Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Exploring the Mechanism of Graphene-Oxide Reduction by Hydrazine in a Multi-Epoxide Environment with DFT Calculations

*Nguyen Tri Hieu, Dénes Szieberth, Eszter Makkos**

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Table S1: Comparison of Electronic Energy Profiles for Hydrazine Reduction via Route 1 using Various Basis Sets at the PBE-D Level (Values in brackets represent differences from the def2-TZVP basis set)

Species	def2-QZVP (kcal/mol)	def2-TZVPP (kcal/mol)	def2-TZVP (kcal/mol)	def2-TZVP and def2-SVP (kcal/mol)	def2-SVP (kcal/mol)
2b + N2H4	0.0 (0.0)	0.0 (0.0)	0.0	0.0 (0.0)	0.0 (0.0)
SC1	-7.7 (0.8)	-8.4 (0.1)	-8.5	-8.7 (-0.2)	-12.1 (-3.6)
ts0	16.3 (1.0)	15.6 (0.3)	15.3	15.8 (0.5)	13.5 (-1.8)
int0	0.1 (0.7)	-0.6 (0.0)	-0.6	-0.5 (0.1)	-3.4 (-2.8)
ts1	8.6 (0.8)	7.6 (-0.2)	7.8	7.7 (-0.1)	1.8 (-6.0)
int1	-17.8 (1.1)	-18.9 (0.0)	-18.9	-19.5 (-0.6)	-28.3 (-9.4)
ts2	-1.8 (0.7)	-2.9 (-0.4)	-2.5	-2.7 (-0.2)	-9.5 (-7.0)
3E + H2O + N2H2	-21.5 (-1.7)	-20.9 (-1.1)	-19.8	-19.7 (0.1)	-12.4 (7.4)
SC1'	0.0 (0.0)	0.0 (0.0)	0.0	0.0 (0.0)	0.0 (0.0)
ts3	19.0 (0.5)	18.8 (0.3)	18.5	18.4 (-0.1)	16.6 (-1.9)
int3	7.9 (0.2)	7.6 (-0.1)	7.7	6.7 (-1.0)	2.6 (-5.1)
ts4	11.1 (0.2)	10.8 (-0.1)	10.9	10.4 (-0.5)	8.2 (-2.7)
2E + H2O + N2H2	-9.2 (-2.2)	-7.9 (-0.9)	-7.0	-6.2 (0.8)	3.4 (10.4)

Table S2: Reaction Profiles of Hydrazine Reduction via Route 1 in Vacuum and Water Solvent at the PBE-D/Def2TZVP Level

	Condition	
Species	In vacuum (kcal/mol)	In water (kcal/mol)
2b + N2H4	0.0	0.0 (0.0)
SC1	-8.5	-6.0 (2.5)
ts0	15.3	14.4 (-0.9)
int0	-0.6	1.8 (2.4)
ts1	7.8	8.6 (0.8)
int1	-18.9	-16.0 (2.9)
ts2	-2.5	-2.5 (0.0)
3E + H2O + N2H2	-19.8	-23.9 (-4.1)
SC1'	0.0	0.0 (0.0)
ts3	18.5	16.4 (-2.1)
int3	7.7	6.8 (-0.9)
ts4	10.9	9.4 (-1.5)
2E + H2O + N2H2	-7.0	-13.2 (-6.2)

Table S3: Basis Set Superposition Error of Various Starting Complexes at the PBE-D/def2-TZVP Level (Values in brackets represent differences compared to def2-TZVP)

	Species	def2TZVP (kcal/mol)	BSSE (kcal/mol)
	2b+N2H4	0.0	0.0 (0.0)
Route 1	SC1	-8.5	-7.2 (1.3)
	int0	-0.6	0.8 (1.4)
Route 2	SC2	-9.2	-7.9 (1.3)
Route 3	SC3	-8.2	-7.2 (1.0)

Table S4: Geometrical Parameters of Different Starting Complexes

Species	O-H	C-O1-C	C-O2-C	C-O3-C	C-O1-C-C	C-O2-C-C	C-O3-C-C	H-N-N-H
SC1	2.23Å	63.0°	63.1°	61.3°	109.9°	110.0°	-109.4°	154.8°
SC1'	2.27Å	N/A	61.4°	61.7°	N/A	110.7°	-107.5°	148.9°
SC2	2.75Å	63.2°	63.2°	61.4°	109.7°	109.5°	-109.8°	153.9°
SC2'	2.44Å	61.5°	61.6°	N/A	111.2°	111.4°	N/A	-144.0°
SC3	2.50Å	62.9°	63.0°	61.8°	109.9°	110.1°	-109.2°	148.8°
SC3'	2.14Å	N/A	60.9°	60.4°	N/A	111.9°	-110.8°	-150.9°

Table S5: Formation Energies in kcal/mol calculated with different reference molecules for the chemical potential of O and H atoms.

Ref1

$$E_f = E_{nE} - (E_{PAH} + n/2\, E_{O_2}) \quad \text{Eq. 1}$$

$$E_f = E_{2E\_2OH} - (E_{PAH} + 2E_{O_2} + E_{H_2}) \quad \text{Eq.2}$$

$$E_f = E_{3E\_1OH\_N_2H_3} - (E_{PAH} + 2E_{O_2} + E_{N_2H_4}) \quad \text{Eq.3}$$

Ref2

$$E_f = E_{2E\_2OH} - (E_{PAH} + 2E_{OH^-} + E_{O_2}) \quad \text{Eq.4}$$

$$E_f = E_{3E\_1OH\_N_2H_3} - \left(E_{PAH} + 1.5E_{O_2} + E_{N_2H_3^-} + E_{OH^-}\right) \quad \text{Eq.5}$$

Ref3

$$E_f = E_{2E\_2OH} - (E_{PAH} + E_{H_2O} + 1.5E_{O_2}) \quad \text{Eq.6}$$

$$E_f = E_{3E\_1OH\_N_2H_3} - \left(E_{PAH} + 1.5E_{O_2} + E_{N_2H_2} + E_{H_2O}\right) \quad \text{Eq.7}$$

	Ref 1	Ref 2	Ref 3
4E	46.8	-	-
3E	43.8	-	-
2E	44.8	-	-
2E_2OH	-42.7	-20.4	11.5
2E_op	28.0	-	-
3E_1OH_N_2H_3	17.6	-22.4	34.4

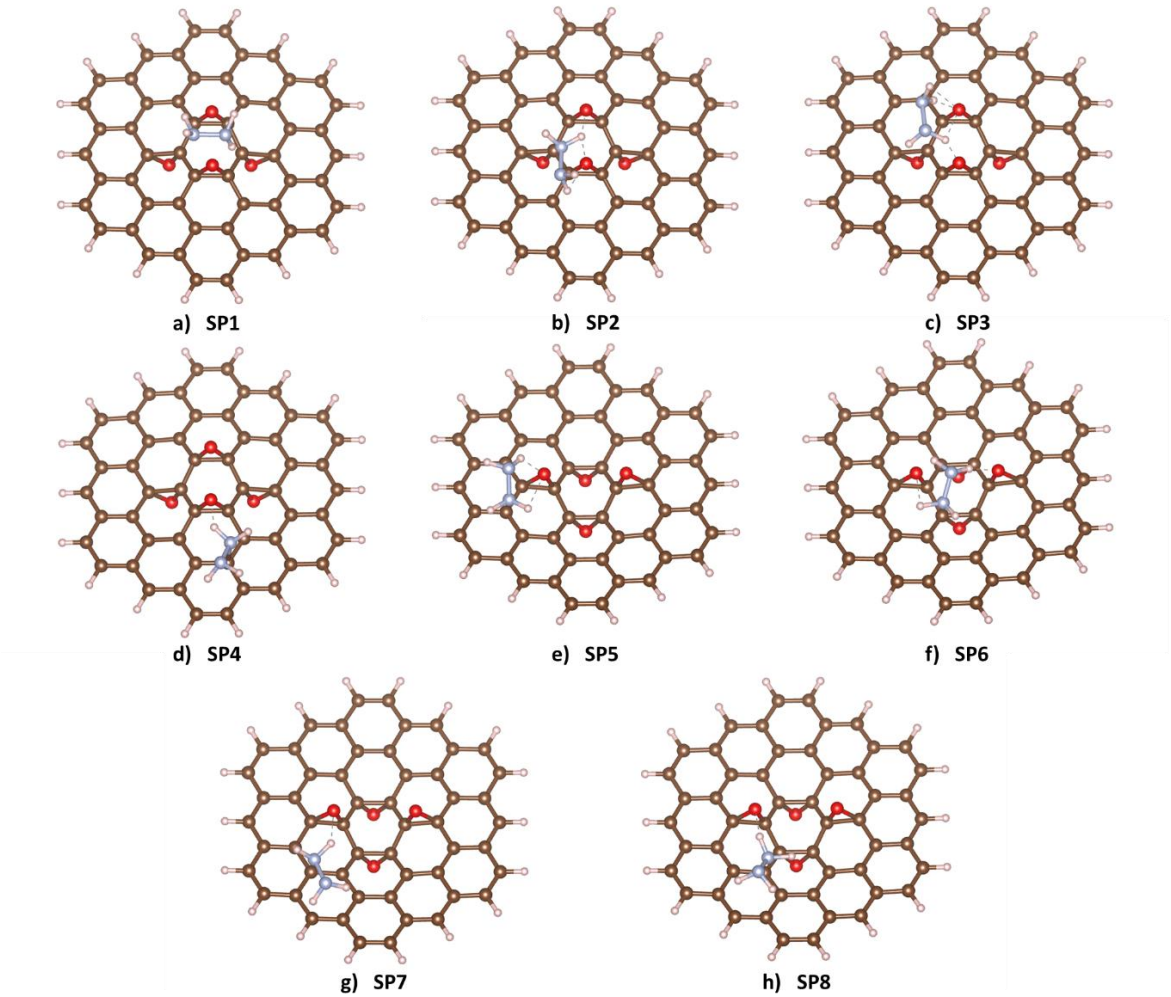

Figure S1: Ball and stick images of the eight different starting positions for the hydrazine to attack the 4E polycyclic aromatic hydrocarbon (red: oxygen, white: hydrogen, brown: carbon)

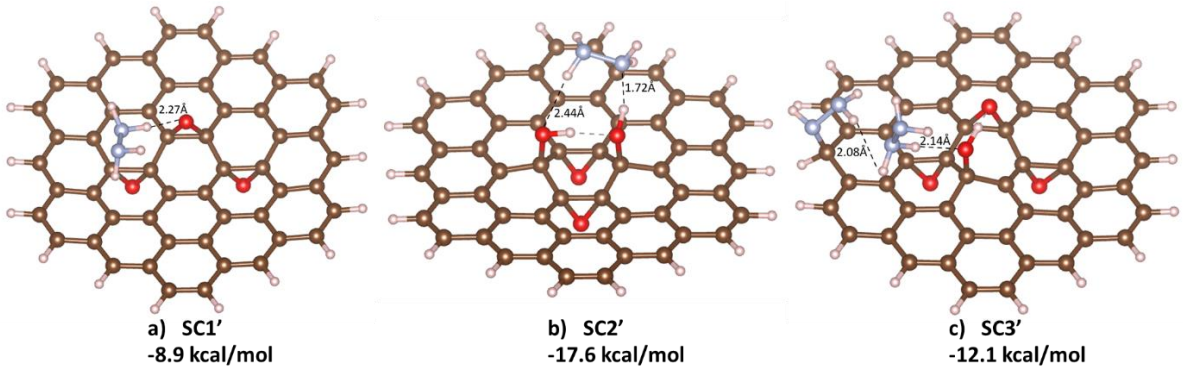

Figure S2: Ball and stick images of the following structures: The optimised starting complexes a) SC1', b) SC2', c) SC3' and their respective interaction energy (red: oxygen, white: hydrogen, brown: carbon)

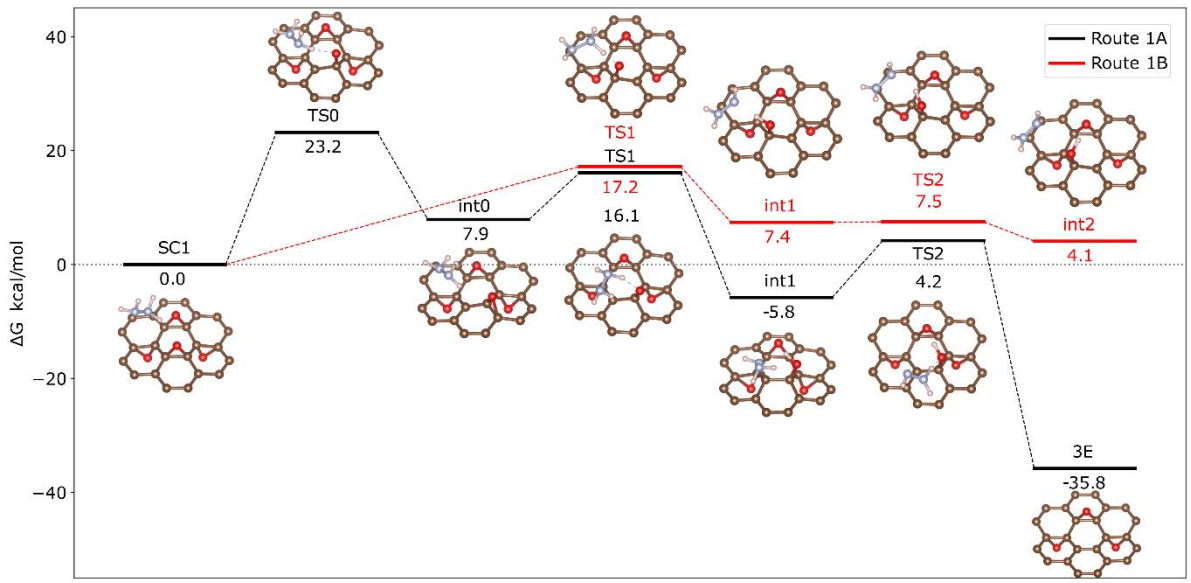

Figure S3 Alternative pathways for Route 1 with (A) and without (B) epoxy migration. Gibbs free energies are calculated at 298 K. The optimised geometries of each reaction step are visualised by ball and stick images of the inner part of the original PAH molecules. (red: oxygen, white: hydrogen, brown: carbon, blue: nitrogen)

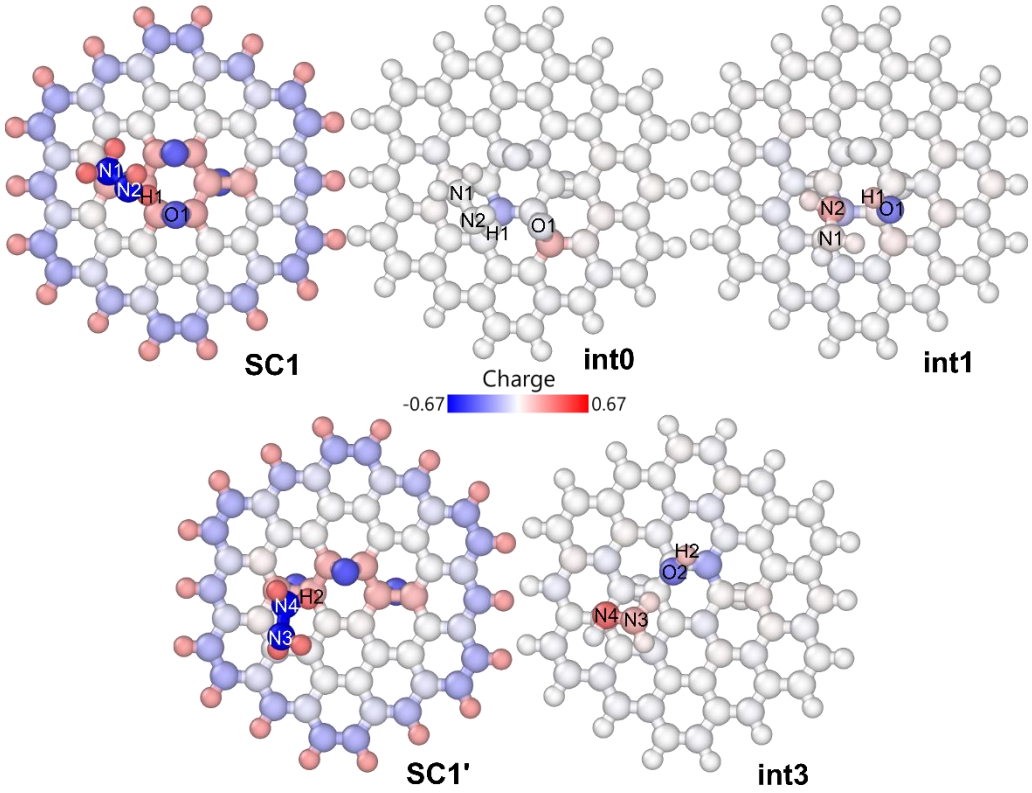

Figure S4: Structure images of the starting complexes and intermediates of Route 1 coloured by the charge transfer within the intermediates referenced to the absolute natural atomic charges of the starting complexes.

Table S6: Calculated natural atomic charges (a.u.) in hydrazine, diazene, the starting complexes and intermediate structures of Route 1 Figure 3.

	N1	N2	Total (N_2H_4 or derivatives)	O1	H1	Total (OH)
N2H4	-0.66	-0.66	0.00	-	-	-
SC1	-0.67	-0.66	0.03	-0.39	-	-
int0	-0.67	-0.66	0.03	-0.41	-	-
int1	-0.63	-0.46	-0.02	-0.69	0.50	-0.19
	N3	**N4**	**total**	**O2**	**H2**	**Total (OH)**
SC1'	-0.66	-0.67	0.04	-0.42	-	-
int3	-0.48	-0.33	0.30	-0.73	0.48	-0.25
N2H2	-0.27	-0.27	0.00	-	-	-

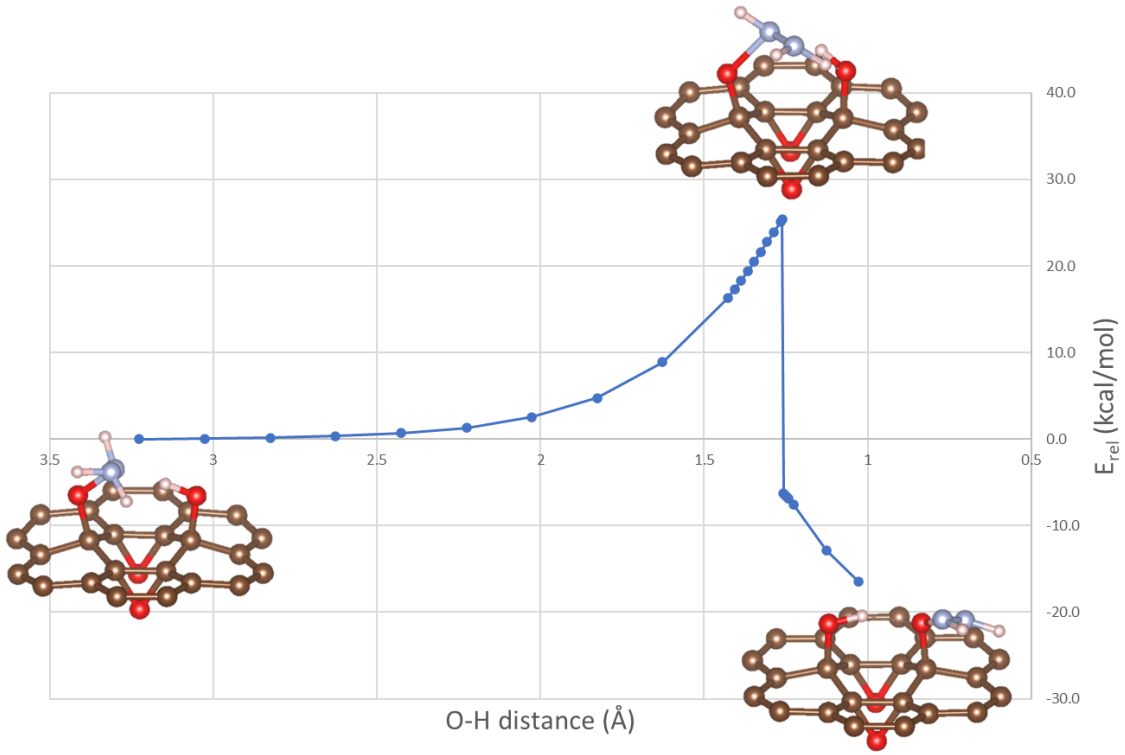

Figure S5: Scan profile of TS2 via Route 2 at the PBE-D Level with a Mixture of Basis Sets (def2-TZVP and def2-SVP)

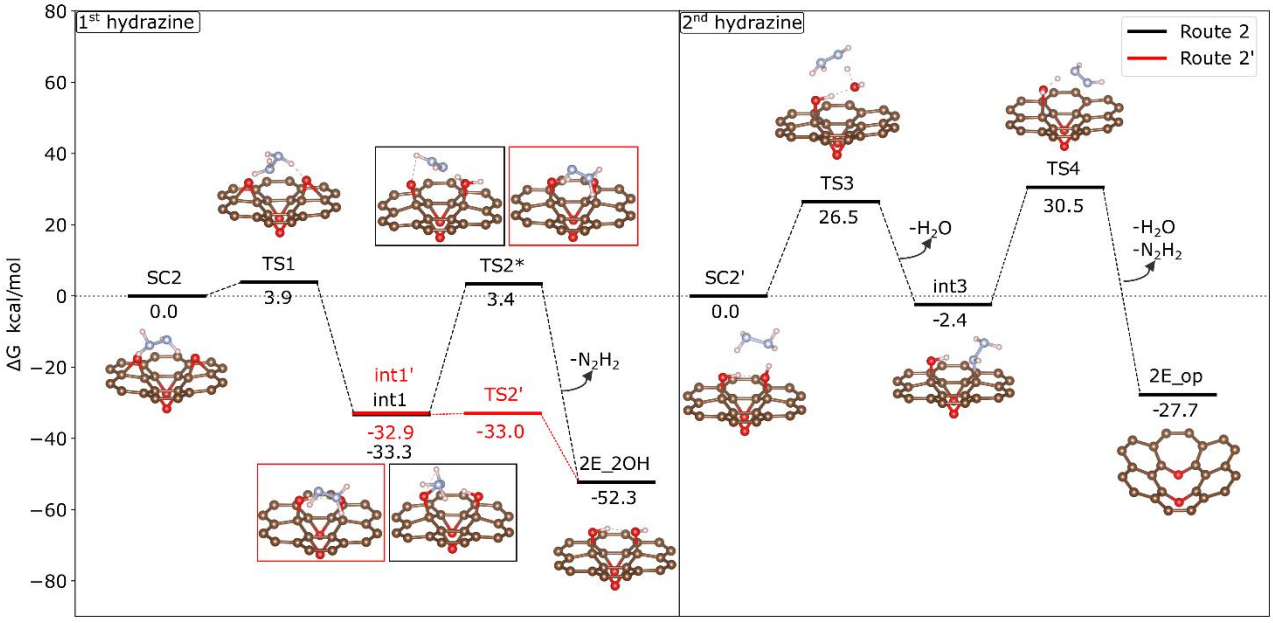

Figure S6: Alternative second protonation step for Route 2. Gibbs free energies are calculated at 298 K. Route 2' represents an analogue pathway where the intermediate structure int1' is energetically almost identical to int1 but does not contain a hydrazinol group (no O-N bond). The second protonation is spontaneous from this structure; the 2E_2OH product forms with a practically zero Gibbs free energy barrier (ΔG(TS2'-int1')= -0.10 kcal·mol^{-1}, the electronic energy difference is ΔE(TS2'-int1')= +0.55 kcal/mol). The optimised geometries of each reaction step are visualised by ball and stick images of the inner part of the original PAH molecules. (red: oxygen, white: hydrogen, brown: carbon, blue: nitrogen)

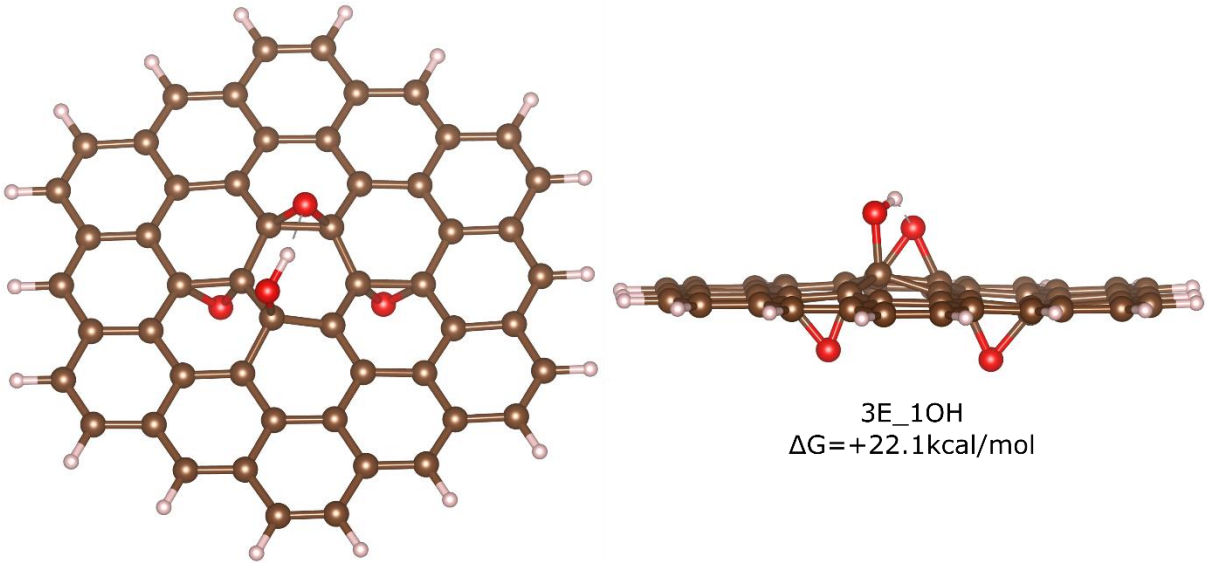

Figure S7: Ball and stick images of 3E_1OH structure (red: oxygen, white: hydrogen, brown: carbon)

Table S7: Calculated Total Energies (E_{tot}), Enthalpies (H), Gibbs Free-Energies (G), and Entropies (S) for Species Concerned in this Study at the Level of PBE-D/def2-TZVP

	species	E_{tot} (a.u.)	H (a.u.)	G (a.u.)	S (cal $K^{-1}mol^{-1}$)
	N_2H_4	-111.7799	-111.7249	-111.7501	55.149
	H_2O	-76.3767	-76.3532	-76.3738	45.152
	N_2H_2	-110.5544	-110.5251	-110.5489	52.216
	4E	-2367.5554	-2366.9950	-2367.0839	189.159
Route 1A	SC1	-2479.3488	-2478.7304	-2478.8325	216.738
	ts0	-2479.3109	-2478.6949	-2478.7955	213.738
	int0	-2479.3363	-2478.7181	-2478.8199	216.184
	ts1	-2479.3228	-2478.7083	-2478.8068	209.340
	int1	-2479.3653	-2478.7466	-2478.8418	202.385
	ts2	-2479.3393	-2478.7277	-2478.8258	208.542
	3E	-2292.4357	-2291.8791	-2291.9669	186.838
	SC1’	-2404.2297	-2403.6147	-2403.7155	214.216
	ts3	-2404.2003	-2403.5924	-2403.6904	208.281
	int3	-2404.2174	-2403.6040	-2403.7012	206.482
	ts4	-2404.2124	-2403.6030	-2403.6997	205.550
	2E	-2217.3098	-2216.7567	-2216.8435	184.586
Route 1B	ts1	-2479.3218	-2478.7070	-2478.8050	208.299
	int1	-2479.3397	-2478.7231	-2478.8207	207.337
	ts2	-2479.3394	-2478.7238	-2478.8205	205.548
	int2	-2479.3451	-2478.7240	-2478.8260	216.685
Route 2	SC2	-2479.3499	-2478.7316	-2478.8337	216.852
	ts1	-2479.3455	-2478.7289	-2478.8275	209.585
	int1	-2479.4115	-2478.7904	-2478.8868	204.813
	ts2	-2479.3473	-2478.8282	-2478.7319	202.700
	2E_2OH	-2368.8639	-2368.2776	-2368.3682	192.656
	SC2’	-2480.6718	-2480.0274	-2480.1269	211.387
	ts3	-2480.6191	-2479.9835	-2480.0847	214.934
	int3	-2404.2810	-2403.6641	-2403.7570	197.546
	ts4	-2404.2145	-2403.6070	-2403.7045	207.252
	2E_op	-2217.3365	-2216.7826	-2216.8686	183.133
	int1’	-2479.4068	-2478.7874	-2478.8861	209.731
	ts2’	-2479.4059	-2478.7882	-2478.8863	208.531
Route 3	SC3	-2479.3483	-2478.7299	-2478.8324	217.747
	ts1	-2479.3233	-2478.7095	-2478.8072	207.600
	int1	-2479.3369	-2478.7200	-2478.8192	210.878
	ts2	-2479.3370	-2478.7211	-2478.8186	207.112
	3E_1OH_N_2H_3	-2479.3817	-2478.7617	-2478.8584	205.515
	SC3’	-2591.1809	-2590.5025	-2590.6101	228.355
	ts3	-2591.1472	-2590.4743	-2590.5805	225.531
	3E_N_2H_3	-2403.6289	-2403.1205	-2403.0245	201.973
	3E_1OH_N_2H_2	-2478.0606	-2477.4668	-2477.5624	203.281
	3E_1OH_N_2H	-2477.0080	-2476.4337	-2476.5263	196.776

Table S8: Calculated Cartesian Coordinates for Species Concerned in this Study at the Level of PBE-D/def2-TZVP

	species	Cartesian coordinates (x, y, z)		
	N_2H_4	N 0.710596	0.100127	0.076494
		N -0.710596	-0.100127	0.076494
		H 1.144907	-0.794567	0.306714
		H 1.064110	0.386855	-0.842172
		H -1.144907	0.794566	0.306715
		H -1.064110	-0.386854	-0.842172
	H_2O	O 0.000000	0.000000	0.119431
		H -0.000000	-0.765881	-0.477724
		H 0.000000	0.765881	-0.477724
	N_2H_2	N 0.121079	-0.621528	0.000000
		N 0.121079	0.621528	-0.000000
		H -0.847555	-1.034067	0.000000
		H -0.847555	1.034067	0.000000
	4E	C 0.544046	6.203650	-0.165578
		C -0.837560	6.171355	-0.163889
		C -1.563470	4.938099	-0.071731
		C -0.817449	3.709039	0.066073
		C 0.640304	3.742953	0.064172
		C 1.327272	5.005793	-0.075318
		C -1.522528	2.492026	0.133678
		C -2.943850	2.427503	-0.003979
		C -3.685721	3.667514	-0.080797
		C -2.978093	4.883388	-0.108242
		C -3.637146	1.187443	-0.035405
		C -5.059545	1.126871	-0.056102
		C -5.780758	2.378338	-0.083971
		C -5.123825	3.587588	-0.115942
		C -2.882155	-0.067836	-0.158794
		C -3.576647	-1.358112	-0.038293
		C -5.000261	-1.365184	-0.059548
		C -5.709470	-0.135271	-0.081676
		C -2.825501	-2.564188	-0.006054
		C -3.507281	-3.837659	-0.087551
		C -4.947494	-3.826107	-0.125176
		C -5.661132	-2.649458	-0.091355
		C -1.402575	-2.560984	0.133678
		C -0.721708	-1.304462	0.469326
		C -1.402398	-0.032205	0.085728
		C -0.785281	1.271158	0.464989
		C -0.639719	-3.742220	0.065264
		C -1.326537	-5.005161	-0.076380
		C -2.742053	-5.018059	-0.115930
		C 0.787690	-1.271367	0.465441
		C 1.402555	0.032561	0.082061
		C 0.724080	1.305831	0.462862
		C 1.402046	2.560307	0.129620
		C 0.818844	-3.706103	0.066823
		C 1.563538	-4.936020	-0.072269

		C 0.838103 -6.169517 -0.165474 C -0.543301 -6.202809 -0.168100 C 1.523377 -2.494115 0.133833 C 2.940513 -2.428147 -0.004891 C 3.634680 -1.187990 -0.037441 C 2.881691 0.067783 -0.162062 C 3.683953 -3.667094 -0.080360 C 5.122075 -3.587673 -0.114654 C 5.779073 -2.378628 -0.082931 C 5.057147 -1.127652 -0.056566 C 3.575863 1.357588 -0.040949 C 4.999495 1.364450 -0.060640 C 5.707798 0.134252 -0.081910 C 2.824562 2.563325 -0.009898 C 3.507015 3.836929 -0.088099 C 4.947276 3.825176 -0.124572 C 5.660794 2.648505 -0.091070 C 2.742792 5.017987 -0.114827 C 2.977207 -4.882522 -0.108144 O -0.029702 1.323151 1.690099 H -6.761942 -2.670873 -0.110167 H -6.809944 -0.161362 -0.118135 H -6.881364 2.347436 -0.101307 H -5.697925 4.526124 -0.164141 H -5.476425 -4.790657 -0.176666 H -3.260424 -5.988108 -0.183328 H -3.542690 5.827441 -0.172820 H -1.069324 -7.166344 -0.255151 H -1.408813 7.109051 -0.248527 H 6.879642 -2.347344 -0.099394 H 6.808324 0.159465 -0.116963 H 6.761620 2.669657 -0.108701 H 5.476174 4.789817 -0.174493 H 5.695651 -4.526548 -0.161715 H 3.541589 -5.826769 -0.172309 H 3.262047 5.987636 -0.180616 H 1.410215 -7.106601 -0.250571 H 1.070601 7.167039 -0.251560 O 0.038674 -1.322845 1.694827 O -1.873240 -0.043243 -1.259181 O 1.871893 0.042401 -1.262661
Route 1A	SC1	C 0.504527 1.366424 0.268562 O -0.204179 1.317249 1.524619 C -0.993328 1.195109 0.323088 C -1.850445 2.345030 0.027049 C -3.264210 2.152780 -0.055039 C -4.116618 3.321281 -0.099454 C -3.522629 4.595914 -0.148447 C -2.118334 4.778040 -0.162397 C -1.260641 3.620701 -0.058489 C 0.187268 3.786735 -0.108316 C 0.753205 5.106993 -0.258523

		C -0.137448 6.229377 -0.316636 C -1.509755 6.072000 -0.271269 C 1.054088 2.678190 -0.076105 C -1.506561 -0.159008 -0.034262 C -2.984818 -0.327122 -0.217654 C -3.844164 0.855339 -0.063101 C -5.255170 0.667253 -0.028454 C -6.086035 1.849165 -0.026378 C -5.542031 3.112489 -0.080410 C -0.700571 -1.364146 0.316974 C 0.797585 -1.190419 0.259350 C 1.283018 0.161654 -0.141469 C 2.737248 0.329289 -0.430797 C 3.317045 1.674753 -0.317233 C 2.465040 2.809067 -0.255617 C 3.028091 4.139139 -0.339712 C 2.160292 5.246716 -0.336862 C 1.627149 -2.342611 -0.097553 C 3.030598 -2.150884 -0.286067 C 3.605088 -0.852897 -0.336114 C 5.015097 -0.665876 -0.387118 C 5.548343 0.649460 -0.414998 C 4.732843 1.810525 -0.367424 C 5.277209 3.148221 -0.401564 C 4.462024 4.257208 -0.409786 C -1.276817 -2.675713 0.013547 C -0.414908 -3.785116 -0.080524 C 1.032830 -3.618951 -0.135385 C 1.881330 -4.776600 -0.298161 C 3.283163 -4.594438 -0.383708 C 3.878668 -3.319497 -0.381870 C 5.302356 -3.110747 -0.455884 C 5.846504 -1.846511 -0.437125 C -0.989592 -5.105572 -0.191184 C -0.105064 -6.228049 -0.310580 C 1.267006 -6.070987 -0.361429 C -2.697690 -2.806846 -0.067777 C -3.264639 -4.137277 -0.118336 C -2.398667 -5.244962 -0.174754 C -3.555316 -1.673557 -0.069205 C -4.972299 -1.808586 -0.034155 C -5.515126 -3.147434 -0.037953 C -4.700393 -4.255359 -0.098182 C -5.790208 -0.647927 -0.028737 O 1.700110 0.217550 -1.504422 O 0.098258 -1.308498 1.515984 O -2.025627 -0.214982 -1.359553 N 2.869721 -0.263438 2.720303 N 1.988270 0.360626 3.669090 H 6.371228 3.266830 -0.442792 H 6.641165 0.774526 -0.474133 H 6.938968 -1.715062 -0.481936

		H 5.957596 -3.993436 -0.521319 H 4.901601 5.265469 -0.463315 H 2.588316 6.259604 -0.407736 H 3.928421 -5.484038 -0.464553 H 0.296811 7.236865 -0.412210 H 1.917286 -6.953494 -0.466833 H -7.179317 1.719663 -0.001768 H -6.884405 -0.772960 -0.021615 H -6.609440 -3.267950 -0.013086 H -5.141875 -5.263865 -0.126857 H -6.199482 3.995659 -0.104350 H -4.171965 5.485318 -0.188011 H -2.830856 -6.257609 -0.219582 H -2.165785 6.954522 -0.331177 H -0.545152 -7.235475 -0.375719 H 1.124147 0.578207 3.166116 H 1.733561 -0.287846 4.421521 H 3.828494 -0.109655 3.035106 H 2.721412 -1.276717 2.657230
	ts0	C 2.049034 -5.360744 -0.212243 C 0.656571 -5.121432 -0.275051 C 0.169664 -3.764080 -0.201696 C 1.087353 -2.707900 -0.057167 C 2.486917 -2.946809 -0.081761 C 2.977233 -4.307654 -0.124057 C 0.581428 -1.361965 0.404946 C -0.835631 -1.093372 -0.061401 C -1.736998 -2.142199 -0.244449 C -1.246708 -3.496308 -0.260551 C -1.263050 0.282477 -0.311789 C -2.734275 0.569899 -0.518438 C -3.657298 -0.560853 -0.379135 C -3.158662 -1.873663 -0.355818 C -0.430036 1.420463 0.162420 C -0.891743 2.784330 -0.109888 C -2.294518 3.016912 -0.221352 C -3.218812 1.937828 -0.282517 C -2.774579 4.380186 -0.198854 C -1.835285 5.431627 -0.181173 C -0.440898 5.196725 -0.153426 C 0.040738 3.837483 -0.081181 C 1.472430 3.577658 -0.027532 C 2.405058 4.677142 -0.098612 C 1.881939 6.013139 -0.159825 C 0.523447 6.260763 -0.178685 C 1.047406 1.160493 0.293784 C 1.974312 2.264334 0.046233 C 3.370933 1.981493 -0.042715 C 4.301253 3.089683 -0.072296 C 3.793971 4.402791 -0.093211 C -4.619399 2.160752 -0.217394 C -5.078597 3.527270 -0.150750

		C -4.198087 4.587609 -0.169367 C -5.063651 -0.286321 -0.304689 C -5.513376 1.049417 -0.252429 C -4.078272 -2.989060 -0.371450 C -5.491763 -2.704422 -0.357523 C -5.964440 -1.414118 -0.303148 C -2.172643 -4.577550 -0.360419 C -3.569823 -4.295690 -0.385890 C 1.478792 -0.218515 -0.057627 C -0.304935 -6.180037 -0.384436 C -1.659939 -5.919542 -0.417720 C 3.411687 -1.864614 -0.058092 C 2.930473 -0.482081 -0.212229 C 3.860890 0.647226 -0.067060 C 4.401168 -4.512078 -0.068369 C 5.280800 -3.456247 0.007550 C 4.815232 -2.089196 -0.003758 C 5.699044 -0.974756 -0.003173 C 5.257675 0.372031 -0.020360 C 5.710178 2.788620 -0.058961 C 6.169178 1.492103 -0.012685 O -1.787940 0.479247 -1.642260 O 0.195044 1.271437 1.449040 O 0.455233 -1.476113 1.766960 O 1.991179 -0.321536 -1.378706 N -2.555168 -0.133624 2.580048 N -2.220911 -1.454805 3.031678 H -7.047849 -1.220777 -0.265548 H -6.597056 1.244293 -0.220045 H -6.163220 3.712891 -0.106496 H -4.577579 5.621120 -0.145740 H -6.194977 -3.551730 -0.371566 H -4.275757 -5.141579 -0.413289 H -2.198596 6.471932 -0.184206 H -2.378574 -6.750615 -0.492985 H 0.155670 7.297805 -0.226269 H 6.365269 -3.640187 0.054939 H 6.783531 -1.169610 0.015857 H 7.250748 1.287878 0.015388 H 6.423908 3.626979 -0.074789 H 4.781715 -5.545422 -0.084767 H 2.414811 -6.399525 -0.239807 H 4.501315 5.247315 -0.112992 H 0.058471 -7.218398 -0.433933 H 2.594063 6.852323 -0.195456 H -1.299163 -1.655585 2.612492 H -2.083400 -1.469410 4.050280 H -3.535526 0.044437 2.800412 H -1.981689 0.595094 3.020677
	int0	C 2.700440 -5.027902 -0.080401 C 1.272835 -4.989042 -0.117948 C 0.598832 -3.732414 -0.044292

		C 1.406806 -2.530967 0.217011 C 2.874327 -2.575227 -0.012136 C 3.501822 -3.871163 -0.063189 C 0.696523 -1.214829 0.213487 C -0.719997 -1.171902 -0.158152 C -1.466632 -2.337786 -0.244168 C -0.804226 -3.632894 -0.160992 C -1.305250 0.120811 -0.479648 C -2.819577 0.217554 -0.602237 C -3.575855 -1.026823 -0.430490 C -2.912748 -2.265549 -0.380222 C -0.616350 1.340432 0.033582 C -1.257876 2.646354 -0.144099 C -2.680254 2.696153 -0.230908 C -3.462024 1.508070 -0.315227 C -3.331819 3.983659 -0.150858 C -2.535301 5.147012 -0.094219 C -1.123647 5.096393 -0.074587 C -0.468895 3.809671 -0.063797 C 0.986767 3.740024 -0.001467 C 1.767542 4.954984 -0.009935 C 1.070622 6.213662 -0.021339 C -0.306127 6.280320 -0.043670 C 0.867736 1.282058 0.176085 C 1.656509 2.504239 0.032539 C 3.079118 2.403618 -0.024285 C 3.854529 3.624332 -0.014876 C 3.176750 4.862818 0.002426 C -4.876702 1.548327 -0.219847 C -5.506601 2.841590 -0.109569 C -4.769335 4.006162 -0.103204 C -5.007348 -0.934988 -0.333009 C -5.621187 0.330814 -0.264664 C -3.679373 -3.491794 -0.357815 C -5.115809 -3.389532 -0.351275 C -5.751815 -2.169535 -0.315877 C -1.596420 -4.832390 -0.261535 C -3.010399 -4.727967 -0.329441 C 1.498297 -0.012888 -0.185302 C 0.467015 -6.168351 -0.226064 C -0.914148 -6.090671 -0.278159 C 3.625049 -1.410002 -0.097722 C 2.963310 -0.094318 -0.264868 C 3.743282 1.144385 -0.081910 C 4.942980 -3.901890 -0.116660 C 5.690449 -2.745054 -0.128161 C 5.066464 -1.444410 -0.123387 C 5.785247 -0.236516 -0.129915 C 5.156182 1.050746 -0.077539 C 5.287049 3.508210 -0.017622 C 5.910796 2.277825 -0.035656 O -1.922507 0.263422 -1.764079

		O 0.005836 1.166374 1.338265 O 1.043530 -1.829160 1.470742 O 2.082702 -0.048874 -1.488452 N -2.437703 -0.354748 2.574188 N -1.839678 -1.530027 3.146385 H -6.851100 -2.118691 -0.274768 H -6.720246 0.385009 -0.212387 H -6.605278 2.884655 -0.047084 H -5.277308 4.981335 -0.042666 H -5.704842 -4.319917 -0.345685 H -3.606061 -5.654697 -0.351646 H -3.031609 6.130007 -0.052721 H -1.513976 -7.011610 -0.346823 H -0.808717 7.260238 -0.047926 H 6.790043 -2.798476 -0.152937 H 6.886033 -0.276781 -0.150432 H 7.010384 2.218078 -0.034032 H 5.888235 4.430790 -0.005915 H 5.443844 -4.882191 -0.146769 H 3.195059 -6.011928 -0.114325 H 3.768951 5.791987 0.018075 H 0.966146 -7.149307 -0.260362 H 1.666161 7.139962 -0.012413 H -1.124137 -1.850291 2.489391 H -1.348261 -1.311106 4.020383 H -3.349550 -0.225997 3.014145 H -1.877962 0.487727 2.744360
	ts1	C -1.415358 -5.490756 -0.217002 C -2.425173 -4.492777 -0.231537 C -2.047733 -3.105948 -0.164687 C -0.670863 -2.776357 -0.043637 C 0.351357 -3.780446 -0.143773 C -0.047578 -5.171226 -0.191500 C -0.308483 -1.381489 0.348125 C -1.310028 -0.337654 -0.085659 C -2.645474 -0.678561 -0.258822 C -3.038918 -2.075373 -0.213185 C -0.857837 1.006191 -0.395867 C -1.909986 2.121983 -0.558794 C -3.312384 1.723715 -0.409855 C -3.661372 0.359936 -0.389597 C 0.468727 1.451350 0.112887 C 0.880521 2.843719 -0.087882 C -0.128901 3.846329 -0.184852 C -1.510040 3.506251 -0.273057 C 0.265364 5.234414 -0.109772 C 1.639300 5.549341 -0.051009 C 2.640997 4.553753 -0.025809 C 2.248670 3.164571 -0.006908 C 3.267922 2.124911 0.051187 C 4.665453 2.487635 0.024156 C 5.009465 3.883953 0.014197

		C 4.044306 4.868458 -0.000636 C 1.515434 0.391918 0.265290 C 2.919720 0.761797 0.084171 C 3.898260 -0.272523 -0.019541 C 5.296898 0.097304 -0.018650 C 5.639936 1.464650 0.016020 C -2.523542 4.496148 -0.186415 C -2.107535 5.873288 -0.078890 C -0.775383 6.226673 -0.069330 C -4.302994 2.762435 -0.313942 C -3.896753 4.108657 -0.238867 C -5.058617 -0.023172 -0.378422 C -6.044679 1.028525 -0.365494 C -5.686983 2.356024 -0.313362 C -4.428138 -2.420307 -0.300594 C -5.402759 -1.384923 -0.354651 C 1.085473 -0.978832 -0.112259 C -3.821540 -4.805117 -0.303243 C -4.781899 -3.810622 -0.328024 C 1.716300 -3.436412 -0.175290 C 2.117340 -2.020799 -0.284028 C 3.530925 -1.644273 -0.109635 C 0.995256 -6.165470 -0.213772 C 2.326385 -5.817273 -0.192587 C 2.740421 -4.434005 -0.175921 C 4.096448 -4.036260 -0.168425 C 4.509500 -2.672164 -0.113471 C 6.272848 -0.958904 -0.043381 C 5.897997 -2.284604 -0.071673 O -1.201171 1.527541 -1.686440 O 0.818538 0.922951 1.418334 O -0.384815 -1.790303 1.683987 O 1.453658 -1.328926 -1.445399 N -3.038934 -0.600821 2.904912 N -1.780263 -0.021836 2.987165 H -6.462386 3.136715 -0.270866 H -4.667366 4.894174 -0.192361 H -2.884606 6.651440 -0.021513 H -0.486215 7.287612 -0.010909 H -7.108441 0.743803 -0.369996 H -6.468272 -1.664598 -0.374066 H 1.941870 6.608246 -0.014349 H -5.848804 -4.077995 -0.383273 H 4.340928 5.929021 -0.006218 H 3.103546 -6.597194 -0.198026 H 4.873768 -4.816928 -0.186041 H 6.664181 -3.075413 -0.078796 H 7.339798 -0.686700 -0.034983 H 0.703216 -7.226863 -0.243864 H -1.717190 -6.549876 -0.246455 H 6.705205 1.746086 0.024628 H -4.123931 -5.863402 -0.338904

		H 6.075851 4.158687 0.015405 H -1.019592 -0.660906 2.549609 H -1.798285 0.894944 2.537798 H -3.463189 -0.577867 1.964819 H -2.976996 -1.570607 3.216005
	int1	C -2.741085 -4.937875 -0.304583 C -3.456788 -3.723598 -0.293014 C -2.743049 -2.482641 -0.065317 C -1.364090 -2.510073 0.121398 C -0.627660 -3.716549 -0.061390 C -1.340124 -4.965430 -0.216854 C -0.619698 -1.322382 0.699181 C -1.447602 0.063802 0.674320 C -2.806487 0.003483 0.013125 C -3.476499 -1.217104 -0.122828 C -0.626788 1.204347 0.068824 C -1.342818 2.477135 -0.270542 C -2.812441 2.482856 -0.214510 C -3.499712 1.240163 -0.203801 C 0.811648 1.315692 0.445273 C 1.532457 2.549463 0.123749 C 0.796763 3.757936 -0.073981 C -0.616965 3.755100 -0.177915 C 1.524540 5.007784 -0.152702 C 2.928981 4.981999 -0.123336 C 3.659166 3.771686 -0.052168 C 2.939924 2.525831 0.080278 C 3.670882 1.268213 0.064075 C 5.108110 1.277740 -0.080849 C 5.783837 2.539432 -0.136324 C 5.089293 3.734445 -0.122458 C 1.570067 0.009393 0.419337 C 2.995196 0.033306 0.091439 C 3.679164 -1.203654 -0.111051 C 5.124842 -1.188632 -0.203190 C 5.796936 0.044823 -0.174731 C -1.354243 4.972508 -0.273668 C -0.611132 6.210395 -0.299608 C 0.763378 6.225179 -0.258820 C -3.501035 3.722252 -0.330682 C -2.767032 4.936809 -0.362873 C -4.930895 1.227516 -0.411724 C -5.615596 2.489053 -0.521754 C -4.937697 3.683984 -0.458117 C -4.900154 -1.231337 -0.400539 C -5.595326 -0.008136 -0.495045 C 0.757935 -1.181803 0.041478 C -4.874668 -3.683903 -0.496636 C -5.565529 -2.491371 -0.549816 C 0.790223 -3.719072 -0.123455 C 1.504004 -2.440657 -0.248980 C 2.975677 -2.431972 -0.185398

		C -0.578600 -6.184183 -0.292530 C 0.795936 -6.171901 -0.267710 C 1.529086 -4.930292 -0.216645 C 2.945786 -4.886471 -0.295725 C 3.673737 -3.673404 -0.262485 C 5.807764 -2.451428 -0.309353 C 5.116044 -3.639618 -0.319865 O -0.825491 1.521294 -1.301088 O 1.205936 0.651591 1.661051 O -0.359809 -1.692883 2.062858 O 0.921773 -1.552680 -1.317992 N -2.726926 -0.149600 2.842023 N -1.658349 0.456007 2.131892 H -5.483050 4.637091 -0.538888 H -3.316922 5.885637 -0.462769 H -1.173003 7.154450 -0.374149 H 1.308986 7.180495 -0.306863 H -6.707998 2.478383 -0.660369 H -6.685249 -0.023932 -0.654791 H 3.482266 5.932776 -0.186194 H -6.652295 -2.489460 -0.727117 H 5.634560 4.688681 -0.191838 H 1.362449 -7.114329 -0.323892 H 3.499864 -5.834732 -0.379169 H 5.657827 -4.595844 -0.387410 H 6.906964 -2.448384 -0.374637 H -1.124563 -7.136541 -0.379106 H -3.293345 -5.883621 -0.424462 H 6.896298 0.055718 -0.247537 H -5.408169 -4.637567 -0.632349 H 6.882127 2.541920 -0.216206 H -0.313553 -0.819603 2.529965 H -1.800350 1.466856 2.170402 H -3.579212 -0.203507 2.268063 H -2.441953 -1.111010 3.046237
	ts2	C -3.934956 -3.980007 -0.391795 C -4.306814 -2.615435 -0.383375 C -3.267569 -1.610900 -0.332938 C -1.923173 -2.009216 -0.250449 C -1.546154 -3.387159 -0.284343 C -2.589400 -4.389626 -0.348421 C -0.928978 -0.994002 0.117667 C -1.253234 0.385120 -0.236670 C -2.587561 0.787049 -0.341108 C -3.623985 -0.212138 -0.293053 C -0.183172 1.353885 -0.457247 C -0.529375 2.838855 -0.552448 C -1.943671 3.198634 -0.389500 C -2.936164 2.197695 -0.376507 C 1.177025 1.052624 0.068455 C 2.240116 2.050299 -0.081479 C 1.874624 3.427022 -0.150437

		C 0.512723 3.829606 -0.235545 C 2.917157 4.423969 -0.050710 C 4.258870 3.999820 0.018477 C 4.621758 2.632930 0.033726 C 3.580018 1.631945 0.017417 C 3.933355 0.217955 0.080216 C 5.322885 -0.172131 0.110768 C 6.323111 0.857947 0.121285 C 5.988863 2.196963 0.090890 C 1.542358 -0.387529 0.202082 C 2.945633 -0.784824 0.080714 C 3.270515 -2.174904 0.032554 C 4.664364 -2.557072 0.103042 C 5.646700 -1.549238 0.144693 C 0.137681 5.194774 -0.126108 C 1.192109 6.173262 -0.005613 C 2.519791 5.806176 0.004504 C -2.272158 4.588918 -0.239863 C -1.241581 5.549755 -0.157602 C -4.331386 2.571332 -0.282151 C -4.651050 3.972962 -0.213932 C -3.668877 4.937252 -0.181184 C -5.003589 0.187419 -0.285286 C -5.321294 1.568962 -0.242774 C 0.492736 -1.360842 -0.208625 C -5.673027 -2.179520 -0.361570 C -6.008569 -0.837286 -0.302051 C -0.191594 -3.797597 -0.228618 C 0.870890 -2.789785 -0.326079 C 2.265862 -3.176005 -0.065557 C -2.198248 -5.776290 -0.326423 C -0.877762 -6.152032 -0.227468 C 0.180913 -5.172100 -0.176088 C 1.550066 -5.530572 -0.091158 C 2.587328 -4.561150 -0.013581 C 4.972574 -3.963230 0.136970 C 3.981926 -4.918962 0.099450 O -0.198585 2.024355 -1.726489 O 1.187908 0.403699 1.383016 O -0.996912 -1.094262 1.828468 O 0.709782 -1.878374 -1.519091 N -3.346812 -0.385352 2.427729 N -3.603973 0.674053 3.064546 H -3.940757 6.001552 -0.102283 H -1.514202 6.614093 -0.079305 H 0.913071 7.236296 0.064511 H 3.305122 6.574870 0.076145 H -5.712067 4.264293 -0.164916 H -6.380645 1.869240 -0.196943 H 5.054943 4.759497 0.078201 H -7.067497 -0.534991 -0.284229 H 6.780647 2.962197 0.106049

		H -0.607139 -7.219103 -0.196323 H 1.819394 -6.598102 -0.067761 H 4.245572 -5.987609 0.137230 H 6.029761 -4.265671 0.198538 H -2.988407 -6.541757 -0.378561 H -4.726323 -4.746770 -0.415727 H 6.707640 -1.842216 0.200119 H -6.466257 -2.943409 -0.385502 H 7.381814 0.556518 0.156240 H -0.315114 -0.424816 2.077545 H -4.628779 0.753295 3.209037 H -4.107905 -1.033066 2.160356 H -2.216574 -0.680060 2.163498
	3E	C 5.718104 -2.480688 -0.213179 C 5.030714 -1.216598 -0.100682 C 3.618146 -1.242108 0.048364 C 2.891784 -2.463266 0.020072 C 3.601188 -3.720317 -0.079984 C 5.036044 -3.676721 -0.181407 C 2.861275 -4.917899 -0.103393 C 1.447652 -4.935034 -0.064238 C 0.730930 -3.681441 -0.023602 C 1.464337 -2.481603 0.018690 C 0.747094 -1.207250 -0.084728 C -0.745934 -1.207856 -0.084859 C -1.462090 -2.482888 0.018358 C -0.727611 -3.682073 -0.023855 C 1.422070 0.037978 0.370475 C 0.700573 1.305957 0.156312 C -0.701744 1.305327 0.156496 C -1.422054 0.036668 0.370489 C -1.435892 2.515112 0.082409 C -0.718090 3.746557 -0.009037 C 0.714691 3.747185 -0.009245 C 1.433617 2.516403 0.082043 C 2.882721 2.504408 0.051653 C 3.585302 3.760700 -0.092646 C 2.853069 4.960545 -0.155849 C 1.438590 4.990511 -0.115934 C -1.443130 4.989240 -0.115429 C -0.694418 6.206640 -0.201115 C 0.688778 6.207235 -0.201363 C 2.924974 0.023291 0.347291 C 3.614113 1.298805 0.103499 C 5.035821 1.272666 -0.070013 C 5.715787 2.538129 -0.192876 C 5.021764 3.726189 -0.188763 C -2.924998 0.020570 0.347401 C -3.615301 1.295529 0.104027 C -2.885005 2.501809 0.052326 C -3.588732 3.757511 -0.091506 C -2.857596 4.958022 -0.154798

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	SC1’	C 4.747792 -3.895052 -0.030400 C 4.406338 -2.499269 -0.158313 C 3.033340 -2.161058 -0.289278 C 2.021487 -3.150564 -0.217829 C 2.381433 -4.543308 -0.103341 C 3.779736 -4.873683 -0.027692 C 0.641703 -2.798922 -0.183745 C 0.280701 -1.377906 -0.086098 C 1.241128 -0.353441 -0.591650 C 2.683822 -0.759352 -0.604830 C -1.157947 -0.991351 -0.037630 C -2.184402 -2.037701 -0.086598 C -1.785919 -3.381002 -0.046840 C -0.378092 -3.763177 -0.093046 C -3.553173 -1.651156 -0.035957 C -3.941769 -0.284652 -0.061172

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	ts4	C 4.568809 -4.066930 0.064628 C 4.284813 -2.662928 -0.084070 C 2.924074 -2.268619 -0.173647 C 1.865563 -3.202896 -0.090184 C 2.173685 -4.607645 0.029329 C 3.555367 -4.998604 0.103692 C 0.494377 -2.790800 -0.110536 C 0.158664 -1.372308 -0.026980 C 1.203078 -0.412683 -0.521127 C 2.622128 -0.863662 -0.511341 C -1.203889 -0.996743 -0.324146 C -2.239893 -1.933031 -0.257057 C -1.925619 -3.324881 -0.117626 C -0.553844 -3.744876 -0.081978 C -3.622845 -1.506739 -0.193899 C -3.962781 -0.141671 -0.165514 C -2.953684 0.880564 -0.482991 C -1.476625 0.411551 -0.600798 C -3.207227 2.280820 -0.108349 C -4.544359 2.659910 0.206953 C -5.561549 1.665224 0.270544 C -5.291994 0.295661 0.130110 C -4.659311 -2.497198 -0.011817 C -6.010042 -2.040180 0.170659 C -6.309465 -0.708885 0.263525 C -0.427532 1.430647 -0.365237 C -0.771247 2.806620 -0.234929 C -2.147824 3.223510 -0.101810 C -2.442222 4.617791 0.130941 C -3.807631 4.994375 0.372414 C -4.813265 4.054674 0.432401 C -2.971594 -4.287086 -0.018402 C -4.318691 -3.851060 0.027558

		C 0.900615 1.027386 -0.357655 C -0.234683 -5.149996 0.011812 C -1.315245 -6.092840 0.071923 C -2.629333 -5.676441 0.064175 C 1.119349 -5.541506 0.075813 C 0.279446 3.772910 -0.156325 C 1.650426 3.359532 -0.214153 C 1.970555 1.969031 -0.304116 C 3.345327 1.534357 -0.318925 C 3.678043 0.147587 -0.293971 C 5.045484 -0.303652 -0.231288 C 5.319315 -1.681173 -0.155166 C -1.388786 5.557330 0.144404 C -0.041510 5.173652 0.000959 C 1.039012 6.120775 0.038113 C 2.355166 5.720325 -0.042577 C 2.712007 4.332916 -0.154345 C 4.052257 3.888663 -0.178266 C 4.391491 2.520647 -0.242046 C 5.757567 2.052932 -0.198649 C 6.069271 0.711618 -0.189488 O -2.292645 0.693586 -1.760526 O 0.289872 -0.937813 1.736145 O 1.851583 -0.725075 -1.775149 N 3.395984 0.067596 2.148760 N 2.247945 0.548043 2.456999 H 7.122027 0.391119 -0.144341 H 6.367727 -2.013851 -0.100839 H 5.620017 -4.387686 0.133990 H 3.791219 -6.070270 0.197867 H 6.562018 2.804320 -0.160206 H 4.860878 4.635332 -0.123759 H 1.359675 -6.613090 0.170404 H 3.163401 6.467646 -0.007058 H -1.072825 -7.165091 0.139405 H -5.847667 4.362154 0.651746 H -6.596169 1.981090 0.478313 H -7.336789 -0.384174 0.448486 H -6.804567 -2.794795 0.278025 H -4.034641 6.059264 0.537103 H -1.626833 6.621948 0.298787 H -5.116604 -4.602086 0.140752 H 0.792184 7.188986 0.141790 H -3.445637 -6.412711 0.127763 H 0.158536 -1.806393 2.158270 H 4.092873 0.832167 2.112369 H 2.090272 1.567114 2.455718 H 1.383712 -0.131920 2.278057
	2E	C -5.679972 2.515138 -0.388605 C -5.006927 1.255756 -0.209659 C -3.601792 1.278941 0.053991 C -2.868088 2.483287 0.038971

		C -3.562249 3.735133 -0.167841 C -4.987754 3.703809 -0.350164 C -2.932894 0.007173 0.396400 C -1.414768 0.004355 0.542711 C -0.692598 1.275116 0.305008 C -1.423112 2.487278 0.148696 C -3.607353 -1.261072 0.051959 C -2.882835 -2.465449 0.035895 C -1.440527 -2.477184 0.146350 C -0.701567 -1.270449 0.302822 C -3.581556 -3.710818 -0.170686 C -5.006748 -3.674061 -0.353057 C -5.693569 -2.483186 -0.391362 C -5.012927 -1.228703 -0.211615 C -5.685468 0.015060 -0.290385 C -0.726075 -3.706236 0.027413 C -1.448193 -4.946381 -0.132341 C -2.855405 -4.914388 -0.218080 C 0.704678 -3.706581 0.028888 C 1.421763 -2.483278 0.148024 C 0.694506 -1.274937 0.304696 C 1.414221 -0.004967 0.541400 C 0.703683 1.270784 0.305995 C 2.932562 -0.009752 0.398422 C 3.598343 -1.280551 0.054096 C 2.862836 -2.481909 0.040449 C 3.554904 -3.729061 -0.166919 C 2.824645 -4.923703 -0.214161 C 1.421402 -4.946808 -0.129545 C 0.678478 -6.161012 -0.234855 C -0.701453 -6.163208 -0.236626 C 4.976631 -3.697181 -0.348372 C 5.665142 -2.514331 -0.388097 C 4.997710 -1.258349 -0.210774 C 5.681341 -0.027538 -0.291741 C 5.014648 1.219627 -0.212159 C 3.610759 1.254928 0.054931 C 2.884865 2.463141 0.039186 C 1.439913 2.474939 0.149377 C 3.587738 3.709563 -0.170455 C 5.012627 3.667381 -0.355688 C 5.696430 2.473647 -0.394696 C -0.702747 3.713126 0.029554 C 0.728005 3.706811 0.029438 C 1.454176 4.945882 -0.130554 C 2.861757 4.913969 -0.217993 C 0.711604 6.166503 -0.235446 C -0.668512 6.172166 -0.234963 C -1.420043 4.957206 -0.129788 C -2.827972 4.934626 -0.215380 O -2.280060 0.006022 1.707525 O 2.277391 -0.008356 1.707871

		H -6.767334 2.509794 -0.562458 H -6.771861 0.017469 -0.472196 H -6.780818 -2.471890 -0.565213 H -5.540200 -4.627516 -0.490695 H -5.517677 4.659276 -0.487496 H -3.367345 5.884611 -0.359082 H -3.400819 -5.860941 -0.362105 H -1.218006 7.120984 -0.337128 H -1.254198 -7.110055 -0.339662 H 6.783277 2.460535 -0.571037 H 6.767252 -0.039192 -0.474809 H 6.744539 -2.508393 -0.560783 H 5.507108 -4.652125 -0.485068 H 5.549103 4.618823 -0.495413 H 3.407131 5.860260 -0.363207 H 3.364109 -5.873474 -0.358376 H 1.268692 7.110844 -0.338006 H 1.234811 -7.105854 -0.336415
Route 1B	ts1	C 0.819482 1.132828 0.365098 O 0.606973 1.219488 1.751854 C -0.606947 1.419556 0.015019 C -1.068848 2.724959 -0.107497 C -2.492053 2.991774 -0.109302 C -2.940959 4.366985 -0.092090 C -1.991116 5.396604 -0.167240 C -0.588050 5.144050 -0.229958 C -0.120136 3.798245 -0.170033 C 1.298869 3.526551 -0.201882 C 2.241806 4.611910 -0.335172 C 1.730595 5.949790 -0.405086 C 0.374458 6.205778 -0.345552 C 1.779946 2.203803 -0.095158 C -1.511529 0.287922 -0.158083 C -2.999062 0.562091 -0.263192 C -3.436802 1.950243 -0.082238 C -4.843337 2.202201 0.054787 C -5.265875 3.582453 0.090722 C -4.359646 4.613579 0.002232 C -1.115073 -1.098316 0.231170 C 0.350531 -1.395293 0.221373 C 1.235048 -0.250581 -0.136421 C 2.671691 -0.537144 -0.368472 C 3.636373 0.559998 -0.197101 C 3.162667 1.912675 -0.200361 C 4.110825 3.001678 -0.309759 C 3.625652 4.320366 -0.365754 C 0.798783 -2.751740 -0.094964 C 2.197179 -2.996252 -0.237197 C 3.140993 -1.928260 -0.266765 C 4.541736 -2.181751 -0.304819 C 5.454162 -1.088781 -0.334613 C 5.033739 0.260602 -0.281771

		C 5.956483 1.371367 -0.324133 C 5.514248 2.675535 -0.352482 C -2.067878 -2.185260 -0.026927 C -1.583314 -3.504538 -0.096797 C -0.153109 -3.787185 -0.143195 C 0.306224 -5.149243 -0.275879 C 1.695946 -5.401566 -0.337880 C 2.653357 -4.366471 -0.323194 C 4.072340 -4.599120 -0.374211 C 4.974891 -3.559397 -0.346989 C -2.532155 -4.591663 -0.157879 C -2.027042 -5.932387 -0.264102 C -0.675432 -6.198704 -0.324192 C -3.463071 -1.885730 -0.037840 C -4.405729 -2.981587 -0.023563 C -3.915110 -4.301299 -0.093323 C -3.936718 -0.544208 -0.017556 C -5.316979 -0.241693 0.105797 C -6.238084 -1.351707 0.165968 C -5.804314 -2.657317 0.080282 C -5.744708 1.120576 0.122609 O 1.695769 -0.314693 -1.486822 O -0.379352 -1.263865 1.463697 O -2.156346 0.329623 -1.447991 N 3.464605 -0.127799 2.410266 N 2.257738 -0.101945 3.095362 H 7.035194 1.152667 -0.366413 H 6.532209 -1.305280 -0.405616 H 6.056049 -3.764909 -0.382542 H 4.430639 -5.638881 -0.434032 H 6.240744 3.501109 -0.414520 H 4.344655 5.153647 -0.439974 H 2.042691 -6.445441 -0.404139 H 2.445224 6.782158 -0.500759 H -0.321747 -7.238315 -0.413939 H -6.342206 3.799179 0.181028 H -6.822483 1.331373 0.201236 H -7.313636 -1.134161 0.260552 H -6.533210 -3.482639 0.100842 H -4.706883 5.658098 0.012961 H -2.339140 6.442344 -0.174412 H -4.632891 -5.137434 -0.094784 H 0.006124 7.243104 -0.393844 H -2.751446 -6.761000 -0.304403 H 1.543765 0.591931 2.567694 H 1.823112 -1.028494 2.997747 H 4.081575 0.628204 2.703827 H 3.939163 -1.031647 2.404961
	int1	C 0.800985 1.133196 0.487383 O 0.819680 1.213925 1.923081 C -0.618991 1.410989 0.055574 C -1.076482 2.710129 -0.089215

		C -2.502532 2.987211 -0.160421 C -2.950660 4.364972 -0.112394 C -2.005965 5.397120 -0.119630 C -0.602461 5.144911 -0.137481 C -0.132822 3.802592 -0.084942 C 1.278275 3.532038 -0.104209 C 2.220854 4.616279 -0.228475 C 1.713949 5.958876 -0.263956 C 0.359736 6.212281 -0.208897 C 1.756635 2.202246 -0.006172 C -1.504190 0.298320 -0.222842 C -3.028805 0.568241 -0.350535 C -3.454896 1.953273 -0.158419 C -4.862974 2.210228 -0.000297 C -5.282913 3.590915 0.039974 C -4.370502 4.615328 -0.036980 C -1.144769 -1.083053 0.205655 C 0.315624 -1.384014 0.281991 C 1.210529 -0.240428 -0.051632 C 2.634518 -0.531703 -0.358484 C 3.617268 0.552318 -0.193525 C 3.133284 1.910580 -0.155374 C 4.077495 2.997344 -0.293665 C 3.602436 4.320658 -0.298331 C 0.771286 -2.745462 -0.015627 C 2.163087 -2.992161 -0.204801 C 3.109317 -1.925642 -0.293110 C 4.502147 -2.180071 -0.406522 C 5.427931 -1.086989 -0.486274 C 5.010790 0.257036 -0.412522 C 5.925245 1.372092 -0.484456 C 5.477368 2.672310 -0.431536 C -2.093793 -2.175529 -0.038682 C -1.611538 -3.498477 -0.050749 C -0.182470 -3.782814 -0.067755 C 0.273973 -5.146358 -0.191962 C 1.659097 -5.400172 -0.280834 C 2.614327 -4.361131 -0.307179 C 4.027803 -4.595861 -0.427658 C 4.931971 -3.556281 -0.459546 C -2.561102 -4.585287 -0.087893 C -2.057323 -5.933323 -0.156230 C -0.708393 -6.200275 -0.215392 C -3.486467 -1.878829 -0.067114 C -4.430233 -2.969754 -0.007903 C -3.940893 -4.294124 -0.037776 C -3.958056 -0.532909 -0.074586 C -5.334110 -0.231327 0.079604 C -6.255873 -1.335873 0.179579 C -5.825947 -2.644134 0.109667 C -5.761852 1.133309 0.086634 O 1.619215 -0.273363 -1.421741

		O -0.469167 -1.196480 1.481349 O -2.165606 0.334110 -1.494837 N 3.859981 -0.154766 2.124930 N 2.801906 -0.390327 2.868641 H 6.998852 1.160743 -0.608563 H 6.497436 -1.309797 -0.622978 H 6.009317 -3.764951 -0.551775 H 4.381838 -5.636319 -0.498243 H 6.195885 3.503119 -0.514212 H 4.323291 5.149965 -0.381074 H 2.005916 -6.443857 -0.349150 H 2.431413 6.791197 -0.336387 H -0.354487 -7.240678 -0.286863 H -6.358352 3.809490 0.130254 H -6.838488 1.345806 0.181352 H -7.328471 -1.113697 0.293127 H -6.554647 -3.468193 0.160674 H -4.711501 5.662216 -0.013552 H -2.354897 6.442229 -0.109099 H -4.660089 -5.128587 -0.012635 H -0.010082 7.249238 -0.235396 H -2.784056 -6.760599 -0.174832 H 1.567297 0.656403 2.304365 H 2.484194 -1.346484 2.647064 H 4.334990 0.729848 2.302889 H 4.444950 -0.893835 1.712732
	ts2	C 0.714636 1.208982 0.442182 O 0.861217 1.295344 1.885617 C -0.734525 1.366793 0.045847 C -1.306110 2.622169 -0.094024 C -2.751353 2.774740 -0.142026 C -3.317281 4.108469 -0.087961 C -2.466077 5.218455 -0.120092 C -1.046403 5.087978 -0.164030 C -0.462066 3.791925 -0.110936 C 0.967721 3.643072 -0.143646 C 1.813386 4.806303 -0.266964 C 1.190005 6.098744 -0.317685 C -0.180867 6.234038 -0.258476 C 1.560001 2.363688 -0.044522 C -1.525526 0.186921 -0.237546 C -3.068542 0.321608 -0.336621 C -3.610605 1.662407 -0.126574 C -5.032408 1.794474 0.058525 C -5.569663 3.133675 0.113162 C -4.751672 4.233729 0.018360 C -1.037083 -1.160017 0.167287 C 0.441270 -1.332158 0.208395 C 1.237587 -0.117032 -0.118206 C 2.685373 -0.281366 -0.383374 C 3.557978 0.883399 -0.175228 C 2.961655 2.192164 -0.152293

		C 3.808976 3.358220 -0.263761 C 3.216257 4.633676 -0.303966 C 1.014618 -2.648418 -0.083995 C 2.425487 -2.772901 -0.252855 C 3.277720 -1.628442 -0.313026 C 4.691927 -1.761383 -0.356776 C 5.520555 -0.593560 -0.356461 C 4.979150 0.710358 -0.289372 C 5.797302 1.900902 -0.322271 C 5.236466 3.157265 -0.326803 C -1.891095 -2.331238 -0.063636 C -1.293676 -3.606158 -0.098964 C 0.154532 -3.764543 -0.133439 C 0.728023 -5.082443 -0.260922 C 2.131587 -5.214808 -0.338547 C 2.994616 -4.098454 -0.344055 C 4.426785 -4.209819 -0.421711 C 5.238799 -3.096635 -0.406628 C -2.144432 -4.772053 -0.134122 C -1.525391 -6.070010 -0.221580 C -0.158528 -6.217669 -0.290502 C -3.304234 -2.157948 -0.067070 C -4.147269 -3.328207 -0.005607 C -3.543607 -4.603839 -0.059617 C -3.892647 -0.858427 -0.054796 C -5.286381 -0.679826 0.127210 C -6.105307 -1.862473 0.232413 C -5.563898 -3.127330 0.139555 C -5.831960 0.642343 0.154276 O 1.674111 -0.105934 -1.478351 O -0.327926 -1.210681 1.434491 O -2.208224 0.175500 -1.498494 N 3.633066 -0.079946 2.257455 N 2.612306 -0.659368 2.825673 H 6.890627 1.782433 -0.379686 H 6.611773 -0.718055 -0.431932 H 6.332975 -3.212086 -0.453910 H 4.871016 -5.215381 -0.487708 H 5.883379 4.046622 -0.389452 H 3.862279 5.523586 -0.375042 H 2.567450 -6.224726 -0.404270 H 1.831718 6.989941 -0.400169 H 0.284290 -7.222695 -0.371408 H -6.657849 3.258379 0.226599 H -6.921140 0.759210 0.269686 H -7.191069 -1.736673 0.366988 H -6.216816 -4.012479 0.193311 H -5.181915 5.246978 0.050466 H -2.903478 6.229700 -0.107973 H -4.186038 -5.498731 -0.032951 H -0.639313 7.234650 -0.293842 H -2.177248 -6.957404 -0.243069

		H 1.123447 0.415593 2.258831 H 2.575854 -1.626432 2.463975 H 3.795850 0.894646 2.509177 H 4.390346 -0.571752 1.765209
	int2	C 0.695168 1.206657 0.396616 O 0.901316 1.199454 1.845264 C -0.755629 1.355441 0.031685 C -1.344447 2.603917 -0.082647 C -2.789632 2.738540 -0.123900 C -3.365247 4.059828 -0.049639 C -2.529148 5.173399 -0.066711 C -1.112596 5.061264 -0.118720 C -0.515516 3.779377 -0.086355 C 0.911018 3.642743 -0.134482 C 1.737359 4.811385 -0.261685 C 1.100490 6.091169 -0.288546 C -0.263415 6.212080 -0.208802 C 1.518093 2.378157 -0.056575 C -1.536384 0.170544 -0.263039 C -3.073528 0.287872 -0.348692 C -3.630648 1.620349 -0.124821 C -5.045901 1.730746 0.068150 C -5.594989 3.058370 0.140274 C -4.795469 4.163424 0.059589 C -1.030180 -1.167482 0.142897 C 0.445848 -1.320776 0.178645 C 1.224581 -0.103441 -0.178959 C 2.668580 -0.252418 -0.412937 C 3.524365 0.926455 -0.230951 C 2.912528 2.220098 -0.187152 C 3.740018 3.392428 -0.302181 C 3.134631 4.654697 -0.321997 C 1.033281 -2.633310 -0.084955 C 2.439958 -2.739338 -0.242160 C 3.274564 -1.588523 -0.315443 C 4.683670 -1.702342 -0.369734 C 5.492952 -0.527462 -0.393285 C 4.934587 0.768583 -0.349777 C 5.734985 1.964884 -0.390345 C 5.162653 3.207760 -0.386571 C -1.870463 -2.348605 -0.069280 C -1.258929 -3.609031 -0.097754 C 0.187860 -3.751456 -0.127255 C 0.773470 -5.056915 -0.240723 C 2.172873 -5.171982 -0.309845 C 3.020180 -4.052166 -0.320869 C 4.448602 -4.144476 -0.398466 C 5.242532 -3.028007 -0.400981 C -2.092043 -4.779081 -0.126098 C -1.459343 -6.064556 -0.202921 C -0.098074 -6.196263 -0.265349 C -3.279173 -2.189458 -0.071557

		C -4.103398 -3.364174 -0.004811 C -3.486723 -4.626036 -0.052477 C -3.880822 -0.902191 -0.063747 C -5.267383 -0.738806 0.124056 C -6.068549 -1.926681 0.231558 C -5.516221 -3.178344 0.140314 C -5.826261 0.572464 0.156925 O 1.662581 -0.111130 -1.537577 O -0.319797 -1.189090 1.421507 O -2.223474 0.155954 -1.521921 N 3.847217 -0.037359 2.281245 N 2.947548 -0.554204 3.040898 H 6.820419 1.861101 -0.458766 H 6.576869 -0.636932 -0.470818 H 6.328976 -3.131028 -0.452800 H 4.902645 -5.136732 -0.454056 H 5.793632 4.097415 -0.454980 H 3.764786 5.545754 -0.393330 H 2.616824 -6.169942 -0.365815 H 1.726436 6.982977 -0.369977 H 0.351981 -7.189220 -0.336814 H -6.675682 3.168241 0.256396 H -6.907974 0.673805 0.277007 H -7.146868 -1.814845 0.366789 H -6.154601 -4.063163 0.195866 H -5.235986 5.162244 0.105972 H -2.974344 6.171784 -0.038275 H -4.113415 -5.521670 -0.019451 H -0.727819 7.200752 -0.227215 H -2.095300 -6.952702 -0.220074 H 0.373874 0.440902 2.177519 H 2.778053 -1.513793 2.690561 H 4.101944 0.933970 2.466669 H 4.418777 -0.545341 1.587342
Route 2	SC2	N -2.901114 -0.135224 2.959925 C -2.791395 0.316109 -0.396263 C -1.361882 0.180377 -0.683473 C -0.467207 1.298153 -0.259392 O -0.703323 1.701396 1.089241 N -1.616449 -0.778769 3.011765 C -3.350920 1.624762 -0.255984 C -4.791129 1.757144 -0.201334 C -5.581227 0.593594 -0.196534 C -5.017870 -0.704260 -0.230144 C -3.585859 -0.845048 -0.345692 C -2.987511 -2.173657 -0.326577 C -3.832605 -3.337907 -0.198575 C -5.252223 -3.149687 -0.135637 C -5.818844 -1.889991 -0.150275 C -0.741966 -1.196264 -0.665733 C -1.590434 -2.350045 -0.357753 C -0.983322 -3.634460 -0.195078

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		H 2.897566 -6.190243 0.053369 H 0.616193 -7.231218 -0.028215 H -1.852364 -6.986235 -0.036100 H 6.640203 -3.163489 0.227314 H 6.882353 -0.658968 0.248275 H -3.886369 -5.505775 -0.082965 H 7.114035 1.817271 0.341790 H -5.894566 -4.040505 -0.056275 H -1.626535 -1.545573 2.336894 H -0.865183 -0.143239 2.719530 H -3.052055 0.296560 3.873403 H -2.903434 0.623276 2.267884
	ts1	N -1.999232 -0.755346 2.769532 C -2.832121 -0.290946 -0.295294 C -1.403495 -0.130002 -0.578130 C -0.764394 1.161448 -0.184869 O -1.080017 1.566808 1.147991 N -0.670197 -0.492702 3.207624 C -3.651472 0.875566 -0.192102 C -5.088948 0.707695 -0.151172 C -5.620870 -0.594825 -0.139528 C -4.800702 -1.750182 -0.166642 C -3.371281 -1.593000 -0.264018 C -2.510946 -2.766694 -0.260964 C -3.092137 -4.081213 -0.153257 C -4.522800 -4.193196 -0.090431 C -5.339150 -3.079742 -0.098780 C -0.517285 -1.336032 -0.575082 C -1.107714 -2.646840 -0.298428 C -0.243866 -3.772846 -0.192336 C -0.833405 -5.089098 -0.121362 C -2.236898 -5.207820 -0.107392 C -1.643052 2.358162 -0.010174 C -3.093401 2.184418 -0.158546 C -3.914209 3.348957 -0.164192 C -5.346217 3.155602 -0.165428 C -5.902941 1.896914 -0.139986 C -1.039852 3.691564 -0.122118 C -1.901682 4.823349 -0.128718 C -3.310525 4.633355 -0.137892 C 0.669238 1.389564 -0.534993 C 1.242882 2.698493 -0.206011 C 0.376864 3.829610 -0.108785 C 0.967461 5.146901 -0.021023 C 0.079430 6.281306 -0.018885 C -1.287433 6.130216 -0.089967 C 2.642747 2.815670 -0.111334 C 3.221982 4.130257 0.035489 C 2.369470 5.260027 0.048003 C 3.504151 1.639227 -0.110153 C 2.970699 0.339072 -0.207805 C 1.550721 0.178747 -0.530972

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		C 3.302328 1.772491 0.027828 C 2.387623 2.906058 0.026827 C 2.904768 4.246767 0.063774 C 4.337170 4.418962 0.156490 C 5.200898 3.347621 0.156648 C 0.453766 1.367258 -0.241794 C 0.989523 2.725275 -0.065948 C 0.083240 3.799130 -0.168497 C 0.603747 5.138500 -0.173503 C 1.999312 5.329335 -0.033848 C 1.756242 -2.261840 -0.298201 C 3.138510 -2.009737 -0.382558 C 4.029133 -3.118814 -0.589267 C 5.449818 -2.854758 -0.607929 C 5.960112 -1.593562 -0.405437 C 1.210532 -3.556070 -0.361550 C 2.096975 -4.666204 -0.577875 C 3.483166 -4.416178 -0.704738 C -0.581285 -1.360653 -0.178675 C -1.110376 -2.718265 0.011308 C -0.211132 -3.792378 -0.140173 C -0.731111 -5.131464 -0.140608 C 0.190984 -6.217438 -0.372713 C 1.532409 -5.996728 -0.593476 C -2.506129 -2.897204 0.130068 C -3.021800 -4.238170 0.177317 C -2.120881 -5.322069 0.047782 C -3.417925 -1.762068 0.144820 C -2.943040 -0.438745 0.020496 C -1.507457 -0.210333 -0.197628 C -0.984508 1.158916 0.207674 C -4.834989 -1.977757 0.224595 C -5.310060 -3.337762 0.337387 C -4.449160 -4.410951 0.312084 C -3.800813 0.677732 -0.069948 C -3.268810 2.020676 -0.271170 C -1.888408 2.271427 -0.242500 C -1.347901 3.564996 -0.326095 O 0.903260 0.758227 -1.474349 C -5.220240 0.458622 -0.020717 C -5.699952 -0.860679 0.147765 C -6.088336 1.600972 -0.189163 C -5.591069 2.865169 -0.397549 C -4.170708 3.131047 -0.432239 C -3.632391 4.430598 -0.556991 C -2.241447 4.677905 -0.491260 C -0.328321 6.227300 -0.354954 C -1.675983 6.007762 -0.518477 O -1.041667 -0.798689 -1.436501 O -1.065251 1.289740 1.628509 H 2.208573 -6.846754 -0.771882 H 4.165072 -5.269291 -0.854776

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	2E_2OH	C 5.431156 -3.067112 -0.113069 C 4.877261 -1.734452 -0.176719

		C 3.446520 -1.586327 -0.136824 C 2.600076 -2.769512 -0.031003 C 3.192018 -4.076710 0.063049 C 4.631883 -4.178699 0.014393 C 2.343732 -5.201652 0.168630 C 0.935224 -5.087647 0.172788 C 0.342861 -3.783298 0.049730 C 1.193877 -2.659879 -0.054523 C 0.603177 -1.336896 -0.306966 C -0.868072 -1.185347 -0.295228 C -1.709407 -2.365749 -0.053852 C -1.102885 -3.636807 0.043914 C -1.433658 0.143153 0.191135 C -2.899219 0.294212 -0.110507 C -3.696594 -0.861837 -0.140283 C -3.107701 -2.191002 -0.043503 C -1.944110 -4.797480 0.152864 C -3.346202 -4.628218 0.128623 C -3.949301 -3.354393 0.023142 C 1.431202 -0.143840 0.149546 C 0.860088 1.191379 -0.295188 C -0.612926 1.335975 -0.280945 C -1.198567 2.660811 -0.035758 C -2.603443 2.769897 -0.015553 C -3.447901 1.587265 -0.122625 C -5.126820 -0.719960 -0.197937 C -5.937253 -1.915369 -0.165604 C -5.379608 -3.166475 -0.047435 C 0.056725 -6.229192 0.281144 C -1.311419 -6.090628 0.269704 C 2.897159 -0.290262 -0.130569 C -4.877682 1.736115 -0.175856 C -5.681475 0.577271 -0.226662 C -3.194225 4.077471 0.067784 C -4.633762 4.180659 0.011910 C -5.431981 3.068854 -0.117922 C 1.706666 2.368565 -0.058396 C 1.098185 3.638783 0.045015 C -0.348079 3.783973 0.057208 C -0.939110 5.089064 0.176268 C -2.346933 5.203747 0.171809 C 1.940305 4.799479 0.151300 C 1.308484 6.093207 0.268261 C -0.059701 6.230206 0.280656 C 3.342871 4.631157 0.124819 C 3.946952 3.358376 0.018177 C 3.105086 2.195492 -0.052679 C 3.695332 0.868245 -0.150963 C 5.377225 3.169747 -0.047620 C 5.936884 1.919103 -0.162562 C 5.125597 0.724378 -0.198946 C 5.679217 -0.574142 -0.222988

		O -0.135342 -1.260555 -1.544692 O -1.407885 0.127376 1.634732 O 0.118981 1.256253 -1.529556 O 1.313669 -0.077529 1.622441 H -6.526980 3.178910 -0.160916 H -6.777540 0.688681 -0.252783 H -7.031625 -1.803135 -0.218394 H -6.025888 -4.057394 -0.009680 H -5.087955 5.182319 0.069083 H -2.800005 6.205929 0.240025 H -3.991647 -5.519548 0.184956 H -0.512261 7.230273 0.370926 H -1.955472 -6.980308 0.351730 H 7.031332 1.806761 -0.210314 H 6.775466 -0.685214 -0.241805 H 6.526257 -3.177215 -0.150274 H 5.086100 -5.180062 0.075665 H 6.023290 4.060746 -0.007285 H 3.987470 5.523059 0.181651 H 2.796642 -6.203661 0.240341 H 1.952653 6.982905 0.348296 H 0.509315 -7.229000 0.372601 H -0.457563 0.033997 1.891263 H 1.856687 -0.804575 1.982425
	SC2’	C -2.078193 5.274526 -0.409741 C -0.677828 5.121261 -0.321174 C -0.125889 3.794214 -0.264752 C -0.998498 2.690829 -0.289560 C -2.394144 2.841917 -0.372583 C -2.952093 4.167231 -0.422715 C 1.311760 3.617035 -0.118174 C 2.173756 4.760663 0.005697 C 1.577907 6.074382 -0.059768 C 0.224411 6.245626 -0.229210 C -0.436807 1.327251 0.003730 C 1.018296 1.182033 -0.420304 C 1.887896 2.331120 -0.133066 C 3.276133 2.120381 0.018076 C 4.133981 3.262714 0.180800 C 3.562864 4.554566 0.159498 C 3.838423 0.780216 0.030762 C 5.253599 0.595064 0.203620 C 6.082460 1.767689 0.359015 C 5.550498 3.035572 0.348666 C 3.016734 -0.360148 -0.104835 C 1.588717 -0.183276 -0.402013 C -1.318554 0.198304 -0.518455 C -0.747378 -1.166487 -0.497510 C 0.671176 -1.315904 0.040643 C 1.252744 -2.676025 -0.227360 C 2.649764 -2.824450 -0.198270 C 3.530579 -1.671807 -0.067976

		C 4.949954 -1.855617 0.064204 C 5.775351 -0.717518 0.204783 C -1.637744 -2.316033 -0.281239 C -1.063116 -3.602070 -0.227442 C 0.382224 -3.777518 -0.275052 C 0.936326 -5.104689 -0.300899 C 2.338872 -5.256798 -0.291810 C 3.210544 -4.148888 -0.227830 C 4.644876 -4.290332 -0.131033 C 5.470677 -3.201989 0.021921 C -3.283045 1.688490 -0.329690 C -2.767712 0.375007 -0.342696 C -3.596215 -0.767273 -0.254980 C -3.033352 -2.107318 -0.224728 C -3.899531 -3.249191 -0.109795 C -3.327505 -4.540553 -0.093844 C -1.931120 -4.746375 -0.162209 C -1.332511 -6.060256 -0.193710 C 0.029445 -6.228677 -0.275531 C -4.708899 1.872712 -0.278392 C -5.540013 0.732966 -0.183971 C -5.019571 -0.581171 -0.157808 C -5.856370 -1.753536 -0.043506 C -5.323376 -3.021163 -0.022772 C -4.389687 4.308023 -0.425492 C -5.225818 3.219963 -0.340016 O 1.343053 0.506128 -1.652603 O 0.592999 -1.268892 1.484655 O -0.360164 1.223977 1.457009 O -0.983694 -0.481388 -1.750380 N -2.625061 0.526751 2.785514 N -2.364254 -0.854887 3.109171 H 0.458053 -7.242908 -0.301415 H 2.765974 -6.272654 -0.296652 H 5.070682 -5.305562 -0.161350 H 6.559248 -3.343618 0.110769 H -3.992463 -5.417196 -0.034010 H 6.862954 -0.858638 0.311958 H -5.986904 -3.896007 0.063510 H 7.166761 1.625892 0.490315 H -4.812117 5.323977 -0.474591 H -2.503542 6.290798 -0.434904 H -0.201378 7.260046 -0.279274 H 2.238528 6.951701 0.023224 H -6.317726 3.361982 -0.322576 H -6.631918 0.873763 -0.136465 H 4.223399 5.430981 0.258786 H -6.946294 -1.611781 0.026089 H 6.207915 3.910594 0.471637 H 0.346223 -0.323141 1.694461 H -1.282908 1.116528 1.885819 H -1.996527 -6.938025 -0.157082

		H -1.628309 -1.190533 2.479398 H -3.194368 -1.424240 2.927014 H -2.830962 1.017024 3.658346 H -3.436651 0.631219 2.167733
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		H 7.081714 -1.249947 0.159475 H -7.083435 -1.240488 0.159696 H 2.516274 6.551987 -1.440645 H 0.004385 6.560940 -1.441641 H -2.507483 6.555242 -1.440726 H -4.647025 5.364555 -1.017579 H 4.654279 5.358535 -1.017350 H 5.872550 3.281447 -0.279973 H -5.868065 3.289202 -0.280091 H 7.083437 1.240486 0.159644 H -7.081713 1.249945 0.159553 H 4.647015 -5.364545 -1.017676
	int1’	N 2.060073 0.452679 2.618257 C 1.957612 -2.068870 -0.261470 C 0.927458 -1.045623 -0.495973 C -0.463402 -1.370876 0.038816 O -0.398601 -1.271429 1.476022 N 1.945366 -0.680605 3.149448 C 1.556093 -3.419265 -0.191033 C 2.566661 -4.439833 -0.114018 C 3.925355 -4.054666 -0.055345 C 4.325921 -2.700941 -0.083554 C 3.316642 -1.681937 -0.200797 C 3.701561 -0.279577 -0.228171 C 5.088910 0.089570 -0.132498 C 6.071788 -0.963879 -0.031766 C 5.708215 -2.290052 -0.008084 C 1.313355 0.381021 -0.517203 C 2.725853 0.747305 -0.307350 C 3.066579 2.120281 -0.266688 C 4.457720 2.484475 -0.209235 C 5.430064 1.460697 -0.142696 C -0.859673 -2.800038 -0.207915 C 0.146595 -3.780719 -0.237038 C -0.228236 -5.169409 -0.248209 C 0.816815 -6.165046 -0.204763 C 2.145521 -5.820677 -0.126377 C -2.225672 -3.131758 -0.195476 C -2.607380 -4.519125 -0.212406 C -1.598380 -5.504415 -0.248584 C -1.518351 -0.371945 -0.423434 C -2.914098 -0.736813 -0.142891 C -3.252498 -2.104007 -0.097934 C -4.637567 -2.471865 0.014731 C -4.976069 -3.875316 -0.015613 C -4.011939 -4.847516 -0.136530 C -3.881138 0.285439 -0.020624 C -5.262891 -0.082773 0.128171 C -5.608381 -1.452229 0.128147 C -3.497601 1.687096 -0.016622 C -2.144773 2.075108 -0.136759 C -1.129720 1.050701 -0.418421

		C 0.293332 1.375114 0.045707 C -4.500013 2.706544 0.135845 C -5.878351 2.297015 0.269807 C -6.241079 0.970787 0.265691 C -1.741217 3.425034 -0.094830 C -0.336028 3.789427 -0.207578 C 0.671539 2.807151 -0.232403 C 2.035501 3.146375 -0.294838 O 1.094969 -0.337129 -1.750097 C -2.746896 4.445539 0.023673 C -4.100976 4.061239 0.141050 C -2.326009 5.826254 -0.008656 C -1.003037 6.174676 -0.142255 C 0.039114 5.178511 -0.231420 C 1.407892 5.517494 -0.293679 C 2.417733 4.533225 -0.314650 C 4.796012 3.887735 -0.240709 C 3.824540 4.859004 -0.304981 O -1.351362 0.352327 -1.669059 O 0.283160 1.239450 1.457467 H -4.299833 -5.910364 -0.157471 H -1.889088 -6.567350 -0.243367 H 0.523568 -7.226637 -0.216839 H 2.918313 -6.603694 -0.078868 H -6.038092 -4.157851 0.057586 H -6.669725 -1.734756 0.217513 H 4.698131 -4.837632 0.007606 H -7.300070 0.688172 0.373882 H 6.480065 -3.071451 0.072844 H -0.711793 7.236516 -0.167307 H 1.696398 6.580965 -0.297358 H 4.111897 5.922054 -0.330403 H 5.860153 4.170016 -0.216724 H -3.097163 6.608656 0.070681 H -4.871047 4.844026 0.233494 H 6.494230 1.743062 -0.095202 H -6.646145 3.078860 0.380710 H 7.134335 -0.681449 0.030702 H -0.225291 -0.278352 1.642854 H 2.352821 -1.378775 2.500609 H 1.629460 1.262427 3.077095 H 2.527425 0.641405 1.708390
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		C 3.297658 -1.711142 -0.197003 C 3.696264 -0.312633 -0.233415 C 5.088202 0.044246 -0.143460 C 6.060760 -1.018548 -0.039976 C 5.684274 -2.341069 -0.009907 C 1.313413 0.368444 -0.516062 C 2.730556 0.723217 -0.315425 C 3.083426 2.092071 -0.279723 C 4.477718 2.444092 -0.228706 C 5.441798 1.411878 -0.160761 C -0.889017 -2.792596 -0.213265 C 0.108929 -3.781656 -0.241160 C -0.278468 -5.166844 -0.256749 C 0.757615 -6.171680 -0.212820 C 2.089203 -5.839191 -0.129834 C -2.257906 -3.111705 -0.202763 C -2.652101 -4.495453 -0.223423 C -1.651737 -5.489544 -0.260952 C -1.524853 -0.358398 -0.420353 C -2.924203 -0.710447 -0.141706 C -3.275153 -2.074616 -0.101445 C -4.663494 -2.429971 0.010948 C -5.014821 -3.830183 -0.023997 C -4.059752 -4.810919 -0.148520 C -3.881493 0.320493 -0.016586 C -5.266410 -0.035353 0.133095 C -5.624583 -1.401597 0.129257 C -3.485087 1.718583 -0.010881 C -2.129169 2.094639 -0.133978 C -1.123878 1.061179 -0.417532 C 0.301479 1.373033 0.047270 C -4.477565 2.746977 0.146162 C -5.859309 2.349800 0.282766 C -6.234358 1.026993 0.275737 C -1.712804 3.440555 -0.090630 C -0.304420 3.792574 -0.207656 C 0.694289 2.801731 -0.234395 C 2.061120 3.127343 -0.303829 O 1.085006 -0.349220 -1.746546 C -2.708670 4.470104 0.032119 C -4.065914 4.097945 0.152851 C -2.275104 5.846962 -0.000521 C -0.949645 6.183631 -0.139836 C 0.083147 5.178254 -0.234059 C 1.454646 5.504296 -0.302934 C 2.455492 4.510733 -0.328050 C 4.828331 3.843980 -0.264752 C 3.865091 4.823793 -0.326095 O -1.351224 0.364328 -1.666703 O 0.292949 1.231971 1.455024 H -4.357758 -5.870912 -0.172615 H -1.951994 -6.549847 -0.258939

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Route 3	SC3	C 3.927439 -4.017198 -0.417697 C 2.569443 -4.411417 -0.339046 C 1.554355 -3.397378 -0.175496 C 1.948094 -2.046051 -0.135129 C 3.306687 -1.641611 -0.312097 C 4.322445 -2.666770 -0.406948 C 0.951792 -1.037412 0.227585 C -0.499706 -1.436068 0.300530 C -0.871710 -2.817881 -0.009125 C 0.148781 -3.781879 -0.116824 C -1.482711 -0.364202 -0.030783 C -2.919131 -0.753852 -0.205374 C -3.276372 -2.172899 -0.066875 C -2.256623 -3.162683 -0.081839 C -1.177049 1.048488 0.337750 C -2.200695 2.057802 0.059328 C -3.569611 1.653808 -0.015784 C -3.946089 0.283486 -0.033015 C -4.589769 2.679607 -0.043435 C -4.196358 4.030045 -0.083854 C -2.836071 4.423375 -0.105823 C -1.811806 3.408841 -0.019563 C -0.406321 3.793247 -0.078826 C -0.048048 5.185536 -0.215816 C -1.099326 6.160047 -0.256402 C -2.431516 5.795651 -0.205041 C 0.275667 1.445420 0.266941 C 0.618811 2.828590 -0.065939 C 1.993269 3.174160 -0.245423 C 2.347522 4.575197 -0.314864 C 1.321292 5.537840 -0.297625 C -5.311720 -0.117071 0.008969

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	ts1	C -1.033524 5.587956 -0.289833 C 0.310359 5.172736 -0.216964

		C 0.611848 3.765410 -0.091585 C -0.457077 2.848360 -0.040086 C -1.814742 3.257703 -0.200514 C -2.103528 4.665410 -0.296845 C -0.173490 1.438856 0.254477 C 1.246374 0.974468 0.213222 C 2.324615 1.949463 -0.020495 C 1.991587 3.317495 -0.060509 C 1.458312 -0.441412 -0.234082 C 2.935758 -0.884426 -0.327577 C 3.985535 0.100996 -0.031461 C 3.667791 1.488760 -0.040235 C 0.445533 -1.450211 -0.081256 C 0.743542 -2.775372 -0.162714 C 2.132853 -3.226886 -0.174458 C 3.196791 -2.316381 -0.138680 C 2.410703 -4.653049 -0.132959 C 1.352780 -5.564970 -0.190836 C -0.015420 -5.143746 -0.235657 C -0.330188 -3.761842 -0.177194 C -1.695908 -3.330560 -0.205431 C -2.764609 -4.292116 -0.355984 C -2.413491 -5.680545 -0.423687 C -1.097282 -6.095054 -0.353727 C -0.926456 -1.015547 0.462466 C -2.012974 -1.957072 -0.069001 C -3.349206 -1.505608 -0.205457 C -4.416530 -2.470244 -0.352071 C -4.097266 -3.838215 -0.407736 C 4.567562 -2.733476 0.018828 C 4.819583 -4.153835 0.054174 C 3.790844 -5.063519 -0.042587 C 5.315402 -0.362610 0.099917 C 5.578597 -1.770986 0.098230 C 4.733416 2.465209 -0.006593 C 6.084421 1.977626 0.095605 C 6.361686 0.629416 0.171496 C 3.062029 4.285765 -0.106942 C 4.401563 3.834129 -0.054340 C -1.184995 0.402022 -0.090076 C 1.413297 6.100503 -0.253474 C 2.719098 5.677664 -0.195997 C -2.877420 2.304181 -0.251699 C -2.566596 0.867864 -0.348707 C -3.668956 -0.101778 -0.214821 C -3.485188 5.065164 -0.372417 C -4.504446 4.140089 -0.376953 C -4.238372 2.720560 -0.335815 C -5.273615 1.756212 -0.408879 C -5.016090 0.362705 -0.349187 C -5.769143 -1.978553 -0.442559 C -6.062228 -0.631989 -0.426591

		O 2.153685 -0.528041 -1.495204 O 0.568848 1.175178 1.467799 O -0.959507 -1.082713 1.918634 O -1.607865 0.513635 -1.454734 N -3.415049 0.473849 2.656229 N -2.607547 -0.444786 3.146084 H 7.403903 0.285156 0.260611 H 6.623920 -2.102840 0.180074 H 5.863264 -4.501789 0.145333 H 4.014149 -6.148871 -0.023612 H 6.905178 2.711316 0.124297 H 5.212638 4.579997 -0.048088 H 1.575639 -6.644114 -0.196460 H 3.535827 6.415736 -0.228036 H -0.848765 -7.161317 -0.404453 H -5.552464 4.473909 -0.436597 H -6.316638 2.099251 -0.505840 H -7.106462 -0.295302 -0.502091 H -6.586371 -2.712743 -0.534545 H -3.716213 6.140642 -0.432046 H -1.254222 6.665708 -0.352476 H -4.914812 -4.579535 -0.501787 H 1.178209 7.174886 -0.333934 H -3.213692 -6.422666 -0.526011 H -2.969554 1.374273 2.444280 H -4.190950 0.176940 1.935804 H -3.147734 -1.326387 3.157746 H -1.561849 -0.784459 2.319216
	int1	C -0.003280 5.712909 -0.128041 C 1.249784 5.068933 -0.064207 C 1.295641 3.627936 0.018002 C 0.085033 2.907975 0.056951 C -1.177646 3.549910 -0.106806 C -1.217430 4.992963 -0.172060 C 0.128970 1.463894 0.308926 C 1.443721 0.760548 0.206234 C 2.665267 1.539432 -0.020631 C 2.582954 2.945107 0.005352 C 1.389807 -0.660105 -0.238794 C 2.771551 -1.357181 -0.360172 C 3.979182 -0.569006 -0.084874 C 3.914156 0.855582 -0.062901 C 0.220247 -1.469017 0.045840 C 0.288375 -2.845517 -0.090075 C 1.576439 -3.524195 -0.158424 C 2.784661 -2.806752 -0.164684 C 1.608689 -4.973217 -0.108065 C 0.406929 -5.691536 -0.121288 C -0.865231 -5.047075 -0.152196 C -0.931527 -3.625478 -0.092381 C -2.203233 -2.961001 -0.140659 C -3.412342 -3.726609 -0.318407

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		H 2.453475 6.896032 -0.115763 H -4.236622 -5.748099 -0.461696 H -3.433395 1.285967 2.372901 H -4.997124 0.744723 1.837923 H -4.496931 -1.311065 2.482607 H -2.048519 -0.925146 2.201304
	ts2	C 0.335410 5.715120 -0.141666 C 1.548680 4.998491 -0.082142 C 1.510041 3.557429 0.000842 C 0.259313 2.910063 0.036030 C -0.964450 3.625639 -0.116578 C -0.919743 5.068639 -0.175646 C 0.217275 1.465648 0.284703 C 1.488213 0.686453 0.201311 C 2.755585 1.392061 -0.016354 C 2.755216 2.800217 -0.000979 C 1.356108 -0.729747 -0.238744 C 2.695912 -1.505902 -0.347421 C 3.944765 -0.789501 -0.061814 C 3.962765 0.636554 -0.045522 C 0.138120 -1.467198 0.038138 C 0.127028 -2.845182 -0.106769 C 1.373811 -3.598479 -0.162604 C 2.622190 -2.953357 -0.152324 C 1.320749 -5.047086 -0.119475 C 0.079417 -5.693852 -0.154049 C -1.152139 -4.975417 -0.198676 C -1.135265 -3.553121 -0.131774 C -2.364531 -2.813139 -0.187785 C -3.616465 -3.506031 -0.372606 C -3.600259 -4.940626 -0.421187 C -2.418950 -5.645575 -0.323840 C -1.111412 -0.715715 0.432051 C -2.363115 -1.399345 -0.073225 C -3.544628 -0.645879 -0.293323 C -4.801795 -1.344289 -0.452190 C -4.808889 -2.751474 -0.471991 C 3.855313 -3.677217 0.016092 C 3.775269 -5.117931 0.060633 C 2.567898 -5.768220 -0.027200 C 5.133496 -1.544387 0.098917 C 5.068089 -2.973185 0.107750 C 5.222709 1.337667 0.028777 C 6.422040 0.553321 0.145339 C 6.377535 -0.823498 0.207372 C 4.019665 3.496487 -0.021316 C 5.216256 2.749928 0.017907 C -1.013232 0.713494 -0.097003 C 2.833179 5.651403 -0.095899 C 4.008870 4.937004 -0.058459 C -2.217974 2.950989 -0.216561 C -2.247383 1.483192 -0.342847

		C -3.540182 0.783116 -0.261104 C -2.166749 5.776777 -0.267558 C -3.371995 5.108811 -0.322124 C -3.436499 3.668944 -0.317762 C -4.675363 2.959658 -0.442712 C -4.742595 1.555042 -0.428539 C -6.007822 -0.554438 -0.556816 C -5.986104 0.823153 -0.537708 O 1.977384 -0.995899 -1.503073 O 0.875585 0.985617 1.475997 O -1.198417 -0.641269 1.884104 O -1.380306 0.945623 -1.457517 N -4.056642 0.468710 2.290132 N -3.881924 -0.773146 2.647975 H 7.308394 -1.400476 0.323134 H 6.006415 -3.541263 0.209103 H 4.709437 -5.692184 0.162002 H 2.529798 -6.868598 -0.002611 H 7.388576 1.077749 0.204715 H 6.177577 3.287324 0.054325 H 0.049289 -6.795228 -0.152468 H 4.975342 5.464958 -0.067671 H -2.427621 -6.746096 -0.363300 H -4.313213 5.675841 -0.396592 H -5.605806 3.538432 -0.553375 H -6.924069 1.392549 -0.632879 H -6.966823 -1.085811 -0.664854 H -2.143811 6.877348 -0.301242 H 0.368426 6.815926 -0.179501 H -5.768742 -3.281842 -0.582014 H 2.857559 6.751546 -0.140405 H -4.556206 -5.474283 -0.540626 H -3.279635 1.108191 2.456726 H -4.921575 0.849477 1.899700 H -4.716089 -1.301963 2.354418 H -2.071512 -1.026191 2.149157
	3E_1OH_N_2H_3	C 2.423469 -5.028559 -0.342061 C 1.021906 -5.005468 -0.251517 C 0.347382 -3.736706 -0.114841 C 1.116979 -2.556938 -0.058723 C 2.529167 -2.571445 -0.219269 C 3.198758 -3.841844 -0.337624 C 0.440545 -1.284070 0.219591 C -1.043829 -1.233565 0.174116 C -1.805781 -2.472886 -0.034436 C -1.108569 -3.695560 -0.073625 C -1.649846 0.066755 -0.229212 C -3.206387 0.073753 -0.288218 C -3.922966 -1.169915 0.009455 C -3.227652 -2.416520 -0.013494 C -0.953263 1.305191 0.048384 C -1.635726 2.509734 -0.057269

		C -3.092128 2.543184 -0.078258 C -3.854454 1.363543 -0.059721 C -3.766119 3.825975 -0.000179 C -3.009819 5.000857 -0.031278 C -1.582644 4.987870 -0.097220 C -0.892799 3.748560 -0.065719 C 0.547542 3.714575 -0.128548 C 1.286290 4.949865 -0.272175 C 0.551879 6.188274 -0.298013 C -0.819567 6.207453 -0.201386 C 0.507668 1.265105 0.422279 C 1.245710 2.494049 -0.049604 C 2.653697 2.444594 -0.196116 C 3.395042 3.679251 -0.313946 C 2.689588 4.903719 -0.341771 C -5.279779 1.377156 0.153202 C -5.926290 2.667031 0.226463 C -5.204635 3.831156 0.128999 C -5.321699 -1.109216 0.218390 C -5.976945 0.163785 0.258100 C -3.971667 -3.650379 0.061642 C -5.396277 -3.569290 0.232379 C -6.039058 -2.353646 0.337624 C -1.862312 -4.926125 -0.098750 C -3.266773 -4.873648 -0.005047 C 1.144279 -0.012125 -0.122081 C 0.226714 -6.212453 -0.277863 C -1.142449 -6.174456 -0.194813 C 3.300954 -1.356939 -0.248147 C 2.599309 -0.057421 -0.340375 C 3.372511 1.196428 -0.222684 C 4.627049 -3.846217 -0.433646 C 5.345405 -2.664667 -0.395001 C 4.693375 -1.395094 -0.303369 C 5.530354 -0.135457 -0.159583 C 4.760416 1.166617 -0.259025 C 4.826196 3.611393 -0.368778 C 5.486070 2.399701 -0.308607 O -2.362000 -0.000191 -1.468332 O -0.339013 -1.207994 1.455960 O 0.693581 1.284231 1.869602 O 1.619222 -0.004983 -1.469407 N 5.466446 -0.201959 2.314719 N 6.271101 -0.113578 1.145626 H -7.128549 -2.317563 0.493513 H -7.069761 0.187470 0.393868 H -7.018937 2.698891 0.358807 H -5.716703 4.804919 0.177221 H -5.971745 -4.505916 0.296165 H -3.833976 -5.817663 0.029495 H -3.527988 5.972740 -0.001496 H -1.723688 -7.109642 -0.210624

		H -1.363170 7.164978 -0.217381 H 6.445444 -2.695495 -0.456942 H 6.332751 -0.142676 -0.930738 H 6.585623 2.361372 -0.310216 H 5.395420 4.550746 -0.447553 H 5.148467 -4.810448 -0.536837 H 2.938738 -5.999066 -0.422964 H 3.256095 5.845900 -0.414827 H 0.749865 -7.177387 -0.365574 H 1.115516 7.129656 -0.391854 H 5.077660 0.726687 2.491440 H 4.669244 -0.841605 2.181800 H 6.928874 -0.894834 1.175234 H 0.200757 0.499422 2.192676
	SC3’	C -5.646156 -1.245788 -0.765495 C -4.708160 -0.171253 -0.651348 C -3.352145 -0.460850 -0.582859 C -2.877134 -1.820324 -0.581121 C -3.829174 -2.892257 -0.764446 C -5.220911 -2.556765 -0.857643 C -3.361681 -4.226089 -0.801848 C -1.996180 -4.535707 -0.673293 C -1.048894 -3.464484 -0.455965 C -1.511726 -2.136917 -0.370653 C -0.584901 -1.082000 0.178606 C 0.859781 -1.382594 -0.121716 C 1.312000 -2.690434 -0.238072 C 0.354615 -3.768292 -0.325585 C -0.947666 0.307551 -0.339310 C -0.040332 1.415525 0.082894 C 1.408551 1.089734 0.109352 C 1.786332 -0.287769 -0.315729 C 2.396431 2.171041 -0.012533 C 1.940080 3.502884 -0.041757 C 0.521332 3.815744 -0.154049 C -0.454740 2.799200 -0.178970 C -1.829542 3.080759 -0.404252 C -2.246308 4.456146 -0.508493 C -1.265487 5.476927 -0.434679 C 0.101026 5.190822 -0.277407 C 2.908460 4.571601 0.015899 C 2.438044 5.934167 -0.070741 C 1.105794 6.228440 -0.220706 C -2.357135 0.629807 -0.618539 C -2.810157 2.033377 -0.506979 C -4.168458 2.329560 -0.615703 C -4.569039 3.699960 -0.694112 C -3.643299 4.727816 -0.666959 C 3.315962 -0.583455 -0.296565 C 4.231189 0.495737 0.085844 C 3.779961 1.850115 0.076634 C 4.733765 2.921053 0.234657

		C 4.271645 4.255513 0.178234 C 2.735812 -2.994190 -0.188594 C 3.700400 -1.977810 -0.086980 C 5.084188 -2.262901 0.196899 C 5.986038 -1.203871 0.383757 C 5.580779 0.169660 0.361378 C 6.507931 1.254590 0.563689 C 6.107243 2.571076 0.472659 C 0.803674 -5.113642 -0.366422 C 2.198187 -5.394260 -0.233504 C 3.155759 -4.381876 -0.124286 C 4.559258 -4.658365 0.075298 C 5.476590 -3.652251 0.252477 C -1.503642 -5.888616 -0.705746 C -0.166226 -6.165951 -0.546805 C -5.221507 1.245073 -0.498777 O 0.640414 1.157111 1.355186 O 2.567746 -0.317709 -1.513242 O -0.839290 -1.106224 1.625865 N -3.814438 -1.944794 3.949072 N -3.829342 -1.478948 2.584746 O -1.345966 0.426796 -1.704357 N -5.929499 1.320734 0.829113 N -5.111502 1.273783 1.985350 H 7.561602 1.011771 0.772032 H 7.046408 -1.434818 0.572691 H 6.535444 -3.890555 0.438245 H 4.879504 -5.711328 0.112028 H 6.841229 3.381908 0.600094 H 5.000499 5.076023 0.276053 H 2.525514 -6.446083 -0.213427 H 3.181567 6.744919 -0.023444 H 0.190133 -7.207556 -0.569611 H -5.641040 3.935253 -0.793961 H -6.023255 1.425870 -1.248244 H -6.719385 -1.004865 -0.786549 H -5.951593 -3.370628 -0.984586 H -3.972111 5.774434 -0.760622 H -1.587260 6.528293 -0.505676 H -4.089303 -5.044019 -0.926356 H 0.775739 7.275998 -0.299228 H -2.226461 -6.705681 -0.856072 H -4.813844 0.297553 2.155308 H -4.258192 1.840849 1.874003 H -6.469128 2.188187 0.864722 H -0.249168 -0.408746 1.988397 H -4.262670 -2.211717 2.019068 H -2.876505 -1.339607 2.226025 H -3.861781 -1.117636 4.547049 H -2.927062 -2.414039 4.158645
	ts3	C -5.553574 -1.849391 -0.737730 C -4.725523 -0.691185 -0.659906

		C -3.339451 -0.843721 -0.704505 C -2.738496 -2.144186 -0.716908 C -3.582893 -3.306169 -0.812234 C -5.001064 -3.113908 -0.852138 C -2.988438 -4.594863 -0.811770 C -1.601954 -4.771736 -0.680730 C -0.753827 -3.609834 -0.534194 C -1.329796 -2.316984 -0.545029 C -0.493978 -1.182449 -0.244296 C 0.915652 -1.342238 -0.253575 C 1.506035 -2.617384 -0.263854 C 0.662316 -3.772347 -0.359002 C -1.021257 0.167295 -0.560912 C -0.230487 1.346162 -0.098816 C 1.241751 1.173487 -0.026560 C 1.777225 -0.163432 -0.406383 C 2.117465 2.346990 -0.139962 C 1.533511 3.625889 -0.198445 C 0.090568 3.795650 -0.318357 C -0.778132 2.687278 -0.348333 C -2.181205 2.835601 -0.513880 C -2.740569 4.161457 -0.570774 C -1.862037 5.273938 -0.531704 C -0.468652 5.122826 -0.421012 C 2.391290 4.785607 -0.143074 C 1.787146 6.093168 -0.240495 C 0.430422 6.253983 -0.378595 C -2.468871 0.348929 -0.770496 C -3.053700 1.694215 -0.569952 C -4.439761 1.849488 -0.563454 C -4.984623 3.171781 -0.600033 C -4.166356 4.288256 -0.636915 C 3.285621 -0.316361 -0.309735 C 4.097690 0.858558 0.042886 C 3.523529 2.162423 -0.015625 C 4.367835 3.325393 0.120530 C 3.778453 4.606679 0.032118 C 2.942405 -2.775301 -0.128745 C 3.804005 -1.663454 -0.047262 C 5.201053 -1.805165 0.252996 C 6.002379 -0.655759 0.401380 C 5.472356 0.670327 0.325721 C 6.292018 1.844891 0.493931 C 5.767678 3.114324 0.369820 C 1.237922 -5.080875 -0.312722 C 2.637301 -5.218502 -0.117429 C 3.491768 -4.110248 -0.008735 C 4.907099 -4.243100 0.231600 C 5.722208 -3.145560 0.376080 C -0.986170 -6.074087 -0.641160 C 0.369336 -6.221328 -0.458746 C -5.329054 0.652193 -0.314210

		O 0.432733 1.166763 1.186689 O 2.582255 -0.156702 -1.593248 O -1.078893 -1.122754 1.770399 N -2.921316 -0.248649 4.520953 N -2.497116 -1.391847 3.851828 O -1.517219 0.323097 -1.909193 N -5.661546 0.587607 1.169166 N -4.535446 0.414117 2.019531 H 7.363904 1.709606 0.707103 H 7.077678 -0.781099 0.604524 H 6.795847 -3.274126 0.584027 H 5.326375 -5.257817 0.317196 H 6.420718 3.994459 0.477191 H 4.422943 5.496223 0.118927 H 3.065418 -6.231290 -0.046026 H 2.446460 6.974449 -0.202500 H 0.816769 -7.226943 -0.422597 H -6.079790 3.296087 -0.619872 H -6.311176 0.781626 -0.815376 H -6.646345 -1.723863 -0.698608 H -5.652100 -3.998027 -0.934625 H -4.605949 5.295711 -0.702078 H -2.287576 6.289259 -0.577596 H -3.638594 -5.480883 -0.889729 H -0.001672 7.264028 -0.454284 H -1.630422 -6.960586 -0.749673 H -4.275132 -0.576287 1.983849 H -3.714244 0.940118 1.676313 H -6.103715 1.470597 1.437967 H -0.404230 -0.466046 2.035450 H -1.847348 -1.897096 4.459957 H -1.975865 -1.242001 2.871102 H -3.630955 0.241019 3.965630 H -2.179031 0.387708 4.834181
	3E_N_2H_3	C 5.401249 2.566720 -0.072662 C 4.725452 1.323214 -0.221420 C 3.329286 1.313099 -0.306111 C 2.575799 2.527268 -0.197349 C 3.271678 3.777174 -0.068846 C 4.698255 3.759286 -0.017478 C 2.529158 4.989011 0.024569 C 1.130290 5.008016 0.025879 C 0.409351 3.756890 -0.060068 C 1.131785 2.530786 -0.174069 C 0.396721 1.312859 -0.235460 C -0.997356 1.309440 -0.194464 C -1.738089 2.520103 -0.089355 C -1.022807 3.751864 -0.018970 C 1.127799 0.038978 -0.463049 C 0.457463 -1.207445 0.029297 C -1.028210 -1.210203 0.075833 C -1.729787 0.031834 -0.378470

		C -1.754264 -2.491136 -0.005782 C -1.017975 -3.691015 0.013675 C 0.440639 -3.689879 -0.037408 C 1.176071 -2.488725 -0.103388 C 2.597069 -2.474868 -0.167482 C 3.302313 -3.730185 -0.114164 C 2.558285 -4.935013 -0.053430 C 1.154344 -4.945212 -0.027330 C -1.732632 -4.943489 0.079618 C -0.975703 -6.171981 0.082412 C 0.395888 -6.174076 0.030504 C 2.615741 0.029190 -0.513320 C 3.341714 -1.244632 -0.253999 C 4.734202 -1.248015 -0.218712 C 5.418154 -2.500793 -0.133856 C 4.731994 -3.701134 -0.101993 C -3.222500 0.014278 -0.300612 C -3.912994 -1.254053 0.019401 C -3.178879 -2.476870 0.041629 C -3.884078 -3.731217 0.158066 C -3.139944 -4.930699 0.162048 C -3.183110 2.503776 -0.013830 C -3.916996 1.290533 -0.045345 C -5.329170 1.263838 0.154025 C -6.008468 0.015620 0.225024 C -5.320950 -1.233645 0.193016 C -6.002023 -2.498432 0.327503 C -5.315657 -3.692590 0.291956 C -1.751423 4.994420 0.107292 C -3.154003 4.962220 0.185165 C -3.886787 3.751646 0.144740 C -5.316679 3.715528 0.277306 C -6.009523 2.523722 0.295127 C 0.371031 6.231439 0.131028 C -1.001924 6.223918 0.169501 C 5.555419 0.044369 -0.295270 O -0.246261 -1.017639 1.278612 O -2.482630 -0.066946 -1.585843 O 1.794121 -0.054183 -1.729398 N 6.637250 0.117405 0.698714 N 6.258011 -0.028456 2.050446 H -7.096447 -2.493865 0.449773 H -7.102414 0.014790 0.352163 H -7.103224 2.520496 0.423416 H -5.856086 4.669536 0.385158 H -5.860086 -4.645803 0.379584 H -3.676147 -5.889768 0.245526 H -3.703600 5.910565 0.298411 H -1.528667 -7.123198 0.129900 H -1.558916 7.169882 0.257474 H 6.519092 -2.507004 -0.106333 H 6.069407 0.043925 -1.287116

		H 6.498492 2.548924 0.004371 H 5.236251 4.715232 0.081053 H 5.282365 -4.654042 -0.061714 H 3.101528 -5.892865 -0.015897 H 3.079991 5.939356 0.110607 H 0.949144 -7.126144 0.035248 H 0.922520 7.182892 0.187826 H 5.880290 0.872792 2.371540 H 5.493999 -0.720785 2.156957 H 7.392514 -0.541801 0.485426
	3E_1OH_N_2H_2	C 4.670032 -1.737879 -0.199929 N 5.569777 -0.722253 1.693091 C 5.503407 -0.490473 0.262616 C 4.883074 0.842234 -0.102383 C 5.692442 2.020661 -0.165567 C 5.117621 3.268087 -0.335700 C 3.693815 3.435035 -0.352380 C 2.867969 2.256067 -0.240551 C 3.498955 0.964006 -0.202774 C 3.270245 -1.574186 -0.232983 C 2.657770 -0.243251 -0.364547 C 1.203029 -0.100673 -0.172117 C 0.660721 1.214570 0.379669 C 1.464826 2.393440 -0.110341 C 0.848651 3.655455 -0.201526 C 1.668717 4.837364 -0.364324 C 3.067091 4.701869 -0.419891 C -0.585034 3.782745 -0.121999 C -1.194236 5.063376 -0.165423 C -0.352611 6.228125 -0.300854 C 1.013785 6.119972 -0.408298 C -1.403721 2.593596 -0.081773 C -0.799930 1.347847 0.035053 C 0.427277 -1.327030 0.177812 C -1.050074 -1.180477 0.162959 C -1.576264 0.155829 -0.233715 C -3.131402 0.262829 -0.273854 C -3.691084 1.592340 -0.047057 C -2.854913 2.721070 -0.088022 C -3.444378 4.045063 -0.018753 C -2.615638 5.170126 -0.079360 C 2.431590 -2.741342 -0.256441 C 1.020595 -2.639262 -0.103702 C 0.175565 -3.766001 -0.158268 C -1.273829 -3.631821 -0.095451 C -1.892169 -2.367868 -0.036034 C -3.306711 -2.220104 0.004506 C -3.920845 -0.931827 0.035102 C -4.127959 -3.403468 0.085476 C -3.503657 -4.668536 0.000609 C -2.106424 -4.811525 -0.118561 C -1.469486 -6.101569 -0.239630

		C -0.105555 -6.223446 -0.345977 C 0.766733 -5.072337 -0.313712 C 2.165140 -5.183363 -0.426396 C 3.016770 -4.051412 -0.428242 C 5.184728 -2.988036 -0.466833 C 4.441234 -4.121178 -0.671364 C -5.108444 1.698557 0.185777 C -5.879932 0.531866 0.307759 C -5.309730 -0.781010 0.264317 C -6.104330 -1.976623 0.394298 C -5.541993 -3.230498 0.277794 C -4.877568 4.142597 0.131492 C -5.669816 3.027516 0.254847 O 0.892044 1.212166 1.828717 O 1.699855 -0.106618 -1.507088 O -0.323836 -1.190603 1.433640 O -2.306558 0.134681 -1.462513 N 4.555442 -0.282118 2.369302 H -7.186669 -1.870900 0.567240 H -6.967132 0.626698 0.457560 H -6.756024 3.130756 0.403213 H -5.326621 5.147197 0.174340 H -6.175551 -4.128407 0.348337 H -4.129686 -5.574539 0.038621 H -3.070565 6.173276 -0.058517 H -2.108487 -6.998220 -0.254978 H -0.832838 7.218725 -0.329531 H 6.535138 -0.589943 -0.114702 H 6.786611 1.919907 -0.096899 H 5.754631 4.161621 -0.427614 H 4.869532 -5.071554 -1.035827 H 2.613458 -6.183509 -0.540626 H 3.692500 5.605696 -0.496596 H 0.353016 -7.218973 -0.453681 H 1.634995 7.022083 -0.522042 H 3.837051 0.351954 1.984481 H 4.480867 -0.595235 3.333052 H 0.342891 0.464679 2.153240
	3E_1OH_N_2H	C 1.113269 0.209751 0.028326 C 2.551804 0.391494 -0.171770 C 0.621914 -1.164912 0.353889 C 3.188088 1.720717 -0.020023 C 3.376362 -0.802207 -0.044251 O 1.587524 0.311891 -1.315558 C 0.298794 1.368051 0.568397 C -0.846845 -1.342563 0.243741 C 1.487742 -2.327803 0.112791 O -0.211666 -1.216243 1.554073 C 2.298499 2.847086 0.027121 C 4.594049 1.878960 -0.046581 C 2.885080 -2.121607 0.006750 C 4.728331 -0.601092 -0.050479

		C 0.886724 2.689867 0.129726 C -1.130207 1.188983 0.127671 O 0.422002 1.398899 2.019552 C -1.616265 -0.141340 -0.190271 C -1.390074 -2.683966 -0.005175 C 0.930208 -3.607558 0.038846 C 2.857292 4.177326 -0.056175 C 5.126559 3.209686 -0.058990 C 5.404188 0.649767 -0.074156 C 3.819092 -3.234567 -0.043451 C 5.682650 -1.647726 -0.060971 C 0.020893 3.793555 0.024682 C -1.971509 2.279067 -0.017372 H 0.038922 0.547521 2.321092 C -3.141305 -0.368111 -0.343175 O -2.230061 -0.300517 -1.474701 C -2.802482 -2.841902 -0.072935 C -0.513393 -3.788138 0.001552 C 1.831279 -4.739530 -0.047686 C 1.978129 5.285363 -0.092379 C 4.287523 4.309469 -0.087396 H 6.218504 3.340181 -0.073306 N 6.724346 0.427496 -0.092477 C 3.226992 -4.536429 -0.061076 C 5.238933 -2.983939 -0.076127 N 6.879464 -0.942620 -0.090110 C -1.413268 3.612854 0.016277 C 0.579130 5.125137 -0.079676 C -3.412560 2.092246 -0.122318 C -3.677207 -1.712274 -0.093474 C -3.987827 0.809945 -0.152305 C -3.349825 -4.176812 -0.041792 C -1.061219 -5.119104 -0.063047 C 1.228186 -6.054702 -0.105730 H 2.400469 6.302109 -0.137202 H 4.716528 5.322700 -0.134411 H 3.884622 -5.420027 -0.097495 H 5.934070 -3.835273 -0.121276 H 7.825684 -1.302358 -0.099141 C -2.276863 4.735597 -0.048372 C -0.331294 6.240198 -0.132898 C -4.271030 3.260654 -0.079820 C -5.079234 -1.863692 0.026476 C -5.408585 0.605733 -0.027692 C -2.461541 -5.280659 -0.058494 C -4.778734 -4.309849 0.037991 C -0.135865 -6.231370 -0.105331 H 1.893222 -6.931334 -0.153432 C -3.693318 4.534812 -0.062457 C -1.694606 6.055148 -0.106138 H 0.088235 7.256630 -0.193688 C -5.699329 3.046911 -0.036300

		C -5.919236 -0.701529 0.029304 C -5.603728 -3.204599 0.099892 C -6.242532 1.785695 0.011685 H -2.881563 -6.299443 -0.055453 H -5.211576 -5.322003 0.067499 H -0.554125 -7.249370 -0.148664 H -4.350213 5.419451 -0.058698 H -2.370628 6.923593 -0.145571 H -6.355405 3.931194 -0.014361 H -7.009425 -0.843685 0.097841 H -6.693556 -3.336692 0.186808 H -7.333793 1.653878 0.077625