000	-0.000874000	8	0.910093000	-3.264117000	-0.566569000
1	2.477148000	-3.355071000	-0.003190000	1	0.058543000	-3.329700000	-0.064118000
pn15''-(COOH)₂				pn16''-(COOH)₂			
6	-2.116465000	-0.116232000	0.104838000	6	-3.335686000	-0.791377000	0.250962000
6	-1.624837000	1.184210000	-0.087231000	6	-2.007447000	-0.418530000	0.130026000
6	-0.188758000	1.396907000	-0.086597000	6	-1.648641000	0.916477000	-0.095886000
6	0.652089000	0.308184000	-0.043920000	6	-2.703772000	1.828627000	-0.211176000
7	0.147914000	-0.980955000	-0.166643000	7	-3.980395000	1.489265000	-0.101051000
6	-1.210629000	-1.261119000	0.118776000	6	-4.286952000	0.217650000	0.133571000
8	-1.565059000	-2.413710000	0.285423000	8	-5.584250000	-0.099003000	0.251713000
6	-3.521271000	-0.286108000	0.203828000	6	-0.975097000	-1.471494000	0.142278000
7	-4.378922000	0.712753000	0.103336000	7	0.330891000	-1.063961000	-0.145793000
6	-3.892323000	1.939424000	-0.102604000	6	0.702766000	0.285389000	-0.049832000
6	-2.548190000	2.232948000	-0.201385000	6	-0.240498000	1.279064000	-0.111338000
8	-4.031357000	-1.497105000	0.401614000	8	-1.255065000	-2.646790000	0.303889000
6	0.400256000	2.697667000	-0.103316000	7	2.046471000	0.591858000	0.115031000
6	1.736835000	2.868719000	-0.152157000	6	2.525847000	1.897300000	-0.115382000
6	2.623441000	1.738179000	-0.082644000	6	1.530119000	2.931728000	-0.215858000
7	2.015358000	0.479215000	0.123380000	6	0.216613000	2.632269000	-0.157867000
8	3.847098000	1.837097000	-0.136899000	8	3.734808000	2.121945000	-0.161268000
1	-4.631667000	2.728911000	-0.188495000	1	-3.618964000	-1.821574000	0.417296000
1	-2.240879000	3.254458000	-0.366729000	1	-2.518651000	2.879293000	-0.403404000
1	-4.992309000	-1.390281000	0.423921000	1	-6.095700000	0.711670000	0.136928000
1	-0.242658000	3.567923000	-0.110558000	1	1.903859000	3.942056000	-0.303859000
1	2.208861000	3.838771000	-0.216360000	1	-0.509802000	3.434481000	-0.185129000
6	2.815915000	-0.604723000	0.764343000	6	2.941449000	-0.388869000	0.787078000
8	2.261052000	-1.426536000	1.420878000	8	2.463681000	-1.259659000	1.443614000
8	4.090914000	-0.508079000	0.558880000	8	4.203113000	-0.160216000	0.606294000
1	4.295540000	0.381635000	0.140249000	1	4.319427000	0.739886000	0.170846000
6	0.977388000	-2.003814000	-0.836236000	6	1.262019000	-2.005788000	-0.799997000
8	1.882862000	-1.658163000	-1.527562000	8	2.122845000	-1.581121000	-1.501806000
8	0.605645000	-3.231160000	-0.624222000	8	1.023087000	-3.264257000	-0.565377000
1	-0.237276000	-3.242721000	-0.101598000	1	0.190985000	-3.367807000	-0.045929000
pn17''-(COOH)₂				pn18''-(COOH)₂			
6	1.347061000	1.537925000	0.000066000	6	1.766330000	-2.487161000	-0.324917000
6	0.544730000	0.352755000	0.000015000	6	0.533084000	-1.977719000	-0.169366000
6	-0.900345000	0.513318000	0.000056000	6	0.331151000	-0.538678000	-0.115701000
6	-1.424392000	1.796707000	0.000160000	6	1.467297000	0.252937000	-0.134893000
7	-0.643488000	2.938427000	0.000221000	7	2.751003000	-0.297083000	-0.059983000
6	0.632905000	2.813604000	0.000176000	6	2.962828000	-1.658837000	-0.301329000
8	1.404295000	3.898056000	0.000230000	8	4.092430000	-2.117951000	-0.411284000

6	-1.791473000	-0.625300000	-0.000011000	6	-0.944213000	0.117499000	-0.111638000
7	-3.162549000	-0.355569000	0.000039000	6	-0.966274000	1.515956000	-0.191801000
6	-3.656185000	0.931124000	0.000167000	7	0.150057000	2.251552000	-0.384539000
6	-2.834891000	1.998155000	0.000224000	6	1.304282000	1.649124000	-0.401661000
8	-1.388980000	-1.798116000	-0.000077000	8	2.379636000	2.337225000	-0.766731000
6	2.711375000	1.492492000	0.000021000	6	-2.196288000	-0.615297000	0.006418000
6	3.401970000	0.244525000	-0.000087000	7	-3.366555000	0.142535000	0.063608000
7	2.581592000	-0.896969000	-0.000101000	6	-3.354892000	1.527671000	0.001657000
6	1.221165000	-0.844921000	-0.000054000	6	-2.212531000	2.218216000	-0.124584000
8	4.637414000	0.137531000	-0.000174000	8	-2.259772000	-1.850783000	0.067549000
1	0.826481000	4.673655000	0.000296000	1	1.944432000	-3.549830000	-0.424475000
1	-4.734245000	0.993460000	0.000203000	1	-0.328649000	-2.625202000	-0.135819000
1	-3.225296000	3.005020000	0.000314000	1	2.116197000	3.258346000	-0.894140000
1	3.315767000	2.388407000	0.000062000	1	-4.334123000	1.978451000	0.059412000
1	0.729321000	-1.804884000	-0.000069000	1	-2.211962000	3.296683000	-0.181527000
6	-4.182680000	-1.429631000	-0.000028000	6	3.773633000	0.460457000	0.680673000
8	-5.333780000	-1.126709000	0.000254000	8	3.442770000	1.309449000	1.442140000
8	-3.698307000	-2.634408000	-0.000480000	8	5.001710000	0.082862000	0.431911000
1	-2.691015000	-2.586962000	-0.000769000	1	4.993002000	-0.778342000	-0.055984000
6	3.169224000	-2.278422000	-0.000142000	6	-4.705431000	-0.468280000	0.195640000
8	2.431348000	-3.208941000	-0.000014000	8	-5.660836000	0.240574000	0.238020000
8	4.462237000	-2.287622000	-0.000275000	8	-4.709731000	-1.767997000	0.254681000
1	4.805499000	-1.322238000	-0.000227000	1	-3.763978000	-2.101512000	0.197654000
pn19''-(COOH)₂				pn20''-(COOH)₂			
6	0.765077000	0.402645000	-0.092506000	6	1.486121000	1.635436000	-0.000089000
6	0.212288000	-0.853083000	0.062610000	6	0.823304000	0.428580000	0.000059000
6	-1.231914000	-1.008489000	0.019019000	6	-0.627667000	0.419313000	-0.000031000
6	-2.044107000	0.118334000	-0.069061000	6	-1.305013000	1.693266000	-0.000274000
7	-1.466138000	1.405581000	-0.054142000	7	-0.608559000	2.887818000	-0.000430000
6	-0.080474000	1.593012000	-0.215557000	6	0.671671000	2.848071000	-0.000322000
8	0.373112000	2.712893000	-0.402642000	8	1.368019000	3.986424000	-0.000420000
7	-1.713624000	-2.268798000	0.013711000	6	-1.410886000	-0.709403000	0.000148000
6	-3.002522000	-2.442510000	-0.108503000	7	-2.766431000	-0.642488000	0.000112000
6	-3.909282000	-1.378567000	-0.279059000	6	-3.473849000	0.579965000	-0.000128000
6	-3.427964000	-0.097691000	-0.260840000	6	-2.674527000	1.750103000	-0.000349000
8	-3.496550000	-3.690528000	-0.094931000	8	-4.716085000	0.577785000	-0.000294000
6	2.212803000	0.581562000	-0.111277000	6	2.906745000	1.714404000	-0.000022000
7	2.969057000	-0.597068000	0.059514000	6	3.617447000	0.570005000	0.000153000
6	2.384445000	-1.828130000	0.217139000	7	2.994028000	-0.661404000	0.000310000
6	1.045419000	-1.993380000	0.219006000	6	1.607638000	-0.804032000	0.000247000
8	2.785252000	1.655285000	-0.257580000	8	1.092063000	-1.925928000	0.000253000
1	-4.959521000	-1.589451000	-0.427830000	1	0.735688000	4.718355000	-0.000576000
1	-4.104039000	0.731349000	-0.391624000	1	-1.009168000	-1.710485000	0.000319000
1	-2.758197000	-4.302040000	0.013961000	1	-3.184781000	2.702539000	-0.000559000
1	3.089061000	-2.639504000	0.334171000	1	3.403609000	2.672457000	-0.000147000
1	0.605743000	-2.971002000	0.334707000	1	4.696026000	0.521993000	0.000192000
6	4.451746000	-0.589376000	0.075669000	6	-3.477333000	-1.958109000	0.000325000
8	5.027811000	-1.620192000	0.226310000	8	-2.829732000	-2.955803000	-0.000114000
8	4.984557000	0.583098000	-0.081227000	8	-4.764772000	-1.845677000	-0.000292000
1	4.249249000	1.267635000	-0.185263000	1	-5.010251000	-0.845079000	-0.000291000
6	-2.315483000	2.549238000	0.308705000	6	3.910613000	-1.832751000	0.000366000
8	-3.370057000	2.366336000	0.834582000	8	5.083414000	-1.638004000	0.000248000
8	-1.821177000	3.717815000	0.011015000	8	3.315798000	-2.986698000	0.000626000
1	-0.871138000	3.605953000	-0.287985000	1	2.320388000	-2.853150000	0.000569000
pn21''-(COOH)₂				pn22''-(COOH)₂			

6	-1.315614000	0.832888000	0.000213000	6	-2.248217000	0.436692000	-0.235911000
6	-0.321524000	-0.162195000	0.000070000	6	-1.605007000	-0.769741000	0.069715000
6	1.049375000	0.253979000	-0.000075000	6	-0.134820000	-0.768931000	0.115445000
6	1.319155000	1.633428000	-0.000121000	6	0.552754000	0.482930000	0.013735000
7	0.358686000	2.575999000	-0.000013000	7	-0.175488000	1.712876000	-0.018249000
6	-0.897080000	2.199941000	0.000160000	6	-1.537139000	1.719456000	-0.304900000
8	-1.805137000	3.163161000	0.000262000	8	-2.144964000	2.758637000	-0.532715000
6	2.155354000	-0.695126000	-0.000150000	6	0.580201000	-1.929600000	0.155639000
7	3.448980000	-0.158745000	-0.000344000	6	2.007626000	-1.955136000	0.095055000
6	3.678612000	1.205500000	-0.000407000	7	2.615078000	-0.710137000	-0.086356000
6	2.674585000	2.094817000	-0.000294000	6	1.906962000	0.459441000	-0.125970000
8	2.008143000	-1.921652000	-0.000091000	8	2.678768000	-2.993745000	0.165337000
6	-2.737522000	0.502552000	0.000400000	6	-3.636863000	0.441563000	-0.374319000
7	-3.046375000	-0.864177000	0.000319000	7	-4.382024000	-0.643221000	-0.223333000
6	-2.061265000	-1.825417000	0.000157000	6	-3.761047000	-1.777189000	0.088533000
6	-0.747248000	-1.532413000	0.000058000	6	-2.379424000	-1.903244000	0.248385000
8	-3.637222000	1.337565000	0.000622000	8	-4.514670000	-2.866003000	0.255142000
1	-1.319269000	4.000150000	0.000174000	1	0.108265000	-2.900218000	0.202907000
1	4.724438000	1.475084000	-0.000554000	1	2.517312000	1.337581000	-0.260684000
1	2.866000000	3.157550000	-0.000339000	1	-4.147449000	1.368837000	-0.608126000
1	-2.438073000	-2.838308000	0.000120000	1	-1.969609000	-2.870542000	0.500760000
1	-0.030270000	-2.332822000	-0.000050000	1	-5.436033000	-2.611994000	0.112068000
6	4.663729000	-0.998940000	-0.000485000	6	4.088868000	-0.574404000	-0.269024000
8	5.730214000	-0.469842000	-0.000623000	8	4.542997000	0.503100000	-0.479007000
8	4.442799000	-2.280999000	-0.000458000	8	4.727370000	-1.698447000	-0.177522000
1	3.452617000	-2.442533000	-0.000358000	1	4.062726000	-2.451104000	-0.012384000
6	-4.435274000	-1.366360000	0.000293000	6	0.495285000	2.935071000	0.431532000
8	-4.623346000	-2.541816000	0.000117000	8	1.544546000	2.874564000	0.991618000
8	-5.345347000	-0.437607000	0.000404000	8	-0.144325000	4.045163000	0.169860000
1	-4.897011000	0.462951000	0.000496000	1	-1.031032000	3.843200000	-0.228173000
pn23''-(COOH) ₂				pn24''-(COOH) ₂			
6	-2.200846000	0.524203000	-0.255344000	6	-2.417080000	0.182597000	0.259217000
6	-1.694485000	-0.744944000	0.076385000	6	-1.645133000	-0.937976000	-0.044653000
6	-0.240166000	-0.909335000	0.137441000	6	-0.186548000	-0.801124000	-0.103021000
6	0.541213000	0.206340000	0.021682000	6	0.367311000	0.522995000	-0.008169000
7	0.006950000	1.501675000	-0.042776000	7	-0.485598000	1.671552000	0.000253000
6	-1.340113000	1.707621000	-0.346962000	6	-1.824607000	1.546595000	0.310351000
8	-1.771193000	2.822155000	-0.597585000	8	-2.541785000	2.511660000	0.533891000
6	0.387093000	-2.190998000	0.239260000	6	0.671467000	-1.866023000	-0.142929000
6	1.728591000	-2.285097000	0.184490000	6	2.091385000	-1.715689000	-0.064553000
7	2.517429000	-1.178065000	-0.052150000	7	2.553634000	-0.411320000	0.120350000
6	1.972536000	0.089021000	-0.250423000	6	1.709400000	0.664028000	0.143228000
8	2.646745000	1.023814000	-0.672544000	8	2.881398000	-2.669005000	-0.123091000
6	-3.578087000	0.680243000	-0.407134000	6	-3.796376000	0.087917000	0.429760000
7	-4.440288000	-0.313845000	-0.251080000	6	-4.375805000	-1.156041000	0.273597000
6	-3.950577000	-1.507509000	0.072921000	7	-3.674679000	-2.245597000	-0.047450000
6	-2.593629000	-1.786007000	0.246791000	6	-2.370696000	-2.145435000	-0.203645000
8	-4.823356000	-2.505449000	0.236929000	8	-1.722976000	-3.269552000	-0.539064000
1	-0.196169000	-3.089431000	0.369913000	1	0.323151000	-2.882628000	-0.208628000
1	2.278408000	-3.208708000	0.287756000	1	2.207896000	1.611051000	0.273169000
1	-3.979841000	1.655939000	-0.657547000	1	-4.377287000	0.968622000	0.662964000
1	-2.296269000	-2.792675000	0.502393000	1	-5.443467000	-1.297234000	0.397941000
1	-5.708434000	-2.149749000	0.082600000	1	-2.387379000	-3.968633000	-0.608881000
6	0.766510000	2.564908000	0.625964000	6	3.995216000	-0.105036000	0.317081000
8	1.558747000	2.284991000	1.464632000	8	4.320132000	1.019621000	0.525928000
8	0.458946000	3.778598000	0.235446000	8	4.760408000	-1.148158000	0.239741000

1	-0.356063000	3.760805000	-0.312000000	1	4.184063000	-1.972342000	0.068804000
6	3.968721000	-1.431984000	-0.166970000	6	0.048309000	2.948924000	-0.490375000
8	4.377616000	-2.528772000	0.046514000	8	1.076300000	2.980534000	-1.087571000
8	4.676647000	-0.392590000	-0.497244000	8	-0.688877000	3.995635000	-0.219698000
1	4.075951000	0.394721000	-0.648860000	1	-1.538331000	3.718439000	0.206136000
pn25''-(COOH)₂				pn26''-(COOH)₂			
6	-2.074030000	-0.671426000	-0.103985000	6	-2.146269000	-0.184350000	-0.143080000
6	-0.862563000	-1.326068000	0.140434000	6	-1.068822000	-1.036552000	0.105926000
6	0.364431000	-0.537619000	0.085797000	6	0.281882000	-0.483872000	0.074104000
6	0.313080000	0.898247000	-0.004531000	6	0.477023000	0.940255000	-0.023513000
7	-0.951636000	1.519320000	-0.004860000	7	-0.665324000	1.783949000	-0.032490000
6	-2.130057000	0.784877000	-0.276991000	6	-1.944295000	1.276284000	-0.281368000
8	-3.153971000	1.366311000	-0.585070000	8	-2.884980000	2.007710000	-0.539052000
6	1.584463000	-1.137720000	0.051849000	6	1.384580000	-1.277504000	0.056830000
7	2.746515000	-0.442443000	-0.051204000	7	2.651616000	-0.783401000	-0.034925000
6	2.750341000	0.959511000	-0.164008000	6	2.890755000	0.591014000	-0.166714000
6	1.475987000	1.602464000	-0.137044000	6	1.739325000	1.438787000	-0.160615000
8	3.820462000	1.566867000	-0.286146000	8	4.046683000	1.016499000	-0.285375000
6	-3.256112000	-1.455578000	-0.115483000	6	-3.442118000	-0.669872000	-0.198754000
7	-3.258555000	-2.757925000	0.108701000	6	-3.613385000	-2.035171000	0.016355000
6	-2.093660000	-3.356737000	0.360735000	7	-2.612034000	-2.864234000	0.285665000
6	-0.878561000	-2.701444000	0.390542000	6	-1.377802000	-2.381003000	0.330303000
8	-4.435977000	-0.889145000	-0.346380000	8	-4.850955000	-2.546098000	-0.037077000
1	1.722046000	-2.208546000	0.088204000	1	1.342557000	-2.356194000	0.100564000
1	1.510212000	2.676194000	-0.211245000	1	1.954816000	2.490305000	-0.247917000
1	-2.144092000	-4.423985000	0.549255000	1	-4.283289000	-0.017882000	-0.388337000
1	0.019950000	-3.257841000	0.614189000	1	-0.603268000	-3.103561000	0.563646000
1	-5.094085000	-1.595664000	-0.288750000	1	-4.786419000	-3.492347000	0.143958000
6	3.994207000	-1.245525000	-0.068988000	6	3.747481000	-1.781864000	-0.026509000
8	3.911962000	-2.429947000	0.028173000	8	3.469601000	-2.935005000	0.083777000
8	5.067115000	-0.533826000	-0.192803000	8	4.926268000	-1.260738000	-0.144861000
1	4.805524000	0.452187000	-0.256600000	1	4.834154000	-0.246716000	-0.225870000
6	-1.042154000	2.942520000	0.359660000	6	-0.500692000	3.205484000	0.326902000
8	-0.166149000	3.458304000	0.977294000	8	0.445909000	3.559180000	0.950972000
8	-2.129127000	3.549323000	-0.038250000	8	-1.456886000	3.995662000	-0.088977000
1	-2.760569000	2.888876000	-0.425970000	1	-2.209461000	3.464704000	-0.448267000
pn27''-(COOH)₂				pn28''-(COOH)₂			
6	-0.729443000	1.882098000	0.124196000	6	1.997070000	2.530751000	-0.290652000
6	-0.255220000	0.580518000	-0.009685000	6	0.737829000	2.075489000	-0.171702000
6	1.151096000	0.363456000	-0.018681000	6	0.473911000	0.657520000	-0.134909000
6	1.968177000	1.481569000	-0.145505000	6	1.542282000	-0.194482000	-0.133194000
7	1.500585000	2.753477000	-0.067816000	7	2.852176000	0.277885000	-0.051538000
6	0.232628000	2.936979000	0.129565000	6	3.143128000	1.631602000	-0.265574000
8	-0.238373000	4.182811000	0.295485000	8	4.298063000	2.026616000	-0.358299000
7	1.736016000	-0.907449000	0.049744000	6	-0.857649000	0.086086000	-0.137979000
6	3.056041000	-1.124303000	-0.371399000	6	-0.989541000	-1.346696000	-0.196079000
6	3.869725000	0.059316000	-0.601322000	7	0.110429000	-2.143362000	-0.405199000
6	3.366437000	1.293520000	-0.432805000	6	1.279146000	-1.603536000	-0.414028000
8	3.508761000	-2.260328000	-0.471824000	8	2.325406000	-2.319486000	-0.804610000
6	-2.132453000	2.142776000	0.221483000	6	-1.995999000	0.830344000	-0.019600000
6	-2.994036000	1.117589000	0.123163000	7	-3.224056000	0.258284000	0.055921000
7	-2.562133000	-0.173987000	-0.147586000	6	-3.409575000	-1.143558000	0.028435000
6	-1.217629000	-0.489442000	-0.315165000	6	-2.234080000	-1.921677000	-0.109483000
8	-0.871724000	-1.584285000	-0.751713000	8	-4.560235000	-1.608791000	0.113160000
1	0.511504000	4.789637000	0.253925000	1	2.235684000	3.583003000	-0.369498000
1	4.901899000	-0.130999000	-0.861947000	1	-0.085391000	2.778976000	-0.153101000

1	3.974162000	2.183376000	-0.547366000	1	2.022384000	-3.222625000	-0.972060000
1	-2.487286000	3.148749000	0.386850000	1	-2.017512000	1.909631000	0.037592000
1	-4.065351000	1.211805000	0.216646000	1	-2.350923000	-2.994903000	-0.156908000
6	1.094908000	-1.900522000	0.925698000	6	3.830685000	-0.553098000	0.675236000
8	0.302447000	-1.544177000	1.740701000	8	3.445241000	-1.388573000	1.425009000
8	1.501641000	-3.124885000	0.741737000	8	5.077970000	-0.248720000	0.427393000
1	2.291591000	-3.125128000	0.137853000	1	5.122778000	0.621353000	-0.041625000
6	-3.632553000	-1.179260000	-0.301899000	6	-4.373066000	1.199643000	0.184714000
8	-4.759555000	-0.854759000	-0.100545000	8	-4.147158000	2.370282000	0.201255000
8	-3.227638000	-2.365162000	-0.654923000	8	-5.514803000	0.606519000	0.264884000
1	-2.238320000	-2.361224000	-0.783566000	1	-5.357587000	-0.418188000	0.219862000
pn29''-(COOH)₂				pn30''-(COOH)₂			
6	2.234337000	0.150276000	-0.174419000	6	3.682403000	-2.134124000	0.248510000
6	1.471775000	-0.981164000	0.135982000	6	2.321371000	-2.203521000	0.384069000
6	0.014488000	-0.872976000	0.150500000	6	1.535120000	-1.052801000	0.166189000
6	-0.571353000	0.428959000	0.023881000	6	2.214196000	0.116458000	-0.174416000
7	0.258885000	1.596307000	-0.012113000	7	3.539193000	0.194765000	-0.322663000
6	1.612473000	1.496825000	-0.285424000	6	4.243802000	-0.894967000	-0.122315000
8	2.308944000	2.471683000	-0.525152000	8	5.570382000	-0.830516000	-0.272532000
6	-0.802269000	-1.967973000	0.194791000	6	0.078044000	-1.045962000	0.191944000
6	-2.222901000	-1.872622000	0.112587000	6	-0.570914000	0.149925000	0.048716000
7	-2.724509000	-0.583036000	-0.094744000	7	0.124072000	1.366342000	-0.022046000
6	-1.918561000	0.520493000	-0.137737000	6	1.485910000	1.411215000	-0.313148000
8	-2.983454000	-2.848840000	0.184148000	8	2.053153000	2.453043000	-0.573337000
6	3.608074000	0.063827000	-0.292529000	6	-0.701110000	-2.243266000	0.292508000
6	4.184635000	-1.189071000	-0.077523000	6	-2.042912000	-2.179380000	0.204785000
7	3.490160000	-2.272379000	0.251132000	7	-2.691253000	-0.991948000	-0.060775000
6	2.171856000	-2.170160000	0.352110000	6	-1.994552000	0.201429000	-0.253618000
8	5.510016000	-1.311337000	-0.194447000	8	-2.548946000	1.206266000	-0.692976000
1	-0.419324000	-2.975897000	0.259879000	1	4.328698000	-2.985969000	0.410960000
1	-2.450016000	1.445673000	-0.292404000	1	1.860245000	-3.141922000	0.663632000
1	4.211811000	0.929771000	-0.525635000	1	5.795330000	0.076953000	-0.517854000
1	1.652579000	-3.080961000	0.627761000	1	-0.235995000	-3.204765000	0.446015000
1	5.740668000	-2.230061000	-0.004963000	1	-2.698995000	-3.031525000	0.302288000
6	-4.176158000	-0.327575000	-0.303179000	6	-0.514078000	2.532368000	0.605816000
8	-4.536110000	0.781801000	-0.533134000	8	-1.344161000	2.370960000	1.438438000
8	-4.907643000	-1.393166000	-0.209998000	8	-0.059921000	3.689501000	0.187904000
1	-4.307521000	-2.195978000	-0.024058000	1	0.757564000	3.560090000	-0.340903000
6	-0.318594000	2.877893000	0.411654000	6	-4.157463000	-1.074919000	-0.210901000
8	-1.363580000	2.906516000	0.979339000	8	-4.698363000	-2.115165000	-0.004601000
8	0.397698000	3.932913000	0.118851000	8	-4.729254000	0.038437000	-0.562250000
1	1.266267000	3.664255000	-0.271516000	1	-4.032956000	0.748086000	-0.699746000
pn31''-(COOH)₂				pn32''-(COOH)₂			
6	2.527760000	2.465401000	-0.217447000	6	2.359823000	0.380744000	-0.292069000
6	1.205577000	2.247491000	-0.098248000	6	1.769568000	-0.841967000	0.042576000
6	0.678502000	0.907914000	-0.099882000	6	0.310416000	-0.927959000	0.116021000
6	1.566262000	-0.136922000	-0.133588000	6	-0.400324000	0.242645000	0.032298000
7	2.934037000	0.082881000	-0.050165000	7	0.222771000	1.500996000	-0.007676000
6	3.478904000	1.366367000	-0.236650000	6	1.555992000	1.627159000	-0.352619000
8	4.686374000	1.525112000	-0.348494000	8	2.064633000	2.707917000	-0.599493000
6	-0.742294000	0.609621000	-0.083586000	6	-0.423571000	-2.158874000	0.182346000
6	-1.108438000	-0.770571000	-0.195395000	6	-1.768711000	-2.142045000	0.115695000
7	-0.189669000	-1.773437000	-0.425594000	7	-2.473198000	-0.975877000	-0.092194000
6	1.054634000	-1.477383000	-0.423165000	6	-1.830021000	0.248145000	-0.240555000
8	1.964327000	-2.375141000	-0.809809000	8	-2.430183000	1.252862000	-0.622060000
6	-1.727070000	1.556829000	0.069328000	6	3.735944000	0.494041000	-0.480763000

6	-3.102509000	1.209071000	0.134793000	6	4.498648000	-0.644316000	-0.317266000
7	-3.398860000	-0.162568000	0.025892000	7	3.974066000	-1.824952000	0.027675000
6	-2.435119000	-1.103259000	-0.139680000	6	2.674228000	-1.921768000	0.204696000
8	-4.022452000	2.035471000	0.282229000	8	2.209121000	-3.127654000	0.569040000
1	2.959051000	3.455897000	-0.270995000	1	0.086844000	-3.098360000	0.299376000
1	0.525505000	3.088493000	-0.051140000	1	-2.385055000	-3.025495000	0.190257000
1	1.508103000	-3.210518000	-0.975249000	1	4.170462000	1.450671000	-0.734769000
1	-1.522730000	2.613102000	0.169287000	1	5.573690000	-0.625420000	-0.455421000
1	-2.778793000	-2.124825000	-0.225929000	1	2.974590000	-3.714887000	0.631782000
6	3.754727000	-0.937202000	0.639494000	6	-0.458088000	2.608323000	0.681997000
8	3.239189000	-1.669925000	1.416097000	8	-1.235372000	2.372159000	1.545606000
8	5.024506000	-0.896308000	0.330859000	8	-0.094438000	3.802874000	0.279112000
1	5.228906000	-0.043614000	-0.124805000	1	0.700584000	3.742432000	-0.291119000
6	-4.805382000	-0.667724000	0.075610000	6	-3.937331000	-1.113165000	-0.227677000
8	-4.990103000	-1.838193000	-0.030368000	8	-4.432165000	-2.182767000	-0.062109000
8	-5.679788000	0.268945000	0.233393000	8	-4.558289000	-0.009145000	-0.521358000
1	-5.188360000	1.175843000	0.287130000	1	-3.892478000	0.734148000	-0.632715000
pn33''-(COOH)₂				pn34''-(COOH)₂			
6	-2.205380000	0.211217000	-0.192469000	6	2.268004000	-0.265953000	-0.150330000
6	-1.561536000	-0.987615000	0.156030000	6	1.366468000	-1.284129000	0.174908000
6	-0.105185000	-1.022927000	0.193446000	6	-0.071144000	-0.969944000	0.164917000
6	0.574813000	0.155566000	0.048112000	6	-0.475704000	0.394140000	0.044795000
7	-0.086720000	1.396758000	-0.026501000	7	0.503201000	1.428103000	0.031459000
6	-1.439357000	1.477659000	-0.321575000	6	1.840615000	1.142671000	-0.263589000
8	-1.985518000	2.535010000	-0.582916000	8	2.631532000	2.035810000	-0.516024000
6	0.643245000	-2.238789000	0.299702000	6	-1.017336000	-1.953860000	0.173379000
6	1.986473000	-2.207632000	0.212634000	6	-2.414725000	-1.675643000	0.070633000
7	2.664588000	-1.038184000	-0.056886000	7	-2.740727000	-0.330135000	-0.113142000
6	1.997711000	0.171703000	-0.252618000	6	-1.799625000	0.662053000	-0.128097000
8	2.577617000	1.163090000	-0.691065000	8	-3.292222000	-2.550124000	0.111095000
6	-3.578357000	0.257855000	-0.332405000	6	3.637986000	-0.620572000	-0.252804000
6	-4.278904000	-0.928314000	-0.107525000	7	4.084073000	-1.843630000	-0.015143000
7	-3.699789000	-2.072792000	0.238429000	6	3.209852000	-2.784532000	0.335410000
6	-2.379464000	-2.101270000	0.361530000	6	1.848131000	-2.566255000	0.437754000
8	-5.609311000	-0.920401000	-0.238982000	8	4.546587000	0.284663000	-0.597396000
1	0.153480000	-3.187603000	0.455336000	1	-0.766936000	-3.003000000	0.224215000
1	2.620818000	-3.075818000	0.313328000	1	-2.203727000	1.651126000	-0.271846000
1	-4.088080000	1.175467000	-0.592580000	1	3.626862000	-3.765517000	0.537288000
1	-1.957680000	-3.059651000	0.642298000	1	1.194476000	-3.376750000	0.723532000
1	-5.930933000	-1.809890000	-0.043371000	1	5.401736000	-0.167281000	-0.590345000
6	0.584670000	2.543276000	0.603034000	6	-4.147613000	0.114553000	-0.330250000
8	1.400206000	2.357344000	1.443854000	8	-4.358846000	1.265170000	-0.537114000
8	0.175185000	3.715026000	0.176789000	8	-5.009962000	-0.850825000	-0.269712000
1	-0.637510000	3.617528000	-0.361768000	1	-4.521667000	-1.727842000	-0.097031000
6	4.128722000	-1.157938000	-0.205252000	6	0.108797000	2.761508000	0.486087000
8	4.643230000	-2.210694000	0.004064000	8	-0.932732000	2.921633000	1.042606000
8	4.728343000	-0.059905000	-0.558861000	8	0.970178000	3.712991000	0.236203000
1	4.050625000	0.666993000	-0.697459000	1	1.784916000	3.330133000	-0.182168000
pn35''-(COOH)₂				pn36''-(COOH)₂			
6	-2.267274000	-0.163476000	-0.155383000	6	-1.430457000	1.662447000	0.098912000
6	-1.485785000	-1.283117000	0.168379000	6	-0.686504000	0.498314000	-0.009768000
6	-0.028113000	-1.138799000	0.177954000	6	0.737217000	0.583180000	-0.028042000
6	0.500336000	0.113465000	0.051259000	6	1.311960000	1.850375000	-0.152327000
7	-0.300490000	1.257073000	0.009775000	7	0.576621000	2.996091000	-0.133892000
6	-1.670715000	1.177734000	-0.281716000	6	-0.703949000	2.900264000	0.047631000
8	-2.303352000	2.183912000	-0.539564000	8	-1.430894000	4.015085000	0.152827000

6	0.858333000	-2.261171000	0.247547000	6	1.599827000	-0.558785000	0.268305000
6	2.187442000	-2.071034000	0.157995000	7	2.964077000	-0.379556000	-0.001247000
7	2.721458000	-0.821158000	-0.082358000	6	3.494740000	0.868038000	-0.282196000
6	1.918027000	0.303792000	-0.252775000	6	2.729417000	1.971774000	-0.316526000
8	2.369322000	1.363179000	-0.677007000	8	1.194341000	-1.595738000	0.782300000
6	-3.666822000	-0.356981000	-0.264888000	6	-2.853065000	1.626047000	0.245008000
7	-4.253946000	-1.522907000	-0.050539000	6	-3.471440000	0.433013000	0.247492000
6	-3.493689000	-2.565664000	0.281889000	7	-2.778789000	-0.742977000	-0.001805000
6	-2.117265000	-2.508079000	0.396601000	6	-1.410783000	-0.755365000	-0.293242000
8	-4.457164000	0.658959000	-0.593518000	8	-0.883207000	-1.726095000	-0.815813000
1	0.484721000	-3.264488000	0.378416000	1	-0.829352000	4.768275000	0.079811000
1	2.920658000	-2.859971000	0.234369000	1	4.563908000	0.866846000	-0.434683000
1	-4.021625000	-3.497088000	0.457338000	1	3.160110000	2.947811000	-0.484208000
1	-1.564250000	-3.396913000	0.660864000	1	-3.411525000	2.539125000	0.384693000
1	-5.361479000	0.316286000	-0.597251000	1	-4.530372000	0.295333000	0.406851000
6	0.228945000	2.455715000	0.670959000	6	3.935135000	-1.479109000	0.095915000
8	1.076997000	2.345238000	1.495277000	8	5.071380000	-1.277949000	-0.199929000
8	-0.330928000	3.578642000	0.292203000	8	3.438564000	-2.611790000	0.505428000
1	-1.126372000	3.388009000	-0.253054000	1	2.469459000	-2.490550000	0.726128000
6	4.189595000	-0.764202000	-0.235249000	6	-3.601297000	-1.963852000	-0.057716000
8	4.825164000	-1.752431000	-0.046522000	8	-4.745546000	-1.905534000	0.264928000
8	4.655231000	0.403239000	-0.568284000	8	-2.972574000	-3.030985000	-0.462650000
1	3.898953000	1.048112000	-0.694935000	1	-2.036910000	-2.795763000	-0.717395000

VII. 3CO₂ complex

pn1...3CO ₂				pn2...3CO ₂			
6	2.969144000	2.959384000	0.218769000	6	-1.328084000	-1.979343000	-0.166148000
6	1.612800000	3.106564000	0.213980000	6	-0.073022000	-1.378831000	-0.314948000
6	0.803417000	1.955285000	0.117251000	6	-0.014934000	0.059958000	-0.337464000
6	1.417340000	0.697907000	0.028566000	6	-1.210873000	0.793845000	-0.152083000
7	2.764772000	0.553136000	0.032455000	7	-2.438580000	0.180068000	0.011299000
6	3.490607000	1.644922000	0.123903000	6	-2.473039000	-1.114379000	-0.008299000
8	4.822406000	1.537916000	0.130704000	8	-3.641333000	-1.746926000	0.133603000
6	-0.632440000	2.004057000	0.092662000	6	1.170724000	0.771528000	-0.532151000
7	-1.411341000	0.972791000	0.006924000	7	1.241504000	2.090044000	-0.518430000
6	-0.831927000	-0.270001000	-0.051335000	6	0.108674000	2.774764000	-0.309447000
6	0.565257000	-0.458983000	-0.062157000	6	-1.134373000	2.188761000	-0.136836000
8	-1.169127000	3.227869000	0.160956000	8	0.210094000	4.112553000	-0.273575000
7	-1.693959000	-1.308362000	-0.099320000	6	-1.408976000	-3.386640000	-0.164442000
6	-1.201720000	-2.522303000	-0.191093000	6	-0.261877000	-4.118259000	-0.304098000
6	0.178772000	-2.824392000	-0.230823000	6	0.957561000	-3.410818000	-0.426897000
6	1.052594000	-1.776865000	-0.157458000	7	1.061617000	-2.100108000	-0.430185000
8	-2.052052000	-3.554904000	-0.248538000	8	2.074867000	-4.136064000	-0.538667000
1	3.655041000	3.791824000	0.290349000	1	-4.341699000	-1.085278000	0.237035000
1	1.146977000	4.081672000	0.282473000	1	2.095465000	0.236010000	-0.717196000
1	5.065086000	0.604150000	0.065348000	1	-2.015869000	2.795574000	0.011512000
1	-2.133071000	3.138382000	0.117596000	1	1.143902000	4.342311000	-0.376934000
1	0.497624000	-3.854367000	-0.309173000	1	-2.373561000	-3.866088000	-0.053255000
1	2.120484000	-1.941166000	-0.173588000	1	-0.249098000	-5.199141000	-0.312761000
1	-2.954640000	-3.209929000	-0.190085000	1	2.829554000	-3.530637000	-0.578430000
6	-4.274587000	-1.089525000	1.077275000	6	3.736408000	2.993547000	-0.137505000
8	-4.125932000	-0.026961000	1.498414000	8	3.379150000	4.094588000	-0.105776000
8	-4.479567000	-2.161323000	0.687991000	8	4.155681000	1.918357000	-0.156692000
6	-4.020690000	1.438388000	-1.009071000	6	3.370348000	-1.322664000	1.149702000
8	-3.905305000	2.528545000	-0.631572000	8	2.771445000	-0.608109000	1.826299000
8	-4.190233000	0.374006000	-1.415401000	8	3.992998000	-2.042165000	0.488122000

6	4.949487000	-2.213205000	-0.097410000	6	-4.903774000	1.592027000	0.379463000
8	5.646849000	-1.291726000	-0.025309000	8	-5.430785000	0.559464000	0.421227000
8	4.267695000	-3.138535000	-0.169954000	8	-4.430747000	2.640334000	0.345229000
pn3...3CO₂				pn4...3CO₂			
6	-2.490451000	0.674034000	0.211429000	6	2.210135000	1.900601000	-0.093515000
6	-1.165281000	1.121219000	0.275585000	6	1.087003000	1.069969000	-0.071069000
6	-0.113495000	0.131183000	0.205516000	6	1.305378000	-0.320882000	0.018675000
6	-0.488268000	-1.214942000	0.080366000	6	2.617816000	-0.802252000	0.080648000
7	-1.801050000	-1.638869000	0.015526000	7	3.674331000	-0.009883000	0.059904000
6	-2.728443000	-0.739725000	0.077584000	6	3.462955000	1.312080000	-0.025993000
8	-4.019343000	-1.099438000	0.019477000	8	4.544059000	2.101291000	-0.046033000
7	1.175102000	0.530452000	0.267317000	6	-0.282388000	1.527644000	-0.124099000
6	2.104057000	-0.381882000	0.214722000	6	-1.313705000	0.565935000	-0.077884000
6	1.856119000	-1.767419000	0.089647000	7	-1.071881000	-0.788160000	-0.023474000
6	0.551657000	-2.172455000	0.020985000	6	0.156114000	-1.189594000	0.028940000
8	3.393550000	0.022840000	0.282515000	8	0.418986000	-2.496808000	0.091695000
6	-3.528217000	1.629540000	0.284261000	6	-0.658151000	2.882378000	-0.213467000
6	-3.206877000	2.950511000	0.419669000	6	-1.980160000	3.230244000	-0.246822000
6	-1.832384000	3.287321000	0.475495000	6	-2.926495000	2.185280000	-0.172604000
7	-0.849999000	2.425534000	0.403406000	7	-2.616953000	0.910907000	-0.085500000
8	-1.521852000	4.584640000	0.611201000	8	-4.218478000	2.530200000	-0.190498000
1	-4.068338000	-2.061714000	-0.071781000	1	2.146273000	2.977343000	-0.158765000
1	2.688184000	-2.457659000	0.052031000	1	2.804845000	-1.868875000	0.149487000
1	0.289889000	-3.218422000	-0.076438000	1	5.332603000	1.542371000	0.008135000
1	3.392881000	0.981823000	0.406835000	1	-0.422168000	-2.978179000	0.069569000
1	-4.558558000	1.300538000	0.234373000	1	0.100396000	3.654526000	-0.258459000
1	-3.949222000	3.733869000	0.484943000	1	-2.319913000	4.253754000	-0.318957000
1	-0.558816000	4.646987000	0.670215000	1	-4.750548000	1.725305000	-0.109507000
6	1.416137000	2.866741000	-1.293718000	6	6.144662000	-1.140524000	0.189484000
8	0.807496000	2.335973000	-2.118903000	8	6.643399000	-0.094667000	0.137661000
8	2.056151000	3.437298000	-0.516570000	8	5.704764000	-2.203581000	0.243731000
6	5.740610000	-1.262917000	0.322806000	6	-2.968917000	-2.666439000	-1.000462000
8	5.222400000	-2.288852000	0.199119000	8	-3.732064000	-1.891607000	-1.380158000
8	6.290721000	-0.255859000	0.447164000	8	-2.234919000	-3.491710000	-0.648143000
6	-2.600825000	-4.380178000	-0.279985000	6	-4.569894000	-0.766530000	1.149693000
8	-3.700406000	-4.013893000	-0.264370000	8	-3.825622000	-1.553552000	1.543150000
8	-1.527520000	-4.796637000	-0.300896000	8	-5.362137000	-0.002534000	0.787700000
pn5...3CO₂				pn6...3CO₂			
6	0.700367000	-0.966677000	0.083768000	6	-1.708884000	1.668273000	0.241927000
6	0.322108000	0.368406000	0.321030000	6	-1.619198000	0.279769000	0.363330000
6	-1.095098000	0.660746000	0.376034000	6	-0.301656000	-0.324356000	0.332741000
6	-1.992182000	-0.405456000	0.236016000	6	0.799140000	0.532846000	0.132708000
7	-1.600073000	-1.716001000	0.015713000	7	0.690455000	1.906338000	-0.010660000
6	-0.334371000	-1.961466000	-0.062899000	6	-0.488906000	2.422165000	0.052451000
8	0.096920000	-3.209277000	-0.286415000	8	-0.658977000	3.747456000	-0.066299000
7	-1.491547000	1.939862000	0.561427000	6	-0.086403000	-1.692046000	0.498699000
6	-2.775590000	2.185229000	0.632311000	6	1.216546000	-2.153998000	0.439360000
6	-3.771823000	1.187843000	0.527999000	7	2.271408000	-1.357559000	0.235547000
6	-3.370493000	-0.103501000	0.324166000	6	2.070666000	-0.058533000	0.089894000
8	-3.185693000	3.453485000	0.805980000	8	1.452302000	-3.469621000	0.594011000
6	2.065927000	-1.270050000	0.017638000	6	-2.985359000	2.266948000	0.298836000
7	3.008674000	-0.357697000	0.172796000	6	-4.085659000	1.472427000	0.464146000
6	2.635710000	0.909113000	0.410444000	6	-3.882539000	0.074801000	0.553167000
6	1.316873000	1.326682000	0.497468000	7	-2.705277000	-0.506296000	0.506812000
8	3.611825000	1.811236000	0.572338000	8	-4.969208000	-0.693984000	0.684240000
1	-0.671158000	-3.793020000	-0.363891000	1	0.207452000	4.160092000	-0.194584000

1	-4.813317000	1.470377000	0.601100000	1	-0.905764000	-2.372141000	0.685874000
1	-4.087210000	-0.909082000	0.226035000	1	2.945312000	0.564011000	-0.067054000
1	-2.405892000	4.025160000	0.802604000	1	2.405683000	-3.616678000	0.525276000
1	2.392700000	-2.288310000	-0.165467000	1	-3.073546000	3.342506000	0.210633000
1	1.077536000	2.358883000	0.710732000	1	-5.092079000	1.864318000	0.515799000
1	4.463693000	1.360527000	0.482705000	1	-4.689754000	-1.620876000	0.678998000
6	5.600407000	-1.167552000	0.007444000	6	4.835387000	-2.242923000	0.125650000
8	5.970166000	-0.086228000	0.204748000	8	4.490059000	-3.335967000	0.301960000
8	5.291586000	-2.259276000	-0.191727000	8	5.241069000	-1.179384000	-0.051661000
6	-3.421723000	-3.913233000	-0.300027000	6	2.903273000	3.686827000	-0.459731000
8	-4.370418000	-3.275163000	-0.161553000	8	3.702363000	2.858855000	-0.466786000
8	-2.499899000	-4.600253000	-0.445820000	8	2.137060000	4.557564000	-0.460856000
6	-0.455861000	3.760236000	-1.354113000	6	-2.938434000	-2.632858000	-1.382274000
8	-0.076356000	2.909450000	-2.032888000	8	-2.114161000	-2.205420000	-2.064153000
8	-0.828287000	4.637324000	-0.695542000	8	-3.775662000	-3.081332000	-0.718240000
pn7...3CO₂				pn8...3CO₂			
6	1.352944000	0.569186000	-0.001400000	6	-1.098742000	-1.293504000	0.087047000
6	0.498719000	-0.560199000	-0.000263000	6	-1.341970000	0.081794000	-0.024100000
6	-0.928663000	-0.293519000	-0.000839000	6	-0.219297000	0.988010000	-0.114450000
6	-1.364458000	1.049772000	-0.002438000	6	1.077292000	0.424697000	-0.078798000
7	-0.501783000	2.128797000	-0.003155000	7	1.297683000	-0.930833000	-0.003647000
6	0.768531000	1.885675000	-0.002701000	6	0.283317000	-1.721673000	0.080471000
8	1.634882000	2.900047000	-0.003361000	8	0.475170000	-3.041316000	0.163763000
6	-1.948431000	-1.280271000	-0.000121000	6	-2.153664000	-2.219400000	0.188682000
7	-3.236424000	-1.017296000	-0.000920000	6	-3.432738000	-1.731422000	0.176013000
6	-3.624506000	0.271411000	-0.002598000	7	-3.706383000	-0.414325000	0.068872000
6	-2.745997000	1.323123000	-0.003375000	6	-2.723332000	0.445066000	-0.026374000
8	-1.595265000	-2.575783000	0.001486000	8	-3.052013000	1.744021000	-0.131033000
6	2.738110000	0.384213000	-0.001107000	6	-0.297428000	2.397013000	-0.232330000
7	3.304345000	-0.809803000	0.000202000	6	0.845719000	3.145256000	-0.297768000
6	2.495718000	-1.876585000	0.001339000	6	2.081768000	2.472092000	-0.228141000
6	1.107421000	-1.817768000	0.001189000	7	2.200287000	1.169510000	-0.117781000
8	3.078578000	-3.081168000	0.002743000	8	3.193083000	3.217308000	-0.276695000
1	1.139543000	3.732574000	-0.003961000	1	1.428473000	-3.212795000	0.129420000
1	-4.697029000	0.434499000	-0.003274000	1	-1.946394000	-3.276376000	0.273245000
1	-3.085865000	2.348394000	-0.004880000	1	-4.295501000	-2.383512000	0.251023000
1	-2.408619000	-3.102431000	0.001797000	1	-4.018855000	1.806229000	-0.114552000
1	3.402142000	1.241984000	-0.002018000	1	-1.260755000	2.880442000	-0.272386000
1	0.544153000	-2.735454000	0.002140000	1	0.830693000	4.222166000	-0.391873000
1	4.038456000	-2.957190000	0.002584000	1	3.957785000	2.630137000	-0.192297000
6	-5.185234000	-2.899077000	0.000335000	6	4.590339000	0.244365000	1.142384000
8	-4.396419000	-3.749500000	0.001424000	8	5.094156000	1.217140000	0.766404000
8	-6.016164000	-2.101329000	-0.000653000	8	4.140118000	-0.735565000	1.549751000
6	6.018359000	-0.953372000	0.000068000	6	3.721614000	-2.095517000	-0.975509000
8	5.975089000	-2.112231000	0.001575000	8	3.297982000	-3.109384000	-0.605695000
8	6.122870000	0.193890000	-0.001441000	8	4.187579000	-1.119357000	-1.371046000
6	-1.336093000	4.903980000	0.004166000	6	-6.339285000	0.280278000	0.079250000
8	-2.465703000	4.683160000	0.006734000	8	-6.671592000	-0.817592000	0.182588000
8	-0.209651000	5.178704000	0.001641000	8	-6.064248000	1.402359000	-0.024655000
pn9...3CO₂				pn10...3CO₂			
6	-1.505728000	-1.734101000	-0.268091000	6	-0.373927000	-3.214576000	-0.615678000
6	-0.183752000	-1.259801000	-0.299644000	6	0.668199000	-2.334806000	-0.627198000
6	0.020637000	0.169862000	-0.224322000	6	0.414809000	-0.958637000	-0.417865000
6	-1.117106000	0.992619000	-0.066193000	6	-0.913341000	-0.572689000	-0.228403000
7	-2.402875000	0.499657000	-0.005604000	7	-1.950603000	-1.436033000	-0.212451000
6	-2.568403000	-0.780216000	-0.114630000	6	-1.679499000	-2.703945000	-0.393322000

8	-3.801378000	-1.294058000	-0.078433000	8	-2.683237000	-3.588101000	-0.379077000
6	1.275053000	0.835184000	-0.321065000	6	1.439591000	0.052821000	-0.409190000
7	1.416833000	2.139239000	-0.240225000	6	1.040223000	1.387538000	-0.249898000
6	0.319571000	2.900245000	-0.060608000	7	-0.276223000	1.762100000	-0.070714000
6	-0.947041000	2.388799000	0.026233000	6	-1.185317000	0.842979000	-0.052309000
8	2.394637000	0.122732000	-0.525333000	8	-2.469449000	1.159773000	0.127624000
6	-1.739269000	-3.121127000	-0.371067000	7	2.734857000	-0.314008000	-0.556530000
6	-0.676665000	-3.971534000	-0.491501000	6	3.644183000	0.629203000	-0.572964000
6	0.614700000	-3.395637000	-0.483380000	6	3.356021000	2.006626000	-0.444536000
7	0.857934000	-2.109114000	-0.392143000	6	2.049615000	2.375462000	-0.276639000
8	1.659949000	-4.225591000	-0.564987000	8	4.935509000	0.280329000	-0.712134000
1	-4.436097000	-0.571056000	0.034001000	1	-0.246806000	-4.277216000	-0.773132000
1	0.500922000	3.967790000	0.005647000	1	1.684372000	-2.661947000	-0.809557000
1	-1.810864000	3.023806000	0.157586000	1	-3.507951000	-3.103662000	-0.225228000
1	3.119980000	0.760683000	-0.607298000	1	-2.542394000	2.118934000	0.232809000
1	-2.757406000	-3.489093000	-0.352156000	1	4.166844000	2.721624000	-0.471652000
1	-0.783630000	-5.043981000	-0.575598000	1	1.765772000	3.414016000	-0.161910000
1	2.467419000	-3.692454000	-0.511675000	1	4.986141000	-0.684738000	-0.723359000
6	2.872626000	-1.668357000	1.472176000	6	-5.139246000	-0.708889000	0.224643000
8	3.584867000	-2.343527000	0.856654000	8	-5.295460000	0.420964000	0.371645000
8	2.193031000	-1.017795000	2.139428000	8	-5.034556000	-1.855013000	0.081327000
6	3.772811000	3.458089000	-0.400726000	6	-1.118394000	4.486346000	0.326319000
8	4.351117000	2.466733000	-0.568052000	8	-2.203659000	4.090850000	0.414762000
8	3.258620000	4.476449000	-0.239671000	8	-0.058726000	4.931090000	0.246142000
6	-4.770172000	2.127892000	0.351396000	6	3.603385000	-2.210616000	1.357684000
8	-4.210145000	3.131455000	0.412478000	8	2.621377000	-2.121816000	1.955045000
8	-5.381589000	1.144142000	0.295896000	8	4.600700000	-2.327115000	0.780420000
pn11...3CO₂				pn12...3CO₂			
6	1.146297000	2.110800000	0.014271000	6	-1.441319000	0.552279000	0.000028000
6	1.516431000	0.760185000	0.007174000	6	-0.633239000	-0.603888000	-0.000007000
6	0.459656000	-0.229245000	0.008167000	6	0.801533000	-0.404178000	-0.000096000
6	-0.858023000	0.244078000	0.015193000	6	1.304513000	0.922327000	-0.000230000
7	-1.212402000	1.569285000	0.019876000	7	0.483664000	2.038148000	-0.000364000
6	-0.256828000	2.437336000	0.020511000	6	-0.794382000	1.845709000	-0.000230000
8	-0.547614000	3.745133000	0.027284000	8	-1.621219000	2.892178000	-0.000267000
6	0.692539000	-1.620156000	0.003164000	6	1.731427000	-1.445792000	0.000074000
6	-0.386548000	-2.462217000	0.005647000	7	3.042781000	-1.267286000	0.000062000
7	-1.668431000	-2.026428000	0.013578000	6	3.501129000	-0.010453000	-0.000130000
6	-1.893417000	-0.737355000	0.018584000	6	2.685676000	1.110693000	-0.000292000
8	-3.155331000	-0.293106000	0.027560000	8	4.830810000	0.156718000	-0.000141000
6	2.160420000	3.093008000	0.014688000	6	-2.831607000	0.409610000	0.000179000
6	3.464428000	2.692834000	0.007842000	7	-3.432830000	-0.768314000	0.000253000
6	3.731145000	1.300590000	0.000657000	6	-2.661153000	-1.863016000	0.000167000
7	2.810289000	0.363681000	0.000303000	6	-1.273013000	-1.842633000	0.000031000
8	5.018973000	0.945779000	-0.006177000	8	-3.281710000	-3.047675000	0.000226000
1	-1.512764000	3.833739000	0.034968000	1	-1.094028000	3.705394000	0.000133000
1	1.700584000	-2.003827000	-0.002391000	1	1.404134000	-2.481079000	0.000228000
1	-0.261941000	-3.539309000	0.001611000	1	3.112110000	2.103307000	-0.000495000
1	-3.744770000	-1.060690000	0.025254000	1	5.247168000	-0.716694000	0.000003000
1	1.887002000	4.140676000	0.020402000	1	-3.471389000	1.285830000	0.000228000
1	4.294929000	3.385197000	0.007649000	1	-0.740423000	-2.782890000	-0.000070000
1	5.081285000	-0.019586000	-0.011137000	1	-4.237438000	-2.893480000	0.000341000
6	4.430870000	-2.784412000	-0.030061000	6	4.601588000	-3.472114000	0.000036000
8	5.270080000	-1.986225000	-0.028192000	8	5.564718000	-2.827060000	0.000065000
8	3.607791000	-3.589358000	-0.031978000	8	3.682028000	-4.167108000	0.000020000
6	-4.232960000	2.820293000	-0.050626000	6	1.435779000	4.753297000	0.000153000
8	-5.013032000	1.979581000	-0.127436000	8	2.552444000	4.475875000	0.000428000

8	-3.487607000	3.706581000	0.025101000	8	0.324276000	5.084846000	0.000230000
6	-3.631009000	-3.888849000	0.017542000	6	-6.153223000	-0.836794000	-0.000127000
8	-2.871021000	-4.755039000	0.010906000	8	-6.139496000	-1.996503000	-0.000117000
8	-4.448305000	-3.066258000	0.024285000	8	-6.226562000	0.312665000	-0.000117000
pn13...3CO₂				pn14...3CO₂			
6	0.287972000	-1.622172000	-0.100796000	6	-3.363006000	2.522918000	0.196965000
6	-0.264421000	-0.349261000	-0.316720000	6	-2.036347000	2.778041000	0.000460000
6	0.608263000	0.799544000	-0.342348000	6	-1.095217000	1.718072000	0.053199000
6	1.983976000	0.573745000	-0.200600000	6	-1.610885000	0.445813000	0.311174000
7	2.525405000	-0.688321000	-0.007289000	7	-2.922124000	0.182273000	0.492703000
6	1.732062000	-1.701492000	0.047635000	6	-3.758188000	1.183547000	0.440365000
8	2.212119000	-2.935737000	0.246079000	8	-5.066196000	0.947105000	0.619935000
7	0.078027000	2.032810000	-0.497302000	6	0.326730000	1.864814000	-0.131849000
6	0.899005000	3.055618000	-0.541430000	6	1.131463000	0.711430000	-0.033780000
6	2.302105000	2.944813000	-0.431998000	7	0.606655000	-0.532851000	0.211883000
6	2.835796000	1.696292000	-0.254654000	6	-0.669959000	-0.655010000	0.384490000
8	0.386314000	4.288010000	-0.692879000	8	-1.191535000	-1.850325000	0.652840000
6	-0.539149000	-2.742745000	-0.044267000	6	0.975309000	3.086133000	-0.408784000
6	-1.899762000	-2.533478000	-0.209749000	6	2.332574000	3.123108000	-0.568200000
7	-2.441344000	-1.332079000	-0.447786000	6	3.039188000	1.907455000	-0.431079000
6	-1.651069000	-0.276231000	-0.502608000	7	2.474788000	0.752929000	-0.169066000
8	-2.738035000	-3.578007000	-0.137564000	8	4.369836000	1.957502000	-0.578157000
1	3.174978000	-2.886442000	0.331434000	1	-4.115592000	3.299506000	0.169211000
1	2.909159000	3.838351000	-0.480424000	1	-1.710730000	3.792761000	-0.191452000
1	3.903567000	1.547754000	-0.153529000	1	-5.180879000	-0.002655000	0.771517000
1	-0.577852000	4.215418000	-0.707968000	1	-0.472295000	-2.499869000	0.639458000
1	-0.145498000	-3.734459000	0.126747000	1	0.403199000	4.001516000	-0.500620000
1	-2.121904000	0.677418000	-0.713064000	1	2.875086000	4.032367000	-0.786014000
1	-3.641062000	-3.248216000	-0.245897000	1	4.725436000	1.068011000	-0.439249000
6	-5.044240000	-0.713174000	-0.113370000	6	4.135555000	-1.205821000	1.076440000
8	-5.337921000	-1.832214000	-0.055361000	8	5.033684000	-0.673802000	0.573606000
8	-4.809777000	0.415267000	-0.160820000	8	3.283405000	-1.769201000	1.609914000
6	5.344849000	-1.184553000	0.317475000	6	1.938086000	-2.884266000	-0.688814000
8	5.655656000	-0.081635000	0.203202000	8	2.789738000	-2.338018000	-1.239927000
8	5.083960000	-2.307158000	0.438870000	8	1.101802000	-3.487054000	-0.159122000
6	-2.165584000	2.725127000	1.172939000	6	-3.997336000	-2.099644000	-0.735790000
8	-2.046236000	1.788867000	1.834647000	8	-3.178506000	-2.167167000	-1.543385000
8	-2.307932000	3.676494000	0.527863000	8	-4.858137000	-2.054995000	0.039261000
pn15...3CO₂				pn16...3CO₂			
6	1.381364000	-0.149573000	-0.015152000	6	2.213398000	-1.971007000	-0.158688000
6	1.087238000	1.224181000	0.083715000	6	1.112959000	-1.121655000	-0.069074000
6	-0.295431000	1.625917000	0.128699000	6	1.283823000	0.269863000	0.036959000
6	-1.286445000	0.625468000	0.064364000	6	2.609006000	0.731853000	0.045049000
7	-0.980712000	-0.705430000	0.005262000	7	3.659689000	-0.066056000	-0.039906000
6	0.265692000	-1.068866000	-0.037901000	6	3.469114000	-1.385857000	-0.139767000
8	0.538793000	-2.367282000	-0.100247000	8	4.558363000	-2.165433000	-0.224143000
6	2.753539000	-0.529201000	-0.075476000	6	-0.252895000	-1.617340000	-0.067849000
7	3.740612000	0.340468000	-0.036191000	7	-1.302777000	-0.874762000	0.009329000
6	3.441318000	1.649076000	0.063617000	6	-1.151551000	0.495407000	0.082300000
6	2.162954000	2.137404000	0.124669000	6	0.111898000	1.113622000	0.118847000
8	3.077614000	-1.815987000	-0.178672000	8	-0.375429000	-2.943799000	-0.147871000
6	-0.728721000	2.965707000	0.225963000	7	-2.303830000	1.193866000	0.117884000
6	-2.062858000	3.256897000	0.248489000	6	-2.236647000	2.501324000	0.222738000
6	-2.966624000	2.173375000	0.155106000	6	-1.028840000	3.227001000	0.289211000
7	-2.606007000	0.915273000	0.060376000	6	0.140267000	2.517939000	0.228827000
8	-4.270248000	2.469987000	0.162481000	8	-3.376752000	3.203518000	0.268531000

1	-0.304456000	-2.845468000	-0.087952000	1	2.099427000	-3.042653000	-0.239816000
1	4.295913000	2.317364000	0.092059000	1	2.835593000	1.790416000	0.121836000
1	2.001097000	3.202548000	0.199856000	1	5.342470000	-1.599647000	-0.198889000
1	4.044507000	-1.871506000	-0.205625000	1	-1.318233000	-3.167503000	-0.117511000
1	-0.007223000	3.770819000	0.285739000	1	-1.058360000	4.303967000	0.377679000
1	-2.445911000	4.264617000	0.325992000	1	1.085638000	3.045372000	0.268743000
1	-4.772447000	1.646913000	0.072723000	1	-4.117944000	2.586290000	0.188879000
6	-4.494675000	-0.851701000	-1.146737000	6	6.092824000	1.130820000	-0.009774000
8	-3.724361000	-1.626488000	-1.513012000	8	5.614325000	2.175408000	0.083777000
8	-5.312940000	-0.102811000	-0.811406000	8	6.628468000	0.107388000	-0.103169000
6	-2.833242000	-2.628444000	1.039893000	6	-3.666793000	-2.153553000	0.972537000
8	-2.086701000	-3.438632000	0.680926000	8	-4.178417000	-1.201543000	1.370627000
8	-3.606993000	-1.866366000	1.425397000	8	-3.195409000	-3.145209000	0.600408000
6	6.371044000	-0.307271000	-0.151958000	6	-4.654525000	0.168604000	-1.129802000
8	6.686121000	0.798796000	-0.078233000	8	-5.199383000	1.116251000	-0.746527000
8	6.116259000	-1.435626000	-0.228817000	8	-4.162315000	-0.787791000	-1.544276000
pn17...3CO₂				pn18...3CO₂			
6	-0.794413000	-1.682799000	0.001812000	6	-1.341687000	-3.304270000	0.339652000
6	-0.731023000	-0.274664000	0.000786000	6	-0.151663000	-2.639715000	0.237306000
6	0.582230000	0.343626000	0.000761000	6	-0.133084000	-1.217542000	0.225342000
6	1.715979000	-0.491644000	0.001649000	6	-1.381216000	-0.590732000	0.324078000
7	1.629273000	-1.874342000	0.002591000	7	-2.557334000	-1.242211000	0.409702000
6	0.461186000	-2.416683000	0.002726000	6	-2.533342000	-2.549191000	0.420308000
8	0.337563000	-3.744324000	0.003742000	8	-3.693324000	-3.215651000	0.508298000
6	0.843725000	1.737697000	-0.000145000	6	1.038106000	-0.373353000	0.121523000
7	2.045283000	2.268249000	-0.000176000	6	0.858989000	1.025399000	0.131914000
6	3.111449000	1.446378000	0.000703000	7	-0.378752000	1.619193000	0.252063000
6	3.002100000	0.080186000	0.001612000	6	-1.422108000	0.860667000	0.347055000
8	-0.199038000	2.587524000	-0.001019000	8	-2.629231000	1.401265000	0.487425000
6	-2.014984000	-2.350154000	0.001945000	6	2.379694000	-0.824923000	0.002292000
6	-3.161767000	-1.572465000	0.001036000	7	3.421880000	-0.035356000	-0.097853000
7	-3.135923000	-0.238489000	0.000043000	6	3.222963000	1.298689000	-0.088113000
6	-1.971858000	0.394144000	-0.000087000	6	1.984157000	1.868901000	0.023274000
8	-4.360204000	-2.173911000	0.001133000	8	2.617739000	-2.150904000	-0.011422000
1	1.221511000	-4.140692000	0.004442000	1	-1.397657000	-4.384555000	0.355869000
1	4.079136000	1.936081000	0.000655000	1	0.772517000	-3.191057000	0.167949000
1	3.871242000	-0.561453000	0.002251000	1	-4.409844000	-2.565933000	0.557291000
1	0.154549000	3.489477000	-0.001678000	1	-2.535175000	2.365287000	0.476682000
1	-2.073188000	-3.429036000	0.002738000	1	4.118653000	1.903993000	-0.174487000
1	-2.020706000	1.473055000	-0.000898000	1	1.848228000	2.940543000	0.029912000
1	-5.045130000	-1.490333000	0.000367000	1	3.574773000	-2.274317000	-0.098620000
6	2.539535000	4.931700000	0.000687000	6	-4.738520000	-0.269650000	-1.070617000
8	3.679295000	4.764803000	0.001663000	8	-4.092948000	0.293181000	-1.841236000
8	1.403635000	5.166624000	0.000094000	8	-5.428937000	-0.842150000	-0.336431000
6	-5.384914000	1.300904000	-0.002604000	6	-0.823097000	4.492274000	0.236901000
8	-6.054108000	0.353525000	-0.002072000	8	-1.948740000	4.256367000	0.381948000
8	-4.771699000	2.275855000	-0.003194000	8	0.282941000	4.777552000	0.093639000
6	3.923755000	-3.661793000	-0.004220000	6	5.977976000	-0.898051000	-0.317426000
8	3.160395000	-4.534538000	-0.002330000	8	5.632713000	-2.005049000	-0.279922000
8	4.718678000	-2.829510000	-0.006150000	8	6.385403000	0.178344000	-0.360163000
pn19...3CO₂				pn20...3CO₂			
6	-0.634613000	-1.041929000	-0.006784000	6	0.880166000	-1.871647000	0.005774000
6	-0.296402000	0.323032000	-0.005239000	6	0.922835000	-0.472965000	0.002889000
6	1.102475000	0.686893000	-0.007484000	6	-0.326288000	0.262185000	0.003324000
6	2.041984000	-0.350745000	-0.010928000	6	-1.532004000	-0.489257000	0.006333000
7	1.699564000	-1.683978000	-0.011833000	7	-1.554083000	-1.874400000	0.008826000

6	0.443627000	-2.007279000	-0.010196000	6	-0.430204000	-2.502675000	0.008811000
8	0.110483000	-3.298048000	-0.011701000	8	-0.409100000	-3.837054000	0.011605000
7	1.447901000	1.999982000	-0.006448000	6	-0.456665000	1.661652000	0.001077000
6	2.722871000	2.293292000	-0.009087000	7	-1.623107000	2.290333000	0.001653000
6	3.758996000	1.327274000	-0.012899000	6	-2.742587000	1.562401000	0.004507000
6	3.411323000	0.008529000	-0.013756000	6	-2.755052000	0.178507000	0.006969000
8	3.106763000	3.579722000	-0.008231000	8	-3.909687000	2.223931000	0.005049000
6	-2.024516000	-1.363270000	-0.004918000	6	2.056807000	-2.639775000	0.005679000
7	-2.970256000	-0.448915000	-0.001875000	6	3.254175000	-1.971247000	0.002624000
6	-2.619980000	0.852348000	-0.000465000	7	3.334337000	-0.626912000	-0.000277000
6	-1.320878000	1.286327000	-0.002028000	6	2.233970000	0.086461000	-0.000170000
8	-2.407273000	-2.639714000	-0.006237000	8	2.365215000	1.421793000	-0.003161000
1	0.926780000	-3.817893000	-0.014928000	1	-1.321627000	-4.163464000	0.013832000
1	4.787710000	1.661458000	-0.014949000	1	0.417450000	2.296426000	-0.001191000
1	4.156609000	-0.776272000	-0.016333000	1	-3.686213000	-0.369116000	0.009105000
1	2.320738000	4.141422000	-0.005221000	1	-3.719523000	3.172524000	0.003207000
1	-3.447005000	1.554879000	0.002070000	1	2.006939000	-3.718918000	0.007979000
1	-1.078513000	2.336185000	-0.000879000	1	4.202337000	-2.496991000	0.002379000
1	-3.375998000	-2.652843000	-0.004595000	1	3.311487000	1.630024000	-0.005049000
6	-5.625759000	-0.988129000	0.004318000	6	-1.569856000	4.995831000	-0.001443000
8	-5.420317000	-2.129278000	0.001980000	8	-0.417884000	5.016147000	-0.002935000
8	-5.894295000	0.132435000	0.006745000	8	-2.728545000	5.045012000	-0.000008000
6	-0.372915000	5.068910000	0.014420000	6	-3.970399000	-3.471012000	-0.014451000
8	-1.487450000	4.777728000	0.019752000	8	-4.697138000	-2.579221000	-0.021274000
8	0.743241000	5.375680000	0.009006000	8	-3.277964000	-4.401664000	-0.007972000
6	3.668787000	-3.823239000	0.022336000	6	5.840229000	0.445145000	-0.006485000
8	4.582952000	-3.122221000	0.034475000	8	5.402093000	1.518935000	-0.008116000
8	2.783296000	-4.569885000	0.010736000	8	6.330305000	-0.597287000	-0.004978000
pn21...3CO₂				pn22...3CO₂			
6	-1.384340000	0.364123000	0.000115000	6	-1.528964000	0.479416000	-0.001169000
6	-0.462323000	-0.707945000	0.000076000	6	-0.986793000	-0.820373000	0.000236000
6	0.948884000	-0.377024000	0.000031000	6	0.465817000	-0.939377000	0.000223000
6	1.318539000	0.984993000	0.000037000	6	1.214835000	0.256065000	-0.001187000
7	0.402523000	2.006411000	0.000095000	7	0.655119000	1.526898000	-0.002444000
6	-0.862797000	1.712959000	0.000136000	6	-0.628770000	1.614363000	-0.002458000
8	-1.739500000	2.708830000	0.000206000	8	-1.228669000	2.811561000	-0.003774000
6	2.022876000	-1.310801000	-0.000029000	6	1.142548000	-2.158738000	0.001417000
7	3.293027000	-0.978174000	-0.000084000	6	2.528481000	-2.141512000	0.001177000
6	3.616054000	0.330298000	-0.000089000	7	3.248764000	-1.018242000	-0.000213000
6	2.685735000	1.332817000	-0.000024000	6	2.611624000	0.142012000	-0.001367000
8	1.751027000	-2.626792000	-0.000013000	8	3.192240000	-3.310587000	0.002340000
6	-2.773524000	0.051259000	0.000131000	6	-2.919516000	0.626489000	-0.001279000
7	-3.230647000	-1.183113000	0.000137000	7	-3.750568000	-0.403057000	-0.000079000
6	-2.342899000	-2.190552000	0.000112000	6	-3.228180000	-1.634602000	0.001281000
6	-0.981010000	-2.021029000	0.000067000	6	-1.864534000	-1.900526000	0.001488000
8	-3.676761000	1.031060000	0.000180000	8	-4.081289000	-2.664915000	0.002471000
1	-1.246429000	3.542759000	0.000209000	1	-0.547579000	3.499748000	-0.004666000
1	4.679016000	0.546738000	-0.000135000	1	0.629696000	-3.110581000	0.002505000
1	2.970014000	2.374718000	-0.000021000	1	3.219243000	1.040704000	-0.002468000
1	2.597849000	-3.098046000	-0.000056000	1	4.140930000	-3.121637000	0.001983000
1	-2.774260000	-3.186469000	0.000094000	1	-3.364511000	1.615754000	-0.002366000
1	-0.331511000	-2.878081000	0.000031000	1	-1.531648000	-2.928708000	0.002615000
1	-4.552260000	0.616185000	0.000208000	1	-4.984666000	-2.316667000	0.002174000
6	5.348422000	-2.740936000	0.000002000	6	-6.430757000	0.094559000	-0.000569000
8	4.611535000	-3.636917000	0.000044000	8	-6.265382000	1.234337000	-0.002131000
8	6.130750000	-1.895585000	-0.000043000	8	-6.654667000	-1.043419000	0.000404000
6	-5.858177000	-1.859899000	-0.000220000	6	2.158058000	3.989684000	0.004393000

8	-6.171477000	-0.743548000	-0.000351000	8	3.190346000	3.480960000	0.007084000
8	-5.608676000	-2.984804000	-0.000105000	8	1.142001000	4.548701000	0.001898000
6	1.152879000	4.842496000	-0.000182000	6	5.967878000	-0.975158000	-0.002738000
8	0.017016000	5.072220000	0.000031000	8	5.995235000	0.176351000	-0.004447000
8	2.290255000	4.663257000	-0.000241000	8	6.004556000	-2.134441000	-0.001007000
pn23...3CO₂				pn24...3CO₂			
6	1.492161000	0.385124000	-0.215037000	6	-1.394983000	1.506909000	-0.000905000
6	0.977133000	-0.909078000	0.009143000	6	-1.310054000	0.108317000	-0.000553000
6	-0.467715000	-1.073222000	-0.003016000	6	0.004991000	-0.513277000	-0.000711000
6	-1.233902000	0.073698000	-0.236769000	6	1.118812000	0.363085000	-0.001183000
7	-0.717834000	1.333138000	-0.431009000	7	1.018020000	1.744670000	-0.001515000
6	0.562844000	1.468815000	-0.423460000	6	-0.154374000	2.267017000	-0.001404000
8	1.101146000	2.680510000	-0.611489000	8	-0.311581000	3.598074000	-0.001819000
6	-1.126969000	-2.303928000	0.198102000	6	0.258264000	-1.889288000	-0.000442000
6	-2.496775000	-2.328995000	0.150448000	6	1.577469000	-2.317957000	-0.000669000
7	-3.250410000	-1.235033000	-0.092166000	7	2.630384000	-1.498591000	-0.001059000
6	-2.649391000	-0.086592000	-0.282769000	6	2.401664000	-0.195539000	-0.001301000
8	-3.386543000	0.998170000	-0.544849000	8	1.821783000	-3.640458000	-0.000350000
6	2.879805000	0.568465000	-0.216058000	6	-2.639642000	2.156487000	-0.000796000
7	3.733316000	-0.419936000	-0.015539000	6	-3.767665000	1.374410000	-0.000321000
6	3.238886000	-1.646669000	0.197832000	7	-3.724294000	0.030283000	0.000039000
6	1.884029000	-1.946354000	0.220593000	6	-2.558512000	-0.575912000	-0.000068000
8	4.117676000	-2.634880000	0.399577000	8	-2.565832000	-1.915557000	0.000273000
1	0.376624000	3.313059000	-0.733544000	1	0.562976000	4.013416000	-0.002360000
1	-0.576389000	-3.215037000	0.387250000	1	-0.531464000	-2.621658000	-0.000065000
1	-3.048683000	-3.249650000	0.303591000	1	3.265438000	0.460785000	-0.001551000
1	-4.318333000	0.736069000	-0.524574000	1	2.780030000	-3.770748000	-0.000584000
1	3.300124000	1.554233000	-0.386325000	1	-2.694208000	3.235304000	-0.001081000
1	1.577331000	-2.967049000	0.398731000	1	-4.761091000	1.809618000	-0.000211000
1	5.011836000	-2.266434000	0.353553000	1	-3.489149000	-2.210434000	0.000570000
6	6.400306000	0.142488000	-0.054238000	6	5.212638000	-2.329448000	0.000531000
8	6.651045000	-0.970783000	0.152928000	8	4.879169000	-3.440150000	0.000858000
8	6.207461000	1.258998000	-0.260564000	8	5.606934000	-1.246914000	0.000256000
6	-1.984064000	3.494794000	0.799539000	6	3.276432000	3.575085000	0.002137000
8	-2.502869000	2.858346000	1.606895000	8	2.498697000	4.435489000	0.001829000
8	-1.461479000	4.183001000	0.025942000	8	4.083557000	2.755086000	0.002457000
6	-5.945904000	-1.530667000	-0.137067000	6	-6.112222000	-1.277508000	0.001320000
8	-5.871254000	-2.657471000	0.091442000	8	-6.702524000	-0.288486000	0.001191000
8	-6.087771000	-0.403348000	-0.368776000	8	-5.569975000	-2.302722000	0.001458000
pn25...3CO₂				pn26...3CO₂			
6	-1.470401000	0.345887000	0.000410000	6	1.037448000	-1.626741000	0.000091000
6	-0.591416000	-0.752982000	-0.001166000	6	0.885591000	-0.229771000	-0.000023000
6	0.828422000	-0.483369000	-0.001180000	6	-0.456491000	0.319357000	-0.000012000
6	1.265479000	0.863732000	0.000477000	6	-1.548756000	-0.580881000	-0.000036000
7	0.386675000	1.923163000	0.001832000	7	-1.378239000	-1.959636000	-0.000046000
6	-0.887564000	1.676290000	0.001803000	6	-0.180342000	-2.431433000	0.000075000
8	-1.730429000	2.700912000	0.003090000	8	0.024318000	-3.748539000	0.000049000
6	1.811771000	-1.478808000	-0.002600000	6	-0.755250000	1.683262000	0.000121000
7	3.110345000	-1.233786000	-0.002474000	7	-1.988143000	2.169795000	0.000188000
6	3.506278000	0.046548000	-0.000802000	6	-3.005910000	1.305704000	0.000132000
6	2.637645000	1.123616000	0.000729000	6	-2.845469000	-0.071541000	-0.000016000
8	4.826924000	0.275476000	-0.000522000	8	-4.248422000	1.813961000	0.000224000
6	-2.867405000	0.072283000	0.000541000	6	2.302019000	-2.206096000	0.000133000
7	-3.357784000	-1.151114000	-0.000779000	6	3.392889000	-1.348095000	0.000042000
6	-2.502547000	-2.187361000	-0.002294000	7	3.276077000	-0.018416000	-0.000148000
6	-1.137564000	-2.051469000	-0.002557000	6	2.067607000	0.522851000	-0.000179000

8	-3.741643000	1.075893000	0.002087000	8	4.630493000	-1.865573000	0.000122000
1	-1.210104000	3.518590000	0.003910000	1	-0.833531000	-4.199900000	0.000165000
1	1.541254000	-2.529791000	-0.003847000	1	0.034717000	2.427995000	0.000168000
1	3.013316000	2.136412000	0.001994000	1	-3.702964000	-0.728772000	-0.000061000
1	5.282309000	-0.577943000	-0.002210000	1	-4.181076000	2.778879000	-0.000006000
1	-2.965055000	-3.169179000	-0.003324000	1	2.438553000	-3.278098000	0.000228000
1	-0.512209000	-2.931893000	-0.003769000	1	2.044876000	1.607711000	-0.000366000
1	-4.629661000	0.688211000	0.001947000	1	5.267063000	-1.136999000	0.000027000
6	4.763944000	-3.368667000	0.002265000	6	-2.252226000	4.856757000	-0.000029000
8	3.873528000	-4.101074000	0.001401000	8	-3.408461000	4.774775000	-0.000116000
8	5.699665000	-2.684885000	0.003676000	8	-1.109030000	5.004789000	0.000081000
6	1.250355000	4.696555000	-0.001636000	6	-3.553137000	-3.858365000	-0.000117000
8	0.127370000	4.984645000	0.001025000	8	-2.745317000	-4.690737000	0.000246000
8	2.376851000	4.460039000	-0.004406000	8	-4.389908000	-3.068744000	-0.000536000
6	-6.004367000	-1.752327000	0.000045000	6	5.391205000	1.689467000	-0.000104000
8	-6.285344000	-0.627516000	0.001479000	8	6.137365000	0.802247000	0.000009000
8	-5.785706000	-2.883716000	-0.001450000	8	4.695139000	2.607838000	-0.000153000
pn27...3CO₂				pn28...3CO₂			
6	0.690881000	-1.718453000	0.000503000	6	1.589075000	-3.330626000	-0.334588000
6	-0.066760000	-0.537064000	0.000017000	6	0.367529000	-2.726153000	-0.235353000
6	0.633530000	0.731200000	-0.000166000	6	0.278327000	-1.312356000	-0.228002000
6	2.041754000	0.689082000	0.000045000	6	1.481743000	-0.614716000	-0.326914000
7	2.773698000	-0.481918000	0.000444000	7	2.692317000	-1.201173000	-0.410206000
6	2.134296000	-1.599415000	0.000684000	6	2.738071000	-2.507760000	-0.416628000
8	2.801493000	-2.763164000	0.001128000	8	3.930971000	-3.114072000	-0.501725000
7	-0.046666000	1.897859000	-0.000482000	6	-0.947733000	-0.553137000	-0.126395000
6	0.632659000	3.017139000	-0.000624000	6	-0.866561000	0.861468000	-0.138904000
6	2.043249000	3.091581000	-0.000491000	7	0.335364000	1.533622000	-0.259634000
6	2.738814000	1.916018000	-0.000142000	6	1.423447000	0.841749000	-0.352089000
8	-0.040420000	4.177664000	-0.000907000	8	2.594567000	1.455057000	-0.493032000
6	0.070517000	-2.980544000	0.000781000	6	-2.219650000	-1.120518000	-0.009732000
6	-1.298869000	-3.014311000	0.000541000	7	-3.335872000	-0.416703000	0.089517000
7	-2.057025000	-1.901347000	0.000010000	6	-3.241465000	0.917530000	0.077845000
6	-1.483893000	-0.718929000	-0.000263000	6	-2.044129000	1.603595000	-0.033549000
8	-2.301577000	0.340984000	-0.000880000	8	-4.384666000	1.614683000	0.179863000
1	3.750707000	-2.575367000	0.001179000	1	1.706462000	-4.405929000	-0.347720000
1	2.525814000	4.059430000	-0.000639000	1	-0.525715000	-3.334134000	-0.165768000
1	3.821146000	1.895970000	0.000015000	1	4.614135000	-2.429221000	-0.550359000
1	-0.986006000	3.973505000	-0.000803000	1	2.440928000	2.411781000	-0.486089000
1	0.664805000	-3.882511000	0.001167000	1	-2.350619000	-2.198340000	0.005939000
1	-1.846180000	-3.950585000	0.000751000	1	-2.023654000	2.683840000	-0.038758000
1	-3.209580000	-0.002915000	-0.000926000	1	-5.116508000	0.986202000	0.247249000
6	-3.727860000	2.786680000	0.001573000	6	-5.635082000	-1.811088000	0.283177000
8	-4.547605000	1.975743000	0.001993000	8	-6.262548000	-0.838326000	0.335689000
8	-2.935214000	3.628482000	0.001154000	8	-5.068704000	-2.814441000	0.235611000
6	-4.739514000	-2.348526000	-0.001208000	6	0.581821000	4.410187000	-0.239435000
8	-4.955229000	-1.209904000	-0.001682000	8	1.721973000	4.259398000	-0.388339000
8	-4.584423000	-3.490960000	-0.000762000	8	-0.541621000	4.611770000	-0.092209000
6	5.666481000	-0.598620000	-0.000377000	6	4.823179000	-0.109241000	1.063200000
8	5.819535000	0.542560000	-0.001034000	8	4.149331000	0.433595000	1.823634000
8	5.565632000	-1.753245000	0.000268000	8	5.540806000	-0.659917000	0.338256000
pn29...3CO₂				pn30...3CO₂			
6	-1.395367000	1.326022000	-0.010275000	6	2.858206000	-2.970650000	0.193911000
6	-1.221158000	-0.070045000	-0.003753000	6	1.497360000	-2.876510000	0.257044000
6	0.128317000	-0.606701000	-0.003068000	6	0.858685000	-1.645650000	-0.032314000
6	1.189332000	0.324454000	-0.008943000	6	1.691811000	-0.575449000	-0.376156000

7	1.003269000	1.701751000	-0.014655000	7	3.036058000	-0.655502000	-0.425971000
6	-0.196319000	2.158068000	-0.015549000	6	3.590359000	-1.808555000	-0.153704000
8	-0.432200000	3.475736000	-0.021666000	8	4.924506000	-1.907890000	-0.197363000
6	0.438268000	-1.966964000	0.002678000	6	-0.571093000	-1.435584000	0.004939000
6	1.774475000	-2.337457000	0.001947000	6	-1.027642000	-0.151899000	-0.318042000
7	2.784756000	-1.465840000	-0.004026000	7	-0.207190000	0.891381000	-0.658384000
6	2.496622000	-0.172929000	-0.009281000	6	1.066043000	0.695184000	-0.694563000
8	2.080959000	-3.646073000	0.007541000	8	1.884043000	1.692079000	-1.043527000
6	-2.672076000	1.875488000	-0.011518000	6	-1.522203000	-2.424485000	0.343604000
6	-3.745199000	0.993325000	-0.006118000	6	-2.849801000	-2.086040000	0.338168000
7	-3.604944000	-0.335178000	0.000114000	7	-3.305827000	-0.855559000	0.015212000
6	-2.384510000	-0.847832000	0.001246000	6	-2.434921000	0.069923000	-0.303001000
8	-4.990504000	1.485404000	-0.007174000	8	-2.873727000	1.286805000	-0.641953000
1	0.415108000	3.944585000	-0.024927000	1	3.390621000	-3.888642000	0.403171000
1	-0.316379000	-2.741152000	0.007489000	1	0.910421000	-3.745662000	0.526108000
1	3.331144000	0.520313000	-0.013850000	1	5.283670000	-1.040440000	-0.436922000
1	3.044485000	-3.731018000	0.006154000	1	1.336902000	2.476424000	-1.201642000
1	-2.832597000	2.944102000	-0.016557000	1	-1.226299000	-3.430620000	0.606812000
1	-2.333877000	-1.931853000	0.006367000	1	-3.614290000	-2.810606000	0.596233000
1	-5.614280000	0.745318000	-0.002857000	1	-3.838981000	1.285262000	-0.566871000
6	5.404320000	-2.184738000	-0.009076000	6	-0.774838000	3.391040000	0.446425000
8	5.751456000	-1.086395000	-0.016389000	8	-1.375722000	2.963540000	1.331209000
8	5.117750000	-3.308573000	-0.001896000	8	-0.156958000	3.867167000	-0.411514000
6	3.148973000	3.648115000	0.028316000	6	4.512366000	1.468807000	0.665957000
8	3.997467000	2.870964000	0.042473000	8	3.656134000	1.844816000	1.338796000
8	2.328029000	4.467175000	0.014482000	8	5.409986000	1.107945000	0.027428000
6	-5.690880000	-2.077435000	0.013009000	6	-5.976287000	-0.426874000	0.095659000
8	-4.981423000	-2.985376000	0.017198000	8	-6.186021000	-1.510849000	0.425453000
8	-6.449529000	-1.200817000	0.009238000	8	-5.833690000	0.675450000	-0.234836000
pn31...3CO ₂				pn32...3CO ₂			
6	2.521806000	-3.226572000	-0.015911000	6	1.405414000	1.372765000	-0.311952000
6	1.173925000	-3.004293000	-0.008203000	6	1.314884000	-0.015068000	-0.122619000
6	0.680375000	-1.679193000	-0.011250000	6	0.005005000	-0.641305000	-0.097003000
6	1.630438000	-0.655212000	-0.021516000	6	-1.094310000	0.217498000	-0.266333000
7	2.960668000	-0.861510000	-0.027143000	7	-0.999359000	1.576552000	-0.427052000
6	3.382504000	-2.102481000	-0.025642000	6	0.167643000	2.111513000	-0.452952000
8	4.698172000	-2.336297000	-0.033664000	8	0.290695000	3.436889000	-0.612972000
6	-0.723770000	-1.323202000	-0.004030000	6	-0.258205000	-2.021685000	0.075567000
6	-1.041131000	0.052304000	-0.008377000	6	-1.561418000	-2.449147000	0.061577000
7	-0.089819000	1.057885000	-0.020524000	7	-2.622406000	-1.634588000	-0.119633000
6	1.153968000	0.723920000	-0.026870000	6	-2.396685000	-0.355051000	-0.281652000
8	2.113855000	1.650802000	-0.039587000	8	-3.433767000	0.467975000	-0.483105000
6	-1.771110000	-2.248579000	0.007315000	6	2.651120000	2.022413000	-0.353707000
6	-3.070596000	-1.771595000	0.014023000	6	3.775598000	1.253143000	-0.202654000
7	-3.382379000	-0.472377000	0.010617000	7	3.728438000	-0.080071000	-0.017182000
6	-2.396237000	0.409369000	-0.000295000	6	2.565186000	-0.685945000	0.022105000
8	-4.085790000	-2.654414000	0.024793000	8	2.573675000	-2.012986000	0.209786000
1	2.950362000	-4.219685000	-0.014792000	1	-0.600130000	3.810549000	-0.693575000
1	0.489432000	-3.843349000	-0.000333000	1	0.541007000	-2.729388000	0.215717000
1	5.155363000	-1.481897000	-0.044444000	1	-1.801100000	-3.498321000	0.195266000
1	1.701431000	2.526729000	-0.037429000	1	-4.242018000	-0.063750000	-0.447994000
1	-1.608897000	-3.317484000	0.011170000	1	2.705499000	3.091471000	-0.500272000
1	-2.669902000	1.459220000	-0.003137000	1	4.769632000	1.686102000	-0.224416000
1	-4.916855000	-2.159667000	0.028371000	1	3.497300000	-2.296619000	0.286653000
6	-5.924991000	0.476216000	0.031029000	6	-2.843734000	3.213069000	0.897666000
8	-5.564791000	1.570297000	0.024027000	8	-3.096474000	2.441316000	1.713943000
8	-6.350304000	-0.602817000	0.038675000	8	-2.599598000	4.034492000	0.115959000

6	-0.698447000	3.886344000	-0.053117000	6	-5.104324000	-2.718202000	-0.097107000
8	-1.841312000	3.748608000	-0.051193000	8	-5.583910000	-1.678556000	-0.282292000
8	0.445187000	4.076511000	-0.055690000	8	-4.691620000	-3.777956000	0.086895000
6	5.329297000	1.456021000	0.080989000	6	6.116932000	-1.357442000	0.265814000
8	4.900102000	2.518484000	0.178435000	8	5.577478000	-2.376686000	0.390127000
8	5.810331000	0.405060000	-0.014416000	8	6.704078000	-0.373566000	0.148556000
pn33...3CO ₂				pn34...3CO ₂			
6	-1.393250000	1.204257000	-0.292314000	6	-1.580642000	0.291642000	0.000434000
6	-1.222603000	-0.181722000	-0.106053000	6	-0.974592000	-0.976064000	0.000021000
6	0.118321000	-0.733066000	-0.089204000	6	0.477758000	-1.042366000	-0.000110000
6	1.171115000	0.172501000	-0.260854000	6	1.181933000	0.176409000	0.000158000
7	1.001424000	1.529841000	-0.419638000	7	0.570663000	1.413161000	0.000585000
6	-0.190055000	2.007097000	-0.438897000	6	-0.720454000	1.465301000	0.000790000
8	-0.384783000	3.322709000	-0.594712000	8	-1.322594000	2.653841000	0.001413000
6	0.427002000	-2.099502000	0.080170000	6	1.202623000	-2.237578000	-0.000488000
6	1.744871000	-2.480409000	0.062789000	6	2.584457000	-2.167760000	-0.000555000
7	2.768392000	-1.620649000	-0.120060000	7	3.263966000	-1.016579000	-0.000283000
6	2.493610000	-0.347961000	-0.280521000	6	2.585420000	0.117080000	0.000053000
8	3.498146000	0.511735000	-0.483502000	8	3.294570000	-3.310074000	-0.000880000
6	-2.667446000	1.762180000	-0.321566000	6	-3.005450000	0.330656000	0.000461000
6	-3.742373000	0.899905000	-0.160990000	7	-3.751426000	-0.755532000	0.000239000
7	-3.607020000	-0.418705000	0.018364000	6	-3.150959000	-1.956786000	-0.000078000
6	-2.392110000	-0.939609000	0.044614000	6	-1.788854000	-2.122684000	-0.000237000
8	-4.985785000	1.396537000	-0.183458000	8	-3.638263000	1.501405000	0.000788000
1	0.483121000	3.746998000	-0.676128000	1	-0.636725000	3.337396000	0.001554000
1	-0.344552000	-2.843447000	0.222076000	1	0.731234000	-3.209971000	-0.000710000
1	2.028797000	-3.518887000	0.193932000	1	3.157822000	1.038524000	0.000252000
1	4.326796000	0.012069000	-0.450402000	1	4.234768000	-3.083031000	-0.001067000
1	-2.821372000	2.822631000	-0.462578000	1	-3.820479000	-2.810755000	-0.000237000
1	-2.347931000	-2.013743000	0.192296000	1	-1.366236000	-3.116514000	-0.000527000
1	-5.610817000	0.668535000	-0.057390000	1	-4.589706000	1.318549000	0.000913000
6	5.286992000	-2.612806000	-0.105583000	6	5.980867000	-0.868339000	0.001107000
8	5.729070000	-1.556887000	-0.291106000	8	6.062343000	-2.025348000	0.000557000
8	4.911412000	-3.686364000	0.078606000	8	5.962843000	0.283328000	0.001659000
6	2.763190000	3.254599000	0.905132000	6	2.035045000	3.930435000	-0.001513000
8	3.069920000	2.486966000	1.706672000	8	1.005947000	4.463792000	0.000442000
8	2.463558000	4.071014000	0.137654000	8	3.078869000	3.444813000	-0.003440000
6	-5.693590000	-2.129919000	0.338907000	6	-6.469239000	-0.761467000	-0.000381000
8	-4.984301000	-3.032831000	0.437706000	8	-6.495986000	0.397513000	0.000058000
8	-6.451695000	-1.257983000	0.246357000	8	-6.502800000	-1.913325000	-0.000840000
pn35...3CO ₂				pn36...3CO ₂			
6	1.543667000	0.203618000	-0.190477000	6	-0.655476000	-1.845799000	-0.341308000
6	0.962320000	-1.057818000	0.040758000	6	-0.763536000	-0.469410000	-0.105893000
6	-0.483122000	-1.169059000	0.017058000	6	0.455156000	0.304416000	-0.016870000
6	-1.202951000	0.000573000	-0.238231000	6	1.670089000	-0.399048000	0.116425000
7	-0.632224000	1.224009000	-0.440397000	7	1.748904000	-1.775082000	0.005628000
6	0.656975000	1.325084000	-0.419667000	6	0.673988000	-2.425976000	-0.284864000
8	1.196454000	2.528888000	-0.612914000	8	0.725861000	-3.741991000	-0.498569000
6	-1.195971000	-2.371370000	0.228642000	6	0.578742000	1.713292000	-0.178135000
6	-2.563496000	-2.341244000	0.169399000	7	1.695648000	2.375302000	0.034418000
7	-3.273523000	-1.219826000	-0.092905000	6	2.811222000	1.684190000	0.333309000
6	-2.626534000	-0.100907000	-0.292352000	6	2.863524000	0.314520000	0.338268000
8	-3.313524000	1.012136000	-0.570896000	8	-0.461639000	2.400183000	-0.656274000
6	2.967266000	0.281191000	-0.174364000	6	-1.794397000	-2.644658000	-0.542111000
7	3.738573000	-0.760888000	0.050478000	6	-3.018648000	-2.032869000	-0.450932000
6	3.164173000	-1.956538000	0.273632000	7	-3.160244000	-0.749521000	-0.070804000

6	1.808125000	-2.158788000	0.278784000	6	-2.094337000	-0.011897000	0.146742000
8	3.563035000	1.450002000	-0.396142000	8	-2.271700000	1.180526000	0.713836000
1	0.464309000	3.149626000	-0.750285000	1	1.644268000	-4.036268000	-0.406175000
1	-0.689256000	-3.303323000	0.435138000	1	3.694322000	2.283934000	0.525909000
1	-3.153515000	-3.236624000	0.329482000	1	3.788305000	-0.222299000	0.491986000
1	-4.256146000	0.791206000	-0.555349000	1	-0.204265000	3.332180000	-0.704382000
1	3.853543000	-2.775060000	0.453054000	1	-1.695592000	-3.699478000	-0.752954000
1	1.411093000	-3.146260000	0.461676000	1	-3.941773000	-2.571645000	-0.633905000
1	4.520023000	1.307063000	-0.344052000	1	-3.223443000	1.322496000	0.821657000
6	-1.872191000	3.356612000	0.850900000	6	1.962905000	5.050577000	-0.244323000
8	-2.334413000	2.695343000	1.673970000	8	0.862611000	5.154852000	-0.595331000
8	-1.405480000	4.066152000	0.062440000	8	3.063492000	5.016627000	0.095400000
6	-5.977754000	-1.402240000	-0.143836000	6	-5.703236000	0.087959000	0.385085000
8	-5.952151000	-2.528347000	0.098579000	8	-6.140469000	-0.903945000	-0.005681000
8	-6.070663000	-0.272853000	-0.389752000	8	-5.322979000	1.105245000	0.791129000
6	6.454173000	-0.674046000	0.092343000	6	4.186135000	-3.304830000	0.325832000
8	6.442614000	0.462668000	-0.135284000	8	4.837375000	-2.413508000	0.651079000
8	6.525639000	-1.801502000	0.319319000	8	3.571852000	-4.233817000	0.002638000

VIII. Dicarboxylic acid-CO₂ complex

pn1''-(COOH) ₂ ...CO ₂				pn2''-(COOH) ₂ ...CO ₂			
6	3.444573000	2.147064000	-0.627979000	6	1.742422000	-1.558379000	-0.330408000
6	2.175305000	2.621455000	-0.439902000	6	0.391626000	-1.246726000	-0.272343000
6	1.115779000	1.705877000	-0.305970000	6	0.015439000	0.156119000	-0.222969000
6	1.388576000	0.341855000	-0.384655000	6	1.008296000	1.184204000	-0.066107000
7	2.637986000	-0.130974000	-0.543818000	7	2.362918000	0.792385000	0.065938000
6	3.619083000	0.745343000	-0.654634000	6	2.769165000	-0.526762000	-0.209762000
8	4.862593000	0.287673000	-0.795775000	8	3.955262000	-0.816749000	-0.299471000
6	-0.226135000	2.182551000	-0.016923000	6	-1.283532000	0.515080000	-0.389336000
7	-1.207064000	1.202036000	0.219605000	7	-1.690566000	1.807489000	-0.384813000
6	-0.988365000	-0.125183000	-0.151145000	6	-0.764177000	2.859307000	-0.257400000
6	0.284497000	-0.594354000	-0.373256000	6	0.609432000	2.491222000	-0.103207000
8	-0.492147000	3.372899000	0.090226000	8	-1.156062000	4.031684000	-0.287549000
7	-2.074281000	-0.970595000	-0.300410000	6	2.119731000	-2.907370000	-0.465766000
6	-1.901667000	-2.374416000	-0.355015000	6	1.146053000	-3.867340000	-0.518783000
6	-0.560192000	-2.848919000	-0.575362000	6	-0.197721000	-3.443122000	-0.417274000
6	0.472332000	-1.984693000	-0.632018000	7	-0.570828000	-2.180650000	-0.299036000
8	-2.875128000	-3.120434000	-0.277513000	8	-1.139080000	-4.381926000	-0.438485000
1	4.306381000	2.790297000	-0.736448000	1	-2.060276000	-0.215867000	-0.552645000
1	1.961990000	3.682125000	-0.384683000	1	1.285517000	3.321598000	0.004507000
1	4.850141000	-0.677593000	-0.724661000	1	3.172041000	-3.157722000	-0.520144000
1	-0.453709000	-3.915287000	-0.715550000	1	1.361817000	-4.921710000	-0.618710000
1	1.477552000	-2.323887000	-0.848824000	1	-2.005996000	-3.964889000	-0.321327000
6	-3.396758000	-0.400645000	-0.678818000	6	-3.148395000	2.036847000	-0.518274000
8	-3.445489000	0.684349000	-1.165235000	8	-3.871680000	1.092871000	-0.593778000
8	-4.395037000	-1.197281000	-0.462945000	8	-3.476819000	3.288630000	-0.536486000
1	-4.047433000	-2.110942000	-0.231502000	1	-2.631193000	3.853364000	-0.444834000
6	-2.348252000	1.515259000	1.107480000	6	3.337283000	1.759212000	0.604206000
8	-2.859031000	0.641624000	1.732336000	8	2.966531000	2.709011000	1.215422000
8	-2.673835000	2.773799000	1.145828000	8	4.588985000	1.479578000	0.351933000
1	-2.010448000	3.312357000	0.642944000	1	4.661005000	0.564177000	-0.026774000
6	3.403814000	-2.110669000	1.349344000	6	-2.992192000	-1.921649000	1.384078000
8	2.403462000	-2.026283000	1.915012000	8	-2.622202000	-0.980927000	1.936309000
8	4.415050000	-2.214282000	0.793593000	8	-3.371704000	-2.871844000	0.840276000
pn3''-(COOH) ₂ ...CO ₂				pn4''-(COOH) ₂ ...CO ₂			
6	-0.476556000	-1.827786000	0.113252000	6	-1.858900000	1.864753000	-0.213919000

6	0.451126000	-0.793705000	-0.038318000	6	-0.833598000	0.931042000	-0.118681000
6	-0.036423000	0.542117000	0.087360000	6	-1.193169000	-0.417358000	0.058243000
6	-1.418891000	0.712380000	-0.024228000	6	-2.542911000	-0.758591000	0.144633000
7	-2.318128000	-0.297587000	-0.003342000	7	-3.517827000	0.132654000	0.064921000
6	-1.854443000	-1.509716000	0.149371000	6	-3.173218000	1.411763000	-0.115084000
8	-2.704807000	-2.532005000	0.298894000	8	-4.154952000	2.308269000	-0.202380000
7	0.760942000	1.687173000	0.282893000	6	0.578725000	1.269916000	-0.106804000
6	0.308838000	2.960587000	-0.076325000	6	1.510163000	0.258036000	-0.044410000
6	-1.115906000	3.095362000	-0.339912000	7	1.134188000	-1.080579000	-0.175692000
6	-1.939287000	2.043155000	-0.242745000	6	-0.195982000	-1.476082000	0.060825000
8	1.058586000	3.931677000	-0.083215000	8	-0.482166000	-2.657543000	0.185755000
6	-0.030206000	-3.186164000	0.251501000	6	1.049084000	2.617851000	-0.123262000
6	1.281564000	-3.467874000	0.277772000	6	2.365534000	2.906976000	-0.149078000
6	2.268410000	-2.434154000	0.026957000	6	3.346955000	1.859385000	-0.050750000
7	1.778587000	-1.152460000	-0.293379000	7	2.848588000	0.552043000	0.151606000
8	3.470111000	-2.669949000	0.017087000	8	4.557734000	2.066038000	-0.079242000
1	-3.611478000	-2.193853000	0.275320000	1	-1.691818000	2.922495000	-0.355023000
1	-1.455192000	4.099409000	-0.555120000	1	-2.827869000	-1.797274000	0.277386000
1	-3.010077000	2.139628000	-0.371533000	1	-5.004873000	1.849527000	-0.119342000
1	-0.778785000	-3.957531000	0.380288000	1	0.327855000	3.424601000	-0.153625000
1	1.677297000	-4.460981000	0.438679000	1	2.751319000	3.914382000	-0.214569000
6	1.976760000	1.548686000	1.078463000	6	3.726613000	-0.451010000	0.821285000
8	2.154785000	0.553257000	1.714922000	8	3.230579000	-1.315904000	1.469996000
8	2.789571000	2.566015000	1.032409000	8	4.992544000	-0.241350000	0.647927000
1	2.371974000	3.303594000	0.503594000	1	5.127299000	0.659381000	0.224524000
6	2.609907000	-0.242387000	-1.085517000	6	2.070807000	-2.021102000	-0.823898000
8	2.088676000	0.608733000	-1.739272000	8	2.964570000	-1.595298000	-1.483913000
8	3.891775000	-0.462450000	-1.017976000	8	1.798809000	-3.278297000	-0.629922000
1	4.060302000	-1.299464000	-0.502598000	1	0.938755000	-3.372030000	-0.148166000
6	-5.209480000	0.006796000	-0.132906000	6	-6.128562000	-0.684134000	0.222312000
8	-5.185020000	1.140219000	-0.334350000	8	-5.830301000	-1.788173000	0.352594000
8	-5.275716000	-1.132306000	0.068979000	8	-6.477388000	0.414937000	0.093498000
pn5''-(COOH) ₂ ...CO ₂				pn6''-(COOH) ₂ ...CO ₂			
6	0.933830000	-0.988656000	-0.159306000	6	-1.663091000	1.566795000	-0.439278000
6	0.325357000	0.295432000	-0.272809000	6	-1.436377000	0.202382000	-0.356729000
6	-1.132072000	0.336069000	-0.379758000	6	-0.050546000	-0.268728000	-0.257679000
6	-1.861592000	-0.847692000	-0.331923000	6	0.991887000	0.692335000	-0.070182000
7	-1.232891000	-2.094032000	-0.026525000	7	0.671159000	2.075470000	0.103261000
6	0.154301000	-2.224268000	-0.048536000	6	-0.594389000	2.551576000	-0.220663000
8	0.705900000	-3.312792000	0.061006000	8	-0.848920000	3.750413000	-0.258385000
7	-1.695324000	1.536836000	-0.608151000	6	0.249080000	-1.584965000	-0.439726000
6	-2.983596000	1.595410000	-0.847054000	6	1.593875000	-2.062506000	-0.444338000
6	-3.792484000	0.448039000	-0.939255000	7	2.574469000	-1.072878000	-0.318240000
6	-3.227176000	-0.772344000	-0.678289000	6	2.278533000	0.252227000	-0.142412000
8	-3.560430000	2.788741000	-1.033106000	8	1.900664000	-3.256680000	-0.572964000
6	2.292614000	-1.083087000	-0.112240000	6	-2.978804000	2.017595000	-0.654969000
7	3.079255000	0.019377000	-0.172089000	6	-3.988033000	1.098857000	-0.758151000
6	2.535810000	1.322618000	-0.297137000	6	-3.651046000	-0.265286000	-0.616956000
6	1.109367000	1.406362000	-0.353280000	7	-2.419515000	-0.704525000	-0.430584000
8	3.287036000	2.300002000	-0.355231000	8	-4.641472000	-1.152038000	-0.673463000
1	-4.835555000	0.547763000	-1.206287000	1	-0.528227000	-2.312546000	-0.623391000
1	-3.831280000	-1.663743000	-0.732962000	1	3.144750000	0.887427000	-0.056690000
1	-2.900285000	3.479239000	-0.881834000	1	-3.164860000	3.082024000	-0.726926000
1	2.809660000	-2.029947000	-0.021693000	1	-5.020495000	1.374757000	-0.922004000
1	0.687940000	2.392313000	-0.484924000	1	-4.284754000	-2.037177000	-0.505501000
6	4.549863000	-0.224386000	-0.102593000	6	4.027921000	-1.397862000	-0.390345000

8	4.935999000	-1.343553000	-0.002757000	8	4.817386000	-0.511284000	-0.334143000
8	5.259649000	0.856952000	-0.161348000	8	4.269220000	-2.664700000	-0.516078000
1	4.642622000	1.659413000	-0.249395000	1	3.385506000	-3.172378000	-0.555044000
6	-2.057860000	-3.169385000	0.529464000	6	1.639595000	2.941811000	0.781045000
8	-3.159321000	-2.941918000	0.922959000	8	2.577596000	2.470815000	1.342992000
8	-1.492716000	-4.348456000	0.547245000	8	1.382090000	4.222134000	0.711095000
1	-0.534493000	-4.270005000	0.297867000	1	0.506988000	4.371220000	0.266777000
6	-1.181598000	3.406981000	1.498380000	6	-2.450382000	-2.795250000	1.546646000
8	-0.657772000	2.613800000	2.150472000	8	-1.594896000	-2.330945000	2.161865000
8	-1.703904000	4.217616000	0.857333000	8	-3.315548000	-3.274424000	0.942100000
pn7''-(COOH)₂...CO₂				pn8''-(COOH)₂...CO₂			
6	1.333751000	0.641538000	-0.000415000	6	-0.994942000	1.348229000	-0.206027000
6	0.604029000	-0.599533000	-0.000151000	6	-1.125136000	-0.026348000	-0.009588000
6	-0.843664000	-0.474336000	-0.000274000	6	0.070521000	-0.857620000	0.037505000
6	-1.409744000	0.802263000	-0.000622000	6	1.299048000	-0.233798000	0.025419000
7	-0.687126000	1.975261000	-0.000818000	7	1.405953000	1.154148000	0.160019000
6	0.605457000	1.887012000	-0.000783000	6	0.331105000	1.984100000	-0.154696000
8	1.343846000	2.986642000	-0.000996000	8	0.473790000	3.189186000	-0.288549000
6	-1.696847000	-1.643137000	-0.000013000	6	-2.107426000	2.182239000	-0.361289000
7	-3.081334000	-1.419843000	-0.000083000	6	-3.350531000	1.599701000	-0.303732000
6	-3.610056000	-0.150909000	-0.000388000	7	-3.517261000	0.284520000	-0.091180000
6	-2.828031000	0.945759000	-0.000678000	6	-2.468937000	-0.493064000	0.054169000
8	-1.267014000	-2.803428000	0.000432000	8	-2.702434000	-1.796011000	0.279161000
6	2.699626000	0.640715000	-0.000331000	6	0.064528000	-2.291999000	0.056218000
7	3.399942000	-0.513449000	-0.000019000	6	1.209846000	-3.001951000	0.127889000
6	2.753275000	-1.774829000	0.000257000	6	2.489730000	-2.356259000	0.073164000
6	1.327580000	-1.768375000	0.000184000	7	2.468847000	-0.959942000	-0.126901000
8	3.439395000	-2.805519000	0.000627000	8	3.560016000	-2.962138000	0.133174000
1	0.763032000	3.764135000	-0.001083000	1	-1.970283000	3.244044000	-0.509110000
1	-4.690020000	-0.120022000	-0.000465000	1	-4.260305000	2.178003000	-0.418030000
1	-3.261418000	1.934294000	-0.000885000	1	-3.662801000	-1.930523000	0.297620000
1	3.290722000	1.547166000	-0.000481000	1	-0.883498000	-2.805673000	0.057292000
1	0.860100000	-2.738249000	0.000470000	1	1.225309000	-4.080392000	0.198632000
6	-4.068235000	-2.522801000	0.000250000	6	3.655463000	-0.313177000	-0.755856000
8	-5.228131000	-2.254956000	0.000087000	8	3.508415000	0.682504000	-1.392488000
8	-3.547838000	-3.712764000	0.000190000	8	4.763293000	-0.952343000	-0.562919000
1	-2.542845000	-3.631591000	0.000060000	1	4.559847000	-1.853077000	-0.152767000
6	4.887590000	-0.381650000	0.000016000	6	2.582984000	1.713148000	0.863632000
8	5.358625000	0.710670000	-0.000334000	8	3.226779000	1.007628000	1.571043000
8	5.503326000	-1.517024000	0.000468000	8	2.785337000	2.982374000	0.660984000
1	4.806455000	-2.271670000	0.000694000	1	2.050022000	3.367519000	0.124891000
6	-1.816264000	4.656912000	0.001026000	6	-6.094028000	-0.635930000	0.040687000
8	-0.720999000	5.037502000	0.001813000	8	-5.705336000	-1.712469000	0.230552000
8	-2.915858000	4.317675000	0.000170000	8	-6.526661000	0.414444000	-0.145591000
pn9''-(COOH)₂...CO₂				pn10''-(COOH)₂...CO₂			
6	-1.624689000	-1.739171000	-0.231991000	6	0.073370000	-2.936714000	-0.569108000
6	-0.355282000	-1.179061000	-0.038034000	6	-0.730420000	-1.871255000	-0.407991000
6	-0.247512000	0.277626000	-0.023293000	6	-0.166678000	-0.569873000	-0.163417000
6	-1.404316000	1.045389000	-0.024189000	6	1.180472000	-0.461828000	-0.012719000
7	-2.669024000	0.439355000	-0.000634000	7	1.997809000	-1.584817000	0.010824000
6	-2.823144000	-0.931054000	-0.267662000	6	1.516508000	-2.838960000	-0.390028000
8	-3.935190000	-1.411594000	-0.470192000	8	2.271003000	-3.793345000	-0.522955000
6	1.056915000	0.926047000	-0.065720000	6	-0.988034000	0.621888000	-0.032093000
7	1.057451000	2.326501000	-0.156895000	6	-0.367265000	1.863793000	0.092375000
6	-0.107586000	3.045574000	-0.212607000	7	1.033712000	1.970708000	-0.112128000
6	-1.319285000	2.464602000	-0.144634000	6	1.845109000	0.845202000	-0.160909000

8	2.133440000	0.326859000	-0.034705000	8	3.038387000	0.903183000	-0.433068000
6	-1.752870000	-3.136841000	-0.336019000	7	-2.321153000	0.446812000	0.080674000
6	-0.639128000	-3.919499000	-0.222953000	6	-3.059499000	1.496137000	0.366109000
6	0.587745000	-3.258884000	0.005581000	6	-2.521481000	2.771608000	0.612757000
7	0.731234000	-1.949985000	0.086866000	6	-1.170869000	2.954368000	0.476641000
8	1.672084000	-4.013089000	0.148801000	8	-4.387484000	1.362934000	0.459661000
1	0.028714000	4.111967000	-0.317135000	1	-0.301005000	-3.924286000	-0.804549000
1	-2.196341000	3.084680000	-0.187724000	1	-1.802096000	-1.955436000	-0.508964000
1	-2.737351000	-3.559335000	-0.494525000	1	-3.179594000	3.577050000	0.907639000
1	-0.662967000	-4.998213000	-0.288144000	1	-0.737770000	3.923667000	0.661783000
1	2.432566000	-3.427974000	0.292370000	1	-4.631015000	0.441072000	0.303975000
6	2.299389000	3.131340000	-0.230266000	6	3.224417000	-1.513864000	0.831468000
8	2.209264000	4.314696000	-0.321700000	8	3.294780000	-0.718596000	1.708953000
8	3.398806000	2.442433000	-0.186743000	8	4.127764000	-2.405137000	0.515395000
1	3.175745000	1.465964000	-0.118075000	1	3.724084000	-3.097307000	-0.062479000
6	-3.835552000	1.215892000	0.467175000	6	1.575753000	3.274503000	-0.541260000
8	-3.678801000	2.179990000	1.146120000	8	0.837269000	4.162787000	-0.830271000
8	-4.987584000	0.744799000	0.078055000	8	2.877347000	3.352281000	-0.557835000
1	-4.859410000	-0.171886000	-0.300598000	1	3.272049000	2.440227000	-0.467851000
6	4.416204000	-1.197924000	0.314823000	6	-4.555347000	-2.362516000	-0.145769000
8	4.895968000	-0.159775000	0.180073000	8	-3.876929000	-3.260661000	-0.393399000
8	3.976520000	-2.259385000	0.456190000	8	-5.238816000	-1.462050000	0.100833000
pn11''-(COOH) ₂ ...CO ₂				pn12''-(COOH) ₂ ...CO ₂			
6	-1.572118000	1.563147000	-0.471456000	6	-1.319863000	0.653822000	-0.130484000
6	-1.462181000	0.177698000	-0.397509000	6	-0.556841000	-0.501117000	0.096693000
6	-0.130052000	-0.412857000	-0.293182000	6	0.895491000	-0.358470000	0.068523000
6	0.934438000	0.422277000	-0.100714000	6	1.502557000	0.947031000	-0.023732000
7	0.776925000	1.802110000	0.089886000	7	0.667380000	2.089929000	-0.011254000
6	-0.419107000	2.439407000	-0.238975000	6	-0.715533000	1.979303000	-0.238325000
8	-0.510782000	3.658224000	-0.257119000	8	-1.398191000	2.968794000	-0.463452000
6	0.087735000	-1.812078000	-0.475783000	6	1.709004000	-1.447260000	0.044723000
6	1.345722000	-2.289109000	-0.476669000	7	3.060593000	-1.358072000	-0.058250000
7	2.435416000	-1.443714000	-0.384401000	6	3.699773000	-0.112962000	-0.189600000
6	2.297465000	-0.058933000	-0.304402000	6	2.856457000	1.041068000	-0.168352000
8	3.255403000	0.696444000	-0.448000000	8	4.927439000	-0.057199000	-0.318149000
6	-2.841288000	2.126414000	-0.693621000	6	-2.709877000	0.549814000	-0.183680000
6	-3.924606000	1.298462000	-0.816744000	7	-3.353390000	-0.595406000	-0.020123000
6	-3.706630000	-0.091205000	-0.692751000	6	-2.622066000	-1.688511000	0.214035000
7	-2.521338000	-0.640215000	-0.499731000	6	-1.228436000	-1.699569000	0.285031000
8	-4.770001000	-0.889247000	-0.775067000	8	-3.267648000	-2.838663000	0.389369000
1	-0.754122000	-2.472799000	-0.616589000	1	1.341097000	-2.462490000	0.090450000
1	1.602949000	-3.332904000	-0.576780000	1	3.377966000	1.979518000	-0.250326000
1	-2.933130000	3.204092000	-0.755238000	1	-3.311207000	1.435689000	-0.358822000
1	-4.928260000	1.662943000	-0.986437000	1	-0.732143000	-2.639203000	0.482733000
1	-4.489828000	-1.801465000	-0.611254000	1	-4.221197000	-2.677479000	0.319866000
6	1.713668000	2.460405000	1.012235000	6	3.806948000	-2.641098000	-0.062880000
8	2.294803000	1.815354000	1.820569000	8	3.195700000	-3.656928000	0.047400000
8	1.793838000	3.761309000	0.863733000	8	5.086224000	-2.496512000	-0.192452000
1	1.065507000	4.080289000	0.287306000	1	5.302324000	-1.502625000	-0.270230000
6	3.760412000	-2.090495000	-0.475806000	6	1.248280000	3.393618000	0.357104000
8	3.818771000	-3.278623000	-0.513813000	8	2.281556000	3.446643000	0.942650000
8	4.766117000	-1.266473000	-0.502769000	8	0.543303000	4.432714000	-0.005569000
1	4.431199000	-0.321440000	-0.492394000	1	-0.342528000	4.140310000	-0.344678000
6	-2.748027000	-2.603820000	1.558165000	6	-6.090554000	-0.646709000	-0.120806000
8	-1.855077000	-2.172692000	2.144193000	8	-6.155791000	0.484234000	-0.325345000
8	-3.648562000	-3.052029000	0.982572000	8	-6.073646000	-1.788412000	0.084160000

pn13''-(COOH) ₂ ...CO ₂				pn14''-(COOH) ₂ ...CO ₂			
6	-0.796524000	-1.573370000	0.156727000	6	2.891103000	2.733304000	0.279231000
6	-0.080757000	-0.356557000	0.022721000	6	1.525745000	2.798370000	0.223907000
6	-0.805838000	0.906283000	0.050675000	6	0.762969000	1.607276000	0.190892000
6	-2.195457000	0.903430000	0.097538000	6	1.479966000	0.418212000	0.234572000
7	-2.917473000	-0.337336000	0.025613000	7	2.817838000	0.339337000	0.267880000
6	-2.287400000	-1.560376000	0.192966000	6	3.500299000	1.457473000	0.287369000
8	-2.900636000	-2.611698000	0.305732000	8	4.835004000	1.402714000	0.321671000
7	-0.072267000	2.024634000	0.101394000	6	-0.680530000	1.561137000	0.039896000
6	-0.684910000	3.177387000	0.227332000	6	-1.319236000	0.345325000	0.087082000
6	-2.076985000	3.289026000	0.365801000	7	-0.622797000	-0.810478000	0.448097000
6	-2.831095000	2.141021000	0.304027000	6	0.775422000	-0.874096000	0.353013000
8	0.063257000	4.289540000	0.247899000	8	1.369807000	-1.931392000	0.460492000
6	-0.150989000	-2.769008000	0.203938000	6	-1.476588000	2.725726000	-0.182456000
6	1.281320000	-2.833816000	0.117267000	6	-2.820307000	2.656721000	-0.274661000
7	1.943797000	-1.598403000	-0.012620000	6	-3.493090000	1.384653000	-0.263050000
6	1.277074000	-0.407204000	-0.051638000	7	-2.666968000	0.242600000	-0.224748000
8	1.921696000	-3.890701000	0.151773000	8	-4.715614000	1.271104000	-0.343054000
1	-2.529360000	4.258584000	0.520401000	1	3.512487000	3.618103000	0.313976000
1	-3.902889000	2.203340000	0.405274000	1	1.042779000	3.766874000	0.213586000
1	0.987116000	4.017097000	0.158361000	1	5.104175000	0.471322000	0.337727000
1	-0.684808000	-3.704479000	0.300391000	1	-0.993006000	3.692526000	-0.242504000
1	1.887001000	0.482815000	-0.133492000	1	-3.451787000	3.525964000	-0.391829000
6	3.424263000	-1.512484000	-0.099310000	6	-3.193328000	-1.038691000	-0.774103000
8	3.931117000	-0.437750000	-0.195941000	8	-2.433670000	-1.830727000	-1.233982000
8	4.020324000	-2.658768000	-0.058311000	8	-4.483085000	-1.142285000	-0.722263000
1	3.321180000	-3.396580000	0.031078000	1	-4.878780000	-0.254604000	-0.461797000
6	-4.316981000	-0.295694000	-0.412140000	6	-1.346630000	-1.868718000	1.188158000
8	-4.751607000	0.677055000	-0.942518000	8	-2.372189000	-1.603685000	1.729208000
8	-5.010210000	-1.379997000	-0.170461000	8	-0.751103000	-3.024540000	1.203982000
1	-4.415083000	-2.103974000	0.146826000	1	0.149922000	-2.949918000	0.799744000
6	4.362142000	2.308022000	-0.181793000	6	4.148167000	-1.762578000	-1.064072000
8	5.502910000	2.178216000	-0.260886000	8	3.288215000	-1.995496000	-1.792538000
8	3.217059000	2.474225000	-0.101563000	8	5.049377000	-1.537590000	-0.368787000
pn15''-(COOH) ₂ ...CO ₂				pn16''-(COOH) ₂ ...CO ₂			
6	1.261334000	-0.219567000	-0.052169000	6	2.169747000	-1.925354000	-0.292565000
6	0.818988000	1.100177000	0.126938000	6	1.009918000	-1.181080000	-0.163196000
6	-0.606661000	1.371302000	0.100120000	6	1.054749000	0.206711000	0.028124000
6	-1.490358000	0.317156000	0.046851000	6	2.328742000	0.777650000	0.101113000
7	-1.041311000	-0.990098000	0.183856000	7	3.449501000	0.077631000	-0.017779000
6	0.309716000	-1.327059000	-0.077100000	6	3.378139000	-1.236039000	-0.219284000
8	0.618645000	-2.493867000	-0.232509000	8	4.520852000	-1.917963000	-0.346906000
6	2.660234000	-0.450199000	-0.128670000	6	-0.283198000	-1.891106000	-0.130652000
7	3.551593000	0.520844000	-0.014581000	7	-1.409147000	-1.117006000	0.163496000
6	3.112555000	1.768294000	0.180581000	6	-1.378853000	0.279821000	0.032274000
6	1.780698000	2.113730000	0.254978000	6	-0.188582000	0.960335000	0.052015000
8	3.119263000	-1.678557000	-0.316262000	8	-0.357067000	-3.100456000	-0.262163000
6	-1.142763000	2.695010000	0.100625000	7	-2.580510000	0.956543000	-0.124031000
6	-2.471896000	2.920144000	0.125116000	6	-2.658166000	2.350289000	0.073357000
6	-3.402486000	1.826087000	0.045060000	6	-1.404641000	3.055628000	0.130058000
7	-2.842196000	0.542333000	-0.145233000	6	-0.234561000	2.388715000	0.063949000
8	-4.621590000	1.974649000	0.078562000	8	-3.749823000	2.915338000	0.128082000
1	3.885916000	2.523975000	0.276994000	1	2.138798000	-2.997154000	-0.432577000
1	1.510545000	3.146763000	0.412658000	1	2.466758000	1.840972000	0.264303000
1	4.088101000	-1.635527000	-0.323622000	1	5.262499000	-1.301119000	-0.264998000
1	-0.465687000	3.538841000	0.115195000	1	-1.469644000	4.132672000	0.192672000

1	-2.905122000	3.908886000	0.176469000	1	0.692799000	2.947412000	0.057839000
6	-3.675000000	-0.511968000	-0.794010000	6	-3.734249000	0.259186000	-0.754210000
8	-3.143026000	-1.358173000	-1.438420000	8	-3.541797000	-0.729424000	-1.389263000
8	-4.948345000	-0.364019000	-0.609456000	8	-4.872105000	0.847393000	-0.565066000
1	-5.124183000	0.534782000	-0.198190000	1	-4.714736000	1.753594000	-0.155637000
6	-1.923309000	-1.975472000	0.843241000	6	-2.557420000	-1.733183000	0.859250000
8	-2.825498000	-1.589630000	1.517324000	8	-3.243047000	-1.060601000	1.560189000
8	-1.598372000	-3.217745000	0.642722000	8	-2.697464000	-3.012331000	0.658986000
1	-0.748172000	-3.266408000	0.134155000	1	-1.944113000	-3.364954000	0.129460000
6	6.249373000	0.132234000	-0.113882000	6	5.794955000	1.454727000	0.140577000
8	6.093557000	-1.006264000	-0.266711000	8	5.237383000	2.450919000	0.299155000
8	6.455299000	1.255846000	0.036248000	8	6.399225000	0.478449000	-0.016480000
pn17''-(COOH)₂...CO₂				pn18''-(COOH)₂...CO₂			
6	-0.937436000	-1.499173000	-0.008547000	6	1.655794000	-3.121655000	-0.483557000
6	-0.808501000	-0.074696000	-0.003843000	6	0.435207000	-2.591947000	-0.298310000
6	0.534615000	0.481621000	-0.005436000	6	0.272622000	-1.156651000	-0.128984000
6	1.614265000	-0.388191000	-0.011046000	6	1.428726000	-0.399154000	-0.078052000
7	1.484073000	-1.768489000	-0.015040000	7	2.696037000	-0.988391000	-0.036010000
6	0.302150000	-2.278700000	-0.014218000	6	2.874249000	-2.331751000	-0.382678000
8	0.133803000	-3.593040000	-0.018533000	8	3.992214000	-2.812010000	-0.518077000
6	0.761680000	1.909693000	-0.001169000	6	-0.983129000	-0.464610000	-0.076527000
7	2.090406000	2.340032000	-0.003399000	6	-0.965116000	0.935734000	-0.038169000
6	3.144892000	1.453845000	-0.009268000	7	0.174470000	1.655148000	-0.171737000
6	2.945139000	0.121991000	-0.012989000	6	1.313894000	1.019680000	-0.240334000
8	-0.159586000	2.739878000	0.004049000	8	2.415522000	1.680551000	-0.555119000
6	-2.153766000	-2.118501000	-0.007723000	6	-2.254483000	-1.170681000	-0.023351000
6	-3.361926000	-1.360005000	-0.002087000	7	-3.404260000	-0.390459000	0.099091000
7	-3.195654000	0.035534000	0.002469000	6	-3.353539000	0.992955000	0.158618000
6	-1.979188000	0.647211000	0.001623000	6	-2.192898000	1.661740000	0.091623000
8	-4.494881000	-1.863901000	-0.001121000	8	-2.351006000	-2.404917000	-0.070524000
1	1.001206000	-4.028572000	-0.022450000	1	1.805659000	-4.177437000	-0.667373000
1	4.118605000	1.920732000	-0.010376000	1	-0.444100000	-3.215603000	-0.324441000
1	3.779311000	-0.563039000	-0.017326000	1	2.220795000	2.628818000	-0.610912000
1	-2.249538000	-3.194861000	-0.011270000	1	-4.319409000	1.464998000	0.257398000
1	-2.012779000	1.725212000	0.005502000	1	-2.169552000	2.740301000	0.132212000
6	2.461115000	3.774306000	0.000239000	6	3.728880000	-0.319820000	0.772980000
8	3.614563000	4.067898000	-0.001983000	8	3.410609000	0.472052000	1.598783000
8	1.452764000	4.592422000	0.005641000	8	4.949810000	-0.708086000	0.506381000
1	0.595120000	4.061571000	0.006075000	1	4.925161000	-1.525828000	-0.050430000
6	-4.377198000	0.960820000	0.008611000	6	-4.759474000	-0.974194000	0.176556000
8	-4.181117000	2.132126000	0.012728000	8	-5.695571000	-0.246205000	0.279742000
8	-5.513963000	0.344246000	0.009406000	8	-4.798108000	-2.273498000	0.122162000
1	-5.348417000	-0.666487000	0.005242000	1	-3.860753000	-2.625221000	0.037378000
6	3.709456000	-3.653238000	0.021182000	6	0.313371000	4.560550000	-0.253213000
8	2.902851000	-4.486293000	0.016445000	8	1.430383000	4.431212000	-0.533741000
8	4.537181000	-2.854084000	0.026423000	8	-0.792123000	4.727740000	0.021287000
pn19''-(COOH)₂...CO₂				pn20''-(COOH)₂...CO₂			
6	-0.941815000	-0.742661000	-0.008826000	6	-1.048093000	-1.659910000	-0.001309000
6	-0.238369000	0.373700000	0.394350000	6	-1.029100000	-0.284035000	-0.000617000
6	1.213743000	0.341813000	0.382338000	6	0.248621000	0.403392000	-0.000637000
6	1.877113000	-0.853263000	0.126812000	6	1.445028000	-0.403876000	-0.001382000
7	1.135739000	-2.031425000	-0.100947000	7	1.391396000	-1.788512000	-0.001895000
6	-0.251660000	-1.991949000	-0.341840000	6	0.238216000	-2.356667000	-0.001888000
8	-0.834244000	-2.983064000	-0.756052000	8	0.140406000	-3.681532000	-0.002615000
7	1.851748000	1.515466000	0.576220000	6	0.408349000	1.767576000	-0.000208000
6	3.158112000	1.537813000	0.509849000	7	1.635108000	2.347699000	-0.000331000

6	3.927962000	0.394427000	0.216967000	6	2.833309000	1.601498000	-0.001072000
6	3.286499000	-0.797909000	0.018961000	6	2.679587000	0.192151000	-0.001579000
8	3.802925000	2.697495000	0.697020000	8	3.928492000	2.187494000	-0.001377000
6	-2.398762000	-0.718830000	-0.079557000	6	-2.265939000	-2.395840000	-0.001339000
7	-3.002710000	0.492022000	0.320653000	6	-3.430387000	-1.718674000	-0.000555000
6	-2.271473000	1.573517000	0.741893000	7	-3.457336000	-0.338637000	0.000261000
6	-0.923245000	1.555850000	0.786303000	6	-2.299961000	0.437218000	0.000250000
8	-3.098019000	-1.654627000	-0.448768000	8	-2.370846000	1.669930000	0.000945000
1	5.002836000	0.481982000	0.135270000	1	1.031743000	-4.065968000	-0.002481000
1	3.857052000	-1.680760000	-0.218890000	1	-0.417722000	2.460977000	0.000277000
1	3.147173000	3.399999000	0.803446000	1	3.581798000	-0.402130000	-0.002175000
1	-2.870381000	2.426868000	1.027749000	1	-2.255192000	-3.474876000	-0.001976000
1	-0.368195000	2.416839000	1.125717000	1	-4.405543000	-2.182073000	-0.000479000
6	-4.473500000	0.679851000	0.319245000	6	1.642862000	3.842740000	0.000231000
8	-4.917022000	1.726180000	0.673593000	8	0.601819000	4.418171000	0.000838000
8	-5.146946000	-0.353763000	-0.082501000	8	2.831751000	4.349522000	-0.000089000
1	-4.503756000	-1.095637000	-0.316972000	1	3.519099000	3.581998000	-0.000689000
6	1.805899000	-3.326750000	0.075119000	6	-4.816085000	0.266108000	0.001144000
8	2.844479000	-3.386504000	0.658282000	8	-5.760556000	-0.455911000	0.001115000
8	1.180223000	-4.345595000	-0.443901000	8	-4.831926000	1.564258000	0.001869000
1	0.275159000	-4.052135000	-0.756325000	1	-3.890055000	1.912886000	0.001657000
6	1.014839000	3.471438000	-1.295879000	6	3.714614000	-3.530380000	0.003024000
8	0.471448000	2.680440000	-1.935742000	8	2.960238000	-4.412194000	0.000930000
8	1.553982000	4.280454000	-0.667669000	8	4.491320000	-2.682544000	0.005288000
pn21''-(COOH) ₂ ...CO ₂				pn22''-(COOH) ₂ ...CO ₂			
6	1.387356000	0.364035000	0.000281000	6	-1.377583000	0.556578000	-0.137426000
6	0.532213000	-0.751661000	-0.000162000	6	-0.779513000	-0.678744000	0.148226000
6	-0.881624000	-0.516942000	-0.000189000	6	0.690475000	-0.741465000	0.149857000
6	-1.330476000	0.815113000	0.000094000	6	1.428153000	0.480094000	0.031136000
7	-0.501099000	1.879256000	0.000101000	7	0.753302000	1.740647000	0.024938000
6	0.797874000	1.669015000	0.000151000	6	-0.613783000	1.807558000	-0.224648000
8	1.585526000	2.726028000	-0.000068000	8	-1.182122000	2.872499000	-0.433376000
6	-1.851309000	-1.605200000	-0.000338000	6	1.355613000	-1.931880000	0.165330000
7	-3.204525000	-1.247814000	-0.000028000	6	2.778556000	-2.018476000	0.061805000
6	-3.612244000	0.072993000	0.000218000	7	3.433380000	-0.799919000	-0.133845000
6	-2.736253000	1.089093000	0.000285000	6	2.775331000	0.399222000	-0.148334000
8	-1.542171000	-2.801540000	-0.000497000	8	3.405623000	-3.085272000	0.108761000
6	2.841030000	0.219310000	0.000823000	6	-2.766732000	0.622526000	-0.234350000
7	3.323502000	-1.097011000	-0.000064000	7	-3.552399000	-0.431203000	-0.061515000
6	2.471431000	-2.176801000	-0.000713000	6	-2.977345000	-1.597405000	0.231615000
6	1.130682000	-2.055371000	-0.000670000	6	-1.595944000	-1.777713000	0.348680000
8	3.628700000	1.160525000	0.002053000	8	-3.765032000	-2.652684000	0.419956000
1	1.030318000	3.521430000	-0.000329000	1	0.844045000	-2.881589000	0.224094000
1	-4.684484000	0.202634000	0.000343000	1	3.418624000	1.251239000	-0.297531000
1	-3.076671000	2.113191000	0.000559000	1	-3.248554000	1.569705000	-0.451710000
1	2.975322000	-3.132868000	-0.001228000	1	-1.220619000	-2.762164000	0.588119000
1	0.523239000	-2.941481000	-0.001096000	1	-4.689346000	-2.380109000	0.311218000
6	-4.296321000	-2.242974000	0.000277000	6	4.905442000	-0.726636000	-0.360287000
8	-5.423727000	-1.860755000	0.000727000	8	5.399127000	0.331420000	-0.579365000
8	-3.905668000	-3.483794000	0.000265000	8	5.497439000	-1.877649000	-0.293268000
1	-2.902419000	-3.510671000	-0.000092000	1	4.806949000	-2.601692000	-0.109960000
6	4.765817000	-1.416554000	-0.000221000	6	1.488684000	2.930104000	0.460535000
8	5.102976000	-2.558311000	-0.000943000	8	2.549815000	2.821018000	0.990109000
8	5.548737000	-0.378759000	0.000372000	8	0.890632000	4.068445000	0.222808000
1	4.986557000	0.456317000	0.001154000	1	-0.013929000	3.908016000	-0.152524000
6	-1.428598000	4.683650000	-0.000608000	6	-6.281812000	-0.154058000	-0.243275000

8	-2.552759000	4.434475000	-0.000508000	8	-6.403248000	-1.282558000	-0.002575000
8	-0.305923000	4.970156000	-0.000743000	8	-6.206536000	0.968742000	-0.484540000
pn23''-(COOH)₂...CO₂				pn24''-(COOH)₂...CO₂			
6	-1.356574000	0.497440000	-0.141336000	6	1.239719000	1.509867000	-0.306604000
6	-0.828087000	-0.770635000	0.162598000	6	1.099394000	0.152610000	-0.023158000
6	0.629284000	-0.920966000	0.173693000	6	-0.248041000	-0.420545000	0.056221000
6	1.395635000	0.203343000	0.042223000	6	-1.365815000	0.483671000	0.006348000
7	0.847588000	1.494131000	0.007848000	7	-1.159801000	1.899207000	0.020592000
6	-0.510442000	1.690087000	-0.250150000	6	0.069590000	2.430225000	-0.311543000
8	-0.960313000	2.802268000	-0.475675000	8	0.238418000	3.624050000	-0.515769000
6	1.271610000	-2.197324000	0.242293000	6	-0.497490000	-1.765548000	0.073430000
6	2.611352000	-2.277748000	0.141875000	6	-1.820813000	-2.305515000	0.016221000
7	3.381409000	-1.160911000	-0.110121000	7	-2.850691000	-1.373094000	-0.123493000
6	2.818525000	0.102589000	-0.277565000	6	-2.617598000	-0.025718000	-0.124442000
8	3.469293000	1.048082000	-0.712141000	8	-2.062537000	-3.520277000	0.054930000
6	-2.738030000	0.640823000	-0.247390000	6	2.493608000	2.086885000	-0.500051000
7	-3.583701000	-0.365573000	-0.071657000	6	3.597521000	1.266655000	-0.385803000
6	-3.077038000	-1.562089000	0.227171000	7	3.503886000	-0.031173000	-0.082828000
6	-1.709734000	-1.821990000	0.353473000	6	2.313582000	-0.572398000	0.096582000
8	-3.926406000	-2.570723000	0.411281000	8	2.279597000	-1.869526000	0.412417000
1	0.701540000	-3.102598000	0.383427000	1	0.292617000	-2.496176000	0.105305000
1	3.172948000	-3.196907000	0.217926000	1	-3.508240000	0.574180000	-0.220000000
1	-3.162932000	1.612731000	-0.476074000	1	2.579440000	3.141650000	-0.717740000
1	-1.393306000	-2.827384000	0.590632000	1	4.603404000	1.646460000	-0.528695000
1	-4.831875000	-2.244110000	0.294907000	1	3.191878000	-2.196481000	0.460319000
6	1.618780000	2.558384000	0.661774000	6	-4.269654000	-1.782993000	-0.292550000
8	2.440027000	2.278110000	1.471863000	8	-5.093658000	-0.943022000	-0.464311000
8	1.287973000	3.772631000	0.292648000	8	-4.447676000	-3.065638000	-0.236783000
1	0.455738000	3.752666000	-0.227937000	1	-3.546253000	-3.521873000	-0.098413000
6	4.830408000	-1.400199000	-0.277199000	6	-2.222624000	2.760929000	0.555079000
8	5.256262000	-2.495002000	-0.088378000	8	-3.128050000	2.289530000	1.165107000
8	5.516883000	-0.351360000	-0.622226000	8	-2.075683000	4.037222000	0.306080000
1	4.904401000	0.431829000	-0.744933000	1	-1.207583000	4.204587000	-0.138466000
6	-6.290133000	0.068232000	-0.268116000	6	5.843498000	-1.449699000	0.156971000
8	-6.479902000	-1.051107000	-0.028454000	8	5.239137000	-2.405852000	0.413729000
8	-6.148432000	1.184670000	-0.508979000	8	6.481916000	-0.524923000	-0.093201000
pn25''-(COOH)₂...CO₂				pn26''-(COOH)₂...CO₂			
6	-1.355528000	0.428787000	-0.132532000	6	-1.069491000	1.511207000	-0.237792000
6	-0.513589000	-0.661636000	0.107336000	6	-0.787171000	0.160595000	-0.018779000
6	0.927537000	-0.435381000	0.068000000	6	0.608252000	-0.267649000	0.003419000
6	1.461637000	0.899993000	0.003199000	6	1.663806000	0.712737000	-0.005082000
7	0.555191000	1.978167000	0.004539000	7	1.313858000	2.089132000	0.018074000
6	-0.815265000	1.784656000	-0.291100000	6	0.018176000	2.516488000	-0.286201000
8	-1.510502000	2.732067000	-0.606625000	8	-0.233220000	3.686327000	-0.518813000
6	1.801580000	-1.476943000	0.028958000	6	0.960429000	-1.579161000	-0.044648000
7	3.146328000	-1.309115000	-0.055838000	7	2.257317000	-1.996398000	-0.086961000
6	3.717861000	-0.026387000	-0.139861000	6	3.317476000	-1.080843000	-0.130837000
6	2.811530000	1.076090000	-0.109395000	6	2.962042000	0.303749000	-0.091154000
8	4.943609000	0.098308000	-0.242297000	8	4.486294000	-1.479779000	-0.205069000
6	-2.755749000	0.193473000	-0.156340000	6	-2.373706000	1.961645000	-0.345015000
7	-3.279279000	-1.005237000	0.050302000	6	-3.386672000	1.012786000	-0.211606000
6	-2.457869000	-2.028407000	0.296466000	7	-3.144196000	-0.272559000	0.028024000
6	-1.083482000	-1.918145000	0.339148000	6	-1.886744000	-0.687955000	0.122701000
8	-3.598467000	1.191294000	-0.377837000	8	-4.657937000	1.409597000	-0.316203000
1	1.494587000	-2.512519000	0.045912000	1	0.243945000	-2.387789000	-0.066955000
1	3.277446000	2.045404000	-0.163193000	1	3.797186000	0.983486000	-0.110627000

1	-2.941614000	-2.984824000	0.468313000	1	-2.600059000	3.005480000	-0.511880000
1	-0.486439000	-2.791174000	0.558333000	1	-1.764274000	-1.746482000	0.328379000
1	-4.499160000	0.833231000	-0.337742000	1	-5.236266000	0.643362000	-0.187916000
6	3.963276000	-2.547980000	-0.082426000	6	2.473852000	-3.462943000	-0.125173000
8	3.407746000	-3.599249000	-0.010894000	8	1.524942000	-4.181974000	-0.091193000
8	5.233893000	-2.329086000	-0.184685000	8	3.721001000	-3.802498000	-0.193800000
1	5.394341000	-1.320804000	-0.229910000	1	4.294621000	-2.958074000	-0.212642000
6	1.041158000	3.313004000	0.389885000	6	2.319886000	3.069746000	0.469456000
8	2.042673000	3.424756000	1.021846000	8	3.241376000	2.719565000	1.131792000
8	0.295899000	4.310904000	-0.005980000	8	2.101934000	4.301864000	0.087401000
1	-0.541273000	3.965845000	-0.412383000	1	1.205652000	4.381906000	-0.321423000
6	-5.965246000	-1.505178000	0.064005000	6	-5.136797000	-2.123071000	0.344947000
8	-5.797073000	-2.623472000	0.282716000	8	-5.937959000	-1.302861000	0.171879000
8	-6.182861000	-0.387714000	-0.155545000	8	-4.375142000	-2.968628000	0.521969000
pn27''-(COOH) ₂ ...CO ₂				pn28''-(COOH) ₂ ...CO ₂			
6	-0.077101000	-1.679359000	0.148636000	6	-2.005478000	-3.085837000	-0.503765000
6	0.480323000	-0.414215000	0.004030000	6	-0.744385000	-2.648045000	-0.345943000
6	-0.384344000	0.716296000	0.006573000	6	-0.477350000	-1.241933000	-0.161797000
6	-1.749248000	0.477643000	-0.104203000	6	-1.542827000	-0.393431000	-0.065830000
7	-2.295251000	-0.766440000	-0.016489000	7	-2.853124000	-0.869162000	-0.023818000
6	-1.503546000	-1.779951000	0.175717000	6	-3.149348000	-2.192146000	-0.375616000
8	-2.004977000	-3.006543000	0.354141000	8	-4.305864000	-2.573624000	-0.499677000
7	0.079117000	2.036593000	0.069709000	6	0.854500000	-0.673886000	-0.109406000
6	-0.721819000	3.109708000	-0.344922000	6	0.988946000	0.756944000	-0.011692000
6	-2.129825000	2.821942000	-0.563157000	7	-0.111378000	1.575317000	-0.138657000
6	-2.625554000	1.585317000	-0.386737000	6	-1.284806000	1.038900000	-0.207240000
8	-0.258554000	4.241497000	-0.449313000	8	-2.335610000	1.772678000	-0.527047000
6	0.755347000	-2.839185000	0.235596000	6	1.990024000	-1.430182000	-0.072773000
6	2.085329000	-2.697136000	0.116592000	7	3.220230000	-0.874747000	0.064941000
7	2.664346000	-1.467203000	-0.165766000	6	3.408639000	0.520469000	0.192867000
6	1.910834000	-0.308849000	-0.323177000	6	2.235346000	1.313969000	0.141430000
8	2.412686000	0.720273000	-0.768258000	8	4.559990000	0.970541000	0.329577000
1	-2.971876000	-2.962363000	0.330387000	1	-2.247135000	-4.123479000	-0.691699000
1	-2.743604000	3.674231000	-0.820898000	1	0.077072000	-3.351151000	-0.406997000
1	-3.682743000	1.374889000	-0.492489000	1	-2.067914000	2.702684000	-0.606221000
1	0.316413000	-3.809713000	0.409931000	1	2.006861000	-2.509306000	-0.133026000
1	2.794037000	-3.507035000	0.201112000	1	2.360705000	2.384776000	0.213669000
6	1.240150000	2.304662000	0.932837000	6	-3.822940000	-0.115527000	0.793269000
8	1.572874000	1.496289000	1.742387000	8	-3.428666000	0.635718000	1.623415000
8	1.794412000	3.468676000	0.744689000	8	-5.073206000	-0.389571000	0.525843000
1	1.218207000	4.017940000	0.147655000	1	-5.124652000	-1.205332000	-0.031430000
6	4.130298000	-1.483800000	-0.343137000	6	4.365775000	-1.827665000	0.088603000
8	4.721543000	-2.498156000	-0.149614000	8	4.136642000	-2.992286000	-0.025449000
8	4.653737000	-0.348458000	-0.706129000	8	5.509408000	-1.250631000	0.234970000
1	3.935206000	0.333701000	-0.823925000	1	5.354909000	-0.227000000	0.303886000
6	-5.150335000	-1.321438000	-0.074597000	6	0.024111000	4.439577000	-0.335011000
8	-4.877015000	-2.424230000	0.152712000	8	-1.104368000	4.411952000	-0.602147000
8	-5.460480000	-0.235864000	-0.301146000	8	1.142777000	4.507934000	-0.075488000
pn29''-(COOH) ₂ ...CO ₂				pn30''-(COOH) ₂ ...CO ₂			
6	1.242602000	1.338205000	-0.239969000	6	-2.679124000	2.865045000	0.515618000
6	1.006317000	-0.016012000	0.026071000	6	-1.315458000	2.741061000	0.502291000
6	-0.371295000	-0.501668000	0.071472000	6	-0.726572000	1.465743000	0.362373000
6	-1.432298000	0.460421000	0.019400000	6	-1.596879000	0.384848000	0.249452000
7	-1.139410000	1.863248000	0.028874000	7	-2.927767000	0.494693000	0.234505000
6	0.130026000	2.326015000	-0.271595000	6	-3.452352000	1.693600000	0.363444000
8	0.370174000	3.506940000	-0.472357000	8	-4.779735000	1.815578000	0.353865000

6	-0.680178000	-1.832972000	0.075707000	6	0.706551000	1.232800000	0.240191000
6	-2.022846000	-2.311515000	0.021991000	6	1.155360000	-0.059353000	0.195416000
7	-3.004660000	-1.323764000	-0.113685000	7	0.291547000	-1.151681000	0.370188000
6	-2.708603000	0.010904000	-0.115448000	6	-1.086333000	-1.015545000	0.240851000
8	-2.327499000	-3.512297000	0.058938000	8	-1.832456000	-1.975748000	0.222355000
6	2.529866000	1.815451000	-0.387787000	6	1.654217000	2.295693000	0.091871000
6	3.572042000	0.895105000	-0.248940000	6	2.951496000	2.010852000	-0.127780000
7	3.373956000	-0.389329000	0.036447000	7	3.385876000	0.712941000	-0.292863000
6	2.129422000	-0.831659000	0.167151000	6	2.508368000	-0.370768000	-0.243171000
8	4.824798000	1.322488000	-0.397135000	8	2.855603000	-1.496646000	-0.592039000
1	0.075589000	-2.604844000	0.085515000	1	-3.176195000	3.818673000	0.631153000
1	-3.570376000	0.650810000	-0.215794000	1	-0.698558000	3.624175000	0.608566000
1	2.726971000	2.859461000	-0.587693000	1	-5.170428000	0.932872000	0.257013000
1	2.034815000	-1.885959000	0.403752000	1	1.352679000	3.329687000	0.158412000
1	5.430227000	0.578276000	-0.260502000	1	3.728975000	2.754710000	-0.219466000
6	-4.444088000	-1.663148000	-0.284668000	6	0.833452000	-2.316331000	1.087687000
8	-5.224374000	-0.782742000	-0.455490000	8	1.774991000	-2.183326000	1.797144000
8	-4.685747000	-2.935160000	-0.232172000	8	0.173233000	-3.431599000	0.887454000
1	-3.809319000	-3.437451000	-0.095336000	1	-0.682463000	-3.242702000	0.445231000
6	-2.165480000	2.787777000	0.527559000	6	4.819019000	0.545626000	-0.607400000
8	-3.114196000	2.371837000	1.112301000	8	5.523127000	1.505403000	-0.606151000
8	-1.940595000	4.052450000	0.278910000	8	5.178545000	-0.678023000	-0.858620000
1	-1.051843000	4.170857000	-0.139217000	1	4.377334000	-1.281297000	-0.821263000
6	5.423174000	-2.192909000	0.264912000	6	-4.474254000	-1.256329000	-1.355251000
8	4.692112000	-3.057710000	0.474698000	8	-5.361307000	-0.975852000	-0.662160000
8	6.193170000	-1.351581000	0.056393000	8	-3.627486000	-1.533469000	-2.083849000
pn31''-(COOH) ₂ ...CO ₂				pn32''-(COOH) ₂ ...CO ₂			
6	-2.830219000	-2.781801000	-0.462260000	6	1.224725000	1.426804000	-0.335634000
6	-1.496652000	-2.671446000	-0.323888000	6	1.147120000	0.065748000	-0.026619000
6	-0.879239000	-1.380107000	-0.167346000	6	-0.170214000	-0.566014000	0.064515000
6	-1.692184000	-0.281175000	-0.074441000	6	-1.271272000	0.251858000	0.025051000
7	-3.071833000	-0.414223000	-0.010548000	7	-1.169039000	1.652753000	0.012489000
6	-3.703578000	-1.625290000	-0.345154000	6	0.008949000	2.279151000	-0.349485000
8	-4.918738000	-1.686273000	-0.468279000	8	0.067818000	3.476708000	-0.573101000
6	0.558241000	-1.182347000	-0.115445000	6	-0.385734000	-1.983985000	0.103447000
6	1.019819000	0.172607000	-0.058349000	6	-1.639696000	-2.473362000	0.055822000
7	0.171582000	1.258863000	-0.175341000	7	-2.736157000	-1.654224000	-0.106492000
6	-1.093614000	1.049589000	-0.212404000	6	-2.604496000	-0.275368000	-0.226562000
8	-1.946682000	2.028703000	-0.499271000	8	-3.547496000	0.438135000	-0.568553000
6	1.471805000	-2.208383000	-0.072967000	6	2.451029000	2.057769000	-0.541296000
6	2.867476000	-1.970300000	0.041482000	6	3.590310000	1.290739000	-0.419942000
7	3.258742000	-0.620625000	0.104168000	7	3.556568000	-0.008246000	-0.099363000
6	2.365748000	0.400612000	0.047768000	6	2.394949000	-0.600066000	0.095232000
8	3.724435000	-2.872293000	0.091285000	8	2.421468000	-1.894333000	0.433741000
1	-3.328552000	-3.726694000	-0.632129000	1	0.442969000	-2.664577000	0.185366000
1	-0.876423000	-3.556885000	-0.380405000	1	-1.876245000	-3.525441000	0.111992000
1	-1.462348000	2.865596000	-0.570910000	1	2.484956000	3.112480000	-0.775234000
1	1.192028000	-3.251567000	-0.101610000	1	4.577952000	1.712578000	-0.571518000
1	2.785068000	1.396771000	0.090045000	1	3.348355000	-2.176767000	0.478030000
6	-3.820616000	0.571512000	0.800215000	6	-2.199947000	2.407471000	0.743244000
8	-3.257068000	1.167825000	1.656224000	8	-2.807892000	1.878470000	1.612766000
8	-5.089448000	0.656207000	0.496734000	8	-2.324239000	3.658325000	0.367291000
1	-5.351645000	-0.118702000	-0.057078000	1	-1.579640000	3.914029000	-0.216571000
6	4.695852000	-0.225528000	0.227291000	6	-4.043826000	-2.330125000	-0.227179000
8	4.962875000	0.932669000	0.269219000	8	-4.095398000	-3.510926000	-0.088516000
8	5.501452000	-1.234173000	0.274530000	8	-5.041458000	-1.534900000	-0.478261000

1	4.949150000	-2.103496000	0.211364000	1	-4.707488000	-0.592929000	-0.574873000
6	1.044560000	3.975995000	-0.372971000	6	5.957336000	-1.311835000	0.148099000
8	-0.057737000	4.268772000	-0.582892000	8	6.551005000	-0.361309000	-0.115177000
8	2.148272000	3.721466000	-0.169602000	8	5.400460000	-2.293177000	0.417836000
pn33''-(COOH)₂...CO₂				pn34''-(COOH)₂...CO₂			
6	-1.225039000	1.264492000	-0.261153000	6	1.423659000	0.353012000	-0.108187000
6	-1.055953000	-0.099910000	0.030916000	6	0.754206000	-0.832089000	0.210612000
6	0.292559000	-0.648305000	0.095840000	6	-0.717229000	-0.829906000	0.181108000
6	1.347869000	0.220197000	0.032089000	6	-1.400183000	0.417131000	0.052444000
7	1.167330000	1.617108000	0.015869000	7	-0.662750000	1.634801000	0.051710000
6	-0.057605000	2.183796000	-0.302202000	6	0.708440000	1.640099000	-0.226453000
8	-0.187144000	3.376466000	-0.513905000	8	1.294703000	2.681572000	-0.467095000
6	0.560905000	-2.053589000	0.147222000	6	-1.432935000	-1.992313000	0.178150000
6	1.831916000	-2.494018000	0.089079000	6	-2.856195000	-2.016754000	0.055700000
7	2.887495000	-1.627716000	-0.098821000	7	-3.457525000	-0.770797000	-0.135595000
6	2.696672000	-0.252606000	-0.237472000	6	-2.748227000	0.398402000	-0.139670000
8	3.604717000	0.489966000	-0.605494000	8	-3.528537000	-3.057383000	0.086357000
6	-2.486293000	1.800233000	-0.425976000	6	2.840267000	0.298738000	-0.198474000
6	-3.572177000	0.932306000	-0.285095000	7	3.526252000	-0.808170000	0.051442000
7	-3.438674000	-0.359393000	0.005982000	6	2.867554000	-1.913242000	0.398434000
6	-2.218801000	-0.861341000	0.154696000	6	1.490630000	-1.985186000	0.484959000
8	-4.803584000	1.417681000	-0.442904000	8	3.535060000	1.372266000	-0.541103000
1	-0.236812000	-2.774641000	0.238106000	1	-0.966669000	-2.964656000	0.233749000
1	2.116579000	-3.533871000	0.152386000	1	-3.350663000	1.279503000	-0.291114000
1	-2.629137000	2.850000000	-0.643197000	1	3.485117000	-2.780936000	0.607927000
1	-2.179200000	-1.919949000	0.387719000	1	1.017615000	-2.913698000	0.767353000
1	-5.443014000	0.702103000	-0.309446000	1	4.475626000	1.134850000	-0.528937000
6	2.173094000	2.422138000	0.724783000	6	-4.923626000	-0.634312000	-0.373180000
8	2.836582000	1.920901000	1.570365000	8	-5.370858000	0.445362000	-0.586387000
8	2.219168000	3.681607000	0.358734000	8	-5.562730000	-1.760471000	-0.321268000
1	1.447192000	3.902892000	-0.202265000	1	-4.902598000	-2.514118000	-0.139778000
6	4.220895000	-2.249738000	-0.225738000	6	-1.336589000	2.852764000	0.502231000
8	4.323886000	-3.424937000	-0.067926000	8	-2.396048000	2.786193000	1.043803000
8	5.181189000	-1.418654000	-0.503580000	8	-0.692772000	3.965886000	0.266000000
1	4.808261000	-0.493459000	-0.612843000	1	0.189888000	3.765850000	-0.141949000
6	-5.559535000	-2.058047000	0.269292000	6	6.254284000	-0.974614000	-0.099645000
8	-4.865649000	-2.952126000	0.485105000	8	6.313921000	0.142394000	-0.403977000
8	-6.295162000	-1.187994000	0.055936000	8	6.240449000	-2.086824000	0.200129000
pn35''-(COOH)₂...CO₂				pn36''-(COOH)₂...CO₂			
6	-1.408955000	0.289695000	-0.112943000	6	-0.572027000	-1.812483000	-0.166513000
6	-0.806257000	-0.938053000	0.199491000	6	-0.782429000	-0.451733000	-0.023124000
6	0.656229000	-1.022041000	0.188982000	6	0.340966000	0.426843000	-0.017962000
6	1.371043000	0.133464000	0.058345000	6	1.613598000	-0.142014000	0.065291000
7	0.756966000	1.387083000	0.029892000	7	1.822886000	-1.489736000	0.015639000
6	-0.612367000	1.522686000	-0.245539000	6	0.793173000	-2.266416000	-0.159539000
8	-1.083022000	2.615772000	-0.494805000	8	0.965887000	-3.577395000	-0.298363000
6	1.358280000	-2.268974000	0.243422000	6	0.218679000	1.857486000	-0.287805000
6	2.699558000	-2.287086000	0.137102000	7	1.361842000	2.626868000	-0.033012000
7	3.418473000	-1.134060000	-0.105908000	6	2.592233000	2.042334000	0.211112000
6	2.797800000	0.102888000	-0.262746000	6	2.756095000	0.708399000	0.219597000
8	3.402636000	1.081367000	-0.689553000	8	-0.786285000	2.369295000	-0.770341000
6	-2.824287000	0.319463000	-0.205943000	6	-1.666374000	-2.723769000	-0.302638000
7	-3.576999000	-0.748137000	0.018898000	6	-2.919235000	-2.239544000	-0.259530000
6	-2.984225000	-1.898407000	0.341876000	7	-3.171351000	-0.905463000	0.026278000
6	-1.615183000	-2.053035000	0.437307000	6	-2.146089000	0.002763000	0.308825000
8	-3.446325000	1.444160000	-0.525167000	8	-2.377235000	1.067934000	0.861865000

1	0.835142000	-3.202992000	0.374908000	1	1.912807000	-3.782571000	-0.254056000
1	3.301941000	-3.180880000	0.201243000	1	3.394288000	2.750362000	0.358791000
1	-3.652687000	-2.733979000	0.524194000	1	3.732400000	0.269529000	0.359782000
1	-1.201420000	-3.016367000	0.694579000	1	-1.484322000	-3.774280000	-0.470407000
1	-4.400524000	1.270742000	-0.518325000	1	-3.808151000	-2.834161000	-0.407619000
6	1.473804000	2.487017000	0.686634000	6	1.353815000	4.095290000	-0.106711000
8	2.303289000	2.243126000	1.501093000	8	2.342446000	4.696122000	0.176934000
8	1.091399000	3.684313000	0.315487000	8	0.220733000	4.616347000	-0.483172000
1	0.269473000	3.621131000	-0.220207000	1	-0.427158000	3.884008000	-0.699870000
6	4.875749000	-1.305562000	-0.277531000	6	-4.593517000	-0.535907000	0.129161000
8	5.351832000	-2.381625000	-0.100275000	8	-5.421792000	-1.329802000	-0.187741000
8	5.513496000	-0.223078000	-0.612633000	8	-4.816498000	0.671468000	0.565870000
1	4.865834000	0.532341000	-0.727804000	1	-3.952687000	1.108769000	0.806896000
6	-6.308106000	-0.731416000	-0.099255000	6	4.424738000	-2.768041000	0.166513000
8	-6.299760000	0.393307000	-0.379687000	8	5.012433000	-1.799480000	0.367767000
8	-6.364213000	-1.848346000	0.177544000	8	3.867489000	-3.764811000	-0.034807000

IX. Tricarboxylic acid

pn1'''-(COOH) ₃				pn2'''-(COOH) ₃			
6	3.567801000	1.894685000	-0.674554000	6	-2.018096000	-0.797259000	-0.390818000
6	2.328553000	2.400308000	-0.517027000	6	-1.218981000	0.259616000	-0.050805000
6	1.226341000	1.529987000	-0.255403000	6	0.215207000	0.048913000	-0.019651000
6	1.421317000	0.178911000	-0.099456000	6	0.737179000	-1.293309000	0.017700000
7	2.724293000	-0.308400000	-0.048714000	7	-0.179614000	-2.367007000	0.033897000
6	3.823614000	0.488367000	-0.466944000	6	-1.504247000	-2.165502000	-0.373242000
8	4.934242000	-0.017176000	-0.586129000	8	-2.244404000	-3.105366000	-0.630215000
6	-0.099685000	2.098764000	-0.107520000	6	1.094778000	1.074607000	-0.208356000
7	-1.133268000	1.202597000	0.204347000	7	2.431267000	0.886786000	-0.275900000
6	-0.974643000	-0.153222000	-0.047221000	6	3.001790000	-0.396314000	-0.150296000
6	0.285536000	-0.709175000	-0.145579000	6	2.087035000	-1.486415000	-0.028737000
8	-0.303215000	3.305514000	-0.155425000	8	4.227648000	-0.532175000	-0.186357000
7	-2.100582000	-0.932475000	-0.224266000	6	-3.392214000	-0.588989000	-0.724956000
6	-2.016947000	-2.348632000	-0.216679000	6	-3.895630000	0.660263000	-0.762051000
6	-0.702308000	-2.902857000	-0.419727000	6	-3.094908000	1.794184000	-0.361872000
6	0.384366000	-2.111285000	-0.429761000	7	-1.783865000	1.517031000	0.112604000
8	-3.032442000	-3.026045000	-0.126940000	8	-3.511568000	2.946322000	-0.373196000
1	4.430618000	2.497194000	-0.921584000	1	0.794043000	2.104342000	-0.343142000
1	2.123875000	3.458926000	-0.623494000	1	2.544204000	-2.460514000	0.013070000
1	-0.656748000	-3.969915000	-0.584963000	1	-3.991212000	-1.454166000	-0.981374000
1	1.350215000	-2.544502000	-0.651522000	1	-4.912675000	0.883912000	-1.052216000
6	-3.360590000	-0.304386000	-0.711023000	6	3.253459000	2.106960000	-0.520413000
8	-3.310099000	0.738195000	-1.281148000	8	2.694528000	3.143270000	-0.683852000
8	-4.424099000	-1.008954000	-0.482833000	8	4.526158000	1.877637000	-0.529693000
1	-4.164534000	-1.919325000	-0.165450000	1	4.688618000	0.883502000	-0.382765000
6	-2.302020000	1.663122000	0.992300000	6	0.259150000	-3.683457000	0.530552000
8	-2.900407000	0.876741000	1.651992000	8	1.238776000	-3.773426000	1.196160000
8	-2.541046000	2.937086000	0.905056000	8	-0.505740000	-4.685315000	0.184344000
1	-1.834860000	3.385345000	0.372994000	1	-1.318307000	-4.356052000	-0.276769000
6	2.999506000	-1.485656000	0.804335000	6	-1.188587000	2.444771000	1.114195000
8	2.199641000	-1.823008000	1.616425000	8	-0.437011000	2.020742000	1.930007000
8	4.144038000	-2.059365000	0.563114000	8	-1.580356000	3.677591000	0.985789000
1	4.700385000	-1.457281000	-0.012885000	1	-2.359034000	3.718654000	0.357594000
pn3'''-(COOH) ₃				pn4'''-(COOH) ₃			
6	0.666969000	-1.757041000	-0.370083000	6	-1.999489000	-1.787563000	0.249106000
6	-0.250708000	-0.797376000	-0.014364000	6	-0.967183000	-0.897595000	0.136443000
6	0.164156000	0.591515000	-0.133658000	6	-1.280170000	0.482383000	-0.073011000

6	1.504607000	0.875192000	-0.049273000	6	-2.578760000	0.879674000	-0.179991000
7	2.451788000	-0.159888000	-0.063791000	7	-3.599132000	-0.005157000	-0.087649000
6	2.079560000	-1.442948000	-0.472793000	6	-3.366895000	-1.384127000	0.143776000
8	2.915364000	-2.291524000	-0.774132000	8	-4.320174000	-2.161148000	0.236248000
7	-0.746107000	1.630170000	-0.358438000	6	0.438347000	-1.266131000	0.120438000
6	-0.410249000	2.964571000	-0.099254000	6	1.394677000	-0.278139000	0.049715000
6	1.006652000	3.236195000	0.025200000	7	1.061351000	1.075594000	0.188101000
6	1.923087000	2.254273000	-0.020971000	6	-0.246401000	1.515615000	-0.072323000
8	-1.260212000	3.848376000	-0.093430000	8	-0.497370000	2.699015000	-0.211259000
6	0.258291000	-3.117314000	-0.543484000	6	0.872744000	-2.627229000	0.123505000
6	-1.033165000	-3.457403000	-0.382733000	6	2.180467000	-2.950768000	0.133990000
6	-2.004052000	-2.489005000	0.080746000	6	3.188566000	-1.927749000	0.036718000
7	-1.513021000	-1.199063000	0.389732000	7	2.720896000	-0.605414000	-0.158056000
8	-3.182975000	-2.765915000	0.262719000	8	4.392240000	-2.162866000	0.060618000
1	1.280277000	4.280588000	0.087054000	1	-1.859482000	-2.846066000	0.412596000
1	2.974022000	2.494754000	-0.003303000	1	-2.859818000	1.914209000	-0.334787000
1	1.011621000	-3.838317000	-0.836360000	1	0.130503000	-3.414660000	0.153126000
1	-1.411485000	-4.456663000	-0.547320000	1	2.540276000	-3.968460000	0.187963000
6	-1.957898000	1.334558000	-1.128057000	6	3.625159000	0.384168000	-0.817341000
8	-2.025650000	0.318846000	-1.752287000	8	3.149245000	1.266067000	-1.457513000
8	-2.879949000	2.249314000	-1.061347000	8	4.885102000	0.144520000	-0.643410000
1	-2.523765000	3.050318000	-0.577290000	1	5.001766000	-0.760516000	-0.227630000
6	-2.274507000	-0.323636000	1.301167000	6	2.022323000	1.975212000	0.853674000
8	-1.699867000	0.532033000	1.898394000	8	2.892241000	1.510740000	1.518516000
8	-3.543256000	-0.592908000	1.376378000	8	1.803160000	3.245228000	0.668602000
1	-3.735186000	-1.444455000	0.884499000	1	0.973083000	3.386391000	0.157208000
6	3.794178000	0.070155000	0.489647000	6	-4.972655000	0.561761000	-0.225170000
8	3.987922000	0.992307000	1.216938000	8	-5.087219000	1.728192000	-0.417035000
8	4.688922000	-0.801896000	0.116038000	8	-5.913476000	-0.321008000	-0.113562000
1	4.251977000	-1.544220000	-0.386523000	1	-5.502502000	-1.233050000	0.047931000
pn5'''-(COOH)₃				pn6'''-(COOH)₃			
6	-0.959572000	0.909605000	0.022778000	6	-1.713172000	1.325451000	0.439162000
6	-0.338744000	-0.380793000	0.010898000	6	-1.439281000	0.042455000	0.072411000
6	1.122381000	-0.395700000	-0.007457000	6	-0.032976000	-0.375356000	0.029696000
6	1.803882000	0.766325000	-0.217164000	6	0.963544000	0.651868000	-0.024042000
7	1.186108000	2.035448000	-0.057633000	7	0.571588000	2.020902000	-0.083709000
6	-0.199927000	2.156355000	0.034198000	6	-0.694370000	2.385584000	0.341293000
8	-0.747149000	3.248356000	0.112843000	8	-1.017301000	3.551483000	0.530087000
7	1.806165000	-1.622502000	-0.060226000	6	0.343966000	-1.669370000	0.239012000
6	3.060898000	-1.741505000	-0.674376000	6	1.716459000	-2.058962000	0.334369000
6	3.695482000	-0.495986000	-1.055026000	7	2.641624000	-1.014708000	0.248963000
6	3.131597000	0.693469000	-0.784505000	6	2.269243000	0.291292000	0.099912000
8	3.591743000	-2.836050000	-0.828686000	8	2.082543000	-3.230046000	0.491618000
6	-2.318067000	1.009379000	-0.026413000	6	-3.042070000	1.697019000	0.827053000
7	-3.107060000	-0.085401000	-0.116886000	6	-4.007573000	0.761516000	0.895557000
6	-2.559070000	-1.386822000	-0.211264000	6	-3.758772000	-0.602276000	0.473025000
6	-1.131242000	-1.480931000	-0.143250000	7	-2.471458000	-0.873977000	-0.051380000
8	-3.301492000	-2.360745000	-0.342489000	8	-4.608671000	-1.481717000	0.508453000
1	4.662814000	-0.583180000	-1.530316000	1	-0.363934000	-2.477625000	0.353155000
1	3.644242000	1.605208000	-1.049027000	1	3.091458000	0.989103000	0.086669000
1	-2.829252000	1.963778000	-0.008136000	1	-3.224500000	2.730714000	1.093725000
1	-0.752833000	-2.489148000	-0.216604000	1	-5.015683000	0.971767000	1.225634000
6	-4.578252000	0.166624000	-0.157364000	6	4.110096000	-1.253273000	0.370751000
8	-4.962199000	1.287874000	-0.082203000	8	4.844023000	-0.319851000	0.339628000
8	-5.286876000	-0.910286000	-0.275445000	8	4.421642000	-2.503151000	0.506336000
1	-4.673240000	-1.715286000	-0.324946000	1	3.572968000	-3.063367000	0.521004000

6	2.050790000	3.158329000	0.325977000	6	1.483413000	2.995185000	-0.686505000
8	3.180996000	2.957803000	0.644976000	8	2.443254000	2.624407000	-1.282896000
8	1.481019000	4.331308000	0.277286000	8	1.148860000	4.248448000	-0.512895000
1	0.502628000	4.229387000	0.135035000	1	0.292800000	4.316588000	-0.023351000
6	1.412361000	-2.640078000	0.931966000	6	-2.331090000	-1.950497000	-1.064198000
8	0.714801000	-2.333209000	1.844699000	8	-1.522002000	-1.835994000	-1.924093000
8	1.891641000	-3.830205000	0.693526000	8	-3.153170000	-2.947203000	-0.893088000
1	2.594172000	-3.771960000	-0.012825000	1	-3.863324000	-2.687520000	-0.244128000
pn7'''-(COOH)₃				pn8'''-(COOH)₃			
6	1.354385000	0.654225000	0.149867000	6	-1.139836000	1.253165000	-0.165217000
6	0.510114000	-0.479667000	-0.105706000	6	-1.204687000	-0.108338000	0.013558000
6	-0.928693000	-0.227312000	-0.060430000	6	0.013879000	-0.895717000	0.052861000
6	-1.409104000	1.070923000	0.039072000	6	1.219974000	-0.221984000	0.029825000
7	-0.536517000	2.175695000	0.028359000	7	1.268686000	1.164943000	0.161112000
6	0.837259000	2.011668000	0.264951000	6	0.153862000	1.947583000	-0.126382000
8	1.555433000	2.970178000	0.502570000	8	0.234342000	3.160224000	-0.252406000
6	-1.860276000	-1.340475000	-0.053092000	6	-2.299692000	2.060073000	-0.317886000
7	-3.213590000	-1.039701000	0.123340000	6	-3.507151000	1.468513000	-0.276973000
6	-3.642715000	0.248664000	0.284412000	7	-3.627752000	0.107350000	-0.069221000
6	-2.799686000	1.300202000	0.242756000	6	-2.530608000	-0.730705000	0.107252000
8	-1.511242000	-2.517637000	-0.191116000	8	-2.695838000	-1.933356000	0.336297000
6	2.707185000	0.508312000	0.217557000	6	0.065512000	-2.332296000	0.076143000
7	3.299945000	-0.693472000	0.035512000	6	1.239273000	-2.992121000	0.144093000
6	2.538369000	-1.851199000	-0.251836000	6	2.493361000	-2.295724000	0.081336000
6	1.113969000	-1.690910000	-0.307938000	7	2.415131000	-0.900365000	-0.127580000
8	3.108435000	-2.928889000	-0.431035000	8	3.586170000	-2.854921000	0.138788000
1	-4.706319000	0.350962000	0.445716000	1	-2.198747000	3.125253000	-0.462267000
1	-3.197947000	2.291705000	0.365669000	1	-4.447124000	1.987074000	-0.390349000
1	3.372009000	1.341275000	0.408928000	1	-0.861612000	-2.881872000	0.085751000
1	0.561687000	-2.593857000	-0.502997000	1	1.298903000	-4.068955000	0.217052000
6	-4.271904000	-2.081534000	0.172173000	6	3.565782000	-0.210653000	-0.778126000
8	-5.397453000	-1.740169000	0.343587000	8	3.368266000	0.775028000	-1.416318000
8	-3.838617000	-3.295104000	0.018530000	8	4.701660000	-0.802006000	-0.598147000
1	-2.840030000	-3.277931000	-0.099413000	1	4.546524000	-1.702818000	-0.173636000
6	4.787345000	-0.715715000	0.133958000	6	2.441108000	1.783044000	0.838224000
8	5.354513000	0.298557000	0.381537000	8	3.121348000	1.110448000	1.541322000
8	5.303696000	-1.884956000	-0.072057000	8	2.586056000	3.054777000	0.614579000
1	4.561603000	-2.551833000	-0.258204000	1	1.818587000	3.407729000	0.101816000
6	-1.051363000	3.489637000	-0.396264000	6	-5.027650000	-0.399493000	-0.036330000
8	-2.046872000	3.558409000	-1.042542000	8	-5.915144000	0.370751000	-0.210966000
8	-0.332646000	4.509955000	-0.011195000	8	-5.139423000	-1.674376000	0.186264000
1	0.528839000	4.198356000	0.366706000	1	-4.227242000	-2.074528000	0.301884000
pn9'''-(COOH)₃				pn10'''-(COOH)₃			
6	-1.783930000	-1.141294000	-0.402217000	6	1.394830000	-2.558172000	-1.263511000
6	-0.456621000	-1.018999000	-0.064266000	6	0.179242000	-2.064221000	-0.981884000
6	0.126835000	0.306254000	-0.047410000	6	0.047243000	-0.780069000	-0.329325000
6	-0.709558000	1.410273000	0.030300000	6	1.189002000	-0.102105000	-0.015971000
7	-2.095965000	1.234321000	0.015693000	7	2.436709000	-0.707269000	-0.101653000
6	-2.651771000	0.017606000	-0.417351000	6	2.615337000	-1.898722000	-0.815468000
8	-3.840258000	-0.067555000	-0.709758000	8	3.730146000	-2.358977000	-1.013660000
6	1.541635000	0.481986000	-0.333060000	6	-1.216388000	-0.120076000	-0.074385000
7	2.031373000	1.783289000	-0.278411000	6	-1.256670000	1.238555000	0.079199000
6	1.193483000	2.853992000	-0.097821000	7	-0.063176000	1.981753000	0.020011000
6	-0.141478000	2.719653000	0.032232000	6	1.183889000	1.365833000	0.087395000
8	2.282750000	-0.451317000	-0.650972000	8	2.224448000	2.008002000	0.051044000
6	-2.345685000	-2.426222000	-0.680007000	7	-2.398375000	-0.868525000	0.001874000

6	-1.564348000	-3.522695000	-0.652131000	6	-3.661466000	-0.243520000	-0.041151000
6	-0.178544000	-3.436632000	-0.244749000	6	-3.665112000	1.178535000	0.203851000
7	0.282193000	-2.162745000	0.166587000	6	-2.521321000	1.878894000	0.321129000
8	0.570272000	-4.404724000	-0.204971000	8	-4.684434000	-0.908068000	-0.178412000
1	1.690933000	3.813202000	-0.095990000	1	1.537889000	-3.485249000	-1.801891000
1	-0.747661000	3.601162000	0.138214000	1	-0.706300000	-2.590171000	-1.314023000
1	-3.395962000	-2.476970000	-0.940088000	1	-4.637853000	1.630240000	0.340783000
1	-1.921553000	-4.513872000	-0.894574000	1	-2.555064000	2.927670000	0.570301000
6	3.467383000	2.107179000	-0.457824000	6	3.454191000	-0.284841000	0.886247000
8	3.809834000	3.241894000	-0.368030000	8	3.107390000	0.245373000	1.888143000
8	4.226584000	1.082392000	-0.704012000	8	4.679870000	-0.591378000	0.549710000
1	3.669322000	0.251090000	-0.743825000	1	4.672008000	-1.235415000	-0.198648000
6	-2.978135000	2.305590000	0.523549000	6	-0.144633000	3.392230000	-0.414547000
8	-2.544717000	3.128689000	1.263187000	8	-1.151056000	3.801100000	-0.901998000
8	-4.208284000	2.240944000	0.096994000	8	0.933845000	4.090871000	-0.208273000
1	-4.356577000	1.379422000	-0.382216000	1	1.692529000	3.481529000	0.014085000
1	1.894060000	-3.768472000	0.445714000	6	-2.331716000	-2.225362000	0.573956000
6	1.414950000	-2.077759000	1.122479000	8	-1.360566000	-2.572287000	1.169574000
8	1.443075000	-1.182536000	1.903982000	8	-3.392381000	-2.948430000	0.350652000
8	2.265608000	-3.055690000	1.032998000	1	-4.125957000	-2.361741000	0.000340000
pn11'''-(COOH)₃				pn12'''-(COOH)₃			
6	-1.624992000	1.361277000	-0.433809000	6	-1.439665000	0.616059000	-0.146017000
6	-1.475000000	0.044585000	-0.093835000	6	-0.649351000	-0.543152000	0.120030000
6	-0.123689000	-0.512932000	-0.037061000	6	0.797844000	-0.356954000	0.083300000
6	0.915766000	0.377248000	0.018100000	6	1.370831000	0.963884000	-0.019224000
7	0.706907000	1.756180000	0.078550000	7	0.511512000	2.091603000	-0.002741000
6	-0.499027000	2.298348000	-0.344197000	6	-0.861156000	1.958786000	-0.252447000
8	-0.642050000	3.497606000	-0.531133000	8	-1.562219000	2.929315000	-0.489984000
6	0.165069000	-1.903056000	-0.232522000	6	1.639887000	-1.424859000	0.051324000
6	1.442570000	-2.312079000	-0.316658000	7	2.986336000	-1.301978000	-0.062196000
7	2.496471000	-1.420221000	-0.288169000	6	3.593720000	-0.039699000	-0.199604000
6	2.293376000	-0.046315000	-0.234674000	6	2.718412000	1.092851000	-0.175165000
8	3.199827000	0.754095000	-0.442451000	8	4.815696000	0.048486000	-0.336597000
6	-2.909967000	1.872009000	-0.805666000	6	-2.796081000	0.510647000	-0.219349000
6	-3.965680000	1.040825000	-0.892708000	7	-3.425675000	-0.673850000	-0.034833000
6	-3.852498000	-0.350549000	-0.507582000	6	-2.707204000	-1.857114000	0.268274000
7	-2.599219000	-0.764915000	0.005824000	6	-1.282421000	-1.731917000	0.338286000
8	-4.787231000	-1.139963000	-0.562822000	8	-3.310988000	-2.914961000	0.449170000
1	-0.618084000	-2.639221000	-0.317448000	1	1.297609000	-2.449464000	0.097485000
1	1.737397000	-3.344133000	-0.434296000	1	3.214300000	2.044849000	-0.263971000
1	-2.985622000	2.925667000	-1.046425000	1	-3.436166000	1.361125000	-0.418483000
1	-4.948761000	1.359090000	-1.211410000	1	-0.763664000	-2.652272000	0.567331000
6	1.637737000	2.558028000	0.891303000	6	3.763197000	-2.569006000	-0.074396000
8	2.254922000	2.034737000	1.756499000	8	3.175471000	-3.597225000	0.038919000
8	1.661782000	3.832068000	0.582159000	8	5.038338000	-2.396076000	-0.212029000
1	0.926382000	4.050758000	-0.028987000	1	5.235873000	-1.402956000	-0.290604000
6	3.843812000	-2.009217000	-0.444955000	6	1.065356000	3.401729000	0.388467000
8	3.951105000	-3.192867000	-0.478739000	8	2.086811000	3.461905000	0.992067000
8	4.809709000	-1.141655000	-0.527773000	8	0.351562000	4.434558000	0.024597000
1	4.439253000	-0.213842000	-0.517638000	1	-0.518931000	4.141253000	-0.342238000
6	-2.567506000	-1.872689000	0.986399000	6	-4.913565000	-0.648249000	-0.145958000
8	-1.734413000	-1.875516000	1.832706000	8	-5.444349000	0.381966000	-0.404932000
8	-3.498454000	-2.767709000	0.808886000	8	-5.471918000	-1.798161000	0.061818000
1	-4.181081000	-2.414906000	0.171295000	1	-4.760296000	-2.489476000	0.259519000
pn13'''-(COOH)₃				pn14'''-(COOH)₃			

6	0.318024000	-1.603741000	0.005782000	6	3.086670000	2.495189000	-0.202940000
6	0.438757000	-0.183608000	0.038342000	6	1.768643000	2.600196000	0.032997000
6	-0.779483000	0.614655000	0.000510000	6	0.925267000	1.424365000	0.048776000
6	-1.976707000	0.001874000	-0.221843000	6	1.541383000	0.210705000	-0.067669000
7	-2.116792000	-1.413656000	-0.088993000	7	2.927502000	0.086262000	-0.119758000
6	-1.019244000	-2.252143000	-0.016958000	6	3.744666000	1.200033000	-0.335658000
8	-1.120415000	-3.467799000	0.036292000	8	4.942480000	1.084321000	-0.550711000
7	-0.709261000	2.017524000	-0.019501000	6	-0.518941000	1.501588000	0.078262000
6	-1.717776000	2.796294000	-0.616730000	6	-1.255223000	0.335521000	0.027405000
6	-2.909462000	2.089201000	-1.017664000	7	-0.616067000	-0.891798000	0.005319000
6	-3.056652000	0.772426000	-0.777812000	6	0.748602000	-0.990144000	-0.333524000
8	-1.585137000	4.011752000	-0.739098000	8	1.206346000	-2.010371000	-0.805961000
6	1.406173000	-2.416376000	-0.019968000	6	-1.231386000	2.733969000	0.215845000
6	2.733292000	-1.874042000	-0.056417000	6	-2.569264000	2.763909000	0.377727000
7	2.801502000	-0.471312000	-0.140291000	6	-3.346968000	1.554141000	0.304301000
6	1.701232000	0.326955000	-0.085548000	7	-2.638237000	0.377943000	-0.033508000
8	3.758339000	-2.559059000	-0.049301000	8	-4.564121000	1.524033000	0.455619000
1	-3.684230000	2.685197000	-1.478980000	1	3.739710000	3.355342000	-0.268865000
1	-3.973962000	0.276511000	-1.056151000	1	1.334311000	3.581768000	0.166685000
1	1.307233000	-3.493085000	-0.032926000	1	-0.683888000	3.666823000	0.240447000
1	1.932008000	1.378232000	-0.171400000	1	-3.124795000	3.676201000	0.542275000
6	4.105417000	0.244549000	-0.313786000	6	-3.369113000	-0.705238000	-0.749024000
8	4.089445000	1.422360000	-0.461494000	8	-2.780263000	-1.389758000	-1.523556000
8	5.135261000	-0.538839000	-0.285158000	8	-4.631790000	-0.765625000	-0.466510000
1	4.829917000	-1.498456000	-0.169719000	1	-4.896927000	0.042135000	0.061889000
6	-3.449692000	-1.918011000	0.274226000	6	-1.304151000	-2.094708000	0.533670000
8	-4.298602000	-1.158915000	0.619403000	8	-2.189372000	-1.954208000	1.313182000
8	-3.596115000	-3.212623000	0.175990000	8	-0.828852000	-3.226705000	0.106978000
1	-2.719160000	-3.647635000	0.026236000	1	-0.047908000	-3.087797000	-0.475675000
6	0.171542000	2.662220000	0.978738000	6	3.523449000	-1.131572000	0.467876000
8	0.641959000	2.010694000	1.857256000	8	2.905447000	-1.759342000	1.262064000
8	0.348103000	3.936193000	0.785407000	8	4.739573000	-1.381958000	0.056830000
1	-0.295174000	4.259701000	0.084844000	1	5.109715000	-0.592130000	-0.402872000
pn15'''-(COOH) ₃				pn16'''-(COOH) ₃			
6	1.353619000	-0.270261000	-0.045487000	6	2.336049000	-1.729906000	-0.341263000
6	0.930881000	1.043540000	0.106898000	6	1.167027000	-1.057796000	-0.195878000
6	-0.476982000	1.348657000	0.088959000	6	1.128791000	0.349562000	0.039900000
6	-1.387781000	0.307507000	0.043435000	6	2.324320000	0.991292000	0.146244000
7	-0.964114000	-0.998052000	0.180523000	7	3.516536000	0.330728000	0.011087000
6	0.388533000	-1.361279000	-0.067214000	6	3.597350000	-1.043965000	-0.256962000
8	0.669419000	-2.535489000	-0.214941000	8	4.688939000	-1.603081000	-0.393132000
6	2.765168000	-0.612912000	-0.141322000	6	-0.097463000	-1.843733000	-0.163713000
7	3.661752000	0.470533000	-0.020408000	7	-1.249390000	-1.137000000	0.172366000
6	3.223403000	1.754448000	0.158854000	6	-1.305209000	0.265159000	0.030236000
6	1.913541000	2.072554000	0.220477000	6	-0.166304000	1.021396000	0.053991000
8	3.199514000	-1.744756000	-0.311578000	8	-0.098704000	-3.048065000	-0.317774000
6	-0.986876000	2.685228000	0.100844000	7	-2.548177000	0.857743000	-0.138543000
6	-2.309511000	2.936672000	0.138865000	6	-2.719146000	2.245840000	0.043432000
6	-3.264486000	1.861180000	0.066466000	6	-1.513945000	3.033274000	0.094334000
7	-2.731963000	0.563687000	-0.136816000	6	-0.302701000	2.444124000	0.044214000
8	-4.476722000	2.031538000	0.117803000	8	-3.844802000	2.737817000	0.089441000
1	4.016156000	2.484919000	0.243788000	1	2.360820000	-2.798698000	-0.506789000
1	1.646504000	3.106312000	0.366953000	1	2.437380000	2.048343000	0.338079000
1	-0.296226000	3.517415000	0.111060000	1	-1.649510000	4.104648000	0.139788000
1	-2.722056000	3.933802000	0.198012000	1	0.586945000	3.062132000	0.032618000
6	-3.591628000	-0.470252000	-0.789256000	6	-3.655552000	0.073681000	-0.750085000

8	-3.078886000	-1.316439000	-1.447420000	8	-3.399637000	-0.913430000	-1.365125000
8	-4.860284000	-0.303780000	-0.590320000	8	-4.828877000	0.588361000	-0.567325000
1	-5.021794000	0.585566000	-0.162611000	1	-4.733089000	1.510042000	-0.174358000
6	-1.873164000	-1.981357000	0.825675000	6	-2.344182000	-1.807267000	0.896037000
8	-2.768322000	-1.581885000	1.499621000	8	-3.047468000	-1.166194000	1.608093000
8	-1.568542000	-3.222404000	0.607669000	8	-2.425191000	-3.095439000	0.709595000
1	-0.704745000	-3.276982000	0.117459000	1	-1.697855000	-3.417133000	0.135322000
6	5.132240000	0.297349000	-0.080132000	6	4.735559000	1.175556000	0.150938000
8	5.825503000	1.258448000	0.031002000	8	4.600727000	2.335884000	0.376295000
8	5.521643000	-0.928100000	-0.252673000	8	5.844277000	0.524094000	0.004446000
1	4.714104000	-1.527714000	-0.313439000	1	5.640845000	-0.452517000	-0.183688000
pn17'''-(COOH)₃				pn18'''-(COOH)₃			
6	1.204738000	1.324824000	-0.251448000	6	1.726568000	-2.869022000	-0.812039000
6	0.719502000	0.006517000	0.002313000	6	0.491358000	-2.354595000	-0.675247000
6	-0.728075000	-0.193321000	0.012607000	6	0.313870000	-0.964527000	-0.294917000
6	-1.580748000	0.890361000	-0.022525000	6	1.446141000	-0.242507000	-0.040738000
7	-1.067156000	2.211590000	-0.015038000	7	2.703690000	-0.830805000	0.022924000
6	0.264847000	2.473047000	-0.326215000	6	2.925859000	-2.119533000	-0.472932000
8	0.661113000	3.595720000	-0.578683000	8	4.054909000	-2.583532000	-0.557808000
6	-1.276523000	-1.535100000	-0.012877000	6	-0.964878000	-0.280898000	-0.170897000
7	-2.659409000	-1.658192000	-0.122622000	6	-1.002582000	1.096922000	-0.017744000
6	-3.472992000	-0.558676000	-0.214690000	7	0.177699000	1.837587000	-0.144172000
6	-2.985264000	0.696660000	-0.166586000	6	1.432144000	1.221308000	-0.123911000
8	-0.567859000	-2.548069000	0.057603000	8	2.461863000	1.857957000	-0.283824000
6	2.528715000	1.604238000	-0.360864000	6	-2.194965000	-1.047754000	-0.079545000
6	3.514611000	0.572808000	-0.208572000	7	-3.361330000	-0.343393000	0.207380000
7	3.003622000	-0.700882000	0.078301000	6	-3.348740000	1.011203000	0.428491000
6	1.665908000	-0.970249000	0.168928000	6	-2.225575000	1.745888000	0.324018000
8	4.728938000	0.770813000	-0.307483000	8	-2.241800000	-2.276221000	-0.234100000
1	-4.523262000	-0.784339000	-0.326840000	1	1.893742000	-3.884536000	-1.146111000
1	-3.668682000	1.524899000	-0.233643000	1	-0.377310000	-2.953677000	-0.894310000
1	2.884280000	2.607971000	-0.548992000	1	-4.308935000	1.431314000	0.689504000
1	1.430441000	-2.001659000	0.374056000	1	-2.275461000	2.804941000	0.502602000
6	-3.346069000	-2.974525000	-0.174322000	6	3.675157000	-0.239414000	0.966841000
8	-4.529065000	-2.994260000	-0.289672000	8	3.283574000	0.441841000	1.856344000
8	-2.553380000	-3.998279000	-0.085761000	8	4.915028000	-0.579221000	0.734655000
1	-1.602609000	-3.678811000	-0.007074000	1	4.941226000	-1.335963000	0.098070000
6	3.905376000	-1.874087000	0.299628000	6	-4.687479000	-1.000803000	0.335761000
8	3.419616000	-2.927215000	0.552991000	8	-5.633069000	-0.328660000	0.593696000
8	5.165178000	-1.592175000	0.185604000	8	-4.672484000	-2.285206000	0.145629000
1	5.275302000	-0.608936000	-0.034523000	1	-3.729623000	-2.579765000	-0.042955000
6	-1.930030000	3.302189000	0.471716000	6	0.084116000	3.268320000	-0.538773000
8	-2.854554000	3.057531000	1.176268000	8	-0.930396000	3.690541000	-0.990014000
8	-1.586748000	4.499327000	0.071568000	8	1.168540000	3.959968000	-0.336949000
1	-0.704757000	4.477993000	-0.369517000	1	1.940664000	3.346710000	-0.200955000
pn19'''-(COOH)₃				pn20'''-(COOH)₃			
6	1.024107000	0.574122000	-0.235042000	6	-1.310187000	1.487122000	-0.215868000
6	0.226476000	-0.506838000	0.096101000	6	-0.969650000	0.176675000	-0.016271000
6	-1.209507000	-0.348284000	0.001819000	6	0.435031000	-0.203465000	0.015055000
6	-1.747490000	0.909008000	0.013528000	6	1.446782000	0.825914000	-0.036468000
7	-0.914028000	2.023618000	-0.119632000	7	1.041307000	2.184316000	-0.009749000
6	0.435731000	1.877472000	-0.526784000	6	-0.274854000	2.545318000	-0.273521000
8	1.042933000	2.829468000	-0.981909000	8	-0.600881000	3.702037000	-0.485484000
7	-2.043814000	-1.476695000	0.019930000	6	0.862014000	-1.504254000	0.003304000
6	-3.401178000	-1.372894000	0.361166000	7	2.174886000	-1.844201000	-0.072548000
6	-3.947798000	-0.029932000	0.349102000	6	3.187253000	-0.878239000	-0.182106000

6	-3.182384000	1.050488000	0.118362000	6	2.760338000	0.484457000	-0.155668000
8	-4.084849000	-2.371839000	0.551483000	8	4.369910000	-1.216977000	-0.292538000
6	2.478794000	0.477721000	-0.202750000	6	-2.660352000	1.913464000	-0.328631000
7	2.990433000	-0.743129000	0.273399000	6	-3.638561000	0.993551000	-0.220284000
6	2.173092000	-1.769941000	0.672954000	7	-3.346082000	-0.334678000	0.005557000
6	0.829490000	-1.697742000	0.592452000	6	-2.043169000	-0.809757000	0.129158000
8	3.239256000	1.376732000	-0.539391000	8	-1.830630000	-2.004173000	0.354136000
1	-5.020830000	0.038252000	0.467058000	1	0.184747000	-2.341945000	0.047920000
1	-3.634330000	2.026612000	0.043158000	1	3.556337000	1.207807000	-0.209853000
1	2.700698000	-2.636049000	1.046971000	1	-2.887161000	2.955466000	-0.494847000
1	0.238902000	-2.537821000	0.923673000	1	-4.693382000	1.212371000	-0.293037000
6	4.445551000	-0.997325000	0.400252000	6	2.469103000	-3.305286000	-0.071056000
8	4.807328000	-2.045389000	0.831059000	8	1.563781000	-4.069921000	0.019162000
8	5.198528000	-0.012132000	0.015718000	8	3.730687000	-3.579973000	-0.174506000
1	4.618868000	0.750844000	-0.291200000	1	4.258350000	-2.713221000	-0.243372000
6	-1.390936000	3.335796000	0.328676000	6	-4.532053000	-1.232212000	0.112191000
8	-2.307335000	3.408045000	1.087931000	8	-5.613945000	-0.756473000	-0.007031000
8	-0.738710000	4.351161000	-0.163709000	8	-4.250659000	-2.480287000	0.329694000
1	0.050113000	4.027952000	-0.679593000	1	-3.257161000	-2.598308000	0.391934000
6	-1.616173000	-2.645124000	-0.765467000	6	2.012651000	3.216061000	0.415133000
8	-0.731954000	-2.536026000	-1.553966000	8	2.960211000	2.912947000	1.061639000
8	-2.276708000	-3.739362000	-0.498097000	8	1.729458000	4.431950000	0.025107000
1	-3.076124000	-3.520789000	0.054881000	1	0.817975000	4.470640000	-0.352825000
pn21'''-(COOH) ₃				pn22'''-(COOH) ₃			
6	-1.379255000	0.391011000	-0.152804000	6	-1.483710000	0.565087000	-0.155893000
6	-0.443767000	-0.616319000	0.064470000	6	-0.889113000	-0.690705000	0.171406000
6	0.967613000	-0.271567000	0.020447000	6	0.583861000	-0.747301000	0.170457000
6	1.349423000	1.068207000	0.007362000	6	1.316724000	0.475662000	0.037625000
7	0.384525000	2.064384000	-0.019683000	7	0.644744000	1.739766000	0.037420000
6	-0.965553000	1.771600000	-0.351541000	6	-0.714319000	1.817556000	-0.237229000
8	-1.698526000	2.669012000	-0.724231000	8	-1.276162000	2.881080000	-0.456537000
6	1.983768000	-1.310611000	-0.040349000	6	1.250659000	-1.935323000	0.182956000
7	3.317457000	-0.894733000	-0.078651000	6	2.676006000	-2.017959000	0.069400000
6	3.652518000	0.432927000	-0.103448000	7	3.324389000	-0.798247000	-0.140006000
6	2.731568000	1.414519000	-0.063005000	6	2.661180000	0.398079000	-0.155637000
8	1.729104000	-2.519352000	-0.069689000	8	3.303456000	-3.081783000	0.118393000
6	-2.812499000	0.129854000	-0.156941000	6	-2.837403000	0.654159000	-0.276962000
7	-3.183572000	-1.203262000	0.089781000	7	-3.640858000	-0.422412000	-0.086749000
6	-2.251606000	-2.174402000	0.328510000	6	-3.120875000	-1.683566000	0.281385000
6	-0.921239000	-1.936408000	0.322710000	6	-1.690736000	-1.765337000	0.399674000
8	-3.676531000	0.980347000	-0.341767000	8	-3.873147000	-2.637839000	0.471505000
1	4.714035000	0.625079000	-0.166779000	1	0.742715000	-2.887101000	0.244198000
1	3.059380000	2.438169000	-0.089204000	1	3.299505000	1.252384000	-0.315611000
1	-2.671456000	-3.152258000	0.520118000	1	-3.339299000	1.582944000	-0.517574000
1	-0.244692000	-2.749860000	0.507330000	1	-1.315331000	-2.742109000	0.669804000
6	4.459633000	-1.843201000	-0.127532000	6	4.794659000	-0.719183000	-0.381476000
8	5.563132000	-1.402805000	-0.159303000	8	5.279348000	0.339850000	-0.612480000
8	4.121043000	-3.096658000	-0.130093000	8	5.394391000	-1.866330000	-0.312714000
1	3.119277000	-3.167094000	-0.110784000	1	4.715616000	-2.593416000	-0.117921000
6	-4.600093000	-1.643860000	0.118735000	6	1.380509000	2.918871000	0.503039000
8	-4.837244000	-2.788744000	0.337674000	8	2.429192000	2.792131000	1.051376000
8	-5.458820000	-0.697761000	-0.107003000	8	0.797009000	4.065738000	0.268906000
1	-4.964957000	0.170049000	-0.249457000	1	-0.094946000	3.926111000	-0.135191000
6	0.743937000	3.438646000	0.391763000	6	-5.104985000	-0.183250000	-0.264504000
8	1.669630000	3.613305000	1.118040000	8	-5.466764000	0.902539000	-0.577988000
8	-0.025500000	4.369815000	-0.094420000	8	-5.836256000	-1.230628000	-0.046904000

1	-0.817461000	3.951541000	-0.535279000	1	-5.249466000	-2.011359000	0.203729000
pn23'''-(COOH)₃				pn24'''-(COOH)₃			
6	-1.459350000	0.525272000	-0.155043000	6	1.434792000	1.322876000	-0.264780000
6	-0.944350000	-0.768082000	0.178673000	6	1.180687000	0.004674000	0.011641000
6	0.515404000	-0.922170000	0.187450000	6	-0.207330000	-0.461280000	0.081544000
6	1.284230000	0.197850000	0.045690000	6	-1.248881000	0.529570000	0.008381000
7	0.751846000	1.498820000	0.014914000	7	-0.927223000	1.922224000	0.014068000
6	-0.597784000	1.713721000	-0.258114000	6	0.346081000	2.343079000	-0.291021000
8	-1.035777000	2.825817000	-0.489557000	8	0.632835000	3.514554000	-0.491034000
6	1.150396000	-2.201828000	0.253609000	6	-0.562654000	-1.782504000	0.107207000
6	2.489478000	-2.288269000	0.145656000	6	-1.926495000	-2.213678000	0.034775000
7	3.263766000	-1.176218000	-0.110993000	7	-2.875561000	-1.201898000	-0.127829000
6	2.707345000	0.089364000	-0.278159000	6	-2.535898000	0.121563000	-0.135456000
8	3.359083000	1.033344000	-0.711570000	8	-2.265578000	-3.402929000	0.080316000
6	-2.803004000	0.700265000	-0.282547000	6	2.749242000	1.814752000	-0.456833000
7	-3.674380000	-0.323624000	-0.095006000	6	3.782393000	0.952113000	-0.349750000
6	-3.236307000	-1.619110000	0.261355000	7	3.581356000	-0.370586000	-0.042072000
6	-1.815869000	-1.794532000	0.382427000	6	2.309460000	-0.911533000	0.171427000
8	-4.050205000	-2.525154000	0.440648000	8	2.186862000	-2.097390000	0.481799000
1	0.576774000	-3.104551000	0.396552000	1	0.166916000	-2.572110000	0.163543000
1	3.046418000	-3.210651000	0.218926000	1	-3.374306000	0.789791000	-0.249074000
1	-3.243337000	1.658887000	-0.527923000	1	2.910716000	2.858442000	-0.678704000
1	-1.505225000	-2.797791000	0.636191000	1	4.818514000	1.226709000	-0.485428000
6	1.532173000	2.543086000	0.688427000	6	-4.322647000	-1.497031000	-0.312969000
8	2.341269000	2.238297000	1.501408000	8	-5.071786000	-0.593380000	-0.500644000
8	1.227394000	3.767875000	0.331690000	8	-4.605064000	-2.759937000	-0.249183000
1	0.414708000	3.775856000	-0.214336000	1	-3.748243000	-3.287715000	-0.094733000
6	4.713148000	-1.424133000	-0.281078000	6	-1.928026000	2.879411000	0.515238000
8	5.130938000	-2.521440000	-0.093517000	8	-2.879836000	2.491234000	1.110784000
8	5.405369000	-0.379158000	-0.625744000	8	-1.670645000	4.134851000	0.252844000
1	4.801701000	0.408548000	-0.747228000	1	-0.782130000	4.229722000	-0.167894000
6	-5.119575000	0.008882000	-0.272259000	6	4.823664000	-1.193947000	0.050939000
8	-5.411933000	1.117756000	-0.578106000	8	5.866951000	-0.667298000	-0.159745000
8	-5.915864000	-0.991706000	-0.062985000	8	4.624960000	-2.437249000	0.361862000
1	-5.377451000	-1.810076000	0.180749000	1	3.642607000	-2.601044000	0.485069000
pn25'''-(COOH)₃				pn26'''-(COOH)₃			
6	-1.466677000	0.377239000	-0.112467000	6	-1.367740000	1.233000000	-0.283735000
6	-0.590157000	-0.668707000	0.094377000	6	-0.868290000	-0.071257000	-0.005113000
6	0.836249000	-0.399463000	0.059308000	6	0.582155000	-0.265818000	0.003960000
6	1.330830000	0.953076000	-0.001318000	6	1.459675000	0.875384000	-0.001977000
7	0.390282000	1.995449000	-0.000161000	7	0.890132000	2.180530000	0.011914000
6	-0.976983000	1.751750000	-0.284904000	6	-0.438293000	2.398610000	-0.347726000
8	-1.702200000	2.671270000	-0.607956000	8	-0.862266000	3.504025000	-0.625615000
6	1.741888000	-1.418417000	0.026449000	6	1.146039000	-1.499242000	-0.059925000
7	3.076642000	-1.212262000	-0.054280000	7	2.494854000	-1.695660000	-0.097138000
6	3.613105000	0.090187000	-0.136051000	6	3.389668000	-0.617324000	-0.121850000
6	2.675938000	1.166756000	-0.105338000	6	2.806452000	0.690417000	-0.081528000
8	4.833094000	0.245598000	-0.235503000	8	4.607509000	-0.812886000	-0.185124000
6	-2.908887000	0.166688000	-0.135552000	6	-2.695712000	1.480172000	-0.405920000
7	-3.326601000	-1.166436000	0.064760000	6	-3.662072000	0.426085000	-0.239714000
6	-2.436725000	-2.180312000	0.285260000	7	-3.130340000	-0.828404000	0.090055000
6	-1.101466000	-1.980013000	0.309494000	6	-1.783409000	-1.056541000	0.197471000
8	-3.744847000	1.045182000	-0.302887000	8	-4.877942000	0.595455000	-0.354771000
1	1.467971000	-2.463172000	0.044977000	1	0.572691000	-2.415490000	-0.098430000
1	3.114918000	2.148809000	-0.153941000	1	3.515996000	1.501060000	-0.096216000
1	-2.894818000	-3.147731000	0.439548000	1	-3.075619000	2.472028000	-0.609894000

1	-0.460284000	-2.824073000	0.507964000	1	-1.535721000	-2.077097000	0.455767000
6	3.929793000	-2.431303000	-0.077908000	6	2.949208000	-3.107415000	-0.154036000
8	3.400353000	-3.495010000	-0.006391000	8	2.130173000	-3.970838000	-0.144260000
8	5.193024000	-2.177098000	-0.176953000	8	4.236212000	-3.238668000	-0.209869000
1	5.328388000	-1.167370000	-0.221752000	1	4.666859000	-2.317587000	-0.210251000
6	0.832545000	3.352824000	0.368075000	6	1.715868000	3.306625000	0.491042000
8	1.833727000	3.502446000	0.992022000	8	2.648891000	3.102145000	1.195112000
8	0.052258000	4.319236000	-0.034101000	8	1.331082000	4.490172000	0.085470000
1	-0.775019000	3.943621000	-0.432835000	1	0.463323000	4.437590000	-0.376807000
6	-4.758934000	-1.561070000	0.064859000	6	-4.003278000	-2.009910000	0.345918000
8	-5.033697000	-2.704389000	0.243259000	8	-3.491025000	-3.042899000	0.633719000
8	-5.584457000	-0.581808000	-0.138052000	8	-5.268704000	-1.763866000	0.219791000
1	-5.064569000	0.273826000	-0.249393000	1	-5.403118000	-0.793595000	-0.034809000
pn27'''-(COOH)₃				pn28'''-(COOH)₃			
6	-0.010134000	-1.677611000	0.385842000	6	-1.974036000	-2.918736000	-0.687936000
6	0.371742000	-0.402005000	0.064251000	6	-0.715348000	-2.458128000	-0.593439000
6	-0.625402000	0.646718000	0.059043000	6	-0.471283000	-1.065259000	-0.298096000
6	-1.950608000	0.303582000	-0.023767000	6	-1.541468000	-0.267494000	-0.055182000
7	-2.330790000	-1.054063000	0.061700000	7	-2.832867000	-0.776894000	0.035558000
6	-1.435248000	-2.021721000	0.506773000	6	-3.127315000	-2.075760000	-0.389366000
8	-1.795529000	-3.138997000	0.852759000	8	-4.278399000	-2.483906000	-0.448848000
7	-0.260341000	1.991524000	0.135253000	6	0.856144000	-0.476779000	-0.219875000
6	-1.158272000	3.017381000	-0.192094000	6	1.005379000	0.942706000	-0.009367000
6	-2.548656000	2.628117000	-0.261211000	7	-0.140376000	1.756691000	-0.174377000
6	-2.935442000	1.345618000	-0.121963000	6	-1.422350000	1.199534000	-0.200175000
8	-0.776249000	4.177297000	-0.316913000	8	-2.412349000	1.864652000	-0.444052000
6	0.940443000	-2.728305000	0.513244000	6	1.969999000	-1.253928000	-0.168630000
6	2.234862000	-2.458387000	0.255143000	7	3.205679000	-0.748923000	0.095101000
7	2.637136000	-1.215976000	-0.195683000	6	3.389237000	0.608827000	0.404916000
6	1.745171000	-0.166366000	-0.390301000	6	2.226420000	1.441897000	0.331827000
8	2.088773000	0.871643000	-0.952096000	8	4.509238000	1.031854000	0.706043000
1	-3.258821000	3.435741000	-0.373805000	1	-2.204552000	-3.942070000	-0.953050000
1	-3.985311000	1.098938000	-0.114329000	1	0.113250000	-3.125566000	-0.793506000
1	0.619677000	-3.713664000	0.815973000	1	1.962188000	-2.325724000	-0.302593000
1	3.036652000	-3.175766000	0.349407000	1	2.406901000	2.485302000	0.525282000
6	0.942871000	2.330339000	0.915039000	6	-3.767649000	-0.076540000	0.940366000
8	1.388488000	1.533861000	1.682724000	8	-3.335133000	0.640194000	1.781546000
8	1.397267000	3.529554000	0.705209000	8	-5.025578000	-0.361217000	0.732528000
1	0.737495000	4.045113000	0.161101000	1	-5.100645000	-1.147406000	0.139301000
6	4.084995000	-1.085168000	-0.495163000	6	4.322941000	-1.724582000	0.098899000
8	4.800107000	-2.005289000	-0.262066000	8	4.087484000	-2.861091000	-0.168963000
8	4.435559000	0.059842000	-1.000252000	8	5.467493000	-1.204639000	0.404412000
1	3.633728000	0.645195000	-1.110988000	1	5.343455000	-0.211035000	0.590925000
6	-3.634883000	-1.468306000	-0.477171000	6	0.049208000	3.179923000	-0.543214000
8	-4.206289000	-0.770042000	-1.252649000	8	1.124166000	3.578024000	-0.853680000
8	-4.066492000	-2.619675000	-0.038077000	8	-1.026171000	3.916977000	-0.479696000
1	-3.359165000	-3.074825000	0.488635000	1	-1.832924000	3.349514000	-0.399010000
pn29'''-(COOH)₃				pn30'''-(COOH)₃			
6	1.436488000	1.146942000	-0.279504000	6	2.890983000	-2.598550000	0.671674000
6	1.074892000	-0.198594000	0.027804000	6	1.548083000	-2.542887000	0.617448000
6	-0.344044000	-0.557400000	0.070986000	6	0.880817000	-1.299989000	0.323062000
6	-1.307574000	0.500900000	0.012421000	6	1.650433000	-0.212072000	0.024429000
7	-0.888076000	1.873660000	0.028510000	7	3.023270000	-0.309897000	-0.101979000
6	0.403763000	2.229027000	-0.308664000	6	3.718358000	-1.447450000	0.336635000
8	0.740342000	3.380061000	-0.528288000	8	4.939007000	-1.464294000	0.381509000
6	-0.776195000	-1.851845000	0.072019000	6	-0.566694000	-1.158423000	0.267883000

6	-2.160735000	-2.200555000	0.016208000	6	-1.094624000	0.097586000	0.141924000
7	-3.043207000	-1.123039000	-0.126520000	7	-0.289029000	1.237353000	0.237026000
6	-2.619481000	0.176339000	-0.129074000	6	1.088536000	1.160924000	0.121979000
8	-2.576556000	-3.364897000	0.053869000	8	1.809015000	2.134106000	0.247263000
6	2.731066000	1.511089000	-0.446821000	6	-1.450150000	-2.284242000	0.231370000
6	3.797030000	0.553262000	-0.304033000	6	-2.768505000	-2.089417000	0.035478000
7	3.395877000	-0.747337000	0.053901000	7	-3.286927000	-0.835292000	-0.203258000
6	2.083976000	-1.095431000	0.199656000	6	-2.479017000	0.300843000	-0.260765000
8	4.985913000	0.828700000	-0.459469000	8	-2.904831000	1.378323000	-0.664998000
1	-0.098070000	-2.693732000	0.079003000	1	3.431342000	-3.497153000	0.937944000
1	-3.414592000	0.897676000	-0.232698000	1	0.964392000	-3.424506000	0.849214000
1	3.011132000	2.531759000	-0.670021000	1	-1.086381000	-3.292665000	0.353352000
1	1.935278000	-2.133379000	0.463509000	1	-3.501130000	-2.882875000	0.020536000
6	-4.508451000	-1.321129000	-0.303780000	6	-0.881526000	2.399798000	0.937915000
8	-5.197626000	-0.368713000	-0.477373000	8	-1.804777000	2.231884000	1.661434000
8	-4.874221000	-2.563251000	-0.250985000	8	-0.292781000	3.542870000	0.690287000
1	-4.056658000	-3.149588000	-0.109036000	1	0.598025000	3.392277000	0.310593000
6	-1.819047000	2.877106000	0.564234000	6	-4.740102000	-0.777578000	-0.473271000
8	-2.778264000	2.534085000	1.176580000	8	-5.379800000	-1.776068000	-0.378844000
8	-1.500025000	4.121634000	0.314792000	8	-5.184427000	0.400984000	-0.793353000
1	-0.627851000	4.176744000	-0.141812000	1	-4.426656000	1.055191000	-0.826763000
6	4.381480000	-1.844556000	0.281474000	6	3.690837000	0.629613000	-1.036793000
8	3.974238000	-2.918280000	0.586501000	8	3.063915000	1.105642000	-1.922112000
8	5.614309000	-1.485863000	0.113049000	8	4.964006000	0.801192000	-0.797797000
1	5.654717000	-0.511207000	-0.147158000	1	5.290028000	0.098548000	-0.188321000
pn31'''-(COOH) ₃				pn32'''-(COOH) ₃			
6	-2.701263000	-2.685015000	-0.686711000	6	1.399723000	1.270822000	-0.288852000
6	-1.367722000	-2.510448000	-0.688046000	6	1.225981000	-0.062181000	0.003889000
6	-0.803680000	-1.217904000	-0.392636000	6	-0.125841000	-0.612272000	0.082693000
6	-1.649532000	-0.208019000	-0.058170000	6	-1.172265000	0.276325000	0.027524000
7	-3.002870000	-0.424321000	0.122147000	7	-0.976179000	1.662936000	0.006625000
6	-3.611608000	-1.618973000	-0.291500000	6	0.246700000	2.206167000	-0.327633000
8	-4.826296000	-1.749576000	-0.271961000	8	0.400204000	3.395443000	-0.551422000
6	0.632264000	-0.951157000	-0.347789000	6	-0.434613000	-2.013749000	0.129106000
6	1.069318000	0.396056000	-0.140265000	6	-1.718455000	-2.416973000	0.072344000
7	0.133289000	1.465329000	-0.265776000	7	-2.758220000	-1.529093000	-0.105169000
6	-1.222900000	1.214375000	-0.202763000	6	-2.537046000	-0.164124000	-0.232403000
8	-2.070277000	2.067995000	-0.404154000	8	-3.424587000	0.609520000	-0.588693000
6	1.549126000	-1.963158000	-0.332094000	6	2.682839000	1.839635000	-0.484921000
6	2.937991000	-1.732486000	-0.084122000	6	3.765356000	1.042403000	-0.372516000
7	3.278269000	-0.410496000	0.224806000	7	3.644299000	-0.291079000	-0.055224000
6	2.370498000	0.611355000	0.189980000	6	2.409399000	-0.904862000	0.170066000
8	3.792144000	-2.627538000	-0.095349000	8	2.357179000	-2.092540000	0.497478000
1	-3.170924000	-3.623948000	-0.947782000	1	0.347102000	-2.745347000	0.228678000
1	-0.718107000	-3.331162000	-0.963581000	1	-2.024280000	-3.450846000	0.133336000
1	1.278415000	-3.002165000	-0.449145000	1	2.777195000	2.890081000	-0.715960000
1	2.783432000	1.578570000	0.426955000	1	4.783417000	1.376348000	-0.510690000
6	-3.707645000	0.467294000	1.074542000	6	-1.976007000	2.501166000	0.701705000
8	-3.077137000	1.045950000	1.895165000	8	-2.619451000	2.031868000	1.577853000
8	-5.003993000	0.486806000	0.925604000	8	-2.023076000	3.742961000	0.284476000
1	-5.288915000	-0.258528000	0.343471000	1	-1.250393000	3.945413000	-0.281701000
6	4.662429000	-0.025003000	0.622336000	6	-4.107073000	-2.121269000	-0.233172000
8	4.875735000	1.101915000	0.930842000	8	-4.234288000	-3.294504000	-0.086526000
8	5.505567000	-1.009032000	0.586928000	8	-5.050363000	-1.266031000	-0.498270000
1	5.024669000	-1.855733000	0.300850000	1	-4.661228000	-0.348959000	-0.600015000
6	0.629991000	2.767575000	-0.747337000	6	4.932616000	-1.035940000	0.042038000

8	1.770253000	2.888922000	-1.062022000	8	5.942853000	-0.451828000	-0.179180000
8	-0.257231000	3.725006000	-0.776841000	8	4.810392000	-2.286282000	0.367364000
1	-1.163101000	3.368836000	-0.597262000	1	3.840112000	-2.505763000	0.498889000
pn33'''-(COOH)₃				pn34'''-(COOH)₃			
6	-1.400167000	1.100069000	-0.280984000	6	1.520364000	0.342476000	-0.113657000
6	-1.122649000	-0.264070000	0.051079000	6	0.848704000	-0.814916000	0.207745000
6	0.268403000	-0.705117000	0.110376000	6	-0.621227000	-0.803686000	0.191233000
6	1.247104000	0.244138000	0.029013000	6	-1.295585000	0.445966000	0.053095000
7	0.961881000	1.628671000	0.010756000	7	-0.549232000	1.654111000	0.058111000
6	-0.291564000	2.104037000	-0.330082000	6	0.825278000	1.646533000	-0.201955000
8	-0.509424000	3.277102000	-0.559658000	8	1.431174000	2.684827000	-0.396489000
6	0.645813000	-2.083475000	0.164340000	6	-1.339666000	-1.964837000	0.193189000
6	1.948295000	-2.420456000	0.095216000	6	-2.764563000	-1.982617000	0.064100000
7	2.928888000	-1.474284000	-0.105159000	7	-3.356918000	-0.734100000	-0.137630000
6	2.627952000	-0.119358000	-0.246210000	6	-2.643672000	0.431822000	-0.144424000
8	3.470614000	0.695214000	-0.615393000	8	-3.439628000	-3.019254000	0.098829000
6	-2.668897000	1.541137000	-0.457481000	6	2.973139000	0.339654000	-0.282651000
6	-3.791554000	0.651672000	-0.309381000	7	3.612995000	-0.878245000	0.030493000
7	-3.472168000	-0.673286000	0.042715000	6	2.918957000	-1.992080000	0.408999000
6	-2.185078000	-1.101251000	0.202513000	6	1.569790000	-2.004935000	0.491966000
8	-4.962211000	0.999184000	-0.464381000	8	3.635363000	1.291330000	-0.671182000
1	-0.090695000	-2.866656000	0.263259000	1	-0.881123000	-2.940280000	0.254314000
1	2.314774000	-3.434579000	0.158532000	1	-3.241292000	1.314910000	-0.303944000
1	-2.882647000	2.574358000	-0.697170000	1	3.539115000	-2.851196000	0.625345000
1	-2.103319000	-2.148672000	0.456314000	1	1.075363000	-2.913520000	0.795561000
6	1.899853000	2.499777000	0.732716000	6	-4.824121000	-0.590106000	-0.383474000
8	2.586698000	2.041699000	1.583513000	8	-5.261171000	0.490892000	-0.606023000
8	1.865093000	3.761370000	0.371562000	8	-5.470459000	-1.711532000	-0.326542000
1	1.105127000	3.934033000	-0.217822000	1	-4.820769000	-2.468667000	-0.137395000
6	4.308752000	-1.989537000	-0.238895000	6	-1.217206000	2.877960000	0.513115000
8	4.503574000	-3.152235000	-0.080871000	8	-2.286023000	2.813845000	1.035187000
8	5.198248000	-1.085024000	-0.522035000	8	-0.557630000	3.984408000	0.299249000
1	4.755861000	-0.192344000	-0.628738000	1	0.333556000	3.778761000	-0.087735000
6	-4.523332000	-1.711252000	0.245561000	6	5.091755000	-1.040971000	-0.041135000
8	-4.184188000	-2.813503000	0.534255000	8	5.560087000	-2.094379000	0.248889000
8	-5.730804000	-1.275868000	0.076843000	8	5.729076000	0.020747000	-0.423496000
1	-5.707696000	-0.295247000	-0.169937000	1	5.069225000	0.758984000	-0.607221000
pn35'''-(COOH)₃				pn36'''-(COOH)₃			
6	-1.508193000	0.298877000	-0.116680000	6	1.001441000	1.612066000	-0.381751000
6	-0.906548000	-0.913677000	0.168332000	6	0.770859000	0.304520000	-0.053330000
6	0.551094000	-1.004354000	0.162053000	6	-0.584748000	-0.188293000	-0.011434000
6	1.267992000	0.153839000	0.048184000	6	-1.634216000	0.706349000	0.076723000
7	0.655302000	1.399146000	0.025383000	7	-1.363523000	2.085324000	0.008993000
6	-0.717923000	1.535992000	-0.244643000	6	-0.127555000	2.552539000	-0.458698000
8	-1.184544000	2.630843000	-0.487210000	8	0.031888000	3.709779000	-0.813582000
6	1.252657000	-2.253298000	0.213942000	6	-0.848591000	-1.590062000	-0.296309000
6	2.594765000	-2.269888000	0.124884000	7	-2.167518000	-2.015032000	-0.113609000
7	3.318358000	-1.114665000	-0.098216000	6	-3.182941000	-1.114034000	0.087659000
6	2.703116000	0.122834000	-0.257240000	6	-2.974574000	0.217584000	0.147059000
8	3.308266000	1.102153000	-0.675710000	8	0.007252000	-2.359254000	-0.726779000
6	-2.958455000	0.407660000	-0.237059000	6	2.317509000	2.114326000	-0.588654000
7	-3.677806000	-0.779325000	0.017189000	6	3.355405000	1.271424000	-0.417965000
6	-3.056247000	-1.956156000	0.328918000	7	3.169732000	-0.016435000	0.047213000
6	-1.711234000	-2.063121000	0.402775000	6	1.906879000	-0.516638000	0.383696000
8	-3.558118000	1.431987000	-0.534212000	8	1.778919000	-1.531086000	1.055318000
1	0.731482000	-3.190125000	0.329977000	1	-4.164444000	-1.559563000	0.163681000

1	3.195829000	-3.164578000	0.189292000	1	-3.817321000	0.874298000	0.267948000
1	-3.731503000	-2.782460000	0.503767000	1	2.467168000	3.138310000	-0.896170000
1	-1.280055000	-3.018831000	0.653083000	1	4.388054000	1.533452000	-0.595711000
6	1.375715000	2.508723000	0.675891000	6	-2.568351000	-3.432318000	-0.232137000
8	2.194881000	2.265345000	1.499553000	8	-3.701355000	-3.727928000	-0.023350000
8	1.001355000	3.700037000	0.285833000	8	-1.602511000	-4.238591000	-0.560668000
1	0.173778000	3.635014000	-0.241915000	1	-0.762867000	-3.712296000	-0.714564000
6	4.779438000	-1.288985000	-0.250331000	6	4.403725000	-0.803898000	0.258229000
8	5.248517000	-2.366840000	-0.071153000	8	5.440980000	-0.356057000	-0.112669000
8	5.425967000	-0.207217000	-0.571494000	8	4.222665000	-1.951363000	0.844484000
1	4.788834000	0.551238000	-0.696254000	1	3.259936000	-2.062282000	1.087049000
6	-5.162572000	-0.836358000	-0.042625000	6	-2.370568000	3.048111000	0.495395000
8	-5.700797000	-1.872547000	0.183518000	8	-3.187130000	2.701439000	1.285318000
8	-5.729295000	0.289747000	-0.344462000	8	-2.266244000	4.250627000	-0.003880000
1	-5.020835000	0.993049000	-0.484149000	1	-1.422732000	4.340498000	-0.514859000

X. Anionic system along with ΔE_{ad}

py⁻				(py-CO₂⁻)_o			$\Delta E_{ad} = -15.7$
6	1.150014000	-1.139498000	0.000000000	6	-1.899630000	1.301514000	-0.263015000
6	-0.099117000	-1.785416000	0.000000000	6	-2.857793000	0.320586000	0.007536000
6	-1.216710000	-0.954135000	0.000000000	6	-2.392361000	-0.967900000	0.216428000
7	-1.213259000	0.371561000	0.000000000	7	-1.109391000	-1.325415000	0.177871000
6	0.000000000	1.041432000	0.000000000	6	-0.192572000	-0.385199000	-0.086249000
6	1.208798000	0.230219000	0.000000000	6	-0.564718000	0.963374000	-0.311968000
1	2.068784000	-1.723198000	0.000000000	1	-2.199182000	2.330296000	-0.436960000
1	-0.199247000	-2.863705000	0.000000000	1	-3.915713000	0.546332000	0.056403000
1	-2.208104000	-1.415156000	0.000000000	1	-3.094395000	-1.771180000	0.432537000
1	2.155009000	0.760543000	0.000000000	1	0.204050000	1.697552000	-0.497454000
8	0.052308000	2.285622000	0.000000000	8	1.049622000	-0.817628000	-0.187352000
				6	2.273805000	0.078914000	0.089730000
				8	3.256205000	-0.421733000	-0.413116000
				8	2.015498000	1.065257000	0.761168000
(py-CO₂⁻)_N				(py-CO₂⁻)_o...CO₂			$\Delta E_{ad} = -30.5$
6	2.516047000	-0.290108000	-0.132002000	6	2.740380000	1.552671000	0.119560000
6	1.748801000	-1.482439000	-0.120426000	6	3.865024000	0.791333000	-0.208059000
6	0.389911000	-1.350409000	-0.026160000	6	3.684330000	-0.576500000	-0.332390000
7	-0.240039000	-0.162394000	0.052730000	7	2.518750000	-1.201336000	-0.163664000
6	0.461083000	1.050421000	0.147631000	6	1.448307000	-0.469215000	0.150493000
6	1.904980000	0.919243000	-0.017040000	6	1.522050000	0.933806000	0.302013000
1	3.597112000	-0.342785000	-0.227193000	1	2.817945000	2.629061000	0.233445000
1	2.201418000	-2.461575000	-0.188391000	1	4.838234000	1.240462000	-0.361604000
1	-0.282675000	-2.199936000	-0.005610000	1	4.525900000	-1.217578000	-0.586064000
1	2.461820000	1.848069000	-0.002379000	1	0.626937000	1.489132000	0.535888000
8	-0.089532000	2.115528000	0.380387000	8	0.340783000	-1.166901000	0.383565000
6	-1.849542000	-0.225275000	-0.060189000	6	-1.018143000	-0.603533000	0.158810000
8	-2.292969000	0.637918000	-0.783699000	8	-1.863102000	-1.264290000	0.738937000
8	-2.283134000	-1.182897000	0.566258000	8	-1.060560000	0.385305000	-0.569919000
				6	-3.734590000	0.473474000	-0.187281000
				8	-3.633256000	1.166531000	0.734054000
				8	-3.969418000	-0.163637000	-1.123499000
(py-CO₂⁻)_N...CO₂				(py... (CO₂⁻)₂)_{N&o}			$\Delta E_{ad} = -26.9$
6	-3.625518000	0.427931000	-0.144920000	6	-0.386296000	2.852195000	0.043377000
6	-2.794425000	1.565975000	0.028510000	6	-1.746024000	2.508840000	0.149980000
6	-1.450767000	1.350863000	0.138626000	6	-2.050804000	1.160057000	0.035879000
7	-0.886967000	0.122907000	0.088040000	7	-1.172124000	0.182908000	-0.170889000
6	-1.656349000	-1.053978000	0.020228000	6	0.164318000	0.486919000	-0.311926000

6	-3.085436000	-0.817935000	-0.161805000	6	0.550627000	1.876583000	-0.177670000
1	-4.698383000	0.554238000	-0.258863000	1	-0.075861000	3.890567000	0.134184000
1	-3.192091000	2.570053000	0.066639000	1	-2.520388000	3.246276000	0.318156000
1	-0.733376000	2.150327000	0.276232000	1	-3.089040000	0.834159000	0.115431000
1	-3.690565000	-1.709050000	-0.272428000	1	1.605859000	2.108180000	-0.260456000
8	-1.175521000	-2.167716000	0.136764000	8	1.001038000	-0.412814000	-0.555674000
6	0.680348000	0.102877000	0.045172000	6	3.315925000	-0.611008000	0.124413000
8	1.138260000	-0.721831000	-0.723759000	8	3.480303000	-1.582082000	-0.483186000
8	1.170183000	0.974772000	0.761774000	8	3.346278000	0.341278000	0.786479000
6	3.633088000	0.063960000	-0.062828000	6	-2.207542000	-2.106371000	0.154728000
8	3.712415000	-0.684029000	0.815223000	8	-3.250590000	-1.734211000	-0.200237000
8	3.694354000	0.815796000	-0.940722000	8	-1.271643000	-2.657523000	0.549645000
nt5⁻				(nt5⁻...CO₂)₀ ΔE_{ad} = -12.1			
6	-0.356780000	-0.582586000	0.000045000	6	-1.517308000	0.342248000	0.024202000
6	0.431615000	0.580437000	0.000071000	6	-0.207531000	0.048989000	-0.388551000
6	-0.203357000	1.837603000	-0.000016000	6	0.140582000	-1.290252000	-0.658851000
6	-1.572792000	1.897483000	-0.000154000	6	-0.802410000	-2.271491000	-0.502432000
7	-2.358935000	0.786039000	-0.000053000	7	-2.075092000	-2.014067000	-0.092971000
6	-1.765641000	-0.374417000	0.000144000	6	-2.393422000	-0.773986000	0.149060000
8	-2.562214000	-1.482327000	0.000104000	8	-3.670536000	-0.523751000	0.553698000
6	0.272570000	-1.849840000	-0.000096000	6	-1.881902000	1.685805000	0.276314000
6	1.654646000	-1.842513000	-0.000131000	6	-0.895226000	2.631270000	0.085457000
7	2.461321000	-0.776036000	-0.000098000	7	0.370161000	2.413911000	-0.297876000
6	1.914928000	0.477258000	0.000047000	6	0.782990000	1.140780000	-0.535251000
8	2.601181000	1.508492000	0.000138000	8	1.952102000	0.863623000	-0.867396000
1	0.413471000	2.727497000	0.000018000	1	1.144253000	-1.512124000	-1.000960000
1	-2.102862000	2.843925000	-0.000345000	1	-0.578370000	-3.313852000	-0.701508000
1	-3.463949000	-1.141936000	-0.000146000	1	-4.100319000	-1.386201000	0.579036000
1	-0.299493000	-2.766537000	0.000233000	1	-2.880051000	1.950213000	0.594840000
1	2.173259000	-2.802831000	-0.000093000	1	-1.142421000	3.679141000	0.259926000
				6	3.327979000	-0.603344000	0.640213000
				8	4.014182000	-0.972381000	-0.216476000
				8	2.725365000	-0.327014000	1.588127000
(nt5-CO₂)_N ΔE_{ad} = -13.6				(nt5-CO₂)_N...CO₂ ΔE_{ad} = -28.0			
6	1.167654000	-0.576563000	0.006250000	6	2.204288000	-0.589271000	0.038247000
6	0.631740000	0.711657000	0.068019000	6	1.720986000	0.719871000	0.035555000
6	1.492249000	1.822826000	0.057622000	6	2.618997000	1.792351000	-0.095911000
6	2.845184000	1.607153000	-0.019540000	6	3.957153000	1.516187000	-0.225876000
7	3.393040000	0.368496000	-0.078229000	7	4.454522000	0.255998000	-0.224881000
6	2.583660000	-0.656314000	-0.063954000	6	3.609816000	-0.732325000	-0.097452000
8	3.136296000	-1.896103000	-0.120385000	8	4.110841000	-1.994027000	-0.093940000
6	0.298794000	-1.708661000	0.020781000	6	1.295446000	-1.683094000	0.176497000
6	-1.038702000	-1.468300000	0.053337000	6	-0.026870000	-1.393090000	0.258404000
7	-1.599092000	-0.229072000	0.072197000	7	-0.540128000	-0.128566000	0.216161000
6	-0.838703000	0.924920000	0.168532000	6	0.267338000	1.001891000	0.194539000
8	-1.302338000	2.036130000	0.346218000	8	-0.143914000	2.137864000	0.318620000
1	1.066846000	2.816326000	0.111568000	1	2.234583000	2.803744000	-0.090623000
1	3.549844000	2.431226000	-0.035081000	1	4.689931000	2.307965000	-0.334846000
1	4.089103000	-1.755204000	-0.162923000	1	5.064869000	-1.898163000	-0.195213000
1	0.689837000	-2.714564000	0.000613000	1	1.648811000	-2.702511000	0.206686000
1	-1.773070000	-2.264193000	0.071053000	1	-0.789042000	-2.153581000	0.368090000
6	-3.219122000	-0.193822000	-0.112075000	6	-2.111469000	-0.035412000	0.139247000
8	-3.576756000	0.730855000	-0.802647000	8	-2.513139000	0.864830000	-0.571525000
8	-3.721792000	-1.154249000	0.449711000	8	-2.646529000	-0.940511000	0.775156000
				6	-5.039575000	-0.150231000	-0.258741000
				8	-5.287727000	0.529584000	0.642882000

				8	-4.922853000	-0.839080000	-1.181207000
((CO₂)...nt5-(CO₂⁻))_{N&O}				ΔE_{ad} =-29.4			
6	-1.866747000	0.519940000	-0.075141000	6	0.385723000	0.581958000	-0.000091000
6	-0.992301000	-0.454488000	0.407888000	6	-0.385720000	-0.581959000	-0.000057000
6	-1.475382000	-1.743623000	0.690802000	6	0.287213000	-1.833747000	-0.000023000
6	-2.804944000	-2.007305000	0.478326000	6	1.662051000	-1.815963000	0.000053000
7	-3.677511000	-1.079648000	0.014212000	7	2.452986000	-0.721692000	0.000023000
6	-3.217030000	0.114960000	-0.242802000	6	1.868905000	0.508762000	-0.000207000
8	-4.093137000	1.043121000	-0.705741000	8	2.549693000	1.564730000	0.000147000
6	-1.379614000	1.830756000	-0.362134000	6	-0.287215000	1.833748000	-0.000034000
6	-0.055196000	2.060795000	-0.178141000	6	-1.662050000	1.815964000	0.000035000
7	0.836188000	1.122693000	0.254410000	7	-2.452986000	0.721689000	0.000041000
6	0.442551000	-0.145637000	0.638801000	6	-1.868909000	-0.508760000	-0.000039000
8	1.187194000	-0.967899000	1.148481000	8	-2.549691000	-1.564731000	0.000051000
1	-0.789927000	-2.491365000	1.066995000	1	-0.286590000	-2.751930000	-0.000004000
1	-3.225770000	-2.986804000	0.676274000	1	2.202467000	-2.767641000	0.000134000
1	-4.945306000	0.595279000	-0.759459000	1	0.286589000	2.751930000	-0.000063000
1	-2.040621000	2.607691000	-0.715265000	1	-2.202468000	2.767640000	0.000071000
1	0.401577000	3.025069000	-0.359445000				
6	2.380431000	1.584745000	0.239295000				
8	3.135618000	0.681370000	-0.055471000				
8	2.471592000	2.776297000	0.484029000				
6	2.841648000	-1.770619000	-0.804738000				
8	2.023990000	-1.509890000	-1.583400000				
8	3.680844000	-2.146539000	-0.105698000				
(nt5-CO₂⁻)_O				(nt5-CO₂⁻)_N			
ΔE_{ad} =-26.9				ΔE_{ad} =-32.5			
6	0.416011000	-0.367180000	-0.092447000	6	-0.665538000	0.696034000	0.056893000
6	1.504534000	0.513446000	-0.027384000	6	-1.200292000	-0.584286000	-0.014871000
6	1.247790000	1.901302000	-0.060518000	6	-0.311148000	-1.704552000	-0.018507000
6	-0.052434000	2.323624000	-0.167592000	6	1.023921000	-1.485396000	0.015779000
7	-1.123010000	1.495790000	-0.253614000	7	1.577998000	-0.224833000	0.038364000
6	-0.905657000	0.201713000	-0.207224000	6	0.800515000	0.919654000	0.132038000
8	-1.911738000	-0.661547000	-0.341532000	8	1.280119000	2.037126000	0.295623000
6	0.669322000	-1.764206000	-0.053998000	6	-1.542425000	1.805041000	0.079905000
6	1.985307000	-2.153009000	0.043400000	6	-2.893262000	1.532744000	0.020481000
7	3.068426000	-1.355000000	0.104935000	7	-3.464526000	0.320637000	-0.049851000
6	2.893179000	-0.004287000	0.074332000	6	-2.664034000	-0.787571000	-0.069092000
8	3.851680000	0.795469000	0.125583000	8	-3.135581000	-1.944224000	-0.129440000
1	2.080757000	2.591051000	-0.003254000	1	-0.722421000	-2.704152000	-0.046395000
1	-0.289148000	3.385610000	-0.198122000	1	1.760384000	-2.277536000	0.035219000
1	-0.145389000	-2.473032000	-0.100186000	1	-1.149092000	2.810608000	0.140710000
1	2.209280000	-3.222072000	0.076489000	1	-3.596653000	2.369495000	0.031217000
6	-3.298931000	-0.328772000	0.155951000	6	3.123459000	-0.168983000	-0.082165000
8	-3.321304000	0.155362000	1.276844000	8	3.678425000	-1.018633000	0.623054000
8	-4.147156000	-0.689643000	-0.651058000	8	3.537824000	0.650087000	-0.889625000
(nt5-(CO₂⁻)₂)_{O&O}				(nt5-(CO₂⁻)₂)_{N&N}			
ΔE_{ad} =-47.6				ΔE_{ad} =-59.3			
6	-0.537171000	-0.448534000	0.000117000	6	0.241164000	-0.646358000	-0.083706000
6	0.537232000	0.448445000	0.000104000	6	-0.240762000	0.646751000	-0.083829000
6	0.268155000	1.839813000	0.000051000	6	0.675563000	1.739242000	-0.100958000
6	-1.043288000	2.231561000	0.000020000	6	2.003397000	1.465706000	-0.077562000
7	-2.109068000	1.393482000	0.000035000	7	2.510058000	0.195339000	-0.032189000
6	-1.881212000	0.096429000	0.000079000	6	1.696442000	-0.927055000	-0.108697000
8	-2.862717000	-0.770321000	0.000047000	8	2.132589000	-2.064967000	-0.219707000
6	-0.268096000	-1.839891000	0.000173000	6	-0.674945000	-1.738862000	-0.100766000
6	1.043350000	-2.231654000	0.000231000	6	-2.002891000	-1.465015000	-0.077672000
7	2.109113000	-1.393570000	0.000241000	7	-2.509316000	-0.194936000	-0.032940000

6	1.881232000	-0.096540000	0.000167000	6	-1.695849000	0.927300000	-0.108825000
8	2.862768000	0.770243000	0.000184000	8	-2.131740000	2.065604000	-0.219297000
1	1.084809000	2.548459000	0.000037000	1	0.301577000	2.752239000	-0.131309000
1	-1.296797000	3.289318000	-0.000013000	1	2.767336000	2.231550000	-0.099986000
1	-1.084752000	-2.548535000	0.000175000	1	-0.301024000	-2.751867000	-0.130992000
1	1.296851000	-3.289413000	0.000283000	1	-2.766801000	-2.230965000	-0.100072000
6	-4.343449000	-0.229548000	-0.000125000	6	4.065729000	0.090379000	0.152262000
8	-4.760807000	-0.119322000	1.133804000	8	4.660408000	0.923251000	-0.532910000
8	-4.760630000	-0.119523000	-1.134143000	8	4.406424000	-0.741970000	0.974026000
6	4.343251000	0.229718000	-0.000212000	6	-4.067783000	-0.090901000	0.152237000
8	4.761057000	0.119880000	1.133640000	8	-4.408180000	0.741768000	0.973232000
8	4.760273000	0.119291000	-1.134287000	8	-4.660334000	-0.925050000	-0.532424000
(nt5-(CO₂)₂)_{O&N}				(nt5-(CO₂)₂)_{N...}(CO₂)_O			
ΔE_{ad} = -53.6				ΔE_{ad} = -50.2			
6	-0.372827000	-0.121169000	0.013099000	6	-1.135210000	0.566992000	0.128109000
6	0.444662000	1.003844000	0.059727000	6	-2.107717000	-0.409636000	-0.041541000
6	-0.147340000	2.283469000	0.061702000	6	-1.701045000	-1.777201000	-0.130646000
6	-1.517433000	2.352836000	0.007005000	6	-0.385701000	-2.082327000	-0.070671000
7	-2.341639000	1.285018000	-0.041978000	7	0.604861000	-1.126966000	0.057145000
6	-1.802157000	0.079143000	-0.036533000	6	0.303089000	0.217061000	0.218341000
8	-2.547758000	-0.998200000	-0.085803000	8	1.154248000	1.073076000	0.452436000
6	0.226044000	-1.420774000	0.025892000	6	-1.531590000	1.919370000	0.234281000
6	1.577065000	-1.503741000	0.047546000	6	-2.884577000	2.178244000	0.154657000
7	2.409383000	-0.412397000	0.045250000	7	-3.865505000	1.278237000	-0.007303000
6	1.924341000	0.883050000	0.129259000	6	-3.538656000	-0.045495000	-0.111373000
8	2.641271000	1.862604000	0.277307000	8	-4.405605000	-0.933194000	-0.259875000
1	0.480658000	3.163213000	0.104815000	1	-2.455276000	-2.544087000	-0.241544000
1	-2.017408000	3.319072000	0.001093000	1	-0.000452000	-3.090984000	-0.111329000
1	-0.395038000	-2.304163000	0.018843000	1	-0.792837000	2.697166000	0.369089000
1	2.110221000	-2.444707000	0.074693000	1	-3.223133000	3.214721000	0.228815000
6	-4.110106000	-0.829736000	-0.035089000	6	3.615324000	1.480354000	-0.148949000
8	-4.502637000	-0.754899000	1.111018000	8	3.997570000	1.263373000	0.922836000
8	-4.584682000	-0.888992000	-1.151018000	8	3.380746000	1.832243000	-1.226905000
6	3.941642000	-0.726602000	-0.098541000	6	2.055319000	-1.657026000	-0.018454000
8	4.523232000	0.011265000	-0.874336000	8	2.172564000	-2.785545000	0.462773000
8	4.266077000	-1.712240000	0.564488000	8	2.845576000	-0.909669000	-0.585821000
(nt5-(CO₂)₂)_{N&N...}(CO₂)_O				(nt5-(CO₂)₂)_{N&N...}CO₂			
ΔE_{ad} = -77.0				ΔE_{ad} = -75.9			
6	1.132007000	-0.921518000	-0.046304000	6	-1.277514000	0.626916000	-0.165528000
6	0.353509000	0.211444000	-0.158027000	6	-0.808351000	-0.667843000	-0.095733000
6	0.979131000	1.488202000	-0.262078000	6	-1.732845000	-1.748697000	-0.003771000
6	2.333428000	1.544381000	-0.211462000	6	-3.056679000	-1.457471000	0.050569000
7	3.129395000	0.442953000	-0.059374000	7	-3.549434000	-0.182592000	0.027068000
6	2.611997000	-0.844657000	-0.042337000	6	-2.729414000	0.922755000	-0.155299000
8	3.309195000	-1.849951000	-0.054267000	8	-3.157647000	2.055939000	-0.326522000
6	0.504300000	-2.199565000	0.027014000	6	-0.352176000	1.706447000	-0.290799000
6	-0.848418000	-2.257346000	0.015293000	6	0.971794000	1.425743000	-0.299198000
7	-1.651798000	-1.146481000	-0.058058000	7	1.469999000	0.150765000	-0.187644000
6	-1.123950000	0.127888000	-0.209352000	6	0.642160000	-0.968415000	-0.157378000
8	-1.808773000	1.126462000	-0.404346000	8	1.061940000	-2.113980000	-0.208916000
1	0.374623000	2.375884000	-0.376128000	1	-1.370195000	-2.765818000	0.021112000
1	2.890845000	2.468012000	-0.294651000	1	-3.827710000	-2.214329000	0.109668000
1	1.111157000	-3.091122000	0.089850000	1	-0.719500000	2.718893000	-0.373926000
1	-1.405367000	-3.182844000	0.056094000	1	1.740803000	2.179139000	-0.399193000
6	4.665273000	0.734347000	0.137681000	6	-5.101422000	-0.048395000	0.264104000
8	5.052199000	1.631485000	-0.610395000	8	-5.724909000	-0.924561000	-0.334232000
8	5.176702000	0.072955000	1.022550000	8	-5.400962000	0.846623000	1.032898000
6	-3.189197000	-1.416881000	0.074278000	6	2.997870000	0.038358000	-0.075499000

8	-3.800076000	-0.535163000	0.659951000	8	3.400873000	-0.780656000	0.738979000
8	-3.504784000	-2.507639000	-0.393916000	8	3.591606000	0.851292000	-0.795307000
6	-4.197039000	1.950512000	0.165234000	6	5.901957000	0.081954000	0.285909000
8	-3.906300000	2.279583000	1.236064000	8	6.125358000	-0.700519000	-0.537023000
8	-4.598246000	1.764010000	-0.904739000	8	5.853786000	0.870461000	1.132887000
(nt5-(CO₂⁻)₂)_{O&O}...CO₂				(nt5-(CO₂⁻)₂)_{N&O}-(CO₂)_O			
ΔE_{ad} = -63.4				ΔE_{ad} = -70.2			
6	-1.580142000	0.498471000	0.110266000	6	-1.205598000	-0.290422000	0.018272000
6	-0.481072000	-0.344238000	0.326216000	6	-0.187412000	0.647483000	0.149555000
6	-0.689204000	-1.747166000	0.348598000	6	-0.519099000	2.014936000	0.236957000
6	-1.966872000	-2.198164000	0.158942000	6	-1.849121000	2.351501000	0.179087000
7	-3.054606000	-1.414308000	-0.047487000	7	-2.863188000	1.470949000	0.050189000
6	-2.886326000	-0.108402000	-0.073262000	6	-2.568840000	0.184678000	-0.026459000
8	-3.886605000	0.708509000	-0.269695000	8	-3.505779000	-0.720180000	-0.156190000
6	-1.370897000	1.896053000	0.079498000	6	-0.867792000	-1.678762000	-0.057655000
6	-0.096668000	2.356693000	0.278748000	6	0.437978000	-2.027063000	-0.026066000
7	0.981320000	1.568761000	0.514860000	7	1.470750000	-1.120314000	0.063122000
6	0.805571000	0.271547000	0.527489000	6	1.237426000	0.236377000	0.217838000
8	1.813911000	-0.552907000	0.812698000	8	2.121362000	1.059242000	0.425972000
1	0.144124000	-2.416175000	0.511717000	1	0.265456000	2.751593000	0.343624000
1	-2.172744000	-3.266024000	0.166134000	1	-2.152109000	3.394635000	0.237707000
1	-2.205704000	2.561399000	-0.094506000	1	-1.647569000	-2.421697000	-0.137483000
1	0.110274000	3.423702000	0.265787000	1	0.779087000	-3.052014000	-0.063021000
6	-5.354514000	0.099961000	-0.362238000	6	-5.015554000	-0.250770000	-0.098064000
8	-5.687292000	-0.018990000	-1.520702000	8	-5.398640000	-0.176942000	1.049804000
8	-5.829120000	-0.031589000	0.744250000	8	-5.469871000	-0.144146000	-1.217334000
6	3.192468000	-0.277223000	0.325866000	6	4.625070000	1.357194000	-0.158561000
8	3.256405000	0.212999000	-0.794066000	8	4.985399000	1.104759000	0.912364000
8	4.034754000	-0.667839000	1.127611000	8	4.402470000	1.727621000	-1.232309000
6	5.920857000	-0.061242000	-0.670859000	6	2.909486000	-1.724058000	-0.053537000
8	5.903899000	-1.113327000	-1.154428000	8	2.967982000	-2.863808000	0.400667000
8	6.103778000	1.000417000	-0.247709000	8	3.712444000	-0.993238000	-0.615750000
pn36⁻				(pn36...CO₂⁻)_O			
ΔE_{ad} = -14.6				ΔE_{ad} = -14.6			
6	-1.456699000	0.696072000	0.070163000	6	-2.419298000	-0.045155000	0.165324000
6	-0.545217000	-0.376296000	-0.012116000	6	-1.103038000	-0.487821000	-0.069045000
6	0.854032000	-0.118949000	0.018229000	6	-0.041872000	0.461719000	-0.140598000
6	1.270429000	1.227294000	-0.103665000	6	-0.395174000	1.827780000	-0.206891000
7	0.363808000	2.277979000	-0.095833000	7	-1.706365000	2.254622000	-0.057042000
6	-0.885759000	2.011417000	0.036764000	6	-2.616507000	1.376730000	0.168113000
8	-1.758970000	3.053134000	0.119591000	8	-3.886371000	1.810015000	0.391625000
6	1.885839000	-1.133971000	0.346600000	6	1.388981000	0.128871000	0.027117000
7	3.189939000	-0.835886000	0.001976000	7	2.310366000	1.075814000	-0.362466000
6	3.504386000	0.422527000	-0.250635000	6	1.905997000	2.321613000	-0.557727000
6	2.635258000	1.511490000	-0.238072000	6	0.603808000	2.787324000	-0.426760000
8	1.598154000	-2.167829000	0.946660000	8	1.753000000	-0.929934000	0.547420000
6	-2.848216000	0.471164000	0.163026000	6	-3.476901000	-0.959871000	0.364005000
6	-3.290985000	-0.821222000	0.122438000	6	-3.191246000	-2.293776000	0.274081000
7	-2.463651000	-1.867851000	-0.118999000	7	-1.977897000	-2.755319000	-0.112495000
6	-1.178182000	-1.652602000	-0.234669000	6	-1.008399000	-1.902194000	-0.327973000
8	-0.430765000	-2.664379000	-0.690531000	8	0.093134000	-2.369112000	-0.923430000
1	-1.208346000	3.843915000	0.072393000	1	-3.835535000	2.772326000	0.344079000
1	4.557510000	0.603612000	-0.473994000	1	2.690586000	3.030219000	-0.825441000
1	2.973750000	2.529925000	-0.369141000	1	0.346848000	3.833560000	-0.516064000
1	-3.528543000	1.305185000	0.268583000	1	-4.472833000	-0.601671000	0.585499000
1	-4.341822000	-1.066458000	0.231372000	1	-3.945961000	-3.050313000	0.459494000
1	-1.019890000	-3.424806000	-0.753359000	1	-0.019398000	-3.324222000	-0.991012000
				6	4.363286000	-0.625176000	0.399139000

				8	4.449675000	-0.156263000	1.454336000
				8	4.440029000	-1.132955000	-0.638107000
(pn36...CO₂⁻)_o				ΔE_{ad} = -13.2			
6	-1.483595000	-1.419939000	0.059327000	6	0.857898000	0.359169000	-0.471439000
6	-0.365606000	-0.588031000	-0.106086000	6	-0.441376000	0.791583000	-0.180780000
6	-0.570644000	0.833980000	-0.029994000	6	-1.469823000	-0.221710000	-0.054156000
6	-1.893415000	1.328625000	-0.048542000	6	-1.130819000	-1.522025000	-0.537248000
7	-2.987607000	0.494774000	0.012082000	7	0.097362000	-1.922535000	-0.916248000
6	-2.769739000	-0.772441000	0.120119000	6	1.141226000	-1.086970000	-0.757888000
8	-3.846460000	-1.581416000	0.252059000	8	2.322321000	-1.435888000	-0.894465000
6	0.430267000	1.836213000	0.156185000	6	-2.718070000	-0.099538000	0.591939000
7	0.217267000	3.130163000	0.058426000	7	-3.676870000	-1.004727000	0.576006000
6	-1.046574000	3.561478000	-0.127263000	6	-3.408778000	-2.165394000	-0.063475000
6	-2.125042000	2.718380000	-0.130658000	6	-2.189044000	-2.476453000	-0.592546000
8	1.660370000	1.472626000	0.555504000	8	-2.960741000	0.985656000	1.365171000
6	-1.341292000	-2.816355000	0.109933000	6	1.904449000	1.287934000	-0.578294000
6	-0.044573000	-3.298252000	-0.003572000	6	1.615795000	2.621689000	-0.428746000
7	1.028674000	-2.576533000	-0.294283000	7	0.358276000	3.077792000	-0.277143000
6	0.898604000	-1.231009000	-0.526753000	6	-0.621834000	2.203716000	-0.204840000
8	1.783478000	-0.588698000	-1.105719000	8	-1.869701000	2.717756000	-0.242741000
1	-4.611620000	-0.993775000	0.242275000	1	-4.226921000	-2.879247000	-0.096594000
1	-1.169478000	4.634987000	-0.228517000	1	-1.979291000	-3.447068000	-1.022276000
1	-3.142769000	3.080060000	-0.196143000	1	-3.850592000	0.845565000	1.708939000
1	-2.191669000	-3.465376000	0.258448000	1	2.902715000	0.933238000	-0.800694000
1	0.134261000	-4.365275000	0.134333000	1	2.390976000	3.380053000	-0.471978000
1	2.191009000	2.278464000	0.533164000	1	-1.745742000	3.672446000	-0.296539000
6	3.863109000	-0.183927000	0.260213000	6	3.965143000	-0.912296000	1.017853000
8	4.285661000	0.607951000	-0.474079000	8	4.847461000	-0.702119000	0.298561000
8	3.576068000	-0.950494000	1.075411000	8	3.164268000	-1.095020000	1.830793000
(pn36-CO₂⁻)_N				ΔE_{ad} = -13.3			
6	-2.396671000	0.304404000	0.039848000	6	-0.035239000	1.573481000	0.047368000
6	-1.201905000	-0.436450000	0.008758000	6	0.055942000	0.189943000	-0.069769000
6	0.048820000	0.248768000	0.051530000	6	1.355547000	-0.414818000	-0.014856000
6	0.031335000	1.643490000	-0.081536000	6	2.489747000	0.421807000	-0.058395000
7	-1.144128000	2.365200000	-0.120945000	7	2.386698000	1.790890000	-0.042523000
6	-2.259551000	1.730781000	-0.012174000	6	1.205249000	2.303658000	0.059128000
8	-3.407302000	2.450066000	0.022297000	8	1.106188000	3.647910000	0.139788000
6	1.326442000	-0.406087000	0.431958000	6	1.630892000	-1.801730000	0.191768000
7	2.473702000	0.309397000	0.063245000	7	2.828188000	-2.337284000	0.123631000
6	2.417366000	1.636529000	-0.151064000	6	3.884588000	-1.518029000	-0.067218000
6	1.254953000	2.354012000	-0.175709000	6	3.778458000	-0.154883000	-0.116229000
8	1.374073000	-1.421080000	1.089978000	8	0.623447000	-2.594182000	0.564443000
6	-3.653339000	-0.338928000	0.097121000	6	-1.296755000	2.222996000	0.117509000
6	-3.668365000	-1.705498000	0.081471000	6	-2.406885000	1.428210000	0.115023000
7	-2.551739000	-2.450838000	-0.095531000	7	-2.366722000	0.093700000	-0.069928000
6	-1.391916000	-1.851140000	-0.180440000	6	-1.182073000	-0.549315000	-0.446324000
8	-0.341507000	-2.579515000	-0.556323000	8	-1.165382000	-1.562885000	-1.105161000
1	-3.136141000	3.374412000	-0.036496000	1	2.011001000	3.981788000	0.108029000
1	3.392484000	2.090494000	-0.282876000	1	4.850318000	-2.007458000	-0.139840000
1	1.248596000	3.426218000	-0.304261000	1	4.643316000	0.490188000	-0.194103000
1	-4.562371000	0.243094000	0.156943000	1	-1.367782000	3.294602000	0.219790000
1	-4.595415000	-2.261967000	0.164869000	1	-3.411683000	1.812508000	0.244806000
1	-0.634328000	-3.496694000	-0.609448000	1	0.972974000	-3.491226000	0.614599000
6	3.931376000	-0.402945000	-0.094401000	6	-3.772791000	-0.722046000	0.116880000
8	4.818539000	0.417498000	0.080313000	8	-4.716086000	0.032800000	-0.052006000
8	3.832580000	-1.567405000	-0.399802000	8	-3.582588000	-1.872042000	0.430328000

(pn36-CO ₂) _N				ΔE _{ad} = -8.1	(pn36-CO ₂) _{N...CO₂}				ΔE _{ad} = -29.4
6	-0.658927000	-1.488453000	-0.235022000		6	2.756546000	0.144373000	-0.048105000	
6	-1.227640000	-0.230970000	-0.020583000		6	1.444296000	-0.350657000	-0.171770000	
6	-0.351782000	0.929803000	-0.032361000		6	0.349435000	0.571896000	-0.145511000	
6	1.041779000	0.695013000	0.067401000		6	0.626682000	1.900153000	0.201816000	
7	1.564645000	-0.561556000	0.025378000		7	1.909841000	2.360884000	0.410411000	
6	0.824408000	-1.667595000	-0.281829000		6	2.888817000	1.543025000	0.241499000	
8	1.320156000	-2.755324000	-0.514929000		8	4.150957000	2.015295000	0.373160000	
6	-0.733528000	2.267953000	-0.265040000		6	-1.003294000	0.242197000	-0.656506000	
7	0.064905000	3.310891000	-0.160543000		7	-2.005742000	1.153006000	-0.304886000	
6	1.358800000	3.066004000	0.118262000		6	-1.706416000	2.398326000	0.114102000	
6	1.900986000	1.811177000	0.203515000		6	-0.434002000	2.832200000	0.337592000	
8	-1.983972000	2.528920000	-0.703600000		8	-1.218180000	-0.699923000	-1.390628000	
6	-1.461350000	-2.632426000	-0.317867000		6	3.879591000	-0.699115000	-0.190450000	
6	-2.814727000	-2.488502000	-0.130071000		6	3.650457000	-2.025969000	-0.423377000	
7	-3.375155000	-1.319432000	0.224866000		7	2.411556000	-2.566513000	-0.401913000	
6	-2.608497000	-0.254511000	0.321010000		6	1.372944000	-1.789214000	-0.226895000	
8	-3.179068000	0.839468000	0.861181000		8	0.201718000	-2.387176000	-0.000890000	
1	1.988885000	3.942525000	0.230088000		1	4.057891000	2.954461000	0.575166000	
1	2.964825000	1.665234000	0.323602000		1	-2.575680000	3.033299000	0.232727000	
1	-2.017724000	3.487286000	-0.806323000		1	-0.221351000	3.849212000	0.631588000	
1	-0.993847000	-3.588320000	-0.511266000		1	4.878813000	-0.291958000	-0.126218000	
1	-3.492765000	-3.331160000	-0.214854000		1	4.464877000	-2.721992000	-0.591296000	
1	-4.091394000	0.588372000	1.047439000		1	0.330199000	-3.333355000	-0.140880000	
6	3.199943000	-0.781053000	0.213885000		6	-3.568457000	0.784036000	-0.401594000	
8	3.790806000	-0.423368000	-0.781943000		8	-4.237996000	1.787051000	-0.587303000	
8	3.432636000	-1.206185000	1.321240000						
(pn36-CO ₂) _{N...CO₂}				ΔE _{ad} = -26.3	pn36 ²⁻				
6	-2.285445000	0.864955000	-0.167835000		6	1.462457000	0.676935000	-0.046207000	
6	-1.131707000	0.101984000	-0.411465000		6	0.567383000	-0.406241000	0.030633000	
6	0.152939000	0.671577000	-0.162081000		6	-0.836715000	-0.147667000	-0.021638000	
6	0.212336000	2.046622000	0.098745000		6	-1.270472000	1.189879000	0.078789000	
7	-0.922565000	2.820524000	0.236479000		7	-0.381165000	2.245562000	0.090304000	
6	-2.072112000	2.244710000	0.164552000		6	0.878762000	1.975295000	-0.015595000	
8	-3.180750000	2.990209000	0.383299000		8	1.730663000	3.056043000	-0.072200000	
6	1.371908000	-0.141986000	0.054169000		6	-1.872050000	-1.174929000	-0.345073000	
7	2.569414000	0.567992000	-0.034283000		7	-3.186552000	-0.880958000	-0.027849000	
6	2.593537000	1.905299000	0.116781000		6	-3.514542000	0.386406000	0.206663000	
6	1.473368000	2.677146000	0.241189000		6	-2.656073000	1.470967000	0.196886000	
8	1.332484000	-1.313507000	0.379387000		8	-1.579920000	-2.214897000	-0.934798000	
6	-3.569591000	0.284732000	-0.254582000		6	2.864916000	0.460713000	-0.165148000	
6	-3.648630000	-1.032568000	-0.614672000		6	3.269834000	-0.857124000	-0.223060000	
7	-2.572889000	-1.751497000	-1.014477000		7	2.500437000	-1.927442000	-0.014766000	
6	-1.389687000	-1.192349000	-0.981912000		6	1.179508000	-1.742734000	0.336127000	
8	-0.376668000	-1.822614000	-1.575685000		8	0.549184000	-2.607154000	0.941012000	
1	-2.862150000	3.878906000	0.583930000		1	1.132006000	3.810193000	-0.025254000	
1	3.596644000	2.313151000	0.157484000		1	-4.576214000	0.564187000	0.406694000	
1	1.529576000	3.741598000	0.414399000		1	-2.996120000	2.490754000	0.329332000	
1	-4.449705000	0.868918000	-0.024697000		1	3.553523000	1.287972000	-0.270648000	
1	-4.598390000	-1.554993000	-0.642963000		1	4.320288000	-1.074160000	-0.440320000	
1	-0.658343000	-2.726015000	-1.764611000						
6	4.014535000	-0.170144000	-0.311038000						
8	4.916192000	0.514835000	0.140009000						
8	3.878895000	-1.190690000	-0.938705000						
6	-0.563608000	-2.751881000	1.494554000						
8	-0.843365000	-1.893775000	2.217564000						
8	-0.354589000	-3.663120000	0.814631000						

8	-3.778089000	-0.398845000	-0.222996000			
6	-2.268153000	-2.061031000	1.072379000			
8	-1.875716000	-1.203022000	1.742796000			
8	-2.627069000	-2.996210000	0.495181000			
(pn36⁻-CO₂⁻)_o				ΔE_{ad} = -18.7		
6	-2.259379000	-0.179748000	0.166005000	6	-2.401284000	0.307421000
6	-0.932207000	-0.511160000	-0.152349000	6	-1.225984000	-0.464691000
6	0.042556000	0.542371000	-0.211891000	6	0.035968000	0.204382000
6	-0.418881000	1.874301000	-0.186102000	6	0.048761000	1.599543000
7	-1.748000000	2.188333000	0.009023000	7	-1.102799000	2.345970000
6	-2.569288000	1.216597000	0.222547000	6	-2.230818000	1.720197000
8	-3.868165000	1.556448000	0.487866000	8	-3.360059000	2.494626000
6	1.491301000	0.374360000	-0.159342000	6	1.319764000	-0.486894000
7	2.321573000	1.393997000	-0.367705000	7	2.489567000	0.243831000
6	1.819787000	2.631628000	-0.487071000	6	2.446269000	1.592728000
6	0.491481000	2.944095000	-0.358629000	6	1.293204000	2.302907000
8	1.973250000	-0.777960000	0.179395000	8	1.365594000	-1.534904000
6	-3.227187000	-1.186027000	0.401587000	6	-3.670748000	-0.309650000
6	-2.766260000	-2.491304000	0.332716000	6	-3.662261000	-1.689109000
7	-1.573192000	-2.876477000	-0.101973000	7	-2.613663000	-2.485926000
6	-0.700153000	-1.921009000	-0.589365000	6	-1.410836000	-1.929004000
8	0.174337000	-2.200503000	-1.400023000	8	-0.556206000	-2.580773000
1	2.553733000	3.416941000	-0.663227000	1	3.424790000	2.047271000
1	0.122181000	3.961761000	-0.380951000	1	1.291783000	3.378765000
1	-4.239872000	-0.937845000	0.685855000	1	-4.574028000	0.277194000
1	-3.432787000	-3.299412000	0.646825000	1	-4.597948000	-2.200065000
6	3.509464000	-0.830607000	0.567965000	1	-3.024833000	3.396278000
8	3.656212000	-0.517459000	1.733123000	6	3.911668000	-0.407109000
8	4.185779000	-1.233501000	-0.351222000	8	3.928773000	-1.560462000
1	-3.864634000	2.520400000	0.466531000	8	4.790184000	0.397651000
(pn36⁻-CO₂⁻)_o... (CO₂)_o				(pn36⁻-CO₂)_o-CO₂⁻		
ΔE_{ad} = -36.8				ΔE_{ad} = -32.3		
6	-2.584314000	0.623325000	-0.181842000	6	-2.784533000	-0.653488000
6	-1.192480000	0.559244000	-0.010432000	6	-1.538947000	-0.586491000
6	-0.579761000	-0.731551000	0.153480000	6	-0.886434000	0.690824000
6	-1.424083000	-1.838475000	0.381782000	6	-1.636888000	1.845999000
7	-2.799809000	-1.740304000	0.325430000	7	-2.905377000	1.772898000
6	-3.307255000	-0.599218000	0.006208000	6	-3.387265000	0.600788000
8	-4.667712000	-0.542146000	-0.118228000	8	-4.610151000	0.544080000
6	0.830377000	-1.045083000	-0.023803000	6	0.495638000	0.934887000
7	1.328033000	-2.235589000	0.290866000	7	0.989896000	2.125086000
6	0.495256000	-3.221562000	0.652065000	6	0.199996000	3.200242000
6	-0.870274000	-3.106812000	0.668380000	6	-1.084034000	3.122917000
8	1.616300000	-0.165830000	-0.579573000	8	1.368399000	-0.097940000
6	-3.226747000	1.844224000	-0.494562000	6	-3.418911000	-1.891972000
6	-2.395814000	2.942858000	-0.636110000	6	-2.722226000	-3.012462000
7	-1.101600000	2.983963000	-0.342798000	7	-1.623113000	-3.010094000
6	-0.498008000	1.862924000	0.185194000	6	-1.101542000	-1.802505000
8	0.527287000	1.940856000	0.858234000	8	-0.373241000	-1.722348000
1	0.972220000	-4.166934000	0.905415000	1	0.657650000	4.159775000
1	-1.527560000	-3.940088000	0.882884000	1	-1.679675000	4.001535000
1	-4.292813000	1.891645000	-0.665122000	1	-4.360422000	-1.959086000
1	-2.821578000	3.880276000	-1.003293000	1	-3.104976000	-4.001202000
6	3.103007000	1.581179000	1.023327000	6	2.502297000	0.056599000
8	2.991367000	0.886501000	1.942434000	8	2.465062000	0.747824000
8	3.313240000	2.351044000	0.185491000	8	3.455810000	-0.661368000
6	2.932335000	-0.738562000	-1.251858000	1	-4.852753000	1.466855000

8	2.672741000	-1.327038000	-2.279746000	6	4.832730000	-0.682277000	0.616363000
8	3.915136000	-0.402445000	-0.624701000	8	4.737606000	-1.516875000	1.477948000
1	-4.956960000	-1.443871000	0.063365000	8	5.617895000	0.103942000	0.149997000
((pn36-CO₂)₂)_{N&N}				(pn36-CO₂)_{N...CO₂}			
ΔE_{ad} = -50.0				ΔE_{ad} = -43.9			
6	1.432738000	1.638938000	-0.014130000	6	1.180134000	1.617174000	0.032257000
6	0.682415000	0.459438000	0.034969000	6	1.026541000	0.228723000	-0.042060000
6	-0.739145000	0.543402000	-0.015628000	6	2.173087000	-0.604113000	0.032117000
6	-1.324771000	1.817708000	0.034664000	6	3.445322000	0.016832000	-0.007661000
7	-0.584017000	2.968562000	0.047740000	7	3.586300000	1.385874000	0.011401000
6	0.705355000	2.858763000	-0.014235000	6	2.512139000	2.105079000	0.072017000
8	1.424402000	4.018492000	-0.053838000	8	2.682906000	3.463950000	0.147860000
6	-1.622357000	-0.626899000	-0.316705000	6	2.133358000	-2.071411000	0.308817000
7	-2.988501000	-0.427310000	-0.021593000	7	3.266197000	-2.806291000	0.004498000
6	-3.501414000	0.821409000	0.087793000	6	4.410844000	-2.159162000	-0.159977000
6	-2.745880000	1.948802000	0.082300000	6	4.602915000	-0.786368000	-0.098005000
8	-1.224193000	-1.621969000	-0.869557000	8	1.158394000	-2.588930000	0.841630000
6	2.862843000	1.611278000	-0.059648000	6	0.041955000	2.491761000	0.069780000
6	3.470240000	0.399998000	-0.086567000	6	-1.190706000	1.941795000	0.048462000
7	2.799342000	-0.777690000	0.013254000	7	-1.405589000	0.594311000	-0.092316000
6	1.430195000	-0.811673000	0.337999000	6	-0.343356000	-0.283879000	-0.406758000
8	0.923857000	-1.737887000	0.918275000	8	-0.512006000	-1.298266000	-1.033264000
1	-4.581638000	0.835062000	0.155484000	1	5.280956000	-2.794443000	-0.349533000
1	-3.189299000	2.932460000	0.143590000	1	5.579803000	-0.327409000	-0.176946000
1	3.430416000	2.528120000	-0.110598000	1	0.174543000	3.560392000	0.154152000
1	4.542313000	0.274663000	-0.164313000	1	-2.104130000	2.515720000	0.113117000
1	0.758733000	4.715564000	-0.029007000	1	3.640363000	3.576614000	0.143877000
6	-4.027332000	-1.618467000	0.076174000	6	-2.863798000	0.136915000	-0.084323000
8	-3.548331000	-2.647116000	0.503517000	8	-3.662277000	1.050306000	-0.354543000
8	-5.157293000	-1.252327000	-0.254627000	8	-3.051041000	-1.028344000	0.232354000
6	3.678127000	-2.093548000	-0.102188000	6	-5.678686000	-0.591193000	0.147859000
8	4.851457000	-1.872947000	0.202857000	8	-5.742489000	-0.299538000	1.267254000
8	3.060802000	-3.051957000	-0.514097000	8	-5.798285000	-0.924311000	-0.954403000
(pn36-CO₂)_{N...CO₂}				(pn36-CO₂)_{N...CO₂}			
ΔE_{ad} = -44.6				ΔE_{ad} = -45.2			
6	-2.939714000	-0.104689000	0.142558000	6	1.338227000	1.951475000	-0.131789000
6	-1.625766000	-0.485647000	-0.189122000	6	0.721763000	0.686756000	-0.129590000
6	-0.594119000	0.500124000	-0.135725000	6	-0.703340000	0.618662000	-0.042763000
6	-0.961385000	1.834305000	0.052068000	6	-1.407216000	1.798339000	0.221385000
7	-2.257878000	2.217008000	0.284937000	7	-0.790206000	3.022120000	0.303768000
6	-3.154784000	1.286061000	0.366816000	6	0.485373000	3.070653000	0.091606000
8	-4.428419000	1.686830000	0.666478000	8	1.065026000	4.310117000	0.112884000
6	0.857851000	0.151825000	-0.059914000	6	-1.491730000	-0.592370000	-0.430582000
7	1.748846000	1.218338000	-0.326694000	7	-2.834803000	-0.594180000	0.012936000
6	1.320071000	2.513390000	-0.240627000	6	-3.459557000	0.566143000	0.343623000
6	0.034002000	2.861338000	-0.011281000	6	-2.823445000	1.760420000	0.421271000
8	1.235569000	-0.937807000	0.308426000	8	-1.063707000	-1.448207000	-1.167141000
6	-3.970659000	-1.071530000	0.250564000	6	2.734151000	2.087333000	-0.348335000
6	-3.587955000	-2.386304000	0.048626000	6	3.431415000	0.918122000	-0.567821000
7	-2.405727000	-2.802917000	-0.393604000	7	2.938966000	-0.315315000	-0.456500000
6	-1.455805000	-1.865235000	-0.745546000	6	1.634711000	-0.493046000	-0.055325000
8	-0.551707000	-2.121667000	-1.531361000	8	1.260280000	-1.568563000	0.411369000
1	2.119579000	3.231920000	-0.351055000	1	-4.521966000	0.448373000	0.510912000
1	-0.261619000	3.896884000	0.088162000	1	-3.353447000	2.672550000	0.658266000
1	-4.973976000	-0.793534000	0.540553000	1	3.202635000	3.060486000	-0.384161000
1	-4.314024000	-3.178343000	0.251500000	1	4.487844000	0.975320000	-0.838938000
1	-4.355970000	2.643518000	0.761440000	1	0.329561000	4.908897000	0.286284000
6	3.269179000	1.026801000	-0.618249000	6	-3.727399000	-1.883233000	0.008016000

8	3.602913000	-0.122014000	-0.862918000	8	-3.118290000	-2.911142000	0.231091000
8	3.888310000	2.093098000	-0.585130000	8	-4.920138000	-1.612022000	-0.171755000
6	3.561125000	-1.807774000	1.076795000	6	3.516708000	-2.852652000	0.402913000
8	3.634746000	-0.992518000	1.898686000	8	3.365857000	-3.351233000	-0.630712000
8	3.578223000	-2.723851000	0.372712000	8	3.805934000	-2.503152000	1.470585000
((pn36-CO₂)₂)_{N&N}-(CO₂)_O				((pn36-CO₂)₂)_{N&N}...CO₂			
ΔE_{ad} = -67.6				ΔE_{ad} = -66.4			
6	-1.134209000	2.117087000	0.030799000	6	2.731728000	1.256953000	0.026729000
6	-0.497511000	0.885104000	-0.152023000	6	1.635385000	0.388283000	0.030426000
6	0.925573000	0.819462000	-0.053730000	6	0.322752000	0.935584000	-0.056821000
6	1.626431000	2.029757000	0.085628000	6	0.185819000	2.329288000	0.003484000
7	0.996209000	3.237852000	0.217081000	7	1.260232000	3.173640000	0.059519000
6	-0.297998000	3.248662000	0.225098000	6	2.444502000	2.648160000	0.030647000
8	-0.907016000	4.456198000	0.404496000	8	3.503872000	3.507231000	0.033760000
6	1.702565000	-0.453216000	0.086896000	6	-0.883169000	0.122399000	-0.407827000
7	3.084392000	-0.333568000	-0.161118000	7	-2.120284000	0.757387000	-0.138204000
6	3.708991000	0.863463000	-0.078669000	6	-2.200020000	2.109326000	-0.017470000
6	3.052985000	2.040249000	0.082877000	6	-1.116172000	2.920081000	0.017514000
8	1.222694000	-1.488274000	0.484290000	8	-0.817482000	-0.936922000	-0.976040000
6	-2.559640000	2.235440000	0.014687000	6	4.073659000	0.761734000	0.022365000
6	-3.286369000	1.107790000	-0.167038000	6	4.249771000	-0.582179000	-0.010508000
7	-2.726736000	-0.108256000	-0.402101000	7	3.227493000	-1.474530000	0.045892000
6	-1.348542000	-0.260780000	-0.621400000	6	1.912567000	-1.061125000	0.326326000
8	-0.895893000	-1.203742000	-1.224963000	8	1.107326000	-1.776061000	0.866407000
1	4.787708000	0.788960000	-0.129948000	1	-3.216820000	2.475635000	0.025440000
1	3.578612000	2.980094000	0.172651000	1	-1.212630000	3.993939000	0.089806000
1	-3.033606000	3.192238000	0.172833000	1	4.912193000	1.441291000	0.007203000
1	-4.368087000	1.089026000	-0.163055000	1	5.223589000	-1.051844000	-0.059178000
1	-0.179653000	5.081825000	0.500685000	1	3.104700000	4.384721000	0.052779000
6	4.019428000	-1.590188000	-0.437612000	6	-3.457482000	-0.009958000	-0.107236000
8	3.464514000	-2.478515000	-1.046124000	8	-3.382465000	-1.165563000	0.271962000
8	5.162078000	-1.388928000	-0.024078000	8	-4.420947000	0.702894000	-0.424492000
6	-3.727856000	-1.321394000	-0.499959000	6	3.630369000	-3.008705000	-0.074675000
8	-4.843205000	-0.958482000	-0.871234000	8	4.798947000	-3.187199000	0.270019000
8	-3.245566000	-2.380949000	-0.146295000	8	2.746465000	-3.702995000	-0.526704000
6	-1.048592000	-2.686901000	1.332928000	6	-6.072688000	-1.285391000	0.232340000
8	-0.792677000	-3.706847000	0.858303000	8	-6.166326000	-0.937547000	1.333079000
8	-1.299127000	-1.714402000	1.912969000	8	-6.135047000	-1.702077000	-0.845273000
((pn36-CO₂)₂)_{N&N}-(CO₂)_N				pn36³⁻			
ΔE_{ad} = -59.7							
6	1.057893000	1.601806000	-0.147033000	6	1.435876000	0.734694000	-0.073939000
6	0.787963000	0.248461000	0.030804000	6	0.591545000	-0.375956000	0.021648000
6	-0.558450000	-0.208475000	-0.018104000	6	-0.836986000	-0.148569000	-0.009810000
6	-1.603094000	0.720449000	0.007758000	6	-1.256795000	1.194034000	0.129237000
7	-1.301117000	2.091007000	-0.001206000	7	-0.429820000	2.286808000	0.148255000
6	-0.032449000	2.510514000	-0.196281000	6	0.888830000	2.121916000	-0.040656000
8	0.208292000	3.779436000	-0.379790000	8	1.681985000	3.104178000	-0.144349000
6	-0.872206000	-1.638203000	-0.325710000	6	-1.848939000	-1.170311000	-0.371277000
7	-2.208577000	-2.009780000	-0.107277000	7	-3.185215000	-0.902818000	-0.093534000
6	-3.170096000	-1.074472000	-0.040176000	6	-3.518583000	0.354250000	0.209034000
6	-2.949880000	0.272114000	-0.017697000	6	-2.662488000	1.433440000	0.274354000
8	-0.064218000	-2.379899000	-0.826732000	8	-1.548372000	-2.220539000	-0.966443000
6	2.398828000	2.084967000	-0.264425000	6	2.841672000	0.544394000	-0.191132000
6	3.399269000	1.170978000	-0.206079000	6	3.305722000	-0.752648000	-0.200451000
7	3.201947000	-0.149150000	0.042914000	7	2.570961000	-1.847902000	0.041288000
6	1.943729000	-0.634049000	0.426946000	6	1.233175000	-1.689703000	0.347548000
8	1.790709000	-1.604960000	1.122272000	8	0.618010000	-2.591537000	0.938949000
1	-4.171186000	-1.487287000	-0.027929000	1	-4.589082000	0.523466000	0.395882000

1	-3.780229000	0.951870000	0.032797000	1	-3.011387000	2.446094000	0.451630000
1	2.594744000	3.133659000	-0.423640000	1	3.487088000	1.405277000	-0.314762000
1	4.443384000	1.429513000	-0.325408000	1	4.370737000	-0.937507000	-0.397399000
1	-0.739514000	4.219046000	-0.448402000				
6	-2.697445000	-3.547499000	-0.042278000				
8	-1.857922000	-4.286006000	0.414544000				
8	-3.857784000	-3.641395000	-0.429593000				
6	4.515033000	-1.078249000	0.019885000				
8	5.525117000	-0.399842000	0.188099000				
8	4.266658000	-2.239994000	-0.201593000				
6	-2.388020000	3.172868000	0.271566000				
8	-3.276658000	2.850354000	1.013137000				
8	-2.131623000	4.249983000	-0.318280000				
(pn36 ²⁻ -CO ₂ ⁻) _o ΔE _{ad} =-38.1				(pn36 ²⁻ -CO ₂ ⁻) _o ΔE _{ad} =-36.6			
6	2.261397000	-0.095246000	-0.207029000	6	-0.557990000	1.770972000	-0.151163000
6	0.968146000	-0.486558000	0.142826000	6	-0.071420000	0.451976000	-0.188280000
6	-0.049194000	0.547923000	0.222993000	6	-1.032689000	-0.621878000	-0.102356000
6	0.424658000	1.889867000	0.223092000	6	-2.342673000	-0.250915000	0.287430000
7	1.714481000	2.275660000	0.017281000	7	-2.803011000	1.032187000	0.424577000
6	2.636629000	1.350097000	-0.303414000	6	-2.000039000	2.057711000	0.116310000
8	3.811011000	1.660980000	-0.625160000	8	-2.398214000	3.254555000	0.091356000
6	-1.477687000	0.372209000	0.157752000	6	-0.806992000	-2.003078000	-0.586984000
7	-2.346885000	1.361670000	0.361691000	7	-1.689080000	-2.994532000	-0.173049000
6	-1.858027000	2.599637000	0.533250000	6	-2.842922000	-2.607872000	0.365618000
6	-0.530512000	2.925315000	0.443897000	6	-3.264940000	-1.306902000	0.559440000
8	-1.969341000	-0.810180000	-0.183261000	8	0.095514000	-2.274641000	-1.390799000
6	3.258274000	-1.078124000	-0.428545000	6	0.323345000	2.860146000	-0.321280000
6	2.881115000	-2.398950000	-0.283506000	6	1.659400000	2.597187000	-0.469429000
7	1.712947000	-2.828751000	0.195233000	7	2.188867000	1.363045000	-0.360573000
6	0.786428000	-1.889266000	0.613458000	6	1.383906000	0.331951000	-0.160873000
8	-0.111342000	-2.200756000	1.404782000	8	1.928166000	-0.829545000	0.154294000
1	-2.604051000	3.375902000	0.718348000	1	-3.520724000	-3.422943000	0.653352000
1	-0.176128000	3.948853000	0.505822000	1	-4.255759000	-1.062094000	0.926125000
1	4.248852000	-0.774393000	-0.740694000	1	-0.087394000	3.862301000	-0.325285000
1	3.592162000	-3.187965000	-0.560190000	1	2.376697000	3.400597000	-0.643885000
6	-3.403822000	-0.889383000	-0.589790000	6	3.384476000	-0.850639000	0.505758000
8	-3.588444000	-0.582097000	-1.767599000	8	3.593832000	-0.575384000	1.686258000
8	-4.143017000	-1.331394000	0.284660000	8	4.108324000	-1.219325000	-0.412628000
(pn36 ²⁻ -CO ₂ ⁻) _o ΔE _{ad} =-39.1				(pn36 ²⁻ -CO ₂ ⁻) _N ΔE _{ad} =-46.1			
6	-0.597881000	0.998950000	-0.174663000	6	2.394825000	0.383840000	-0.077878000
6	0.787628000	0.845961000	0.002906000	6	1.268495000	-0.435963000	0.031035000
6	1.334954000	-0.479204000	-0.048552000	6	-0.031631000	0.199626000	0.058745000
6	0.423831000	-1.553314000	-0.038711000	6	-0.035581000	1.599951000	0.183169000
7	-0.941823000	-1.395295000	-0.147426000	7	1.057012000	2.405799000	0.193112000
6	-1.411208000	-0.193495000	-0.258707000	6	2.277383000	1.867103000	-0.013879000
8	-2.724183000	0.001039000	-0.549400000	8	3.308570000	2.580227000	-0.114828000
6	2.772460000	-0.799790000	-0.295493000	6	-1.286203000	-0.499417000	-0.295763000
7	3.209359000	-2.078208000	0.001403000	7	-2.493614000	0.210497000	0.002056000
6	2.293569000	-3.037125000	0.166900000	6	-2.461710000	1.559462000	0.227735000
6	0.926496000	-2.881431000	0.085592000	6	-1.312830000	2.265350000	0.301520000
8	3.540537000	0.019061000	-0.815870000	8	-1.340228000	-1.551768000	-0.904083000
6	-1.161844000	2.301689000	-0.290808000	6	3.679628000	-0.200971000	-0.234962000
6	-0.285925000	3.361733000	-0.227643000	6	3.742938000	-1.577561000	-0.281435000
7	1.015848000	3.295274000	0.082441000	7	2.728901000	-2.416609000	-0.044907000
6	1.557365000	2.069266000	0.403126000	6	1.501758000	-1.886781000	0.305729000
8	2.603185000	1.988856000	1.057516000	8	0.657156000	-2.582919000	0.883222000

1	2.696723000	-4.038362000	0.361827000	1	-3.441514000	2.010106000	0.312241000
1	0.232285000	-3.709971000	0.159586000	1	-1.320171000	3.338004000	0.452739000
1	-2.220434000	2.424656000	-0.473576000	1	4.545233000	0.436808000	-0.359270000
1	-0.666247000	4.371193000	-0.422378000	1	4.702750000	-2.058216000	-0.510398000
6	-3.812316000	-0.662755000	0.165272000	6	-3.873223000	-0.425234000	-0.051111000
8	-3.585634000	-0.986452000	1.327388000	8	-4.761983000	0.355713000	-0.453894000
8	-4.832503000	-0.725356000	-0.534097000	8	-3.952950000	-1.578871000	0.356513000
(pn36²⁻-CO₂⁻)_N				(pn36²⁻-CO₂⁻)_N			
ΔE_{ad}=-44.3				ΔE_{ad}=-41.6			
6	0.039585000	1.544733000	-0.109357000	6	-0.763129000	-1.435854000	-0.128870000
6	-0.086034000	0.163254000	-0.023073000	6	-1.254031000	-0.139987000	0.019626000
6	-1.406171000	-0.406646000	-0.017593000	6	-0.327221000	0.970808000	-0.029531000
6	-2.476363000	0.513028000	0.119189000	6	1.043213000	0.685661000	0.043375000
7	-2.357955000	1.872589000	0.107969000	7	1.504574000	-0.628814000	0.032329000
6	-1.153071000	2.431709000	-0.092613000	6	0.689402000	-1.711013000	-0.144973000
8	-0.996274000	3.678303000	-0.218205000	8	1.149406000	-2.855505000	-0.259115000
6	-1.716737000	-1.824650000	-0.323067000	6	-0.721547000	2.363819000	-0.350140000
7	-2.982411000	-2.301134000	-0.007713000	7	0.191863000	3.374695000	-0.088790000
6	-3.928952000	-1.406040000	0.275951000	6	1.457532000	3.030641000	0.132518000
6	-3.786567000	-0.033858000	0.295264000	6	1.975278000	1.748830000	0.142127000
8	-0.902827000	-2.562714000	-0.896098000	8	-1.804768000	2.630754000	-0.890075000
6	1.336230000	2.150038000	-0.186947000	6	-1.654877000	-2.534883000	-0.247568000
6	2.440843000	1.372904000	-0.168161000	6	-3.002522000	-2.245884000	-0.214823000
7	2.377137000	0.007844000	-0.006185000	7	-3.538625000	-1.055058000	0.073444000
6	1.149599000	-0.628210000	0.304654000	6	-2.695914000	-0.010669000	0.400979000
8	1.133157000	-1.678884000	0.911276000	8	-3.113951000	0.956813000	1.048263000
1	-4.920213000	-1.828460000	0.489736000	1	2.148712000	3.865265000	0.299617000
1	-4.621325000	0.637662000	0.464503000	1	3.034346000	1.557589000	0.250278000
1	1.397343000	3.224899000	-0.289695000	1	-1.265226000	-3.532234000	-0.403463000
1	3.449310000	1.754862000	-0.245963000	1	-3.723204000	-3.047620000	-0.416874000
6	3.711766000	-0.730176000	0.014469000	6	3.020869000	-0.897940000	0.122491000
8	4.652439000	-0.036322000	0.449649000	8	3.603082000	-0.868757000	-0.963386000
8	3.700096000	-1.865456000	-0.447795000	8	3.428528000	-1.065796000	1.274350000
(pn36⁻-CO₂)₂⁻)_{O&O}				((pn36⁻-CO₂)₂⁻)_{O&O}			
ΔE_{ad}=-69.5				ΔE_{ad}=-66.9			
6	0.716142000	-1.005323000	-0.067708000	6	-2.208202000	-0.678749000	-0.441418000
6	-0.426015000	-0.183530000	-0.142715000	6	-0.958755000	-0.114168000	-0.152517000
6	-0.239290000	1.238065000	-0.067468000	6	0.107262000	-1.024750000	0.236850000
6	1.036582000	1.695624000	0.322488000	6	-0.306172000	-2.336617000	0.599402000
7	2.130876000	0.869622000	0.493314000	7	-1.557870000	-2.851676000	0.450031000
6	1.992981000	-0.390671000	0.243863000	6	-2.494164000	-2.126301000	-0.179595000
6	-1.217726000	2.256256000	-0.540251000	8	-3.613811000	-2.589789000	-0.496724000
7	-1.061231000	3.555070000	-0.083942000	6	1.527289000	-0.799834000	0.136840000
6	0.115049000	3.900691000	0.430829000	7	2.428596000	-1.642292000	0.643482000
6	1.215027000	3.077571000	0.586606000	6	1.986796000	-2.794080000	1.166205000
8	-2.094115000	1.977201000	-1.360278000	6	0.681378000	-3.206529000	1.145164000
6	0.610348000	-2.405866000	-0.247562000	8	1.967984000	0.236238000	-0.543345000
6	-0.638741000	-2.925593000	-0.443299000	6	-3.264041000	0.129860000	-0.907647000
7	-1.774789000	-2.203162000	-0.366924000	6	-3.041073000	1.478758000	-1.010267000
6	-1.702650000	-0.900082000	-0.155856000	7	-1.917196000	2.080379000	-0.594090000
8	-2.797938000	-0.245049000	0.139923000	6	-0.926347000	1.339678000	-0.109878000
1	0.201329000	4.950249000	0.734165000	8	0.065882000	1.945460000	0.495610000
1	2.176310000	3.435548000	0.932553000	1	2.758030000	-3.438350000	1.592914000
1	1.502128000	-3.017001000	-0.223450000	1	0.371775000	-4.186393000	1.489819000
1	-0.775806000	-3.989787000	-0.631989000	1	-4.207679000	-0.337782000	-1.156487000
6	-4.056694000	-1.056153000	0.420297000	1	-3.808145000	2.144723000	-1.407473000
8	-4.129801000	-1.391838000	1.596357000	6	-0.157619000	3.409048000	0.890981000
8	-4.790484000	-1.152278000	-0.550318000	8	-0.768522000	3.501582000	1.948868000

8	3.023459000	-1.244067000	0.404980000	8	0.368565000	4.195727000	0.123934000
6	4.387401000	-0.958464000	-0.104116000	6	3.424611000	0.204234000	-0.991933000
8	5.236104000	-1.540234000	0.573741000	8	3.568844000	-0.441623000	-2.024748000
8	4.437469000	-0.276844000	-1.119288000	8	4.159248000	0.881109000	-0.292077000
((pn36-CO₂)₂)_{N&N}				((pn36-CO₂)₂)_{N&N}			
ΔE_{ad}= -85.8				ΔE_{ad}= -81.4			
6	1.400922000	1.658057000	-0.080892000	6	-2.136151000	0.810733000	-0.140806000
6	0.690980000	0.468255000	0.002964000	6	-0.829395000	1.267293000	0.018172000
6	-0.749218000	0.533020000	0.027961000	6	0.251241000	0.302325000	0.013989000
6	-1.305045000	1.824099000	0.132462000	6	-0.075981000	-1.048486000	0.071895000
7	-0.622400000	2.991350000	0.127200000	7	-1.389271000	-1.475783000	0.055730000
6	0.715297000	2.974949000	-0.056568000	6	-2.452882000	-0.633166000	-0.135400000
6	-1.625725000	-0.618091000	-0.286458000	6	1.651345000	0.677430000	-0.303037000
7	-3.008280000	-0.432145000	0.010859000	7	2.623274000	-0.322621000	-0.030621000
6	-3.510345000	0.822522000	0.201257000	6	2.250687000	-1.624431000	0.116166000
6	-2.740243000	1.930973000	0.247246000	6	0.961279000	-2.034891000	0.143362000
8	-1.251298000	-1.623592000	-0.854815000	8	1.964326000	1.710937000	-0.857635000
6	2.830226000	1.646465000	-0.161278000	6	-3.204369000	1.728167000	-0.285224000
6	3.484278000	0.463994000	-0.158897000	6	-2.872299000	3.069111000	-0.277962000
7	2.837248000	-0.735626000	-0.015810000	7	-1.671886000	3.574544000	0.004211000
6	1.459714000	-0.786912000	0.299418000	6	-0.654442000	2.708961000	0.362727000
8	0.983907000	-1.741227000	0.874396000	8	0.324635000	3.109011000	0.996482000
1	-4.588806000	0.848343000	0.284586000	1	3.083005000	-2.311825000	0.178490000
1	-3.173320000	2.915093000	0.372119000	1	0.717389000	-3.084231000	0.224110000
1	3.351729000	2.588922000	-0.250082000	1	-4.211759000	1.366213000	-0.439165000
1	4.558620000	0.369993000	-0.239805000	1	-3.649717000	3.807902000	-0.503480000
8	1.388307000	4.027367000	-0.165395000	8	-3.602529000	-1.065951000	-0.248266000
6	3.725212000	-1.989945000	-0.044528000	6	4.135129000	-0.042907000	-0.027805000
8	3.210840000	-2.981075000	-0.542214000	8	4.802476000	-1.001780000	-0.454686000
8	4.870612000	-1.780220000	0.392946000	8	4.467123000	1.037265000	0.438885000
6	-4.030301000	-1.572026000	0.012019000	6	-1.701611000	-2.996017000	0.155978000
8	-5.154214000	-1.214512000	-0.390846000	8	-1.670647000	-3.576354000	-0.927030000
8	-3.631743000	-2.639185000	0.457077000	8	-1.886515000	-3.377598000	1.310061000
((pn36-CO₂)₂)_{N&N}				((pn36-CO₂)₂)_{O&N}			
ΔE_{ad}= -81.2				ΔE_{ad}= -79.3			
6	0.194133000	-1.267574000	0.158838000	6	1.653352000	1.038038000	0.080221000
6	0.490763000	0.078658000	0.030829000	6	0.274916000	1.274128000	-0.019757000
6	-0.577649000	1.042744000	0.035475000	6	-0.608061000	0.139947000	-0.018745000
6	-1.894813000	0.556368000	-0.049705000	6	-0.024540000	-1.127192000	-0.108680000
7	-2.160289000	-0.804228000	-0.013647000	7	1.326695000	-1.356511000	-0.1111003000
6	-1.198390000	-1.754605000	0.173616000	6	2.122052000	-0.335055000	0.029641000
6	-0.388332000	2.486234000	0.313336000	6	-2.059656000	0.233504000	0.307390000
7	-1.432449000	3.346517000	0.005804000	7	-2.823772000	-0.923988000	0.000919000
6	-2.628642000	2.816622000	-0.213008000	6	-2.212270000	-2.135414000	-0.170395000
6	-2.961750000	1.472352000	-0.186807000	6	-0.869762000	-2.285911000	-0.199911000
8	0.638143000	2.913520000	0.849835000	8	-2.557009000	1.166388000	0.901220000
6	1.235145000	-2.245960000	0.248016000	6	2.554481000	2.124905000	0.227467000
6	2.523308000	-1.840077000	0.204289000	6	1.995051000	3.384639000	0.286537000
7	2.877903000	-0.530424000	-0.000298000	7	0.714706000	3.690390000	0.065078000
6	1.904855000	0.438706000	-0.337620000	6	-0.153936000	2.680495000	-0.295988000
8	2.190953000	1.417098000	-0.990591000	8	-1.211206000	2.926577000	-0.879457000
1	-3.429449000	3.536590000	-0.414469000	1	-2.905046000	-2.961840000	-0.249795000
1	-3.981276000	1.131380000	-0.301074000	1	-0.408199000	-3.258065000	-0.309233000
1	0.968370000	-3.285210000	0.377210000	1	3.614433000	1.947751000	0.341744000
1	3.367925000	-2.508919000	0.292131000	1	2.643765000	4.236948000	0.516297000
8	-1.477657000	-2.952971000	0.295878000	8	3.438475000	-0.496860000	0.118725000
6	4.386131000	-0.231967000	-0.032470000	6	-4.358809000	-0.933510000	0.000572000
8	4.705811000	0.884923000	0.348145000	8	-4.835005000	-2.017655000	0.383522000

8	5.064077000	-1.210839000	-0.391907000	8	-4.890061000	0.083326000	-0.422852000
6	-3.631718000	-1.294761000	-0.106122000	6	4.056598000	-1.863226000	-0.035840000
8	-4.205085000	-1.337296000	0.980427000	8	4.257403000	-2.166065000	-1.204742000
8	-3.996238000	-1.526604000	-1.257889000	8	4.336797000	-2.371475000	1.043704000
((pn36-CO₂)₂)_{O&N} $\Delta E_{ad}=-78.1$				((pn36-CO₂)₂)_{O&N} $\Delta E_{ad}=-76.5$			
6	-0.318315000	-0.860457000	0.179139000	6	1.742409000	-1.667753000	0.265736000
6	0.469629000	0.282620000	0.037501000	6	0.978779000	-0.493013000	0.186728000
6	-0.167532000	1.560703000	0.054683000	6	-0.445521000	-0.638962000	-0.030117000
6	-1.579967000	1.570789000	0.023222000	6	-0.870921000	-1.913116000	-0.450775000
7	-2.351327000	0.438871000	0.132740000	7	-0.117586000	-3.038740000	-0.503675000
6	-1.751246000	-0.705465000	0.252305000	6	1.144685000	-3.002571000	-0.032588000
6	0.533327000	2.859633000	0.273647000	6	-1.435501000	0.383784000	0.365744000
7	-0.144541000	4.018683000	-0.057806000	7	-2.766756000	0.137694000	-0.068468000
6	-1.464710000	3.948822000	-0.227332000	6	-3.101733000	-1.018012000	-0.709532000
6	-2.247700000	2.816325000	-0.127376000	6	-2.240621000	-2.044721000	-0.883224000
8	1.652033000	2.906899000	0.790161000	8	-1.172754000	1.358260000	1.043252000
6	0.288606000	-2.158932000	0.255674000	6	3.117908000	-1.605338000	0.574480000
6	1.634340000	-2.255259000	0.200513000	6	3.683416000	-0.368817000	0.739501000
7	2.454319000	-1.171981000	-0.002115000	7	3.029553000	0.783604000	0.512516000
6	1.913407000	0.088035000	-0.340263000	6	1.749502000	0.746102000	0.170174000
8	2.539185000	0.890177000	-0.995382000	8	1.191692000	1.846142000	-0.279880000
1	-1.955662000	4.903581000	-0.447086000	1	-4.133352000	-1.052291000	-1.036989000
1	-3.326935000	2.835798000	-0.210919000	1	-2.552991000	-2.977643000	-1.334423000
1	-0.334069000	-3.031012000	0.390517000	1	3.673576000	-2.529560000	0.667396000
1	2.170196000	-3.190650000	0.280231000	1	4.730061000	-0.263564000	1.026906000
8	-2.450566000	-1.825735000	0.518230000	8	1.841114000	-4.033644000	0.105953000
6	3.966166000	-1.455192000	-0.026827000	6	-3.973909000	1.003160000	0.328823000
8	4.675089000	-0.529250000	0.340453000	8	-4.013525000	1.354251000	1.501115000
8	4.233112000	-2.620445000	-0.367353000	8	-4.779496000	1.147225000	-0.606308000
6	-3.749569000	-2.134044000	-0.130779000	6	2.115822000	3.001281000	-0.638692000
8	-4.474348000	-2.782583000	0.625788000	8	2.158389000	3.865291000	0.222887000
8	-3.852168000	-1.771837000	-1.295288000	8	2.584623000	2.881600000	-1.764901000
((pn36-CO₂)₂)_{O&N} $\Delta E_{ad}=-75.9$				((pn36-CO₂)₂)_{O&N} $\Delta E_{ad}=-74.2$			
6	-1.187004000	1.742202000	0.268794000	6	-1.289066000	1.620245000	-0.221551000
6	-0.467190000	0.599166000	-0.036874000	6	-0.003440000	1.217700000	0.131534000
6	0.969299000	0.725090000	-0.193077000	6	0.285566000	-0.206418000	0.192453000
6	1.466252000	2.056965000	-0.267406000	6	-0.804252000	-1.098299000	0.178366000
7	0.742781000	3.187905000	-0.062745000	7	-2.100451000	-0.645373000	-0.001026000
6	-0.542632000	3.087511000	0.317612000	6	-2.407640000	0.650108000	-0.311063000
6	1.951760000	-0.332898000	-0.145470000	6	1.594386000	-0.812437000	0.117834000
7	3.237709000	-0.136522000	-0.433879000	7	1.793987000	-2.118019000	0.286392000
6	3.645696000	1.119145000	-0.672326000	6	0.723412000	-2.908614000	0.422996000
6	2.849153000	2.226762000	-0.573435000	6	-0.578920000	-2.483737000	0.339977000
8	1.589114000	-1.526966000	0.266807000	8	2.623792000	-0.060618000	-0.202037000
6	-2.599475000	1.675701000	0.482172000	6	-1.576193000	2.984150000	-0.452258000
6	-3.230264000	0.486195000	0.359002000	6	-0.518865000	3.867543000	-0.322254000
7	-2.582527000	-0.655530000	-0.022413000	7	0.685508000	3.571906000	0.156747000
6	-1.232222000	-0.623118000	-0.444369000	6	0.921224000	2.283517000	0.608105000
8	-0.787413000	-1.471506000	-1.186413000	8	1.815774000	2.052251000	1.422789000
1	4.702715000	1.224682000	-0.924443000	1	0.937906000	-3.966724000	0.573689000
1	3.230717000	3.234406000	-0.691872000	1	-1.408708000	-3.176737000	0.372699000
1	-3.125812000	2.579403000	0.753885000	1	-2.568828000	3.285148000	-0.757641000
1	-4.291428000	0.350451000	0.518656000	1	-0.663489000	4.913449000	-0.615706000
8	-1.229542000	4.082454000	0.648780000	8	-3.559529000	0.990732000	-0.586208000
6	-3.455644000	-1.921299000	-0.133017000	6	-3.270634000	-1.666205000	0.034652000
8	-2.895945000	-2.965500000	0.161968000	8	-3.483772000	-2.211463000	-1.046233000

8	-4.630129000	-1.665409000	-0.451875000	8	-3.766292000	-1.796822000	1.152934000
6	2.694724000	-2.525600000	0.582730000	6	3.943060000	-0.744115000	-0.506189000
8	2.931631000	-3.289342000	-0.339641000	8	4.055078000	-1.014969000	-1.697390000
8	3.087702000	-2.420585000	1.739253000	8	4.682197000	-0.826031000	0.463215000
((pn36⁻-CO₂)₂)_{N&N}				(pn36²⁻-CO₂)_{N...}(CO₂)_O			
ΔE_{ad}=-73.1				ΔE_{ad}=-64.1			
6	-0.199819000	1.568065000	-0.319835000	6	1.082460000	1.753648000	-0.049117000
6	0.508626000	0.361131000	-0.266101000	6	0.704631000	0.430151000	0.126856000
6	-0.234233000	-0.876784000	-0.207674000	6	1.725642000	-0.578988000	0.142669000
6	-1.611349000	-0.800562000	0.064708000	6	3.020603000	-0.153753000	-0.248632000
7	-2.271831000	0.423175000	0.123413000	7	3.385299000	1.135292000	-0.507933000
6	-1.671816000	1.612349000	-0.154368000	6	2.491813000	2.124251000	-0.337475000
6	0.303969000	-2.190472000	-0.627786000	6	1.557702000	-1.936173000	0.714734000
7	-0.385611000	-3.328037000	-0.228769000	7	2.523842000	-2.890619000	0.430100000
6	-1.634139000	-3.178638000	0.187059000	6	3.675105000	-2.469486000	-0.093895000
6	-2.339834000	-1.988912000	0.284656000	6	4.019632000	-1.166688000	-0.391323000
8	1.293940000	-2.282905000	-1.358525000	8	0.618911000	-2.208775000	1.476274000
6	0.470554000	2.797697000	-0.485782000	6	0.101051000	2.793384000	0.037278000
6	1.838546000	2.773306000	-0.547228000	6	-1.189237000	2.486306000	0.280018000
7	2.571039000	1.662479000	-0.351387000	7	-1.643716000	1.180566000	0.348360000
6	1.958270000	0.506551000	-0.142769000	6	-0.761389000	0.108455000	0.048240000
8	2.668683000	-0.515254000	0.269433000	8	-1.169869000	-0.960226000	-0.361146000
1	-2.153302000	-4.104860000	0.456729000	1	4.418509000	-3.257019000	-0.276123000
1	-3.387443000	-1.962679000	0.550166000	1	5.005956000	-0.890477000	-0.747699000
1	-0.109694000	3.708527000	-0.555259000	1	0.430609000	3.819764000	-0.052010000
1	2.408705000	3.686166000	-0.718741000	1	-1.970554000	3.218332000	0.415710000
8	-2.305226000	2.671608000	-0.212038000	8	2.795239000	3.343314000	-0.457332000
6	-3.802665000	0.451456000	0.393532000	6	-3.129418000	1.006976000	0.616368000
8	-4.482682000	0.327346000	-0.622835000	8	-3.515461000	-0.142017000	0.831786000
8	-4.085004000	0.560105000	1.585658000	8	-3.765920000	2.075170000	0.617588000
6	4.112102000	-0.256054000	0.673292000	6	-3.465599000	-1.864335000	-1.003221000
8	4.205574000	0.082356000	1.847569000	8	-3.597360000	-1.108299000	-1.875041000
8	4.911875000	-0.506415000	-0.215003000	8	-3.458098000	-2.757888000	-0.268201000
((pn36⁻-CO₂)₂)_{O&N}				((pn36⁻-CO₂)₂)_{O&N}			
ΔE_{ad}=-62.5				ΔE_{ad}=-59.4			
6	-2.770545000	0.219525000	0.175084000	6	-0.388412000	1.195416000	0.176502000
6	-1.564276000	-0.359492000	-0.217043000	6	1.009728000	1.055578000	0.111775000
6	-0.380409000	0.480568000	-0.205788000	6	1.568791000	-0.241743000	-0.101249000
6	-0.608267000	1.878492000	-0.076536000	6	0.729994000	-1.358937000	0.038675000
7	-1.792163000	2.466014000	0.190309000	7	-0.635818000	-1.183495000	0.219869000
6	-2.873741000	1.688233000	0.437158000	6	-1.201249000	0.012966000	0.216944000
6	0.968206000	0.001887000	-0.143387000	6	2.954502000	-0.493982000	-0.600926000
7	2.007951000	0.878897000	-0.334290000	7	3.482015000	-1.757635000	-0.414777000
6	1.765824000	2.219469000	-0.362344000	6	2.645574000	-2.753762000	-0.130722000
6	0.525372000	2.739114000	-0.213086000	6	1.276216000	-2.665232000	0.029004000
8	1.209783000	-1.237881000	0.152900000	8	3.581398000	0.369506000	-1.217830000
6	-3.936174000	-0.575875000	0.263207000	6	-0.974926000	2.488059000	0.261602000
6	-3.804325000	-1.915391000	-0.057146000	6	-0.107608000	3.555217000	0.251282000
7	-2.725069000	-2.490636000	-0.581280000	7	1.229035000	3.494464000	0.326117000
6	-1.623008000	-1.700253000	-0.860744000	6	1.827729000	2.265875000	0.461906000
8	-0.767561000	-2.069477000	-1.670368000	8	2.966483000	2.151160000	0.923965000
1	2.659904000	2.814378000	-0.474263000	1	3.109482000	-3.741215000	-0.039435000
1	0.365462000	3.809691000	-0.176388000	1	0.656149000	-3.536962000	0.183633000
1	-4.863362000	-0.136565000	0.606141000	1	-2.047951000	2.618140000	0.275231000
1	-4.657466000	-2.584910000	0.106818000	1	-0.523574000	4.565993000	0.201740000
8	-3.958849000	2.175455000	0.815590000	8	-2.509497000	0.062115000	0.413623000
6	2.236741000	-1.622016000	1.280854000	6	-1.544294000	-2.479113000	0.489342000
8	2.593400000	-0.665025000	1.943401000	8	-1.963337000	-2.977224000	-0.540367000

8	2.398701000	-2.821529000	1.281844000	8	-1.597863000	-2.743400000	1.680530000
6	3.517925000	0.465274000	-0.612250000	6	-3.440444000	0.683359000	-0.640575000
8	4.282900000	1.419981000	-0.454025000	8	-2.938030000	0.777289000	-1.743080000
8	3.659187000	-0.676490000	-0.998512000	8	-4.520946000	0.940367000	-0.131963000
(pn36-(CO₂)₃)³⁻_{N&N&N}				(pn36-(CO₂)₃)³⁻_{O&O&N}			
ΔE_{ad}=-115.1				ΔE_{ad}=-96.5			
6	1.094504000	1.598230000	-0.134621000	6	0.953090000	-1.721805000	-0.620016000
6	0.835076000	0.245129000	-0.016171000	6	-0.064575000	-0.841563000	-0.245366000
6	-0.536268000	-0.209964000	-0.010885000	6	0.304374000	0.528520000	0.089702000
6	-1.539781000	0.757565000	0.050018000	6	1.667673000	0.792461000	0.328777000
7	-1.253122000	2.101703000	0.030773000	7	2.643038000	-0.165023000	0.112587000
6	0.010193000	2.598934000	-0.141648000	6	2.389346000	-1.367132000	-0.473336000
6	-0.915180000	-1.613654000	-0.304471000	6	-0.563481000	1.681809000	0.035122000
7	-2.264485000	-1.944065000	-0.018589000	7	-0.179066000	2.881006000	0.478580000
6	-3.197881000	-0.968323000	0.117606000	6	1.088231000	3.035720000	0.865419000
6	-2.910550000	0.355669000	0.129044000	6	2.061385000	2.070606000	0.778731000
8	-0.175845000	-2.408362000	-0.842587000	8	-1.729805000	1.570900000	-0.536149000
6	2.433937000	2.088587000	-0.215949000	6	0.659767000	-3.021949000	-1.070407000
6	3.453685000	1.200046000	-0.185026000	6	-0.659130000	-3.401547000	-1.078829000
7	3.260948000	-0.139591000	-0.005194000	7	-1.650684000	-2.655790000	-0.579261000
6	1.987716000	-0.654128000	0.325855000	6	-1.380917000	-1.445917000	-0.091037000
8	1.860874000	-1.685619000	0.943371000	8	-2.289679000	-0.836481000	0.610376000
1	-4.209908000	-1.343628000	0.188516000	1	1.346367000	4.027260000	1.236898000
1	-3.696357000	1.092698000	0.202605000	1	3.095535000	2.277622000	1.016016000
1	2.600505000	3.149994000	-0.326572000	1	1.467832000	-3.670538000	-1.379988000
1	4.495027000	1.479447000	-0.269145000	1	-0.955747000	-4.375821000	-1.466762000
8	0.223956000	3.806949000	-0.248396000	6	-3.525549000	-1.693520000	1.050743000
6	4.537362000	-1.021712000	-0.020211000	8	-3.284226000	-2.290089000	2.086462000
8	4.370264000	-2.152451000	-0.444053000	8	-4.476657000	-1.540075000	0.314685000
8	5.543859000	-0.399775000	0.351879000	6	-2.492309000	2.891854000	-0.856425000
6	-2.785280000	-3.403629000	0.033048000	8	-2.189062000	3.304936000	-1.964369000
8	-3.953932000	-3.500235000	-0.371230000	8	-3.272807000	3.202703000	0.019351000
8	-2.003502000	-4.209087000	0.509243000	8	3.287638000	-2.142767000	-0.795773000
6	-2.420462000	3.146661000	0.122997000	6	4.142566000	0.187367000	0.400312000
8	-2.919703000	3.403586000	-0.966518000	8	4.491300000	-0.115922000	1.536867000
8	-2.655358000	3.492332000	1.275559000	8	4.697068000	0.740634000	-0.542681000
(pn36-(CO₂)₃)³⁻_{O&O&O}				((pn36-(CO₂)₂)₂)⁻_{O&O}-CO₂⁻			
ΔE_{ad}=-92.9				ΔE_{ad}=-90.9			
6	-1.380245000	1.070530000	-0.385615000	6	2.519258000	-0.468075000	1.046866000
6	-0.081697000	0.604619000	-0.129744000	6	1.432385000	0.009533000	0.307413000
6	0.071520000	-0.793648000	0.225003000	6	0.688421000	-0.963848000	-0.473034000
6	-1.109815000	-1.493787000	0.556028000	6	1.355393000	-2.202797000	-0.719504000
7	-2.382123000	-0.984945000	0.416795000	7	2.489718000	-2.623506000	-0.109088000
6	-2.516580000	0.193063000	-0.106075000	6	3.019013000	-1.875541000	0.878240000
6	1.279020000	-1.593011000	0.128320000	6	-0.646488000	-0.873212000	-0.925627000
7	1.345666000	-2.831355000	0.615741000	7	-1.208033000	-1.694254000	-1.789586000
6	0.228256000	-3.399747000	1.085892000	6	-0.481046000	-2.751848000	-2.183500000
6	-1.012075000	-2.819553000	1.042524000	6	0.748041000	-3.070280000	-1.666114000
8	2.301376000	-1.124416000	-0.528835000	8	-1.475715000	0.102331000	-0.418474000
6	-1.600987000	2.388088000	-0.840945000	6	3.236631000	0.411133000	1.872930000
6	-0.502841000	3.197227000	-0.972362000	6	2.861932000	1.734612000	1.879452000
7	0.733680000	2.851626000	-0.589055000	7	1.935374000	2.251436000	1.062966000
6	0.952755000	1.633784000	-0.101444000	6	1.284005000	1.441160000	0.238256000
8	2.081287000	1.386701000	0.491779000	8	0.521741000	1.976374000	-0.698782000
1	0.350134000	-4.407079000	1.484488000	1	-0.953143000	-3.396734000	-2.923411000
1	-1.916865000	-3.333283000	1.340592000	1	1.263679000	-3.987402000	-1.926317000
1	-2.604837000	2.719637000	-1.064710000	1	4.058926000	0.026081000	2.461737000
1	-0.603193000	4.206995000	-1.369134000	1	3.351724000	2.447307000	2.542788000

6	3.001524000	2.621143000	0.796366000	6	1.071123000	3.186484000	-1.450680000
8	2.706812000	3.115702000	1.870742000	8	2.258360000	3.083765000	-1.730101000
8	3.844381000	2.786199000	-0.058828000	8	0.193329000	3.999702000	-1.685598000
6	3.432502000	-2.135290000	-0.889930000	6	-2.593486000	-0.350695000	0.247313000
8	3.197121000	-2.681212000	-1.955753000	8	-2.674119000	-1.452617000	0.728086000
8	4.338014000	-2.125906000	-0.081957000	8	-3.480388000	0.600520000	0.282735000
8	-3.702898000	0.706813000	-0.367614000	8	3.951393000	-2.272188000	1.602568000
6	-4.972507000	-0.113753000	-0.088308000	6	-4.786966000	0.298904000	1.058389000
8	-5.434020000	0.129311000	1.013990000	8	-4.676185000	0.530948000	2.247227000
8	-5.311919000	-0.767136000	-1.060257000	8	-5.679654000	-0.041106000	0.301433000
(pn36-(CO₂)₃)³⁻_{N&N&N...}(CO₂)₀ ΔE_{ad}=-134.2				(pn36-(CO₂)₃)³⁻_{N&N&N...}(CO₂)₀ ΔE_{ad}=-133.5			
6	-0.584295000	2.206973000	0.105505000	6	-2.548457000	0.847315000	0.155569000
6	-0.640719000	0.823723000	0.125622000	6	-1.575314000	-0.124129000	0.017796000
6	0.598993000	0.076420000	0.163121000	6	-0.186415000	0.275015000	-0.002726000
6	1.791140000	0.785761000	0.005998000	6	0.098360000	1.636695000	-0.059427000
7	1.813837000	2.153743000	-0.108063000	7	-0.886348000	2.584736000	-0.016022000
6	0.697240000	2.934746000	0.010475000	6	-2.211188000	2.284764000	0.176647000
6	0.663353000	-1.343411000	0.572242000	6	0.910749000	-0.672020000	0.276538000
7	1.907830000	-1.984400000	0.367601000	7	2.223370000	-0.175810000	-0.027132000
6	3.030980000	-1.259370000	0.127611000	6	2.452588000	1.171511000	-0.178389000
6	3.037200000	0.084524000	-0.031715000	6	1.461513000	2.081403000	-0.170807000
8	-0.251721000	-1.922809000	1.123594000	8	0.774587000	-1.744984000	0.809381000
6	-1.769650000	3.000321000	0.140535000	6	-3.928869000	0.498484000	0.238804000
6	-2.966535000	2.373143000	0.208715000	6	-4.267638000	-0.812119000	0.188812000
7	-3.087022000	1.016007000	0.173847000	7	-3.356071000	-1.805198000	-0.007424000
6	-1.981581000	0.186530000	-0.100992000	6	-2.015818000	-1.512681000	-0.331413000
8	-2.132159000	-0.911652000	-0.589751000	8	-1.321074000	-2.290397000	-0.944298000
1	3.934277000	-1.853116000	0.103369000	1	3.491620000	1.441192000	-0.292726000
1	3.962787000	0.618887000	-0.186201000	1	1.684938000	3.133389000	-0.268126000
1	-1.683122000	4.076758000	0.137576000	1	-4.665489000	1.278467000	0.361538000
1	-3.913935000	2.891878000	0.265094000	1	-5.284936000	-1.170354000	0.271422000
8	0.760279000	4.163671000	-0.004497000	8	-3.059396000	3.162707000	0.309684000
6	-4.536219000	0.458116000	0.299747000	6	-3.914750000	-3.263744000	0.005237000
8	-4.618971000	-0.600927000	0.895374000	8	-3.132898000	-4.095732000	0.427082000
8	-5.376812000	1.232009000	-0.179107000	8	-5.094240000	-3.310835000	-0.366079000
6	2.097244000	-3.513919000	0.498086000	6	3.366737000	-1.075628000	-0.056213000
8	3.232563000	-3.818287000	0.887173000	8	4.436255000	-0.472889000	0.392707000
8	1.134656000	-4.185534000	0.156471000	8	3.276802000	-2.194991000	-0.474085000
6	3.186274000	2.899761000	-0.286116000	6	-0.504686000	4.116559000	-0.099639000
8	3.735407000	3.145190000	0.781212000	8	-0.207419000	4.585054000	0.990440000
8	3.483129000	3.066984000	-1.463112000	8	-0.532974000	4.539338000	-1.247229000
6	-0.992270000	-3.325227000	-1.195193000	6	5.850153000	-1.127047000	0.063874000
8	-0.287213000	-2.734713000	-1.899189000	8	6.365911000	-1.537069000	1.079324000
8	-1.745337000	-3.978984000	-0.610091000	8	6.117622000	-0.997087000	-1.110183000
(pn36-(CO₂)₃)³⁻_{N&N&N}-CO₂ ΔE_{ad}=-133.2				(pn36-(CO₂)₃)³⁻_{N&N&N...}(CO₂)₀ ΔE_{ad}=-132.5			
6	0.126751000	1.735624000	-0.126781000	6	0.222993000	-2.093053000	-0.210046000
6	0.010181000	0.364733000	-0.020440000	6	-0.123715000	-0.756417000	-0.204709000
6	-1.296980000	-0.237502000	-0.014587000	6	0.919446000	0.239603000	-0.134668000
6	-2.400402000	0.618237000	0.049859000	6	2.220825000	-0.203418000	0.107848000
7	-2.259489000	1.982157000	0.042253000	7	2.525830000	-1.539561000	0.208291000
6	-1.057419000	2.614988000	-0.123915000	6	1.616707000	-2.536652000	-0.018359000
6	-1.513147000	-1.673696000	-0.308297000	6	0.709199000	1.647156000	-0.551162000
7	-2.816490000	-2.149433000	-0.034078000	7	1.756428000	2.537560000	-0.207683000
6	-3.850374000	-1.284039000	0.102498000	6	2.987142000	2.063987000	0.110105000
6	-3.715680000	0.065483000	0.121992000	6	3.278913000	0.748048000	0.249586000
8	-0.678927000	-2.378429000	-0.834006000	8	-0.229788000	2.010722000	-1.225624000

6	1.407500000	2.370598000	-0.227366000	6	-0.770438000	-3.105919000	-0.376656000
6	2.522910000	1.619937000	-0.220898000	6	-2.058978000	-2.736376000	-0.538474000
7	2.470089000	0.248962000	-0.037970000	7	-2.478258000	-1.432961000	-0.450210000
6	1.250243000	-0.408129000	0.310614000	6	-1.578545000	-0.417356000	-0.050248000
8	1.258923000	-1.439181000	0.928976000	8	-1.946318000	0.607424000	0.479598000
1	-4.814427000	-1.770829000	0.167564000	1	3.735243000	2.838355000	0.214611000
1	-4.580099000	0.708636000	0.192145000	1	4.285745000	0.423060000	0.465688000
1	1.447054000	3.443071000	-0.348795000	1	-0.465500000	-4.141705000	-0.407719000
1	3.518294000	2.017819000	-0.344331000	1	-2.864752000	-3.430868000	-0.725096000
8	-0.970140000	3.837747000	-0.221184000	8	1.938408000	-3.724912000	-0.016247000
6	3.724110000	-0.492373000	-0.038062000	6	-3.989695000	-1.195022000	-0.682577000
8	3.778726000	-1.632223000	-0.403324000	8	-4.318923000	-0.023293000	-0.808629000
8	4.706034000	0.266175000	0.370233000	8	-4.635439000	-2.247923000	-0.742676000
6	-3.172918000	-3.667275000	0.024789000	6	1.616078000	4.083044000	-0.287493000
8	-4.323189000	-3.888044000	-0.374948000	8	2.676884000	4.632050000	-0.619635000
8	-2.300364000	-4.370722000	0.500266000	8	0.523759000	4.512248000	0.039711000
6	-3.539992000	2.901307000	0.149021000	6	4.004887000	-1.980504000	0.504000000
8	-4.070974000	3.095082000	-0.936128000	8	4.687890000	-2.066766000	-0.509538000
8	-3.788908000	3.217710000	1.304361000	8	4.224108000	-2.120864000	1.701508000
6	6.196872000	-0.200704000	0.048175000	6	-4.282245000	1.430258000	1.303451000
8	6.428016000	-0.098795000	-1.135852000	8	-4.373507000	0.537544000	2.039806000
8	6.775864000	-0.476023000	1.074404000	8	-4.291345000	2.412722000	0.696241000
(pn36-(CO₂)₃)³⁻_{N&N&N}... (CO₂)₀ ΔE_{ad}=-132.5				(pn36-(CO₂)₃)³⁻_{N&N&N}-CO₂ ΔE_{ad}=-131.6			
6	-0.589010000	1.387875000	-0.341387000	6	-2.632930000	-0.262674000	-0.112789000
6	0.625542000	0.765824000	-0.114905000	6	-1.399843000	0.356264000	-0.026201000
6	0.683518000	-0.676175000	-0.085276000	6	-0.205491000	-0.458022000	-0.037441000
6	-0.520179000	-1.379311000	-0.128701000	6	-0.362688000	-1.838201000	0.038952000
7	-1.728842000	-0.730781000	-0.260600000	7	-1.595719000	-2.431235000	0.043345000
6	-1.839491000	0.619742000	-0.440638000	6	-2.765476000	-1.733152000	-0.114208000
6	1.953544000	-1.429301000	-0.243510000	6	1.126026000	0.093225000	-0.376362000
7	1.877014000	-2.807417000	0.078386000	7	2.228755000	-0.781964000	-0.086008000
6	0.676718000	-3.438403000	0.108742000	6	2.019617000	-2.130602000	0.080459000
6	-0.514859000	-2.805330000	-0.019976000	6	0.795521000	-2.686348000	0.117203000
8	2.962825000	-0.946750000	-0.706398000	8	1.301790000	1.140350000	-0.944734000
6	-0.681552000	2.808687000	-0.457748000	6	-3.837436000	0.499777000	-0.159541000
6	0.451442000	3.541426000	-0.357445000	6	-3.748100000	1.850756000	-0.123870000
7	1.666777000	2.988854000	-0.072891000	7	-2.565585000	2.510685000	0.022134000
6	1.777811000	1.632928000	0.304831000	6	-1.370863000	1.817580000	0.304085000
8	2.676267000	1.240084000	1.010959000	8	-0.442802000	2.346264000	0.871544000
1	0.754790000	-4.512116000	0.214515000	1	2.927491000	-2.709450000	0.160142000
1	-1.437788000	-3.363793000	-0.046024000	1	0.682632000	-3.754909000	0.225178000
1	-1.642991000	3.261379000	-0.649627000	1	-4.784616000	-0.012075000	-0.242739000
1	0.480582000	4.617190000	-0.464015000	1	-4.605245000	2.508292000	-0.178637000
8	-2.933370000	1.156272000	-0.646345000	8	-3.850788000	-2.301844000	-0.202206000
6	2.872064000	3.968802000	-0.026273000	6	-2.644401000	4.070989000	0.001478000
8	3.939760000	3.474983000	-0.344335000	8	-1.662782000	4.615807000	-0.467887000
8	2.528495000	5.121165000	0.274445000	8	-3.734162000	4.484436000	0.417756000
6	3.131054000	-3.701047000	0.284071000	6	3.633871000	-0.370929000	-0.138210000
8	2.941858000	-4.866884000	-0.092421000	8	4.467027000	-1.230624000	-0.371066000
8	4.069250000	-3.144128000	0.826905000	8	3.834929000	0.854583000	0.136749000
6	-3.063850000	-1.542540000	-0.295447000	6	-1.706445000	-4.002816000	0.137131000
8	-3.217630000	-2.178641000	-1.329228000	8	-1.618701000	-4.545742000	-0.955992000
8	-3.721494000	-1.417701000	0.736128000	8	-1.813254000	-4.394456000	1.291714000
6	-5.152279000	0.779467000	0.697055000	6	5.461547000	1.272898000	0.186354000
8	-4.704581000	1.161335000	1.693994000	8	5.842260000	1.172395000	1.322663000
8	-5.756640000	0.481125000	-0.244887000	8	5.817748000	1.610490000	-0.908850000

(pn36-(CO ₂) ₃) ³⁻ _{N&N&N} -CO ₂ $\Delta E_{ad}=-131.2$				(pn36-(CO ₂) ₃) ³⁻ _{N&N&N} -CO ₂ $\Delta E_{ad}=-130.6$			
6	-0.255108000	-1.974890000	0.093389000	6	-0.788170000	-1.783113000	-0.269764000
6	-0.036262000	-0.617774000	-0.023512000	6	-1.237768000	-0.493340000	-0.060778000
6	-1.159325000	0.282812000	-0.002027000	6	-0.298221000	0.605420000	-0.093758000
6	-2.438675000	-0.280392000	-0.026474000	6	1.058908000	0.311339000	-0.153464000
7	-2.632775000	-1.638025000	-0.008505000	7	1.489354000	-1.004039000	-0.270312000
6	-1.615042000	-2.542102000	0.129650000	6	0.644589000	-2.086624000	-0.410754000
6	-1.013307000	1.731017000	0.277720000	6	-0.722783000	2.010745000	-0.308717000
7	-2.172582000	2.505887000	0.038796000	7	0.282538000	2.979640000	-0.077769000
6	-3.388251000	1.915191000	-0.057257000	6	1.589283000	2.631769000	-0.057078000
6	-3.583439000	0.573155000	-0.066823000	6	2.034746000	1.349655000	-0.121982000
8	-0.016168000	2.216870000	0.765555000	8	-1.807632000	2.319456000	-0.748054000
6	0.837336000	-2.899563000	0.162710000	6	-1.692101000	-2.886566000	-0.319853000
6	2.098911000	-2.437035000	0.124970000	6	-3.015707000	-2.640844000	-0.173322000
7	2.383005000	-1.095917000	-0.060455000	7	-3.512010000	-1.401004000	0.096607000
6	1.347591000	-0.170669000	-0.400671000	6	-2.653921000	-0.324873000	0.408966000
8	1.575378000	0.815701000	-1.047525000	8	-3.011148000	0.597513000	1.101839000
1	-4.208182000	2.619889000	-0.098320000	1	2.264979000	3.475318000	-0.009641000
1	-4.579123000	0.157281000	-0.105201000	1	3.094489000	1.132929000	-0.114592000
1	0.622011000	-3.950859000	0.285571000	1	-1.308655000	-3.879917000	-0.499190000
1	2.974635000	-3.061579000	0.214630000	1	-3.776476000	-3.407585000	-0.229130000
8	-1.823365000	-3.750234000	0.234010000	8	1.084573000	-3.216225000	-0.586829000
6	3.811126000	-0.762335000	-0.118268000	6	-5.066150000	-1.289514000	0.199179000
8	4.076696000	0.454925000	0.125019000	8	-5.514110000	-0.205562000	-0.125526000
8	4.595118000	-1.674597000	-0.324983000	8	-5.585693000	-2.359113000	0.543343000
6	-2.156594000	4.064904000	-0.025460000	6	-0.030726000	4.507398000	0.048424000
8	-3.205243000	4.556318000	0.411787000	8	0.868747000	5.203213000	-0.436624000
8	-1.159492000	4.536973000	-0.539749000	8	-1.061847000	4.758205000	0.644416000
6	-4.098478000	-2.219967000	-0.070162000	6	2.939030000	-1.276574000	-0.411180000
8	-4.627101000	-2.282862000	1.031795000	8	3.409798000	-1.412135000	-1.510030000
8	-4.453681000	-2.465315000	-1.215356000	8	3.519395000	-1.300240000	0.734007000
6	5.750848000	0.777729000	0.184504000	6	5.173722000	-1.291881000	0.711451000
8	6.125591000	1.073463000	-0.913782000	8	5.579360000	-2.364829000	1.075378000
8	6.104657000	0.667653000	1.325820000	8	5.555823000	-0.195395000	0.394162000
(pn36-(CO ₂) ₃) ³⁻ _{O&O&N...} (CO ₂) _o $\Delta E_{ad}=-120.9$				(pn36-(CO ₂) ₃) ³⁻ _{O&O&N...} (CO ₂) _o $\Delta E_{ad}=-120.2$			
6	1.994282000	1.139956000	0.290288000	6	1.623982000	-0.999294000	-0.167153000
6	0.635273000	0.798583000	0.205251000	6	0.430542000	-0.343304000	0.092186000
6	0.300511000	-0.590731000	0.017572000	6	0.461913000	1.087828000	0.264954000
6	1.351321000	-1.458444000	-0.288887000	6	1.737708000	1.682165000	0.391759000
7	2.674607000	-1.102079000	-0.323588000	7	2.920396000	1.010406000	0.211903000
6	2.991846000	0.113209000	0.019183000	6	2.870252000	-0.244646000	-0.123864000
6	-1.019528000	-1.161243000	0.389478000	6	-0.667694000	1.996272000	0.205429000
7	-1.256833000	-2.486677000	-0.046867000	7	-0.566147000	3.271106000	0.564488000
6	-0.221978000	-3.269745000	-0.469955000	6	0.652292000	3.765066000	0.835866000
6	1.052422000	-2.830498000	-0.575592000	6	1.819769000	3.059420000	0.716985000
8	-1.802074000	-0.579840000	1.112781000	8	-1.801758000	1.560234000	-0.272640000
6	2.385249000	2.462186000	0.600781000	6	1.638868000	-2.407541000	-0.414846000
6	1.389845000	3.383878000	0.787490000	6	0.473023000	-3.090024000	-0.353225000
7	0.086096000	3.139609000	0.569298000	7	-0.714593000	-2.516351000	0.008045000
6	-0.292161000	1.925743000	0.195671000	6	-0.767698000	-1.174298000	0.434712000
8	-1.500552000	1.741218000	-0.253377000	8	-1.664270000	-0.755158000	1.133407000
1	-0.514621000	-4.289630000	-0.675940000	1	0.673054000	4.813593000	1.132168000
1	1.858591000	-3.488498000	-0.868722000	1	2.796094000	3.504707000	0.858932000
1	3.434341000	2.705619000	0.692586000	1	2.568458000	-2.898834000	-0.659192000
1	1.627990000	4.402106000	1.091917000	1	0.393595000	-4.150295000	-0.546380000
6	-2.322706000	2.982946000	-0.698358000	6	-4.115533000	-0.384671000	0.013291000

8	-1.860975000	3.501658000	-1.697842000	8	-4.567760000	-0.412401000	1.079337000
8	-3.301650000	3.131610000	0.009316000	8	-3.780872000	-0.359170000	-1.092196000
6	-4.141518000	0.264107000	0.092067000	6	-2.845104000	2.593684000	-0.762256000
8	-4.571015000	0.315195000	1.166755000	8	-2.475353000	3.183934000	-1.761143000
8	-3.832451000	0.243061000	-1.021044000	8	-3.857155000	2.547032000	-0.085306000
8	4.247154000	0.505962000	0.092597000	8	3.960253000	-0.932300000	-0.403940000
6	5.388259000	-0.517398000	-0.073719000	6	5.344556000	-0.286211000	-0.214408000
8	5.880097000	-0.457466000	-1.187538000	8	5.725023000	-0.353088000	0.941217000
8	5.625113000	-1.105792000	0.966242000	8	5.815831000	0.077281000	-1.278898000
6	-2.638786000	-3.186569000	0.073176000	6	-1.942040000	-3.476645000	0.090990000
8	-3.601043000	-2.438499000	0.104811000	8	-1.599731000	-4.665766000	0.130913000
8	-2.538526000	-4.422290000	0.079997000	8	-3.028932000	-2.927111000	0.066861000
(pn36-(CO₂)₃)³⁻_{O&O&N...}-(CO₂)_O ΔE_{ad}=-113.1				(pn36-(CO₂)₃)²⁻_{O&O&O}-CO₂⁻ ΔE_{ad}=-111.4			
6	0.658169000	-1.455211000	-0.282818000	6	2.050961000	0.725066000	0.673754000
6	-0.538286000	-0.766297000	-0.074363000	6	0.770313000	0.718667000	0.109631000
6	-0.465821000	0.659108000	0.219196000	6	0.361841000	-0.473876000	-0.607003000
6	0.783544000	1.182090000	0.601986000	6	1.389188000	-1.386942000	-0.953646000
7	1.937692000	0.412394000	0.550027000	7	2.676245000	-1.319475000	-0.480296000
6	1.973726000	-0.834900000	0.008616000	6	2.971597000	-0.377683000	0.366155000
6	-1.514829000	1.626206000	-0.012265000	6	-0.959892000	-0.890882000	-0.932917000
7	-1.410715000	2.894511000	0.392116000	7	-1.239212000	-1.875581000	-1.756760000
6	-0.251825000	3.299260000	0.913050000	6	-0.223911000	-2.618736000	-2.222187000
6	0.882023000	2.529355000	1.007762000	6	1.075787000	-2.458051000	-1.816830000
8	-2.558190000	1.273569000	-0.705786000	8	-2.030715000	-0.292094000	-0.335742000
6	0.661018000	-2.801858000	-0.690049000	6	2.489785000	1.825409000	1.434200000
6	-0.558022000	-3.417532000	-0.826588000	6	1.632974000	2.894268000	1.539548000
7	-1.720300000	-2.851866000	-0.483266000	7	0.471451000	2.997739000	0.884104000
6	-1.734088000	-1.597566000	-0.034076000	6	0.061445000	1.986535000	0.119326000
8	-2.812470000	-1.143624000	0.528659000	8	-0.935552000	2.162935000	-0.689802000
1	-0.225267000	4.336208000	1.246994000	1	-0.498647000	-3.409240000	-2.916723000
1	1.816043000	2.929072000	1.375566000	1	1.870500000	-3.129151000	-2.116841000
1	1.603158000	-3.300608000	-0.870581000	1	3.468890000	1.811300000	1.890861000
1	-0.625837000	-4.441737000	-1.192178000	1	1.898734000	3.753281000	2.154115000
6	-3.917878000	-2.205073000	0.884409000	6	-1.282179000	3.682777000	-1.071409000
8	-3.685451000	-2.711800000	1.967878000	8	-0.452821000	4.110160000	-1.848147000
8	-4.791760000	-2.251563000	0.046672000	8	-2.315378000	4.036091000	-0.557345000
6	-3.506209000	2.418460000	-1.197507000	6	-2.914572000	-1.147113000	0.317533000
8	-3.144203000	2.832624000	-2.285923000	8	-2.558789000	-2.196484000	0.789214000
8	-4.430774000	2.610385000	-0.436853000	8	-4.086358000	-0.604441000	0.344592000
8	3.029929000	-1.451168000	-0.151242000	8	4.141128000	-0.312640000	0.948505000
6	5.350056000	-0.611236000	-0.996779000	6	5.253710000	-1.351672000	0.567659000
8	5.893441000	-0.886578000	-0.011589000	8	5.885495000	-0.979482000	-0.400241000
8	4.968091000	-0.395333000	-2.068276000	8	5.295726000	-2.255701000	1.377479000
6	3.294047000	1.037284000	0.994121000	6	-5.202888000	-1.394931000	1.134675000
8	3.404925000	1.130894000	2.210269000	8	-5.152007000	-1.162030000	2.322476000
8	4.012889000	1.357499000	0.048678000	8	-5.908706000	-2.011563000	0.362548000
(pn36-(CO₂)₃)²⁻_{O&O&O}-CO₂⁻ ΔE_{ad}=-110.8				(pn36-(CO₂)₃)²⁻_{O&O&O}-CO₂⁻ ΔE_{ad}=-110.2			
6	-2.192407000	0.647848000	-0.588422000	6	-0.628730000	1.021112000	-0.110606000
6	-0.876416000	0.764404000	-0.122787000	6	0.701339000	0.576863000	0.003823000
6	-0.284523000	-0.402924000	0.505014000	6	0.919141000	-0.815965000	0.316502000
6	-1.168272000	-1.452324000	0.854813000	6	-0.198720000	-1.561650000	0.747314000
7	-2.491601000	-1.505230000	0.492364000	7	-1.485525000	-1.062114000	0.767954000
6	-2.960722000	-0.558850000	-0.264451000	6	-1.674805000	0.113998000	0.296571000
6	1.104145000	-0.685003000	0.713984000	6	2.144637000	-1.577156000	0.101009000
7	1.551068000	-1.698991000	1.421912000	7	2.284053000	-2.817127000	0.570708000
6	0.664801000	-2.593253000	1.887872000	6	1.228746000	-3.430689000	1.120281000

6	-0.672612000	-2.545649000	1.602743000	6	-0.029224000	-2.892419000	1.192469000
8	2.025029000	0.077804000	0.099224000	8	3.079601000	-1.072733000	-0.635251000
6	-2.805249000	1.708339000	-1.284679000	6	-0.924609000	2.333450000	-0.543300000
6	-2.075842000	2.861164000	-1.436433000	6	0.142103000	3.155273000	-0.797539000
7	-0.880320000	3.074773000	-0.875170000	7	1.418326000	2.836632000	-0.541623000
6	-0.308110000	2.104335000	-0.163660000	6	1.715163000	1.629534000	-0.064682000
8	0.723112000	2.378929000	0.569012000	8	2.886568000	1.412713000	0.431003000
1	1.084885000	-3.403226000	2.479102000	1	1.416409000	-4.438515000	1.489060000
1	-1.365680000	-3.320496000	1.903587000	1	-0.888755000	-3.439052000	1.556751000
1	-3.810406000	1.594992000	-1.664250000	1	-1.949844000	2.653108000	-0.661156000
1	-2.477163000	3.695904000	-2.009675000	1	-0.017466000	4.156994000	-1.193268000
6	1.057256000	3.933989000	0.775762000	6	3.814599000	2.705031000	0.662536000
8	0.398159000	4.373433000	1.695459000	8	3.570032000	3.187539000	1.748877000
8	1.924277000	4.299695000	0.019548000	8	4.578195000	2.867506000	-0.257455000
6	3.332630000	-0.452365000	0.007840000	6	4.263604000	-2.058423000	-1.066677000
8	3.390786000	-1.351920000	-0.916318000	8	3.981762000	-2.598647000	-2.116908000
8	4.210846000	0.006055000	0.680966000	8	5.190238000	-2.001709000	-0.293740000
8	-4.180192000	-0.594512000	-0.741157000	8	-2.935655000	0.653247000	0.308922000
6	-5.126625000	-1.778501000	-0.354225000	6	-4.032735000	-0.074588000	-0.136192000
8	-5.727727000	-1.541326000	0.674610000	8	-5.094299000	0.451431000	0.389159000
8	-5.121181000	-2.637691000	-1.213510000	8	-3.937522000	-0.989189000	-0.906647000
6	4.826147000	-2.000814000	-1.189837000	6	-6.500844000	-0.006928000	-0.193242000
8	5.010311000	-2.954904000	-0.469409000	8	-7.081969000	-0.694385000	0.617522000
8	5.375221000	-1.425989000	-2.103890000	8	-6.701489000	0.491861000	-1.278016000
(pn36-(CO₂)₃)²⁻_{O&O&O}-CO₂⁻ ΔE_{ad}=-110.1				(pn36-(CO₂)₃)²⁻_{O&O&O}-CO₂⁻ ΔE_{ad}=-109.9			
6	-0.644382000	-0.879532000	0.473341000	6	1.387092000	-1.206135000	-0.615025000
6	0.683735000	-0.524972000	0.175584000	6	0.399111000	-0.239529000	-0.359768000
6	0.951952000	0.854148000	-0.160870000	6	0.817545000	1.005492000	0.251399000
6	-0.161110000	1.680468000	-0.422651000	6	2.119997000	1.031529000	0.796833000
7	-1.466811000	1.293890000	-0.193755000	7	3.045438000	0.021544000	0.655660000
6	-1.666729000	0.120343000	0.278383000	6	2.737294000	-0.998570000	-0.083432000
6	2.242331000	1.532506000	-0.116885000	6	0.109974000	2.269384000	0.205995000
7	2.400998000	2.756214000	-0.620474000	7	0.518376000	3.327106000	0.907980000
6	1.324229000	3.440362000	-1.027212000	6	1.682855000	3.250700000	1.562444000
6	0.034272000	2.995069000	-0.904687000	6	2.535358000	2.177381000	1.513660000
8	3.229270000	0.974123000	0.505635000	8	-0.899037000	2.398861000	-0.601149000
6	-0.971390000	-2.182800000	0.910505000	6	1.078064000	-2.391020000	-1.309640000
6	0.056905000	-3.085503000	0.986368000	6	-0.222974000	-2.588280000	-1.689258000
7	1.307830000	-2.843748000	0.572058000	7	-1.220092000	-1.763546000	-1.329880000
6	1.625527000	-1.642034000	0.093363000	6	-0.943704000	-0.681543000	-0.641550000
8	2.742342000	-1.481668000	-0.530590000	8	-1.978265000	-0.007970000	-0.118753000
1	1.527983000	4.428212000	-1.438768000	1	1.955638000	4.139663000	2.130733000
1	-0.829067000	3.598992000	-1.150189000	1	3.515075000	2.179619000	1.972784000
1	-1.989794000	-2.434163000	1.169003000	1	1.861438000	-3.106549000	-1.515898000
1	-0.121294000	-4.090216000	1.366500000	1	-0.520804000	-3.460812000	-2.264169000
6	3.599577000	-2.814113000	-0.828195000	6	-3.221022000	-0.688190000	-0.075135000
8	3.276953000	-3.266246000	-1.906034000	8	-3.220742000	-1.565472000	0.869330000
8	4.399224000	-3.023706000	0.050403000	8	-4.106723000	-0.351273000	-0.807266000
6	4.483121000	1.903461000	0.831804000	6	-1.405305000	3.878886000	-0.882348000
8	4.303890000	2.477924000	1.887679000	8	-0.765428000	4.369738000	-1.792184000
8	5.352126000	1.786964000	0.000283000	8	-2.348280000	4.167580000	-0.182679000
8	-2.921674000	-0.242639000	0.693898000	8	3.599658000	-1.948646000	-0.358274000
6	-4.050151000	0.046005000	-0.065598000	6	5.075524000	-1.815621000	0.139761000
8	-4.010087000	0.210979000	-1.253092000	8	5.239839000	-2.417597000	1.182566000
8	-5.072471000	0.042193000	0.730331000	8	5.758015000	-1.216205000	-0.667456000
6	-6.516127000	0.071141000	0.059470000	6	-4.586305000	-2.391985000	1.077428000

8	-6.804480000	-1.016935000	-0.385749000	8	-5.244727000	-1.882715000	1.955439000
8	-7.024157000	1.159684000	0.213779000	8	-4.609113000	-3.361630000	0.356931000
(pn36-(CO₂)₃)²⁻_{N&N&N}-CO₂⁻...CO₂ ΔE_{ad}=-150.1				(pn36-(CO₂)₃)²⁻_{N&N&N}-CO₂⁻...CO₂ ΔE_{ad}=-149.9			
6	2.267444000	1.343173000	-0.183733000	6	-0.373732000	-1.475257000	-0.173226000
6	1.825323000	0.043677000	-0.026600000	6	-0.602457000	-0.121018000	-0.044089000
6	0.403584000	-0.218781000	-0.018776000	6	0.510083000	0.792731000	-0.045973000
6	-0.462083000	0.868810000	0.008693000	6	1.795346000	0.248473000	-0.009990000
7	0.003817000	2.157590000	-0.051412000	7	1.998698000	-1.111229000	-0.039035000
6	1.327342000	2.479414000	-0.234988000	6	0.992095000	-2.028461000	-0.200124000
6	-0.151409000	-1.561653000	-0.281235000	6	0.349923000	2.240306000	-0.319139000
7	-1.549056000	-1.698421000	0.009525000	7	1.494289000	3.026553000	-0.054083000
6	-2.358789000	-0.594944000	0.129467000	6	2.715310000	2.451981000	0.054956000
6	-1.880968000	0.663626000	0.104390000	6	2.929778000	1.111487000	0.053443000
8	0.457375000	-2.468116000	-0.791954000	8	-0.644555000	2.715899000	-0.822220000
6	3.659101000	1.644206000	-0.257660000	6	-1.454982000	-2.410620000	-0.267645000
6	4.544075000	0.621072000	-0.180420000	6	-2.722560000	-1.962785000	-0.234585000
7	4.166995000	-0.669019000	0.036093000	7	-3.012211000	-0.625831000	-0.029064000
6	2.833663000	-0.996849000	0.354030000	6	-1.991123000	0.310736000	0.317399000
8	2.550175000	-1.989158000	0.984378000	8	-2.245603000	1.296979000	0.955671000
1	-3.410130000	-0.816810000	0.233819000	1	3.525256000	3.166708000	0.116674000
1	-2.555226000	1.504804000	0.178016000	1	3.931460000	0.710178000	0.105482000
1	3.973885000	2.667833000	-0.395557000	1	-1.227362000	-3.457222000	-0.406095000
1	5.615433000	0.750584000	-0.254933000	1	-3.588371000	-2.595992000	-0.351828000
8	1.691298000	3.641166000	-0.381599000	8	1.219539000	-3.229643000	-0.314189000
6	5.317611000	-1.729267000	0.053194000	6	-4.413757000	-0.222113000	-0.002919000
8	4.987202000	-2.830198000	-0.345378000	8	-4.753677000	0.875809000	-0.341684000
8	6.391885000	-1.237609000	0.419183000	8	-5.168290000	-1.210010000	0.393197000
6	-2.168761000	-3.017556000	0.058299000	6	1.452619000	4.588202000	0.027380000
8	-3.386759000	-2.968903000	-0.406659000	8	2.499323000	5.098462000	-0.388362000
8	-1.588167000	-3.965380000	0.506045000	8	0.439169000	5.035275000	0.531242000
6	-1.000000000	3.328634000	-0.005815000	6	3.438424000	-1.661080000	0.025590000
8	-1.473359000	3.620181000	-1.101797000	8	3.997972000	-1.722327000	-1.067215000
8	-1.211610000	3.752141000	1.128552000	8	3.821374000	-1.907957000	1.167384000
6	-4.356781000	-4.201160000	-0.076432000	6	-6.741288000	-1.119133000	0.096751000
8	-4.596409000	-4.819628000	-1.087402000	8	-7.349738000	-1.013894000	1.136144000
8	-4.680611000	-4.181529000	1.089036000	8	-6.955185000	-1.253017000	-1.086244000
6	-3.303948000	5.095525000	0.155796000	6	6.287559000	-2.209036000	0.195937000
8	-4.001970000	4.182062000	0.292055000	8	6.522036000	-1.080667000	0.308483000
8	-2.757636000	6.109342000	0.031784000	8	6.238406000	-3.361985000	0.096352000
(pn36-(CO₂)₃)²⁻_{N&N&N}-(CO₂)₂²⁻ ΔE_{ad}=-148.7				(pn36-(CO₂)₃)²⁻_{O&O&O}-(CO₂)₂²⁻ ΔE_{ad}=-126.5			
6	1.357894000	1.923177000	-0.161591000	6	2.050894000	-0.605517000	-1.009109000
6	0.788662000	0.674355000	-0.030951000	6	0.784647000	-0.383554000	-0.448240000
6	-0.647379000	0.553491000	-0.001280000	6	0.707522000	0.512871000	0.686896000
6	-1.393237000	1.729902000	0.065013000	6	1.926580000	0.804443000	1.344786000
7	-0.806762000	2.961577000	0.029869000	7	3.167142000	0.455878000	0.871427000
6	0.537088000	3.150333000	-0.168260000	6	3.246003000	-0.122108000	-0.293799000
6	-1.334993000	-0.721917000	-0.278089000	8	4.380866000	-0.372282000	-0.872833000
7	-2.733741000	-0.721359000	0.020336000	6	-0.430940000	1.236688000	1.127045000
6	-3.423497000	0.454597000	0.177695000	7	-0.479010000	1.918087000	2.248177000
6	-2.823551000	1.660307000	0.178061000	6	0.651186000	2.022202000	2.964360000
8	-0.817706000	-1.677634000	-0.802248000	6	1.866419000	1.541988000	2.545329000
6	2.775469000	2.087559000	-0.270089000	8	-1.536192000	1.293384000	0.330196000
6	3.568298000	1.000238000	-0.244248000	6	2.176047000	-1.369506000	-2.177490000
7	3.056717000	-0.265311000	-0.040931000	6	1.032565000	-1.912711000	-2.713352000
6	1.690351000	-0.471625000	0.302452000	7	-0.159571000	-1.860705000	-2.102042000
8	1.340993000	-1.447306000	0.914113000	6	-0.267234000	-1.186141000	-0.982758000

1	-4.491050000	0.335469000	0.287770000	8	-1.424880000	-1.327028000	-0.286979000
1	-3.407824000	2.562989000	0.275166000	1	0.564799000	2.569577000	3.899748000
1	3.177095000	3.080493000	-0.406976000	1	2.785799000	1.731883000	3.083960000
1	4.640368000	1.034147000	-0.365312000	1	3.153199000	-1.519045000	-2.615417000
8	1.024848000	4.268376000	-0.296994000	1	1.059349000	-2.467220000	-3.647355000
6	3.995515000	-1.391497000	-0.032889000	6	-1.759279000	-2.640526000	0.080073000
8	3.656684000	-2.476620000	-0.413713000	8	-0.920470000	-3.504427000	0.138564000
8	5.162766000	-1.009036000	0.387361000	8	-3.010870000	-2.696003000	0.350324000
6	-3.490776000	-1.973629000	0.050639000	6	-1.895313000	2.569294000	-0.114893000
8	-4.695814000	-1.788445000	-0.399704000	8	-1.102214000	3.476562000	-0.133411000
8	-3.002674000	-2.980883000	0.479994000	8	-3.121769000	2.550792000	-0.499765000
6	-1.707314000	4.271132000	0.137250000	6	5.757299000	0.055286000	-0.126672000
8	-2.173121000	4.598401000	-0.942908000	8	6.154351000	-0.860709000	0.551948000
8	-1.793958000	4.669996000	1.287712000	8	6.094763000	1.154422000	-0.494513000
6	-5.804621000	-2.936130000	-0.069056000	6	-3.680270000	3.931873000	-1.115603000
8	-6.097562000	-3.515061000	-1.085058000	8	-4.244519000	4.566333000	-0.254502000
8	-6.113918000	-2.878137000	1.095812000	8	-3.460817000	3.981514000	-2.302353000
6	6.439141000	-1.984100000	0.071207000	8	-4.000871000	-4.764432000	-0.058031000
8	6.841094000	-2.459321000	1.102507000	6	-3.550709000	-4.143339000	0.873841000
8	6.706569000	-1.928654000	-1.103218000	8	-3.426825000	-4.220058000	2.070561000
(pn36-(CO₂)₃)³⁻_{N&N&N... ((CO₂)₃)_{O&O&O} ΔE_{ad}=-167.4}				(pn36-(CO₂)₃)⁻_{N&N&N-(CO₂)₂²⁻... CO₂ ΔE_{ad}=-164.7}			
6	-1.687769000	1.422711000	0.089039000	6	1.174409000	1.849995000	-0.208712000
6	-0.361655000	1.033703000	0.161085000	6	1.031553000	0.487384000	-0.057707000
6	-0.054281000	-0.378357000	0.237553000	6	-0.290500000	-0.088000000	-0.036404000
6	-1.109079000	-1.265529000	0.439728000	6	-1.376960000	0.782132000	0.002864000
7	-2.418042000	-0.843623000	0.454732000	7	-1.210144000	2.139773000	-0.053033000
6	-2.788022000	0.448034000	0.202624000	6	0.005890000	2.749885000	-0.243831000
6	1.278749000	-0.919821000	-0.100281000	6	-0.527913000	-1.521603000	-0.294616000
7	1.498540000	-2.276239000	0.235170000	7	-1.854053000	-1.966097000	-0.002792000
6	0.444749000	-3.082736000	0.544553000	6	-2.887444000	-1.074162000	0.126732000
6	-0.836103000	-2.657284000	0.619283000	6	-2.710243000	0.261839000	0.106763000
8	2.114287000	-0.262984000	-0.696097000	8	0.276234000	-2.265190000	-0.800133000
6	-2.053114000	2.794250000	-0.046788000	6	2.465597000	2.458050000	-0.310249000
6	-1.067861000	3.720567000	-0.105213000	6	3.563384000	1.680508000	-0.258167000
7	0.250087000	3.403415000	0.025421000	7	3.480368000	0.322290000	-0.034198000
6	0.664397000	2.106323000	0.378807000	6	2.248238000	-0.304203000	0.304779000
8	1.728892000	1.912771000	0.925071000	8	2.220109000	-1.329380000	0.933983000
1	0.726811000	-4.112720000	0.706203000	1	-3.860785000	-1.529625000	0.232583000
1	-1.633141000	-3.347469000	0.850641000	1	-3.557713000	0.927343000	0.185823000
1	-3.097436000	3.059042000	-0.117838000	1	2.531428000	3.524976000	-0.462378000
1	-1.248965000	4.779973000	-0.226367000	1	4.570034000	2.053135000	-0.372124000
8	-3.973712000	0.782322000	0.140487000	8	0.106036000	3.962405000	-0.385958000
6	1.252718000	4.598909000	-0.089464000	6	4.732338000	-0.445109000	0.001198000
8	2.314387000	4.313123000	-0.609861000	8	4.758833000	-1.587761000	-0.361796000
8	0.757283000	5.656723000	0.319466000	8	5.709718000	0.296480000	0.418686000
6	2.889036000	-2.955104000	0.232517000	6	-2.166708000	-3.398750000	0.050179000
8	2.821737000	-4.183033000	0.327879000	8	-3.360136000	-3.621783000	-0.404518000
8	3.844822000	-2.189305000	0.161921000	8	-1.378964000	-4.181712000	0.502720000
6	-3.570763000	-1.878997000	0.680341000	6	-2.455504000	3.062352000	0.008585000
8	-4.156980000	-2.172395000	-0.358341000	8	-2.989115000	3.237362000	-1.082400000
8	-3.668555000	-2.236420000	1.846089000	8	-2.736440000	3.423083000	1.147392000
6	3.727756000	0.152035000	1.536814000	6	-4.029792000	-5.090816000	-0.069627000
8	2.986313000	-0.355401000	2.269252000	8	-4.078926000	-5.739944000	-1.081715000
8	4.545160000	0.676922000	0.912380000	8	-4.365298000	-5.119821000	1.086738000
6	3.917416000	-1.263837000	-2.275537000	6	7.246553000	-0.237101000	0.131091000
8	4.740000000	-0.488339000	-2.038503000	8	7.752475000	-0.554131000	1.175290000

8	3.167268000	-2.055084000	-2.673049000	8	7.497069000	-0.106699000	-1.039456000
6	-5.928510000	-0.411446000	-1.125825000	6	-5.124531000	4.216958000	0.206632000
8	-6.578284000	-0.518451000	-0.173122000	8	-5.564542000	3.155295000	0.344393000
8	-5.438540000	-0.273476000	-2.165485000	8	-4.845349000	5.333829000	0.082923000
(pn36-(CO₂)₃)_{o&o&o}-(CO₂)₂²⁻... CO₂ ΔE_{ad}=-141.8							
6	1.233731000	-0.726712000	-1.102516000				
6	0.000012000	-0.438454000	-0.500344000				
6	0.003416000	0.477380000	0.621263000				
6	1.254229000	0.729450000	1.230416000				
7	2.461536000	0.316946000	0.714690000				
6	2.463067000	-0.284600000	-0.432476000				
8	3.574300000	-0.605751000	-1.052412000				
6	-1.088446000	1.255420000	1.091007000				
7	-1.062822000	1.954233000	2.201830000				
6	0.097105000	2.025648000	2.872591000				
6	1.275459000	1.490415000	2.415566000				
8	-2.216465000	1.346554000	0.334764000				
6	1.284321000	-1.512094000	-2.262874000				
6	0.098441000	-2.008332000	-2.749197000				
7	-1.067466000	-1.892922000	-2.097351000				
6	-1.106434000	-1.199909000	-0.984773000				
8	-2.240006000	-1.279533000	-0.246107000				
1	0.068535000	2.591705000	3.800090000				
1	2.222970000	1.652085000	2.912734000				
1	2.236124000	-1.713866000	-2.734027000				
1	0.066297000	-2.575878000	-3.674968000				
6	-2.622323000	-2.576181000	0.148657000				
8	-1.816549000	-3.472506000	0.189484000				
8	-3.862650000	-2.573122000	0.460007000				
6	-2.545110000	2.634126000	-0.111962000				
8	-1.715762000	3.507170000	-0.168027000				
8	-3.782262000	2.658544000	-0.450630000				
6	4.915989000	-0.251376000	-0.415643000				
8	5.351140000	-1.156050000	0.276595000				
8	5.334971000	0.829274000	-0.794689000				
6	-4.310778000	4.064921000	-1.073576000				
8	-4.825680000	4.723416000	-0.202137000				
8	-4.118471000	4.087732000	-2.264022000				
8	-4.946688000	-4.614785000	0.108847000				
6	-4.449749000	-4.007235000	1.023008000				
8	-4.291252000	-4.067116000	2.214590000				
6	7.691257000	0.187242000	0.354335000				
8	7.461556000	0.721315000	1.353955000				
8	8.084095000	-0.325156000	-0.607579000				

XI. CO₂ complexes of Li⁺-incorporated anionic systems

HCl				LiCl			
1	0.000000000	0.000000000	-1.210684000	3	0.000000000	0.000000000	-1.717778000
17	0.000000000	0.000000000	0.071217000	17	0.000000000	0.000000000	0.303137000
py-Li complex				nt5-2Li complex			
6	2.625563000	-0.021524000	-0.000145000	6	0.278437000	0.630658000	0.000000000
6	2.028090000	-1.302493000	-0.000448000	6	-0.278430000	-0.630668000	0.000009000
6	0.671110000	-1.377567000	-0.000345000	6	0.564323000	-1.774446000	-0.000017000
7	-0.137389000	-0.275028000	-0.000146000	6	1.902171000	-1.588559000	-0.000049000
6	0.406538000	1.001591000	0.000197000	7	2.490550000	-0.339615000	-0.000052000

6	1.839449000	1.088227000	0.000191000	6	1.731681000	0.802185000	-0.000031000
1	3.705189000	0.077408000	-0.000142000	8	2.201871000	1.959560000	-0.000048000
1	2.616546000	-2.208346000	-0.000690000	6	-0.564316000	1.774435000	0.000022000
1	0.127828000	-2.311260000	-0.000387000	6	-1.902166000	1.588544000	0.000051000
1	2.243719000	2.091308000	0.000499000	7	-2.490539000	0.339603000	0.000061000
8	-0.286603000	2.045939000	0.000630000	6	-1.731672000	-0.802190000	0.000042000
3	-2.049659000	2.103396000	0.001948000	8	-2.201867000	-1.959569000	0.000044000
6	-1.682792000	-0.605266000	-0.000188000	1	0.139527000	-2.766627000	-0.000013000
8	-1.912157000	-1.784730000	0.001944000	1	2.616891000	-2.397514000	-0.000074000
8	-2.415031000	0.397301000	-0.002533000	1	-0.139523000	2.766617000	0.000016000
				1	-2.616885000	2.397501000	0.000070000
				6	-4.074221000	0.371055000	0.000101000
				8	-4.519917000	1.485390000	0.000116000
				8	-4.599921000	-0.753422000	0.000094000
				3	-3.931727000	-2.362655000	0.000129000
				6	4.074187000	-0.371047000	-0.000088000
				8	4.519938000	-1.485366000	-0.000184000
				8	4.599880000	0.753438000	-0.000071000
				3	3.931751000	2.362677000	-0.000099000
pn36-3Li complex							
6	-0.759482000	-1.777596000	-0.267211000				
6	-0.725368000	-0.422174000	-0.033378000				
6	0.544773000	0.253317000	-0.005979000				
6	1.698665000	-0.507757000	0.130172000				
7	1.632828000	-1.894884000	0.066353000				
6	0.489276000	-2.549303000	-0.279009000				
8	0.459569000	-3.771993000	-0.516655000				
6	0.650614000	1.662824000	-0.336843000				
7	1.872138000	2.266345000	-0.108806000				
6	2.967204000	1.507333000	0.197476000				
6	2.947216000	0.156029000	0.273574000				
8	-0.309194000	2.256071000	-0.867912000				
6	-1.993517000	-2.454888000	-0.437261000				
6	-3.133675000	-1.734105000	-0.335342000				
7	-3.140236000	-0.418275000	0.058279000				
6	-1.969680000	0.242558000	0.366836000				
8	-1.933946000	1.299148000	1.018791000				
1	3.868997000	2.083451000	0.344339000				
1	3.858421000	-0.383038000	0.472530000				
1	-2.011343000	-3.509377000	-0.666179000				
1	-4.118040000	-2.137482000	-0.520811000				
6	2.153460000	3.811996000	-0.209185000				
8	3.238641000	4.117753000	0.204282000				
8	1.217485000	4.469369000	-0.696667000				
3	-0.315489000	3.960237000	-1.346584000				
6	-4.580222000	0.222199000	0.162784000				
8	-5.424357000	-0.445649000	-0.368761000				
8	-4.610416000	1.304802000	0.771243000				
3	-3.354817000	2.198492000	1.588883000				
6	2.911293000	-2.732181000	0.424676000				
8	3.413799000	-2.408318000	1.463964000				
8	3.180347000	-3.588828000	-0.439174000				
3	1.933670000	-4.710136000	-0.976101000				

XII. CO₂ complexes of anionic systems in presence of trimethyl phosphonium cation

(CH ₃) ₄ P ⁺ (OH) ⁻	H ₂ O
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15	0.402796000	-0.000026000	0.000114000	8	0.000000000	0.000000000	0.116610000
6	-0.138183000	1.534830000	-0.761204000	1	0.000000000	0.761593000	-0.466439000
1	0.237818000	2.381395000	-0.183928000	1	0.000000000	-0.761593000	-0.466439000
1	0.238151000	1.587883000	-1.784359000				
1	-1.236944000	1.459290000	-0.724064000				
6	2.223334000	-0.000261000	0.000334000				
1	2.595706000	0.064980000	-1.023270000				
1	2.595776000	0.853504000	0.568701000				
1	2.595618000	-0.919397000	0.455589000				
6	-0.139177000	-0.108116000	1.709588000				
1	0.236251000	0.751785000	2.267171000				
1	-1.237913000	-0.102952000	1.624426000				
1	0.236810000	-1.031106000	2.154564000				
6	-0.138535000	-1.426455000	-0.948610000				
1	-1.237267000	-1.355827000	-0.901862000				
1	0.237307000	-2.339243000	-0.482946000				
8	-2.380891000	0.000056000	-0.000202000				
1	-3.338299000	-0.000430000	-0.000389000				
1	0.237532000	-1.349926000	-1.970375000				
py-(CO₂)⁻...*(P(CH₃)₄)				nt5-(CO₂)⁻...*(P(CH₃)₄)			
6	4.188176000	1.044008000	0.044781000	6	3.153847000	0.320353000	-0.001281000
6	4.255797000	-0.372349000	0.076773000	6	2.135204000	-0.631968000	0.028468000
6	3.082605000	-1.061604000	0.055620000	6	2.456906000	-2.000537000	0.043961000
7	1.876414000	-0.438018000	0.024315000	6	3.782176000	-2.355867000	0.018093000
6	1.742371000	0.945938000	-0.097984000	7	4.790577000	-1.454426000	-0.012359000
6	2.987264000	1.678162000	-0.034095000	6	4.481497000	-0.185968000	-0.019384000
1	5.103230000	1.625966000	0.071669000	8	5.482402000	0.718059000	-0.045197000
1	5.197396000	-0.899952000	0.114973000	6	2.839503000	1.715950000	0.001730000
1	3.024059000	-2.142434000	0.061596000	6	1.536755000	2.068932000	-0.003170000
1	2.904153000	2.755647000	-0.087299000	7	0.513896000	1.148791000	-0.032407000
8	0.643081000	1.476813000	-0.277359000	6	0.720952000	-0.211552000	0.064290000
6	0.640213000	-1.333547000	0.108114000	8	-0.194126000	-1.019861000	0.198048000
8	0.684802000	-2.308223000	-0.626004000	1	1.664936000	-2.736006000	0.074836000
8	-0.207233000	-0.931213000	0.912523000	1	4.086358000	-3.396214000	0.023301000
15	-2.679114000	0.186476000	-0.013256000	1	3.621332000	2.460150000	0.011394000
6	-4.233648000	0.931344000	-0.593479000	1	1.196601000	3.095301000	0.016399000
1	-4.764009000	0.230918000	-1.240324000	6	-0.902444000	1.711374000	-0.136963000
1	-4.867968000	1.185865000	0.256829000	8	-1.622476000	1.096530000	-0.931069000
1	-4.013053000	1.839232000	-1.157452000	8	-1.103268000	2.680832000	0.577682000
6	-3.151233000	-1.305867000	0.882860000	15	-3.785459000	-0.515711000	0.021933000
1	-3.805872000	-1.039083000	1.714314000	6	-5.138600000	-1.573492000	0.618794000
1	-3.680206000	-1.976173000	0.203127000	1	-5.715623000	-1.955640000	-0.224552000
1	-2.234421000	-1.774556000	1.240593000	1	-4.724565000	-2.414676000	1.177283000
6	-1.713711000	-0.192142000	-1.490176000	1	-5.797082000	-1.001305000	1.274057000
1	-1.320012000	-1.208076000	-1.423062000	6	-2.813484000	-1.549639000	-1.083738000
1	-2.347467000	-0.082892000	-2.370994000	1	-2.371641000	-2.361786000	-0.504723000
1	-0.868066000	0.499974000	-1.520061000	1	-3.477098000	-1.948363000	-1.853931000
6	-1.941685000	1.404451000	1.085745000	1	-2.011161000	-0.944821000	-1.502143000
1	-1.660585000	2.281275000	0.501208000	6	-4.574855000	0.843774000	-0.861701000
1	-2.679383000	1.668070000	1.846808000	1	-5.169152000	0.444351000	-1.685331000
1	-1.038070000	0.975816000	1.514476000	1	-5.225609000	1.383885000	-0.171725000
				1	-3.784606000	1.498181000	-1.229316000
				6	-2.897266000	0.053848000	1.486997000
				1	-3.469855000	-0.204471000	2.378470000
				1	-1.918322000	-0.431221000	1.493513000
				1	-2.743638000	1.133155000	1.428726000

				1	6.308292000	0.218853000	-0.054188000
pn36-(CO ₂) ⁻ ...*(P(CH ₃) ₄) ₄				(nt5-(CO ₂) ₂) ²⁻ ...*(P(CH ₃) ₄) ₂			
6	-3.662077000	-0.669429000	0.162466000	6	0.498487000	-0.476556000	0.038018000
6	-2.275405000	-0.675550000	-0.064538000	6	-0.498521000	0.476426000	-0.038758000
6	-1.570737000	0.574304000	-0.051889000	6	-0.171419000	1.862240000	-0.078014000
6	-2.323885000	1.750810000	-0.015688000	6	1.134438000	2.212396000	-0.059248000
7	-3.690846000	1.752035000	0.133951000	7	2.141743000	1.280406000	-0.032925000
6	-4.292816000	0.621116000	0.273122000	6	1.911196000	-0.075160000	0.088449000
6	-0.117482000	0.673184000	0.124628000	8	2.819722000	-0.890566000	0.254401000
7	0.430291000	1.914699000	-0.200445000	6	0.171388000	-1.862369000	0.077243000
6	-0.327645000	3.044659000	-0.240327000	6	-1.134474000	-2.212522000	0.058461000
6	-1.676258000	3.015800000	-0.116774000	7	-2.141765000	-1.280530000	0.032184000
8	0.567675000	-0.217361000	0.605532000	6	-1.911229000	0.075038000	-0.089119000
6	-4.400276000	-1.867445000	0.227000000	8	-2.819781000	0.890449000	-0.254936000
6	-3.725485000	-3.039496000	0.017577000	1	-0.956557000	2.602056000	-0.119012000
7	-2.423670000	-3.075491000	-0.338056000	1	1.483223000	3.235993000	-0.062943000
6	-1.745532000	-1.959878000	-0.418849000	1	0.956524000	-2.602188000	0.118206000
8	-0.518252000	-2.042531000	-0.958008000	1	-1.483258000	-3.236122000	0.062103000
1	0.244834000	3.955780000	-0.354190000	6	3.566567000	1.815844000	-0.113629000
1	-2.266918000	3.919440000	-0.114049000	8	4.285255000	1.201357000	-0.911219000
1	-5.461444000	-1.845977000	0.430205000	8	3.781039000	2.771167000	0.616861000
1	-4.222602000	-4.000169000	0.084285000	6	-3.566604000	-1.815945000	0.113011000
8	-5.617251000	0.614252000	0.496808000	8	-4.285084000	-1.201663000	0.910949000
6	1.936086000	2.061596000	-0.389586000	8	-3.781273000	-2.771030000	-0.617723000
8	2.404004000	3.084048000	0.085135000	15	-6.374475000	0.507881000	-0.016460000
8	2.445046000	1.117692000	-1.006551000	6	-7.682392000	1.630023000	-0.598655000
15	4.044549000	-0.863982000	0.227357000	1	-8.232146000	2.038091000	0.250721000
6	5.036886000	-2.152382000	1.042736000	1	-7.233460000	2.451366000	-1.159767000
1	4.425759000	-2.664950000	1.787651000	1	-8.373622000	1.091452000	-1.248636000
1	5.385813000	-2.879035000	0.307639000	6	-5.353346000	1.492575000	1.089658000
1	5.897989000	-1.701744000	1.538483000	1	-4.867761000	2.279766000	0.511584000
6	2.708933000	-1.743196000	-0.598493000	1	-5.999579000	1.923535000	1.857484000
1	3.154009000	-2.534314000	-1.206595000	1	-4.583402000	0.847906000	1.509366000
1	2.039247000	-2.161366000	0.154229000	6	-7.220818000	-0.815225000	0.870310000
1	2.138172000	-1.034199000	-1.194919000	1	-7.789744000	-0.391015000	1.699435000
6	3.537291000	0.276770000	1.532426000	1	-7.900704000	-1.323492000	0.184258000
1	2.465849000	0.143207000	1.696505000	1	-6.457997000	-1.505732000	1.230031000
1	4.105110000	0.059440000	2.437941000	6	-5.533235000	-0.100312000	-1.492856000
1	3.706307000	1.305013000	1.208310000	1	-6.115882000	0.168659000	-2.374699000
6	5.146986000	-0.076499000	-0.963560000	1	-4.539653000	0.353945000	-1.520237000
1	5.995129000	0.356632000	-0.430400000	1	-5.410611000	-1.183097000	-1.427399000
1	5.506681000	-0.823488000	-1.673302000	15	6.374466000	-0.507718000	0.017244000
1	4.578383000	0.703619000	-1.469276000	6	5.532656000	0.100404000	1.493334000
1	-5.901052000	1.537203000	0.523364000	1	6.115102000	-0.168453000	2.375347000
1	-0.411196000	-2.969046000	-1.209238000	1	5.409878000	1.183173000	1.427881000
				1	4.539162000	-0.354051000	1.520468000
				6	7.220974000	0.815424000	-0.869317000
				1	6.458275000	1.505938000	-1.229289000
				1	7.900715000	1.323697000	-0.183127000
				1	7.790101000	0.391181000	-1.698293000
				6	7.682365000	-1.629593000	0.600025000
				1	8.373129000	-1.090914000	1.250412000
				1	7.233325000	-2.451077000	1.160847000
				1	8.232660000	-2.037479000	-0.249088000
				6	5.354017000	-1.492761000	-1.089186000
				1	4.868443000	-2.280058000	-0.511250000

				1	4.584079000	-0.848358000	-1.509292000
				1	6.000710000	-1.923594000	-1.856700000
(pn-(CO ₂) ₂) ² -...*(P(CH ₃) ₄) ₂				(pn-(CO ₂) ₃) ³ -...*(P(CH ₃) ₄) ₃			
6	1.007177000	-3.371953000	-0.110038000	6	1.213475000	-1.391077000	-0.163366000
6	1.204269000	-2.016360000	0.102685000	6	0.446730000	-0.294211000	0.135732000
6	2.514097000	-1.484915000	0.101075000	6	0.994624000	1.022106000	0.089466000
6	3.587020000	-2.378766000	0.066038000	6	2.364773000	1.167448000	-0.048762000
7	3.401676000	-3.727559000	-0.042164000	7	3.156472000	0.045477000	-0.155707000
6	2.188395000	-4.173140000	-0.171749000	6	2.664870000	-1.237315000	-0.325802000
6	2.747592000	-0.044483000	-0.094886000	6	0.101488000	2.160010000	-0.106735000
7	4.050699000	0.385553000	0.140521000	7	0.693614000	3.420935000	-0.040459000
6	5.081550000	-0.513530000	0.208714000	6	2.053095000	3.535364000	-0.041202000
6	4.913424000	-1.855999000	0.142309000	6	2.912261000	2.483313000	-0.072614000
8	1.869108000	0.688048000	-0.521808000	8	-1.077124000	1.986130000	-0.385366000
6	-0.321481000	-3.895499000	-0.285589000	6	0.597287000	-2.675714000	-0.349133000
6	-1.356072000	-3.031786000	-0.303867000	6	-0.748714000	-2.762674000	-0.308857000
7	-1.194367000	-1.683263000	-0.032724000	7	-1.534601000	-1.679485000	0.056909000
6	0.020734000	-1.216149000	0.505793000	6	-0.920610000	-0.551085000	0.640076000
8	0.066295000	-0.324078000	1.314546000	8	-1.429341000	0.055708000	1.549430000
1	6.051583000	-0.042859000	0.290746000	1	2.394770000	4.561116000	-0.055819000
1	5.757762000	-2.529300000	0.158544000	1	3.975135000	2.649856000	-0.151783000
1	-0.474262000	-4.948292000	-0.469510000	1	1.209502000	-3.528369000	-0.603391000
1	-2.375704000	-3.317429000	-0.514365000	1	-1.307913000	-3.655623000	-0.543990000
8	2.009574000	-5.497019000	-0.352864000	8	3.411200000	-2.178874000	-0.574471000
6	-2.345937000	-0.779550000	-0.131495000	6	-2.987279000	-1.759482000	-0.018693000
8	-2.109410000	0.426177000	-0.222482000	8	-3.620076000	-0.697185000	0.004882000
8	-3.460940000	-1.355402000	-0.143672000	8	-3.446627000	-2.922178000	-0.140622000
6	4.429549000	1.892786000	0.220930000	6	-0.125626000	4.759241000	-0.087923000
8	5.614867000	2.092688000	0.035879000	8	0.585555000	5.729331000	-0.265710000
8	3.474386000	2.629863000	0.482987000	8	-1.338037000	4.612574000	0.080189000
15	0.756441000	3.754615000	-0.197779000	6	4.659762000	0.171965000	-0.204575000
6	-0.875821000	4.466796000	-0.564617000	8	5.116082000	0.715014000	-1.203936000
1	-1.539542000	3.658594000	-0.878813000	8	5.226013000	-0.318801000	0.783716000
1	-1.284797000	4.935998000	0.331430000	15	7.589166000	-1.531979000	0.168325000
1	-0.800287000	5.209907000	-1.359520000	6	6.545346000	-2.037056000	-1.212434000
6	0.476461000	2.571128000	1.112998000	1	5.520770000	-2.202287000	-0.867221000
1	0.004992000	3.108275000	1.940581000	1	6.522669000	-1.234329000	-1.951234000
1	-0.178191000	1.773782000	0.751938000	1	6.960795000	-2.946696000	-1.648975000
1	1.432843000	2.144413000	1.406156000	6	7.894710000	0.248497000	0.302272000
6	1.367441000	3.121509000	-1.765352000	1	7.257718000	0.759090000	-0.422758000
1	0.771534000	2.256747000	-2.056381000	1	7.592922000	0.580972000	1.294019000
1	1.286956000	3.923216000	-2.503189000	1	8.952122000	0.450149000	0.125522000
1	2.397308000	2.803677000	-1.623077000	6	7.060384000	-2.299260000	1.714137000
6	1.814918000	5.106150000	0.354955000	1	6.052776000	-1.954094000	1.938868000
1	1.890006000	5.858540000	-0.431981000	1	7.077321000	-3.383266000	1.587000000
1	1.389269000	5.557276000	1.252792000	1	7.751948000	-2.017601000	2.510167000
1	2.796198000	4.676741000	0.569650000	6	9.225989000	-2.258131000	-0.171678000
15	-5.681000000	0.082815000	0.088014000	1	9.148957000	-3.344491000	-0.234636000
6	-4.690858000	0.499629000	1.544296000	1	9.604868000	-1.873857000	-1.120480000
1	-5.261453000	1.159312000	2.198461000	1	9.925870000	-1.993367000	0.622610000
1	-4.424603000	-0.421628000	2.060166000	15	-4.014273000	3.088351000	0.053692000
1	-3.763484000	0.970957000	1.212012000	6	-5.577861000	2.164705000	0.108537000
6	-6.284187000	-1.618418000	0.123801000	1	-5.317362000	1.104088000	0.044370000
1	-5.431076000	-2.289115000	0.052588000	1	-6.096164000	2.358272000	1.048841000
1	-6.825518000	-1.780654000	1.057646000	1	-6.220380000	2.445363000	-0.727186000
1	-6.965695000	-1.769686000	-0.715263000	6	-3.104132000	2.551335000	1.495400000

6	-7.189241000	1.095136000	0.239263000	1	-3.741751000	2.747107000	2.362407000
1	-7.704275000	0.865562000	1.173359000	1	-2.885553000	1.485809000	1.402004000
1	-6.921695000	2.153450000	0.234289000	1	-2.175550000	3.115353000	1.544358000
1	-7.860776000	0.896863000	-0.597605000	6	-3.341815000	2.774009000	-1.581546000
6	-4.966925000	0.545853000	-1.509266000	1	-3.081321000	1.718142000	-1.654637000
1	-5.614574000	1.269628000	-2.005161000	1	-4.114503000	3.046234000	-2.305366000
1	-3.966650000	0.946741000	-1.332451000	1	-2.441245000	3.372828000	-1.698166000
1	-4.856900000	-0.354055000	-2.112486000	6	-4.378430000	4.851052000	0.186941000
1	2.889693000	-5.894092000	-0.360196000	1	-5.012081000	5.166972000	-0.643227000
				1	-4.882657000	5.054151000	1.132930000
				1	-3.416504000	5.370194000	0.153074000
				15	-6.028878000	-3.371125000	-0.045285000
				6	-5.642196000	-2.551701000	1.521592000
				1	-6.543109000	-2.480420000	2.131485000
				1	-4.872732000	-3.127445000	2.034093000
				1	-5.224872000	-1.566148000	1.304624000
				6	-5.323845000	-5.029389000	-0.165624000
				1	-4.240092000	-4.945639000	-0.192610000
				1	-5.645555000	-5.610894000	0.700319000
				1	-5.698178000	-5.505393000	-1.073818000
				6	-7.827786000	-3.666938000	0.017414000
				1	-8.078356000	-4.280339000	0.884356000
				1	-8.353761000	-2.713600000	0.095893000
				1	-8.156885000	-4.177726000	-0.888982000
				6	-5.779078000	-2.378828000	-1.538591000
				1	-6.735448000	-2.213583000	-2.035745000
				1	-5.302113000	-1.440398000	-1.248712000
				1	-5.088358000	-2.908193000	-2.193481000

XIII. Anionic systems in presence of trimethyl phosphonium cation

py ⁻ ...*P(CH ₃) ₄				nt5 ⁻ ...*P(CH ₃) ₄			
6	-3.610506000	0.788763000	0.000047000	6	1.675991000	-0.662352000	0.000974000
6	-3.787522000	-0.601916000	0.000276000	6	2.315709000	0.580198000	0.001011000
6	-2.648253000	-1.382702000	0.000152000	6	1.537596000	1.771020000	0.003065000
7	-1.397620000	-0.902861000	-0.000109000	6	0.181484000	1.622985000	0.003901000
6	-1.219032000	0.433367000	-0.000247000	7	-0.497075000	0.443591000	0.003099000
6	-2.339737000	1.311059000	-0.000238000	6	0.203312000	-0.725257000	0.003055000
1	-4.470045000	1.450789000	0.000079000	8	-0.372972000	-1.835326000	0.005176000
1	-4.770022000	-1.054145000	0.000519000	6	2.448954000	-1.840097000	-0.000917000
1	-2.732021000	-2.466721000	0.000237000	6	3.814747000	-1.725367000	-0.002886000
1	-2.152918000	2.377165000	-0.000473000	7	4.460204000	-0.531394000	-0.002987000
8	-0.021946000	0.936340000	-0.000430000	6	3.738273000	0.553742000	-0.001092000
15	1.891451000	-0.025443000	-0.000028000	8	4.376457000	1.746955000	-0.001249000
6	1.295817000	-0.716650000	1.573713000	1	2.005335000	2.744686000	0.003574000
1	0.940323000	0.104755000	2.194257000	1	-0.436122000	2.518346000	0.005099000
1	0.441782000	-1.357445000	1.352098000	1	1.950939000	-2.800219000	-0.000730000
1	2.088144000	-1.270369000	2.075951000	1	4.455253000	-2.599916000	-0.004427000
6	2.359861000	1.735670000	-0.000044000	15	-3.198562000	0.049425000	-0.000830000
1	1.917881000	2.209047000	0.874943000	6	-3.061156000	1.859356000	-0.021227000
1	3.442958000	1.846769000	0.000476000	1	-2.518024000	2.184430000	0.864838000
1	1.918746000	2.209043000	-0.875472000	1	-2.494982000	2.162096000	-0.900666000
6	3.596294000	-0.771803000	0.000120000	1	-4.052829000	2.311999000	-0.039373000
1	4.152315000	-0.459144000	0.887175000	6	-2.652400000	-0.699967000	1.554466000
1	3.530554000	-1.862750000	0.000361000	1	-1.976160000	-1.522660000	1.308533000
1	4.152197000	-0.459552000	-0.887163000	1	-2.084783000	0.037897000	2.118151000

6	1.295912000	-0.717553000	-1.573380000	1	-3.522494000	-1.039193000	2.117462000
1	0.442096000	-1.358484000	-1.351247000	6	-5.004497000	-0.243246000	0.002751000
1	0.939786000	0.103632000	-2.193896000	1	-5.456690000	0.203381000	0.889912000
1	2.088368000	-1.271038000	-2.075617000	1	-5.459131000	0.191988000	-0.888754000
				1	-5.200164000	-1.317300000	0.010015000
				6	-2.654096000	-0.727548000	-1.542874000
				1	-3.526765000	-1.024234000	-2.125526000
				1	-2.036043000	-0.020274000	-2.092252000
				1	-2.023069000	-1.581022000	-1.283292000
				1	5.320870000	1.549426000	-0.003676000
pn36-...P(CH₃)₄				nt5²⁻...(P(CH₃)₄)₂			
6	-3.316416000	-0.216286000	0.119816000	6	0.245525000	-0.425700000	0.029003000
6	-1.949708000	-0.520607000	-0.002336000	6	-0.446356000	0.778633000	0.037600000
6	-0.999742000	0.551755000	-0.001283000	6	0.273748000	1.999810000	0.033537000
6	-1.490369000	1.860169000	-0.135544000	6	1.638874000	1.921533000	0.023814000
7	-2.841176000	2.150030000	-0.097109000	7	2.360948000	0.772666000	0.015954000
6	-3.667877000	1.181931000	0.085478000	6	1.711606000	-0.423965000	0.017894000
6	0.425739000	0.380084000	0.283795000	8	2.358723000	-1.503092000	0.009784000
7	1.278430000	1.405229000	-0.048545000	6	-0.483204000	-1.645518000	0.026809000
6	0.759605000	2.611441000	-0.324022000	6	-1.843345000	-1.578402000	0.047332000
6	-0.579487000	2.924002000	-0.312576000	7	-2.567857000	-0.419463000	0.068334000
8	0.867194000	-0.644216000	0.835738000	6	-1.915970000	0.781474000	0.040123000
6	-4.287442000	-1.232379000	0.218548000	8	-2.556206000	1.856229000	0.011452000
6	-3.857997000	-2.530028000	0.142309000	1	-0.256660000	2.941409000	0.037304000
7	-2.576574000	-2.855414000	-0.133918000	1	2.225553000	2.841125000	0.021149000
6	-1.682192000	-1.907377000	-0.250327000	1	0.045398000	-2.588334000	0.013834000
8	-0.484515000	-2.277148000	-0.741001000	1	-2.417672000	-2.499587000	0.049503000
1	1.483683000	3.395521000	-0.546190000	15	-4.970727000	-0.155135000	-0.029486000
1	-0.944079000	3.930077000	-0.462342000	6	-6.804834000	0.089732000	-0.203750000
1	-5.330929000	-0.981758000	0.347188000	1	-7.329212000	-0.194852000	0.710180000
1	-4.543554000	-3.362568000	0.250031000	1	-7.019623000	1.139643000	-0.416141000
8	-4.981105000	1.463471000	0.209568000	1	-7.187602000	-0.513719000	-1.029971000
15	3.935356000	-0.260865000	0.045000000	6	-4.725731000	0.857016000	1.456691000
6	5.445170000	-1.273102000	0.122900000	1	-4.774932000	1.906350000	1.169286000
1	5.204601000	-2.249108000	0.548209000	1	-5.538588000	0.610766000	2.144161000
1	5.855011000	-1.414132000	-0.878035000	1	-3.753522000	0.667007000	1.897228000
1	6.192124000	-0.786969000	0.751743000	6	-4.939905000	-1.936697000	0.330455000
6	2.834839000	-1.137298000	-1.080414000	1	-5.944372000	-2.281893000	0.573880000
1	3.448902000	-1.539138000	-1.890041000	1	-4.573775000	-2.476044000	-0.543270000
1	2.305752000	-1.923205000	-0.542788000	1	-4.262838000	-2.120266000	1.162326000
1	2.091333000	-0.439715000	-1.461240000	6	-4.475328000	0.367936000	-1.700320000
6	3.440893000	-0.022629000	1.759352000	1	-5.361349000	0.589954000	-2.295203000
1	2.986853000	-0.939201000	2.133205000	1	-3.837908000	1.246694000	-1.586942000
1	4.340923000	0.235526000	2.323968000	1	-3.889049000	-0.430901000	-2.151145000
1	2.691943000	0.764763000	1.795862000	15	5.241319000	-0.129784000	-0.016782000
6	4.427692000	1.316846000	-0.679473000	6	4.575265000	-0.720302000	1.548475000
1	5.180529000	1.791271000	-0.047998000	1	5.342860000	-0.560248000	2.310246000
1	4.839872000	1.148729000	-1.675759000	1	3.663110000	-0.170606000	1.767088000
1	3.531454000	1.933664000	-0.736073000	1	4.320638000	-1.774552000	1.450804000
1	-5.060219000	2.423562000	0.145165000	6	5.381557000	1.670012000	-0.015212000
1	-0.558118000	-3.229254000	-0.884670000	1	4.372690000	2.077602000	-0.002633000
				1	5.935075000	1.989194000	0.869549000
				1	5.913963000	1.992297000	-0.911736000
				6	6.958925000	-0.740720000	-0.035780000
				1	7.493975000	-0.390865000	0.848059000
				1	6.954667000	-1.832268000	-0.037246000

				1	7.475270000	-0.388373000	-0.929702000
				6	4.542820000	-0.714575000	-1.570086000
				1	4.291707000	-1.769591000	-1.471707000
				1	3.625656000	-0.165063000	-1.767148000
				1	5.294018000	-0.550231000	-2.347147000
pn²⁻...*(P(CH₃)₄)₂				pn³⁻...*(P(CH₃)₄)₃			
6	-0.858918000	2.300563000	-0.949559000	6	-0.771229000	0.995233000	1.339881000
6	-0.317567000	1.124803000	-0.424996000	6	0.260003000	0.371799000	0.646335000
6	0.544546000	1.207068000	0.711415000	6	-0.070556000	-0.485245000	-0.459516000
6	1.081979000	2.462175000	1.037624000	6	-1.399445000	-0.932578000	-0.543444000
7	0.643475000	3.621805000	0.426843000	7	-2.428329000	-0.400701000	0.199008000
6	-0.307854000	3.530279000	-0.440034000	6	-2.175406000	0.602278000	1.067333000
6	0.797082000	0.089217000	1.624848000	6	0.849018000	-0.799167000	-1.545414000
7	1.893071000	0.151356000	2.429142000	7	0.597301000	-1.896224000	-2.322781000
6	2.500907000	1.337776000	2.588911000	6	-0.613183000	-2.460535000	-2.229299000
6	2.112249000	2.524957000	2.002499000	6	-1.653918000	-2.007904000	-1.441463000
8	0.002293000	-0.882633000	1.682048000	8	1.845320000	-0.063797000	-1.782119000
6	-1.892081000	2.237588000	-1.919225000	6	-0.468790000	2.002763000	2.284821000
6	-2.303602000	0.981714000	-2.296434000	6	0.858658000	2.306233000	2.476745000
7	-1.691220000	-0.171137000	-1.949607000	7	1.888151000	1.598777000	1.961238000
6	-0.574581000	-0.112694000	-1.180504000	6	1.613671000	0.517124000	1.191873000
8	0.235847000	-1.072193000	-1.143463000	8	2.505404000	-0.356211000	0.980787000
1	3.350240000	1.334922000	3.270105000	1	-0.769666000	-3.336489000	-2.859248000
1	2.575489000	3.471461000	2.245126000	1	-2.616411000	-2.503562000	-1.455324000
1	-2.347407000	3.136444000	-2.309587000	1	-1.268947000	2.518852000	2.797249000
1	-3.164118000	0.873090000	-2.954983000	1	1.140172000	3.144861000	3.113038000
8	-0.811975000	4.670443000	-0.964664000	8	-3.108047000	1.192616000	1.667890000
15	3.199369000	-1.661431000	-0.761637000	15	2.793827000	-3.272503000	0.562497000
6	2.308209000	-2.438228000	0.583089000	6	3.399967000	-2.463520000	-0.915715000
1	2.573936000	-3.497895000	0.591316000	1	4.422023000	-2.810483000	-1.086661000
1	2.567375000	-1.954344000	1.529656000	1	2.747964000	-2.704436000	-1.761129000
1	1.241345000	-2.283317000	0.413817000	1	3.346400000	-1.384954000	-0.757863000
6	4.952640000	-2.084516000	-0.546768000	6	3.049052000	-5.055323000	0.304102000
1	5.307352000	-1.660477000	0.394315000	1	2.440461000	-5.381173000	-0.541391000
1	5.073127000	-3.168293000	-0.516299000	1	4.098821000	-5.254107000	0.083579000
1	5.543428000	-1.678105000	-1.368792000	1	2.755047000	-5.613544000	1.194072000
6	2.667628000	-2.349517000	-2.340985000	6	3.786353000	-2.807913000	1.995093000
1	2.816674000	-3.430603000	-2.336179000	1	4.834361000	-3.044923000	1.803270000
1	1.607117000	-2.107294000	-2.448882000	1	3.649193000	-1.732360000	2.134496000
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6	3.128480000	0.134781000	-0.840396000	6	1.045798000	-3.093181000	0.949478000
1	2.149744000	0.424771000	-1.217133000	1	0.878656000	-2.103259000	1.368448000
1	3.273435000	0.563383000	0.154464000	1	0.446432000	-3.201741000	0.041730000
1	3.919289000	0.472133000	-1.514363000	1	0.785684000	-3.873184000	1.669310000
15	-3.330019000	-1.580253000	0.613943000	15	-5.481669000	0.128901000	-0.176584000
6	-4.167655000	-2.343818000	2.030526000	6	-5.220205000	-0.669282000	1.415130000
1	-3.478218000	-2.351596000	2.877015000	1	-5.253143000	0.086840000	2.198393000
1	-5.057153000	-1.771265000	2.296319000	1	-6.011325000	-1.414161000	1.538553000
1	-4.452642000	-3.368707000	1.789888000	1	-4.225136000	-1.110618000	1.406626000
6	-2.918548000	0.096374000	1.123490000	6	-7.277229000	0.429699000	-0.248925000
1	-3.702361000	0.445895000	1.798749000	1	-7.817761000	-0.512947000	-0.151925000
1	-1.946881000	0.055580000	1.627657000	1	-7.567865000	1.089505000	0.570538000
1	-2.857634000	0.751966000	0.254203000	1	-7.544192000	0.899718000	-1.196244000
6	-1.945829000	-2.641616000	0.197328000	6	-4.729337000	1.729034000	-0.515234000
1	-1.143213000	-2.448468000	0.915384000	1	-4.794908000	2.364358000	0.365794000
1	-2.296242000	-3.675531000	0.236639000	1	-3.678030000	1.570489000	-0.745670000

1	-1.574866000	-2.384841000	-0.796617000	1	-5.263427000	2.160618000	-1.366015000
6	-4.494253000	-1.546269000	-0.765674000	6	-5.109902000	-0.973774000	-1.553575000
1	-4.881232000	-2.550436000	-0.946278000	1	-4.029528000	-0.973871000	-1.698131000
1	-5.318756000	-0.866907000	-0.545001000	1	-5.446821000	-1.985389000	-1.321510000
1	-3.938956000	-1.197953000	-1.639155000	1	-5.619650000	-0.615004000	-2.449667000
1	-0.331093000	5.393110000	-0.542326000	15	3.007843000	3.131579000	-0.805493000
				6	3.578448000	4.045554000	-2.268313000
				1	3.354985000	3.453363000	-3.157647000
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				1	4.654758000	4.212512000	-2.209671000
				6	1.238832000	2.887902000	-1.029432000
				1	0.857944000	3.711692000	-1.636746000
				1	1.109594000	1.920963000	-1.530550000
				1	0.734506000	2.869183000	-0.062176000
				6	4.001406000	1.643423000	-0.720629000
				1	3.713519000	0.993728000	-1.550876000
				1	5.050647000	1.944540000	-0.773210000
				1	3.784022000	1.102227000	0.205440000
				6	3.345575000	4.164568000	0.636331000
				1	4.390200000	4.480454000	0.623140000
				1	2.694221000	5.039817000	0.628315000
				1	3.143507000	3.549078000	1.516545000