

SUPPLEMENTARY INFORMATION

DFT Study of Dihydrogen Addition to Molybdenum π -Heteroaromatic Complexes: Prerequisite Step for the Catalytic Hydrodenitrogenation Process

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**Table of the cartesian coordinates of all the stationary points considered in the
manuscript (see Table 1 and Scheme 1)**

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XYZ file for : **1-N**

6	-1.10044515	1.24749969	2.31515411
6	-1.52266964	-0.07230418	2.62337506
6	-0.52558432	-1.09596215	2.71075883
7	0.83040540	-0.87028103	2.67165006
6	1.23521765	0.46327405	2.57240533
6	0.30749644	1.56950441	2.41169198
1	-2.57969397	-0.32382503	2.70469142
1	-0.81938600	-2.13169961	2.89676168
1	-1.82970121	2.05472584	2.22051905
42	-0.20249105	-0.10624818	0.72709220
15	-1.32817262	1.31794066	-0.89371107
15	-1.30465293	-2.06092864	-0.16779269
15	1.75420247	-0.46334338	-0.73212656
6	-0.36066098	-3.67287567	0.03123712
6	-2.91703018	-2.57267361	0.64666656
6	-1.86286406	-2.30071441	-1.94738467
6	-1.02955414	3.16686522	-0.73336707
6	-1.13560353	1.23011751	-2.76428096
6	-3.20229898	1.33975267	-0.80977121
1	-3.29514826	-3.51285705	0.21758572
1	-2.76853291	-2.71052275	1.72572724
1	-3.66406136	-1.78087135	0.49915134
1	-0.97859407	-4.54364987	-0.23669950
1	0.53053181	-3.65681904	-0.61131317
1	-0.02304881	-3.76271856	1.07262851

1	-2.27272945	-3.31203889	-2.09233364
1	-2.64256922	-1.56685714	-2.19356020
1	-1.01851583	-2.15420641	-2.63271271
1	-3.62969359	2.11129341	-1.46885816
1	-3.59695470	0.35732553	-1.10255489
1	-3.50828059	1.53357317	0.22736872
1	-1.57627356	3.72853080	-1.50611731
1	-1.36045733	3.50699434	0.25647290
1	0.04561377	3.37257396	-0.82271542
1	-1.80005685	1.95211520	-3.26348091
1	-0.09633755	1.46890278	-3.03119525
1	-1.36369626	0.22039244	-3.12729581
6	3.10708670	-1.54311529	-0.02491989
6	1.71221829	-1.20966863	-2.45599522
6	2.72425832	1.08705465	-1.11773219
1	2.71801900	-1.20935128	-2.90360098
1	1.35371702	-2.24699198	-2.40165120
1	1.03075476	-0.63906428	-3.09967916
1	3.65883246	0.85122786	-1.64942203
1	2.11208448	1.75380929	-1.74077064
1	2.95337973	1.60674299	-0.17786428
1	3.97342635	-1.58704841	-0.70239469
1	3.41526848	-1.14265633	0.94745072
1	2.71354682	-2.55534957	0.13661311
6	2.62610565	0.76953504	2.71142296
6	3.08452758	2.07235890	2.65839574
1	3.30489063	-0.06126935	2.91044005
1	4.15008714	2.27624153	2.78190518
6	2.18137543	3.14835040	2.45584406
1	2.55275039	4.17318321	2.41141971
6	0.82649507	2.89371092	2.32996399
1	0.12240152	3.72133292	2.21404216
1	0.41863983	-2.79484795	-6.09093962
1	0.53018341	-2.41253872	-5.45314049

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XYZ file for : **TS1-N**

6	-0.71676125	1.10019137	1.63279218
6	-1.32439221	-0.13304942	2.08239147
6	-0.41492084	-1.21507327	2.27835834
7	0.95289402	-1.04342679	2.13269461
6	1.43124392	0.25984724	2.44277158
6	0.61502281	1.40077141	2.19459880
1	-2.39699269	-0.24515666	2.23740837
1	-0.76287855	-2.21093320	2.56830456
1	-1.37065261	1.95765205	1.44617195

42	-0.18317726	-0.50500994	0.18626944
15	-1.37159206	0.86964546	-1.41911770
15	-1.77857686	-2.27852852	-0.24273718
15	2.07614905	0.11697627	-1.02694064
6	-1.07359965	-3.99617907	0.04960433
6	-3.31410656	-2.41553681	0.82158911
6	-2.59312575	-2.61466822	-1.90000342
6	-0.74924353	2.63745757	-1.57562207
6	-1.57627527	0.55213418	-3.26671098
6	-3.16881703	1.25053751	-1.02246546
1	-3.88696703	-3.31183138	0.54215810
1	-3.04055746	-2.48675592	1.88230952
1	-3.94268904	-1.52587366	0.68227553
1	-1.86643217	-4.75769560	0.00100630
1	-0.31486154	-4.21760736	-0.71216081
1	-0.58774555	-4.03108291	1.03368598
1	-3.15545173	-3.56017227	-1.86746813
1	-3.28629730	-1.80123523	-2.15206579
1	-1.82413556	-2.67741466	-2.68139779
1	-3.58916583	2.00147218	-1.70881332
1	-3.76309536	0.32915481	-1.09432996
1	-3.24138242	1.62171570	0.00906414
1	-1.45252095	3.25973431	-2.14954454
1	-0.60462698	3.07065209	-0.57736108
1	0.21988108	2.63657188	-2.09344186
1	-2.10782857	1.38225010	-3.75840274
1	-0.58448217	0.43872434	-3.72504070
1	-2.13287520	-0.37758894	-3.43565492
6	3.44338981	-1.05232120	-0.54151381
6	2.28488078	0.11361885	-2.88439275
6	2.86349701	1.74712507	-0.59977948
1	3.34233679	0.24831735	-3.15806712
1	1.92366008	-0.83892902	-3.29479373
1	1.69578128	0.92983599	-3.32350574
1	3.85264931	1.82352115	-1.07548430
1	2.22703418	2.57239311	-0.94305614
1	2.97162923	1.82473586	0.48932088
1	4.40482910	-0.74401980	-0.97897316
1	3.51398552	-1.06667295	0.55386041
1	3.19525150	-2.06747392	-0.88085507
6	2.72060623	0.43773469	2.96915849
6	3.20800179	1.72817346	3.23116463
1	3.32812888	-0.44701430	3.17031318
1	4.21639839	1.85397174	3.63035009
6	2.40759360	2.85123866	2.98286508
1	2.79043612	3.85339476	3.18384092

6	1.11213532	2.68443007	2.46905048
1	0.48094597	3.55672049	2.27656015
1	1.03943636	-2.56834300	-1.42498408
1	0.51618631	-1.99947496	-1.53220029

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XYZ file for : 2-N

6	-0.28029133	1.35946134	1.36214283
6	-1.26706421	0.35594227	1.72695470
6	-0.70060884	-0.91548351	2.01645586
7	0.67211590	-1.07358170	1.97753944
6	1.39790382	0.03840851	2.50024919
6	0.94477488	1.34190748	2.19545928
1	-2.34228379	0.53097714	1.77163029
1	-1.32726314	-1.76674965	2.30152875
1	-0.64324469	2.34710711	1.06610652
42	-0.21977267	-0.44545654	-0.14182029
15	-1.66085782	0.99841883	-1.47719757
15	-1.54962332	-2.49012064	-0.40193335
15	2.00957168	0.28445994	-0.98523784
6	-0.86911318	-3.98237402	0.49131099
6	-3.33316306	-2.53845037	0.16217564
6	-1.70801889	-3.22905175	-2.10339310
6	-0.88380970	2.43884946	-2.39088792
6	-2.65947572	0.29011124	-2.88705867
6	-3.04427652	1.92914350	-0.61845159
1	-3.75867169	-3.54754687	0.05483384
1	-3.39687557	-2.23365639	1.21597162
1	-3.92289232	-1.82939514	-0.43472238
1	-1.55459915	-4.83954309	0.41608242
1	0.09559222	-4.23629185	0.03204274
1	-0.67881624	-3.74688831	1.54599539
1	-2.22352656	-4.19996089	-2.06006807
1	-2.26218292	-2.55060331	-2.76297859
1	-0.69881753	-3.36444217	-2.51383660
1	-3.57263867	2.57787751	-1.33266703
1	-3.75545931	1.20683252	-0.19484572
1	-2.65070673	2.54878851	0.19773284
1	-1.63461185	3.01816427	-2.94949183
1	-0.38742464	3.09394456	-1.66232177
1	-0.12714537	2.05919031	-3.09068844
1	-3.23621323	1.07929150	-3.39161021
1	-1.98107258	-0.18496422	-3.60816053
1	-3.35449049	-0.46952099	-2.50466445
6	3.45826328	-0.59401095	-0.21901886
6	2.32256279	-0.09189058	-2.78233415

6	2.60640204	2.04869750	-0.89581606
1	3.35293357	0.17293971	-3.06282214
1	2.15619338	-1.16445250	-2.94680079
1	1.61708649	0.46577885	-3.41200728
1	3.63656797	2.12813868	-1.27472746
1	1.94960267	2.69482830	-1.49247704
1	2.57569173	2.38183061	0.15008992
1	4.39808822	-0.28526361	-0.70036687
1	3.49646493	-0.36274057	0.85306318
1	3.31097776	-1.67578745	-0.33295357
6	2.53922628	-0.13971150	3.28718054
6	3.25231394	0.98233616	3.75105915
1	2.87166574	-1.15480006	3.51400263
1	4.15847749	0.84025567	4.34307314
6	2.80652619	2.27250753	3.45102777
1	3.36242921	3.14178695	3.80728723
6	1.63923085	2.45337616	2.68424872
1	1.28433695	3.46249227	2.45568450
1	0.72187251	-1.78972890	-0.71768225
1	-0.29410323	-0.71974622	-1.84883281

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XYZ file for : **TS2-N**

6	-0.04901840	1.50908991	1.43429574
6	-1.19675221	0.68910411	1.77982691
6	-0.87196430	-0.66813411	2.05194282
7	0.47660663	-1.07795893	1.99471527
6	1.40730786	-0.11238708	2.52231405
6	1.16353110	1.25179929	2.24841960
1	-2.22224059	1.04807292	1.86785131
1	-1.62418488	-1.39177189	2.37706082
1	-0.23992557	2.54857978	1.15473943
42	-0.29344107	-0.27247878	-0.05834596
15	-1.73103770	0.95234346	-1.62896266
15	-1.51126594	-2.39878319	-0.31310358
15	1.85793745	0.44102038	-1.03481678
6	-0.94894920	-3.82321886	0.76756204
6	-3.35144402	-2.44477764	0.04768769
6	-1.48236023	-3.28798468	-1.94975225
6	-1.13474518	2.57313160	-2.37479383
6	-2.36570993	0.15444192	-3.19494556
6	-3.34885995	1.59054141	-0.92922605
1	-3.74619799	-3.47134683	0.00264810
1	-3.54396232	-2.02797391	1.04609133
1	-3.87903629	-1.82291422	-0.68869074
1	-1.62679958	-4.68451451	0.67280352

1	0.06080373	-4.11570477	0.44848923
1	-0.88820051	-3.51403584	1.81889095
1	-2.05563933	-4.22576075	-1.89714461
1	-1.89696014	-2.64727020	-2.73711545
1	-0.43651800	-3.50767489	-2.20126115
1	-3.94470632	2.10749165	-1.69688826
1	-3.92702970	0.75266521	-0.51730659
1	-3.13419248	2.29428400	-0.11300602
1	-1.91903260	3.06647417	-2.96993800
1	-0.82177675	3.24270016	-1.56147945
1	-0.26395105	2.38449905	-3.01779254
1	-2.92716584	0.87514989	-3.80800290
1	-1.51675985	-0.23571774	-3.77236641
1	-3.02682800	-0.68417369	-2.93803627
6	3.37343992	-0.42590356	-0.37537621
6	2.11505177	0.13883601	-2.85776009
6	2.43877534	2.21446206	-0.93481572
1	3.11117674	0.48025459	-3.17775313
1	2.00953523	-0.93663694	-3.05114536
1	1.34556173	0.66739015	-3.43615142
1	3.42411721	2.32981501	-1.41137655
1	1.71272135	2.86775404	-1.43604395
1	2.50992445	2.50970743	0.11974507
1	4.28042992	-0.07594257	-0.89103053
1	3.46550033	-0.23391764	0.70152889
1	3.25390722	-1.50699263	-0.52803976
6	2.50427325	-0.51048937	3.28450991
6	3.40875868	0.46020654	3.75782609
1	2.65737088	-1.57284806	3.48446020
1	4.28827231	0.15209504	4.32561597
6	3.17949069	1.81263150	3.49292896
1	3.88060083	2.56653296	3.85632560
6	2.04665983	2.21171285	2.75765045
1	1.86223403	3.27327385	2.57086981
1	0.74512876	-1.56108781	0.66124267
1	0.00529621	-1.00602919	-1.61252078

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XYZ file for : 3-N

6	0.19736993	1.70220509	1.32710985
6	-1.07327731	1.07701676	1.63938145
6	-1.03166728	-0.29167884	2.01784827
7	0.32479828	-0.81261053	2.06112637
6	1.35327397	0.00307283	2.64012411
6	1.33069536	1.34278157	2.18987980
1	-2.02131717	1.61381909	1.66151706

1	-1.83008021	-0.82947049	2.52568108
1	0.16969102	2.73095749	0.96365183
42	-0.38389611	-0.14640389	-0.10165543
15	-1.93441735	1.16954214	-1.37023133
15	-1.30292287	-2.35930115	-0.43274516
15	1.77514268	0.09041182	-1.21244161
6	-0.86215043	-3.66295935	0.86086587
6	-3.16281044	-2.63941157	-0.43067601
6	-0.88402777	-3.35727064	-1.95845295
6	-1.70261125	3.03844336	-1.36656843
6	-2.13958906	0.91371110	-3.20940764
6	-3.75514986	1.15434327	-0.88269485
1	-3.42236989	-3.70970113	-0.46164542
1	-3.59521830	-2.18180128	0.47006560
1	-3.59491837	-2.14017403	-1.30910775
1	-1.30339789	-4.63853880	0.60800036
1	0.23075726	-3.77359708	0.91320173
1	-1.24397581	-3.36625849	1.84940432
1	-1.38715447	-4.33643059	-1.96038014
1	-1.18486182	-2.78829222	-2.84854919
1	0.20356585	-3.50627580	-1.99938397
1	-4.34013967	1.88486631	-1.46299167
1	-4.16568912	0.14953779	-1.04740016
1	-3.85241503	1.38842559	0.18690212
1	-2.47980609	3.54275138	-1.96102454
1	-1.74733140	3.41511991	-0.33501654
1	-0.71282046	3.28079438	-1.77618530
1	-2.89403964	1.59358595	-3.63282538
1	-1.17297610	1.08534070	-3.70238953
1	-2.43984546	-0.12693434	-3.39402594
6	3.29003753	-0.43375719	-0.24393432
6	2.12694498	-0.80838322	-2.81229020
6	2.31542611	1.80842939	-1.72065688
1	3.14262710	-0.59461391	-3.17932077
1	2.02031278	-1.88912287	-2.64742763
1	1.39010187	-0.50205635	-3.56686895
1	3.32322023	1.79996084	-2.16508673
1	1.59735477	2.20573742	-2.45109184
1	2.30731043	2.45766594	-0.83536775
1	4.20480788	-0.26796205	-0.83294455
1	3.35044101	0.13732303	0.69102428
1	3.20563596	-1.50093740	0.00337080
6	2.34562119	-0.48189728	3.48618322
6	3.39174341	0.37493257	3.87552240
1	2.33004394	-1.52351804	3.81809285
1	4.19003817	0.00041477	4.51744138

6	3.40378999	1.70031799	3.42721916
1	4.21741000	2.36558525	3.72235698
6	2.37494455	2.18636829	2.60346486
1	2.38565128	3.22745839	2.27171278
1	0.37842299	-1.79698379	2.31255977
1	-0.43697321	-0.58513130	-1.76427264

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XYZ file for : 4-N

6	0.19013782	1.80856443	1.44162305
6	-1.07741826	1.19140876	1.78125193
6	-1.03183642	-0.16876997	2.18821434
7	0.32455776	-0.68990973	2.23046823
6	1.35936948	0.13800927	2.77986104
6	1.33273188	1.46724879	2.29982968
1	-2.02494851	1.72915240	1.80207908
1	-1.82571432	-0.69494085	2.71491793
1	0.15816436	2.82971478	1.05765045
42	-0.40588909	-0.06943705	0.05966258
15	-1.96397418	1.22339878	-1.22337351
15	-1.33050048	-2.28896966	-0.21020068
15	1.74307566	0.14476703	-1.07445085
6	-0.91557033	-3.55129140	1.13138406
6	-3.19117058	-2.56097660	-0.23009253
6	-0.89191084	-3.33821007	-1.69572047
6	-1.73119325	3.09169116	-1.25257605
6	-2.17907343	0.93747848	-3.05691648
6	-3.78188340	1.21692216	-0.72529946
1	-3.45546242	-3.63056058	-0.23634844
1	-3.63533270	-2.07721156	0.65103452
1	-3.60625420	-2.08363016	-1.12868198
1	-1.36325903	-4.53066146	0.90617844
1	0.17559581	-3.67135054	1.19886406
1	-1.30449036	-3.21807119	2.10528253
1	-1.39491060	-4.31712512	-1.67120492
1	-1.18184357	-2.79983946	-2.60817731
1	0.19622195	-3.48785876	-1.71696809
1	-4.37000666	1.93906721	-1.31289192
1	-4.19402989	0.21010743	-0.87281108
1	-3.87252328	1.46663693	0.34136412
1	-2.51137581	3.58578814	-1.85165894
1	-1.77034096	3.48667354	-0.22770992
1	-0.74363965	3.32621343	-1.67201739
1	-2.93708461	1.60940397	-3.48665770
1	-1.21569551	1.10332834	-3.55809423
1	-2.47851454	-0.10631599	-3.22389722

6	3.25611313	-0.42085341	-0.12613561
6	2.06235103	-0.73932621	-2.68915864
6	2.31324485	1.85764248	-1.56643793
1	3.08118702	-0.54707320	-3.05935074
1	1.92677381	-1.81911601	-2.54076577
1	1.33027110	-0.40040274	-3.43452578
1	3.31499572	1.83342641	-2.02366929
1	1.59485360	2.28002366	-2.28230863
1	2.33094785	2.49503908	-0.67276536
1	4.17015051	-0.26083658	-0.71791662
1	3.33177412	0.13413329	0.81749423
1	3.15477403	-1.49034643	0.10437271
6	2.35995431	-0.32814663	3.62689174
6	3.41041277	0.53661089	3.98601126
1	2.34704836	-1.36180490	3.98289260
1	4.21481631	0.17625860	4.62840813
6	3.41883325	1.85123354	3.50713464
1	4.23558658	2.52257322	3.77892646
6	2.38182749	2.31907120	2.68306874
1	2.38923461	3.35258231	2.32829815
1	0.37972152	-1.66809308	2.50460663
1	-0.48282222	-0.55501890	-1.58900239
1	-0.93405778	-1.62127950	-5.98065687
1	-0.58914976	-1.65521321	-5.31336821

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XYZ file for : **TS3-N**

6	0.22750653	2.77868592	2.19786761
6	-0.95153616	2.12814646	1.90748288
6	-1.08431306	0.69263021	1.89968250
7	0.20002720	0.00896770	2.05808322
6	1.26857364	0.63416848	2.78405021
6	1.34012905	2.04989587	2.76638354
1	-1.84530831	2.70878542	1.66799589
1	-1.95219880	0.21245166	2.36425732
1	0.30502952	3.86141559	2.08947869
42	-0.32137082	0.29463321	-0.14318569
15	-2.34728488	1.04953441	-1.23997560
15	-1.00471620	-1.92229967	-0.24095488
15	1.98523414	-0.15116519	-0.95570038
6	-0.25521341	-3.14665280	1.00805413
6	-2.79757526	-2.41127811	0.10577687
6	-0.74950514	-2.96784053	-1.78773110
6	-2.34069838	2.79563642	-1.93318402
6	-2.99129237	0.17391836	-2.75966738
6	-3.94281742	1.16715132	-0.25128943

1 -2.92226541 -3.50477247 0.13659582
1 -3.10164839 -1.98867342 1.07437725
1 -3.46218972 -2.00514672 -0.66821966
1 -0.55286256 -4.18128442 0.78021364
1 0.84112260 -3.08275669 1.00342648
1 -0.61882082 -2.91902765 2.02370062
1 -1.18463183 -3.97490459 -1.68764266
1 -1.20414506 -2.45204848 -2.64432656
1 0.32860841 -3.06021051 -1.98160151
1 -4.76865679 1.55414931 -0.86747444
1 -4.21365545 0.17711720 0.13764312
1 -3.79361638 1.84090061 0.60393433
1 -3.30843291 3.04550339 -2.39374069
1 -2.12679272 3.50898153 -1.12563284
1 -1.54421024 2.87766328 -2.68479711
1 -3.90434046 0.66049861 -3.13426521
1 -2.21094774 0.20500080 -3.53137048
1 -3.21090714 -0.87715220 -2.53290167
6 2.96965871 -1.61105900 -0.31467961
6 2.23009317 -0.36650674 -2.78752692
6 3.25084896 1.18998355 -0.61037224
1 3.28982073 -0.54258402 -3.02693540
1 1.62282240 -1.20950402 -3.14037181
1 1.87995841 0.54205368 -3.29424233
1 4.24528606 0.90957140 -0.99011654
1 2.92594361 2.12422395 -1.08691440
1 3.31131266 1.35980739 0.47379393
1 3.99302953 -1.60512822 -0.72032190
1 3.02000819 -1.55993804 0.78188684
1 2.47316259 -2.54747696 -0.60263463
6 2.24909329 -0.13191435 3.41527320
6 3.36026116 0.49471680 4.00296250
1 2.16339701 -1.22224795 3.42731354
1 4.13368890 -0.10832100 4.48035415
6 3.47028274 1.89042371 3.96074954
1 4.33620348 2.38342772 4.40560654
6 2.46798367 2.65701157 3.35588960
1 2.54393774 3.74680577 3.34300518
1 0.09640337 -0.96966436 2.32039760
1 -0.35864447 0.37261227 -1.90434806
1 0.57281468 3.01766494 -0.87778314
1 0.39334602 2.33234011 -1.17713200

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XYZ file for : 5-N

6 0.55715322 2.03675093 1.29316003

6	-0.83927191	1.69725194	1.39291868
6	-1.00097208	0.30590969	1.78233662
7	-0.14661527	-0.17327566	2.83605306
6	1.10835904	0.35669933	3.05353521
6	1.49694415	1.48919535	2.27588728
1	-1.63547430	2.44468205	1.43894568
1	-2.02652924	-0.03693254	1.94154000
1	0.80682011	3.03620314	0.92315203
42	-0.29747778	0.58560279	-0.41796443
15	-2.58700598	1.27794426	-1.02245752
15	-0.96062495	-1.79555408	-0.39836391
15	2.10595878	-0.10878596	-0.71138803
6	0.08778960	-3.02431613	0.54782675
6	-2.64017438	-2.32634056	0.24714934
6	-1.04540516	-2.68580008	-2.04184740
6	-2.75606379	3.08700507	-1.46741555
6	-3.39170491	0.53144615	-2.53306880
6	-4.02595687	1.16395642	0.18011350
1	-2.75212141	-3.41753882	0.16381231
1	-2.76051025	-2.03468775	1.29854282
1	-3.43425429	-1.84799648	-0.34131464
1	-0.41031297	-4.00339640	0.60801589
1	1.05075455	-3.15054127	0.03626772
1	0.28664799	-2.64514854	1.55837573
1	-1.29765093	-3.74946463	-1.91244731
1	-1.80468680	-2.20155412	-2.66986012
1	-0.08261736	-2.59300557	-2.55869298
1	-4.93301587	1.60620325	-0.25774818
1	-4.22854520	0.11616335	0.43666141
1	-3.78251734	1.70236356	1.10657989
1	-3.79879094	3.35769417	-1.69260383
1	-2.39201318	3.70030565	-0.63136903
1	-2.12815516	3.29254942	-2.34530693
1	-4.35268687	1.01813226	-2.75715991
1	-2.70591153	0.64765507	-3.38250566
1	-3.56299008	-0.54234244	-2.37619266
6	3.17415165	-1.00014724	0.54353772
6	2.45699686	-1.18033950	-2.20505349
6	3.26885135	1.30036567	-1.10621506
1	3.54015545	-1.25682285	-2.38391640
1	2.05716136	-2.19122714	-2.04631709
1	1.96213649	-0.74420632	-3.08239528
1	4.29371096	0.93468353	-1.26994964
1	2.91546906	1.81368913	-2.01112505
1	3.26867838	2.01109781	-0.27012470
1	4.16795736	-1.19763287	0.11341746

1	3.28343963	-0.38043004	1.44152415
1	2.71206070	-1.95115324	0.83462055
6	1.99314272	-0.18320461	4.00622313
6	3.24960758	0.39199418	4.21647867
1	1.68613721	-1.05810574	4.58651425
1	3.92380325	-0.04021042	4.95782420
6	3.63428156	1.52636327	3.48354464
1	4.60694037	1.98974272	3.65541328
6	2.75777918	2.06301177	2.53364924
1	3.04822353	2.95610799	1.97278884
1	-0.33453538	-1.09444504	3.21674820
1	-0.43205673	0.16168106	-2.12181939
1	-0.19088857	2.15063167	-1.35751970
1	0.65692369	1.89100312	-1.27827589

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XYZ file for : **TS4-N**

6	-0.19604321	1.74577362	1.64700629
6	-1.06461075	0.57460516	1.82031505
6	-0.27333657	-0.62492683	1.98154968
7	0.86663839	-0.55277802	2.85532042
6	1.57362176	0.61743251	3.01817530
6	1.06214004	1.80929734	2.43060678
1	-2.11756510	0.66377422	2.09012212
1	-0.81941291	-1.55482773	2.16352531
1	-0.72190375	2.70775153	1.59217956
42	-0.29720409	0.24287066	-0.19775797
15	-2.30027675	1.43853929	-0.99136883
15	-1.24449951	-2.00767868	-0.63375154
15	2.05415725	-0.48250613	-0.52842221
6	-0.30448349	-3.55318058	-0.12531333
6	-2.88405265	-2.42828332	0.17943547
6	-1.61760166	-2.50147033	-2.39303549
6	-1.91079113	3.08655345	-1.79307513
6	-3.38959020	0.74526764	-2.34483076
6	-3.63862577	1.98987948	0.19660796
1	-3.19947280	-3.45964131	-0.04079529
1	-2.79601575	-2.30494782	1.26824678
1	-3.65208634	-1.72810280	-0.17619913
1	-0.89164203	-4.46295293	-0.32271815
1	0.63528535	-3.60702588	-0.69168225
1	-0.06185275	-3.50686262	0.94488290
1	-2.04029133	-3.51631028	-2.43883081
1	-2.32193517	-1.78923483	-2.83791734
1	-0.68596390	-2.46168009	-2.97264897
1	-4.39456425	2.60132300	-0.31779098

1	-4.12677773	1.10886486	0.63636420
1	-3.20006384	2.58134917	1.01253067
1	-2.81714510	3.59004043	-2.16257490
1	-1.40643531	3.73309055	-1.06144225
1	-1.21831068	2.91009741	-2.62713020
1	-4.16128723	1.47278789	-2.63843812
1	-2.76165361	0.50916207	-3.21432041
1	-3.88115871	-0.17584695	-2.00362764
6	2.96496060	-1.72871194	0.53554205
6	2.43119369	-1.18776629	-2.21943176
6	3.33432676	0.88221974	-0.49384992
1	3.51080034	-1.35401481	-2.35778803
1	1.89756289	-2.13952421	-2.34879363
1	2.05941726	-0.48492526	-2.97639362
1	4.34457253	0.49209021	-0.69046324
1	3.07552764	1.62719993	-1.25864442
1	3.31387315	1.37199575	0.48936725
1	3.92861330	-1.99202049	0.07396472
1	3.16188989	-1.28185539	1.51863756
1	2.36455016	-2.63810328	0.66510314
6	2.78405220	0.66094416	3.74500965
6	3.47416054	1.86235246	3.90092209
1	3.17079710	-0.25782469	4.19468074
1	4.40754300	1.87715571	4.46654391
6	2.97020961	3.04779663	3.33785753
1	3.50545253	3.98969817	3.46442957
6	1.77501987	3.00736408	2.61474902
1	1.37854687	3.92491796	2.17005629
1	1.37303032	-1.41663871	3.02003012
1	-0.38167683	0.08738439	-1.95521668
1	0.31304805	1.91204322	0.15671139
1	0.55999599	1.65272567	-0.86297826

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XYZ file for : **6-N**

6	-0.12840266	1.81151951	1.58628218
6	-0.93331675	0.54814179	1.75235797
6	-0.06488143	-0.59618072	1.91897929
7	1.11694053	-0.43410971	2.72574061
6	1.65413880	0.78984929	3.03901919
6	1.04057236	1.96404120	2.52844080
1	-1.95124673	0.60561505	2.13953006
1	-0.54651908	-1.54702617	2.16495998
1	-0.76683176	2.70675897	1.59496402
42	-0.27339287	0.10833937	-0.28353981
15	-2.19245252	1.47113577	-1.03639756

15	-1.34954645	-2.06133854	-0.54359336
15	2.04346835	-0.60360940	-0.69196800
6	-0.40562875	-3.64056036	-0.15282844
6	-2.85941516	-2.38154379	0.52904276
6	-2.02849046	-2.58746456	-2.19673426
6	-1.77820108	3.24756393	-1.47425840
6	-3.10100647	1.01559941	-2.60313601
6	-3.65995806	1.78112223	0.08290646
1	-3.23128297	-3.41126578	0.41509170
1	-2.61476279	-2.20382840	1.58569057
1	-3.65014110	-1.67489807	0.24158876
1	-1.05890947	-4.52522371	-0.20093731
1	0.40495436	-3.75566593	-0.88562138
1	0.03858079	-3.57155890	0.84914291
1	-2.50692122	-3.57586004	-2.13070822
1	-2.75824928	-1.85135223	-2.55397005
1	-1.20145854	-2.62455309	-2.91821712
1	-4.39652042	2.43997010	-0.40087691
1	-4.13850160	0.82536826	0.33667146
1	-3.32364771	2.25185451	1.01727954
1	-2.67055906	3.81479529	-1.78052031
1	-1.31233681	3.74382963	-0.61160396
1	-1.04606996	3.23615993	-2.29282169
1	-3.78584964	1.81987370	-2.91151386
1	-2.36738474	0.82640718	-3.39759144
1	-3.68234079	0.09890388	-2.43607525
6	2.92309993	-2.03266754	0.14705779
6	2.44395094	-1.00851070	-2.46928246
6	3.32524341	0.72241288	-0.37438093
1	3.52340462	-1.17030034	-2.61088855
1	1.89413846	-1.91171994	-2.76681293
1	2.10252219	-0.17769354	-3.09989059
1	4.33685713	0.37796294	-0.63846998
1	3.06660022	1.60468902	-0.97512900
1	3.30356791	1.00869102	0.68615398
1	3.94865659	-2.13606769	-0.23881141
1	2.97355351	-1.84246419	1.22712256
1	2.37790365	-2.96963327	-0.02029450
6	2.80117280	0.91274963	3.85966327
6	3.30787671	2.16964908	4.18113228
1	3.28141202	0.01003866	4.24687407
1	4.19098196	2.24299728	4.81887151
6	2.68935892	3.33599533	3.69903972
1	3.08217387	4.31939568	3.95903388
6	1.56517116	3.21606983	2.87566451
1	1.08247899	4.11506417	2.48130417

1 1.66005220 -1.26007721 2.94750869
1 -0.48486980 -0.37576307 -1.93570700
1 0.34229376 1.85638568 0.50552327
1 0.49611283 1.13732981 -1.45900826

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XYZ file for : 7-N

6 -0.25152677 1.83694409 1.17368720
6 -1.12668584 0.61863147 1.32926300
6 -0.31932878 -0.54579402 1.62995059
7 0.78499968 -0.38541183 2.54217725
6 1.35349147 0.83152292 2.83108747
6 0.84040645 1.99519184 2.20277056
1 -2.16792532 0.74106814 1.63330808
1 -0.85163682 -1.46843218 1.87320049
1 -0.84435482 2.75634925 1.08396060
42 -0.29921991 0.03155568 -0.61195051
15 -2.07019720 1.36913402 -1.67881066
15 -1.49568106 -2.06936724 -0.88648566
15 2.00716612 -0.80831745 -0.75262656
6 -0.60502056 -3.70855816 -0.66731727
6 -2.94621393 -2.40319196 0.26203830
6 -2.32721633 -2.44525210 -2.51428682
6 -2.04644809 3.23344206 -1.45140894
6 -2.08472404 1.32474295 -3.54261246
6 -3.88903382 1.09441389 -1.31902225
1 -3.40421194 -3.37990557 0.04503884
1 -2.61864358 -2.39393132 1.31061219
1 -3.69698193 -1.61196704 0.13574713
1 -1.28605463 -4.56406879 -0.79490930
1 0.20294914 -3.77620010 -1.40888250
1 -0.16185555 -3.74495871 0.33725871
1 -2.84230387 -3.41654180 -2.47852732
1 -3.05720929 -1.66084776 -2.75346610
1 -1.56517750 -2.45989806 -3.30484547
1 -4.52092570 1.81728390 -1.85753413
1 -4.18024740 0.07724527 -1.61385739
1 -4.06000208 1.20066363 -0.23851317
1 -2.79093004 3.71949295 -2.09969715
1 -2.27257290 3.49210072 -0.40790317
1 -1.04478627 3.61128416 -1.69771397
1 -2.87950412 1.96592861 -3.95283965
1 -1.10501636 1.66925802 -3.89926155
1 -2.22461642 0.29240092 -3.88675698
6 2.70627029 -2.26336992 0.20297889
6 2.56652459 -1.28412603 -2.46778617

6	3.32365368	0.45361560	-0.33462086
1	3.64104550	-1.52134538	-2.48662942
1	1.99030088	-2.15435025	-2.80962538
1	2.35477825	-0.44763265	-3.14594064
1	4.33485792	0.04849475	-0.49312674
1	3.17351956	1.33353151	-0.97465525
1	3.21703225	0.76758716	0.71268114
1	3.76388765	-2.42460506	-0.05569594
1	2.63747889	-2.06219788	1.28009179
1	2.13712539	-3.17378095	-0.02218786
6	2.43050918	0.95505011	3.74077263
6	2.96636507	2.20717041	4.03318539
1	2.83240353	0.05836796	4.22016076
1	3.79471461	2.28265389	4.74034314
6	2.44493237	3.36643663	3.43388921
1	2.85941596	4.34677958	3.67091137
6	1.38965434	3.24370889	2.52421983
1	0.98399447	4.13635292	2.03922141
1	1.28775770	-1.21843001	2.82543787
1	-0.33622369	-0.61663828	-2.22292611
1	0.30199788	1.80796804	0.13374926
1	0.61465221	0.96713144	-1.76831514
1	-1.17308440	-1.99238183	5.13870937
1	-0.79634423	-1.46767854	4.75221968

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XYZ file for : **TS5-N**

6	-0.01542429	2.32455703	1.12899072
6	-1.02955531	1.23721844	0.75603457
6	-0.88647947	-0.05695564	1.37744712
7	0.26905502	-0.22990030	2.22875922
6	0.67616627	0.83910795	3.03285453
6	0.51284501	2.15534401	2.54020307
1	-2.06447771	1.59582812	0.71218136
1	-1.80007350	-0.50473999	1.79576535
1	-0.47040995	3.32164815	1.02135552
42	-0.82181985	-0.33184213	-0.90284543
15	-1.22784006	1.59828980	-2.36824713
15	-1.13530411	-2.66505827	-0.24696206
15	1.50026730	-0.55571118	-1.39089934
6	-1.01918583	-3.97326278	-1.57600935
6	-0.19779648	-3.52659211	1.13676284
6	-2.86902311	-3.05322642	0.36046577
6	-0.29768013	3.22589212	-2.30667037
6	-1.18179685	1.28076507	-4.20838206
6	-2.96580186	2.29432767	-2.24511021

1	-0.42687999	-4.60273770	1.16144321
1	0.88474967	-3.38779316	1.01874601
1	-0.50274210	-3.08993913	2.09896018
1	-1.37643578	-4.94724328	-1.20915517
1	-1.62934685	-3.64961481	-2.42948560
1	0.01943343	-4.07444490	-1.91439797
1	-2.95489586	-4.10772807	0.66324560
1	-3.12008184	-2.41222021	1.21704174
1	-3.58342134	-2.84776326	-0.44765226
1	-3.10275344	3.13870343	-2.93732588
1	-3.68745093	1.50380097	-2.48982059
1	-3.15748605	2.63607435	-1.21866699
1	-0.66096413	3.91261009	-3.08637590
1	-0.44464207	3.69083533	-1.32330979
1	0.77831812	3.05946502	-2.44806205
1	-1.53834724	2.15482865	-4.77387347
1	-0.15638977	1.04283275	-4.51855514
1	-1.81623747	0.41145849	-4.42530780
6	2.24627120	-2.24971162	-1.67605834
6	2.22407627	0.25683181	-2.91397000
6	2.70587734	0.08632883	-0.10675961
1	3.30884559	0.08208283	-2.97129182
1	1.74332342	-0.16509567	-3.80702550
1	2.03877412	1.33817319	-2.88842153
1	3.73847986	-0.16554914	-0.39050740
1	2.61686745	1.17777327	-0.02169570
1	2.46444489	-0.35367536	0.86946487
1	3.32566289	-2.17160478	-1.87431694
1	2.09173099	-2.88551329	-0.79483725
1	1.75372794	-2.71345989	-2.54135241
6	1.28045707	0.63559828	4.28989599
6	1.69572324	1.72537925	5.05894229
1	1.41222148	-0.38308566	4.66541544
1	2.15629485	1.55071399	6.03329964
6	1.50476959	3.03355491	4.59383281
1	1.81473974	3.88666737	5.19871322
6	0.91423370	3.23261923	3.33876002
1	0.77624929	4.24899859	2.95899205
1	0.34026241	-1.13972927	2.67406742
1	-1.94990482	-0.94852080	-2.04573195
1	0.84436433	2.31349987	0.43708312
1	-0.30300617	-1.05746865	-2.42384171
1	-3.65292334	-0.30472387	-0.70822744
1	-4.07516998	-0.04023016	-0.13933850

XYZ file for : **8-N**

6	0.25005281	2.40628059	1.03065640
6	-0.86250162	1.39338309	0.74303977
6	-0.73787611	0.08229293	1.30143142
7	0.46051648	-0.19319510	2.06993261
6	1.01183463	0.83550503	2.84322270
6	0.90506386	2.16781081	2.37792696
1	-1.86792918	1.81400365	0.79951003
1	-1.63372034	-0.35975084	1.74788551
1	-0.15276275	3.43076091	0.99608701
42	-0.81164923	-0.17237126	-1.00909411
15	-1.87067128	1.60795052	-2.27192487
15	-1.45007730	-2.54406527	-0.50130814
15	1.69746549	-0.70076431	-0.96182091
6	-1.02114098	-3.81507785	-1.79756972
6	-0.92693500	-3.46064930	1.04682122
6	-3.28760897	-2.81101809	-0.37840566
6	-1.43171319	3.39119198	-1.96122335
6	-1.59488730	1.51993563	-4.11137875
6	-3.72934398	1.71685908	-2.20884809
1	-1.34568124	-4.47819983	1.06291020
1	0.16688567	-3.52300114	1.10586185
1	-1.29741721	-2.91406920	1.92573742
1	-1.44395200	-4.80100008	-1.55310949
1	-1.41592649	-3.46659449	-2.76093587
1	0.06987007	-3.89926487	-1.89121360
1	-3.52779457	-3.87521358	-0.23341109
1	-3.67570772	-2.22145993	0.46239449
1	-3.75532670	-2.44031954	-1.29920371
1	-4.11055765	2.51333522	-2.86548261
1	-4.14565939	0.74803574	-2.51408646
1	-4.03710771	1.91035826	-1.17261438
1	-1.96131651	4.04980506	-2.66561379
1	-1.70713190	3.66476781	-0.93464979
1	-0.34763512	3.51982105	-2.07699687
1	-2.12682752	2.32795989	-4.63556422
1	-0.51735062	1.59214924	-4.30936540
1	-1.94434082	0.54422975	-4.47295189
6	2.36059391	-2.25070216	-0.14902731
6	2.43477626	-0.90762081	-2.65867890
6	2.91804156	0.52013190	-0.25656609
1	3.52348859	-1.05681360	-2.60006447
1	1.96427534	-1.76637341	-3.15408055
1	2.21007980	-0.00961911	-3.24859081
1	3.94233726	0.13888500	-0.38296363
1	2.81792541	1.47256222	-0.79478793

1	2.72436545	0.69044253	0.80906340
1	3.44553398	-2.33578492	-0.31053096
1	2.16349231	-2.19902107	0.92990579
1	1.86938805	-3.14021933	-0.56559721
6	1.70867613	0.56690761	4.03923333
6	2.27398489	1.60858213	4.77798720
1	1.79425648	-0.46496108	4.39198096
1	2.80458117	1.38376902	5.70529084
6	2.14518923	2.93452288	4.34187483
1	2.57473367	3.75206998	4.92236605
6	1.45990827	3.19734008	3.14867959
1	1.36439622	4.22739241	2.79376124
1	0.44751403	-1.09346156	2.54125537
1	-0.23312429	-0.83592282	-2.50969079
1	1.02752429	2.36875214	0.25041794
1	0.28203299	1.01279322	-1.70877745
1	-2.46181466	-0.13335127	-0.46904217
1	-1.86881018	-0.84405412	-2.17183004

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XYZ file for : **TS6-N**

6	0.23610122	2.38577206	0.99165759
6	-0.95265562	1.43549408	0.85594023
6	-1.04978402	0.34949578	1.74028374
7	-0.08513442	0.17595276	2.74126645
6	0.68165108	1.25141642	3.20240487
6	0.81842871	2.39904683	2.39327018
1	-1.90693409	1.85946387	0.54886839
1	-2.03084575	-0.06890908	1.95256880
1	-0.07178937	3.40616769	0.71496927
42	-0.90638021	-0.44692687	-0.76139851
15	-1.45838952	1.37271447	-2.35891783
15	-1.31272755	-2.80910564	-0.66382043
15	1.59210218	-0.51544271	-0.87802508
6	-1.15630447	-3.78889220	-2.24631683
6	-0.37787961	-3.94006633	0.50091711
6	-3.05178544	-3.28972406	-0.17300765
6	-0.60231962	3.04029975	-2.42656186
6	-1.34829478	0.91272425	-4.16146168
6	-3.22945505	1.96595191	-2.28560376
1	-0.71076149	-4.98403156	0.39657221
1	0.70021287	-3.88114776	0.30224062
1	-0.55294281	-3.60456517	1.53265594
1	-1.46379580	-4.83539050	-2.09967871
1	-1.78960919	-3.31705958	-3.00894962
1	-0.11613304	-3.75506587	-2.59496479

1 -3.19104496 -4.38177000 -0.17897457
1 -3.25778365 -2.89223981 0.82972000
1 -3.75077106 -2.81437980 -0.87296943
1 -3.44150788 2.72362850 -3.05545658
1 -3.88594129 1.09635262 -2.41753257
1 -3.43079311 2.38867942 -1.29145667
1 -1.01849813 3.66006369 -3.23545841
1 -0.73662153 3.56774663 -1.47298686
1 0.47295921 2.89840645 -2.59708698
1 -1.72596905 1.72208229 -4.80423633
1 -0.30121769 0.69763721 -4.41262755
1 -1.93390533 -0.00074333 -4.32631559
6 2.34632980 -2.02243068 -1.69422471
6 2.54658238 0.76806237 -1.87179792
6 2.64533395 -0.49838622 0.67657064
1 3.62690998 0.55483083 -1.89137232
1 2.15768070 0.76815344 -2.90009837
1 2.38866113 1.76804999 -1.44387676
1 3.70892976 -0.64534442 0.43437734
1 2.53288825 0.45398220 1.21106300
1 2.30726969 -1.30420273 1.34287689
1 3.44464232 -1.95308679 -1.71907692
1 2.05672075 -2.92812718 -1.14557654
1 1.95991254 -2.10038824 -2.71928026
6 1.30201695 1.19880269 4.46505035
6 2.03909102 2.28886515 4.93150847
1 1.19514710 0.30279789 5.08205087
1 2.51607534 2.23493081 5.91157766
6 2.15458759 3.44726378 4.15184619
1 2.72250050 4.30422042 4.51581456
6 1.53959605 3.49030018 2.89491198
1 1.63554235 4.38524943 2.27430863
1 -0.22437491 -0.59274166 3.38741904
1 -2.05643223 -0.93681058 -1.92482261
1 1.03402211 2.11747751 0.27868433
1 -0.20838869 -0.96962517 -2.25522248
1 -2.59736775 -0.33303926 -0.28921062
1 -0.78687550 -1.19836682 0.83469748

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XYZ file for : **9-N**

6 0.52679173 2.19572721 0.95453177
6 -0.69795615 1.29442320 0.74605071
6 -0.74950753 0.13192611 1.69018656
7 0.35277617 0.07659230 2.65441801
6 0.72462106 1.29217975 3.25389541

6	0.80493790	2.43002994	2.42211310
1	-1.62410130	1.87346881	0.79586068
1	-1.73300822	0.03785656	2.17428056
1	0.39306389	3.15653089	0.43705409
42	-0.84979205	-0.42774733	-0.76107603
15	-1.40665307	1.39781797	-2.28167456
15	-1.36771508	-2.81464659	-0.62937992
15	1.64148272	-0.62275366	-1.07519957
6	-1.27308861	-3.79990511	-2.20734735
6	-0.43884863	-3.95111365	0.53819100
6	-3.11305519	-3.23074612	-0.10249127
6	-0.38263255	2.95126236	-2.49413474
6	-1.60356542	0.93252240	-4.07499271
6	-3.07035511	2.18090805	-1.96097474
1	-0.82951458	-4.97950300	0.49482651
1	0.62882686	-3.95469876	0.28082839
1	-0.54176559	-3.57485640	1.56627976
1	-1.61831741	-4.83260310	-2.04783222
1	-1.90457061	-3.30760768	-2.95831492
1	-0.24083461	-3.80621284	-2.57830827
1	-3.29405126	-4.31657246	-0.09403972
1	-3.28967567	-2.81635364	0.89934045
1	-3.80782583	-2.73751654	-0.79471673
1	-3.29956936	2.96379369	-2.69978890
1	-3.83333913	1.39286697	-1.99502951
1	-3.07652561	2.61513620	-0.95223261
1	-0.83518690	3.61045725	-3.25060845
1	-0.32466668	3.49093478	-1.54062325
1	0.63537857	2.68692635	-2.80719764
1	-1.96752927	1.78321503	-4.67019380
1	-0.63368562	0.59585631	-4.46510845
1	-2.31092954	0.09639341	-4.14713556
6	2.21561573	-2.07097711	-2.11101699
6	2.64155349	0.70236313	-1.96309931
6	2.77195793	-0.89575466	0.39891150
1	3.70605702	0.43013579	-2.03571970
1	2.23090738	0.82347652	-2.97579429
1	2.55023478	1.66140439	-1.43551854
1	3.81480030	-1.02986381	0.07304096
1	2.71323887	-0.05129979	1.09684934
1	2.44018685	-1.79506105	0.93683838
1	3.31116586	-2.07405315	-2.21779718
1	1.89888628	-3.00950156	-1.63645353
1	1.74803076	-2.00973438	-3.10267607
6	1.06048961	1.38973979	4.61568064
6	1.45988597	2.61960506	5.14988722

1	1.00387992	0.50446494	5.25503881
1	1.71737439	2.68655066	6.20852475
6	1.51021559	3.76076346	4.33965654
1	1.80712084	4.72243436	4.76037201
6	1.18015999	3.65607593	2.98075780
1	1.23299040	4.53796638	2.33666460
1	0.24476449	-0.67914819	3.32855463
1	-2.14512672	-0.83856469	-1.78740674
1	1.42234367	1.72686345	0.51293128
1	-0.35299308	-0.95142012	-2.33086232
1	-2.48073271	-0.21044987	-0.17122859
1	-0.67762661	-0.92017017	1.12918245

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XYZ file for : **10-N**

6	0.73643129	2.49137578	1.44171516
6	-0.43319976	1.82105348	0.70067609
6	-1.25976695	0.89743594	1.54019950
7	-0.79077550	0.68311483	2.91348957
6	0.57725299	0.71774187	3.19496307
6	1.39687335	1.62096092	2.48006700
1	-1.06108719	2.62566833	0.29585605
1	-2.32490704	1.16290694	1.58078712
1	0.33997570	3.38657206	1.96811586
42	-0.52163130	0.01322777	-0.69711655
15	-2.06713646	1.43281107	-1.88933962
15	-0.93217024	-2.45821298	-0.53742080
15	1.94005159	-0.45503266	-0.55677057
6	0.28216444	-3.75689154	0.04906475
6	-2.34706245	-2.91645995	0.59723474
6	-1.49596615	-3.24786728	-2.12399963
6	-1.40732844	3.04799964	-2.55688902
6	-2.81564777	0.73533030	-3.44422381
6	-3.61971605	2.05063428	-1.04021138
1	-2.56181550	-3.99426529	0.54564561
1	-2.08122142	-2.65553766	1.63151923
1	-3.24021427	-2.34658147	0.31075576
1	-0.18185916	-4.75299884	-0.00483804
1	1.18919426	-3.75515151	-0.56800636
1	0.56344492	-3.54854399	1.08980663
1	-1.78895782	-4.29599267	-1.96079043
1	-2.34380674	-2.67511230	-2.51967001
1	-0.67832751	-3.19456478	-2.85411200
1	-4.21139973	2.70104445	-1.70189083
1	-4.22518237	1.18431750	-0.73954637
1	-3.35094269	2.61847823	-0.13767726

1	-2.19619200	3.63315965	-3.05291518
1	-0.97551065	3.63682334	-1.73663804
1	-0.60704370	2.81911528	-3.27292835
1	-3.44864168	1.47889929	-3.95105227
1	-2.00107566	0.41917437	-4.10857687
1	-3.41649124	-0.14766266	-3.18824290
6	2.87282142	-1.37538181	0.78805589
6	2.52626917	-1.42743201	-2.04919853
6	3.10354687	0.99114910	-0.76076719
1	3.61569074	-1.58554439	-2.02477304
1	2.01760719	-2.39889485	-2.09911882
1	2.24753747	-0.86094890	-2.94723813
1	4.13130527	0.62744364	-0.90892552
1	2.78698615	1.57658403	-1.63330312
1	3.07835897	1.62987316	0.12803514
1	3.94000757	-1.46255637	0.53130413
1	2.76871581	-0.83044347	1.73455323
1	2.45830526	-2.38185430	0.91968089
6	1.13040529	-0.06175795	4.22980750
6	2.47776617	0.07402069	4.57653987
1	0.49394145	-0.76738667	4.77112938
1	2.89022534	-0.53464950	5.38333166
6	3.29403253	0.97868073	3.88623657
1	4.34637237	1.08827434	4.15119294
6	2.74287567	1.73943899	2.84540485
1	3.37192420	2.45508158	2.30865512
1	-1.27342032	-0.07975713	3.38542662
1	-0.32430895	-0.56550319	-2.31847273
1	1.48043689	2.87937296	0.72978508
1	0.44204646	1.01828389	-1.70665676
1	-1.27745249	-0.19914383	1.06987632
1	-2.13736927	-0.58653499	-1.03587218
1	2.19077756	5.04094556	-2.01678378
1	1.89139213	4.37216845	-1.84770577

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XYZ file for : **TS7-N**

6	0.97851515	1.48069423	2.15416118
6	-0.31421321	1.22450196	1.34955864
6	-1.38427120	0.87014705	2.39146906
7	-1.02752765	-0.36480633	3.10617623
6	0.26670457	-0.47165527	3.62193665
6	1.29357565	0.38909178	3.16255092
1	-0.64858169	2.20874613	0.94010008
1	-1.49591944	1.70353351	3.12485479
1	0.87424828	2.43328596	2.71801190

42	-0.40869285	0.62647586	-0.87249452
15	-2.20682261	0.93568825	-2.43085681
15	-0.84221263	-1.71144324	-0.44202466
15	2.13541492	0.55966219	-1.03585869
6	0.43169097	-2.73042797	0.47221165
6	-2.35262908	-2.15392451	0.56214221
6	-1.09276761	-2.83921255	-1.90829231
6	-1.89280774	0.59518570	-4.24288503
6	-3.84020669	0.04762929	-2.23453868
6	-2.86150103	2.68664196	-2.55893484
1	-2.47367151	-3.24650128	0.61634012
1	-2.21089850	-1.74896974	1.57258014
1	-3.24481519	-1.70186282	0.11147675
1	0.05169159	-3.74411904	0.67203634
1	1.33786433	-2.80396241	-0.14380565
1	0.68344385	-2.23545387	1.41840736
1	-1.31346748	-3.86594881	-1.58016389
1	-1.91997041	-2.47155791	-2.52958851
1	-0.17989067	-2.83670205	-2.51892969
1	-3.70177327	2.75179886	-3.26685932
1	-3.19226118	3.01770720	-1.56511454
1	-2.05307226	3.34859199	-2.89873005
1	-2.78146695	0.81069445	-4.85507988
1	-1.05177579	1.21795106	-4.57504484
1	-1.60672285	-0.45793325	-4.36692255
1	-4.54151563	0.33727568	-3.03134872
1	-3.68854511	-1.03933802	-2.27259287
1	-4.26775169	0.30454644	-1.25626053
6	3.28495970	-0.41536565	0.07424080
6	2.73787612	-0.07918828	-2.68118453
6	3.01188391	2.21752044	-1.04311750
1	3.83408785	-0.01492407	-2.75079759
1	2.42338614	-1.12511937	-2.79477870
1	2.27559180	0.50813254	-3.48442383
1	4.08799114	2.09740844	-1.23924412
1	2.56431351	2.83982451	-1.83019878
1	2.87743577	2.72913594	-0.08035439
1	4.33493015	-0.15898747	-0.13307027
1	3.06303804	-0.23702541	1.13303362
1	3.13762975	-1.48556541	-0.12237917
6	0.57062168	-1.46441516	4.57880249
6	1.86394173	-1.60179308	5.08411374
1	-0.22453023	-2.13271342	4.92109738
1	2.07317921	-2.37525364	5.82565481
6	2.88567573	-0.75116517	4.64119184
1	3.89942415	-0.84962088	5.03137653

6	2.58432225	0.22880538	3.68770244
1	3.37337050	0.90331049	3.34138356
1	-1.74017434	-0.67994334	3.76088127
1	0.01816055	-0.46893136	-2.11820196
1	1.85343532	1.63096853	1.50511116
1	0.20089945	1.33409441	-2.34368938
1	-2.35933798	0.71377162	1.91105215
1	-2.03160786	0.77212036	-0.24798811
1	0.19387785	3.48025403	-0.73164729
1	-0.25178572	3.25863638	-1.30225470

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XYZ file for : **11-N**

6	0.86900826	1.64896368	2.25203268
6	-0.42893261	1.34123048	1.46330413
6	-1.38436505	0.67669991	2.46179666
7	-0.83088486	-0.57124813	3.01061281
6	0.46834700	-0.52205229	3.52664798
6	1.34458022	0.52840135	3.16114149
1	-0.90348590	2.31730242	1.28037140
1	-1.59231194	1.38197846	3.30122705
1	0.70076266	2.53887024	2.89552210
42	-0.43846704	0.74796824	-0.88799077
15	-2.18807935	1.00113130	-2.54348461
15	-0.94533581	-1.66572507	-0.38900586
15	2.11073060	0.54145532	-0.93861648
6	0.28628479	-2.74411802	0.50656789
6	-2.50706751	-2.10929442	0.53312464
6	-1.18524680	-2.75250109	-1.89205408
6	-1.80325396	0.55586458	-4.31651076
6	-3.83887090	0.14527284	-2.35683645
6	-2.80165285	2.74708930	-2.78236200
1	-2.66641394	-3.19778498	0.51400566
1	-2.40816733	-1.77583754	1.57144822
1	-3.36397803	-1.60139355	0.07284841
1	-0.13530321	-3.74470365	0.68662891
1	1.18422986	-2.84577218	-0.11778563
1	0.56124659	-2.27807883	1.45937749
1	-1.43207964	-3.78352298	-1.59705675
1	-1.99060287	-2.35738033	-2.52497488
1	-0.25860547	-2.75067962	-2.48148856
1	-3.58662686	2.80002550	-3.55185358
1	-3.19637453	3.11539285	-1.82593858
1	-1.95446389	3.38053417	-3.07860486
1	-2.65842922	0.75951400	-4.97811936
1	-0.93364870	1.14176856	-4.64224429

1	-1.53757949	-0.50812763	-4.37456109
1	-4.50991115	0.40317177	-3.18979038
1	-3.70604816	-0.94437375	-2.33244864
1	-4.29125231	0.46128085	-1.40744300
6	3.16300121	-0.47058885	0.22670648
6	2.74585815	-0.14152224	-2.55435851
6	3.05022215	2.15802419	-0.92861928
1	3.84583257	-0.12924604	-2.58195641
1	2.38702388	-1.17268206	-2.67294135
1	2.34428335	0.45878326	-3.38050004
1	4.12587457	1.99623311	-1.09524437
1	2.64508966	2.79471774	-1.72719058
1	2.90741926	2.67522530	0.02962428
1	4.22997788	-0.25038655	0.07109383
1	2.89211695	-0.27804178	1.27143317
1	2.99004621	-1.53376379	0.01669922
6	0.92794276	-1.54238284	4.38833653
6	2.22653774	-1.52147770	4.89834172
1	0.24812947	-2.35654840	4.65584132
1	2.55680446	-2.31943191	5.56624016
6	3.09767083	-0.47881773	4.55460432
1	4.11368804	-0.45016850	4.95049386
6	2.64336383	0.52651253	3.69317300
1	3.31618386	1.34487582	3.41884649
1	-1.47098591	-1.05686053	3.63655800
1	-0.01454485	-0.36433748	-2.12312233
1	1.69606420	1.93847875	1.58587076
1	0.22746449	1.37395794	-2.35577887
1	-2.34726859	0.44420479	1.98613568
1	-2.06397971	0.96290260	-0.28234430
1	0.12749756	2.47668757	-0.66486540
1	-0.70627603	2.55884054	-0.94928742

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XYZ file for : **TS8-N**

6	0.48653668	2.08304625	2.43011982
6	-0.69724083	1.52008367	1.61899131
6	-1.38468350	0.46168635	2.48351062
7	-0.47468637	-0.62810095	2.83920998
6	0.79385482	-0.28656031	3.31715152
6	1.32795547	1.00769829	3.09388947
1	-1.44460945	2.32068394	1.50416186
1	-1.75298113	0.96383152	3.40883924
1	0.09147191	2.74728192	3.22542052
42	-0.48008830	0.52903417	-0.85745067
15	-2.08043516	1.01687550	-2.56364588

15	-1.16362753	-1.84659512	-0.51294072
15	2.04865508	0.25784442	-0.71280809
6	0.00485320	-3.09001604	0.26259327
6	-2.70925538	-2.25677066	0.46867561
6	-1.55466812	-2.82062815	-2.06129142
6	-1.64642564	0.59208626	-4.33240087
6	-3.83190459	0.36302877	-2.50653650
6	-2.46531173	2.83370249	-2.76616749
1	-2.96047043	-3.32360090	0.37135928
1	-2.55042229	-2.02978000	1.53021413
1	-3.54570251	-1.64597772	0.10369276
1	-0.47440979	-4.07403612	0.38313896
1	0.88285153	-3.19856078	-0.38907785
1	0.33340236	-2.70882427	1.23756003
1	-1.84511236	-3.85319027	-1.81510077
1	-2.36905676	-2.34065702	-2.61898670
1	-0.66255811	-2.83117831	-2.70146877
1	-3.19268850	3.00873244	-3.57353961
1	-2.86410403	3.21444402	-1.81645734
1	-1.53032943	3.36544193	-2.98666117
1	-2.42271080	0.93503495	-5.03290173
1	-0.68787129	1.06819898	-4.57817345
1	-1.52044033	-0.49495189	-4.42435570
1	-4.40808768	0.70524165	-3.37936738
1	-3.83152200	-0.73475782	-2.48701911
1	-4.30887181	0.72401543	-1.58549260
6	2.98659313	-0.91744078	0.39606167
6	2.78677726	-0.23763301	-2.35168358
6	3.02669176	1.82058657	-0.40546720
1	3.88561471	-0.25180519	-2.29586532
1	2.41706523	-1.23496390	-2.62374984
1	2.46018702	0.47156142	-3.12257396
1	4.10106868	1.65478691	-0.57614237
1	2.65914314	2.60477975	-1.08079608
1	2.88048289	2.15203965	0.63045649
1	4.07110256	-0.79332628	0.25575194
1	2.72988263	-0.73349886	1.44575498
1	2.70892800	-1.94929837	0.14565066
6	1.57843824	-1.25062118	3.98737910
6	2.86726227	-0.94861800	4.42864142
1	1.16537267	-2.25000191	4.15067095
1	3.45282689	-1.71248236	4.94356218
6	3.40605350	0.32564548	4.20532332
1	4.41402406	0.56988763	4.54239729
6	2.62829084	1.28201640	3.54242475
1	3.03593453	2.28251607	3.37035801

1	-0.91272401	-1.37265001	3.37682307
1	0.01575665	-0.56751331	-2.10011248
1	1.12940250	2.72854119	1.80900989
1	0.29457475	1.27548356	-2.18773296
1	-2.25772614	0.04501108	1.96745914
1	-2.13155577	0.88682820	-0.40055608
1	-0.24475567	1.96638338	0.21888181
1	-0.31122890	2.32448877	-0.72733453

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XYZ file for : **12-N**

6	0.93938422	2.66090155	3.15116391
6	-0.15985670	2.94027546	2.11659902
6	-1.21329024	1.84085256	2.13737237
7	-0.58393879	0.53614164	1.77188575
6	0.48841033	0.18518697	2.66440582
6	1.26011804	1.18370200	3.29621990
1	-0.63649480	3.91216828	2.31346496
1	-1.66542490	1.75732703	3.14470317
1	0.62695547	3.03668666	4.14151797
42	-0.46808272	0.22818671	-0.74172105
15	-2.10088893	0.69060575	-2.41934665
15	-0.91075624	-2.21267355	-0.50622824
15	2.04878135	0.37237458	-0.76637416
6	0.48539027	-3.43379265	-0.17823122
6	-2.15597040	-2.83125076	0.76637866
6	-1.61134993	-3.10539698	-1.99604228
6	-1.72990122	0.22591086	-4.19346874
6	-3.86143881	0.06822715	-2.29662062
6	-2.46956020	2.50723358	-2.65058296
1	-2.27886629	-3.92409360	0.71808196
1	-1.84878164	-2.56442446	1.78855092
1	-3.12122707	-2.34515700	0.56625660
1	0.12771881	-4.47421914	-0.12483541
1	1.20864756	-3.34245489	-1.00146870
1	1.00482322	-3.17735477	0.75459616
1	-1.74560452	-4.17815002	-1.78910239
1	-2.57810499	-2.66978033	-2.27733465
1	-0.91580481	-2.97884338	-2.83642891
1	-3.21843310	2.67226307	-3.44043691
1	-2.83134122	2.91205594	-1.69667798
1	-1.53344271	3.02113076	-2.90387396
1	-2.51284897	0.58650626	-4.87773559
1	-0.76277737	0.66506258	-4.47249799
1	-1.64670566	-0.86598244	-4.27457481
1	-4.45373268	0.38998229	-3.16665290

1 -3.87928291 -1.02734231 -2.23398248
1 -4.30569178 0.47134054 -1.37698623
6 3.21148044 -0.56110083 0.36732193
6 2.80228180 -0.10143737 -2.40520368
6 2.77640270 2.08432052 -0.57331214
1 3.88776908 0.07941483 -2.40839906
1 2.60337040 -1.16396462 -2.59697234
1 2.32361274 0.48558482 -3.19937894
1 3.86151600 2.09076652 -0.75921701
1 2.26693296 2.75826386 -1.27437547
1 2.58453007 2.44413391 0.44667511
1 4.25914062 -0.32663349 0.12316559
1 3.01728062 -0.29385284 1.41334593
1 3.04532027 -1.64021126 0.24941573
6 0.75669118 -1.17026517 2.92503673
6 1.79962467 -1.54949084 3.76930227
1 0.14074620 -1.93286311 2.44689418
1 1.98962628 -2.60814648 3.95351931
6 2.60041828 -0.56770348 4.36838279
1 3.42851569 -0.84934137 5.02013221
6 2.31834844 0.77849712 4.13017072
1 2.92389718 1.55122744 4.61148997
1 -1.30426036 -0.18806649 1.81509967
1 0.04264690 -0.78179096 -2.04209480
1 1.85686511 3.21756887 2.89855194
1 0.15889578 1.09052047 -2.07233466
1 -1.99712631 2.03263489 1.39684844
1 -2.13910233 0.44294422 -0.21593065
1 0.24796050 2.97093757 1.09487613
1 -0.45402093 1.97484906 -0.59300337

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XYZ file for : 13

42 -0.30291559 0.08881096 -0.99563048
15 -2.29359186 0.90567196 -2.03663203
15 -0.75501998 -2.32760017 -0.75901256
15 2.13251548 0.16409998 -1.34486427
6 -0.49905633 -2.88899217 1.01407207
6 -2.43591862 -3.09822044 -1.06644824
6 0.28922116 -3.59201668 -1.65693281
6 -2.33139805 0.99603329 -3.90027770
6 -3.96352122 0.12110465 -1.74158260
6 -2.69379772 2.67257123 -1.60422431
1 -2.44303943 -4.16928542 -0.81165251
1 -3.18655914 -2.57121549 -0.46333525
1 -2.69269175 -2.97976254 -2.12850238

1 -0.68134789 -3.96939377 1.11778625
1 0.53040059 -2.66910153 1.33079946
1 -1.18925074 -2.34007745 1.66921954
1 -0.02373034 -4.62199478 -1.42606548
1 0.20569407 -3.41606864 -2.73805635
1 1.34016408 -3.45773926 -1.36742112
1 -3.59551360 3.02150870 -2.13032977
1 -2.83648610 2.73945246 -0.51817496
1 -1.83207542 3.29669667 -1.87238703
1 -3.26401974 1.45423188 -4.26181592
1 -1.47133800 1.58641978 -4.24265328
1 -2.23631940 -0.01950219 -4.30767364
1 -4.75593591 0.70455972 -2.23459976
1 -3.97028592 -0.90037862 -2.14229330
1 -4.15212704 0.07932962 -0.66102303
6 3.08440635 -0.27171228 0.20861523
6 3.02334110 -0.87384147 -2.61705178
6 2.87774204 1.82872021 -1.73592557
1 4.10595721 -0.67397265 -2.62067450
1 2.84431801 -1.93757363 -2.41471717
1 2.60407822 -0.63902120 -3.60508730
1 3.97744654 1.79178768 -1.76402409
1 2.49493640 2.16123410 -2.71042355
1 2.53838384 2.54508075 -0.97681908
1 4.16198984 -0.09879481 0.06789216
1 2.72840251 0.35260084 1.04016891
1 2.91947383 -1.32778516 0.46218805
1 -0.27682486 -0.62494416 -2.55656033
1 -0.00127756 1.19528313 -2.25176378
1 -1.71550784 0.28567800 0.03286940
1 -0.07608688 1.73988766 -0.44661408

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XYZ file for : 14

6 0.86092629 2.64643096 3.24635230
6 -0.09440030 2.89576483 2.06926967
6 -1.24102859 1.88167476 2.10489578
7 -0.68965663 0.53384206 1.99681051
6 0.40473603 0.18192359 2.79273616
6 1.21795852 1.17665456 3.39081372
1 -0.49880042 3.91827214 2.10786119
1 -1.82232781 2.01869041 3.04045263
1 0.38684546 3.00156502 4.17903755
6 0.74352925 -1.17798901 2.96217162
6 1.86327483 -1.55040379 3.70541833
1 0.11857230 -1.94348463 2.49409788

1	2.10209222	-2.60904629	3.82311664
6	2.67712920	-0.57219529	4.29259327
1	3.55763635	-0.85522831	4.87037103
6	2.34389028	0.77584272	4.12336618
1	2.97168616	1.54881358	4.57575816
1	-1.37948845	-0.20447859	1.89221126
1	1.77920896	3.24271281	3.12573647
1	-1.92823363	2.04188144	1.26046927
1	0.44362448	2.78698691	1.11409749