

On the role of resonantly stabilized radicals in polycyclic aromatic hydrocarbon (PAH)

formation: Pyrene and fluoranthene formation from benzyl-indenyl addition

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Supplementary material

Table S1: Rate constants for the elementary reactions. The units are cm, s, mol and cal.

REACTIONS	A	n	E
Benzyl + Indenyl → IS1	8.1E+11	-0.369	1171.9
IS1 → Benzyl + Indenyl	9.1E+11	0.749	41187.1
IS1 → IS2 + H	1.3E+11	0.770	4354.4
IS2 + H → IS1	9.1E+11	0.140	25588.4
IS2 → IS3	8.1E+11	0.038	11810.2
IS3 → IS2	9.1E+11	0.347	4109.7
IS3 → IS4	6.3E+11	0.439	14799.0
IS4 → IS3	9.8E+10	0.513	29006.1
IS4 → IS5	2.8E+11	0.101	58117.8
IS5 → IS4	5.5E+11	0.424	7957.2
IS5 → IS6	9.6E+11	0.430	52316.1
IS6 → IS5	9.6E+11	0.396	40102.8
IS6 → IS7	1.6E+11	0.580	10385.7
IS7 → IS6	9.7E+11	-0.006	77287.5
IS7 → IS8 + H	9.6E+11	0.361	33569.4
IS8 + H → IS7	4.9E+11	0.490	5592.6
IS8 + H → IS9 + H2	8.0E+11	0.670	13222.6
IS9 + H2 → IS8 + H	1.4E+11	0.597	8697.3
IS9 → IS10	4.2E+11	0.159	11625.5
IS10 → IS9	9.2E+11	0.413	28439.2
IS10 → IS11	7.9E+11	0.349	36065.3
IS11 → IS10	9.6E+11	0.284	28523.3
IS11 → IS12	6.6E+11	0.566	39777.6
IS12 → IS11	3.6E+10	0.328	6618.8
IS12 → IS13	8.5E+11	-0.119	2297.2
IS13 → IS12	9.3E+11	0.605	46781.9
IS12 → IS12' + C ₂ H ₂	8.1E+11	1.004	41908.7
IS12' + C ₂ H ₂ → IS12	9.1E+11	0.396	8304.4
IS13 → Pyrene + H	6.8E+11	0.508	18658.5
Pyrene + H → IS13	7.6E+11	0.444	8062.4
IS2 → IS7	7.4E+11	0.101	29784.5

IS7 $\rightarrow$ IS2	3.9E+11	0.359	40530.2
IS4 $\rightarrow$ IS22 + H	6.6E+11	0.392	28227.9
IS22 + H $\rightarrow$ IS4	1.7E+11	0.632	6476.2
IS8 + H $\rightarrow$ IS14 + H2	7.1E+11	0.704	12158.7
IS14 + H2 $\rightarrow$ IS8 + H	3.2E+10	0.785	6625.9
IS14 $\rightarrow$ IS15	2.8E+11	0.213	13445.2
IS15 $\rightarrow$ IS14	4.6E+10	0.839	33648.1
IS15 $\rightarrow$ IS16 + H	9.7E+10	0.840	28282.1
IS16 + H $\rightarrow$ IS15	8.2E+11	0.459	5465.4
IS10 $\rightarrow$ IS16 + H	6.9E+11	0.548	25832.1
IS16 + H $\rightarrow$ CA10	3.2E+11	0.567	5610.0
IS16 + H $\rightarrow$ A + H2	8.1E+11	0.693	11926.5
A + H2 $\rightarrow$ IS16 + H	9.1E+11	0.378	6719.4
A $\rightarrow$ B	1.3E+11	0.997	57767.4
B $\rightarrow$ A	9.1E+11	0.670	40985.1
B $\rightarrow$ C	6.6E+11	0.566	39777.6
C $\rightarrow$ B	3.6E+10	0.328	6618.8
C $\rightarrow$ D	6.3E+11	0.006	2897.2
D $\rightarrow$ C	9.8E+10	0.886	44076.3
C $\rightarrow$ C' + C ₂ H ₂	1.3E+11	1.187	41711.9
C' + C ₂ H ₂ $\rightarrow$ C	9.1E+11	0.260	9479.8
D $\rightarrow$ E + H	2.8E+11	0.620	18070.1
E + H $\rightarrow$ D	9.1E+11	0.417	8435.3
E+H $\rightarrow$ F *	3.1E+14	0	700.0
F (+M) $\rightarrow$ E+H (+M) *	4.30E+12	0.6	77313.0
IS1 + H $\rightarrow$ IS17 + H2	9.5E+11	0.710	14813.1
IS17 + H2 $\rightarrow$ IS1 + H	3.4E+10	0.787	5644.7
IS17 $\rightarrow$ IS18	4.4E+11	0.096	20567.9
IS18 $\rightarrow$ IS17	3.8E+11	0.454	9319.4
IS17 $\rightarrow$ IS2	7.7E+11	0.271	30302.1
IS2 $\rightarrow$ IS17	8.0E+11	0.219	59602.5
IS18 $\rightarrow$ IS19	1.9E+11	0.545	2464.8
IS19 $\rightarrow$ IS18	4.9E+11	-0.053	33691.5
IS19 $\rightarrow$ IS20	4.5E+11	0.132	9801.6
IS20 $\rightarrow$ IS19	6.5E+11	0.437	10063.0
IS20 $\rightarrow$ IS21	7.1E+11	0.300	10348.1
IS21 $\rightarrow$ IS20	7.5E+11	0.267	31202.2
IS21 $\rightarrow$ IS22 + H	2.8E+11	0.652	29580.3
IS22 + H $\rightarrow$ IS21	6.8E+11	0.539	3638.6
IS19 $\rightarrow$ IS23	6.6E+11	0.053	13396.1
IS23 $\rightarrow$ IS19	1.6E+11	0.589	3569.7
IS23 $\rightarrow$ IS24	1.2E+11	0.566	4742.7
IS24 $\rightarrow$ IS23	5.0E+11	0.338	39088.5
IS24 $\rightarrow$ IS22 + H	9.6E+11	1.091	-310382.7

IS22 + H → IS24	3.4E+11	0.050	346237.5
IS22 + H → IS25 + H2	5.9E+11	0.705	12626.2
IS25 + H2 → IS22 + H	2.2E+11	0.476	7524.8
IS25 → IS26	7.5E+11	0.177	33652.3
IS26 → IS25	2.6E+11	0.512	15132.7
IS26 → IS27	5.1E+11	0.473	41723.9
IS27 → IS26	7.0E+11	0.432	42479.6
IS27 → IS28	8.9E+11	0.353	16106.4
IS28 → IS27	9.6E+11	0.166	31094.8
IS28 → IS29	5.5E+11	0.390	23076.7
IS29 → IS28	1.4E+11	0.569	23082.5
IS29 → IS9	1.5E+11	0.460	8368.4
IS9 → IS29	2.6E+11	0.411	9197.2
IS25 → IS28	8.4E+11	0.456	42367.7
IS28 → IS25	2.5E+11	0.627	39484.6
IS1 → IS30 + H2	8.1E+11	0.507	106219.2
IS30 + H2 → IS1	2.4E+11	0.313	90138.3
IS30 → IS31 + H	9.3E+11	0.622	8114.3
IS31 + H → IS30	3.5E+11	0.167	14846.0
IS31 → IS32	2.0E+11	0.368	38061.9
IS32 → IS31	2.5E+11	0.542	1784.7
IS32 → IS25	6.2E+11	0.345	3796.0
IS25 → IS32	4.7E+11	0.598	50287.1
IS31 → IS28	3.5E+11	0.263	49946.1
IS28 → IS31	8.3E+11	0.601	57712.3
IS1 → IS33 + H2	5.9E+11	0.759	98208.7
IS33 + H2 → IS1	5.5E+11	0.190	9933.0
IS33 → IS22	9.2E+11	0.124	878.6
IS22 → IS33	2.9E+11	0.697	95123.0
IS33 → IS34	7.6E+11	0.456	14765.5
IS34 → IS33	7.5E+11	0.294	7555.7
IS34 → IS8	3.8E+11	0.347	278.1
IS8 → IS34	5.7E+11	0.876	99698.9

For the reactions with “*” and the reactions involving barrierless H-addition on the radicals site, the rate constants were already present in the base mechanism, and the same were used in flame simulations.

Table S2: The energies (in hartree), molecular geometries (in Å) and vibrational frequencies (in cm⁻¹) of intermediate species (IS) obtained using B3LYP/6-311++G(d,p).

Species	E1	Cartesian coordinate (Å)				Vibrational Frequency
IS1	-618.03245	C	-2.53009500	0.89992200	-0.21701600	30 40 58 110 138 226 238 294 354 408 414 439 475 541
		C	-1.82981400	-0.32287600	-0.17743800	561 568 595 634 636 712 728 736 749 763 794 812 842 855
		C	-2.50107100	-1.50923000	0.07798200	870 879 919 930 951 968 983 986 1000 1002 1017 1041
		C	-3.88378700	-1.47258000	0.29505200	1050 1058 1089 1100 1134 1170 1177 1182 1186 1202 1215
		C	-4.57768300	-0.26163400	0.25385000	1223 1244 1290 1315 1337 1342 1346 1363 1392 1482 1485
		C	-3.90720000	0.93611400	-0.00320700	1488 1490 1526 1598 1622 1631 1643 1646 2995 3032 3075
		C	-1.56598800	1.96598600	-0.50486000	3149 3154 3156 3161 3166 3173 3175 3185 3187 3189 3216
		C	-0.33489000	1.44108900	-0.63672000	
		C	-0.36055800	-0.06170500	-0.44875900	
		H	-1.97317700	-2.45712700	0.10938100	
		H	-4.42089900	-2.39276500	0.49602100	
		H	-5.64871800	-0.25242800	0.42347300	
		H	-4.45102700	1.87425600	-0.03583600	
		H	-1.82381600	3.01383600	-0.59768300	
		H	0.57186900	1.98960000	-0.85383600	
		H	-0.06496300	-0.54747300	-1.38952300	
		C	0.58196800	-0.58371700	0.67000100	
		H	0.39637400	-1.65461500	0.79936100	
		H	0.30593800	-0.09856500	1.61029100	
		C	2.05078300	-0.36011600	0.38313800	
		C	2.75747700	0.67889400	0.99754100	
		C	2.73553200	-1.18456700	-0.51833500	
		C	4.10711700	0.89254500	0.71844600	
		H	2.24656800	1.32450100	1.70476000	
		C	4.08317900	-0.97499100	-0.80160700	
		H	2.20970400	-2.00433700	-0.99887300	
		C	4.77433100	0.06706700	-0.18402800	
		H	4.63694200	1.70181200	1.20894300	
		H	4.59537400	-1.62786100	-1.49989500	
		H	5.82403300	0.22996400	-0.40081400	
IS2	-617.39836	C	-2.78169300	0.70151000	0.06433600	14 51 59 142 163 207 235 304 354 406 414 451 483 540 544
		C	-1.68546000	-0.13421100	-0.22685100	576 582 626 637 679 704 727 748 754 772 791 825 841 868
		C	-1.85062400	-1.50587000	-0.34171700	872 892 902 951 961 974 976 986 987 992 1037 1040 1080
		C	-3.13082600	-2.04593400	-0.17330200	1086 1119 1136 1170 1176 1182 1190 1207 1222 1234 1264
		C	-4.22062600	-1.21904500	0.10872000	1299 1329 1340 1351 1384 1435 1478 1483 1488 1502 1574
		C	-4.05662400	0.16228000	0.23076500	1593 1597 1629 1643 3030 3150 3158 3158 3163 3165 3174
		C	-2.29758600	2.08302300	0.13446100	3174 3183 3186 3188 3191 3215
		C	-0.97530000	2.11508000	-0.10672300	
		C	-0.42932100	0.71592500	-0.36765600	
		H	-1.00624000	-2.15277100	-0.55546600	
		H	-3.27813500	-3.11652200	-0.26119000	
		H	-5.20484900	-1.65611500	0.23601200	
		H	-4.90623700	0.79958800	0.45168200	
		H	-2.92484200	2.94033900	0.34576200	
		H	-0.34255100	2.99256900	-0.11527200	
		H	-0.06995700	0.66097400	-1.40191500	
		C	0.66402800	0.33531100	0.58669900	
		H	0.36852900	0.26776300	1.62971100	
		C	2.01834200	0.08433900	0.27481300	
		C	2.55604000	0.14855300	-1.04363500	
		C	2.92513300	-0.25756200	1.32285800	
		C	3.89501100	-0.11250600	-1.28502100	
		H	1.91288500	0.40660000	-1.87623900	
		C	4.25953500	-0.51579800	1.06894500	
		H	2.54651900	-0.31395900	2.33806500	
		C	4.76025400	-0.44676400	-0.23753000	
		H	4.27497400	-0.05569300	-2.29939100	
		H	4.92184500	-0.77355300	1.88824800	
		H	5.80635200	-0.64920800	-0.43498300	
IS3	-617.38636	C	-2.41075400	0.82496600	0.10582300	43 68 73 152 176 249 268 366 376 408 414 447 526 536 547
		C	-1.84916100	-0.37151900	-0.44542200	590 626 633 648 707 712 747 755 765 798 823 837 848 852
		C	-2.60088900	-1.53028600	-0.53319400	869 876 922 945 964 977 978 994 1000 1013 1032 1050
		C	-3.92372500	-1.52190500	-0.06861900	1057 1062 1100 1120 1160 1168 1182 1192 1205 1209 1233

		C	-4.47801800	-0.36068900	0.49079300	1247 1294 1314 1330 1347 1354 1383 1399 1458 1484 1498
		C	-3.73788900	0.80955300	0.58916300	1526 1584 1607 1616 1640 3147 3156 3158 3159 3164
		C	-1.45423700	1.86473200	0.05268000	3166 3170 3175 3177 3187 3189 3207
		C	-0.19197400	1.34823100	-0.50287600	
		C	-0.43675000	-0.11133600	-0.83305900	
		H	-2.17717600	-2.43552700	-0.95527400	
		H	-4.52393100	-2.42178000	-0.13943900	
		H	-5.50193700	-0.37938500	0.84767100	
		H	-4.17563300	1.70468500	1.01748400	
		H	-1.60035200	2.87902100	0.39919200	
		H	0.46337500	1.97744800	-1.09340600	
		H	-0.00346700	-0.58976000	-1.70355900	
		C	0.51305000	0.23100400	0.31636400	
		H	0.11273400	0.07508400	1.31227700	
		C	1.97445300	0.02092300	0.19818400	
		C	2.66597700	0.14275200	-1.01789800	
		C	2.71297800	-0.30944100	1.34464900	
		C	4.04198400	-0.05878000	-1.08141400	
		H	2.13044700	0.39708300	-1.92615700	
		C	4.08898000	-0.51188000	1.28138900	
		H	2.19877000	-0.40895100	2.29498200	
		C	4.76167200	-0.38741700	0.06695500	
		H	4.55417900	0.04067200	-2.03221600	
		H	4.63586900	-0.76755100	2.18231200	
		H	5.83293100	-0.54449600	0.01502500	
IS4	-617.40925	C	2.14454700	0.74639300	0.17305200	24 34 77 161 177 250 273 290 370 402 414 453 505 524 535
		C	1.69561200	-0.45275300	-0.48396500	555 615 633 640 707 711 716 751 760 773 788 819 849 855
		C	2.60194200	-1.55032200	-0.56594300	862 904 926 944 952 974 984 995 1001 1017 1040 1049
		C	3.87351600	-1.46590700	-0.03488300	1082 1100 1137 1163 1176 1181 1194 1202 1205 1228 1252
		C	4.30088200	-0.28855400	0.60320300	1295 1317 1339 1342 1360 1409 1428 1456 1481 1499 1521
		C	3.43529800	0.79999700	0.70034300	1558 1600 1622 1638 1664 2910 3145 3151 3155 3158 3160
		C	1.22527700	1.86665900	0.26511300	3161 3169 3169 3174 3177 3187 3188
		C	-0.01946300	1.82421200	-0.23699400	
		C	0.40440000	-0.51505700	-1.01601700	
		H	2.27392800	-2.46016700	-1.05776000	
		H	4.54720000	-2.31235500	-0.11016400	
		H	5.30002600	-0.22726900	1.01840200	
		H	3.76475600	1.70911300	1.19378600	
		H	1.57583700	2.76575400	0.76376900	
		H	-0.67708000	2.68245700	-0.14390500	
		H	0.07627300	-1.42672800	-1.50506000	
		C	-0.58202000	0.61561300	-0.94387000	
		H	-0.82941500	0.92100700	-1.97602300	
		C	-1.91408600	0.16542800	-0.32513500	
		C	-1.96879500	-0.25663500	1.00812500	
		C	-3.08964100	0.16243600	-1.07891900	
		C	-3.17235900	-0.67015300	1.57241400	
		H	-1.06260200	-0.25874300	1.60437900	
		C	-4.29771300	-0.25243600	-0.51663300	
		H	-3.06213100	0.48720600	-2.11459100	
		C	-4.34203100	-0.66993200	0.81105600	
		H	-3.19879800	-0.99344000	2.60731300	
		H	-5.20111600	-0.24826100	-1.11665300	
		H	-5.27907700	-0.99251500	1.25083100	
IS5	-617.32947	C	2.08176100	0.74515400	0.20638400	66 90 131 149 182 283 313 350 391 425 455 475 504 531
		C	1.28611900	-0.42352000	0.03647800	549 566 585 610 666 679 694 716 753 766 792 806 842 880
		C	1.89304500	-1.66357100	-0.12128400	889 912 923 942 958 965 979 980 990 993 1033 1055 1071
		C	3.28590300	-1.77429800	-0.12737000	1098 1119 1145 1149 1166 1177 1183 1199 1215 1235 1240
		C	4.07426600	-0.63945800	0.04841100	1284 1303 1328 1338 1354 1371 1393 1418 1429 1480 1493
		C	3.47514600	0.60728500	0.21958000	1530 1590 1620 1638 1642 2915 2928 3002 3149 3150 3154
		C	1.45103500	2.07296700	0.36617300	3156 3161 3167 3173 3176 3187 3188
		C	0.17535200	2.32722200	0.01193300	
		C	-0.18259200	-0.14864400	0.14551500	
		H	1.27821700	-2.54963100	-0.23997400	
		H	3.75078600	-2.74449000	-0.26243200	
		H	5.15515500	-0.72369300	0.05253300	
		H	4.09449600	1.48844600	0.35446400	
		H	2.08255100	2.87172200	0.74363200	
		H	-0.24874400	3.32302400	0.08100900	
		H	-0.42205000	0.00302100	1.20612000	
		C	-0.54956100	1.16499500	-0.58903800	
		H	-0.19644000	1.05203200	-1.63023400	
		C	-1.96704900	0.64706700	-0.55053400	
		C	-3.20275200	1.03286900	-0.14520300	
		C	-1.47380100	-0.79055300	-0.50653100	

		C	-4.11720600	0.02719600	0.28248100	
		H	-3.47484500	2.08128100	-0.07034000	
		C	-2.41382300	-1.73351400	0.16353200	
		H	-1.20157300	-1.15414600	-1.51185800	
		C	-3.68059800	-1.31173400	0.47358000	
		H	-5.12923600	0.30006800	0.55599400	
		H	-2.11722900	-2.76307100	0.33586700	
		H	-4.38254900	-2.02133800	0.90057600	
IS6	-617.31008	C	-2.09030500	0.73666900	-0.22730500	68 81 128 160 173 271 288 361 396 414 462 473 501 514
		C	-1.31267800	-0.43928200	-0.01729200	537 572 591 614 661 670 700 741 750 765 787 798 812 864
		C	-1.93427600	-1.66480400	0.18264000	875 886 940 946 958 961 976 979 991 1034 1045 1055
		C	-3.32928000	-1.75266800	0.19261200	1090 1107 1124 1146 1152 1160 1171 1183 1212 1220 1237
		C	-4.10108300	-0.61317900	-0.02162900	1269 1290 1304 1315 1338 1347 1360 1366 1407 1418 1481
		C	-3.48465000	0.61943600	-0.23524800	1490 1521 1572 1588 1628 1642 2890 2905 2977 3146 3149
		C	-1.43139200	2.04621300	-0.43040200	3151 3156 3163 3169 3174 3174 3184 3187
		C	-0.15509800	2.28711000	-0.06165700	
		C	0.15298600	-0.16263500	-0.14030200	
		H	-1.33051500	-2.55281500	0.33593600	
		H	-3.80890800	-2.71008300	0.36295500	
		H	-5.18306200	-0.68209600	-0.02238300	
		H	-4.09160400	1.50427300	-0.39932500	
		H	-2.04154300	2.84336200	-0.84447700	
		H	0.28723600	3.27335100	-0.15391000	
		H	0.31243200	0.04618200	-1.21459900	
		C	0.52440000	1.12991400	0.60226900	
		H	0.10956300	1.06533000	1.61844300	
		C	2.00334100	0.58904000	0.76423400	
		C	3.27714500	0.98570900	0.08542600	
		C	1.49278700	-0.75661500	0.27414900	
		C	4.10255800	-0.01815400	-0.33970400	
		H	3.59717600	2.02233200	0.06994800	
		C	2.33251300	-1.72878900	-0.19722900	
		C	3.69647000	-1.38982500	-0.36771000	
		H	5.09437100	0.22610300	-0.70719900	
		H	1.96225600	-2.67939400	-0.57039900	
		H	4.40436900	-2.14105900	-0.69791100	
		H	2.22761500	0.57567400	1.84582100	
IS7	-617.41560	C	2.19788100	0.40887800	-0.19106700	29 35 66 154 171 243 262 298 379 413 426 475 482 513 530
		C	1.07072800	-0.17245100	0.44593700	559 614 631 647 686 713 723 755 769 792 795 806 841 855
		C	1.05866900	-1.54697800	0.68077300	882 925 935 960 966 984 986 996 1002 1017 1049 1059
		C	2.12583600	-2.35763600	0.29984900	1094 1100 1138 1176 1180 1181 1193 1202 1205 1233 1233
		C	3.23500100	-1.79210700	-0.33748900	1273 1304 1338 1341 1361 1387 1435 1465 1481 1511 1522
		C	3.26803100	-0.42899300	-0.57849200	1549 1593 1623 1625 1639 2944 3151 3153 3156 3160 3160
		C	2.24326900	1.82293800	-0.42458700	3169 3172 3173 3177 3182 3187 3187
		C	1.18746400	2.65368600	-0.01692700	
		C	0.07562900	2.15347900	0.60698300	
		H	0.19502800	-1.99403200	1.16241700	
		H	2.09241000	-3.42354400	0.49445400	
		H	4.06689400	-2.41796200	-0.64074200	
		H	4.12750700	0.01654300	-1.06904900	
		H	3.11196200	2.24492100	-0.91669100	
		H	1.25594500	3.72114900	-0.20138300	
		H	-0.72826100	2.81479200	0.91089000	
		C	-0.11228700	0.68572400	0.89123100	
		H	-0.20240400	0.57190300	1.98321100	
		C	-1.44733300	0.19807800	0.31271200	
		C	-1.64527800	0.14363200	-1.07197200	
		C	-2.49692700	-0.17577700	1.15452100	
		C	-2.86177900	-0.27957900	-1.59875000	
		H	-0.83949500	0.43145100	-1.73863600	
		C	-3.71912800	-0.59956700	0.62961100	
		H	-2.35923200	-0.13723000	2.23083900	
		C	-3.90445700	-0.65311600	-0.74899900	
		H	-2.99820400	-0.31848700	-2.67397300	
		H	-4.52223500	-0.88784300	1.29903200	
		H	-4.85182400	-0.98293300	-1.16036500	
IS8	-616.86950	C	-2.37285200	0.38762600	0.04516500	43 75 83 168 181 244 292 314 409 415 443 478 503 530 569
		C	-1.04589600	-0.15085200	-0.03151900	582 631 633 664 710 717 746 776 794 806 816 842 860 879
		C	-0.90262400	-1.55141300	-0.23183500	924 938 973 978 987 990 997 1002 1016 1043 1051 1080
		C	-2.00073200	-2.37415600	-0.32154400	1100 1138 1168 1181 1185 1203 1207 1234 1272 1309 1313
		C	-3.30633000	-1.84303900	-0.21816600	1350 1365 1388 1424 1462 1476 1490 1524 1544 1611 1615
		C	-3.48389700	-0.49246200	-0.04389700	1631 1640 1658 3157 3159 3160 3165 3168 3170 3175 3180
		C	-2.55195600	1.78715300	0.19276500	3183 3185 3189 3199
		C	-1.46728800	2.62558800	0.25301700	

		C	-0.15860800	2.09973600	0.18815000	
		H	0.09056900	-1.97110100	-0.32553500	
		H	-1.86534100	-3.43844700	-0.47884700	
		H	-4.16415100	-2.50259100	-0.28665900	
		H	-4.48301200	-0.07414300	0.02232200	
		H	-3.56050900	2.18274800	0.25208900	
		H	-1.60693300	3.69519700	0.36286200	
		H	0.68793500	2.77308100	0.26405100	
		C	0.07257600	0.74299100	0.06255200	
		C	1.47961700	0.24913700	0.03217600	
		C	1.96568500	-0.61995900	1.01945000	
		C	2.36193000	0.68404600	-0.96562200	
		C	3.29347300	-1.04026300	1.00836600	
		H	1.30134900	-0.95341800	1.80885300	
		C	3.68988700	0.26069700	-0.97961300	
		H	1.99839900	1.34947000	-1.74088200	
		C	4.16036300	-0.60285300	0.00745400	
		H	3.65292800	-1.70500400	1.78619400	
		H	4.35527200	0.60408800	-1.76408600	
		H	5.19341700	-0.93173500	-0.00175200	
IS9	-616.19553	C	-2.37406300	0.37574600	0.03052200	51 74 87 168 181 240 292 316 411 416 452 471 499 525 563
		C	-1.02864700	-0.13790500	-0.02069000	577 628 630 644 710 711 746 764 779 799 818 842 854 882
		C	-0.92839000	-1.52204700	-0.20830900	921 935 959 969 982 989 999 1015 1040 1051 1083 1103
		C	-1.94910400	-2.40570100	-0.32604000	1130 1165 1182 1188 1204 1208 1237 1303 1311 1345 1352
		C	-3.26968500	-1.87666800	-0.26249200	1361 1397 1452 1458 1478 1507 1525 1587 1611 1629 1639
		C	-3.46576400	-0.52734600	-0.09025600	1651 3157 3159 3160 3167 3167 3172 3177 3180 3184 3186
		C	-2.56370600	1.77272800	0.18270700	3191
		C	-1.48389400	2.61668400	0.27491900	
		C	-0.16763100	2.10900400	0.22738800	
		H	-1.78553300	-3.46871000	-0.46625700	
		H	-4.11724900	-2.54750800	-0.35443300	
		H	-4.47292300	-0.12659100	-0.04806600	
		H	-3.57520900	2.16335400	0.22172700	
		H	-1.63637600	3.68347500	0.39450400	
		H	0.66638800	2.79407800	0.32808300	
		C	0.08420100	0.75656900	0.08728500	
		C	1.48047200	0.24971400	0.04658400	
		C	1.87915200	-0.85239400	0.81761400	
		C	2.44118200	0.88209400	-0.75601200	
		C	3.19586600	-1.30477900	0.78690900	
		H	1.15864800	-1.34313900	1.46078900	
		C	3.75727400	0.42785600	-0.78858400	
		H	2.14675200	1.72136000	-1.37612700	
		C	4.14006400	-0.66789700	-0.01680700	
		H	3.48569000	-2.15261400	1.39774400	
		H	4.48162200	0.92503700	-1.42429100	
		H	5.16422800	-1.02269000	-0.04209400	
IS10	-616.22213	C	2.29519600	-0.00976200	-0.08899400	89 97 169 191 238 267 347 408 422 463 476 490 517 558
		C	0.89856600	0.00028300	0.08902700	564 589 621 632 644 684 735 758 773 785 807 813 837 877
		C	0.13260600	1.17846100	0.18942200	895 912 922 965 970 974 982 989 1023 1053 1064 1071
		C	0.76631600	2.39651500	0.10101800	1129 1147 1163 1179 1193 1208 1234 1250 1275 1287 1320
		C	2.17422100	2.41735100	-0.09319300	1361 1382 1395 1419 1434 1457 1480 1518 1521 1593 1609
		C	2.92570900	1.26087000	-0.18011500	1626 1646 2831 3154 3157 3158 3159 3168 3172 3175
		C	2.91012100	-1.28972600	-0.17040200	3181 3183 3189
		C	2.14053700	-2.44072300	-0.08532600	
		C	0.73692200	-2.41164700	0.07349500	
		H	0.22339600	3.33248500	0.17682100	
		H	2.67269800	3.37742100	-0.17257700	
		H	3.99923800	1.32071200	-0.32474000	
		H	3.98420000	-1.36519400	-0.30189500	
		H	2.63375600	-3.40481400	-0.14878900	
		H	0.18281600	-3.34209100	0.12344400	
		C	0.09888500	-1.17830400	0.16075300	
		C	-1.27643600	-0.75464400	0.25568800	
		C	-1.29979200	0.75515900	0.48359300	
		C	-2.46072300	-1.43796700	0.03820900	
		C	-2.49466700	1.42553800	-0.12615600	
		H	-1.41267900	0.89580500	1.58118700	
		C	-3.64098900	-0.72722700	-0.20169300	
		H	-2.46136300	-2.52025500	-0.04635800	
		C	-3.61682200	0.69572000	-0.36313400	
		H	-2.48122800	2.49961400	-0.27562100	
		H	-4.56411600	-1.26373400	-0.38588100	
		H	-4.51461400	1.19066300	-0.71873700	

IS11	-616.21032	C	2.16445300	0.07597800	-0.01485800	83 109 171 203 245 272 313 382 410 439 473 489 520 541 554 605 608 629 674 699 722 753 771 789 800 816 834 848 871 884 912 924 952 971 984 991 1025 1056 1080 1088 1104 1128 1143 1166 1184 1200 1226 1237 1250 1280 1303 1357 1365 1380 1398 1432 1450 1478 1518 1549 1569 1593 1626 1637 2855 3158 3160 3166 3170 3173 3183 3185 3188 3201 3218
		C	0.74416800	0.17920700	-0.05467200	
		C	0.11067400	1.46820000	0.19353900	
		C	0.94354100	2.56766300	0.51705300	
		C	2.33226200	2.44437500	0.55203500	
		C	2.94335500	1.23184800	0.28042100	
		C	2.76990600	-1.18418700	-0.24361200	
		C	1.99865300	-2.30332700	-0.47887400	
		C	0.59870800	-2.21148300	-0.48944500	
		H	0.48062500	3.52742200	0.72002000	
		H	2.93847700	3.31155900	0.79006200	
		H	4.02376600	1.14260100	0.30527800	
		H	3.85203100	-1.25705600	-0.22358600	
		H	2.47318000	-3.26217500	-0.65568900	
		H	0.00301500	-3.09751200	-0.67739300	
		C	-0.03824200	-0.99201900	-0.27903000	
		C	-1.48616100	-0.85102500	-0.21470300	
		C	-1.27397300	1.61698000	0.08060900	
		C	-2.46025800	-1.71072600	0.17549800	
		C	-2.10932900	0.50173000	-0.45984200	
		H	-1.72811700	2.58537600	0.26114700	
		C	-3.73177600	-0.99455800	0.25667600	
		H	-2.32689800	-2.75168700	0.44102400	
		C	-3.54823900	0.30573100	-0.05543500	
		H	-2.14597100	0.63361800	-1.56425100	
		H	-4.67237700	-1.45401700	0.53346200	
		H	-4.30371900	1.07799300	-0.10638600	
IS12	-616.15887	C	2.24748500	0.08006500	0.05057300	25 64 142 166 173 206 244 275 348 391 445 454 473 486 507 530 541 597 624 654 675 688 750 760 769 798 818 826 829 843 872 898 906 920 928 981 987 996 1051 1070 1106 1131 1144 1184 1204 1224 1240 1261 1283 1315 1334 1383 1394 1413 1442 1477 1492 1534 1548 1610 1617 1626 1634 1666 3055 3159 3161 3163 3167 3168 3180 3185 3198 3204 3256
		C	0.83928100	0.31329300	-0.02861600	
		C	0.36379800	1.66213300	-0.00576100	
		C	1.26329000	2.71192200	0.10922300	
		C	2.64806200	2.47453100	0.20487300	
		C	3.13099300	1.18845800	0.17366900	
		C	2.73146300	-1.24741000	0.00111700	
		C	1.85189000	-2.29910400	-0.12831000	
		C	0.46941200	-2.07081700	-0.19853500	
		H	0.88951200	3.73036800	0.12095000	
		H	3.33073800	3.31160200	0.29748700	
		H	4.19689700	0.99862500	0.24029000	
		H	3.80010600	-1.42346400	0.06013900	
		H	2.22319000	-3.31666400	-0.17614500	
		H	-0.17956900	-2.93065900	-0.30142500	
		C	-0.06938400	-0.78831300	-0.14076800	
		C	-1.53126500	-0.52236800	-0.16534600	
		C	-1.05738800	1.88975400	-0.14397100	
		C	-2.45294100	-1.53362200	-0.14640700	
		C	-1.93702200	0.86983100	-0.22129900	
		H	-1.40631500	2.91576200	-0.20220000	
		C	-3.91305900	-1.46264800	-0.09407800	
		H	-2.09042300	-2.55445000	-0.18379500	
		C	-4.71523400	-0.52894000	0.38654000	
		H	-2.98872200	1.08301400	-0.35557100	
		H	-4.40306000	-2.36386400	-0.47312200	
		H	-4.68998300	0.41347300	0.90953200	
IS12'	-538.77210	C	2.30212000	0.08513900	0.00746900	53 156 202 208 313 337 411 441 472 475 498 498 526 562 591 606 653 682 747 759 773 791 806 812 830 835 907 922 976 980 986 993 1058 1103 1121 1141 1179 1202 1222 1240 1258 1290 1360 1390 1409 1427 1462 1490 1533 1560 1616 1626 1629 1667 3159 3161 3162 3168 3175 3185 3187 3189 3258
		C	0.89073800	0.30519900	-0.04394900	
		C	0.39645300	1.64813800	-0.07073700	
		C	1.28893200	2.70768500	-0.04647900	
		C	2.68036800	2.48651200	0.00435500	
		C	3.17782400	1.20635100	0.03079500	
		C	2.79204700	-1.24188000	0.03379900	
		C	1.91919100	-2.30721900	0.01006700	
		C	0.53265700	-2.09182000	-0.04039400	
		H	0.90702600	3.72297100	-0.06700200	
		H	3.35617100	3.33408000	0.02247500	
		H	4.24761300	1.03129000	0.06988900	
		H	3.86339100	-1.40729200	0.07278500	
		H	2.29898100	-3.32255000	0.03025200	
		H	-0.12921500	-2.94950900	-0.05811200	
		C	-0.00055300	-0.81041600	-0.06777700	
		C	-1.47239900	-0.56306800	-0.12116000	
		C	-1.03784800	1.85892900	-0.12294100	
		C	-2.38763000	-1.53064600	-0.14619700	
		C	-1.90990300	0.83400300	-0.14651000	
		H	-1.40049200	2.88153800	-0.14289400	

		H	-2.46152000	-2.60598700	-0.14095500	
		H	-2.97709100	1.01597000	-0.18541200	
IS13	-616.22903	C	1.41432800	-1.24664900	-0.01626300	81 133 193 216 245 338 383 397 442 457 488 499 506 522
		C	0.72714500	0.00937700	0.06982600	538 550 581 651 674 679 706 733 761 774 799 812 819 844
		C	1.47692900	1.22618000	0.02606400	850 912 947 960 971 978 987 990 1062 1074 1093 1098
		C	2.88835600	1.15998500	-0.02024600	1142 1168 1174 1188 1198 1217 1231 1256 1260 1294 1335
		C	3.53540400	-0.05845700	-0.05964000	1371 1398 1414 1419 1426 1458 1477 1520 1554 1584 1622
		C	2.79860900	-1.25832400	-0.07647100	1628 1682 2749 3148 3154 3156 3158 3165 3168 3171 3174
		C	0.62141600	-2.46531400	-0.12703300	3182 3184
		C	-0.71157900	-2.46345000	0.00882700	
		C	-1.46505200	-1.21734800	0.39588900	
		H	3.45771100	2.08343600	-0.03521300	
		H	4.61820400	-0.09602800	-0.09882500	
		H	3.31996500	-2.20695400	-0.15238600	
		H	1.14741900	-3.38853500	-0.35012100	
		H	-1.28086500	-3.38255400	-0.08938700	
		H	-1.55199300	-1.27849100	1.50893000	
		C	-0.68287000	0.05324700	0.13955200	
		C	-1.36540000	1.27915500	0.04716600	
		C	0.76617100	2.46175600	0.01841300	
		C	-2.78617000	1.28493400	-0.07518200	
		C	-0.60003700	2.48666900	0.00525200	
		H	1.33083700	3.38806000	-0.00198500	
		C	-3.49972300	0.07762100	-0.22967700	
		H	-3.30313700	2.23410400	-0.15865800	
		C	-2.88726000	-1.13681100	-0.08601800	
		H	-1.12812800	3.43347000	-0.04217600	
		H	-4.55297300	0.11994800	-0.48769900	
		H	-3.43864800	-2.06188500	-0.21522100	
IS14	-616.19432	C	-2.38223900	0.38071100	0.02921300	45 70 88 169 179 247 292 314 409 423 443 478 501 529 560
		C	-1.05720700	-0.16493400	-0.03250800	577 622 630 656 703 713 743 751 791 806 812 841 856 876
		C	-0.92205900	-1.57377900	-0.16088800	925 946 970 974 987 987 991 994 1042 1047 1082 1119
		C	-2.02373700	-2.39598700	-0.19939200	1139 1169 1175 1186 1207 1230 1248 1272 1305 1321 1361
		C	-3.32655400	-1.85602800	-0.11626600	1387 1423 1434 1469 1473 1493 1543 1564 16121626 1633
		C	-3.49730100	-0.49773600	-0.00918700	1658 3157 3157 3160 3163 3169 3172 3174 3183 3186 3186
		C	-2.55921200	1.78534200	0.11878700	3198
		C	-1.47360800	2.62408800	0.14206800	
		C	-0.16723800	2.09400900	0.08959700	
		H	0.06796800	-2.00419200	-0.23446900	
		H	-1.89214300	-3.46759600	-0.29952100	
		H	-4.18718900	-2.51480600	-0.14531000	
		H	-4.49393600	-0.07188800	0.04433400	
		H	-3.56705600	2.18384800	0.16898400	
		H	-1.61066400	3.69712800	0.21439000	
		H	0.67841000	2.77008700	0.14316100	
		C	0.06277200	0.73269100	0.01068500	
		C	1.46819100	0.24631000	-0.02082700	
		C	1.95209300	-0.77052000	0.78130300	
		C	2.43348300	0.83830700	-0.86303800	
		C	3.24295900	-1.23221700	0.84179400	
		C	3.76095000	0.41373400	-0.85051600	
		H	2.12428000	1.62708300	-1.54102400	
		C	4.17562000	-0.61431200	-0.00410600	
		H	3.53830500	-2.03222100	1.51195200	
		H	4.47665300	0.88618300	-1.51374800	
		H	5.21038300	-0.93976300	0.00118800	
IS15	-616.22719	C	-2.26624600	0.50333900	0.02282000	95 114 158 198 229 279 341 408 432 466 472 491 535 544
		C	-0.93488900	0.19850400	-0.27489200	556 602 616 630 673 690 738 756 759 775 797 815 842 876
		C	-0.37795300	-1.19174600	-0.29548500	885 895 954 957 967 975 987 1023 1044 1068 1072 1104
		C	-1.14570400	-2.09864800	0.62275400	1132 1157 1172 1179 1191 1197 1227 1231 1285 1292 1317
		C	-2.45952100	-1.79184100	0.90560300	1322 1359 1380 1420 1463 1468 1490 1502 1525 1607 1615
		C	-3.07087000	-0.57121500	0.53816500	1619 1645 2847 3153 3158 3159 3164 3172 3175 3176
		C	-2.62811200	1.86812000	-0.04677300	3183 3184 3187
		C	-1.66438600	2.83629900	-0.32796500	
		C	-0.31090000	2.50838400	-0.49740300	
		H	-0.55276100	-1.59096100	-1.31789200	
		H	-0.71475700	-3.04026000	0.94325500	
		H	-3.05381300	-2.51208400	1.45932200	
		H	-4.11278700	-0.39675400	0.78124200	
		H	-3.64988400	2.16787700	0.16099900	
		H	-1.96277200	3.87807100	-0.37099600	
		H	0.42383700	3.29287600	-0.63903600	
		C	0.05777500	1.15974100	-0.44528500	
		C	1.35406000	0.45698900	-0.42340900	

		C	1.12073700	-0.92712000	-0.23763700	
		C	2.65819000	0.94153500	-0.50779800	
		C	2.18248800	-1.81318200	-0.13650100	
		C	3.72239900	0.04572000	-0.39258100	
		H	2.84898000	1.99936900	-0.65256500	
		C	3.48917000	-1.31760700	-0.20293800	
		H	2.01062800	-2.87612600	-0.00218100	
		H	4.74125400	0.41253800	-0.44794800	
		H	4.32776000	-1.99827600	-0.10821600	
IS16	-615.68805	C	2.32869200	-0.02050600	-0.03128700	101 120 164 207 254 295 356 434 436 465 477 493 570 571
		C	0.92781700	-0.01853100	-0.05951600	572 627 628 648 684 746 752 777 783 789 816 827 880 906
		C	0.13264100	1.15294700	-0.10272000	916 925 951 976 985 985 989 1037 1043 1060 1105 1123
		C	0.76953500	2.37508000	-0.11824300	1161 1182 1184 1208 1234 1253 1292 1317 1340 1395 1402
		C	2.19102000	2.40563400	-0.09029300	1441 1453 1470 1484 1504 1521 1612 1639 1641 1644 1656
		C	2.95783400	1.25604100	-0.04818300	3159 3160 3160 3166 3170 3171 3176 3183 3184 3188
		C	2.95304000	-1.29882200	0.01082300	
		C	2.18191300	-2.44624800	0.02183500	
		C	0.76054800	-2.41168800	-0.00752500	
		H	0.21800400	3.30844700	-0.15101900	
		H	2.68762200	3.36965800	-0.10262400	
		H	4.04023800	1.32661000	-0.02800500	
		H	4.03517400	-1.37244500	0.03427800	
		H	2.67489700	-3.41167000	0.05404000	
		H	0.20551700	-3.34349900	0.00282600	
		C	0.12824200	-1.18776000	-0.04851600	
		C	-1.27343700	-0.72803500	-0.08737900	
		C	-1.27075800	0.69718000	-0.12043900	
		C	-2.47509900	-1.42602700	-0.09538200	
		C	-2.46978700	1.39855800	-0.16099500	
		C	-3.67547900	-0.70991600	-0.13626400	
		H	-2.48881800	-2.51032400	-0.07043900	
		C	-3.67285200	0.68583800	-0.16870200	
		H	-2.47943500	2.48288800	-0.18645800	
		H	-4.61877500	-1.24434400	-0.14286000	
		H	-4.61413200	1.22292500	-0.20021800	
IS17	-617.35139	C	-2.52280700	0.91452800	-0.21196500	26 38 57 104 133 224 246 279 351 400 413 439 476 538 546
		C	-1.82536300	-0.31298500	-0.19208300	565 586 630 636 711 725 739 755 765 809 835 843 853 863
		C	-2.49843300	-1.50204300	0.03847900	877 900 930 949 980 984 987 998 1017 1040 1049 1053
		C	-3.88269200	-1.46594300	0.25152800	1100 1111 1164 1168 1175 1182 1192 1200 1203 1223 1237
		C	-4.57216900	-0.25330900	0.23083800	1302 1314 1338 1343 1360 1362 1478 1483 1484 1490 1526
		C	-3.89920700	0.94946600	-0.00175500	1595 1623 1625 1637 1643 3016 3038 3080 3149 3157 3158
		C	-1.55729000	2.00326800	-0.47986800	3164 3167 3175 3176 3186 3187 3206
		C	-0.36138100	1.43188800	-0.60417800	
		C	-0.33918000	-0.06287800	-0.45268400	
		H	-1.97191600	-2.45084100	0.05329500	
		H	-4.42227000	-2.38858400	0.43311100	
		H	-5.64375200	-0.24389000	0.39699900	
		H	-4.44137400	1.88866000	-0.01834400	
		H	-1.80910500	3.05256100	-0.55726000	
		H	-0.03993300	-0.52677100	-1.40110000	
		C	0.59654300	-0.58738000	0.66632600	
		H	0.41728300	-1.66007100	0.78352900	
		H	0.31047900	-0.11088300	1.60790400	
		C	2.06243900	-0.34680600	0.38126300	
		C	2.69836100	0.81963800	0.81989500	
		C	2.80976600	-1.27697600	-0.34984800	
		C	4.04230600	1.05254400	0.53319800	
		H	2.13572600	1.55069200	1.39119400	
		C	4.15359100	-1.04826500	-0.63963400	
		H	2.33702500	-2.19325800	-0.69101900	
		C	4.77434900	0.11953500	-0.19910700	
		H	4.51803700	1.96163100	0.88436400	
		H	4.71632000	-1.78336100	-1.20451800	
		H	5.82048100	0.29842100	-0.42058700	
IS18	-617.33447	C	-1.93640200	0.75806800	-0.35206500	57 65 98 152 215 270 275 309 368 404 426 458 500 526 565
		C	-1.88621900	-0.61350800	0.01230500	581 598 614 651 661 719 746 762 765 774 802 824 847 856
		C	-3.05119500	-1.30594400	0.31257000	873 885 917 947 952 967 969 972 987 997 1004 1040 1050
		C	-4.26959800	-0.61874300	0.30601500	1098 1106 1124 1143 1164 1173 1184 1200 1204 1228 1255
		C	-4.31851900	0.73661100	-0.03038200	1289 1306 1326 1333 1367 1406 1452 1464 1477 1489 1536
		C	-3.15774000	1.43390900	-0.36824300	1592 1599 1621 1641 3054 3060 3135 3152 3153 3156 3162
		C	-0.57054000	1.23479800	-0.61281200	3170 3171 3173 3185 3194 3195
		C	0.25738900	0.17092100	-0.57588700	
		C	-0.46398900	-1.07326300	-0.13518900	
		H	-3.02118100	-2.36010300	0.56861600	

		H	-5.18355900	-1.14029500	0.56717600	
		H	-5.27290500	1.25174000	-0.03329800	
		H	-3.20792100	2.48245000	-0.64169100	
		H	-0.28598600	2.27801700	-0.66947300	
		H	-0.37198400	-1.94560700	-0.78832600	
		C	0.64440800	-1.11417200	0.98489900	
		H	1.06088800	-2.09430600	1.22092500	
		H	0.33730000	-0.59377400	1.89158200	
		C	1.60498600	-0.16096000	0.09094500	
		C	2.28262200	0.94362000	0.82630300	
		C	2.54758300	-0.96203900	-0.75344200	
		C	3.63211500	1.15119900	0.76531400	
		H	1.65455100	1.58578900	1.43517000	
		C	3.89011000	-0.71847400	-0.78403700	
		H	2.12585800	-1.76162400	-1.35357100	
		C	4.46651000	0.33132600	-0.02907600	
		H	4.07312500	1.96306000	1.33475100	
		H	4.52894500	-1.33615900	-1.40701000	
		H	5.53374000	0.51071300	-0.06814700	
IS19	-617.38429	C	-1.87698000	-0.85014000	0.08099300	39 57 92 105 121 169 227 277 283 293 367 413 441 476 517
		C	-1.93311400	0.55649800	0.08698300	540 560 582 609 634 647 679 703 752 762 778 790 819 847
		C	-3.15115400	1.21734100	0.09812500	871 885 899 927 952 981 988 989 998 1008 1015 1040 1052
		C	-4.32855200	0.45994400	0.11452800	1095 1103 1126 1173 1182 1186 1201 1208 1209 1262 1280
		C	-4.27595800	-0.93609600	0.11636900	1300 1320 1333 1358 1381 1454 1473 1488 1489 1524 1598
		C	-3.05089700	-1.60486900	0.09935300	1614 1632 1637 1643 3005 3140 3158 3160 3164 3167 3174
		C	-0.47665600	-1.25152300	0.06362700	3179 3184 3186 3191 3193 3249
		C	0.33554000	-0.16712300	0.05797000	
		C	-0.52167000	1.11783800	0.07092700	
		H	-3.19655000	2.30134100	0.09275100	
		H	-5.29001400	0.96091200	0.12621100	
		H	-5.19849400	-1.50594800	0.12929100	
		H	-3.01579900	-2.68908300	0.09865000	
		H	-0.14633900	-2.28267700	0.08909700	
		H	-0.33289500	1.65605400	1.00937200	
		C	-0.25492200	2.02625200	-1.08704600	
		H	0.40703100	2.87757800	-0.99671700	
		H	-0.60489600	1.74758000	-2.07345500	
		C	1.80251800	-0.15709000	0.06058300	
		C	2.53635000	-1.25785400	-0.41817700	
		C	2.52291000	0.94604900	0.54953100	
		C	3.92590600	-1.26172600	-0.39121000	
		H	2.00949000	-2.10899800	-0.83365600	
		C	3.91488700	0.94261700	0.57529200	
		H	1.99103600	1.80996700	0.92996400	
		C	4.62446400	-0.16122600	0.10720400	
		H	4.46720200	-2.12162200	-0.77022000	
		H	4.44586200	1.80449000	0.96417700	
		H	5.70833400	-0.16293000	0.12422100	
IS20	-617.38389	C	-1.82851700	0.42663700	0.62756200	26 62 81 172 187 257 280 336 372 394 416 448 482 544 553
		C	-1.89298400	-0.46181800	-0.49337600	579 596 633 651 674 713 725 747 770 774 793 840 857 862
		C	-3.07323800	-0.62774200	-1.19462600	871 913 930 937 959 964 976 986 1002 1016 1028 1032
		C	-4.21598500	0.07769900	-0.78662900	1053 1058 1102 1111 1124 1167 1181 1191 1195 1201 1233
		C	-4.16993100	0.93221700	0.32422500	1254 1270 1320 1347 1350 1355 1404 1454 1474 1476 1497
		C	-2.99276300	1.11196400	1.03904400	1527 1583 1605 1617 1642 3118 3157 3158 3163 3164
		C	-0.51207000	0.45124600	1.13692200	3165 3173 3175 3179 3187 3188 3203 3209
		C	0.36324700	-0.48353500	0.37686700	
		C	-0.56242700	-1.09782600	-0.68847600	
		H	-3.12178200	-1.29489400	-2.04893300	
		H	-5.14448700	-0.04168700	-1.33318900	
		H	-5.06645400	1.46345700	0.62438600	
		H	-2.96183600	1.78172600	1.89158000	
		H	-0.16361700	1.04462300	1.97211000	
		H	-0.19358900	-1.31418500	-1.68410600	
		C	-0.04826900	-1.95268500	0.45440600	
		H	0.70671800	-2.68801700	0.20139300	
		H	-0.74344200	-2.25276100	1.22963700	
		C	1.78900100	-0.10001000	0.11442300	
		C	2.06826100	1.08025300	-0.58925700	
		C	2.86188200	-0.86773300	0.57765800	
		C	3.38110100	1.47359800	-0.83171900	
		H	1.24560600	1.68863500	-0.94987000	
		C	4.17891400	-0.47587300	0.33620200	
		H	2.66703000	-1.77482700	1.13865900	
		C	4.44303900	0.69455400	-0.37067500	
		H	3.57682800	2.38718300	-1.38243000	

		H	4.99727800	-1.08459800	0.70491300	
		H	5.46616800	0.99967800	-0.55946200	
IS21	-617.41698	C	1.81057100	0.54576100	-0.10891300	36 57 104 123 172 236 269 282 334 411 413 451 476 510
		C	2.33475100	-0.77629000	0.11501100	542 549 563 620 636 691 694 704 737 758 762 773 846 850
		C	3.75074000	-0.93764300	0.17398200	853 908 919 926 937 950 972 972 983 1000 1014 1038 1053
		C	4.59653400	0.13987600	0.01164300	1059 1107 1140 1163 1183 1198 1205 1214 1229 1278 1289
		C	4.07451600	1.42721000	-0.21516800	1312 1337 1347 1359 1390 1428 1450 1452 1476 1503 1527
		C	2.69646300	1.61575800	-0.27201700	1558 1600 1609 1634 1649 2918 2949 3154 3156 3157 3160
		C	0.37844500	0.73235600	-0.14628400	3161 3168 3174 3181 3187 3188 3192
		C	-0.51866700	-0.27205500	0.00293300	
		C	1.45067900	-1.84379000	0.26068900	
		H	4.15478700	-1.92985600	0.34613600	
		H	5.67034400	-0.00456000	0.05731000	
		H	4.74416100	2.26956700	-0.34326500	
		H	2.29433000	2.60951200	-0.44300500	
		H	0.02526900	1.74465600	-0.31495800	
		H	1.84534300	-2.84145100	0.42542700	
		C	-0.03254300	-1.69518600	0.17075300	
		H	-0.51389700	-2.14357100	1.05493900	
		H	-0.40248800	-2.31261700	-0.66656600	
		C	-1.97752100	-0.02729300	0.00090900	
		C	-2.51202300	1.20765300	0.41402700	
		C	-2.88493600	-1.02424600	-0.39846500	
		C	-3.88173800	1.44295400	0.39965100	
		H	-1.84738100	1.98263800	0.77649900	
		C	-4.25761600	-0.78842800	-0.41382200	
		H	-2.51969400	-1.99165800	-0.72046700	
		C	-4.76474500	0.44666500	-0.01817900	
		H	-4.26341200	2.40286300	0.72988000	
		H	-4.93149300	-1.57412800	-0.73734900	
		H	-5.83332400	0.62879500	-0.02507600	
IS22	-616.87330	C	1.79408600	-0.54322300	0.11317400	52 62 92 172 185 261 276 338 401 416 433 485 514 527 554
		C	2.29732800	0.76993400	-0.14613700	569 632 642 665 709 711 753 772 780 786 833 854 868 871
		C	3.70077000	0.97521400	-0.18074700	910 934 957 967 982 985 992 1001 1015 1036 1043 1063
		C	4.57000300	-0.06779300	0.03530600	1103 1153 1173 1181 1182 1205 1218 1255 1289 1298 1315
		C	4.07351200	-1.36705600	0.29693200	1352 1378 1396 1403 1458 1480 1497 1527 1541 1602 1616
		C	2.71925700	-1.59816000	0.33551500	1639 1640 1666 3156 3159 3159 3161 3164 3167 3174 3175
		C	0.39203400	-0.74969600	0.14753200	3181 3183 3187 3190
		C	-0.50279500	0.28237900	-0.06255500	
		C	1.36521800	1.81865100	-0.35975800	
		H	4.07911800	1.97254800	-0.38028400	
		H	5.64057400	0.10121300	0.00727500	
		H	4.76868400	-2.18155700	0.46701800	
		H	2.33852600	-2.59434600	0.53612300	
		H	0.02367000	-1.74552000	0.37069500	
		H	1.73789000	2.81628400	-0.56857100	
		C	0.01391300	1.58497400	-0.31799400	
		H	-0.67747600	2.39801500	-0.50731200	
		C	-1.96918000	0.05111400	-0.02299000	
		C	-2.53420600	-1.10125600	-0.58990300	
		C	-2.82858200	0.97889400	0.58480800	
		C	-3.90829000	-1.32135000	-0.54525000	
		H	-1.89292200	-1.81771500	-1.09067000	
		C	-4.20280800	0.75907400	0.63021800	
		H	-2.41446200	1.86757300	1.04767700	
		C	-4.74920800	-0.39231100	0.06555200	
		H	-4.32377900	-2.21511300	-0.99757500	
		H	-4.84683700	1.48503000	1.11419000	
		H	-5.81929700	-0.56274700	0.09922200	
IS23	-617.36870	C	-1.80194000	-0.67383800	-0.27433700	39 56 109 152 173 260 286 312 350 411 419 431 485 522
		C	-1.78975400	0.80950500	-0.19211400	548 563 631 636 668 677 698 709 715 764 774 807 829 840
		C	-2.99218800	1.45004900	0.34484500	845 875 915 920 932 937 961 970 979 994 998 1009 1027
		C	-4.13862300	0.72231800	0.45423700	1034 1051 1073 1100 1124 1158 1181 1199 1205 1214 1232
		C	-4.17664800	-0.67132900	0.12483600	1268 1301 1326 1348 1358 1371 1402 1442 1467 1474 1509
		C	-3.01660100	-1.36030800	-0.20768500	1523 1537 1599 1606 1632 3113 3151 3155 3159 3160 3167
		C	-0.46372900	-1.14766800	-0.25270400	3173 3180 3186 3187 3191 3200 3210
		C	0.43052600	-0.11552300	-0.04458300	
		C	-0.31370300	1.18811000	-0.02034500	
		H	-2.97483200	2.50861800	0.58218600	
		H	-5.04704800	1.19980600	0.80506700	
		H	-5.11660000	-1.20488400	0.20402300	
		H	-3.04145000	-2.43729900	-0.34054300	
		H	-0.19702000	-2.18938500	-0.37504700	
		H	-0.01558700	1.98360000	0.65335300	

		C	-0.99717200	1.54804200	-1.31166800	
		H	-1.28169100	2.58227100	-1.46843200	
		H	-0.75122700	0.98409600	-2.20406000	
		C	1.87774200	-0.20585000	0.09000100	
		C	2.53126300	-1.44689800	0.24543600	
		C	2.67907200	0.95287200	0.06752400	
		C	3.91184300	-1.52165200	0.36412200	
		H	1.94699000	-2.35832900	0.28803100	
		C	4.06329300	0.87502000	0.18784800	
		H	2.21270100	1.92231400	-0.06097900	
		C	4.68944700	-0.36098700	0.33574900	
		H	4.38726900	-2.48880200	0.48588600	
		H	4.65483800	1.78366800	0.16311300	
		H	5.76746800	-0.42198200	0.43097900	
IS24	-617.42251	C	-1.80289900	-0.34823600	-0.23778200	39 57 88 125 175 228 257 272 327 412 416 446 501 515 529
		C	-2.21357100	1.00393200	-0.12225900	557 598 620 637 698 705 711 740 752 756 783 800 855 862
		C	-3.57080600	1.31352700	-0.18863700	868 929 932 941 962 983 984 987 1001 1016 1051 1056
		C	-4.53157500	0.32017800	-0.36941000	1097 1106 1136 1179 1182 1201 1202 1203 1228 1258 1292
		C	-4.13352200	-1.01549000	-0.48851500	1302 1311 1338 1355 1361 1397 1446 1474 1476 1513 1523
		C	-2.78931500	-1.34319200	-0.42404900	1571 1595 1615 1626 1641 2942 2958 3148 3158 3158 3164
		C	-0.41223800	-0.68618400	-0.16924300	3169 3172 3174 3179 3181 3187 3189
		C	0.58706700	0.29326000	0.02642000	
		C	0.23228500	1.61858900	0.14697800	
		H	-3.88339600	2.34990800	-0.09905400	
		H	-5.58195200	0.58352700	-0.41863300	
		H	-4.87542700	-1.79330000	-0.63086600	
		H	-2.47664900	-2.37834600	-0.51575600	
		H	-0.12686500	-1.72385800	-0.29624300	
		H	0.99673600	2.36481200	0.33367500	
		C	-1.18330300	2.09615200	0.06362700	
		H	-1.42534500	2.67900800	0.96613300	
		H	-1.27435800	2.82625700	-0.75754300	
		C	2.01695100	-0.11757600	0.10886800	
		C	2.39934100	-1.24209500	0.85408600	
		C	3.01570100	0.60952900	-0.55389400	
		C	3.73616000	-1.62367800	0.93846200	
		H	1.64526300	-1.80858200	1.38900000	
		C	4.35281700	0.22845800	-0.47084900	
		H	2.73780900	1.46726500	-1.15605700	
		C	4.71905100	-0.88991300	0.27616300	
		H	4.01086400	-2.49148500	1.52802100	
		H	5.10821700	0.80056800	-0.99830500	
		H	5.75959700	-1.18748000	0.34040100	
IS25	-616.19797	C	1.79682500	-0.56463300	0.08346000	40 59 94 164 183 262 278 322 407 414 433 494 502 521 547
		C	2.30957000	0.76675800	-0.10703600	568 630 639 650 706 709 749 763 776 782 824 852 871 872
		C	3.71487500	0.95372200	-0.12063600	930 936 961 972 984 992 1000 1015 1035 1044 1072 1105
		C	4.56974600	-0.11007900	0.04970000	1143 1173 1178 1182 1205 1236 1260 1282 1313 1343 1357
		C	4.06061400	-1.41665800	0.24117200	1363 1393 1445 1476 1489 1516 1529 1577 1613 1636 1640
		C	2.70516200	-1.64259000	0.25746100	1658 3157 3160 3161 3167 3169 3176 3179 3181 3183 3190
		C	0.40578900	-0.68248700	0.08293800	3191
		C	-0.52172200	0.30706300	-0.05959100	
		C	1.38268100	1.83057800	-0.27749100	
		H	4.10721100	1.95484500	-0.26788600	
		H	5.64203700	0.04915800	0.03812300	
		H	4.74853500	-2.24384800	0.37464800	
		H	2.30939200	-2.64083800	0.40285500	
		H	1.76648000	2.83275900	-0.43646500	
		C	0.02699900	1.61725800	-0.25684500	
		H	-0.64954000	2.45021800	-0.41340400	
		C	-1.98170900	0.05571300	-0.01964000	
		C	-2.49529500	-1.18855800	-0.41711500	
		C	-2.88227800	1.03575200	0.42184900	
		C	-3.86219200	-1.44237300	-0.37801000	
		H	-1.81112500	-1.95219200	-0.76958600	
		C	-4.25115400	0.78179000	0.45921100	
		H	-2.51206000	1.99591800	0.76182800	
		C	-4.74782300	-0.45706400	0.05848400	
		H	-4.23822400	-2.40891700	-0.69476700	
		H	-4.92970400	1.55146600	0.80999100	
		H	-5.81353700	-0.65370500	0.08719000	
IS26	-616.16924	C	1.19557300	-0.30321400	-0.19404000	62 95 138 161 194 292 321 346 408 431 453 494 517 535
		C	2.09833500	0.80084100	0.02612500	544 588 598 645 672 685 695 756 759 772 803 824 841 871
		C	3.47727400	0.51526100	0.18406100	886 892 934 962 963 971 974 991 999 1009 1039 1107 1120
		C	3.94740500	-0.77791800	0.13038200	1130 1158 1167 1178 1206 1229 1239 1278 1287 1319 1358

		C	3.05688100	-1.85562300	-0.08661100	1371 1383 1411 1420 1466 1472 1525 1550 1570 1598 1623 1660 2930 3149 3156 3157 3160 3165 3169 3177 3185 3186 3188
		C	1.71084200	-1.62537500	-0.24490800	
		C	-0.15252500	0.05277100	-0.34454700	
		C	-0.60511600	1.36955500	-0.27334800	
		C	1.60711700	2.14323700	0.07685600	
		H	4.16562200	1.33805700	0.34854600	
		H	5.00614300	-0.97533500	0.25425500	
		H	3.44288900	-2.86806300	-0.12716500	
		H	1.02689400	-2.45033900	-0.41058700	
		H	2.33002900	2.93604600	0.24067000	
		C	0.27338400	2.45601300	-0.06813900	
		H	-0.06930800	3.48287200	-0.01967900	
		C	-1.99581000	0.95715600	-0.38645200	
		C	-1.56750100	-0.48919600	-0.66010500	
		C	-3.25789200	1.29537700	0.03648500	
		C	-2.39711200	-1.48389700	0.09041400	
		H	-1.61925900	-0.73025700	-1.73551400	
		C	-4.13123600	0.24034100	0.36809700	
		H	-3.54316300	2.32374600	0.23475500	
		C	-3.65249100	-1.10709800	0.47238000	
		H	-2.06208000	-2.50871900	0.21092800	
		H	-5.14346400	0.46005400	0.68652500	
		H	-4.32036000	-1.84772000	0.90140900	
IS27	-616.17034	C	-0.00179400	-0.02269000	-0.00106300	68 83 141 164 196 279 314 363 405 435 453 491 514 541 546 587 601 638 663 689 705 745 766 776 807 818 825 874 885 903 952 955 959 965 970 977 993 1039 1061 1103 1124 1140 1154 1173 1182 1200 1214 1231 1276 1285 1309 1355 1369 1379 1412 1423 1461 1477 1521 1548 1571 1591 1622 1658 2932 3149 3157 3157 3161 3166 3169 3178 3181 3185 3188
		C	0.00502900	0.00749100	1.43731200	
		C	1.26119100	-0.00839600	2.09903600	
		C	2.43843700	-0.05136200	1.38816500	
		C	2.42080800	-0.08003300	-0.02479600	
		C	1.22352900	-0.06536100	-0.70518500	
		C	-1.28940400	-0.01146100	-0.59457000	
		C	-2.46171400	0.05334700	0.16303900	
		C	-1.21716100	0.05008100	2.17370700	
		H	1.28009200	0.01431900	3.18382300	
		H	3.38763800	-0.06268700	1.91198600	
		H	3.35624100	-0.11241700	-0.57197800	
		H	1.20829700	-0.08230500	-1.78924000	
		H	-1.15385700	0.06559800	3.25688500	
		C	-2.46069100	0.07721800	1.55741100	
		H	-3.37139300	0.11372800	2.14443000	
		C	-3.35035800	0.11455600	-1.10144200	
		C	-2.02845200	-0.13677500	-1.83597800	
		C	-4.43754000	-0.81434400	-1.54238500	
		C	-1.96696300	-0.72426200	-3.07994000	
		H	-3.69932700	1.15226100	-1.23676500	
		C	-4.33855400	-1.36386200	-2.78686900	
		H	-5.33360300	-0.94309500	-0.94427800	
		C	-3.16154500	-1.25165100	-3.60137000	
		H	-1.02587600	-0.89592700	-3.59254500	
		H	-5.17103900	-1.93841900	-3.18111900	
		H	-3.16288700	-1.71011000	-4.58330100	
IS28	-616.19383	C	-2.15834800	0.47617400	0.90724800	43 72 84 167 189 242 281 311 411 416 439 479 500 527 561 570 628 630 655 709 714 744 769 789 791 804 836 858 878 934 953 966 975 986 998 1002 1016 1044 1050 1092 1106 1133 1161 1179 1182 1203 1222 1238 1290 1310 1321 1353 1381 1408 1442 1465 1474 1523 1530 1587 1609 1620 1639 1651 3155 3159 3160 3167 3169 3177 3178 3183 3185 3190 3200
		C	-0.97217300	0.23842300	0.13306200	
		C	-0.98879000	0.58021800	-1.24563300	
		C	-2.09870400	1.15389400	-1.82147200	
		C	-3.25382700	1.41662100	-1.05208900	
		C	-3.28055100	1.07891300	0.27893300	
		C	-2.20762800	0.09636100	2.27559200	
		C	-1.12828900	-0.51748800	2.87658500	
		C	-0.00563200	-0.71895300	2.08051400	
		H	-0.11669500	0.37103100	-1.85117800	
		H	-2.08974100	1.40019800	-2.87748500	
		H	-4.12003300	1.87330200	-1.51722200	
		H	-4.16997600	1.26220700	0.87283500	
		H	-3.11357200	0.28801000	2.84219600	
		H	-1.15628400	-0.82059800	3.91707400	
		C	0.17047600	-0.36626400	0.77771000	
		C	1.47449300	-0.60019300	0.09604800	
		C	2.05157200	-1.87709500	0.10595100	
		C	2.17442200	0.44699100	-0.51924900	
		C	3.28846200	-2.10408500	-0.49315500	
		H	1.51933000	-2.69309400	0.58124900	
		C	3.41272100	0.22012300	-1.11511600	
		H	1.75570400	1.44682000	-0.51184300	
		C	3.97263700	-1.05680400	-1.10764600	
		H	3.71680500	-3.10022000	-0.48062500	

		H	3.94396300	1.04375400	-1.57924800	
		H	4.93592700	-1.23260000	-1.57303200	
IS29	-616.19433	C	0.02522000	-0.06752500	-0.01077200	44 70 88 168 179 246 291 314 409 423 442 478 501 529 560
		C	0.00394400	-0.01433800	1.42239600	577 622 630 656 703 713 743 751 791 806 812 841 856 876
		C	1.24877500	0.04149300	2.10567300	925 945 970 974 986 987 991 994 1042 1047 1082 1119
		C	2.44084300	0.01944600	1.42033100	1139 1169 1175 1186 1207 1230 1248 1272 1305 1321 1361
		C	2.45736100	-0.05518800	0.00967000	1387 1423 1434 1469 1473 1493 1543 1564 1612 1626 1633
		C	1.27412700	-0.09291200	-0.68611400	1658 3157 3157 3160 3163 3169 3172 3174 3183 3186 3186
		C	-1.19707100	-0.08533100	-0.73051900	3198
		C	-2.39709200	-0.04743700	-0.06638100	
		C	-2.42575500	-0.00309700	1.34342700	
		H	1.25518900	0.10754700	3.18567500	
		H	3.37643100	0.06482200	1.96650100	
		H	3.40364400	-0.07438400	-0.51920300	
		H	1.27559700	-0.13926600	-1.77024600	
		H	-1.16591900	-0.12993100	-1.81408500	
		H	-3.33031100	-0.06495400	-0.61795000	
		C	-1.26475300	0.00716400	2.09462800	
		C	-1.37383000	0.03405900	3.57791800	
		C	-0.67737800	-0.81368200	4.41923100	
		C	-2.25269000	0.92086600	4.23573200	
		C	-0.76878300	-0.87940200	5.78688200	
		H	-3.38330700	-0.00790400	1.85151100	
		C	-2.38998300	0.90558700	5.62264600	
		H	-2.81610600	1.63510900	3.64424900	
		C	-1.65825100	0.01198900	6.40451100	
		H	-0.18917400	-1.58667300	6.37011900	
		H	-3.07021700	1.60358300	6.09740700	
		H	-1.77010800	0.00484400	7.48345500	
IS30	-616.83834	C	-2.62857700	0.88073700	0.15558700	40 52 86 143 182 204 271 307 355 415 424 441 508 548 570
		C	-1.82720800	-0.27203100	-0.02523800	587 632 648 659 705 728 737 762 767 805 813 846 855 872
		C	-2.41951300	-1.50901900	-0.24276300	879 905 941 946 951 980 987 1002 1014 1037 1044 1052
		C	-3.81593200	-1.59595800	-0.26943000	1095 1107 1131 1179 1183 1201 1205 1212 1257 1296 1328
		C	-4.60529400	-0.45824500	-0.08807500	1343 1355 1371 1419 1473 1480 1489 1523 1563 1609 1623
		C	-4.01688100	0.79186600	0.12537400	1635 1641 1669 3131 3157 3159 3163 3166 3174 3176 3186
		C	-1.73115700	2.01781700	0.36127400	3188 3199 3202 3241
		C	-0.44418500	1.59779000	0.29444800	
		C	-0.40868100	0.15011800	0.04732800	
		H	-1.82103400	-2.40178000	-0.39123300	
		H	-4.28977300	-2.55706400	-0.43414800	
		H	-5.68569200	-0.54625100	-0.11477200	
		H	-4.63434300	1.67322100	0.26257500	
		H	-2.05786200	3.03077400	0.55768800	
		H	0.42623900	2.21594100	0.45101700	
		C	0.65239000	-0.68583700	-0.05561300	
		H	0.42719000	-1.74812500	-0.12182000	
		C	2.08238100	-0.37449800	-0.05749900	
		C	2.98260000	-1.34083900	0.42860400	
		C	2.61362600	0.82762300	-0.55921200	
		C	4.35141900	-1.09909800	0.45826000	
		H	2.59514800	-2.28425400	0.79905400	
		C	3.98395000	1.06462400	-0.53729500	
		H	1.95267400	1.56043300	-1.00332900	
		C	4.85851900	0.10846700	-0.02073600	
		H	5.02362600	-1.85460000	0.84930800	
		H	4.37308500	1.99406300	-0.93802900	
		H	5.92600800	0.29654400	-0.00639400	
IS31	-616.18190	C	-2.87119400	0.65359200	0.00000000	16 47 60 138 155 210 272 302 313 405 421 462 494 529 562
		C	-1.67716700	-0.10271400	-0.00000100	567 586 623 652 676 677 731 747 752 764 805 820 858 872
		C	-1.70912700	-1.48889500	-0.00000100	883 888 944 953 977 982 985 986 1029 1032 1041 1088
		C	-2.95324700	-2.12894500	-0.00000100	1098 1122 1170 1174 1179 1192 1208 1276 1288 1302 1344
		C	-4.13672000	-1.38655000	0.00000000	1346 1385 1450 1473 1483 1487 1556 1570 1585 1623 1639
		C	-4.10640700	0.01086600	0.00000100	1859 3159 3164 3166 3169 3176 3186 3187 3191 3196 3199
		C	-2.51241600	2.07416400	0.00000100	3230
		C	-1.16711600	2.20408300	0.00000000	
		C	-0.54004900	0.86074000	-0.00000100	
		H	-0.79130100	-2.06693600	-0.00000200	
		H	-2.99941100	-3.21211300	-0.00000100	
		H	-5.09081800	-1.90181400	0.00000100	
		H	-5.02980500	0.58024300	0.00000200	
		H	-3.22717300	2.88686600	0.00000200	
		H	-0.59937100	3.12324900	0.00000000	
		C	0.74267400	0.58514500	-0.00000100	
		C	2.05975800	0.21718000	0.00000000	

		C	2.77617000	0.02310800	1.22709500	
		C	2.77617100	0.02311000	-1.22709500	
		C	4.10892500	-0.34016400	1.21119900	
		H	2.25302100	0.16644600	2.16457000	
		C	4.10892700	-0.34016300	-1.21119800	
		H	2.25302300	0.16644900	-2.16457100	
		C	4.78956600	-0.52568700	0.00000100	
		H	4.63219800	-0.48275400	2.15033600	
		H	4.63220100	-0.48275100	-2.15033500	
		H	5.83495700	-0.81010800	0.00000100	
IS32	-616.12436	C	2.20694300	-0.82220800	0.20509900	34 47 74 145 182 214 295 360 403 413 427 445 510 530 548
		C	1.78291000	0.27939100	-0.63394100	580 594 631 680 696 699 722 745 764 770 790 848 854 863
		C	2.43280200	1.50458300	-0.58911000	881 918 926 944 968 975 982 995 1010 1030 1043 1058
		C	3.52887700	1.65720500	0.26366100	1101 1103 1143 1169 1182 1195 1215 1239 1257 1292 1319
		C	3.96355100	0.59551600	1.07713400	1332 1352 1367 1434 1472 1492 1514 1569 1601 1602 1628
		C	3.31490000	-0.62844000	1.06310600	1725 3084 3161 3163 3170 3170 3180 3181 3187 3190 3192
		C	1.36722000	-1.94939700	0.03719200	3193
		C	0.36929400	-1.67096800	-1.01563500	
		C	0.58982400	-0.19215800	-1.30933000	
		H	2.10763800	2.32404400	-1.21955200	
		H	4.05543800	2.60419800	0.29489200	
		H	4.82376800	0.73928800	1.72143000	
		H	3.65822400	-1.44060600	1.69482100	
		H	1.55771400	-2.92289900	0.47173300	
		H	0.22315000	-2.40643600	-1.80556400	
		C	-0.63416000	-0.51292000	-0.91794400	
		C	-1.88441000	-0.12056200	-0.34639700	
		C	-2.68237000	-1.05636300	0.33855000	
		C	-2.34548300	1.20584300	-0.47243900	
		C	-3.88966600	-0.66801700	0.90614400	
		H	-2.33665800	-2.08005800	0.42253500	
		C	-3.56135500	1.58053500	0.08292700	
		H	-1.74230500	1.92643900	-1.01257500	
		C	-4.33616500	0.64833000	0.77775300	
		H	-4.49098600	-1.39439500	1.44123600	
		H	-3.90827200	2.60254700	-0.02122000	
		H	-5.28398600	0.94565200	1.21163900	
IS33	-616.72324	C	-2.58443100	0.81901300	-0.16472600	36 39 54 129 162 195 234 305 395 402 413 431 476 518 540
		C	-1.74769200	-0.31505000	-0.21601200	559 588 627 636 696 725 743 752 773 792 836 853 866 876
		C	-2.24742600	-1.57564100	0.07788800	898 912 949 953 963 987 992 1006 1010 1040 1041 1060
		C	-3.59913900	-1.70038800	0.40870800	1087 1098 1133 1145 1176 1182 1186 1197 1221 1254 1284
		C	-4.43087600	-0.57635600	0.46087200	1308 1318 1344 1350 1385 1462 1478 1490 1503 1571 1592
		C	-3.93205700	0.69389100	0.17932200	1619 1622 1646 2929 3159 3160 3166 3170 3176 3179 3186
		C	-1.78536100	1.98640200	-0.50805300	3187 3190 3193 3232
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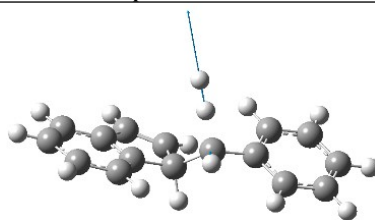
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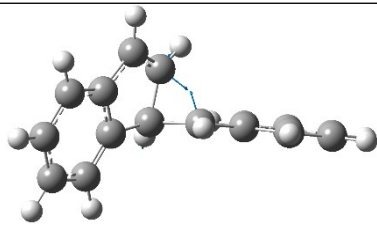
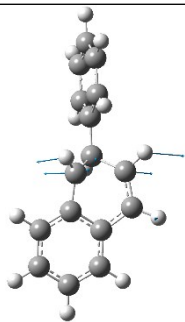
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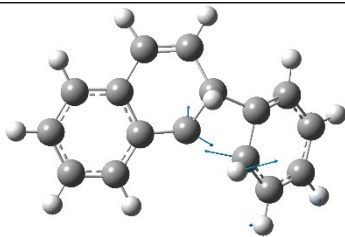
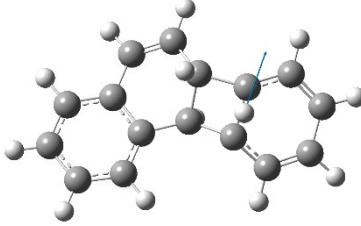
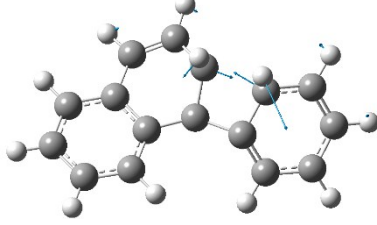
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		C	0.60125300	2.46409200	-1.94161200	
		C	-0.73076300	2.78261600	-2.16840800	
		H	-2.78939600	2.17903800	-1.91773600	
		H	1.38321500	3.13566400	-2.27948700	
		H	-0.98343500	3.70262600	-2.68300400	
ISF	-615.033956	C	1.71636100	-1.10741000	0.07944600	96 150 215 245 259 355 398 407 461 480 502 506 516 549
		C	0.34364900	-0.78210300	-0.12681500	552 576 596 661 699 718 740 757 764 798 809 825 827 856
		C	-0.01960200	0.41930600	-0.80661900	908 918 975 979 984 990 1011 1087 1107 1112 1165 1183
		C	0.99895000	1.29837700	-1.28167700	1197 1218 1228 1251 1261 1312 1341 1364 1390 1423 1443
		C	2.37364700	0.94455500	-1.05945100	1450 1454 1513 1526 1591 1606 1627 1639 1657 3155 3156
		C	2.71602200	-0.20001700	-0.41186200	3160 3162 3169 3175 3177 3184 3191
		C	2.04251300	-2.29537500	0.75111200	
		C	1.04834600	-3.15237800	1.21424300	
		C	-0.29729900	-2.85162200	1.02220900	
		H	3.14263700	1.61784600	-1.42354500	
		H	3.76009700	-0.44949000	-0.25387800	
		H	3.08719600	-2.54235500	0.90774700	
		H	1.32439800	-4.06481000	1.73056500	
		H	-1.06914800	-3.52046700	1.38373400	
		C	-0.66923800	-1.67581400	0.35656600	
		C	-2.00169600	-1.26771700	0.10462500	
		C	-1.39277100	0.75244900	-1.01725500	
		C	-2.40702600	-0.15728000	-0.52490600	
		C	-1.71481400	1.93951500	-1.68828200	
		C	0.62899500	2.47616800	-1.94833600	
		H	-3.45458700	0.08293400	-0.67775700	
		C	-0.71160400	2.78953700	-2.14731000	
		H	-2.75747900	2.19218300	-1.84803600	
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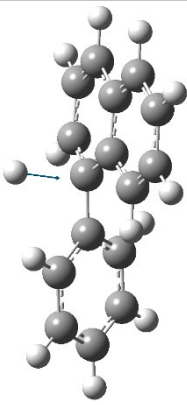
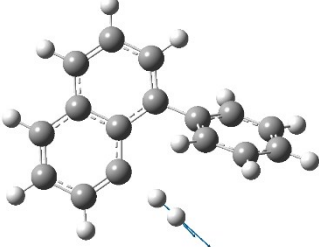
Table S3: The energies (in hartree), molecular geometries (in Å), displacement vectors and vibrational frequencies (in cm⁻¹) of transition structures (TS) obtained using B3LYP/6-311++G(d,p).

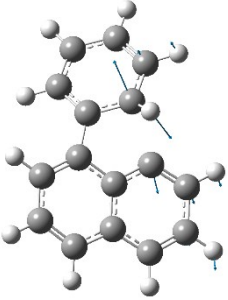
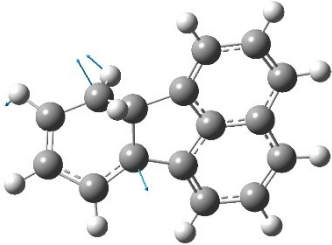
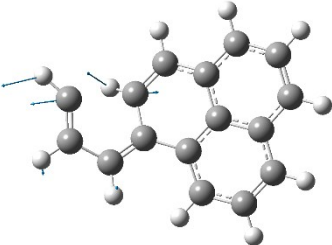
Species	E1	Cartesian coordinate (Å)			Displacement Vector	Frequency
TS2	-618.52821	C	-2.58800700	0.89166400	-0.12783200	-1216 28 46 78 104 143
		C	-1.84145300	-0.29690300	-0.24839400	220 240 250 269 331 403
		C	-2.45737400	-1.53168800	-0.11196200	414 420 442 505 542 562
		C	-3.83211300	-1.57705000	0.14804300	577 619 635 643 710 725
		C	-4.57257700	-0.39923900	0.26642200	736 750 768 796 825 836
		C	-3.95743100	0.84649800	0.12842200	855 870 881 922 935 952
		C	-1.67758600	2.02219800	-0.32397900	968 984 987 992 1000 1016
		C	-0.43068600	1.57138900	-0.54670800	1042 1049 1071 1089 1103
		C	-0.39271400	0.05523600	-0.53882500	1135 1165 1175 1182 1183
		H	-1.89434200	-2.45478200	-0.20582900	1203 1206 1221 1234 1260
		H	-4.32655600	-2.53564000	0.25795800	1285 1305 1318 1343 1349
		H	-5.63664900	-0.45401400	0.46786500	1369 1393 1410 1480 1486
		H	-4.53667700	1.75906800	0.22002200	1489 1523 1598 1614 1632
		H	-1.98083700	3.06162800	-0.30136500	1637 1646 2954 3080 3155

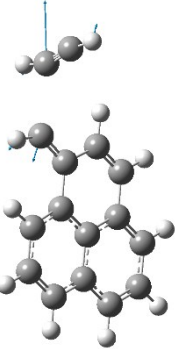
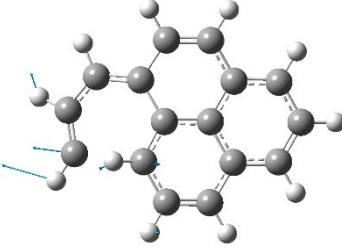
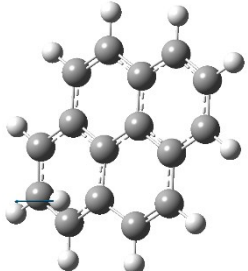


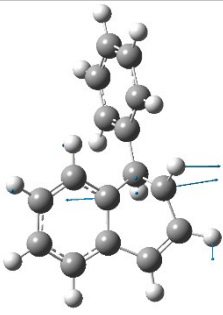
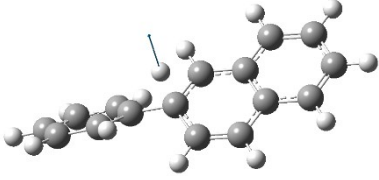
		H	0.43622400	2.18298200	-0.75195400		3156 3163 3163 3173 3174 3182 3186 3190 3192 3225
		H	-0.13870400	-0.28511200	-1.55675200		
		C	0.61095000	-0.62180000	0.40798500		
		H	0.40886300	-1.69329800	0.46344100		
		H	0.28126100	-0.22904100	1.58873200		
		C	2.06820900	-0.35616400	0.23578000		
		C	2.63941100	0.89003800	0.53756600		
		C	2.91747100	-1.38085300	-0.20938000		
		C	4.00468800	1.10859100	0.37568900		
		H	2.01343500	1.68473200	0.92611000		
		C	4.28270300	-1.16176500	-0.37823300		
		H	2.50039000	-2.35825400	-0.43011200		
		C	4.83149800	0.08617700	-0.08944700		
		H	4.42622000	2.07701400	0.62174500		
		H	4.91745400	-1.96725400	-0.73072400		
		H	5.89451500	0.25795000	-0.21486600		
		H	0.00545900	0.07604600	2.49485000		
TS3	-617.37978	C	-2.43369800	0.85037500	-0.03995700		-507 57 60 73 157 172 246 256 366 407 408 416 491 509 542 557 591 631 634 697 715 737 754 763 779 823 839 843 846 873 878 903 916 944 951 976 983 990 1004 1036 1043 1068 1083 1101 1123 1151 1174 1180 1188 1201 1227 1234 1250 1296 1327 1344 1351 1369 1381 1414 1474 1482 1500 1518 1596 1600 1621 1628 3117 3157 3158 3162 3164 3173 3175 3179 3187 3188 3190 3207 3232
TS4	-617.36251	C	2.35278500	0.79219200	-0.08782900		-644 36 67 75 159 179 251 270 367 390 414 416 460 520 532 548 578 626 635 663 687 692 711 752 766 769 808 851 854 857 873 913 929 949 980 982 982 1000 1016 1042 1050 1094 1113 1126 1160 1179 1182 1186 1205 1206 1226 1233 1251 1297 1318 1347 1351 1363 1417 1434 1481 1486 1498 1527 1596 1615 1622 1644 3050 3156 3158 3160 3162 3163 3170 3174 3177 3179 3181 3187 3188
		C	1.83455200	-0.46323900	0.34432300		
		C	2.67493400	-1.56925300	0.42109200		
		C	4.01302400	-1.45446000	0.02665600		
		C	4.51434100	-0.23420800	-0.43246400		
		C	3.69229900	0.89082600	-0.48171400		
		C	1.40103900	1.86001700	0.11227800		
		C	0.08257200	1.47095600	0.33875000		
		C	0.40608900	-0.43218400	0.67025900		
		H	2.29317700	-2.52160000	0.77377700		
		H	4.66339700	-2.32017700	0.08015700		
		H	5.55281700	-0.15681000	-0.73399600		
		H	4.09448600	1.84674100	-0.80094300		
		H	1.72412200	2.88030700	0.28551800		
		H	-0.61717100	2.10029100	0.87758400		
		H	-0.00490000	-0.92507500	1.54337200		
		C	-0.48649900	0.21646800	-0.31866500		
		H	-0.15781300	0.09989400	-1.35372500		
		C	-1.96902200	0.01793700	-0.19198000		
		C	-2.63024800	0.09192000	1.04146400		
		C	-2.72813200	-0.24892300	-1.33667900		
		C	-4.00748000	-0.09837300	1.12490100		
		H	-2.06948900	0.30163400	1.94609400		
		C	-4.10630300	-0.44028900	-1.25571700		
		H	-2.23332300	-0.30835000	-2.30056800		
		C	-4.75179700	-0.36583500	-0.02347200		
		H	-4.50034000	-0.03724900	2.08898200		
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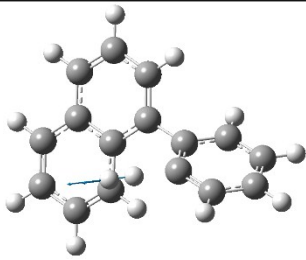
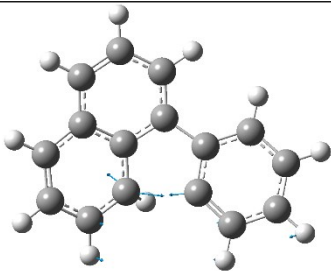
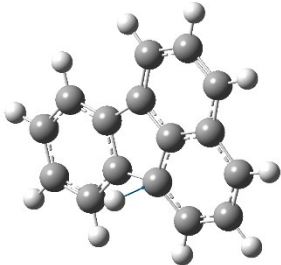
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		C	-1.36045900	-0.44762300	-0.09272500		
		C	-1.99220300	-1.68950000	-0.08410800		
		C	-3.38414400	-1.77815800	-0.06545600		
		C	-4.15632400	-0.61713100	-0.08103000		
		C	-3.53842400	0.63021900	-0.11832500		
		C	-1.49063800	2.06663800	-0.20770500		
		C	-0.18924100	2.25242600	0.08524400		
		C	0.10189200	-0.20810000	-0.18268400		
		H	-1.38891400	-2.59095500	-0.08303000		
		H	-3.86385300	-2.75025800	-0.04265200		
		H	-5.23841600	-0.68354300	-0.07143100		
		H	-4.14383800	1.53080400	-0.14850400		
		H	-2.11423900	2.90475700	-0.50335300		
		H	0.27435800	3.23209900	0.04230400		
		H	0.47412100	-0.20208000	-1.20794200		
		C	0.52475700	1.03771000	0.59293900		
		H	0.18782100	0.88312600	1.63513600		
		C	1.95830000	0.59692100	0.53169200		
		C	3.06939800	1.09409800	-0.08946200		
		C	1.74136800	-0.84441800	0.69380200		
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		H	3.15152600	2.15327700	-0.31078500		
		C	2.75425200	-1.72265600	0.17871400		
		H	1.20964000	-1.17362600	1.58683000		
		C	3.88594900	-1.18754900	-0.41996700		
		H	4.97878300	0.58366800	-0.98878000		
		H	2.65246900	-2.79595300	0.29432500		
		H	4.65581700	-1.85563000	-0.79186900		
TS6	-617.24493	C	-2.11084400	0.73358700	-0.22039100		-2359 71 91 128 168 176 281 309 346 377 404 419 473 502 530 540 569 589 617 669 679 701 716 751 781 795 795 808 847 882 903 933 941 956 958 975 979 991 995 1038 1056 1084 1123 1139 1162 1171 1183 1191 1197 1217 1237 1262 1280 1304 1320 1339 1359 1390 1407 1412 1475 1483 1494 1508 1558 1588 1630 1643 2189 2909 2930 3149 3151 3155 3156 3163 3173 3174 3177 3186 3190
		C	-1.32252100	-0.43560400	-0.01949500		
		C	-1.93280700	-1.66380800	0.19882500		
		C	-3.32632200	-1.76112700	0.23154600		
		C	-4.10924400	-0.62759500	0.02250600		
		C	-3.50507700	0.60755800	-0.20687900		
		C	-1.46527900	2.04617800	-0.43812900		
		C	-0.18225600	2.29738100	-0.10345400		
		C	0.14020000	-0.15533500	-0.16841500		
		H	-1.31979000	-2.54610700	0.34882500		
		H	-3.79718200	-2.72033700	0.41573000		
		H	-5.19061300	-0.70392800	0.03913500		
		H	-4.12032500	1.48753600	-0.36608900		
		H	-2.08795100	2.83830800	-0.84284000		
		H	0.25274500	3.28497600	-0.21050600		
		H	0.30000500	0.07016100	-1.23847600		
		C	0.52645000	1.15560400	0.55727500		
		H	0.15054000	1.11612600	1.59355700		
		C	1.97805000	0.64311900	0.57136300		
		C	3.31811400	0.99448100	0.25542700		
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		C	4.18266300	0.00378400	-0.13577700		
		H	3.65093300	2.02558300	0.32496400		
		C	2.40090100	-1.71070900	-0.32099500		
		H	1.85815600	-0.26207700	1.41897300		
		C	3.71350000	-1.34835900	-0.42502500		
		H	5.22458500	0.23717900	-0.31813300		
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		H	4.43342500	-2.06189000	-0.81008200		
TS7	-617.29290	C	-2.16980100	0.68778800	-0.28616100		-541 60 80 148 170 183 268 329 381 406 414 462 469 498 518 561 575 604 645 669 682 710 732 749 776 791 811 823 850 886 913 921 956 966 969 980 989 1006 1026 1049 1059 1088 1094 1131 1151 1162 1178 1183 1189 1221 1253 1264 1287 1305 1318 1336 1359 1362 1400 1433 1447 1479 1490 1526 1573 1587 1616 1640 2924 3038 3069 3144 3149 3155 3156 3162 3168 3172 3173 3186 3187
		C	-1.28778100	-0.37798500	0.04900700		
		C	-1.79281400	-1.63001900	0.37512000		
		C	-3.17323800	-1.85086400	0.37934300		
		C	-4.04594600	-0.82049000	0.03611800		
		C	-3.54623100	0.43831100	-0.29722000		
		C	-1.62568000	2.02774000	-0.57871300		
		C	-0.38214600	2.40920300	-0.20064900		
		C	0.15103400	0.01513000	-0.10492700		
		H	-1.11018000	-2.43488500	0.62637100		
		H	-3.56301300	-2.82745800	0.64407300		
		H	-5.11603500	-0.99453800	0.03018400		
		H	-4.23102500	1.24010400	-0.55499700		
		H	-2.30109900	2.74915900	-1.03006400		
		H	-0.05586000	3.43906900	-0.30148800		
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		C	0.40466300	1.37694400	0.51776900		

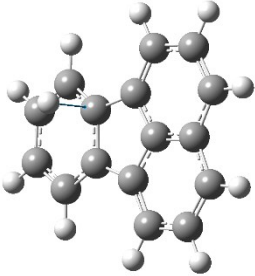
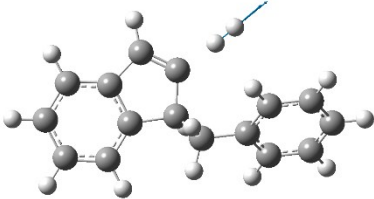
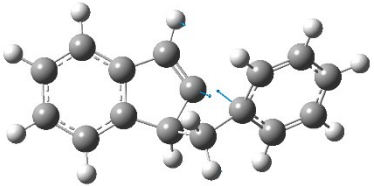
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		C	2.17931200	0.57834800	0.82679400		
		C	3.56023100	0.77807000	0.44247100		
		C	1.50044600	-0.58263000	0.22896300		
		C	4.22699800	-0.20321200	-0.26511200		
		H	4.09386000	1.65299900	0.79787800		
		C	2.20045300	-1.54875500	-0.45431500		
		C	3.58945800	-1.40162100	-0.64590700		
		H	5.27667900	-0.06668100	-0.50397000		
		H	1.67331000	-2.35810800	-0.95116000		
		H	4.14911900	-2.16544300	-1.17271600		
		H	2.00951000	0.78226100	1.88304800		
TS8	-617.36341	C	-2.37354000	0.36084100	-0.00714400		-804 45 78 81 173 180 241
		C	-1.04586300	-0.17297900	-0.04270700		289 319 391 415 417 441
		C	-0.87797600	-1.56892700	0.12347900		486 499 527 545 566 579
		C	-1.96363100	-2.40145700	0.28788300		633 636 659 710 715 744
		C	-3.27394000	-1.87818400	0.29152700		773 789 805 816 843 858
		C	-3.47071500	-0.52499600	0.15089200		881 919 937 973 977 987
		C	-2.56878100	1.76450200	-0.09729600		989 998 1002 1016 1045
		C	-1.49385400	2.62014700	-0.17499600		1051 1085 1101 1133 1166
		C	-0.18614800	2.11205500	-0.21944000		1182 1184 1200 1203 1235
		H	0.12098500	-1.98472900	0.12827700		1267 1303 1312 1341 1354
		H	-1.80995700	-3.46671300	0.41902600		1378 1418 1461 1474 1483
		H	-4.12109300	-2.54340500	0.41492000		1523 1541 1593 1609 1616
		H	-4.47364700	-0.11119000	0.16737600		1639 1651 3159 3160 3162
		H	-3.58126100	2.15334300	-0.07318600		3166 3170 3174 3176 3181
		H	-1.65085200	3.69231100	-0.20936600		3184 3188 3189 3201
		H	0.65198700	2.79443900	-0.30062500		
		C	0.06531600	0.73506000	-0.24899000		
		H	-0.05735600	0.65663300	-2.14507400		
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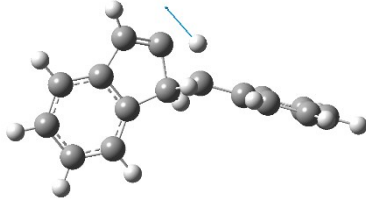
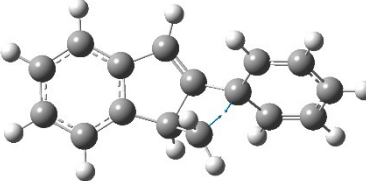
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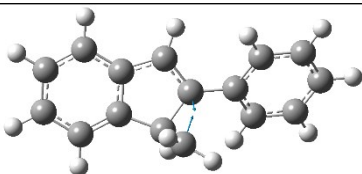
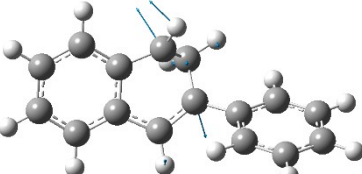
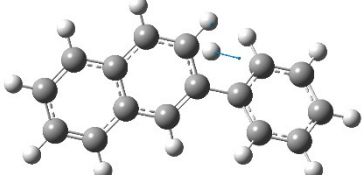
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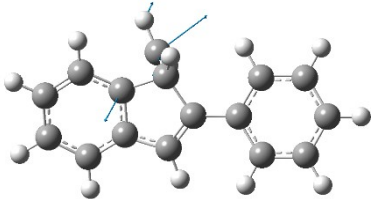
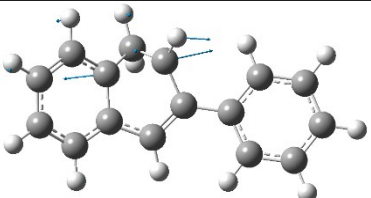
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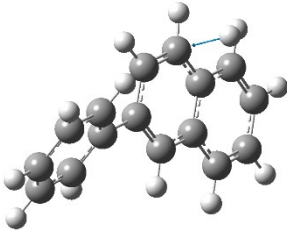
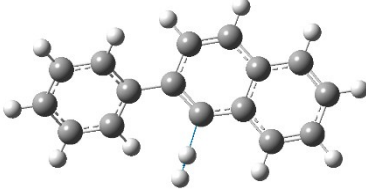
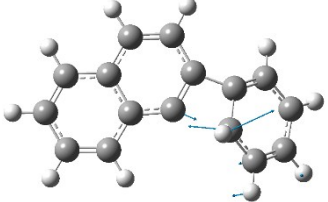
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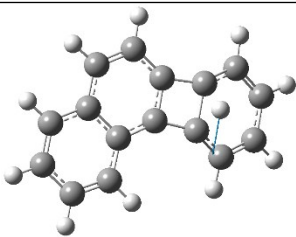
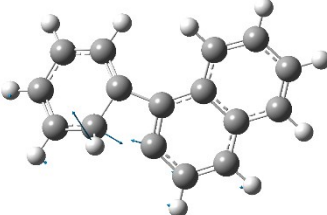
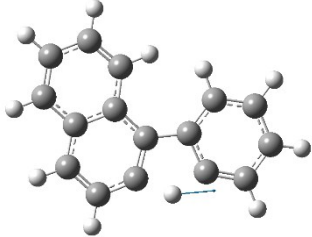
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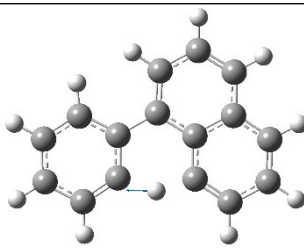
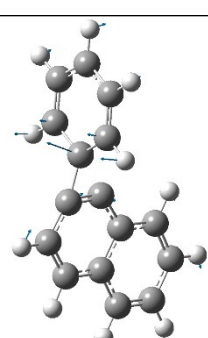
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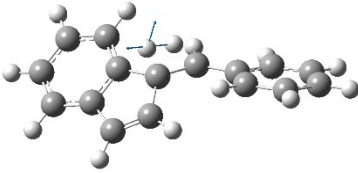
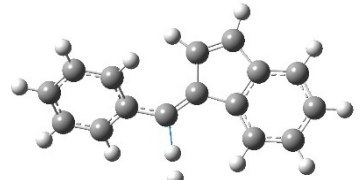
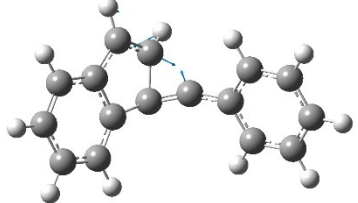
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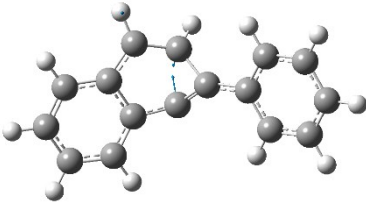
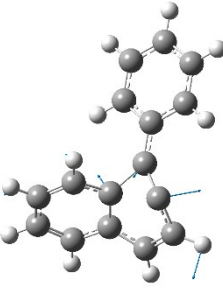
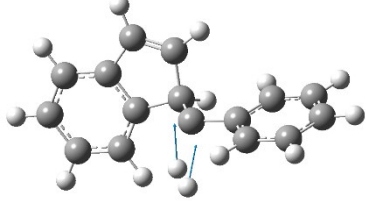
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		C	4.74715100	-0.40702400	-0.09891400		
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		H	5.81712800	-0.57665900	-0.13899000		
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		C	-1.73145700	0.76836600	0.02459800		263 286 305 331 406 412
		C	-2.93227400	1.46509700	0.34494800		440 498 536 565 590 620
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		C	-4.17732800	-0.59535700	-0.03482700		749 771 776 835 840 844
		C	-3.00577500	-1.31881100	-0.24680100		878 890 920 938 956 968
		C	-0.42759700	-1.15970700	-0.15665600		979 995 1012 1022 1036
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		H	-2.90713300	2.51988700	0.59635300		1241 1264 1300 1338 1341
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		C	-0.69582400	1.67766600	-1.24578000		
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		H	2.00814200	-2.36254400	0.40738600		
		C	4.10064900	0.87204800	0.08948300		
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		C	4.73956700	-0.35404900	0.25924600		
		H	4.45789000	-2.47532000	0.50731800		
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		C	-1.94339900	0.87355500	-0.39562600		283 295 321 369 410 414
		C	-3.12895900	1.42901800	0.18345100		450 485 528 546 583 632
		C	-4.17275400	0.60358500	0.54449100		641 666 700 706 715 732
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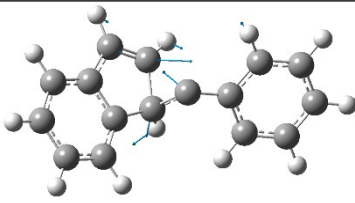
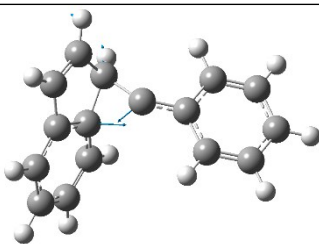
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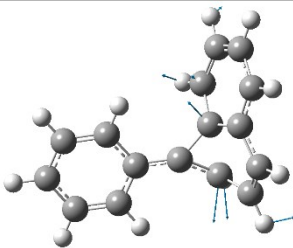
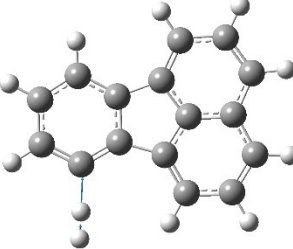
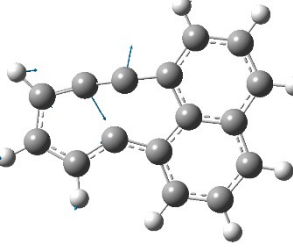
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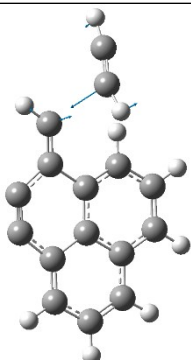
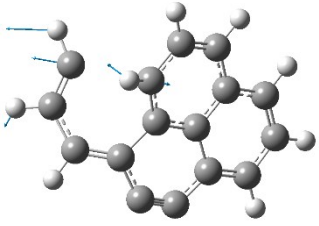
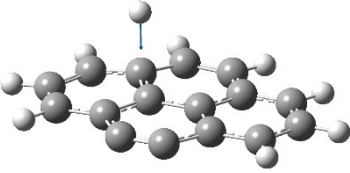
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		H	-4.56307000	1.52084700	0.89197100		
		H	-2.03096400	2.96808500	0.83042100		
		H	0.40536600	2.32959000	0.10584100		
		H	-0.46736100	0.62143000	-1.90570500		
		C	0.64543500	-0.68028600	-0.03207900		
		H	0.19083400	-0.20677400	-1.35945400		
		H	0.32972800	-1.70322600	0.12285600		
		C	2.06381800	-0.38301800	0.00989800		
		C	2.94153300	-1.33243800	0.58233800		
		C	2.64610200	0.78517200	-0.53073400		
		C	4.31039000	-1.11577300	0.63289200		
		H	2.52722400	-2.24538500	0.99783800		
		C	4.02314900	0.99203700	-0.48293200		
		H	2.03010600	1.52974900	-1.02013400		
		C	4.86665700	0.05250700	0.10389300		
		H	4.95186400	-1.86293200	1.08809000		
		H	4.43748500	1.89767000	-0.91331500		
		H	5.93627800	0.22126000	0.14502000		
TS40	-617.32868	C	2.62397200	0.89694800	-0.20710800		-1166 46 49 70 120 163 191 223 256 309 383 401 412 422 448 515 544 565 591 627 635 659 702 708 735 759 764 788 804 851 853 871 883 931 943 954 983 986 989 1002 1011 1038 1045 1051 1092 1102 1127 1174 1179 1183 1197 1203 1210 1260 1309 1313 1345 1353 1388 1468 1477 1488 1511 1567 1600 1621 1626 1639 1656 1757 3160 3164 3171 3171 3182 3182 3188 3193 3194 3199 3233
		C	1.84294900	-0.26148100	0.02649500		
		C	2.45638100	-1.47147400	0.32527900		
		C	3.85415100	-1.52607900	0.37338800		
		C	4.62311500	-0.38521700	0.13732400		
		C	4.01281000	0.83840600	-0.15328800		
		C	1.71423000	2.01108000	-0.47841100		
		C	0.43483600	1.57750500	-0.40936400		
		C	0.41850100	0.13386900	-0.09336100		
		H	1.87317000	-2.36304600	0.52070900		
		H	4.34407800	-2.46610700	0.60049500		
		H	5.70459300	-0.44875900	0.18334900		
		H	4.61364300	1.72400800	-0.33067100		
		H	2.03087100	3.02016900	-0.70883100		
		H	-0.45555100	2.16278300	-0.58538100		
		C	-0.67398200	-0.63631100	0.00947700		
		H	-0.44701900	-1.99137600	0.07034200		
		C	-2.09164400	-0.35779300	0.03438500		
		C	-2.99108300	-1.16269200	-0.69155500		
		C	-2.61197600	0.69403700	0.81618100		
		C	-4.35509500	-0.89923100	-0.66821300		
		H	-2.60729700	-1.98801200	-1.28008000		
		C	-3.97856600	0.94929200	0.83744800		
		H	-1.93580000	1.29444000	1.41272000		
		C	-4.85447500	0.15853100	0.09333700		
		H	-5.03243300	-1.52195400	-1.24164600		
		H	-4.36265900	1.76248900	1.44322300		
		H	-5.91975000	0.35791500	0.11511000		
		H	-0.35060200	-2.89889100	0.08858000		
TS41	-616.12101	C	-2.31285600	0.79520400	0.13868200		-389 29 45 74 140 184 218 331 362 407 412 425 473 521 538 546 578 594 630 692 718 733 743 752 757 788 804 838 867 868 893 907 951 976 981 990 1000 1017 1032 1041 1064 1101 1105 1151 1171 1180 1196 1227 1249 1263 1305 1306 1335 1352 1377 1452 1465 1496 1504 1576 1585 1612 1622 1739 3160 3164 3169 3171 3178 3184 3189 3189 3195 3198 3213
		C	-1.73882700	-0.28847500	-0.61179600		
		C	-2.21841400	-1.59047700	-0.48176300		
		C	-3.30942800	-1.81908400	0.34988600		
		C	-3.90743900	-0.76166000	1.06425900		
		C	-3.42016000	0.53032100	0.97402300		
		C	-1.58357100	1.99893200	-0.08880800		
		C	-0.56187000	1.75557000	-1.04694500		
		C	-0.60491200	0.28546700	-1.31530400		
		H	-1.76875100	-2.40400300	-1.03955500		
		H	-3.71250300	-2.82095700	0.44431100		
		H	-4.76456600	-0.96863600	1.69549300		
		H	-3.88271800	1.33463500	1.53597600		
		H	-1.87493800	2.97738700	0.26983600		
		H	-0.16982600	2.49921700	-1.72553700		
		C	0.65222300	0.46942100	-0.95583700		

		C	1.88025000	0.13281500	-0.34773400		
		C	2.46109500	0.96367400	0.63849400		
		C	2.57649600	-1.03341700	-0.74992700		
		C	3.67187100	0.61730900	1.21956600		
		H	1.94400900	1.86756100	0.93665700		
		C	3.79430800	-1.35501800	-0.16852100		
		H	2.14985600	-1.66874900	-1.51694500		
		C	4.34876600	-0.53823500	0.82022300		
		H	4.09865800	1.25743600	1.98363100		
		H	4.31571200	-2.25144100	-0.48551600		
		H	5.29987800	-0.79653100	1.27064600		
TS42	-616.11816	C	-2.33569100	0.83375300	0.07191000		-561 46 51 79 149 190 236 308 339 404 415 446 466 512 520 541 574 600 632 680 699 703 730 745 769 772 816 842 854 861 873 933 950 978 987 1000 1003 1013 1031 1044 1094 1104 1131 1151 1175 1182 1195 1228 1263 1297 1309 1325 1336 1352 1393 1440 1475 1493 1519 1566 1599 1609 1633 1762 3032 3161 3163 3170 3172 3179 3180 3182 3185 3191 3192
TS43	-616.10261	C	-1.93202700	1.29606900	-0.01006600		-507 48 60 66 156 185 190 261 376 403 413 424 452 535 538 548 579 594 630 682 697 708 715 740 750 764 813 833 846 850 878 918 954 967 975 983 996 1008 1019 1038 1057 1079 1103 1127 1177 1181 1193 1207 1245 1269 1310 1320 1354 1381 1402 1453 1469 1473 1512 1530 1595 1603 1621 1757 3153 3163 3164 3170 3178 3181 3187 3188 3192 3193 3214
TS44	-617.87815	C	-2.55827500	0.85026300	0.26534900		-624 41 52 59 130 161 183 227 252 345 392 407 414 436 472 522 532 548 567 592 629 639 696 724 745 751 778 788 833 855 866 874 897 936 946 951 960 968 988 995 1009 1014 1035 1042 1049 1086 1096 1105 1135 1176 1182 1185 1190 1201 1220 1239 1282

		H	-4.30545500	-2.44961000	-0.70272900		1311 1321 1347 1352 1386 1470 1484 1489 1512 1585 1602 1625 1627 1646 2949 3114 3160 3160 3168 3169 3178 3178 3185 3188 3190 3191 3227
		H	-5.59698400	-0.63717100	0.36511100		
		H	-4.48990800	1.49855300	0.98864000		
		H	-1.95978700	2.92553600	0.92065100		
		H	0.44713800	2.31864500	0.09987400		
		H	-0.08414700	0.25971900	-1.55605800		
		C	0.58690600	-0.41636300	0.45856500		
		H	0.31238900	-2.42295900	-0.09959300		
		H	0.25399400	-1.89038000	0.51827700		
		C	2.02204300	-0.29446100	0.16362200		
		C	2.91659800	-0.88152100	1.08421200		
		C	2.57357400	0.43732600	-0.90879900		
		C	4.29086000	-0.76196400	0.93407300		
		H	2.49683300	-1.42898900	1.92076800		
		C	3.95007400	0.58779100	-1.04299300		
		H	1.92306300	0.90021500	-1.64148000		
		C	4.81131400	-0.01867000	-0.12842400		
		H	4.95936200	-1.22824000	1.64900400		
		H	4.35459300	1.16760800	-1.86538000		
		H	5.88445000	0.09131500	-0.23983000		
TS45	-616.72202	C	-2.62732100	0.85004800	-0.19595300		-245 51 53 82 138 173 243 262 342 408 418 433 494 498 536 549 589 628 631 701 723 747 753 767 789 806 842 847 859 878 897 929 940 959 984 992 999 1007 1038 1043 1072 1091 1103 1114 1137 1178 1180 1190 1196 1229 1261 1290 1310 1343 1347 1357 1398 1454 1466 1488 1507 1525 1594 1609 1622 1641 2965 3157 3162 3164 3169 3174 3178 3181 3188 3189 3193 3238
TS46	-616.69969	C	-1.93059800	1.30185400	-0.15387100		-506 39 50 62 149 165 215 267 352 394 409 409 477 490 522 534 592 597 626 684 692 720 732 753 758 808 812 829 838 865 897 931 947 957 970 974 985 985 1022 1032 1043 1067 1097 1109 1126 1156 1175 1179 1190 1206 1232 1288 1298 1335 1346 1369 1416 1431 1457 1476 1496 1541 1568 1582 1596 1598 3049 3158 3159 3165 3165 3177 3180 3185 3189 3191 3192 3216

TS47	-616.71144	H	5.39479400	-1.47869900	-0.77071800		-367 40 66 68 172 176 197 264 365 394 411 422 456 487 519 534 580 615 625 685 686 712 724 739 753 770 804 830 834 858 897 905 913 936 964 970 978 988 991 1012 1033 1082 1098 1108 1114 1131 1173 1175 1193 1195 1257 1262 1306 1311 1349 1374 1397 1431 1464 1481 1520 1543 1559 1571 1581 1601 3108 3155 3159 3164 3165 3177 3178 3180 3184 3189 3191 3201
		C	-1.89892800	1.29034400	-0.01671800		
		C	-1.12918300	0.06210700	-0.32064800		
		C	-1.66960800	-1.19671300	0.16422400		
		C	-2.71521000	-1.19701100	1.05026500		
		C	-3.30157700	0.01951900	1.48978400		
		C	-2.90244200	1.24104800	0.94332400		
		C	-1.64495700	2.34180800	-0.96988100		
		C	-0.93462600	1.89771400	-2.03581600		
		C	-0.44048600	0.50733000	-1.88750600		
		H	-1.18595700	-2.12180000	-0.12830500		
		H	-3.09173000	-2.13757900	1.43684100		
		H	-4.10602800	-0.00766000	2.21546600		
		H	-3.43189900	2.15065500	1.20955900		
		H	-2.05747400	3.33820100	-0.87399100		
		H	-0.73161500	2.47431400	-2.93054800		
		H	-0.45527700	-0.18498400	-2.72760300		
		C	0.28991500	0.18677100	-0.68619200		
		C	1.53108300	-0.29156800	-0.24926500		
		C	1.71397000	-0.77385600	1.07824600		
		C	2.66038400	-0.28774600	-1.11701900		
		C	2.95182100	-1.22762600	1.49972600		
		H	0.86938000	-0.77414600	1.75733500		
		C	3.89027300	-0.74750500	-0.67929000		
		H	2.54175700	0.08237900	-2.12922700		
		C	4.04901200	-1.22167500	0.62906300		
		H	3.07236600	-1.58948500	2.51507300		
		H	4.73824300	-0.73816400	-1.35557000		
		H	5.01503500	-1.57870300	0.96634100		
TSA	-616.17264	C	2.33675400	-0.01826000	-0.03118900		-862 99 106 163 179 197 255 255 292 359 431 458 468 477 494 560 566 573 623 629 641 664 733 757 772 779 785 816 827 895 903 917 919 929 967 975 978 987 1016 1031 1060 1071 1094 1127 1165 1177 1205 1216 1248 1266 1286 1329 1393 1396 1422 1450 1454 1467 1496 1518 1563 1635 1637 1639 1656 2357 3160 3161 3162 3170 3172 3176 3183 3184 3188
		C	0.93568200	-0.02239100	-0.05927500		
		C	0.13681000	1.14624800	-0.10248500		
		C	0.76851100	2.37147100	-0.11820100		
		C	2.18939900	2.40768700	-0.09041600		
		C	2.96035100	1.26068600	-0.04827700		
		C	2.96701400	-1.29355300	0.01099800		
		C	2.20189200	-2.44498100	0.02226100		
		C	0.78052800	-2.41863400	-0.00690400		
		H	0.21284900	3.30229000	-0.15099800		
		H	2.68223300	3.37356300	-0.10288500		
		H	4.04244900	1.33539900	-0.02821500		
		H	4.04948900	-1.36156100	0.03432800		
		H	2.69968800	-3.40783300	0.05453500		
		H	0.22716800	-3.35055300	0.00352800		
		C	0.14418100	-1.19680700	-0.04796900		
		C	-1.25817300	-0.74347800	-0.08669000		
		C	-1.26575000	0.68928900	-0.12013200		
		C	-2.47339500	-1.38924400	-0.09619100		
		C	-2.46882700	1.38514000	-0.16062300		
		C	-3.68531100	-0.72273000	-0.13614700		
		H	-2.53622200	-2.88606200	-0.06277900		
		C	-3.67551200	0.67814400	-0.16853400		
		H	-2.47827400	2.46927800	-0.18606700		
		H	-4.62406600	-1.26583100	-0.14246200		
		H	-4.61617000	1.21714600	-0.20006500		
		H	-2.60895800	-3.73284300	-0.04466000		
TSB	-614.92083	C	2.27074700	0.19836200	-0.02191200		-274 61 101 172 191 232 274 293 389 421 435 483 491 511 534 543 573 591 603 631 662 672 738 749 774 802 808 813 845 855 871 882 957 963 968 1020 1066 1072 1084 1122 1142 1177 1187 1229 1241 1269 1340 1356 1364 1389 1398 1444 1460 1486 1510 1516 1558 1581 1600 1979 3161 3164 3177 3180 3186 3191 3198 3220 3236
		C	0.86020000	0.17629100	0.08397700		
		C	0.11170100	1.33047600	0.44140100		
		C	0.77848700	2.54570300	0.69050400		
		C	2.17394100	2.56363900	0.58986000		
		C	2.91665300	1.43339200	0.25351200		
		C	2.89806400	-1.01265500	-0.40634200		
		C	2.13105100	-2.14273500	-0.68190200		
		C	0.73414000	-2.14245200	-0.59976700		
		H	0.23029400	3.43999000	0.95728300		
		H	2.69462800	3.49510500	0.78331900		
		H	3.99735200	1.49539900	0.19186800		
		H	3.97799700	-1.05365000	-0.49403900		
		H	2.63176800	-3.05708800	-0.98158000		
		H	0.17750700	-3.03910800	-0.84255100		
		C	0.07433300	-0.96042200	-0.20605700		
		C	-1.33450900	-0.77817800	-0.03754100		
		C	-1.24366700	1.00790500	0.47691900		
		C	-2.41495700	-1.64889100	-0.12698400		

		C	-2.43870300	0.77434800	0.08795700		
		C	-3.69979300	-1.11544200	-0.13042200		
		H	-2.21274400	-2.70790300	-0.23427400		
		C	-3.70975700	0.28415800	0.02314200		
		H	-4.60123100	-1.70788900	-0.19557500		
		H	-4.57892800	0.90900500	0.16271800		
TSC'	-614.78879	C	2.24503300	-0.38964200	0.59880300		-392 21 55 96 114 175 205
		C	0.88772100	-0.57449600	0.19627700		215 220 308 324 387 416
		C	0.07088300	0.57560400	-0.09552800		439 451 479 522 539 553
		C	0.65737300	1.83274800	-0.04543900		562 578 610 613 652 666
		C	1.99731100	2.00766400	0.34420400		691 761 764 773 782 793
		C	2.77441900	0.92252000	0.67372100		804 826 909 936 940 956
		C	3.04952900	-1.52695500	0.89804100		983 995 1043 1072 1105
		C	2.55217900	-2.80153400	0.79051600		1127 1175 1196 1211 1242
		C	1.22155300	-3.01625500	0.36991100		1262 1352 1361 1394 1457
		H	0.06958600	2.69862500	-0.32118600		1473 1522 1554 1607 1624
		H	2.41340700	3.00822200	0.37672300		1645 1921 2109 3163 3166
		H	3.80794200	1.05366800	0.97577500		3181 3182 3196 3200 3240
		H	4.07597700	-1.36432500	1.20853200		3382 3474
		H	3.18223200	-3.65309300	1.01999400		
		H	0.83410500	-4.02253300	0.26911100		
		C	0.40826500	-1.94416900	0.07615400		
		C	-0.94821500	-1.92190900	-0.37185100		
		C	-1.39585900	0.43966600	-0.46371900		
		C	-1.66881900	-0.97020400	-0.63346500		
		C	-2.29562500	1.42143500	-0.54519500		
		C	-2.70427600	4.30372600	0.12057000		
		C	-2.22910700	3.33886700	0.69160300		
		H	-3.33776600	1.37388400	-0.82182300		
		H	-3.13826900	5.03336200	-0.52091500		
		H	-1.78810000	2.78200800	1.48767600		
TSD	-614.85006	C	1.70042500	-1.08045400	0.07529000		-275 77 129 191 209 229
		C	0.32805600	-0.69999900	-0.01310700		274 323 378 396 413 427
		C	-0.01542300	0.63556600	-0.41953200		454 488 504 531 547 576
		C	1.01147900	1.58553200	-0.55604200		612 614 617 651 697 752
		C	2.37421800	1.19562700	-0.45207200		774 784 798 819 830 840
		C	2.70769800	-0.10289000	-0.18450300		893 912 918 960 976 985
		C	2.03094600	-2.40287600	0.45510100		1039 1051 1088 1122 1152
		C	1.05181300	-3.32315900	0.77385500		1177 1193 1210 1235 1263
		C	-0.30575800	-2.96579900	0.73558500		1276 1324 1360 1375 1380
		H	3.14657100	1.94767200	-0.56628000		1443 1451 1500 1518 1579
		H	3.74866500	-0.39907600	-0.10877300		1608 1615 1631 2095 3041
		H	3.07771400	-2.68261700	0.50614900		3162 3165 3177 3180 3181
		H	1.33023400	-4.32835500	1.06866500		3196 3197 3220
		H	-1.07105800	-3.68290300	1.00586900		
		C	-0.67468900	-1.68585100	0.35710000		
		C	-1.96799700	-1.09781700	0.24438500		
		C	-1.41704800	1.01808200	-0.71639000		
		C	-2.26833600	0.02602700	-0.14121300		
		C	-1.79996400	1.97480400	-1.62550300		
		C	0.37806000	2.70879800	-2.59389200		
		C	-0.95064200	2.63271200	-2.59385000		
		H	-2.86718400	2.10684800	-1.76200500		
		H	1.10289600	3.12927000	-3.27710400		
		H	-1.48611100	3.04169300	-3.45655200		
		H	0.76610400	2.63421500	-0.47205100		
TSE	-614.89158	C	1.68802200	-1.08173700	0.09410300		-1026 93 150 214 258 259
		C	0.30934100	-0.76690300	-0.09726300		353 384 397 402 433 464
		C	-0.06176100	0.44968400	-0.75947700		488 513 517 536 543 554
		C	0.95916100	1.40558400	-1.11908600		577 585 602 634 708 724
		C	2.34993500	0.99886500	-0.99165600		766 777 795 811 821 844
		C	2.68747000	-0.17047700	-0.40430000		902 916 971 981 986 991
		C	2.04049500	-2.27777100	0.73671000		1001 1070 1085 1118 1168
		C	1.07273400	-3.16956600	1.18760800		1191 1195 1199 1223 1244
		C	-0.28238600	-2.90321100	1.00141200		1291 1296 1327 1369 1403
		H	3.11219100	1.67897200	-1.35540200		1415 1440 1446 1513 1528
		H	3.73062400	-0.44910500	-0.29896100		1576 1603 1626 1653 2091
		H	3.09161500	-2.50585900	0.87700900		3162 3165 3168 3180 3181
		H	1.37537300	-4.08544500	1.68208200		3184 3197 3198
		H	-1.03617800	-3.60273900	1.34079100		
		C	-0.67758400	-1.72709900	0.36640100		
		C	-1.97465900	-1.25365000	0.04642000		
		C	-1.43769000	0.79634900	-1.04127700		
		C	-2.28902500	-0.21663600	-0.52986500		
		C	-1.75326200	1.95942200	-1.74432800		

		C	0.59346200	2.51507700	-1.93862700		
		C	-0.73131600	2.79236500	-2.21418900		
		H	-2.79112200	2.19016700	-1.94905400		
		H	1.37764400	3.17241200	-2.29697000		
		H	-0.98512200	3.66447400	-2.80589000		
		H	0.94846400	2.28528900	0.37280100		