

Supporting Information for

Reaction Kinetics of Hydrogen Abstraction from Polycyclic Aromatic Hydrocarbons by

H atoms

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In this supporting information, we present:

- **Table S1.** Comparison of single point energy by CCSD(T)-F12a/cc-PVTZ with geometries optimized by different DFT method and basis sets.
- **Eq.(1) ~ Eq.(4)** CCSD(T)/CBS extrapolation equations
- **Table S2.** Comparison of bond dissociation energy (BDE) of C-H bond in benzene (A1) and naphthalene (A2) obtained by experiments and calculated at CCSD(T)/CBS level.
- **Table S3.** The barrier height (ΔE_0^\ddagger) and reaction energy (ΔH_{298}) of R1 calculated using several compound methods and the error deviated from the benchmark CCSD(T)/CBS value. (units: kcal/mol)
- **Table S4.** The barrier height (ΔE_0^\ddagger) and reaction energy (ΔH_{298}) of R2 calculated using several compound methods and the error deviated from the benchmark CCSD(T)/CBS value. (units: kcal/mol)
- **Table S5.** Total energies, relative energies, zero-point energies, expectation values of S2 operator (projected values are in parentheses), vibrational frequencies, rotational constants for all optimized structures at B3LYP/6-311G(d,p) level in this work.
- **Table S6.** Cartesian coordinates of optimized structures at B3LYP/6-311G(d,p) level for all species in this work.

Table S1. Comparison of single point energy by CCSD(T)-F12a/cc-PVTZ with geometries optimized by different DFT method and basis sets. (Energy unit: kcal/mol; Single point energy obtained by CCSD(T)-F12a/cc-PVTZ//B3LYP/6-311g(d,p) are taken as reference values)

DFT methods/basis set	C ₆ H ₆ (R)	C ₆ H ₇ (TS)	C ₆ H ₅ (P)
B3LYP/6-311g(d,p)	0.0	0.0	0.0
B3LYP/6-311++g(d,p)	0.0	0.0	0.0
B3LYP/6-311+g(3df,2p)	0.0	0.1	0.0
B3LYP/6-311++g(3df,2p)	0.0	0.0	0.0
B3LYP/def2TZVP	0.0	0.1	0.0
M06-2X/6-311g(d,p)	0.0	0.0	0.0
M06-2X/6-311++g(d,p)	0.0	0.0	0.0
M06-2X/6-311+g(3df,2p)	0.1	0.1	0.1
M06-2X/6-311++g(3df,2p)	0.1	0.1	0.1
M06-2X/def2TZVP	0.1	0.1	0.1
M06-L/6-311g(d,p)	0.0	-0.5	0.1
M06-L/6-311++g(d,p)	0.0	-0.5	0.1
M06-L/6-311+g(3df,2p)	0.1	-0.5	0.1
M06-L/6-311++g(3df,2p)	0.1	-0.5	0.1
M06-L/def2TZVP	0.2	-0.4	0.2

Three kinds of density functional methods and five basis sets containing different number of basis functions were combined to optimize geometries and calculate harmonic vibrational frequencies of the reactants, transition states and products of R1. Table S1 shows the single-point energy of C₆H₆, TS (C₆H₇), and C₆H₅ calculated by CCSD(T)-F12a/cc-PVTZ using different geometries relative to the single-point energy obtained by CCSD(T)-F12a/cc-PVTZ//B3LYP/6-311g(d,p). It is clear that differences are small, within 0.5 kcal/mol for any given species, so geometries are not sensitive of the chosen density functional methods or basis sets.

In addition, we have investigated the spin contamination of wave function. All $\langle S^2 \rangle$ values for the TS (C₆H₇) are very close to 0.75 regardless of the DFT methods used for optimization, indicating only mild spin contamination. More specifically,

the $\langle S^2 \rangle$ of the TS and C₆H₅ are 0.7604 and 0.7571 respectively, by B3LYP/6-311g(d,p), which is the most closest to 0.75 among the three DFT methods. Considering the limited influence of the level of theory on the optimized geometries and the good performance of B3LYP/6-311g(d,p) on spin contamination of radicals, we employed it to optimize geometries and calculate frequencies for all of the reaction systems.

Eq.(1) ~ Eq.(4) CCSD(T)/CBS extrapolation equations

The benchmark energy calculations in our work were performed using CCSD(T)/CBS (extrapolation to the limit of a complete basis set), based on the following equations^(1, 2)

$$E(\text{CCSD(T) / CBS}) = E_{\text{CBS}}^{\text{corr}} + E_{\text{CBS}}^{\text{HF}} \quad (1)$$

$$E_{\text{CBS}}^{\text{corr}} = \frac{X^3 E_X^{\text{corr}} - (X-1)^3 E_{X-1}^{\text{corr}}}{X^3 - (X-1)^3} \quad (2)$$

$$E_{\text{CBS}}^{\text{HF}} = \frac{E_{X-1}^{\text{HF}} - \lambda E_X^{\text{HF}}}{1 - \lambda} \quad (3)$$

where

$$\lambda = \frac{X}{X+1} \exp[9(\sqrt{X} - \sqrt{X-1})] \quad (4)$$

In the above equations, X and X-1 represent a pair of basis sets with successive cardinalities, which are cc-PVTZ (X = 3) and cc-PVDZ (X - 1 = 2) respectively in our study. “corr” stands for correlation energies, and “HF” represents Hartree-Fock energies. Eq.(3) is derived from the Karton-Martin two-point formula,⁽³⁾ which has also been employed in the extrapolation of CCSD(T) results to the CBS limits.^(1, 2) Energies computed at CCSD(T)/CBS level are believed to be accurate within 1 kcal/mol, and are often regarded as benchmark value to test various of density functional methods,^(1, 2, 4) especially when experimental results are not available. Unfortunately, this gold standard method can hardly be applied to a system with more than 10 non-hydrogen atoms due to its enormous computational cost.⁽⁵⁾

Table S2. Comparison of bond dissociation energy (BDE) of C-H bond in benzene (A1) and naphthalene (A2) obtained by experiments and calculated at CCSD(T)/CBS level.

	BDE of C-H (kcal/mol)	
	A1	A2 (α)
CCSD(T)/CBS	111.4	111.9
experiment	112.0 \pm 0.6 ⁽⁶⁾	112.3 \pm 1.3 ⁽⁷⁾

Note: A2- α represents the same site as A2-1 in Fig. 2.

Table S3. The barrier height (ΔE_0^\ddagger) and reaction energy (ΔH_{298}) of R1 calculated using several compound methods and the error deviated from the benchmark CCSD(T)/CBS value. (units: kcal/mol)

Methods	ΔE_0^\ddagger	ΔH_{298}	Error	
			ΔE_0^\ddagger	ΔH_{298}
CCSD(T)/CBS	15.6	7.9	0.0	0.0
G4	15.7	7.5	0.1	-0.4
G4MP2	15.8	7.3	0.2	-0.6
G3	16.9	9.2	1.3	1.3
G3(MP2,CC)	17.1	8.8	1.5	0.9
CBS-QB3	17.3	9.5	1.7	1.6
G3MP2	17.9	9.8	2.3	1.9
G3MP2B3	18.0	9.4	2.4	1.5

Table S4. The barrier height (ΔE_0^\ddagger) and reaction energy (ΔH_{298}) of R2 calculated using several compound methods and the error deviated from the benchmark CCSD(T)/CBS value. (units: kcal/mol)

Methods	ΔE_0^\ddagger	ΔH_{298}	Error	
			ΔE_0^\ddagger	ΔH_{298}
CCSD(T)/CBS	15.7	8.3	0.0	0.0
G3MP2B3	15.6	7.2	0.1	-1.1
G3	15.4	8.2	-0.3	-0.1
G3MP2	15.2	7.6	-0.5	-0.7
CBS-QB3	14.9	7.4	-0.8	-0.9
G4	13.6	5.7	-2.1	-2.6
G4MP2	12.1	3.9	-3.6	-4.4
G3(MP2,CC)	21.1	13.1	5.4	4.8

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Table S5. Total energies, relative energies, zero-point energies, expectation values of S2 operator (projected values are in parentheses), vibrational frequencies, rotational constants for all optimized structures at B3LYP/6-311G(d,p) level in this work.

Species	Symmetry number	Total Energy (hartrees)	ZPE (unscaled) (hartrees)	$\langle S^2 \rangle$	Frequencies (unscaled) (cm-1)	Rotational constants (GHz)
H	1	-0.502155	0	0.75 (0.75)		
H2	1	-1.169626	0.010069	0	4420.0	1811.2
A1	12	-232.209591	0.100179	0	412.3 412.5 623.0 623.1 688.5 723.2 861.7 862.8 980.9 981.7 1013.7 1016.5 1023.4 1060.1 1060.4 1174.6 1197.3 1197.6 1335.8 1381.4 1512.7 1513.2 1637.7 1638.0 3155.8 3165.2 3165.7 3181.0 3181.6 3191.9	5.7 5.7 2.9
A1-TS	2	-232.694656	0.097997	0.760391 (0.75)	-850.1 179.4 227.1 402.0 426.0 602.7 612.4 687.6 722.7 831.1 884.8 920.3 968.1 970.7 999.5 1016.7 1023.3 1049.0 1089.4 1178.6 1182.0 1319.6 1328.3 1468.4 1479.0 1585.7 1630.5 2376.1 3156.5 3162.2 3172.5 3176.3 3187.7	5.6 4.9 2.6
A1-P	2	-231.533449	0.087045	0.750029 (0.75)	400.3 426.4 601.8 620.3 673.0 721.0 812.4 892.1 964.2 988.9 992.8 1017.2 1049.6 1073.3 1175.3 1176.0 1302.4 1324.3 1462.8 1470.8 1575.9 1629.9 3156.2 3162.1 3174.3 3176.9 3188.3	6.3 5.6 3.0
A2	4	-385.839809	0.146929	0	173.6 186.5 365.7 395.8 479.6 488.3 519.0 519.9 634.9 636.1 729.3 773.3 786.9 798.5 808.8 849.6 896.9 951.0 957.1 974.4 992.6 999.9 1035.6 1046.3 1151.1	3.1 1.2 0.9

					1169.2	1171.9	1185.2	1232.3	1270.0	
					1287.1	1391.3	1398.7	1418.0	1490.6	
					1491.7	1548.6	1614.0	1641.4	1671.2	
					3156.1	3157.8	3160.2	3163.6	3174.2	
					3175.5	3187.0	3188.2			
A2-TS-1	1	-386.324243	0.144902	0.761759 (0.75)	-857.3	148.1	170.8	204.3	232.8	
					375.5	400.6	467.8	506.5	508.8	2.9
					521.2	616.5	620.5	739.1	765.5	1.2
					775.1	796.3	802.9	865.0	899.1	0.9
					912.3	924.6	966.5	980.1	999.1	
					1023.6	1040.0	1069.8	1138.0	1169.5	
					1179.7	1205.6	1237.5	1273.4	1366.8	
					1384.6	1391.1	1457.5	1485.2	1525.8	
					1586.3	1637.4	1662.9	2360.4	3157.8	
					3159.3	3168.1	3169.8	3181.3	3182.3	
					3192.1					
A2-P-1	1	-385.163358	0.133972	0.759055 (0.75)	169.4	186.5	361.6	400.6	462.4	
					507.3	508.4	521.6	611.0	631.4	3.3
					730.9	772.8	774.2	789.9	800.0	1.2
					865.5	893.0	932.4	964.6	976.2	0.9
					998.8	1033.1	1046.2	1138.7	1169.0	
					1175.8	1197.7	1235.8	1270.3	1360.4	
					1378.1	1389.5	1451.3	1483.5	1520.4	
					1582.9	1637.4	1662.7	3158.1	3159.6	
					3169.7	3170.8	3181.7	3182.7	3193.1	
A2-TS-2	1	-386.324694	0.144765	0.760923 (0.75)	-846.8	142.6	179.8	219.1	221.8	
					372.7	389.2	475.0	488.1	509.7	3.1
					516.2	616.0	631.1	746.4	766.9	1.2
					769.4	783.1	811.9	851.9	890.1	0.8
					910.0	931.8	960.6	972.5	997.8	
					1021.2	1041.4	1053.3	1146.7	1163.0	
					1174.6	1212.3	1254.9	1279.2	1353.3	
					1387.4	1395.5	1462.9	1470.0	1533.9	
					1598.8	1619.1	1658.7	2384.8	3155.8	
					3158.3	3159.4	3164.5	3176.3	3177.5	
					3188.6					
A2-P-2	1	-385.163452	0.133803	0.757847 (0.75)	174.6	192.0	368.9	387.0	471.8	
					485.5	511.3	520.6	611.2	628.2	3.2
					744.9	755.0	767.4	794.0	805.9	1.3
					845.0	887.9	936.2	956.7	970.6	0.9
					996.6	1039.6	1049.2	1141.3	1161.1	
					1172.1	1207.9	1249.9	1276.7	1335.1	
					1385.9	1394.3	1457.1	1468.4	1529.9	
					1592.5	1620.1	1656.7	3155.1	3158.9	
					3160.1	3164.7	3176.5	3179.6	3188.7	
A3	4	-539.464229	0.193332	0	92.1	121.1	235.9	236.3	269.3	
					387.9	396.1	398.1	480.3	485.4	2.2
					506.1	535.9	591.1	617.8	642.5	0.5
					661.6	741.9	759.2	763.5	770.3	0.4
					782.7	821.0	846.4	867.2	897.2	
					913.2	918.8	929.4	968.6	973.4	
					995.8	996.8	1026.9	1031.6	1127.4	
					1158.7	1173.6	1189.1	1190.5	1210.5	
					1289.9	1290.7	1294.5	1339.5	1375.9	
					1414.8	1415.0	1427.9	1482.2	1487.6	
					1517.2	1579.8	1594.1	1624.7	1668.4	
					1670.7	3154.4	3156.5	3157.6	3158.5	
					3162.7	3164.2	3175.3	3175.6	3187.0	
					3187.5					
A3-TS-1	2	-539.947828	0.191552	0.766132 (0.75)	-852.6	90.0	118.8	145.3	233.8	
					234.3	264.2	267.2	390.7	395.8	2.0
					398.5	476.8	502.1	502.2	540.1	0.5
					581.0	615.0	624.7	656.3	746.1	0.4
					750.0	751.1	768.0	772.4	830.9	
					851.5	866.7	897.3	900.4	910.6	
					930.2	970.3	972.7	997.0	997.7	
					1026.5	1030.1	1063.2	1126.7	1166.8	
					1169.2	1189.7	1198.7	1240.1	1268.3	
					1290.9	1323.5	1366.6	1374.8	1398.0	
					1413.4	1475.6	1484.2	1510.3	1569.4	
					1570.8	1620.4	1659.0	1667.4	2356.0	
					3157.6	3159.5	3162.1	3170.4	3170.7	
					3182.9	3183.1	3193.0	3193.4		

A3-TS-2	1	-539.948722	0.191281	0.763398 (0.75)	-857.0 234.7 404.3 577.7 754.8 854.5 915.1 1016.7 1177.5 1293.0 1425.0 1586.3 3154.9 3174.7	91.1 264.1 478.8 605.6 759.2 879.1 925.8 1029.1 1179.9 1328.2 1451.9 1622.2 3159.5 3177.7	109.5 270.0 489.4 634.6 772.9 895.4 972.3 1063.8 1194.7 1364.1 1481.9 1659.0 3159.9 3182.8	173.4 390.8 511.2 656.9 781.8 895.9 978.8 1110.6 1247.1 1386.0 1503.3 1669.8 3164.6 3189.5	209.6 395.6 530.8 735.3 820.5 910.6 997.6 1163.1 1287.8 1402.7 1550.5 2358.8 3168.6	2.0 0.4 0.4
A3-TS-3	1	-539.949148	0.191156	0.762207 (0.75)	-847.2 243.0 399.9 580.5 751.9 844.3 916.8 1014.2 1170.5 1290.5 1423.8 1589.3 3155.7 3164.8	87.7 253.9 472.5 609.7 761.8 863.8 924.0 1029.2 1188.4 1310.3 1455.6 1608.2 3157.6 3176.9	117.6 279.3 482.0 640.1 775.8 882.1 968.6 1049.2 1204.2 1370.2 1472.1 1645.3 3158.4 3179.3	174.9 381.8 506.1 654.3 792.9 896.0 972.9 1129.3 1270.5 1372.8 1505.9 1669.1 3160.1 3188.9	204.1 394.8 530.6 736.2 819.9 908.3 997.3 1157.8 1286.0 1412.5 1571.5 2383.9 3160.8	2.1 0.4 0.4
A3-P-1	2	-538.787320	0.180630	0.765395 (0.75)	89.7 383.2 504.6 657.7 772.8 905.9 997.6 1166.6 1291.9 1412.5 1571.3 3158.7 3182.3	118.4 391.3 536.7 743.5 829.2 932.0 1024.9 1188.4 1323.4 1473.7 1620.7 3163.0 3192.7	231.9 397.9 580.8 749.1 851.9 970.3 1028.4 1196.4 1361.8 1483.7 1658.5 3169.8 3193.2	232.9 472.6 613.6 759.2 865.8 972.4 1124.7 1233.8 1371.5 1508.9 1665.6 3170.2	263.4 501.2 637.3 767.3 896.6 997.2 1165.6 1267.8 1390.2 1564.0 3157.6 3182.1	2.2 0.4 0.4
A3-P-2	1	-538.787867	0.180341	0.761482 (0.75)	90.5 390.5 511.6 655.1 779.6 901.2 997.5 1173.5 1291.1 1424.2 1586.0 3158.9 3177.4	122.5 394.9 525.9 724.3 822.1 910.9 1023.9 1177.4 1324.3 1447.0 1622.0 3159.5 3182.2	233.2 400.4 573.7 754.9 854.6 925.2 1031.3 1193.3 1360.2 1481.4 1659.8 3164.5 3189.0	235.3 474.9 617.0 762.2 871.4 971.2 1112.8 1242.0 1380.0 1501.3 1669.6 3169.4	265.8 486.2 638.3 769.2 900.5 974.5 1162.1 1285.9 1399.1 1547.1 3154.4 3175.2	2.2 0.5 0.4
A3-P-3	1	-538.787928	0.180190	0.759734 (0.75)	93.4 379.5 505.4 658.0 788.1 901.1 997.1 1166.6 1288.1 1422.3 1588.0 3157.1 3176.0	122.3 396.2 533.6 724.4 819.7 910.4 1029.2 1187.9 1304.1 1450.7 1610.5 3158.0 3180.0	237.5 398.8 578.3 751.2 834.4 924.6 1038.3 1202.0 1364.3 1471.0 1642.2 3159.4 3187.8	238.1 464.7 608.5 760.1 860.5 965.0 1124.6 1261.9 1369.8 1504.7 1668.9 3160.6	273.4 481.6 639.0 774.2 894.1 972.2 1156.3 1284.2 1410.6 1565.1 3154.8 3164.4	2.2 0.5 0.4
A3-p	2	-539.471930	0.193652	0	95.1 399.9 507.7 723.5 801.8 888.6	100.2 411.5 542.3 725.8 827.4 947.6	229.4 436.9 557.4 727.2 843.4 961.1	242.4 446.9 599.5 747.7 876.8 977.0	248.5 506.2 632.9 765.8 881.1 992.5	1.6 0.6 0.4

					993.0 1165.7 1242.5 1375.0 1535.8 1661.2 3169.9 3206.0	1017.3 1173.4 1266.5 1445.2 1563.3 3155.4 3175.5	1061.2 1186.4 1304.7 1450.9 1609.0 3159.2 3183.4	1062.4 1189.2 1325.4 1472.1 1644.5 3160.0 3186.0	1115.4 1225.0 1368.5 1490.9 1656.5 3168.9 3193.9	
A3-p-TS-1	1	-539.956368	0.191638	0.761646 (0.75)	-859.8 239.2 436.7 548.1 732.5 848.2 950.2 1050.2 1178.0 1292.8 1445.8 1596.5 3155.6 3185.2	93.8 247.5 446.5 587.9 752.4 870.9 962.0 1061.1 1189.4 1305.6 1472.9 1638.8 3161.7 3190.9	98.0 258.1 509.3 631.3 760.5 870.9 991.4 1062.5 1198.2 1349.1 1482.0 1646.8 3167.0 3195.1	150.9 395.4 516.0 707.8 795.0 883.7 994.8 1117.2 1219.6 1364.4 1517.7 1652.5 3171.1 3205.8	236.8 407.9 532.8 722.8 833.0 912.0 1015.5 1161.0 1263.0 1385.4 1563.0 2355.6 3178.6	1.5 0.5 0.4
A3-p-TS-2	1	-539.956221	0.191675	0.761348 (0.75)	-855.6 228.5 446.1 550.7 723.1 837.0 954.2 1034.4 1182.3 1286.7 1430.6 1589.9 3159.9 3185.2	89.1 240.2 448.1 587.6 756.4 879.0 970.3 1060.7 1187.3 1321.0 1458.9 1637.2 3162.1 3189.3	97.7 266.6 502.4 624.0 758.5 884.3 982.5 1078.3 1214.2 1354.1 1482.5 1652.4 3164.5 3194.1	173.4 405.2 503.4 712.1 806.8 889.4 994.4 1103.8 1224.7 1369.5 1514.1 1655.9 3170.3 3207.5	224.3 414.7 550.4 712.2 829.6 910.2 996.9 1165.7 1246.3 1414.9 1547.4 2364.1 3176.6	1.6 0.5 0.4
A3-p-TS-3	1	-539.956537	0.191476	0.760675 (0.75)	-840.7 228.0 431.5 555.2 726.4 823.5 945.2 1023.0 1177.1 1294.6 1444.7 1594.9 3157.1 3177.2	91.4 261.3 448.9 589.9 754.2 871.8 960.4 1059.0 1183.8 1314.1 1457.5 1622.5 3160.0 3185.4	93.9 261.8 503.6 621.5 769.2 880.6 979.7 1064.5 1206.2 1356.7 1477.6 1649.5 3161.4 3191.6	170.6 393.3 504.7 712.9 811.9 884.0 993.7 1119.0 1237.5 1371.8 1524.6 1659.6 3169.4 3204.9	205.5 409.8 538.8 713.7 820.3 903.7 1008.4 1161.7 1260.8 1398.7 1541.6 2399.7 3171.3	1.6 0.5 0.4
A3-p-TS-4	1	-539.956842	0.191458	0.760845 (0.75)	-848.1 238.2 431.0 551.9 721.9 839.6 955.0 1029.1 1174.7 1285.0 1441.3 1600.0 3155.5 3179.2	89.7 249.8 449.3 585.0 752.0 865.4 959.5 1060.6 1186.5 1313.6 1456.4 1614.4 3158.7 3180.7	99.1 265.2 501.0 628.4 786.0 878.9 980.4 1071.0 1215.6 1357.2 1473.6 1651.2 3161.2 3187.4	171.9 396.9 501.2 712.4 791.2 886.2 993.9 1114.7 1240.4 1365.2 1515.1 1659.4 3171.0 3202.3	203.5 410.4 547.9 719.0 818.8 900.0 997.1 1159.1 1253.1 1417.2 1552.3 2383.0 3177.2	1.6 0.5 0.4
A3-p-TS-5	1	-539.955838	0.191814	0.761077 (0.75)	-950.8 239.9 447.3 559.3 724.2 834.7 961.4 1055.8 1174.0	71.9 253.7 453.5 590.4 750.1 881.8 972.7 1059.5 1185.2	99.1 370.5 499.1 620.6 775.7 882.3 983.4 1093.6 1199.9	173.2 405.1 504.3 712.9 801.4 893.7 996.1 1123.3 1231.2	227.3 409.1 555.5 713.6 830.8 911.0 1012.6 1166.6 1244.1	1.5 0.5 0.4

					1287.0	1318.0	1355.1	1365.7	1425.2	
					1432.8	1455.3	1479.0	1524.6	1538.5	
					1588.0	1638.2	1652.2	1657.7	2242.4	
					3156.4	3160.2	3161.0	3169.1	3171.9	
					3176.2	3183.8	3187.2	3220.4		
A3-p-P-1	1	-538.795584	0.180707	0.758892 (0.75)	95.5	99.0	230.6	243.5	245.8	
					393.9	403.6	435.8	446.0	499.7	
					512.2	532.7	553.8	586.7	630.8	
					717.9	722.3	730.0	746.9	761.8	
					794.4	837.1	838.1	873.6	875.7	
					880.8	949.9	962.1	990.5	995.5	1.7
					1014.8	1058.7	1062.2	1113.8	1160.2	0.6
					1175.2	1187.5	1191.4	1218.0	1261.2	0.4
					1292.2	1300.0	1344.8	1359.4	1375.6	
					1444.6	1473.1	1481.4	1513.4	1563.3	
					1594.1	1640.0	1645.5	1654.0	3157.0	
					3161.7	3166.5	3171.6	3178.1	3185.1	
					3190.4	3195.0	3205.5			
A3-p-P-2	1	-538.795397	0.180752	0.758461 (0.75)	94.9	101.1	225.6	239.2	245.6	
					404.4	413.5	447.0	447.4	498.2	
					499.6	551.7	553.3	584.2	631.3	
					707.4	720.4	723.8	748.5	758.1	
					805.1	831.2	835.6	878.6	882.7	
					883.8	952.6	966.9	983.5	994.3	1.6
					1006.3	1059.9	1061.4	1104.0	1165.5	0.6
					1179.4	1186.3	1206.5	1223.3	1243.9	0.4
					1285.0	1320.3	1348.3	1368.6	1409.7	
					1428.6	1457.4	1481.3	1508.2	1544.4	
					1587.7	1637.2	1652.7	1655.0	3159.9	
					3160.7	3164.4	3170.9	3177.3	3185.6	
					3189.6	3194.6	3207.6			
A3-p-P-3	1	-538.795186	0.180545	0.757478 (0.75)	93.2	103.4	227.3	250.1	251.8	
					391.2	413.8	430.3	447.4	502.0	
					503.2	535.1	552.1	588.5	626.6	
					709.1	716.7	725.7	751.3	762.8	
					806.1	816.5	831.0	869.5	880.1	
					885.0	942.1	959.0	979.4	993.2	1.6
					1009.2	1059.7	1066.1	1116.1	1156.9	0.6
					1175.6	1181.9	1203.8	1236.8	1258.4	0.4
					1290.0	1308.8	1348.1	1371.1	1394.2	
					1442.6	1456.6	1474.4	1522.7	1536.5	
					1591.0	1620.8	1648.9	1659.4	3156.9	
					3160.3	3161.5	3169.6	3172.0	3177.0	
					3185.1	3191.1	3204.1			
A3-p-P-4	1	-538.795603	0.180541	0.757735 (0.75)	97.8	100.0	235.4	240.1	250.7	
					396.0	409.5	429.3	448.5	499.0	
					507.3	546.4	557.4	581.8	623.0	
					706.7	718.3	723.2	750.6	778.7	
					788.6	827.0	836.9	858.6	880.0	
					885.9	952.7	957.4	979.0	993.8	1.7
					1006.6	1059.1	1069.0	1110.9	1154.9	0.6
					1174.1	1185.9	1212.9	1239.4	1250.5	0.4
					1275.1	1312.5	1345.8	1364.8	1413.7	
					1438.1	1455.8	1471.1	1509.2	1551.6	
					1595.1	1613.8	1651.0	1658.5	3154.2	
					3158.2	3160.8	3169.9	3177.1	3180.6	
					3182.1	3187.5	3199.7			
A3-p-P-5	1	-538.798446	0.180606	0.758241 (0.75)	99.7	116.1	222.1	225.8	247.9	
					406.9	410.2	447.6	451.2	494.8	
					500.2	555.4	556.0	588.2	629.1	
					706.8	720.9	725.3	743.1	770.2	
					802.6	828.1	835.7	884.4	889.1	
					889.3	963.1	968.3	981.4	996.6	1.7
					1012.9	1050.5	1065.4	1099.6	1162.4	0.6
					1172.1	1179.7	1190.0	1230.4	1242.7	0.4
					1281.7	1314.2	1355.5	1367.4	1424.1	
					1431.6	1450.0	1476.4	1515.7	1533.4	
					1585.8	1637.4	1650.5	1655.7	3155.6	
					3159.1	3159.8	3167.2	3170.0	3174.9	
					3178.2	3182.5	3189.3			
A4	4	-693.086295	0.239594	0	56.7	89.8	150.3	163.3	191.7	1.6
					271.7	305.1	317.8	318.2	383.2	0.2
					448.2	474.4	478.4	483.8	505.6	0.2

					518.9	562.7	567.2	618.6	634.8	
					645.1	734.0	745.7	757.3	758.3	
					762.9	769.4	778.2	788.4	844.3	
					854.7	864.9	867.8	892.1	910.6	
					916.3	917.1	945.3	972.2	973.6	
					995.8	996.4	1020.7	1023.3	1146.9	
					1150.3	1152.0	1186.5	1189.6	1204.1	
					1223.2	1224.1	1291.0	1298.8	1315.6	
					1318.1	1359.9	1367.8	1411.9	1418.1	
					1424.3	1432.4	1479.6	1482.1	1501.6	
					1557.5	1578.3	1583.8	1609.0	1648.6	
					1663.2	1677.4	3154.6	3156.4	3156.7	
					3158.3	3159.7	3159.8	3163.4	3164.5	
					3175.4	3176.4	3186.4	3188.4		
A4-TS-1	1	-693.569969	0.237771	0.775722 (0.75)	-853.3	55.8	87.2	139.4	151.3	
					162.0	192.6	262.7	270.3	305.9	
					313.8	318.9	385.1	450.7	472.0	
					475.6	502.8	505.1	515.3	560.4	
					562.4	616.3	627.3	636.9	723.4	
					745.3	747.1	756.9	759.2	763.6	
					772.7	780.8	845.1	855.0	873.4	
					876.8	897.9	901.1	908.8	913.9	
					943.4	972.7	973.9	996.6	997.0	1.6
					1020.7	1022.6	1062.6	1145.6	1149.3	0.2
					1163.4	1185.8	1191.5	1209.7	1220.8	0.2
					1246.9	1275.3	1301.1	1316.1	1355.7	
					1359.3	1381.3	1391.6	1416.6	1426.7	
					1473.7	1479.2	1498.0	1535.0	1563.4	
					1579.7	1605.7	1637.0	1660.8	1674.4	
					2354.0	3155.5	3158.8	3159.9	3162.6	
					3164.8	3170.6	3176.3	3178.1	3183.2	
					3189.4	3193.4				
A4-TS-2	1	-693.570864	0.237519	0.766127 (0.75)	-858.1	56.2	83.6	148.9	157.9	
					158.5	202.4	234.5	271.1	311.4	
					316.3	324.3	385.3	449.8	474.6	
					479.0	495.1	500.6	513.2	556.7	
					560.4	612.9	622.3	642.0	722.1	
					748.8	753.7	754.4	761.4	772.8	
					776.9	786.9	848.9	862.8	868.0	
					872.4	891.9	892.3	908.8	915.8	
					921.6	935.0	973.7	978.5	996.9	
					1011.7	1021.9	1062.1	1131.2	1151.1	1.6
					1154.5	1180.6	1188.4	1210.1	1222.0	0.2
					1271.9	1298.3	1305.0	1314.0	1340.9	0.2
					1360.4	1393.3	1407.4	1412.5	1429.4	
					1451.6	1479.0	1492.1	1540.5	1558.2	
					1581.0	1606.7	1646.3	1657.2	1674.0	
					2354.9	3155.2	3157.8	3159.2	3160.2	
					3160.4	3164.8	3168.1	3176.1	3177.2	
					3182.7	3189.0				
A4-P-1	1	-692.409487	0.226848	0.779153 (0.75)	55.6	88.1	148.4	161.5	188.1	
					269.5	299.9	311.9	317.8	385.4	
					441.2	467.6	474.7	503.7	505.9	
					514.4	560.4	562.4	617.4	631.7	
					640.7	720.8	744.9	754.3	756.5	
					759.4	763.7	772.8	782.1	844.0	
					854.2	873.3	874.5	902.5	904.0	
					909.9	944.2	972.5	973.7	996.5	
					997.1	1018.5	1023.4	1144.7	1148.4	1.7
					1161.0	1184.2	1190.4	1207.8	1219.4	0.2
					1241.7	1274.3	1299.4	1316.0	1354.3	0.2
					1359.6	1372.5	1385.8	1416.0	1425.0	
					1472.2	1479.1	1497.3	1530.1	1561.8	
					1579.7	1605.9	1637.0	1659.8	1673.3	
					3155.0	3158.4	3158.9	3163.9	3164.7	
					3170.6	3175.8	3177.5	3182.8	3187.7	
					3193.6					
A4-P-2	1	-692.410042	0.226569	0.765545 (0.75)	55.9	90.9	148.5	163.3	190.6	
					269.8	304.8	313.2	319.2	385.0	
					447.1	472.2	478.0	492.8	498.2	1.7
					510.6	554.0	563.2	611.0	632.3	0.2
					642.4	713.8	745.0	752.9	757.9	0.2
					761.5	769.2	776.4	786.5	848.8	

					858.1	867.7	871.7	889.2	896.9	
					915.5	919.3	936.5	972.8	973.9	
					996.8	1016.7	1022.4	1132.5	1150.9	
					1153.3	1173.6	1188.1	1209.1	1221.1	
					1267.9	1296.7	1302.8	1312.3	1334.5	
					1358.6	1388.5	1403.3	1410.7	1429.1	
					1447.5	1478.3	1491.0	1537.3	1557.5	
					1580.8	1606.6	1645.8	1658.0	1674.2	
					3154.7	3157.6	3159.0	3160.0	3160.2	
					3164.7	3169.5	3176.5	3177.1	3182.4	
					3189.0					
A4-py	4	-615.706615	0.206405	0	98.4	152.3	214.0	249.3	262.6	
					359.4	402.1	412.1	462.6	500.4	
					507.1	508.7	513.6	538.5	554.3	
					586.0	595.4	687.8	704.1	726.2	
					749.6	756.9	783.5	814.7	814.9	
					834.5	846.6	859.3	902.4	916.3	
					973.6	979.9	980.8	982.0	991.0	1.0
					1014.9	1091.3	1114.0	1127.1	1165.4	0.6
					1168.1	1198.3	1204.4	1232.1	1262.7	0.4
					1264.2	1268.3	1342.7	1351.6	1400.0	
					1427.5	1434.3	1457.8	1459.5	1483.3	
					1515.6	1535.7	1596.4	1626.1	1635.8	
					1646.0	1670.8	3155.9	3156.2	3159.4	
					3160.1	3167.2	3168.1	3175.3	3175.4	
					3184.3	3184.8				
A4-py-TS-1	2	-616.191567	0.204209	0.760424 (0.75)	-850.0	91.9	150.3	168.8	216.2	
					218.3	245.6	282.6	366.2	395.2	
					408.2	462.9	496.7	506.4	507.3	
					516.2	530.6	553.6	569.9	594.6	
					679.1	681.8	718.0	753.4	766.0	
					789.9	806.8	807.2	831.6	844.2	
					864.8	878.5	908.8	913.3	977.1	1.0
					980.6	981.9	989.7	1008.7	1041.7	0.5
					1083.2	1105.5	1132.0	1165.9	1169.5	0.4
					1202.5	1214.1	1250.5	1255.9	1266.7	
					1331.8	1346.0	1377.9	1413.8	1417.8	
					1445.3	1450.3	1477.3	1500.6	1528.3	
					1556.1	1620.6	1621.3	1645.8	1666.4	
					2378.9	3157.5	3157.6	3160.8	3162.6	
					3163.5	3168.4	3176.6	3176.8	3185.3	
A4-py-TS-2	1	-616.190568	0.204434	0.762727 (0.75)	-843.6	95.6	134.6	175.8	214.4	
					230.8	255.5	264.8	368.1	405.7	
					410.8	460.3	488.7	504.8	509.9	
					514.4	539.6	547.2	573.8	596.3	
					685.6	701.3	715.9	740.1	765.6	
					788.6	799.0	820.2	831.7	839.4	
					857.3	893.1	911.5	947.7	969.1	1.0
					978.1	981.6	990.5	999.3	1034.3	0.5
					1095.8	1121.2	1137.9	1165.5	1178.4	0.4
					1199.5	1209.4	1241.2	1260.1	1267.1	
					1330.5	1336.2	1391.2	1400.7	1425.2	
					1440.7	1451.7	1474.9	1490.3	1526.4	
					1586.1	1607.6	1628.9	1641.4	1666.2	
					2390.1	3156.9	3158.9	3160.1	3163.8	
					3168.6	3173.9	3177.0	3184.7	3187.3	
A4-py-TS-3	1	-616.191076	0.204383	0.762092 (0.75)	-861.3	95.3	142.3	158.4	227.6	
					235.0	253.9	268.1	358.0	398.3	
					407.8	459.8	493.2	504.3	507.5	
					522.1	548.9	552.5	582.1	592.6	
					668.7	695.6	727.6	736.6	767.0	
					782.4	807.9	824.4	829.2	836.8	
					867.8	902.1	915.7	917.5	975.6	1.0
					976.7	983.9	989.9	1012.7	1047.0	0.6
					1090.8	1108.5	1115.7	1166.5	1189.1	0.4
					1198.7	1228.4	1229.6	1254.4	1263.2	
					1318.1	1345.1	1376.5	1395.4	1425.4	
					1447.2	1453.5	1458.6	1515.5	1530.0	
					1594.0	1612.7	1631.8	1639.3	1661.6	
					2351.9	3155.5	3157.7	3161.4	3163.7	
					3169.8	3176.3	3178.1	3185.5	3191.8	
A4-py-P-1	2	-615.030381	0.193272	0.757117 (0.75)	100.8	149.9	214.6	244.9	271.6	1.0
					362.5	393.1	413.3	460.8	494.9	0.6

					504.7	507.9	515.7	526.4	550.1	0.4
					565.7	594.7	674.0	697.2	713.9	
					751.6	764.8	798.0	800.6	800.6	
					832.0	842.3	865.4	867.7	912.5	
					976.4	980.0	984.3	988.9	1007.7	
					1084.8	1105.6	1129.9	1165.8	1166.9	
					1201.3	1207.8	1250.2	1253.7	1266.7	
					1319.8	1344.6	1371.9	1413.7	1415.0	
					1443.9	1448.7	1476.2	1501.5	1528.0	
					1544.9	1618.9	1620.1	1646.8	1665.5	
					3158.0	3158.1	3161.2	3163.8	3165.2	
					3168.8	3177.2	3177.4	3185.8		
A4-py-P-2	1	-615.029483	0.193560	0.760432 (0.75)	98.2	154.2	211.1	252.3	259.8	1.0
					361.4	406.0	410.8	462.3	486.0	0.6
					501.6	510.3	514.5	538.8	551.9	0.4
					572.3	596.5	684.9	700.0	714.4	
					744.8	764.2	782.6	802.8	821.7	
					831.4	836.5	855.8	909.9	940.2	
					971.8	977.3	982.0	990.2	1005.4	
					1095.6	1117.5	1135.0	1163.8	1175.7	
					1196.9	1205.5	1239.6	1259.2	1266.3	
					1325.5	1334.5	1386.8	1399.4	1422.0	
					1440.2	1450.0	1469.6	1485.8	1525.7	
					1585.2	1604.8	1629.7	1640.8	1665.1	
					3157.1	3159.5	3160.8	3164.2	3169.3	
					3175.7	3177.8	3185.5	3189.8		
A4-py-P-3	1	-615.030254	0.193478	0.759530 (0.75)	97.3	151.9	217.7	247.4	261.2	1.0
					355.7	397.2	407.5	461.6	485.6	0.6
					504.3	507.0	516.7	550.3	551.8	0.4
					582.2	596.9	663.2	700.4	726.6	
					741.6	764.9	782.1	809.8	820.3	
					826.8	837.5	860.4	906.0	916.5	
					976.3	976.4	983.8	989.8	1012.2	
					1089.0	1108.6	1113.4	1166.0	1184.2	
					1197.3	1219.1	1229.7	1252.4	1262.2	
					1313.0	1342.6	1365.4	1392.2	1424.7	
					1445.6	1452.0	1455.4	1516.4	1528.8	
					1595.1	1609.3	1630.5	1642.8	1661.0	
					3156.4	3157.7	3161.6	3163.9	3170.3	
					3176.6	3178.8	3185.6	3193.3		
A4-p	2	-693.091929	0.240553	0	80.2	83.9	127.3	175.4	208.2	0.8
					258.9	279.5	323.3	378.7	418.9	0.4
					439.1	440.5	478.9	519.6	524.9	0.3
					526.7	553.1	588.1	590.5	632.4	
					686.3	690.1	706.6	756.2	761.7	
					769.5	769.7	811.2	817.7	827.1	
					853.0	865.8	883.2	889.2	962.5	
					965.5	970.1	978.8	981.4	993.6	
					1006.5	1015.1	1055.8	1072.1	1130.1	
					1153.8	1168.4	1178.9	1182.2	1190.4	
					1217.9	1235.9	1239.1	1254.5	1279.2	
					1325.7	1352.2	1368.0	1385.4	1397.3	
					1449.6	1449.7	1456.2	1484.3	1532.3	
					1534.3	1557.9	1596.9	1638.2	1647.5	
					1648.7	1667.3	3157.5	3158.8	3160.1	
					3161.3	3169.9	3170.4	3177.2	3179.4	
					3186.5	3187.2	3213.4	3231.2		
A4-p-TS-1	1	-693.575980	0.238336	0.761741 (0.75)	-1076.4	78.2	84.9	126.4	173.1	0.8
					199.1	205.0	270.3	273.7	329.2	0.4
					373.0	383.2	434.2	435.1	443.8	0.2
					487.2	512.3	521.8	527.2	551.6	
					577.3	598.9	621.4	677.6	683.8	
					702.7	753.7	758.5	761.9	773.3	
					813.4	819.4	824.9	851.9	858.0	
					886.5	897.4	958.0	963.2	965.9	
					976.9	979.3	986.3	1003.7	1010.4	
					1052.5	1064.3	1111.5	1125.4	1149.0	
					1173.4	1177.8	1184.8	1192.4	1218.2	
					1238.0	1244.1	1264.8	1307.4	1343.6	
					1361.9	1380.8	1394.4	1417.2	1442.2	
					1453.9	1469.2	1510.3	1527.4	1544.5	
					1580.9	1631.7	1640.5	1648.8	1665.1	
					2067.6	3158.1	3159.2	3160.2	3161.5	

					3167.6 3186.7	3171.2 3215.4	3177.3	3179.6	3183.8	
A4-p-P-1	1	-692.426278	0.226870	0.758905 (0.75)	46.6 253.2 428.1 521.6 672.0 760.7 851.1 959.0 1015.4 1173.2 1240.2 1362.4 1455.5 1580.6 3121.4 3167.4 3187.3	79.1 276.5 440.1 548.6 688.3 766.9 860.0 965.8 1056.3 1179.2 1243.5 1380.5 1467.3 1633.0 3157.2 3172.1	143.5 317.2 492.1 568.6 708.5 808.7 880.0 974.0 1063.6 1183.2 1262.1 1399.5 1502.2 1645.3 3158.2 3176.5	167.2 381.9 507.9 595.7 744.1 816.8 889.3 983.9 1119.2 1187.5 1303.3 1416.9 1528.9 1649.6 3159.3 3179.2	174.8 417.4 510.4 626.9 746.8 829.2 956.4 994.2 1149.8 1218.4 1338.5 1444.4 1542.0 1668.5 3161.0 3182.3	0.8 0.4 0.2
A5	4	-846.707249	0.285786	0	38.5 193.3 349.4 473.1 525.7 647.3 752.3 795.6 876.4 922.2 995.6 1144.2 1207.2 1295.3 1376.5 1434.6 1557.9 1642.1 3157.0 3162.1 3188.7	71.2 238.4 362.2 478.5 553.7 715.8 753.0 837.7 889.4 923.6 995.6 1158.5 1210.2 1312.4 1411.0 1477.4 1576.8 1673.0 3158.5 3164.1 3188.9	102.3 240.8 380.3 479.9 579.5 725.3 762.2 842.9 890.3 936.5 1016.7 1184.9 1242.5 1319.0 1417.5 1478.6 1578.9 1673.8 3158.7 3165.1	119.2 263.6 454.3 491.0 616.6 744.6 771.4 842.9 902.8 973.3 1019.4 1188.5 1251.2 1333.8 1419.3 1493.4 1594.0 3155.3 3159.5 3176.9	149.1 293.9 471.6 512.9 639.5 746.7 775.1 848.8 917.8 973.8 1134.0 1200.0 1294.4 1358.7 1427.2 1542.5 1633.7 3156.6 3161.2 3176.9	1.3 0.1 0.1
A5-TS-1	2	-847.191324	0.283728	0.836254 (0.75)	-857.1 126.0 263.3 381.5 493.2 579.3 724.8 752.5 837.5 899.1 937.4 1017.7 1164.5 1219.9 1307.8 1379.7 1474.0 1574.5 1670.4 3160.0 3176.5	38.1 163.0 273.5 460.9 503.2 611.9 737.5 769.4 849.4 901.9 973.8 1019.8 1179.9 1242.5 1330.4 1418.0 1487.9 1588.6 2343.1 3163.4 3178.1	70.2 193.4 292.8 467.9 509.0 633.3 744.9 770.3 856.2 910.5 974.0 1063.1 1190.1 1264.0 1353.1 1422.9 1507.1 1616.9 3155.4 3164.7 3178.2	102.0 230.0 341.6 472.1 524.9 637.8 749.8 792.7 889.2 914.5 996.3 1136.6 1193.0 1278.4 1370.0 1426.6 1529.9 1636.7 3156.1 3165.0 3189.4	119.0 239.1 360.3 473.6 550.2 705.8 750.7 817.9 891.9 921.7 996.3 1148.1 1205.1 1301.1 1375.7 1472.1 1574.2 1670.4 3159.8 3176.3 3189.6	1.3 0.1 0.1
A5-TS-2	1	-847.191233	0.283798	0.814992 (0.75)	-855.8 139.9 256.7 381.6 490.7 578.3 718.4 757.1 838.9 894.5 931.8 1017.3	38.3 151.0 271.9 451.8 501.0 614.4 737.5 764.0 847.7 905.8 972.9 1019.2	68.9 192.3 293.5 466.7 516.6 628.2 746.7 773.1 856.4 915.4 974.0 1064.0	100.9 237.1 346.1 473.1 521.7 642.3 748.3 799.2 876.8 918.0 996.0 1140.9	118.6 239.8 364.9 475.9 548.6 707.6 751.8 829.3 891.2 918.9 996.3 1146.4	1.3 0.1 0.1

					1155.8	1181.1	1188.8	1197.6	1207.5	
					1236.5	1238.4	1253.0	1278.8	1303.2	
					1310.5	1328.7	1353.3	1371.6	1382.1	
					1389.0	1406.0	1418.3	1429.8	1471.6	
					1475.6	1490.5	1510.2	1542.5	1565.1	
					1576.3	1590.3	1620.6	1638.7	1666.4	
					1671.6	2346.1	3155.6	3157.8	3158.8	
					3160.1	3160.4	3162.9	3164.9	3170.6	
					3177.3	3178.1	3183.1	3189.1	3193.4	
A5-TS-3	1	-847.191926	0.283651	0.776766 (0.75)	-858.1	38.4	67.3	101.9	117.7	
					135.7	176.1	192.9	215.6	242.5	
					254.0	272.4	293.9	346.8	367.1	
					381.9	453.2	470.3	474.3	478.8	
					491.7	495.0	510.6	515.3	545.6	
					573.9	606.5	632.1	645.8	709.0	
					723.0	738.9	741.7	749.9	759.6	
					760.8	771.6	774.3	794.6	836.7	
					842.2	845.9	865.1	879.4	889.5	
					890.3	900.1	901.3	911.2	917.7	1.3
					926.3	930.5	974.2	978.3	996.4	0.1
					1008.8	1018.2	1061.4	1127.5	1139.7	0.1
					1155.0	1179.6	1187.0	1201.0	1205.4	
					1229.2	1246.7	1283.1	1294.7	1309.4	
					1313.4	1326.0	1350.4	1357.1	1396.8	
					1403.8	1411.7	1417.3	1431.4	1450.2	
					1476.1	1486.1	1532.3	1543.2	1557.3	
					1577.6	1592.0	1631.0	1640.3	1663.8	
					1673.2	2353.6	3155.4	3156.7	3158.5	
					3159.2	3159.7	3161.6	3162.8	3165.1	
					3168.1	3176.3	3177.2	3182.8	3189.0	
A5-TS-4	1	-847.192313	0.283528	0.775798 (0.75)	-850.1	38.2	70.5	99.1	117.3	
					143.1	169.7	206.1	210.2	246.9	
					250.8	263.3	295.0	352.4	365.7	
					376.4	455.0	461.2	471.8	476.3	
					479.4	487.3	510.5	523.4	549.1	
					573.4	610.6	637.1	646.9	706.3	
					718.4	739.2	743.2	749.6	761.5	
					761.6	774.0	781.2	794.6	833.2	
					837.6	845.9	852.7	875.1	884.7	
					890.7	891.0	900.6	909.9	918.0	1.3
					926.2	930.9	971.2	974.1	996.3	0.1
					1007.6	1018.1	1047.3	1131.7	1146.5	0.1
					1157.9	1186.4	1194.1	1201.9	1205.7	
					1237.3	1247.7	1289.1	1293.6	1299.2	
					1315.9	1323.5	1335.7	1357.7	1395.2	
					1404.8	1416.6	1422.9	1430.0	1449.7	
					1469.7	1486.6	1539.1	1552.6	1565.9	
					1577.6	1588.0	1624.3	1633.3	1651.6	
					1673.2	2377.2	3155.8	3156.7	3157.6	
					3158.3	3158.6	3159.9	3160.7	3162.0	
					3163.6	3165.2	3177.2	3180.4	3189.0	
A5-P-1	2	-846.030956	0.272776	0.859238 (0.75)	38.1	69.9	101.9	118.3	148.6	
					191.9	235.3	238.6	262.6	292.4	
					339.4	360.6	381.3	453.8	463.1	
					470.7	473.1	491.7	504.8	506.2	
					524.8	550.4	578.7	616.0	637.1	
					641.9	702.3	724.0	735.2	744.6	
					751.0	752.4	756.6	769.5	770.1	
					792.4	823.6	833.8	849.2	855.3	
					888.6	896.1	899.9	901.5	911.2	
					921.3	936.7	973.4	973.5	995.9	1.4
					995.9	1018.2	1020.0	1137.4	1146.0	0.1
					1163.3	1176.6	1189.7	1190.2	1204.6	0.1
					1214.6	1242.3	1261.9	1277.2	1299.7	
					1305.4	1329.8	1354.2	1361.7	1369.8	
					1374.8	1417.6	1421.2	1422.9	1471.4	
					1472.8	1483.5	1500.9	1529.0	1573.1	
					1573.5	1587.9	1614.8	1634.8	1668.9	
					1669.6	3155.1	3155.6	3159.5	3159.7	
					3164.2	3164.4	3165.8	3176.3	3176.5	
					3177.9	3178.1	3189.2	3189.3		
A5-P-2	1	-846.030853	0.272841	0.832661 (0.75)	38.0	70.4	100.9	118.5	146.0	1.4
					191.6	236.0	236.8	263.2	292.9	0.1

					345.0	357.0	381.4	446.6	462.1	0.1
					471.8	475.5	490.7	503.9	513.7	
					520.9	548.5	578.9	613.7	636.8	
					643.1	705.5	721.4	742.0	744.6	
					747.3	751.2	758.5	763.9	773.1	
					798.2	832.2	836.3	847.4	857.7	
					876.3	890.6	891.8	912.9	917.5	
					920.3	932.7	972.4	973.7	995.6	
					996.1	1016.0	1018.9	1139.7	1144.3	
					1155.0	1178.3	1188.1	1195.9	1206.5	
					1233.4	1238.3	1249.5	1276.8	1301.8	
					1310.0	1328.0	1352.5	1369.8	1373.4	
					1383.6	1402.5	1417.8	1429.1	1469.8	
					1475.3	1489.5	1502.1	1541.0	1563.6	
					1575.8	1589.7	1619.4	1638.1	1664.6	
					1671.0	3155.4	3157.8	3158.6	3160.0	
					3160.3	3163.8	3164.8	3170.6	3177.2	
					3177.9	3182.7	3189.0	3193.4		
A5-P-3	1	-846.031153	0.272676	0.781544 (0.75)	38.3	71.8	101.6	119.4	149.2	1.4
					191.8	237.9	238.5	264.3	293.3	0.1
					344.1	361.4	381.5	453.3	467.8	0.1
					473.8	478.6	491.7	494.0	507.1	
					510.1	544.1	572.4	615.9	636.6	
					645.7	704.0	721.8	731.4	744.6	
					749.8	757.3	761.0	768.3	774.2	
					796.2	836.9	840.8	846.0	861.6	
					874.8	889.0	891.9	900.9	905.3	
					917.4	925.3	931.1	972.7	974.1	
					996.3	1013.2	1018.7	1128.6	1138.9	
					1155.0	1172.7	1186.7	1200.2	1204.2	
					1227.1	1246.3	1280.6	1294.0	1308.5	
					1310.7	1323.1	1343.5	1356.1	1392.1	
					1400.5	1408.4	1416.5	1431.0	1446.2	
					1475.4	1485.6	1529.0	1540.6	1555.6	
					1577.5	1591.0	1630.0	1639.9	1663.5	
					1672.9	3155.1	3156.4	3158.0	3158.9	
					3159.4	3161.0	3162.1	3164.8	3169.4	
					3177.0	3177.2	3182.5	3189.0		
A5-P-4	1	-846.031154	0.272548	0.779037 (0.75)	39.0	71.8	103.6	120.2	150.0	1.3
					194.8	239.8	242.3	263.8	292.8	0.1
					350.9	363.5	374.8	450.9	454.6	0.1
					471.6	475.9	479.1	488.8	512.1	
					522.3	548.3	576.7	608.9	635.8	
					646.7	698.8	721.6	733.0	741.8	
					749.5	760.0	761.1	773.6	776.3	
					794.2	822.0	837.9	845.7	849.4	
					873.6	889.1	892.8	897.9	900.8	
					917.0	924.3	931.3	967.0	973.9	
					996.1	1017.9	1027.7	1129.6	1144.0	
					1155.0	1185.6	1189.9	1200.5	1204.9	
					1235.0	1246.7	1278.6	1292.1	1296.1	
					1314.8	1320.6	1332.7	1357.1	1392.3	
					1402.3	1416.1	1420.6	1428.9	1444.9	
					1468.8	1486.1	1537.3	1549.8	1559.5	
					1577.4	1591.0	1622.5	1633.4	1649.6	
					1673.0	3155.5	3156.2	3157.5	3158.1	
					3158.7	3159.7	3160.7	3161.8	3163.6	
					3165.1	3177.0	3182.4	3188.9		
A5-p	2	-846.713599	0.286801	0	65.0	71.8	90.2	121.1	169.5	0.4
					174.6	229.3	245.9	276.0	312.8	0.3
					343.2	399.1	420.0	420.9	451.2	0.2
					471.3	477.5	496.2	527.1	537.4	
					545.3	552.2	576.7	611.3	635.2	
					659.9	679.2	691.7	724.7	736.1	
					753.5	765.7	779.0	785.6	798.4	
					805.2	817.3	840.1	856.6	866.8	
					884.2	884.9	937.6	949.7	960.8	
					967.4	969.4	978.2	981.5	997.5	
					998.8	1047.3	1058.8	1082.9	1094.8	
					1151.3	1166.3	1172.0	1179.6	1183.4	
					1184.7	1208.0	1225.1	1234.4	1239.1	
					1249.3	1286.1	1297.9	1343.9	1357.0	
					1364.7	1374.2	1398.0	1412.0	1448.2	

					1448.7	1466.1	1472.6	1515.1	1526.6	
					1547.1	1555.0	1590.3	1623.0	1647.5	
					1649.1	1655.8	1661.5	3157.5	3157.9	
					3159.7	3160.2	3162.2	3170.8	3171.0	
					3177.0	3177.9	3180.8	3186.3	3186.6	
					3217.8	3218.5				
A5-p-TS-1	1	-847.197221	0.284594	0.761983 (0.75)	-1015.3	62.4	74.2	90.4	120.4	
					158.2	165.8	207.2	235.7	244.9	
					277.2	309.9	342.0	362.2	398.6	
					420.3	426.1	449.9	472.2	482.4	
					499.5	520.8	536.3	545.2	556.3	
					569.6	613.9	623.7	653.4	671.3	
					690.7	720.6	729.8	754.7	763.9	
					775.2	784.4	793.1	805.9	819.8	
					838.2	855.6	859.9	882.3	893.1	
					935.4	940.7	945.6	960.6	965.5	0.4
					971.2	978.0	981.8	994.9	1042.6	0.3
					1053.8	1076.9	1080.9	1108.9	1146.7	0.2
					1166.2	1173.6	1179.0	1184.4	1192.6	
					1209.5	1224.6	1234.6	1241.9	1262.2	
					1292.2	1336.9	1347.1	1361.6	1375.2	
					1390.6	1408.8	1422.2	1444.2	1452.0	
					1468.8	1502.3	1513.0	1537.8	1545.5	
					1576.4	1616.6	1641.6	1648.1	1651.8	
					1660.4	2153.4	3157.8	3158.3	3159.8	
					3160.3	3162.6	3167.9	3171.1	3177.2	
					3178.0	3181.2	3183.2	3186.6	3223.4	
A5-p-TS-2	1	-847.198594	0.284602	0.760989 (0.75)	-847.6	63.8	70.5	88.6	119.3	
					147.6	169.0	198.7	217.1	238.9	
					250.1	282.6	313.4	345.3	400.3	
					414.9	419.9	450.0	470.3	477.3	
					495.8	520.8	531.1	542.3	553.3	
					569.0	612.4	631.0	652.9	676.6	
					691.0	719.2	727.9	757.3	772.0	
					776.0	779.3	791.6	810.1	824.1	
					840.1	854.8	860.3	880.8	884.9	
					915.4	926.1	944.6	956.1	963.0	0.4
					969.3	977.6	981.8	998.7	1025.5	0.3
					1045.3	1062.3	1085.3	1093.3	1147.8	0.2
					1162.2	1173.3	1178.9	1184.1	1202.3	
					1216.2	1230.3	1234.3	1244.6	1274.4	
					1288.5	1328.2	1349.6	1360.2	1374.3	
					1391.7	1406.4	1414.1	1445.2	1451.5	
					1467.3	1502.8	1513.6	1538.4	1549.2	
					1585.3	1612.7	1621.7	1648.4	1654.0	
					1660.7	2382.1	3155.6	3158.3	3160.3	
					3161.0	3163.0	3172.1	3177.7	3178.7	
					3179.8	3181.5	3187.3	3202.6	3217.7	
A5-p-P-1	1	-846.043028	0.273615	0.759823 (0.75)	52.5	70.4	92.1	121.3	159.1	
					182.4	224.1	235.8	274.2	304.6	
					348.3	398.7	419.7	425.8	450.0	
					472.1	475.0	504.5	518.2	532.9	
					543.3	553.2	568.3	615.9	627.3	
					651.0	675.0	691.7	718.9	727.6	
					750.5	758.9	775.0	784.5	794.6	
					805.7	822.4	838.1	856.4	861.4	
					881.6	888.0	936.7	942.4	960.9	
					964.6	968.7	977.1	982.0	992.7	0.4
					1048.6	1058.7	1080.8	1088.5	1147.1	0.3
					1166.6	1173.9	1179.9	1183.6	1187.1	0.2
					1209.5	1226.6	1235.2	1241.7	1260.2	
					1290.2	1333.3	1348.2	1360.0	1377.4	
					1389.0	1410.8	1421.0	1445.8	1451.3	
					1467.5	1493.7	1513.8	1535.3	1545.9	
					1574.4	1616.2	1644.3	1646.2	1654.0	
					1661.7	3156.5	3158.0	3158.5	3160.5	
					3162.4	3167.0	3171.3	3176.4	3178.1	
					3180.5	3181.3	3186.5	3221.9		
A5-p-P-2	1	-846.037373	0.273653	0.758026 (0.75)	65.1	72.0	90.4	120.6	172.0	
					177.6	230.9	245.0	278.7	312.4	0.5
					343.3	399.4	413.0	419.6	449.8	0.3
					469.9	477.1	496.7	518.4	537.7	0.2
					545.3	552.1	567.4	611.7	626.5	

					650.8	673.6	691.4	717.5	727.5	
					756.8	764.2	774.2	782.2	791.4	
					809.2	820.8	838.4	856.8	859.9	
					881.2	884.9	931.7	944.7	951.4	
					962.4	968.9	976.3	981.5	998.4	
					1047.6	1062.7	1081.9	1091.4	1143.2	
					1160.7	1172.6	1178.5	1183.7	1201.0	
					1215.0	1228.3	1233.3	1244.3	1267.8	
					1286.8	1321.9	1343.2	1359.4	1374.1	
					1389.3	1402.9	1414.3	1442.3	1450.6	
					1466.9	1496.7	1513.7	1536.1	1549.2	
					1582.9	1610.4	1621.6	1648.2	1653.6	
					1660.6	3154.3	3158.6	3160.3	3161.1	
					3163.1	3172.1	3178.0	3179.0	3181.0	
					3181.7	3187.4	3200.3	3218.3		
A5-a	2	-846.732352	0.286748	0	41.5	54.6	106.5	115.7	125.3	
					185.3	215.0	251.4	282.0	305.3	
					310.5	408.5	413.6	415.7	433.2	
					442.8	501.9	524.8	528.9	530.3	
					534.7	567.0	569.1	580.2	606.7	
					663.9	677.7	723.1	730.7	735.7	
					753.5	757.3	779.7	786.0	789.3	
					799.2	815.2	828.4	869.1	876.6	
					877.4	879.3	898.4	907.1	952.3	
					955.0	978.6	979.2	981.5	991.2	0.7
					992.4	1018.7	1060.8	1068.2	1126.5	0.2
					1133.5	1168.6	1179.3	1182.3	1189.8	0.1
					1198.0	1224.9	1239.0	1248.1	1260.4	
					1290.4	1292.8	1310.4	1330.7	1353.4	
					1362.9	1377.4	1411.7	1445.5	1455.6	
					1456.7	1466.4	1484.3	1508.9	1526.0	
					1549.5	1589.5	1599.9	1634.6	1649.1	
					1651.2	1660.3	1666.2	3155.6	3157.4	
					3158.7	3160.2	3160.6	3169.6	3169.9	
					3177.0	3177.6	3184.1	3185.0	3193.5	
					3196.4	3222.8				
A5-a-TS-1	2	-847.212400	0.285370	0.764090 (0.75)	-1087.9	46.2	55.2	103.1	108.9	
					146.8	195.2	212.7	235.1	284.1	
					306.6	309.6	310.1	400.6	408.5	
					424.1	430.5	449.2	456.9	510.7	
					526.4	529.2	537.6	550.4	567.8	
					574.4	581.6	604.1	655.2	673.8	
					714.8	718.9	738.5	756.3	761.1	
					777.0	779.2	798.8	798.8	813.9	
					828.2	872.0	881.4	883.2	901.5	
					903.4	960.2	960.5	979.8	981.9	0.7
					987.0	988.4	994.8	995.4	1016.9	0.2
					1059.0	1066.9	1115.1	1121.9	1154.3	0.1
					1167.5	1177.8	1180.7	1187.7	1211.6	
					1225.9	1228.4	1240.4	1261.7	1285.7	
					1299.0	1321.5	1350.2	1353.6	1362.1	
					1402.4	1422.2	1431.4	1446.1	1462.4	
					1482.9	1502.0	1518.5	1536.2	1579.0	
					1586.1	1624.3	1645.9	1647.5	1655.0	
					1663.0	1987.2	3157.0	3157.7	3160.3	
					3160.8	3162.6	3171.8	3171.9	3177.1	
					3177.7	3187.3	3187.5	3221.1	3221.4	
A5-a-TS-2	1	-847.216440	0.284977	0.761025 (0.75)	-945.4	40.9	51.6	93.6	113.3	
					122.7	161.0	204.8	214.8	248.2	
					287.5	303.8	311.0	375.4	412.8	
					413.7	424.7	433.5	448.7	503.3	
					521.9	528.4	533.1	534.3	562.3	
					577.1	577.1	598.5	656.7	669.1	
					716.8	726.2	731.0	756.1	761.7	
					777.1	786.7	790.1	797.1	816.4	0.7
					829.9	868.6	876.7	882.4	891.2	0.2
					895.6	906.0	914.3	955.7	972.2	0.1
					978.9	980.9	984.9	993.0	1016.0	
					1057.7	1065.8	1107.8	1122.0	1133.9	
					1167.4	1178.8	1184.9	1193.8	1200.3	
					1227.6	1239.5	1255.8	1277.9	1290.9	
					1305.6	1320.3	1340.2	1359.9	1372.9	
					1408.0	1435.3	1438.0	1449.7	1456.7	

					1472.7	1500.3	1518.5	1538.6	1559.6	
					1594.9	1630.8	1641.9	1648.8	1659.6	
					1664.4	2243.2	3156.2	3157.7	3159.3	
					3160.6	3161.2	3169.7	3170.5	3177.1	
					3177.8	3184.3	3185.1	3196.2	3241.9	
A5-a-TS-3	1	-847.217244	0.284537	0.760909 (0.75)	-848.6	40.0	54.1	105.5	113.1	
					118.6	171.6	185.9	209.5	227.9	
					263.2	284.0	305.0	312.5	408.6	
					411.3	413.6	433.7	439.6	499.3	
					521.2	524.5	528.3	533.2	557.8	
					571.2	579.9	603.2	661.1	667.9	
					716.8	727.9	734.5	755.5	766.0	
					771.7	784.6	785.2	795.2	820.1	
					835.9	860.8	869.5	872.3	879.2	
					889.5	897.7	907.5	954.4	957.0	0.6
					972.9	980.7	983.8	992.8	1006.6	0.2
					1028.4	1062.4	1073.7	1126.4	1132.9	0.1
					1163.2	1176.8	1185.1	1196.1	1218.2	
					1235.4	1241.6	1254.7	1280.8	1289.1	
					1299.3	1321.5	1347.6	1359.6	1374.2	
					1398.9	1426.3	1446.3	1449.5	1456.3	
					1474.4	1502.0	1506.6	1540.6	1581.4	
					1596.6	1609.0	1639.9	1650.3	1658.2	
					1665.6	2384.2	3155.6	3156.7	3158.6	
					3160.6	3161.3	3170.5	3177.7	3178.4	
					3179.4	3180.7	3185.3	3195.6	3221.1	
A5-a-P-1	2	-846.061463	0.273859	0.760209 (0.75)	48.4	55.7	106.0	112.8	143.6	
					192.2	213.0	221.4	293.7	304.9	
					306.6	401.9	417.8	423.4	427.7	
					448.3	503.7	525.4	528.1	532.3	
					545.7	555.1	571.7	579.1	603.1	
					661.5	669.0	706.6	728.3	742.1	
					757.0	761.4	776.2	782.2	792.6	
					794.2	812.7	827.5	875.6	881.6	
					883.8	897.6	902.6	959.2	960.9	
					979.0	981.1	985.2	993.9	994.8	0.7
					1016.6	1056.1	1058.2	1122.1	1131.4	0.2
					1164.2	1174.2	1174.4	1183.0	1202.4	0.1
					1227.9	1229.0	1241.0	1265.5	1286.4	
					1297.0	1320.2	1352.0	1355.5	1359.7	
					1416.9	1421.3	1421.5	1447.9	1464.1	
					1481.5	1498.7	1522.8	1534.4	1578.9	
					1584.9	1626.6	1643.1	1647.5	1656.8	
					1659.4	3156.4	3156.8	3159.7	3159.8	
					3163.4	3167.2	3167.6	3175.8	3176.4	
					3178.3	3178.7	3189.7	3189.9		
A5-a-P-2	1	-846.059146	0.273752	0.758203 (0.75)	46.0	57.4	110.3	110.9	135.1	
					190.0	212.3	238.8	288.5	305.4	
					310.6	406.0	414.4	425.2	432.0	
					448.8	504.0	516.7	524.7	533.3	
					533.3	561.8	576.2	576.8	603.4	
					662.4	664.8	714.2	728.0	736.0	
					746.2	756.9	774.1	787.1	791.3	
					797.0	814.4	828.1	873.7	878.9	
					888.2	892.9	902.7	906.1	956.1	
					966.5	978.1	980.4	983.1	992.8	
					1016.1	1060.9	1066.7	1113.1	1129.3	0.7
					1166.3	1177.3	1182.4	1189.3	1195.8	0.2
					1228.3	1239.9	1256.1	1273.2	1290.0	0.1
					1297.5	1317.8	1337.8	1359.1	1371.6	
					1409.6	1434.4	1438.7	1444.9	1455.6	
					1469.8	1496.2	1515.7	1534.0	1557.5	
					1593.8	1628.9	1641.5	1646.9	1659.1	
					1662.7	3156.0	3157.3	3159.0	3159.9	
					3160.6	3170.1	3170.1	3176.5	3177.3	
					3182.8	3183.1	3189.1	3202.1		
A5-a-P-3	1	-846.055973	0.273650	0.757829 (0.75)	42.1	54.3	106.0	116.8	128.3	
					184.9	217.8	253.2	282.6	304.7	
					311.7	406.9	410.1	413.6	433.3	0.7
					438.7	502.3	518.5	528.2	530.3	0.2
					534.3	555.6	570.6	579.0	601.6	0.1
					658.5	664.8	714.6	728.6	732.9	
					755.5	763.2	772.3	782.6	785.5	

					794.2	819.3	834.5	855.6	871.1	
					873.4	880.0	891.4	907.3	952.4	
					954.3	975.9	980.3	982.6	992.6	
					1012.1	1062.5	1072.2	1123.2	1130.6	
					1161.2	1176.0	1184.7	1195.8	1215.7	
					1234.1	1239.7	1254.1	1274.6	1288.8	
					1296.0	1320.6	1341.1	1357.9	1373.6	
					1394.6	1425.1	1442.2	1449.8	1455.7	
					1473.6	1497.3	1505.0	1539.2	1578.1	
					1595.4	1607.0	1639.6	1649.8	1657.9	
					1665.1	3154.6	3156.5	3158.6	3160.6	
					3161.3	3170.3	3177.6	3178.7	3180.0	
					3182.0	3185.1	3195.1	3220.6		
A2R5	2	-462.037053	0.158745	0	160.5	212.2	229.3	375.6	423.1	
					461.5	470.8	518.9	561.4	583.1	
					615.7	668.6	675.1	695.8	741.2	
					767.0	788.4	818.0	848.5	879.5	1.5
					917.6	929.4	935.4	975.8	985.6	1.2
					1027.5	1034.8	1056.5	1102.6	1113.1	0.7
					1176.1	1203.3	1224.5	1246.4	1273.1	
					1331.5	1385.5	1419.5	1447.3	1457.4	
					1489.7	1515.5	1540.4	1636.4	1652.4	
					1660.6	3159.6	3160.0	3169.0	3169.7	
					3183.1	3184.0	3201.8	3221.9		
A2R5-TS-1	1	-462.516676	0.157075	0.766166 (0.75)	-731.9	128.9	160.6	180.3	213.3	
					244.2	368.0	422.3	458.3	489.7	
					515.7	554.2	562.8	619.1	650.5	
					665.2	684.2	760.7	772.4	799.5	
					814.1	839.3	849.0	860.9	922.7	1.4
					929.8	952.0	977.3	987.6	1015.1	1.2
					1032.4	1057.3	1092.8	1169.8	1198.3	0.7
					1207.9	1239.7	1257.7	1266.5	1376.7	
					1403.0	1447.4	1451.2	1473.5	1512.0	
					1517.9	1630.7	1645.0	1655.9	2652.9	
					3161.5	3163.4	3171.9	3174.8	3184.7	
					3187.4	3218.2				
A2R5-TS-2	1	-462.521830	0.156654	0.761780 (0.75)	-886.6	131.5	190.5	220.6	221.1	
					230.1	377.8	427.8	463.7	477.2	
					513.5	554.2	573.3	610.5	670.0	
					671.0	689.8	736.5	765.4	792.0	
					792.9	841.0	871.5	917.3	924.4	1.5
					935.2	958.4	983.1	1016.0	1025.8	1.2
					1045.1	1080.4	1104.5	1132.8	1170.9	0.7
					1202.9	1238.1	1255.1	1320.2	1343.2	
					1401.3	1437.4	1445.4	1479.6	1497.0	
					1535.6	1608.0	1633.8	1651.7	2306.4	
					3160.5	3161.5	3170.3	3176.8	3185.3	
					3208.5	3229.4				
A2R5-TS-3	1	-462.522164	0.156566	0.761056 (0.75)	-855.7	137.9	187.7	222.3	226.1	
					233.8	370.0	424.3	463.6	471.1	
					512.2	557.4	565.5	607.0	662.3	
					669.5	690.9	735.7	773.8	793.2	
					816.9	853.9	869.7	892.9	906.6	1.5
					924.3	938.3	982.4	1018.7	1030.0	1.2
					1049.8	1055.5	1098.8	1106.6	1187.4	0.7
					1214.3	1216.9	1259.2	1326.6	1357.2	
					1397.9	1408.1	1454.3	1471.6	1502.1	
					1538.0	1601.1	1643.4	1651.2	2369.0	
					3161.4	3162.6	3167.2	3172.1	3184.6	
					3205.1	3225.1				
A2R5-TS-4	1	-462.521153	0.156757	0.763041 (0.75)	-851.7	147.5	158.9	216.8	219.3	
					251.7	381.4	436.5	453.7	470.2	
					508.8	557.8	568.0	611.2	670.8	
					672.0	684.9	736.3	780.6	806.9	
					809.7	841.1	862.6	892.4	924.4	1.4
					934.8	949.2	984.3	1011.6	1018.7	1.2
					1038.9	1069.0	1101.9	1122.7	1189.2	0.7
					1216.4	1221.8	1261.1	1326.7	1365.2	
					1388.8	1415.2	1447.0	1482.0	1493.3	
					1537.6	1615.2	1636.1	1652.9	2373.5	
					3158.7	3164.0	3173.5	3176.6	3190.6	
					3204.4	3224.2				
A2R5-P-1	1	-461.353890	0.146077	0.764581	158.1	211.9	234.8	366.1	422.2	1.6

				(0.75)	455.7 618.2 770.4 920.9 1031.6 1205.6 1401.5 1520.5 3164.0 3223.1	485.1 642.6 796.9 928.9 1056.2 1235.8 1447.5 1630.0 3171.9	516.2 671.1 813.0 976.4 1090.2 1252.6 1448.9 1643.6 3176.2	552.7 688.3 840.1 986.8 1167.6 1263.5 1471.5 1655.0 3184.3	554.1 754.2 872.7 1012.2 1194.6 1373.4 1512.8 3161.1 3188.3	1.2 0.7
A2R5-P-2	1	-461.361025	0.145909	0.759038 (0.75)	162.2 463.9 608.3 760.5 922.7 1042.5 1201.5 1396.3 1533.7 3161.1 3230.7	215.5 472.0 667.5 788.0 934.7 1078.3 1235.3 1433.3 1604.9 3170.3	223.3 517.9 669.7 806.8 954.0 1103.4 1253.8 1441.4 1630.9 3176.7	376.3 556.2 691.9 836.4 981.9 1126.5 1308.7 1480.2 1649.0 3184.6	427.3 571.7 733.6 872.6 1019.3 1166.5 1339.7 1493.6 3160.1 3209.5	1.5 1.3 0.7
A2R5-P-3	1	-461.361018	0.145662	0.758066 (0.75)	163.0 463.8 602.9 771.1 884.7 1036.3 1205.6 1391.0 1537.3 3164.0 3225.0	216.4 471.1 665.9 800.8 922.7 1050.1 1214.9 1410.4 1591.0 3168.2	227.4 516.7 667.9 811.0 937.2 1098.5 1258.8 1454.4 1641.8 3171.6	368.7 558.9 690.6 854.2 981.8 1105.9 1321.1 1466.6 1650.4 3184.0	422.4 560.0 732.0 871.8 1027.2 1185.9 1348.5 1501.7 3160.9 3204.8	1.5 1.3 0.7
A2R5-P-4	1	-461.360000	0.145873	0.760817 (0.75)	156.6 448.7 609.0 779.4 923.5 1032.6 1210.1 1376.5 1536.3 3163.7 3223.7	212.5 471.3 670.9 797.9 932.7 1060.3 1218.4 1414.8 1606.3 3173.4	236.5 508.5 674.2 808.4 944.3 1100.4 1259.4 1444.3 1634.8 3176.9	381.4 559.1 690.5 834.1 984.4 1119.1 1326.5 1479.1 1651.7 3191.9	428.4 564.5 733.5 867.9 1015.8 1187.5 1356.7 1490.2 3158.9 3203.8	1.6 1.2 0.7

Table S6. Cartesian coordinates of optimized structures at B3LYP/6-311G(d,p) level for all species in this work.

Species Name	Geometry (Å)			Species Name	Geometry (Å)				
H	H	0.000000	0.000000	0.000000	H2	H	0.000000	0.000000	0.372063
						H	0.000000	0.000000	-0.372063
A1	C	-0.560604	1.275909	0.000000	A1-TS	C	-1.479586	0.000001	-0.000002
	C	-1.385360	0.152438	-0.000024		C	-0.787696	-1.210891	-0.000001
	C	-0.824752	-1.123457	0.000017		C	0.611599	-1.219542	0.000000
	C	0.560655	-1.275887	-0.000004		C	1.255910	-0.000001	0.000001
	C	1.385354	-0.152493	-0.000015		C	0.611600	1.219542	0.000001
	C	0.824707	1.123489	0.000019		C	-0.787695	1.210892	-0.000001
	H	-0.996827	2.268652	0.000002		H	-2.563677	0.000001	-0.000003
	H	-2.463188	0.271274	-0.000013		H	-1.332091	-2.149302	-0.000002
	H	-1.466376	-1.997609	0.000019		H	1.162556	-2.153779	0.000001
	H	0.996752	-2.268686	0.000008		H	2.754443	-0.000001	0.000004
	H	2.463197	-0.271195	-0.000011		H	1.162558	2.153778	0.000002
	H	1.466439	1.997562	0.000032		H	-1.332089	2.149303	-0.000001
						H	3.603501	0.000000	0.000006
A1-P	C	0.000003	1.321868	0.000000	A2	C	2.429422	0.707398	0.000002
	C	-1.211527	0.631299	-0.000008		C	1.243505	1.400219	-0.000003
	C	-1.223490	-0.770372	0.000019		C	0.000014	0.715613	0.000000
	C	0.000005	-1.396249	0.000001		C	-0.000016	-0.715608	-0.000001
	C	1.223487	-0.770377	-0.000020		C	1.243484	-1.400222	-0.000003
	C	1.211522	0.631310	0.000006		C	2.429406	-0.707419	0.000002
	H	-0.000010	2.405807	0.000001		H	-1.241815	2.485397	-0.000006
	H	-2.149897	1.175978	-0.000009		H	3.372260	1.242768	0.000004
	H	-2.157261	-1.321324	0.000020		H	1.241851	2.485384	-0.000001
	H	2.157273	-1.321305	-0.000016		C	-1.243489	1.400230	0.000000

	H 2.149902 1.175970 0.000010		C -1.243508 -1.400225 0.000000 H 1.241821 -2.485390 0.000000 H 3.372240 -1.242795 0.000005 C -2.429417 -0.707402 0.000000 C -2.429402 0.707416 0.000003 H -1.241838 -2.485389 -0.000004 H -3.372268 -1.242753 0.000002 H -3.372241 1.242785 0.000002
A2-TS-1	C -2.425779 0.750079 0.000028 C -1.216459 1.401006 0.000181 C -0.002877 0.665406 0.000108 C -0.051918 -0.771607 -0.000129 C -1.322280 -1.403905 -0.000280 C -2.479275 -0.663506 -0.000205 H 1.376916 2.744651 0.000505 H -3.347937 1.320065 0.000085 H -1.171153 2.483770 0.000357 C 1.277217 1.246597 0.000253 C 1.166360 -1.502505 -0.000200 H -1.364574 -2.488292 -0.000457 H -3.442128 -1.161792 -0.000323 C 2.382837 -0.864341 -0.000049 C 2.447878 0.555441 0.000187 H 1.120276 -2.586399 -0.000377 H 3.302596 -1.439201 -0.000106 H 3.407594 1.061055 0.000307 H 1.464185 3.590153 0.000646	A2-P-1	C -2.394156 0.728899 0.000019 C -1.190969 1.391503 0.000195 C 0.035536 0.677138 0.000124 C -0.014529 -0.761272 -0.000138 C -1.273595 -1.416546 -0.000312 C -2.436064 -0.685616 -0.000236 H 1.330165 2.406984 0.000489 H -3.321788 1.290018 0.000077 H -1.161568 2.476282 0.000387 C 1.301882 1.322702 0.000295 C 1.226562 -1.408644 -0.000194 H -1.296076 -2.499809 -0.000509 H -3.394889 -1.191376 -0.000371 C 2.446428 -0.820580 -0.000029 C 2.473049 0.604393 0.000221 H 3.369470 -1.389592 -0.000093 H 3.429824 1.115633 0.000354
A2-TS-2	C 2.456667 -0.813656 0.000030 C 1.236635 -1.445175 0.000185 C 0.031960 -0.695858 0.000113 C 0.104012 0.735039 -0.000124 C 1.382417 1.352485 -0.000279 C 2.530530 0.598651 -0.000204 H -1.322261 -2.401571 0.000445 H 3.370176 -1.397682 0.000086 H 1.178530 -2.528543 0.000363 C -1.251387 -1.318331 0.000268 C -1.097320 1.493785 -0.000197 H 1.438269 2.436080 -0.000456 H 3.499815 1.084192 -0.000325 C -2.328411 0.875098 -0.000045 C -2.354324 -0.524435 0.000184 H -1.031979 2.577431 -0.000375 H -3.245352 1.453830 -0.000101 H -3.696758 -1.194512 0.000344 H -4.455106 -1.574852 0.000433	A2-P-2	C 2.341936 -0.789945 0.000000 C 1.125068 -1.426615 0.000001 C -0.086688 -0.686652 0.000000 C -0.017508 0.744692 -0.000001 C 1.255138 1.371753 0.000001 C 2.406806 0.622818 -0.000001 H -1.395072 -2.412161 0.000002 H 3.258819 -1.368278 0.000000 H 1.073581 -2.510409 0.000001 C -1.355613 -1.327125 0.000000 C -1.235611 1.493112 0.000001 H 1.303819 2.455522 0.000000 H 3.373426 1.114005 -0.000001 C -2.395684 0.795275 0.000001 C -2.524432 -0.593525 -0.000002 H -1.201596 2.577825 0.000001 H -3.493451 -1.079237 0.000000
A3	C 3.654601 0.712031 0.000029 C 3.654601 -0.712031 0.000005 C 1.221845 0.721546 0.000018 C 0.000002 1.401456 0.000024 C -1.221848 0.721545 0.000006 C -1.221848 -0.721545 -0.000018 C 0.000002 -1.401456 -0.000024 C 1.221845 -0.721546 -0.000006 C -2.476556 1.404877 0.000012 C -2.476555 -1.404877 -0.000036 C -3.654602 -0.712028 -0.000029 C -3.654602 0.712028 -0.000005 H -2.475917 2.489905 0.000030 H -0.000002 2.487340 0.000042 H -0.000002 -2.487340 -0.000042 H -2.475917 -2.489905 -0.000054 C 2.476558 -1.404878 -0.000012 C 2.476558 1.404878 0.000036 H 2.475915 -2.489907 -0.000030 H 2.475915 2.489907 0.000054 H -4.599200 -1.244481 -0.000043 H -4.599200 1.244481 -0.000001 H 4.599202 -1.244477 0.000001 H 4.599203 1.244477 0.000043	A3-TS-1	C 3.658011 -0.754447 -0.000030 C 3.661757 0.669914 -0.000006 C 1.224827 -0.764638 -0.000019 C 0.000000 -1.440523 -0.000024 C -1.224827 -0.764638 -0.000007 C -1.233240 0.685702 0.000017 C 0.000000 1.316595 0.000022 C 1.233240 0.685702 0.000006 C -2.479742 -1.446641 -0.000012 C -2.488033 1.369354 0.000035 C -3.661757 0.669914 0.000029 C -3.658011 -0.754447 0.000005 H -2.478160 -2.531772 -0.000030 H 0.000000 -2.526084 -0.000042 H 0.000000 2.822711 0.000049 H -2.488311 2.452888 0.000053 C 2.488033 1.369354 0.000011 C 2.479742 -1.446641 -0.000036 H 2.488311 2.452888 0.000029 H 2.478160 -2.531772 -0.000054 H 0.000000 3.672688 0.000064 H 4.608201 1.198549 -0.000002 H 4.601726 -1.288001 -0.000043 H -4.608201 1.198549 0.000042 H -4.601726 -1.288001 0.000001
A3-TS-2	C 3.697652 -0.678012 -0.000030 C 3.670642 0.746238 -0.000006	A3-TS-3	C -3.728875 0.656719 -0.000031 C -3.701336 -0.767357 -0.000006

	C 1.265966 -0.733934 -0.000019 C 0.058536 -1.440057 -0.000024 C -1.177725 -0.788248 -0.000007 C -1.199588 0.661547 0.000017 C 0.005924 1.368756 0.000023 C 1.238698 0.708594 0.000005 C -2.421192 -1.494519 -0.000013 C -2.478980 1.265719 0.000034 C -3.655571 0.597458 0.000029 C -3.617481 -0.833551 0.000004 H -2.396394 -2.579033 -0.000031 H 0.081906 -2.525755 -0.000042 H -0.017581 2.452949 0.000040 H -2.551954 2.764591 0.000060 C 2.479721 1.416281 0.000011 C 2.533263 -1.393286 -0.000036 H 2.457303 2.500945 0.000029 H 2.553043 -2.478079 -0.000054 H -4.607319 1.117873 0.000042 H -4.550043 -1.387146 0.000000 H 4.605027 1.295922 -0.000002 H 4.652338 -1.191682 -0.000043 H -2.625519 3.611504 0.000075		C -1.297163 0.711873 -0.000019 C -0.088892 1.415774 -0.000024 C 1.146778 0.760940 -0.000007 C 1.172093 -0.683437 0.000018 C -0.034636 -1.387878 0.000023 C -1.269359 -0.730336 0.000006 C 2.383282 1.479799 -0.000013 C 2.446681 -1.344965 0.000035 C 3.566447 -0.586914 0.000028 C 3.585790 0.822205 0.000005 H 2.353055 2.564890 -0.000031 H -0.110847 2.501296 -0.000043 H -0.013495 -2.473316 0.000042 H 2.483683 -2.429850 0.000054 C -2.510443 -1.437796 0.000011 C -2.564334 1.371721 -0.000037 H -2.488859 -2.522545 0.000030 H -2.583811 2.456547 -0.000055 H 4.887399 -1.297405 0.000047 H 4.522936 1.367387 0.000001 H -4.635691 -1.317275 -0.000002 H -4.683640 1.170297 -0.000044 H 5.633075 -1.702107 0.000057
A3-P-1	C 3.660137 0.680374 0.000029 C 3.663744 -0.743896 0.000005 C 1.226072 0.697721 0.000018 C 0.000002 1.372919 0.000023 C -1.226076 0.697719 0.000006 C -1.237197 -0.755264 -0.000019 C 0.000002 -1.364381 -0.000023 C 1.237193 -0.755265 -0.000007 C -2.483125 1.375654 0.000011 C -2.489449 -1.442886 -0.000036 C -3.663746 -0.743893 -0.000030 C -3.660139 0.680371 -0.000006 H -2.485213 2.460839 0.000030 H -0.000002 2.458292 0.000041 H -2.484270 -2.526326 -0.000054 C 2.489453 -1.442888 -0.000012 C 2.483129 1.375657 0.000035 H 2.484267 -2.526328 -0.000031 H 2.485211 2.460841 0.000053 H -4.609935 -1.273111 -0.000044 H -4.604193 1.213629 -0.000001 H 4.609937 -1.273108 0.000001 H 4.604196 1.213624 0.000042	A3-P-2	C 3.618544 0.738901 0.000029 C 3.643124 -0.685066 0.000005 C 1.186103 0.707154 0.000017 C -0.045585 1.370692 0.000023 C -1.258457 0.676703 0.000006 C -1.225589 -0.775197 -0.000019 C 0.003351 -1.440393 -0.000024 C 1.211193 -0.735662 -0.000007 C -2.528637 1.335157 0.000011 C -2.484706 -1.406818 -0.000035 C -3.690016 -0.804375 -0.000030 C -3.700311 0.631243 -0.000006 H -2.545053 2.419720 0.000030 H -0.059971 2.456591 0.000041 H 0.014817 -2.524686 -0.000043 C 2.477151 -1.397783 -0.000012 C 2.428933 1.411600 0.000035 H 2.494020 -2.482544 -0.000031 H 2.409550 2.496396 0.000053 H -4.621794 -1.359122 -0.000044 H -4.652749 1.150396 -0.000001 H 4.596707 -1.200852 0.000000 H 4.553875 1.287168 0.000042
A3-P-3	C -3.589801 -0.757020 0.000029 C -3.614900 0.666568 0.000005 C -1.157749 -0.721420 0.000017 C 0.076053 -1.379371 0.000023 C 1.286999 -0.679819 0.000006 C 1.258437 0.765623 -0.000019 C 0.026243 1.424064 -0.000024 C -1.183130 0.720867 -0.000007 C 2.547475 -1.356283 0.000012 C 2.510236 1.475426 -0.000036 C 3.640815 0.742599 -0.000029 C 3.729684 -0.658165 -0.000005 H 2.555653 -2.441939 0.000030 H 0.094347 -2.464988 0.000041 H 0.006791 2.509503 -0.000042 H 2.511209 2.560777 -0.000054 C -2.449801 1.381203 -0.000013 C -2.399234 -1.428030 0.000035 H -2.469403 2.465990 -0.000031 H -2.378558 -2.512853 0.000053 H 4.685415 -1.169606 -0.000001 H -4.568844 1.182076 0.000000 H -4.524562 -1.306415 0.000042	A3-p	C -3.555755 -0.296446 0.000046 C -2.833856 0.877021 0.000045 C -1.421157 0.865035 0.000005 C -0.728221 -0.379583 -0.000034 C -1.498252 -1.564282 -0.000041 C -2.877871 -1.527262 0.000000 C -0.678184 2.091367 -0.000005 C 0.728222 -0.379603 -0.000075 C 1.421185 0.864958 -0.000094 C 0.678251 2.091317 -0.000054 H -1.228829 3.026266 0.000022 H -3.345107 1.834160 0.000073 H -1.005697 -2.527978 -0.000083 H 1.228909 3.026214 -0.000066 C 2.833867 0.876987 -0.000152 C 1.498142 -1.564313 -0.000141 H 1.005606 -2.528001 -0.000833 C 3.555757 -0.296485 0.000227 C 2.877879 -1.527268 0.000298 H 3.345165 1.834083 -0.000513 H 4.639572 -0.272621 0.000546 H 3.440557 -2.454056 0.000632 H -4.639557 -0.272746 0.000075 H -3.440659 -2.453964 -0.000006
A3-p-TS-1	C 3.532452 -0.429416 0.000040 C 2.845913 0.765171 0.000037 C 1.433981 0.785078 0.000021	A3-p-TS-2	C 3.512341 -0.455833 0.000030 C 2.796621 0.705141 0.000028 C 1.400571 0.793748 0.000016

	C 0.699548 -0.442398 0.000006		C 0.668198 -0.435309 0.000004
	C 1.441034 -1.644294 0.000010		C 1.400746 -1.644852 0.000006
	C 2.821460 -1.641094 0.000026		C 2.781179 -1.662985 0.000018
	C 0.683610 1.990300 0.000017		C 0.703591 2.046729 0.000015
	C -0.758168 -0.402019 -0.000011		C -0.786877 -0.383203 -0.000009
	C -1.428494 0.856274 -0.000013		C -1.435279 0.885285 -0.000009
	C -0.656377 2.073372 0.000001		C -0.652103 2.086474 0.000003
	H 3.379465 1.708301 0.000048		H 1.285761 2.960483 0.000024
	H 0.924951 -2.595652 -0.000001		H 0.874326 -2.590139 -0.000003
	H -1.174583 3.027395 -0.000001		H -1.172393 3.038457 0.000002
	C -2.839574 0.899215 -0.000030		C -2.846726 0.946172 -0.000022
	C -1.553962 -1.569493 -0.000025		C -1.597130 -1.540893 -0.000021
	H -1.082096 -2.543415 -0.000024		H -1.138300 -2.521055 -0.000021
	C -3.584825 -0.260078 -0.000044		C -3.608776 -0.201545 -0.000034
	C -2.932671 -1.504067 -0.000041		C -2.974471 -1.455401 -0.000033
	H -3.330663 1.866601 -0.000032		H -3.324312 1.920424 -0.000022
	H -4.667876 -0.213664 -0.000057		H -4.691041 -0.140002 -0.000043
	H -3.514075 -2.419058 -0.000052		H -3.569336 -2.361788 -0.000042
	H 4.616331 -0.435901 0.000053		H 4.596824 -0.460881 0.000040
	H 3.359656 -2.582183 0.000028		H 3.309559 -2.610284 0.000019
	H 1.434690 3.287902 0.000032		H 3.590677 1.979961 0.000041
	H 1.830647 4.040373 0.000040		H 4.066943 2.683646 0.000048
	C 3.444623 -0.283060 0.000020		C -3.534588 -0.096067 -0.000043
	C 2.771453 0.902341 0.000030		C -2.749014 1.041563 -0.000047
	C 1.352554 0.879187 0.000020		C -1.337265 0.959667 -0.000029
	C 0.669240 -0.372372 0.000000		C -0.694963 -0.313362 -0.000005
	C 1.439041 -1.558613 -0.000010		C -1.516716 -1.470579 0.000000
	C 2.823433 -1.527106 0.000000		C -2.873349 -1.319498 -0.000019
	C 0.603903 2.101312 0.000030		C -0.540780 2.152420 -0.000034
	C -0.787873 -0.379822 -0.000010		C 0.758912 -0.376742 0.000014
	C -1.487719 0.860879 0.000000		C 1.503992 0.837318 0.000008
	C -0.752562 2.091398 0.000020		C 0.814333 2.094059 -0.000016
	H 1.148889 3.039221 0.000045		H -1.049904 3.110346 -0.000052
	H 3.289494 1.856178 0.000045		H -3.213854 2.022598 -0.000066
	H 0.947264 -2.523087 -0.000025		H -1.079118 -2.461242 0.000018
	H -1.308919 3.022892 0.000028		H 1.404209 3.004570 -0.000020
	C -2.900536 0.866061 -0.000009		C 2.915890 0.787805 0.000027
	C -1.552327 -1.568206 -0.000029		C 1.475717 -1.594226 0.000038
	H -1.056380 -2.530056 -0.000037		H 0.941647 -2.535556 0.000043
	C -3.616536 -0.310748 -0.000028		C 3.585640 -0.416103 0.000050
	C -2.932030 -1.537816 -0.000038		C 2.855431 -1.616770 0.000056
	H -3.416188 1.820732 -0.000001		H 3.468288 1.721681 0.000022
	H -4.700360 -0.292674 -0.000034		H 4.669393 -0.439532 0.000063
	H -3.489776 -2.467496 -0.000053		H 3.377685 -2.566781 0.000074
	H 3.397222 -2.447109 -0.000008		H -4.616849 -0.032765 -0.000057
	H 4.946991 -0.242098 0.000030		H -3.706582 -2.566162 -0.000013
	H 5.793794 -0.217118 0.000036		H -4.174363 -3.274072 -0.000009
A3-p-TS-3	C 3.444623 -0.283060 0.000020	A3-p-TS-4	C -3.534588 -0.096067 -0.000043
	C 2.771453 0.902341 0.000030		C -2.749014 1.041563 -0.000047
	C 1.352554 0.879187 0.000020		C -1.337265 0.959667 -0.000029
	C 0.669240 -0.372372 0.000000		C -0.694963 -0.313362 -0.000005
	C 1.439041 -1.558613 -0.000010		C -1.516716 -1.470579 0.000000
	C 2.823433 -1.527106 0.000000		C -2.873349 -1.319498 -0.000019
	C 0.603903 2.101312 0.000030		C -0.540780 2.152420 -0.000034
	C -0.787873 -0.379822 -0.000010		C 0.758912 -0.376742 0.000014
	C -1.487719 0.860879 0.000000		C 1.503992 0.837318 0.000008
	C -0.752562 2.091398 0.000020		C 0.814333 2.094059 -0.000016
	H 1.148889 3.039221 0.000045		H -1.049904 3.110346 -0.000052
	H 3.289494 1.856178 0.000045		H -3.213854 2.022598 -0.000066
	H 0.947264 -2.523087 -0.000025		H -1.079118 -2.461242 0.000018
	H -1.308919 3.022892 0.000028		H 1.404209 3.004570 -0.000020
	C -2.900536 0.866061 -0.000009		C 2.915890 0.787805 0.000027
	C -1.552327 -1.568206 -0.000029		C 1.475717 -1.594226 0.000038
	H -1.056380 -2.530056 -0.000037		H 0.941647 -2.535556 0.000043
	C -3.616536 -0.310748 -0.000028		C 3.585640 -0.416103 0.000050
	C -2.932030 -1.537816 -0.000038		C 2.855431 -1.616770 0.000056
	H -3.416188 1.820732 -0.000001		H 3.468288 1.721681 0.000022
	H -4.700360 -0.292674 -0.000034		H 4.669393 -0.439532 0.000063
	H -3.489776 -2.467496 -0.000053		H 3.377685 -2.566781 0.000074
	H 3.397222 -2.447109 -0.000008		H -4.616849 -0.032765 -0.000057
	H 4.946991 -0.242098 0.000030		H -3.706582 -2.566162 -0.000013
	H 5.793794 -0.217118 0.000036		H -4.174363 -3.274072 -0.000009
	C -3.566380 -0.297395 -0.000009		C 3.580955 -0.213801 0.000049
	C -2.859033 0.885016 -0.000032		C 2.850286 0.954239 0.000067
	C -1.446451 0.888986 -0.000026		C 1.438705 0.917129 0.000044
	C -0.742401 -0.348790 0.000006		C 0.748305 -0.337066 0.000006
	C -1.494686 -1.543921 0.000026		C 1.536486 -1.509208 -0.000020
	C -2.874717 -1.520554 0.000019		C 2.915825 -1.451770 0.000002
	C -0.716712 2.122833 -0.000055		C 0.632137 2.077545 0.000051
	C 0.711606 -0.332300 0.000013		C -0.710645 -0.348669 -0.000013
	C 1.399461 0.923410 -0.000022		C -1.429466 0.883575 -0.000012
	C 0.639585 2.139304 -0.000055		C -0.704120 2.134040 0.000023
	H -1.277359 3.051676 -0.000079		H 3.342836 1.919336 0.000097
	H -3.381415 1.836009 -0.000055		H 1.057778 -2.480031 -0.000064
	H -0.984916 -2.496829 0.000046		H -1.256531 3.068295 0.000023
	H 1.179270 3.080553 -0.000080		C -2.840942 0.872068 -0.000039
	C 2.812636 0.953402 -0.000022		C -1.461828 -1.545294 -0.000030
	C 1.534350 -1.467557 0.000051		C -0.952607 -2.500215 -0.000021
	H 1.064169 -2.861270 0.000137		C -3.540933 -0.315295 -0.000059
	C 3.557780 -0.205459 0.000013		C -2.842083 -1.533408 -0.000052
	C 2.901455 -1.453475 0.000053		H -3.368951 1.819783 -0.000042
	H 3.307936 1.918496 -0.000051		H -4.625032 -0.310138 -0.000079
	H 4.641392 -0.164381 0.000011		H -3.387911 -2.470032 -0.000060
	H 3.469081 -2.377739 0.000088		H 4.664342 -0.180122 0.000067
	H -4.650377 -0.286114 -0.000014		H 3.489986 -2.371387 -0.000018
	H -3.427220 -2.453344 0.000035		
	H 0.920485 -3.708066 0.000192		
A3-p-P-2	C 3.619616 -0.188314 0.000061	A3-p-P-3	C 3.541192 -0.319042 0.000064

	C 2.819715 0.910043 0.000075		C 2.898010 0.877280 0.000074
	C 1.427110 0.931654 0.000049		C 1.476037 0.863698 0.000045
	C 0.771650 -0.341587 0.000008		C 0.783186 -0.383202 0.000011
	C 1.577913 -1.503979 -0.000015		C 1.541179 -1.577355 -0.000007
	C 2.957280 -1.438788 0.000010		C 2.928244 -1.561631 0.000021
	C 0.659522 2.142657 0.000056		C 0.737058 2.091541 0.000045
	C -0.684052 -0.374200 -0.000014		C -0.674105 -0.378746 -0.000012
	C -1.405757 0.854298 -0.000016		C -1.364340 0.867414 -0.000023
	C -0.696137 2.100942 0.000019		C -0.619504 2.091916 0.000007
	H 1.190903 3.086800 0.000089		H 1.289391 3.025134 0.000072
	H 1.110802 -2.479882 -0.000063		H 3.425293 1.825720 0.000102
	H -1.273261 3.019596 0.000021		H 1.040421 -2.537371 -0.000051
	C -2.818253 0.831358 -0.000048		H -1.168404 3.027875 0.000002
	C -1.424520 -1.577598 -0.000032		C -2.777092 0.883980 -0.000057
	H -0.908053 -2.528594 -0.000018		C -1.448504 -1.560809 -0.000023
	C -3.511467 -0.359325 -0.000071		H -0.960568 -2.526778 0.000001
	C -2.804584 -1.573603 -0.000060		C -3.502761 -0.286883 -0.000075
	H -3.352738 1.775619 -0.000053		C -2.827939 -1.519298 -0.000055
	H -4.595480 -0.361484 -0.000097		H -3.284947 1.842861 -0.000067
	H -3.344886 -2.513542 -0.000071		H -4.586417 -0.260036 -0.000103
	H 4.702000 -0.127507 0.000081		H -3.393040 -2.444566 -0.000060
	H 3.542501 -2.352354 -0.000010		H 3.494302 -2.486007 0.000006
	C 3.603007 -0.431137 0.000046		C 3.558712 -0.368206 0.000039
	C 2.900489 0.762548 0.000056		C 2.855024 0.818602 0.000048
	C 1.486275 0.785315 0.000035		C 1.440944 0.841019 0.000032
	C 0.748243 -0.435174 0.000006		C 0.719563 -0.393868 0.000006
	C 1.480041 -1.654634 -0.000015		C 1.507329 -1.541091 -0.000004
	C 2.838165 -1.586652 0.000009		C 2.866075 -1.603461 0.000010
	C 0.782070 2.034842 0.000040		C 0.699961 2.069709 0.000044
	C -0.705943 -0.388202 -0.000010		C -0.728370 -0.389403 -0.000014
	C -1.356626 0.879151 -0.000014		C -1.414158 0.855362 -0.000003
	C -0.573631 2.079899 0.000012		C -0.658366 2.075400 0.000027
	H 1.362408 2.951457 0.000064		H 1.253297 3.003142 0.000065
	H 3.437517 1.706258 0.000079		H 3.388201 1.763174 0.000069
	H 0.970730 -2.610157 -0.000054		H -1.200849 3.015099 0.000036
	H -1.092443 3.032629 0.000012		C -2.826671 0.860650 -0.000024
	C -2.768359 0.935906 -0.000040		C -1.479470 -1.583060 -0.000046
	C -1.512398 -1.548121 -0.000022		H -0.953022 -2.530999 -0.000058
	H -1.050340 -2.526968 -0.000006		C -3.539279 -0.319958 -0.000051
	C -3.527067 -0.214097 -0.000056		C -2.858952 -1.551173 -0.000062
	C -2.889879 -1.466682 -0.000044		H -3.346013 1.813372 -0.000016
	H -3.248863 1.908754 -0.000044		H -4.623241 -0.301379 -0.000066
	H -4.609521 -0.155431 -0.000077		H -3.421183 -2.478152 -0.000083
	H -3.482422 -2.374539 -0.000050		H 4.643447 -0.363142 0.000051
	H 4.686602 -0.449776 0.000062		H 3.405308 -2.544244 0.000000
A3-p-P-4	C 4.880889 -0.714776 0.000011	A3-p-P-5	C 4.871917 -0.770692 -0.000036
	C 4.880889 0.714776 0.000035		C 4.882572 0.658330 -0.000012
	C 3.706615 1.407260 0.000041		C 2.436894 -0.770407 -0.000024
	H 3.705811 2.492293 0.000059		C 1.217787 -1.439670 -0.000030
	C 2.446292 0.725014 0.000024		C -0.015991 -0.758472 -0.000013
	C 2.446292 -0.725014 -0.000001		C -0.017190 0.699166 0.000012
	C 3.706615 -1.407260 -0.000006		C 1.230808 1.323481 0.000016
	H 3.705811 -2.492293 -0.000024		C 2.452287 0.687203 0.000000
	C -0.000227 0.725011 0.000012		C -1.253177 -1.429880 -0.000018
	C -1.233530 1.404315 0.000018		C -1.247035 1.384911 0.000029
	C -2.446606 0.724778 0.000001		C -2.459662 0.704793 0.000023
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	C -3.706486 1.407369 0.000006		C -4.897401 -0.727950 0.000011
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	C -4.880793 -0.714200 -0.000035		C -3.717560 1.390614 0.000040
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	H -3.706134 2.492316 0.000024		H 1.212803 -2.525121 -0.000048
	H -1.234424 2.490067 0.000036		H 1.239358 2.828737 0.000043
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	C 1.233969 -1.404444 -0.000018		C 3.715757 1.363485 0.000006
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	H 1.233811 -2.490201 -0.000036		H 3.721894 2.446981 0.000024
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	H 5.826670 -1.244812 0.000006		H -5.838022 1.233745 0.000048
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A4		A4-TS-1	

	H -5.826470 -1.245021 -0.000049 H -5.826470 1.245021 -0.000007		H 1.245010 3.678792 0.000059 H 5.832458 1.180734 -0.000007 H 5.813947 -1.307185 -0.000049
A4-TS-2	C 4.846117 -0.816876 -0.000036 C 4.873579 0.619442 -0.000012 C 2.404165 -0.790343 -0.000024 C 1.181682 -1.450462 -0.000029 C -0.042900 -0.753570 -0.000012 C -0.025726 0.696308 0.000012 C 1.214335 1.364434 0.000017 C 2.415878 0.666751 0.000000 C -1.284412 -1.418010 -0.000018 C -1.250750 1.390863 0.000029 C -2.471648 0.725826 0.000023 C -2.488957 -0.723626 -0.000001 C -3.756815 -1.390855 -0.000006 H -3.769457 -2.475754 -0.000024 C -4.922749 -0.683864 0.000011 C -4.905646 0.745153 0.000034 C -3.722935 1.423643 0.000040 H -1.297913 -2.503604 -0.000035 H 1.166391 -2.536202 -0.000047 H -1.237392 2.476385 0.000046 H -3.709077 2.508507 0.000058 C 3.695909 1.278893 0.000005 C 3.658193 -1.486450 -0.000041 H 3.758810 2.777314 0.000031 H 3.641799 -2.571118 -0.000059 H -5.844839 1.286688 0.000048 H -5.874727 -1.202630 0.000007 H 5.822489 1.145153 -0.000007 H 5.783689 -1.361991 -0.000049 H 3.826035 3.625033 0.000045 H 1.230273 2.448664 0.000035	A4-P-1	C 4.900785 0.673845 -0.000011 C 4.899934 -0.755802 -0.000036 C 3.727302 -1.450934 -0.000042 H 3.718189 -2.534315 -0.000060 C 2.471570 -0.760184 -0.000024 C 2.464939 0.700405 0.000000 C 3.729992 1.372890 0.000006 H 3.735527 2.458055 0.000024 C -0.006063 -0.752031 -0.000013 C -1.238083 -1.432078 -0.000018 C -2.446344 -0.743031 -0.000001 C -2.438884 0.706733 0.000023 C -1.224005 1.385199 0.000029 C 0.009434 0.708112 0.000012 C -3.708743 -1.419496 -0.000007 C -3.695214 1.394467 0.000041 C -4.873276 0.706822 0.000034 C -4.880365 -0.721101 0.000011 H -3.713347 -2.504346 -0.000025 H -1.236889 -2.516253 -0.000036 H -1.224545 2.471102 0.000047 H -3.690554 2.479380 0.000059 C 1.250543 1.378836 0.000018 C 1.241196 -1.364093 -0.000029 H 1.253853 2.464083 0.000036 H 5.847873 1.201490 -0.000007 H 5.845776 -1.285428 -0.000049 H -5.816006 1.242649 0.000048 H -5.828187 -1.247773 0.000006
A4-P-2	C 4.859809 -0.688043 0.000010 C 4.843805 0.741083 0.000035 C 3.661820 1.420784 0.000041 H 3.649120 2.505692 0.000059 C 2.409729 0.724316 0.000023 C 2.425978 -0.725162 -0.000001 C 3.693211 -1.393757 -0.000007 H 3.704432 -2.478666 -0.000025 C -0.036611 0.697819 0.000012 C -1.276403 1.367851 0.000017 C -2.484282 0.681763 0.000000 C -2.459896 -0.777646 -0.000024 C -1.243903 -1.449406 -0.000030 C -0.020027 -0.752201 -0.000013 C -3.756033 1.346326 0.000006 C -3.727574 -1.400462 -0.000041 C -4.926223 -0.791439 -0.000036 C -4.928303 0.649452 -0.000011 H -3.766334 2.430955 0.000024 H -1.284633 2.453713 0.000036 H -1.239207 -2.533652 -0.000048 C 1.220881 -1.418144 -0.000018 C 1.189448 1.390521 0.000029 H 1.232325 -2.503700 -0.000036 H 1.177657 2.476154 0.000047 H 5.811373 -1.207533 0.000006 H 5.783549 1.281704 0.000048 H -5.862210 -1.339030 -0.000050 H -5.878627 1.172432 -0.000007	A4-py	C 3.518205 0.000000 0.000368 C 2.828903 -1.208574 0.000306 C 1.427079 -1.234372 0.000158 C 0.712474 0.000000 0.000072 C 1.427078 1.234373 0.000133 C 2.828900 1.208575 0.000280 C 0.679174 -2.460718 0.000092 C -0.712474 0.000000 -0.000075 C -1.427077 -1.234373 -0.000137 C -0.679171 -2.460719 -0.000050 C -2.828901 -1.208575 -0.000280 H -3.375035 -2.145968 -0.000327 C -3.518205 -0.000003 -0.000359 C -2.828902 1.208574 -0.000300 C -1.427080 1.234373 -0.000157 C -0.679174 2.460719 -0.000094 C 0.679171 2.460720 0.000043 H 1.227053 3.397296 0.000084 H -1.227058 3.397295 -0.000157 H 1.227056 -3.397296 0.000155 H 4.602471 0.000002 0.000483 H 3.375038 -2.145966 0.000375 H 3.375039 2.145965 0.000326 H -1.227055 -3.397295 -0.000101 H -4.602471 -0.000001 -0.000470 H -3.375039 2.145964 -0.000363
A4-py-TS-1	C -3.573544 0.000000 -0.000349 C -2.883687 -1.208009 -0.000293 C -1.481859 -1.233796 -0.000154 C -0.765908 0.000000 -0.000072 C -1.481859 1.233796 -0.000131 C -2.883687 1.208008 -0.000270 C -0.736716 -2.461071 -0.000094 C 0.659724 0.000000 0.000065 C 1.370096 -1.239036 0.000121 C 0.621604 -2.464380 0.000038	A4-py-TS-2	C 3.553375 0.172423 -0.000361 C 2.797016 1.340195 -0.000307 C 1.396073 1.286888 -0.000162 C 0.753256 0.013435 -0.000072 C 1.536041 -1.179054 -0.000129 C 2.934025 -1.073400 -0.000273 C 0.581476 2.470108 -0.000102 C -0.668723 -0.068901 0.000070 C -1.449529 1.132279 0.000123 C -0.774884 2.400325 0.000034

	C 2.777910 -1.220648 0.000257 H 3.333330 -2.152932 0.000302 C 3.413559 0.000000 0.000332 C 2.777909 1.220648 0.000279 C 1.370096 1.239036 0.000144 C 0.621604 2.464380 0.000085 C -0.736716 2.461071 -0.000047 H -1.286074 3.396806 -0.000085 H 1.168263 3.401442 0.000147 H -1.286074 -3.396806 -0.000153 H -4.657749 0.000000 -0.000454 H -3.429304 -2.145686 -0.000356 H -3.429304 2.145686 -0.000310 H 1.168263 -3.401442 0.000086 H 4.912696 -0.000001 0.000470 H 3.333330 2.152933 0.000342 H 5.761467 -0.000001 0.000545		C -2.829174 0.974444 0.000262 H -3.694387 2.207960 0.000317 C -3.484121 -0.236870 0.000347 C -2.716842 -1.403801 0.000294 C -1.315396 -1.341658 0.000156 C -0.497285 -2.522848 0.000100 C 0.858723 -2.445554 -0.000035 H 1.458590 -3.349657 -0.000070 H -0.990229 -3.489347 0.000167 H 1.077559 3.435031 -0.000166 H 4.635896 0.233936 -0.000470 H 3.289322 2.306890 -0.000375 H 3.532471 -1.978264 -0.000312 H -1.374295 3.303124 0.000082 H -4.567603 -0.289568 0.000453 H -3.206144 -2.372534 0.000361 H -4.205364 2.884360 0.000350
A4-py-TS-3	C -3.501712 -0.187472 0.000208 C -2.868628 1.051535 0.000365 C -1.469735 1.132303 0.000283 C -0.693971 -0.071924 0.000036 C -1.358665 -1.333411 -0.000121 C -2.760666 -1.364715 -0.000031 H -1.506325 3.633796 0.000699 H -4.584764 -0.235171 0.000274 H -3.451473 1.964869 0.000553 C -0.733864 2.349670 0.000430 C 0.731168 -0.010296 -0.000052 H -3.266598 -2.324315 -0.000152 C 1.403356 1.249388 0.000105 C 0.606372 2.453434 0.000355 H 1.106374 3.417254 0.000479 H -1.916290 4.378982 0.000855 C -0.561188 -2.528097 -0.000369 C 1.493345 -1.216166 -0.000298 C 0.795686 -2.471746 -0.000453 C 2.804034 1.277501 0.000013 C 2.893483 -1.137923 -0.000382 C 3.537426 0.094636 -0.000228 H 3.314573 2.234520 0.000133 H 4.620893 0.135273 -0.000297 H 3.473569 -2.054543 -0.000571 H 1.381743 -3.384820 -0.000642 H -1.070362 -3.486154 -0.000490	A4-py-P-1	C 3.471322 -0.000001 0.000358 C 2.781158 -1.207792 0.000298 C 1.379299 -1.233500 0.000156 C 0.662840 0.000000 0.000072 C 1.379301 1.233501 0.000135 C 2.781155 1.207793 0.000278 C 0.634947 -2.461195 0.000094 C -0.763229 0.000000 -0.000078 C -1.472261 -1.240443 -0.000139 C -0.723237 -2.465500 -0.000047 C -2.882969 -1.225083 -0.000293 H -3.439080 -2.156549 -0.000343 C -3.498316 -0.000003 -0.000373 C -2.882966 1.225082 -0.000317 C -1.472266 1.240444 -0.000165 C -0.723238 2.465502 -0.000097 C 0.634945 2.461196 0.000048 H 1.185134 3.396395 0.000098 H -1.269845 3.402488 -0.000162 H 1.185136 -3.396393 0.000161 H 4.555454 0.000001 0.000464 H 3.326612 -2.145504 0.000361 H 3.326615 2.145502 0.000326 H -1.269844 -3.402486 -0.000093 H -3.439087 2.156543 -0.000390
A4-py-P-2	C -3.482453 -0.126150 0.000361 C -2.846470 1.111448 0.000299 C -1.447329 1.198118 0.000156 C -0.681375 -0.005350 0.000072 C -1.340573 -1.270327 0.000137 C -2.742338 -1.304203 0.000281 C -0.755539 2.457882 0.000091 C 0.741836 0.053619 -0.000076 C 1.396697 1.329390 -0.000140 C 0.600862 2.525249 -0.000050 C 2.779119 1.291379 -0.000286 C 3.566698 0.168262 -0.000375 C 2.915056 -1.070728 -0.000312 C 1.514011 -1.147474 -0.000162 C 0.817400 -2.404353 -0.000093 C -0.539588 -2.462758 0.000050 H -1.046094 -3.422099 0.000098 H 1.404292 -3.316806 -0.000158 H -1.347077 3.367346 0.000157 H -4.565642 -0.172790 0.000469 H -3.432788 2.024079 0.000363 H -3.248022 -2.263901 0.000330 H 1.111133 3.480984 -0.000099 H 4.649512 0.225047 -0.000492 H 3.498601 -1.985875 -0.000380	A4-py-P-3	C 3.536849 -0.109276 -0.000347 C 2.869088 1.111551 -0.000314 C 1.467906 1.167957 -0.000177 C 0.725300 -0.049138 -0.000070 C 1.428084 -1.298838 -0.000108 C 2.829389 -1.307255 -0.000245 C 0.745659 2.409810 -0.000142 C -0.701729 -0.024308 0.000070 C -1.386908 1.226900 0.000103 C -0.611991 2.436807 -0.000008 C -2.789225 1.237299 0.000243 H -3.310721 2.188402 0.000269 C -3.509130 0.047612 0.000348 C -2.852002 -1.179373 0.000316 C -1.452499 -1.239489 0.000178 C -0.732026 -2.495882 0.000144 C 0.606224 -2.452151 0.000005 H -1.290010 -3.426958 0.000223 H 1.313285 3.334459 -0.000224 H 4.620769 -0.127516 -0.000450 H 3.433417 2.037969 -0.000394 H 3.350719 -2.256824 -0.000270 H -1.140599 3.384227 0.000018 H -4.593022 0.075150 0.000457 H -3.421766 -2.102267 0.000399
A4-p	C 2.402486 1.890068 0.345564 C 1.216441 2.534133 0.192120 C 0.000041 1.810241 0.000052 C -0.000001 0.394764 0.000139	A4-p-TS-1	C -2.383921 1.936993 -0.318023 C -1.196526 2.572333 -0.137571 C 0.017282 1.841373 0.043264 C 0.011009 0.426668 0.028757

	C 1.287810 -0.279825 -0.055455 C 2.479911 0.474616 0.186304 C -1.216341 2.534163 -0.192123 C -1.287835 -0.279744 0.055706 C -2.479908 0.474696 -0.186285 C -2.402402 1.890144 -0.345592 C -3.737297 -0.173262 -0.190728 H -4.621003 0.418513 -0.405743 C -3.851832 -1.511258 0.107019 C -2.700094 -2.235816 0.460392 C -1.458432 -1.636113 0.437570 H -1.166445 3.616945 -0.236243 H 3.316003 2.444305 0.532571 H 1.166602 3.616924 0.236071 H -3.315870 2.444417 -0.532733 H -4.822755 -1.993294 0.109465 H -2.787500 -3.270302 0.773213 H -0.606231 -2.206586 0.773943 C 1.458351 -1.636183 -0.437386 C 3.737312 -0.173302 0.190478 H 0.606087 -2.206744 -0.773486 H 4.621044 0.418502 0.405291 C 2.699997 -2.235848 -0.460432 C 3.851783 -1.511320 -0.107162 H 2.787396 -3.270301 -0.773360 H 4.822730 -1.993299 -0.110077		C -1.278279 -0.240310 0.062186 C -2.471580 0.518557 -0.194283 C 1.242048 2.554548 0.220947 C 1.288906 -0.259839 -0.047556 C 2.492451 0.486032 0.156737 C 2.427853 1.900414 0.330821 C 3.743753 -0.172080 0.114513 H 4.640205 0.410699 0.298887 C 3.833608 -1.510676 -0.188943 C 2.662662 -2.229602 -0.489000 C 1.428448 -1.620427 -0.418282 H 1.201233 3.637001 0.278874 H -3.292163 2.499108 -0.507372 H -1.142881 3.655519 -0.161643 H 3.349838 2.447500 0.496246 H 4.799602 -2.001037 -0.229063 H 2.729143 -3.269194 -0.789342 H 0.550030 -2.188653 -0.685595 C -1.502324 -1.587634 0.403679 C -3.727409 -0.131573 -0.255738 H -0.565927 -2.352710 1.163193 H -4.603491 0.466054 -0.483820 C -2.717866 -2.213555 0.393098 C -3.855945 -1.476730 0.003074 H -2.810821 -3.247016 0.709704 H -4.826516 -1.958308 -0.040009 H -0.113267 -2.865924 1.703869
A4-p-P-1	C 2.433687 1.905224 -0.000028 C 1.232477 2.539769 -0.000013 C 0.000999 1.814729 0.000003 C -0.004297 0.400546 0.000002 C 1.278209 -0.277595 0.000001 C 2.500751 0.481270 -0.000020 C -1.227181 2.543953 0.000019 C -1.283670 -0.288012 -0.000002 C -2.490193 0.480651 0.000010 C -2.425642 1.905263 0.000024 C -3.743770 -0.174558 0.000002 H -4.642912 0.432837 0.000010 C -3.831615 -1.547188 -0.000014 C -2.652006 -2.312757 -0.000022 C -1.418849 -1.697388 -0.000014 H -1.180052 3.627667 0.000035 H 3.359900 2.470101 -0.000044 H 1.185737 3.623555 -0.000016 H -3.353197 2.467833 0.000034 H -4.799160 -2.036200 -0.000024 H -2.710269 -3.395420 -0.000030 H -0.523814 -2.309908 -0.000024 C 1.475648 -1.658447 0.000024 C 3.748896 -0.187635 -0.000010 H 4.651379 0.414136 -0.000018 C 2.653404 -2.336446 0.000020 C 3.838190 -1.561624 0.000015 H 2.696991 -3.420211 0.000048 H 4.805170 -2.052900 0.000031	A5	C -6.107570 0.715774 0.000017 C -6.107570 -0.715774 0.000041 C -4.934793 -1.408406 0.000047 H -4.934727 -2.493389 0.000065 C -3.672386 -0.726676 0.000029 C -3.672386 0.726675 0.000005 C -4.934793 1.408406 -0.000001 H -4.934726 2.493389 -0.000019 C -1.224402 -0.727460 0.000018 C -0.000012 -1.406654 0.000024 C 1.224429 -0.727459 0.000007 C 1.224429 0.727459 -0.000018 C -0.000012 1.406654 -0.000024 C -1.224402 0.727460 -0.000006 C 2.464011 -1.406141 0.000012 C 2.464011 1.406141 -0.000035 C 3.672406 0.726659 -0.000029 C 3.672406 -0.726659 -0.000005 C 4.934774 -1.408397 0.000001 H 4.934737 -2.493379 0.000019 C 6.107575 -0.715761 -0.000016 C 6.107575 0.715761 -0.000041 C 4.934774 1.408397 -0.000047 H 2.464697 -2.491824 0.000030 H 0.000001 -2.492239 0.000042 H 0.000000 2.492239 -0.000042 H 2.464697 2.491824 -0.000053 H 4.934737 2.493379 -0.000065 C -2.464035 1.406145 -0.000012 C -2.464035 -1.406145 0.000035 H -2.464678 2.491830 -0.000030 H -2.464678 -2.491830 0.000053 H 7.053507 1.245462 -0.000054 H 7.053507 -1.245462 -0.000012 H -7.053510 1.245463 0.000012 H -7.053510 -1.245462 0.000054
A5-TS-1	C 6.116064 0.684372 -0.000017 C 6.112702 -0.746396 -0.000041 C 4.937847 -1.436529 -0.000047 H 4.935073 -2.521467 -0.000065 C 3.677736 -0.751934 -0.000030 C 3.681161 0.700657 -0.000006 C 4.944286 1.379707 0.000000 H 4.945929 2.464574 0.000018 C 1.228322 -0.754703 -0.000019 C 0.000000 -1.429539 -0.000024	A5-TS-2	C 6.104822 0.657083 -0.000017 C 6.093373 -0.773841 -0.000041 C 4.916101 -1.459756 -0.000047 H 4.909441 -2.544868 -0.000065 C 3.657495 -0.772928 -0.000030 C 3.673698 0.688042 -0.000006 C 4.939590 1.362954 0.000000 H 4.946641 2.446454 0.000018 C 1.202347 -0.760517 -0.000018 C -0.026150 -1.430807 -0.000023

	C -1.228322 -0.754703 -0.000007		C -1.248094 -0.745337 -0.000007
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	C 0.000000 1.338652 0.000022		C -0.018126 1.388249 0.000023
	C 1.236551 0.708075 0.000006		C 1.202044 0.702297 0.000006
	C -2.467721 -1.431085 -0.000012		C -2.489311 -1.419734 -0.000012
	C -2.475200 1.386691 0.000035		C -2.480085 1.392230 0.000034
	C -3.681161 0.700657 0.000029		C -3.691498 0.716686 0.000029
	C -3.677736 -0.751934 0.000005		C -3.696221 -0.736103 0.000005
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	H -2.468123 -2.516912 -0.000030		H -2.493566 -2.505382 -0.000029
	H 0.000000 -2.514879 -0.000042		H -0.031891 -2.516534 -0.000041
	H 0.000000 2.840819 0.000049		H -2.476589 2.477809 0.000052
	H -2.476865 2.470932 0.000052		H -4.946829 2.487888 0.000063
	H -4.945929 2.464574 0.000064		C 2.455987 1.325198 0.000011
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	C 2.467721 -1.431085 -0.000036		H 2.466544 2.828729 0.000037
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	H -7.063130 1.211936 0.000053		H -7.078872 -1.243362 0.000013
	H -7.057360 -1.278315 0.000012		H 7.055334 1.178354 -0.000013
	H 7.063130 1.211936 -0.000013		H 7.035465 -1.310231 -0.000054
	H 7.057360 -1.278315 -0.000054		H 2.473777 3.679349 0.000053
	H 0.000000 3.691619 0.000065		H -0.013011 2.472368 0.000040
	C 6.095922 0.633705 -0.000017		C -6.159601 -0.743069 -0.000017
	C 6.073880 -0.805092 -0.000041		C -6.168282 0.688467 -0.000041
	C 4.890072 -1.479191 -0.000047		C -4.999688 1.388159 -0.000047
	H 4.878082 -2.563913 -0.000065		H -5.005827 2.473122 -0.000066
	C 3.630892 -0.788533 -0.000030		C -3.733298 0.713855 -0.000030
	C 3.637208 0.672378 -0.000005		C -3.724458 -0.739387 -0.000005
	C 4.917192 1.288742 0.000000		C -4.982703 -1.428748 0.000000
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	C 1.181864 -0.761503 -0.000018		C -1.285485 0.729031 -0.000018
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	C -1.266979 -0.740737 -0.000006		C 1.163132 0.743279 -0.000007
	C -1.254911 0.713981 0.000017		C 1.172329 -0.711307 0.000018
	C -0.024616 1.382948 0.000023		C -0.047665 -1.397815 0.000023
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	C -6.137691 0.743759 0.000040		C 6.017512 -0.625550 0.000039
	C -4.959120 1.426527 0.000046		C 4.893497 -1.369763 0.000046
	H -2.521779 -2.494614 -0.000029		H 2.390594 2.515941 -0.000030
	H -0.057105 -2.515772 -0.000041		H -0.071232 2.501083 -0.000042
	H -2.479618 2.488915 0.000052		H -0.041277 -2.483335 0.000041
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	C 2.437253 1.365260 0.000012		H 4.918082 -2.455011 0.000065
	C 2.415061 -1.453002 -0.000035		C -2.511838 -1.411742 0.000012
	H 2.449428 2.449525 0.000029		C -2.528834 1.400506 -0.000036
	H 2.404101 -2.538773 -0.000053		H -2.506030 -2.497390 0.000030
	H -7.079296 1.281090 0.000053		H -2.535782 2.486163 -0.000054
	H -7.100177 -1.209162 0.000013		H 7.329085 -1.349970 0.000058
	H 7.043273 1.162216 -0.000012		H 6.999603 1.321209 0.000011
	H 7.013949 -1.345855 -0.000055		H -7.102485 -1.278175 -0.000013
	H 5.040345 3.634877 0.000041		H -7.117551 1.212144 -0.000055
	H -0.015000 2.468340 0.000040		H 8.070238 -1.763814 0.000068
	C 6.118197 -0.733838 0.000016		C 6.135335 -0.756334 0.000016
	C 6.115699 0.696569 0.000040		C 6.136124 0.674529 0.000041
	C 4.941073 1.387667 0.000046		C 4.966013 1.373664 0.000047
	H 4.939427 2.472620 0.000065		H 4.972007 2.458808 0.000065
	C 3.680273 0.704671 0.000029		C 3.699824 0.701688 0.000030
	C 3.683135 -0.748078 0.000005		C 3.706346 -0.762040 0.000005
	C 4.945420 -1.428000 -0.000001		C 4.963471 -1.451746 -0.000001
	H 4.945926 -2.512894 -0.000019		H 4.955384 -2.535195 -0.000019
	C 1.229767 0.715159 0.000018		C 1.241999 0.710756 0.000018
A5-TS-3		A5-TS-4	
A5-P-1		A5-P-2	

	C 0.000003 1.389614 0.000023		C 0.017132 1.387476 0.000023
	C -1.229772 0.715157 0.000006		C -1.209587 0.709323 0.000006
	C -1.240675 -0.750000 -0.000019		C -1.216708 -0.745563 -0.000018
	C 0.000002 -1.358596 -0.000023		C 0.003393 -1.434371 -0.000024
	C 1.240670 -0.750000 -0.000007		C 1.226859 -0.754895 -0.000007
	C -2.471359 1.387234 0.000012		C -2.445621 1.392799 0.000012
	C -2.476196 -1.433308 -0.000036		C -2.458317 -1.418779 -0.000036
	C -3.683138 -0.748076 -0.000030		C -3.664867 -0.733996 -0.000030
	C -3.680276 0.704669 -0.000005		C -3.658170 0.718536 -0.000005
	C -4.941070 1.387666 0.000000		C -4.916767 1.406050 0.000000
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	C -6.115700 0.696566 -0.000017		C -6.093102 0.718421 -0.000017
	C -6.118199 -0.733835 -0.000041		C -6.099644 -0.712475 -0.000041
	C -4.945417 -1.427998 -0.000047		C -4.929424 -1.410419 -0.000047
	H -2.475164 2.473095 0.000030		H -2.441674 2.478457 0.000030
	H -0.000002 2.474722 0.000042		H 0.017477 2.473246 0.000041
	H -2.471257 -2.517454 -0.000054		H -2.463083 -2.504355 -0.000054
	H -4.945927 -2.512892 -0.000066		H -4.933762 -2.495367 -0.000065
	C 2.476200 -1.433309 -0.000012		C 2.478712 -1.366795 -0.000012
	C 2.471364 1.387236 0.000035		C 2.488273 1.380133 0.000035
	H 2.471255 -2.517454 -0.000030		H 2.492613 2.465431 0.000053
	H 2.475162 2.473096 0.000053		H -7.047990 -1.237810 -0.000054
	H -7.064820 -1.262217 -0.000055		H -7.036690 1.252302 -0.000012
	H -7.060686 1.227974 -0.000012		H 7.081252 -1.285783 0.000012
	H 7.064821 -1.262216 0.000012		H 7.083316 1.201953 0.000054
	H 7.060688 1.227971 0.000054		H 0.005217 -2.518458 -0.000043
A5-P-3	C 6.159438 -0.781206 0.000017		C -6.062273 0.689394 0.000016
	C 6.156948 0.661584 0.000041		C -6.053091 -0.742077 0.000041
	C 4.983751 1.354991 0.000047		C -4.875695 -1.426955 0.000047
	H 4.991322 2.439584 0.000065		H -4.868129 -2.511922 0.000065
	C 3.711970 0.687040 0.000030		C -3.617965 -0.736771 0.000029
	C 3.692068 -0.775392 0.000005		C -3.627210 0.716407 0.000005
	C 4.963696 -1.393987 0.000000		C -4.894019 1.389817 -0.000001
	C 1.262207 0.696046 0.000018		H -4.900898 2.474775 -0.000019
	C 0.042917 1.384022 0.000023		C -1.170155 -0.720943 0.000017
	C -1.187205 0.714552 0.000006		C 0.059044 -1.391873 0.000023
	C -1.198551 -0.740311 -0.000018		C 1.278405 -0.703986 0.000006
	C 0.020683 -1.429463 -0.000024		C 1.269852 0.750457 -0.000019
	C 1.250177 -0.759409 -0.000007		C 0.041197 1.421357 -0.000024
	C -2.420997 1.402761 0.000012		C -1.179153 0.733821 -0.000007
	C -2.442915 -1.409374 -0.000035		C 2.521902 -1.375605 0.000011
	C -3.646359 -0.720484 -0.000030		C 2.505768 1.437497 -0.000036
	C -3.635038 0.732559 -0.000005		C 3.716601 0.764569 -0.000030
	C -4.891829 1.424225 0.000000		C 3.727972 -0.691447 -0.000006
	H -4.883134 2.509179 0.000018		C 4.987689 -1.382388 0.000000
	C -6.069990 0.740545 -0.000017		H 4.981893 -2.468019 0.000019
	C -6.081143 -0.690884 -0.000041		C 6.173157 -0.699648 -0.000016
	C -4.913702 -1.392691 -0.000047		C 6.101797 0.709306 -0.000040
	H -2.413369 2.488419 0.000030		C 4.985852 1.456620 -0.000047
	H 0.051229 2.469617 0.000041		H 2.527411 -2.461208 0.000029
	H -2.452173 -2.495044 -0.000053		H 0.066609 -2.477449 0.000041
	H -4.921732 -2.477635 -0.000065		H 0.033835 2.506877 -0.000042
	C 2.482180 -1.451469 -0.000013		H 2.500246 2.522933 -0.000054
	C 2.505393 1.369051 0.000035		H 5.000736 2.541808 -0.000065
	H 2.482062 -2.535674 -0.000031		C -2.423072 1.404035 -0.000013
	H 2.510693 2.454886 0.000053		C -2.404814 -1.408119 0.000035
	H -7.031243 -1.213043 -0.000054		H -2.431031 2.489677 -0.000031
	H -7.011861 1.277422 -0.000012		H -2.397988 -2.493794 0.000053
	H 7.097194 -1.325871 0.000012		H 7.124050 -1.219527 -0.000012
	H 7.105974 1.186901 0.000055		H -7.011774 1.212686 0.000012
	H 0.012848 -2.514986 -0.000042		H -6.995699 -1.277660 0.000054
A5-p	C -0.722534 0.782028 -0.055369		C -0.718414 0.811915 -0.047796
	C -1.365435 2.017765 -0.331991		C -1.366202 2.049633 -0.301557
	C -0.648498 3.239917 -0.209218		C -0.643916 3.268375 -0.179652
	C 0.648071 3.240033 0.208205		C 0.662112 3.259777 0.208572
	C 1.365144 2.017989 0.331257		C 1.378284 2.035172 0.308780
	C 0.722417 0.782120 0.054790		C 0.725402 0.803200 0.040708
	C 1.584915 -0.368357 -0.189052		C 1.570939 -0.355236 -0.214422
	C 2.961155 -0.305793 0.188237		C 2.952668 -0.302545 0.140225
	C 2.747904 2.045809 0.694593		C 2.768502 2.054184 0.642873
	C 3.501946 0.916458 0.691408		C 3.512735 0.918440 0.625671
	C 1.165525 -1.512837 -0.912325		C 1.125414 -1.502507 -0.914628
	C 3.800994 -1.424421 -0.026885		C 3.776465 -1.432913 -0.072811
A5-p-TS-1			

	H 4.834819 -1.363697 0.297018 C 3.338115 -2.547735 -0.671797 C 2.014412 -2.572231 -1.148538 C -1.584883 -0.368428 0.189022 C -2.748250 2.045330 -0.695152 H -3.182316 2.998531 -0.977875 C -3.502163 0.915893 -0.691578 C -2.961179 -0.306147 -0.188091 C -3.800842 -1.424803 0.027540 C -1.165223 -1.512590 0.912625 H -4.834727 -1.364329 -0.296219 C -3.337716 -2.547840 0.672771 C -2.013936 -2.572018 1.149318 H 4.543492 0.942176 0.993368 H 3.181812 2.999124 0.977170 H 1.172259 4.171184 0.394292 H -1.172814 4.170975 -0.395408 H -4.543756 0.941421 -0.993391 H -3.994977 -3.392545 0.845157 H -1.658839 -3.424840 1.716783 H 1.659514 -3.425277 -1.715792 H 3.995510 -3.392411 -0.843814 H -0.159679 -1.550328 1.305452 H 0.160080 -1.550830 -1.305356		H 4.816100 -1.379958 0.233260 C 3.288523 -2.561371 -0.690286 C 1.957760 -2.576620 -1.145961 C -1.577709 -0.340446 0.182826 C -2.752202 2.078960 -0.651785 H -3.191107 3.035800 -0.913788 C -3.503134 0.947080 -0.672193 C -2.959142 -0.285509 -0.198965 C -3.786067 -1.421984 -0.024751 C -1.200728 -1.502339 0.876730 H -4.817043 -1.362993 -0.356874 C -3.321013 -2.561379 0.590790 C -2.003077 -2.584641 1.098329 H 4.560017 0.936421 0.907771 H 3.215303 3.004124 0.916364 H 1.193293 4.188027 0.389279 H -1.168074 4.202903 -0.347604 H -4.544483 0.975673 -0.974680 H -3.970713 -3.418553 0.729183 H -1.645496 -3.433300 1.671649 H 1.584211 -3.433861 -1.694613 H 3.932313 -3.417249 -0.858314 H 0.117927 -1.531358 -1.301437 H -0.014605 -1.542358 1.700840 H 0.609162 -1.618803 2.294785
A5-p-TS-2	C 0.746417 0.799919 0.054233 C 1.407338 2.018595 0.361049 C 0.710262 3.254432 0.261724 C -0.584621 3.285382 -0.159533 C -1.321294 2.078110 -0.310828 C -0.697812 0.826453 -0.061658 C -1.578933 -0.313548 0.156517 C -2.956552 -0.222473 -0.215656 C -2.702823 2.135982 -0.673700 C -3.475816 1.019660 -0.692927 C -1.174962 -1.484870 0.858826 C -3.823664 -1.326333 -0.024099 H -4.856636 -1.235075 -0.345309 C -3.389161 -2.482163 0.592220 C -2.069837 -2.496486 1.038322 C 1.590290 -0.359415 -0.209724 C 2.788362 2.015976 0.731598 H 3.236628 2.955660 1.036390 C 3.523103 0.874162 0.708768 C 2.964927 -0.328056 0.177321 C 3.786906 -1.456201 -0.055784 C 1.156112 -1.480954 -0.959765 H 4.819339 -1.420241 0.275986 C 3.308922 -2.557732 -0.726625 C 1.988342 -2.549655 -1.212368 H -4.516706 1.069762 -0.993590 H -3.121255 3.101680 -0.936455 H -1.092822 4.228857 -0.326543 H 1.248859 4.172557 0.470002 H 4.563078 0.875854 1.017039 H 3.952461 -3.410277 -0.911355 H 1.622790 -3.384974 -1.798743 H -4.054189 -3.324268 0.746774 H 0.153185 -1.493442 -1.360927 H -0.173512 -1.558494 1.259758 H -1.605978 -3.701384 1.800732 H -1.348279 -4.380925 2.238776	A5-p-P-1	C 0.742726 0.782975 0.120975 C 1.440731 2.005316 0.307383 C 0.747457 3.244260 0.231529 C -0.572136 3.275919 -0.103660 C -1.318617 2.071904 -0.223996 C -0.701380 0.819285 0.031773 C -1.580189 -0.328883 0.199626 C -2.937228 -0.241893 -0.235488 C -2.695509 2.132965 -0.605952 C -3.456003 1.010876 -0.684420 C -1.199805 -1.505280 0.893565 C -3.783965 -1.369855 -0.126400 H -4.801325 -1.290009 -0.495036 C -3.350275 -2.529743 0.475082 C -2.058627 -2.577900 1.026876 C 1.550660 -0.406765 -0.102687 C 2.857218 2.011516 0.504622 H 3.337063 2.962727 0.709334 C 3.595680 0.875146 0.414726 C 2.977137 -0.359202 0.054266 C 3.752654 -1.517835 -0.197990 C 1.067540 -1.625974 -0.577003 H 4.826194 -1.457199 -0.055062 C 3.180655 -2.690913 -0.636912 C 1.780334 -2.751899 -0.842602 H -4.487260 1.059862 -1.017253 H -3.113192 3.102519 -0.855535 H -1.082597 4.220470 -0.257900 H 1.305943 4.162645 0.376323 H 4.670264 0.897740 0.562183 H 3.794506 -3.563000 -0.835549 H 1.308774 -3.659813 -1.203019 H -1.737279 -3.454292 1.578196 H -4.013711 -3.382508 0.564307 H -0.241730 -1.543270 1.389136
A5-p-P-2	C -0.704086 0.768089 -0.052382 C -1.328849 2.016506 -0.311576 C -0.593275 3.226138 -0.173878 C 0.704513 3.202225 0.238740 C 1.404768 1.968554 0.342131 C 0.741031 0.745922 0.054119 C 1.585048 -0.411975 -0.209268 C 2.968120 -0.376142 0.154592 C 2.789667 1.972132 0.695931 C 3.528054 0.832807 0.669797	A5-a	C -3.652531 1.724671 -0.000049 C -3.715639 0.288279 -0.000016 C -4.960989 -0.374421 0.000014 C -1.222406 1.658919 -0.000055 C 0.000003 2.333022 -0.000057 C 1.222410 1.658920 -0.000034 C 1.229744 0.226913 -0.000010 C 0.000003 -0.439104 0.000003 C -1.229742 0.226911 -0.000023 C 2.466284 2.377602 -0.000024

	C 1.139191 -1.549217 -0.947541 C 3.802866 -1.496635 -0.080981 H 4.840319 -1.445585 0.235096 C 3.332702 -2.622308 -0.731572 C 2.012315 -2.567186 -1.154858 C -1.582026 -0.372957 0.177669 C -2.711648 2.069497 -0.671563 H -3.132218 3.032663 -0.940304 C -3.481636 0.950900 -0.682671 C -2.957739 -0.285678 -0.197239 C -3.812840 -1.395201 0.003698 C -1.178080 -1.532546 0.885350 H -4.845956 -1.315844 -0.318232 C -3.364877 -2.533553 0.632674 C -2.041437 -2.583118 1.107802 H 4.572116 0.841121 0.963396 H 3.239266 2.914888 0.988615 H 1.242736 4.123101 0.435118 H -1.104432 4.167215 -0.345566 H -4.523047 0.995517 -0.982673 H -4.033545 -3.371524 0.793235 H -1.697734 -3.449054 1.662082 H 3.971050 -3.478085 -0.917672 H -0.173180 -1.590120 1.277345 H 0.133924 -1.581821 -1.344300		C 2.512775 -0.473121 0.000018 C 3.715642 0.288276 0.000031 C 3.652536 1.724670 0.000010 C 4.960988 -0.374427 0.000062 H 2.432807 3.461966 -0.000040 H 0.000003 3.418779 -0.000073 H 0.000005 -1.518859 0.000048 C -2.512774 -0.473120 -0.000013 C -2.466278 2.377602 -0.000071 H -2.432800 3.461966 -0.000100 C -5.036131 -1.751898 0.000048 C -2.623494 -1.879509 -0.000008 C 2.623486 -1.879506 0.000030 C 5.036124 -1.751906 0.000064 H -1.731694 -2.492719 -0.000036 H 6.000073 -2.247749 0.000072 C -3.854317 -2.507924 0.000022 C 3.854310 -2.507927 0.000044 H -4.585638 2.278218 -0.000064 H -5.867167 0.222484 0.000007 H -6.000081 -2.247738 0.000095 H -3.904424 -3.590931 0.000020 H 1.731683 -2.492713 0.000005 H 3.904408 -3.590934 0.000043 H 5.867170 0.222473 0.000072 H 4.585644 2.278214 0.000025
A5-a-TS-1	C -3.654540 1.741812 0.026715 C -3.722572 0.305986 0.033341 C -4.968667 -0.353954 0.038272 C -1.224014 1.671605 -0.037725 C 0.000001 2.342766 -0.053966 C 1.224016 1.671606 -0.037729 C 1.240352 0.234393 0.016187 C 0.000001 -0.391363 0.086464 C -1.240351 0.234392 0.016188 C 2.467560 2.390947 -0.029620 C 2.523020 -0.460081 0.000793 C 3.722573 0.305986 0.033336 C 3.654542 1.741812 0.026703 C 4.968668 -0.353956 0.038267 H 2.431228 3.474938 -0.056701 H 0.000000 3.428070 -0.069026 C -2.523019 -0.460081 0.000790 C -2.467558 2.390947 -0.029610 H -2.431226 3.474938 -0.056689 C -5.045885 -1.731092 -0.009661 C -2.633891 -1.863772 -0.084229 C 2.633889 -1.863773 -0.084215 C 5.045884 -1.731095 -0.009657 H -1.741308 -2.466218 -0.170517 H 6.010988 -2.224753 -0.008514 C -3.867453 -2.488158 -0.082543 C 3.867451 -2.488160 -0.082528 H -4.585279 2.298818 0.047625 H -5.873619 0.243826 0.070592 H -6.010990 -2.224750 -0.008520 H -3.921692 -3.568860 -0.148974 H 1.741305 -2.466219 -0.170493 H 3.921689 -3.568862 -0.148949 H 5.873620 0.243824 0.070581 H 4.585281 2.298817 0.047609 H 0.000009 -1.657082 0.715063 H -0.000036 -2.367093 1.233485	A5-a-TS-2	C -3.636124 -1.765242 -0.000043 C -3.708018 -0.329178 -0.000023 C -4.957002 0.328332 -0.000035 C -1.205196 -1.690930 -0.000012 C 0.019618 -2.360394 -0.000014 C 1.238946 -1.680382 -0.000008 C 1.240658 -0.248275 -0.000003 C 0.009326 0.415060 0.000001 C -1.214852 -0.259607 0.000003 C 2.485952 -2.393880 -0.000010 C 2.520374 0.457336 -0.000003 C 3.726258 -0.298632 -0.000004 C 3.669078 -1.735358 -0.000008 C 4.968613 0.369617 -0.000003 H 2.457366 -3.478368 -0.000013 H 0.024133 -3.446073 -0.000024 H -0.002679 1.493431 0.000003 C -2.498128 0.434466 0.000011 C -2.446943 -2.412783 -0.000033 H -2.410300 -3.496997 -0.000045 C -5.048251 1.704850 -0.000009 C -2.667783 1.823947 0.000043 C 2.622802 1.864406 -0.000001 C 5.036455 1.747436 -0.000001 H 5.997894 2.248170 0.000000 C -3.870845 2.476890 0.000043 C 3.850927 2.497948 0.000000 H -4.567066 -2.322425 -0.000066 H -5.858040 -0.275711 -0.000064 H -6.016294 2.193422 -0.000018 H -3.917690 3.560463 0.000088 H 1.727500 2.472507 0.000000 H 3.896073 3.581131 0.000002 H 5.877706 -0.222824 -0.000004 H 4.604594 -2.284876 -0.000009 H -1.582048 2.816366 0.000205 H -1.046340 3.488029 0.000600
A5-a-TS-3	C 3.595018 -1.816767 -0.000039 C 3.682669 -0.381171 -0.000027 C 4.943694 0.254273 -0.000030 C 1.166150 -1.712308 -0.000022 C -0.067444 -2.365711 -0.000020 C -1.278200 -1.670963 -0.000006 C -1.262421 -0.238879 0.000006 C -0.022113 0.406725 0.000004 C 1.195687 -0.280718 -0.000010 C -2.533816 -2.369139 -0.000004	A5-a-P-1	C -3.662428 1.706003 -0.000043 C -3.715561 0.268136 -0.000022 C -4.945587 -0.422313 -0.000019 C -1.226237 1.676891 -0.000030 C 0.000000 2.349571 -0.000034 C 1.226237 1.676891 -0.000018 C 1.239949 0.236278 0.000004 C 0.000000 -0.362889 0.000006 C -1.239949 0.236278 -0.000009 C 2.482721 2.374875 -0.000023

	C -2.533651 0.482418 0.000021 C -3.748531 -0.259133 0.000022 C -3.708853 -1.696476 0.000009 C -4.982897 0.423736 0.000036 H -2.518278 -3.453862 -0.000014 H -0.085797 -3.451248 -0.000029 H -0.003917 1.486440 0.000012 C 2.489301 0.397220 -0.000013 C 2.398422 -2.450331 -0.000036 H 2.348060 -3.533949 -0.000045 C 5.054763 1.634148 -0.000019 C 2.620320 1.808192 -0.000002 C -2.620755 1.890436 0.000034 C -5.035146 1.802215 0.000049 H 1.746189 2.447534 0.000009 H -5.990695 2.314004 0.000060 C 3.870792 2.359795 -0.000006 C -3.841078 2.538841 0.000048 H 4.518617 -2.385757 -0.000050 H 5.837684 -0.361625 -0.000041 H 6.023424 2.120871 -0.000022 H -1.719152 2.489136 0.000034 H -3.873533 3.622464 0.000058 H -5.898732 -0.158174 0.000037 H -4.650957 -2.234543 0.000010 H 3.964072 3.856617 0.000007 H 4.011567 4.703670 0.000013		C 2.505983 -0.475969 0.000020 C 3.715561 0.268136 0.000014 C 3.662428 1.706003 -0.000007 C 4.945587 -0.422313 0.000030 H 2.465688 3.459811 -0.000039 H 0.000000 3.434893 -0.000051 C -2.505983 -0.475969 -0.000006 C -2.482721 2.374875 -0.000047 H -2.465687 3.459811 -0.000063 C -4.985031 -1.802504 0.000001 C -2.571162 -1.882767 0.000015 C 2.571162 -1.882767 0.000041 C 4.985031 -1.802504 0.000051 H -1.646413 -2.448714 0.000028 H 5.937796 -2.319682 0.000063 C -3.787867 -2.537155 0.000018 C 3.787867 -2.537155 0.000057 H -4.599801 2.252382 -0.000056 H -5.867033 0.150694 -0.000031 H -5.937796 -2.319682 0.000004 H -3.818921 -3.620840 0.000034 H 1.646413 -2.448714 0.000045 H 3.818921 -3.620840 0.000073 H 5.867033 0.150694 0.000026 H 4.599801 2.252382 -0.000012
A5-a-P-2	C -3.679999 1.694800 -0.000047 C -3.733715 0.257257 -0.000021 C -4.959754 -0.443459 -0.000013 C -1.242176 1.658174 -0.000036 C -0.019319 2.331536 -0.000042 C 1.201571 1.651619 -0.000025 C 1.211835 0.217610 0.000001 C -0.016995 -0.448652 0.000008 C -1.237289 0.229795 -0.000010 C 2.446224 2.369448 -0.000031 C 2.494901 -0.480862 0.000019 C 3.697289 0.280607 0.000012 C 3.632822 1.716867 -0.000013 C 4.942388 -0.382494 0.000030 H 2.413140 3.453826 -0.000050 H -0.014728 3.417235 -0.000061 H -0.050157 -1.530539 0.000028 C -2.506662 -0.475674 -0.000003 C -2.497595 2.359054 -0.000054 H -2.478969 3.443826 -0.000074 C -5.004273 -1.824296 0.000011 C -2.642399 -1.858585 0.000023 C 2.603203 -1.887343 0.000042 C 5.016097 -1.760112 0.000054 H 5.979751 -2.256570 0.000068 C -3.803300 -2.570578 0.000032 C 3.833934 -2.515882 0.000060 H -4.617012 2.241953 -0.000061 H -5.882711 0.126408 -0.000028 H -5.957158 -2.342455 0.000016 H -3.820927 -3.654745 0.000051 H 1.709741 -2.498046 0.000047 H 3.883853 -3.598871 0.000078 H 5.849058 0.213657 0.000025 H 4.565390 2.271346 -0.000018	A5-a-P-3	C -3.700216 1.647439 -0.000044 C -3.745745 0.209750 -0.000019 C -4.988694 -0.460864 -0.000012 C -1.269712 1.616053 -0.000034 C -0.055755 2.305390 -0.000040 C 1.175143 1.646915 -0.000023 C 1.201873 0.214888 0.000001 C -0.018818 -0.466956 0.000008 C -1.256497 0.184060 -0.000010 C 2.409428 2.382000 -0.000028 C 2.493972 -0.468256 0.000018 C 3.686421 0.309158 0.000014 C 3.604045 1.744575 -0.000010 C 4.940557 -0.336650 0.000031 H 2.361737 3.465783 -0.000046 H -0.069568 3.391006 -0.000058 H -0.005457 -1.546783 0.000028 C -2.528777 -0.532166 -0.000003 C -2.523295 2.316988 -0.000051 H -2.505606 3.401586 -0.000069 C -5.063341 -1.845777 0.000009 C -2.616376 -1.949385 0.000020 C 2.623275 -1.872960 0.000038 C 5.034016 -1.712999 0.000052 H -1.724983 -2.564108 0.000032 H 6.004460 -2.195937 0.000066 C -3.853695 -2.517544 0.000025 C 3.862454 -2.484754 0.000055 H -4.640257 2.188865 -0.000056 H -5.900155 0.129148 -0.000025 H -6.017078 -2.360416 0.000015 H 1.739979 -2.498341 0.000040 H 3.926996 -3.566955 0.000071 H 5.838650 0.272298 0.000028 H 4.529722 2.310429 -0.000013
A2R5	C -2.386699 0.320693 0.000046 C -1.160109 0.949932 0.000238 C 0.000000 0.140288 0.000022 C -0.000002 -1.253900 -0.000208 C -1.281320 -1.877466 -0.000376 C -2.425544 -1.102630 -0.000279 H -3.317313 0.878559 0.000195 C 1.160112 0.949933 0.000075 C 1.281322 -1.877467 -0.000245 H -1.358948 -2.959622 -0.000586 H -3.393152 -1.592278 -0.000403	A2R5-TS-1	C 2.345714 -0.418349 0.000027 C 1.347950 0.530912 0.000032 C -0.001366 0.089982 0.000001 C -0.393115 -1.248367 -0.000033 C 0.658947 -2.208659 -0.000037 C 1.976962 -1.792650 -0.000008 H 3.394880 -0.144536 0.000049 C -0.889200 1.194167 0.000012 C -1.798730 -1.486546 -0.000059 H 0.425444 -3.268102 -0.000063 H 2.764773 -2.537550 -0.000012

	C 2.425542 -1.102633 -0.000084 C 2.386698 0.320695 0.000066 H 1.358946 -2.959623 -0.000391 H 3.393152 -1.592277 -0.000119 H 3.317316 0.878555 0.000100 C 0.680573 2.342157 0.000012 C -0.680572 2.342156 0.000741 H 1.314982 3.218073 0.001230 H -1.314982 3.218072 -0.000077		C -2.678682 -0.422037 -0.000050 C -2.242401 0.934075 -0.000014 H -2.176544 -2.503466 -0.000086 H -3.744904 -0.619746 -0.000070 H -2.978821 1.730578 -0.000009 C -0.040892 2.407144 0.000051 C 1.245307 1.991152 0.000062 H -0.399095 3.426960 0.000068 H 2.451725 2.974649 0.000103 H 3.079577 3.516268 0.000125
A2R5-TS-2	C -2.309346 0.038043 0.000019 C -1.195235 0.827886 0.000154 C 0.043568 0.128615 0.000025 C 0.182015 -1.259545 -0.000223 C -1.024560 -2.018863 -0.000351 C -2.248663 -1.369615 -0.000231 C 1.114566 1.052640 0.000182 C 1.520354 -1.748980 -0.000318 H -0.987015 -3.103376 -0.000543 H -3.166801 -1.947219 -0.000329 C 2.580894 -0.862744 -0.000167 C 2.398294 0.548474 0.000084 H 1.706585 -2.817655 -0.000509 H 3.592747 -1.252370 -0.000242 H 3.267538 1.197838 0.000194 C 0.499868 2.389167 0.000419 C -0.855073 2.258610 0.000403 H 1.044757 3.323200 0.000580 H -1.574594 3.065049 0.000547 H -3.667805 0.651441 0.000130 H -4.455502 0.980960 0.000188	A2R5-TS-3	C 2.252219 0.725359 -0.000040 C 0.933887 1.144058 -0.000145 C -0.080484 0.154704 -0.000026 C 0.137282 -1.223967 0.000192 C 1.506602 -1.642661 0.000298 C 2.463973 -0.666879 0.000178 H 3.088740 1.416533 -0.000120 C -1.354661 0.768836 -0.000160 C -1.029054 -2.042253 0.000281 H 1.767679 -2.696131 0.000468 C -2.280818 -1.456863 0.000151 C -2.466685 -0.045523 -0.000072 H -0.934895 -3.122829 -0.000448 H -3.158889 -2.093230 0.000220 H -3.473281 0.359071 -0.000166 C -1.105946 2.220466 -0.000374 C 0.236655 2.441467 -0.000365 H -1.873805 2.982074 -0.000515 H 0.722534 3.407401 -0.000497 H 3.888110 -1.125442 0.000294 H 4.695990 -1.387911 0.000362
A2R5-TS-4	C 2.243211 0.864991 0.000012 C 0.909870 1.216411 -0.000130 C -0.059362 0.184438 -0.000029 C 0.221532 -1.187081 0.000207 C 1.604394 -1.476288 0.000341 C 2.585181 -0.523170 0.000255 H 3.035131 1.606932 -0.000054 C -1.362640 0.735905 -0.000208 C -0.902150 -2.061922 0.000269 H 3.631399 -0.810907 0.000370 C -2.179029 -1.534369 0.000097 C -2.432412 -0.133299 -0.000145 H -0.754437 -3.135583 0.000449 H -3.026045 -2.211332 0.000146 H -3.457719 0.221335 -0.000274 C -1.180900 2.197223 -0.000433 C 0.150555 2.478418 -0.000386 H -1.983080 2.922505 -0.000606 H 0.590052 3.466516 -0.000517 H 2.049193 -2.912330 0.000612 H 2.326006 -3.714678 0.000770	A2R5-P-1	C 2.367856 0.595989 0.000016 C 1.086983 1.100599 -0.000132 C -0.000726 0.185902 -0.000033 C 0.139511 -1.201419 0.000202 C 1.475240 -1.695987 0.000349 C 2.541190 -0.815990 0.000257 H 3.236191 1.245122 -0.000049 C -1.239478 0.875978 -0.000202 C -1.073745 -1.950936 0.000266 H 1.656253 -2.765642 0.000534 H 3.550849 -1.211064 0.000371 C -2.288715 -1.295213 0.000102 C -2.394766 0.126031 -0.000134 H -1.041221 -3.035262 0.000445 H -3.202617 -1.878972 0.000155 H -3.376799 0.586744 -0.000252 C -0.912392 2.322958 -0.000414 C 0.433246 2.406523 -0.000381 H -1.627880 3.132463 -0.000576
A2R5-P-2	C 2.318022 0.611066 0.000110 C 1.063708 1.137073 0.000028 C 0.023658 0.160850 0.000019 C 0.216198 -1.221509 0.000159 C 1.566418 -1.680181 0.000273 C 2.606972 -0.762285 0.000227 C -1.234768 0.807029 -0.000185 C -0.969295 -2.011318 0.000171 H 1.782866 -2.743617 0.000376 H 3.635265 -1.106956 0.000300 C -2.209304 -1.399946 0.000014 C -2.363754 0.013666 -0.000183 H -0.898795 -3.093838 0.000292 H -3.100695 -2.017271 0.000015 H -3.361199 0.440775 -0.000341 C -0.954084 2.249888 -0.000407 C 0.393548 2.444791 -0.000018 H -1.704447 3.028461 -0.000686 H 0.903101 3.397705 -0.001216	A2R5-P-3	C -2.461045 -0.149913 -0.000043 C -1.360051 0.691696 0.000047 C -0.069736 0.104710 -0.000005 C 0.196250 -1.266143 -0.000198 C -0.950332 -2.129993 -0.000328 C -2.168467 -1.521611 -0.000232 H -3.482753 0.214803 -0.000018 C 0.919717 1.115412 0.000192 C 1.571295 -1.637716 -0.000243 H -0.838433 -3.209272 -0.000472 C 2.548814 -0.660661 -0.000081 C 2.242869 0.729304 0.000149 H 1.851015 -2.685723 -0.000402 H 3.591069 -0.960275 -0.000113 H 3.051052 1.452994 0.000296 C 0.192812 2.396467 0.000447 C -1.145175 2.148749 0.000162 H 0.656638 3.373508 0.000657 H -1.930297 2.892160 0.000861
A2R5-P-4	C -2.429230 0.065768 -0.000146 C -1.258019 0.794075 0.000117		

C	-0.026180	0.096243	0.000018		
C	0.115775	-1.299195	-0.000219		
C	-1.124703	-1.964356	-0.000421		
C	-2.348030	-1.364570	-0.000422		
H	-3.404968	0.540946	0.000005		
C	1.055840	1.008993	0.000191		
C	1.447955	-1.801045	-0.000212		
H	-3.261234	-1.950095	-0.000517		
C	2.509896	-0.917226	0.000006		
C	2.335152	0.495656	0.000228		
H	1.623120	-2.870363	-0.000387		
H	3.519997	-1.311397	-0.000044		
H	3.208999	1.138681	0.000266		
C	0.449297	2.350522	-0.000025		
C	-0.905785	2.224069	0.000817		
H	1.000515	3.280900	-0.000165		
H	-1.618226	3.037717	0.001247		