

ESI for

**Confinement Effects on the Structure and Reactivity of Encapsulated
Buckybowl in Cycloparaphenylene**

Shan Li^a, Zi-Yang Qiu^a, Jing-Shuang Dang^{*a}, Hidehiro Sakurai^b

a. Key Laboratory for Macromolecular Science of Shaanxi Province, School of Chemistry and Chemical Engineering, Shaanxi Normal University, Xi'an 710119, China

b. Department of Applied Chemistry, Graduate School of Engineering, Osaka University, Osaka 565-0871, Japan.

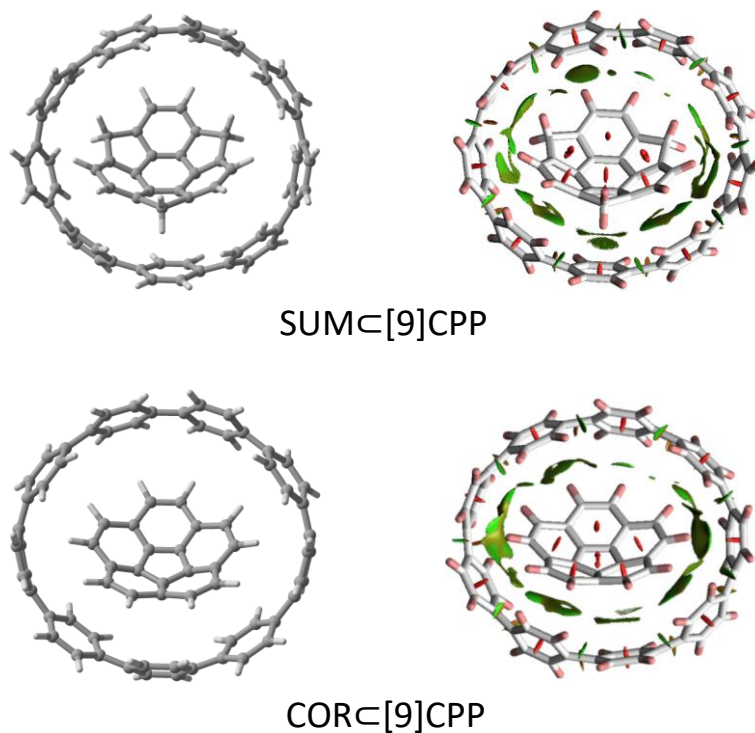


Fig. S1. Structures and non-covalent interaction diagrams of SUMC[9]CPP and CORC[9]CPP.

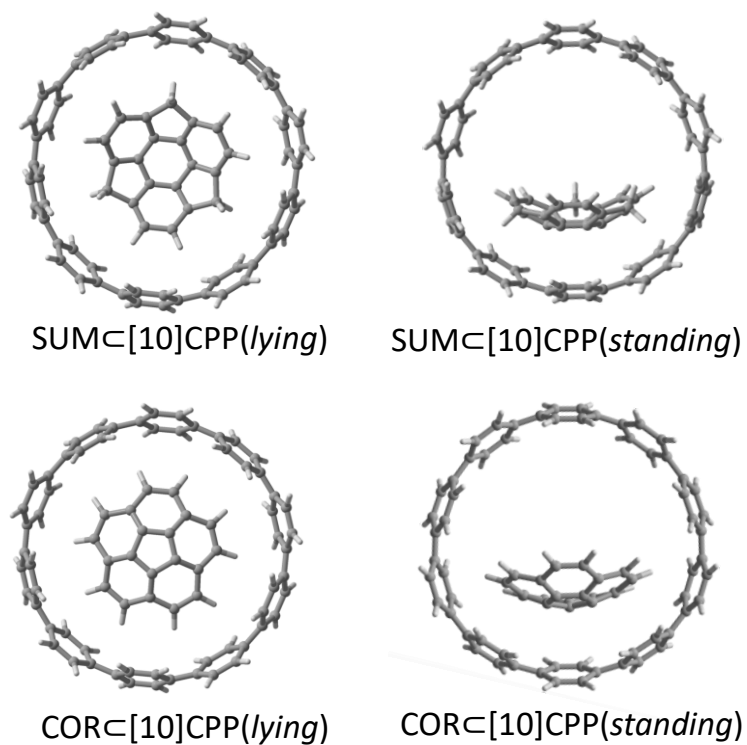


Fig. S2. Structures of SUMC[10]CPP and CORC[10]CPP in *lying* and *standing* orientations.

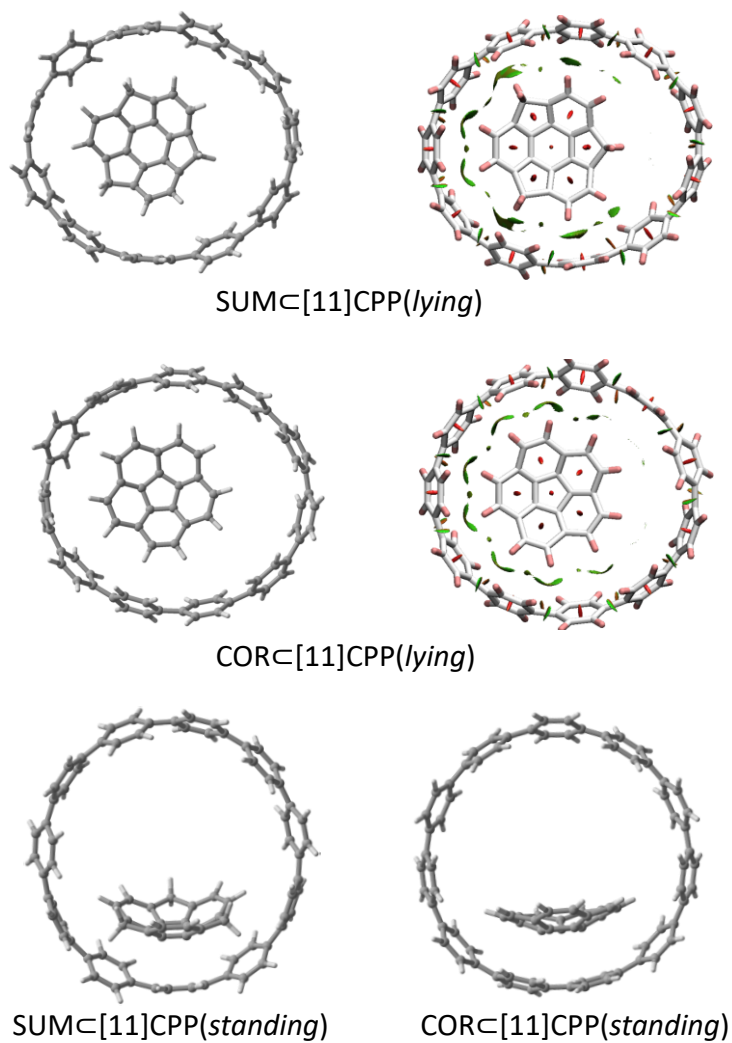


Fig. S3. Structures of SUMC[11]CPP and CORC[11]CPP in *lying* and *standing* orientations and the non-covalent interaction diagrams of complexes in a more stable lying orientation.

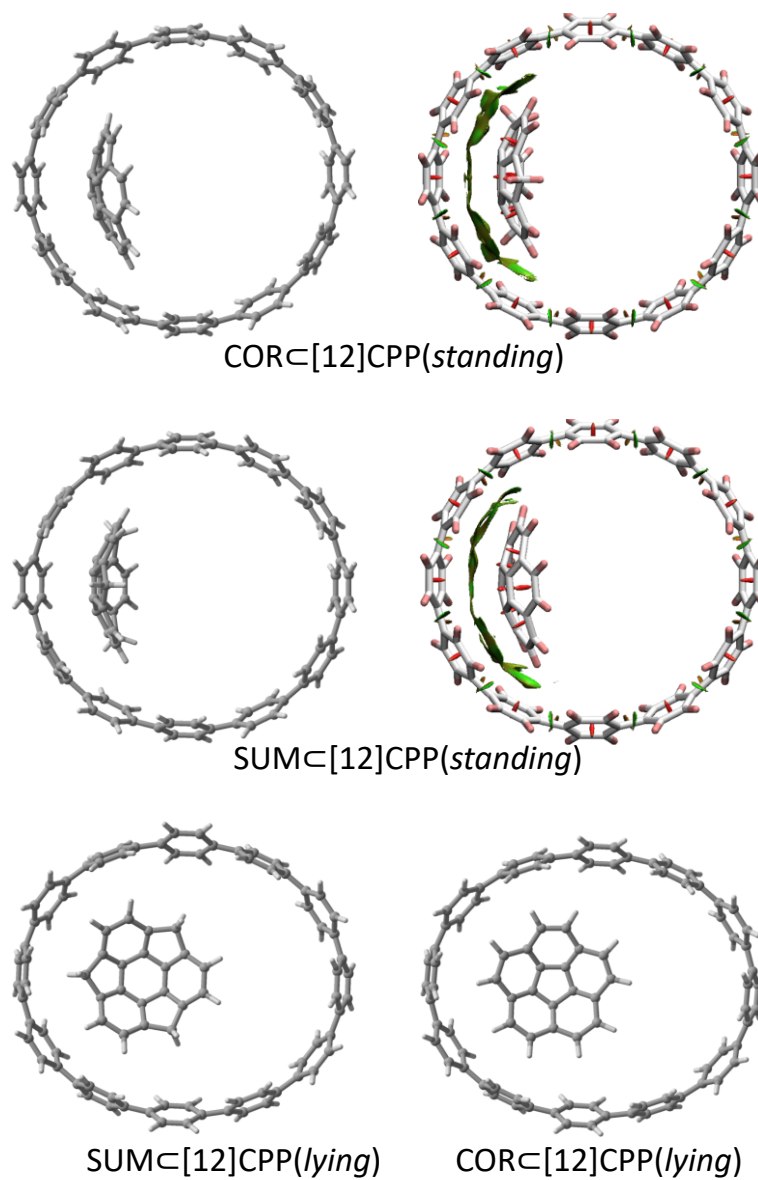


Fig. S4. Structures of SUMC[12]CPP and CORC[12]CPP in *lying* and *standing* orientations and the non-covalent interaction diagrams of complexes in a more stable *standing* orientation.

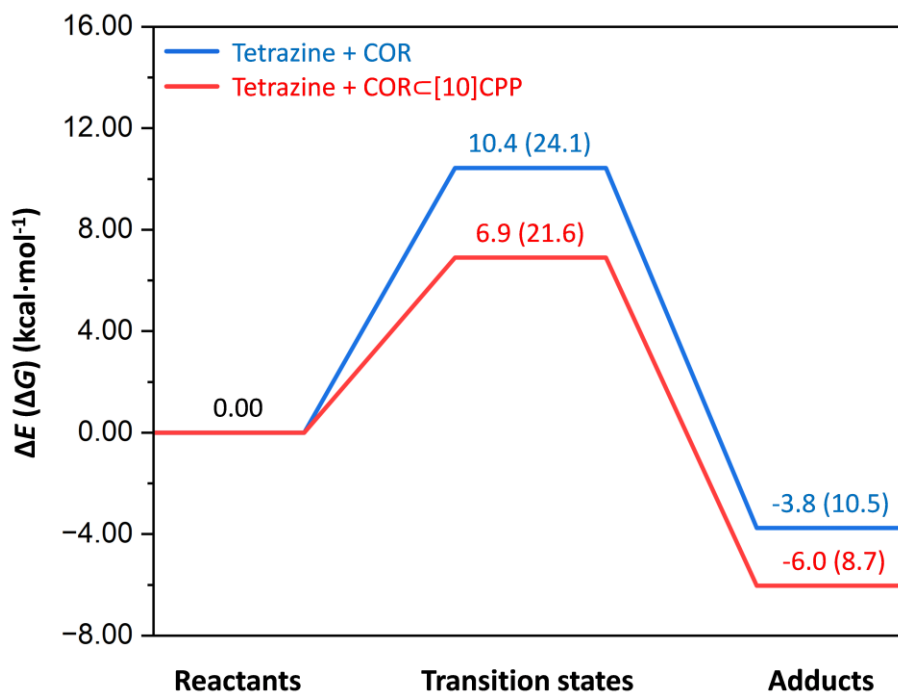


Fig. S5. Energy profiles of the DA reactions Tetrazine + COR and Tetrazine + COR<[10]CPP.

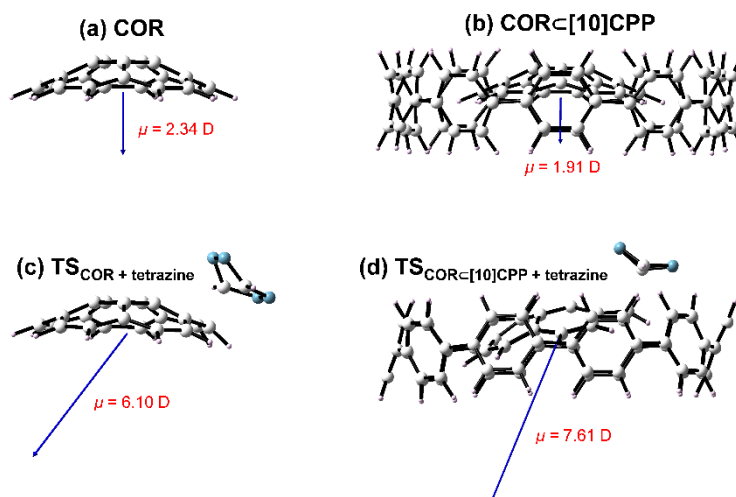


Fig. S6. Calculated dipole moments of (a) corannulene, (b) COR<[10]CPP, (c) TS of the DA reaction COR + tetrazine, and (d) TS of the DA reaction COR<[10]CPP + tetrazine.

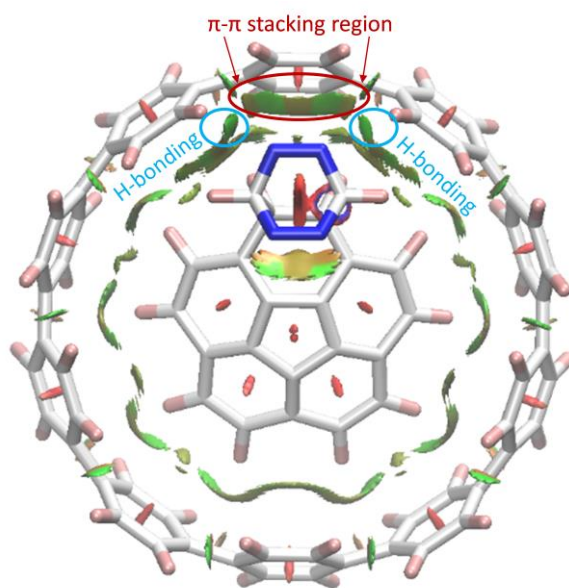


Fig. S7. non-covalent interaction diagrams of the transition state configuration of the DA reaction between CORC[10]CPP and tetrazine.

Table S1. Calculated binding energies of buckybowl⊂[n]CPP.

Buckybowl	Orientation	ΔE_b^a (ΔG_b^b) (kcal·mol ⁻¹)			
		[9]CPP	[10]CPP	[11]CPP	[12]CPP
Sumanene	<i>lying</i>	-28.4 (-14.7)	-30.0 (-15.3)	-24.1 (-11.4)	-18.9 (-6.6)
	<i>standing</i>		-25.0 (-10.8)	-23.9 (-9.9)	-22.6 (-8.7)
Corannulene	<i>lying</i>	-26.0 (-11.6)	-31.7 (-16.6)	-24.0 (-11.2)	-19.2 (-6.7)
	<i>standing</i>		-24.3 (-10.7)	-23.3 (-9.3)	-22.0 (-8.9)

a. ΔE_b represents the change of zero-point energy (ZPE)-corrected electronic energies.

b. ΔG_b represents the change of Gibbs free energies at room temperature.

Table S2. Calculated distortion energies of [n]CPP (E_{d-CPP}) in buckybowl⊂[n]CPP

Buckybowl	Orientation	E_{d-CPP} (kcal·mol ⁻¹)			
		[9]CPP	[10]CPP	[11]CPP	[12]CPP
Sumanene	<i>lying</i>	1.4	0.4	1.2	1.5
	<i>standing</i>		0.7	0.5	0.6
Corannulene	<i>lying</i>	4.2	0.1	0.9	2.2
	<i>standing</i>		0.5	0.8	0.6

S1. Computational Details.

Density functional theory (DFT) calculations were carried out by applying the Gaussian 16 program.^{S1} Geometrical optimizations of all relevant structures were performed using the B97D3 functional in conjunction with the basis sets of 6-311G(d,p). Frequency analyses were performed at the same level of theory to confirm the nature of stationary points. The zero-point energy (ZPE)-corrected energies as well as Gibbs free energies were used to estimate the binding strength between host and guest molecules and the free energy barriers were used to evaluate the reactivity kinetically. The implicit solvent effect was considered using the polarizable continuum model (PCM), with dichloromethane and toluene, as utilized in relevant experiments,^{S2-S3} chosen as the solvents. To further examine the thermal stability of newly-designed host-guest compounds, ab initio molecular dynamics (AIMD) simulations were conducted using the CP2K 9.1 program.^{S4} The Grimme's D3-corrected PBE functional was employed. The AIMD simulations under the NVT ensemble was set to a time step of 1 fs at a fluctuant temperature around 300 K with a CSVN thermostat method.

References:

S1. Gaussian 16, Revision A.03, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.;

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S2. Matsuno, T.; Fujita, M.; Fukunaga, K.; Sato, S.; Isobe, H., Concyclic CH- π Arrays for Single-Axis Rotations of a Bowl in a Tube. *Nat. Commun.* **2018**, *9*, 3779.

S3. Iwamoto, T.; Watanabe, Y.; Sadahiro, T.; Haino, T.; Yamago, S., *Angew. Chem. Int. Ed.* **2011**, *50*, 8342.

S4. CP2K Developer Group. CP2K home page.<http://www.cp2k.org/>.

S2. Cartesian coordinates of all relevant structures and the imaginary frequency of all transition states (TSs).

Corannulene (COR)

C	0.27	-0.89	3.05	C	-0.10	2.46	-0.65	H	0.67	-1.48	3.88
C	0.27	0.50	3.16	C	-0.67	1.22	-0.36	H	0.66	0.95	4.07
C	-0.11	1.34	2.05	C	-0.67	0.68	0.96	H	0.66	3.32	2.60
C	0.27	2.72	1.79	C	-0.67	-0.75	0.85	H	0.67	4.25	0.35
C	0.27	3.25	0.50	C	-0.66	-1.08	-0.53	H	0.69	-3.60	2.07
C	-0.10	-1.57	1.82	C	-0.08	-2.26	-1.01	H	0.70	-4.18	-0.29
C	0.29	-2.88	1.36	C	0.31	-2.22	-2.41	H	0.70	1.74	-3.94
C	0.30	-3.21	0.01	C	0.31	-1.03	-3.14	H	0.69	3.60	-2.36
C	0.30	1.57	-2.94	C	-0.08	0.23	-2.55	H	0.72	-3.11	-2.87
C	0.29	2.63	-2.04	C	-0.66	0.13	-1.28	H	0.72	-1.04	-4.15

Sumanene (SUM)

C	4.86	-1.43	3.08	C	3.64	-1.31	0.58	H	4.04	2.41	-3.39
C	4.37	-0.20	2.64	C	4.24	-2.53	0.95	H	5.72	2.03	-2.99
C	3.70	-0.18	1.40	C	4.79	-2.59	2.24	H	5.37	-0.66	-4.26
C	3.75	1.13	0.81	C	4.76	-2.08	-2.74	H	5.31	-3.49	2.57
C	3.74	1.27	-0.57	C	4.22	-2.28	-1.46	H	5.27	-2.89	-3.26
C	4.44	2.31	-1.22	C	4.46	-3.34	-0.35	H	5.47	-3.75	-0.40
C	4.68	1.86	-2.69	C	4.71	1.28	2.99	H	3.76	-4.18	-0.44
C	4.82	-0.77	-3.33	C	4.46	2.02	1.65	H	4.08	1.67	3.80
C	4.33	0.35	-2.64	C	5.05	3.13	1.03	H	5.75	1.38	3.31
C	3.68	0.11	-1.42	C	5.04	3.28	-0.39	H	5.65	3.83	1.61
C	3.63	-1.16	-0.85	H	5.42	-1.51	4.00	H	5.63	4.08	-0.82

[9]CPP

C	-8.94	-5.51	3.16	C	-8.46	2.33	6.08	C	-7.97	-1.61	-5.80
C	-8.98	-6.02	1.86	C	-8.92	-1.83	5.51	C	-6.78	-2.14	-5.26
C	-9.20	-5.42	-1.06	C	-8.63	0.98	6.38	C	-7.93	2.65	-5.65
C	-9.12	-3.63	-5.05	C	-8.98	-3.05	4.85	C	-8.04	-0.16	-6.08
C	-9.22	-4.96	-2.37	C	-7.79	-4.87	3.65	C	-6.91	0.59	-6.48
C	-9.11	-2.44	-5.77	C	-6.62	-4.95	2.86	C	-7.74	3.95	-4.95
C	-9.18	0.56	-5.66	C	-7.87	-5.90	0.99	C	-6.51	4.21	-4.32
C	-8.82	4.80	-4.62	C	-6.66	-5.45	1.56	C	-6.86	1.97	-6.27
C	-9.12	1.93	-5.45	C	-8.06	-4.98	-3.18	C	-7.54	5.83	-2.81
C	-8.72	5.72	-3.57	C	-8.01	-5.91	-0.48	C	-6.41	5.13	-3.28
C	-8.66	6.19	-0.61	C	-6.91	-6.12	-1.35	C	-7.32	6.42	1.41
C	-8.16	5.90	3.75	C	-7.98	-4.06	-4.33	C	-7.52	6.37	-1.43
C	-8.56	6.21	0.78	C	-6.78	-3.33	-4.54	C	-6.34	6.79	-0.80
C	-8.12	5.02	4.84	C	-6.94	-5.67	-2.66	C	-7.13	5.92	2.79

C	-5.98	5.16	3.08	H	-10.12	-4.46	-2.73	H	-5.15	5.15	2.37
C	-6.23	6.81	0.59	H	-10.03	-2.11	-6.25	H	-5.09	3.61	4.24
C	-7.06	4.11	5.00	H	-10.07	0.02	-5.36	H	-5.07	2.40	5.93
C	-5.94	4.28	4.15	H	-9.77	4.69	-5.14	H	-5.37	0.03	6.34
C	-7.54	0.08	6.36	H	-9.97	2.42	-4.98	H	-5.76	-2.04	6.73
C	-7.19	2.86	5.79	H	-9.60	6.30	-3.31	H	-5.85	-4.18	5.55
C	-6.08	2.02	6.04	H	-9.60	5.88	-1.06	H	-5.71	-4.47	3.22
C	-7.73	-1.37	6.11	H	-9.04	6.53	3.62	H	-5.78	-5.35	0.94
C	-6.67	-2.30	6.20	H	-9.42	5.93	1.37	H	-6.01	-6.59	-0.97
C	-6.26	0.66	6.29	H	-8.97	5.00	5.52	H	-5.47	5.19	-2.73
C	-7.85	-3.88	4.75	H	-9.35	2.94	5.97	H	-5.64	3.59	-4.55
C	-6.72	-3.52	5.53	H	-9.78	-1.16	5.43	H	-5.95	2.51	-6.53
H	-9.84	-5.56	3.77	H	-9.64	0.60	6.52	H	-6.04	0.09	-6.90
H	-9.91	-6.45	1.48	H	-9.87	-3.29	4.28	H	-5.87	-1.55	-5.27
H	-10.07	-5.25	-0.43	H	-5.46	7.03	-1.39	H	-5.88	-3.63	-4.01
H	-10.04	-4.21	-4.99	H	-5.28	7.06	1.05	H	-6.05	-5.79	-3.28

CORC[9]CPP

C	-6.33	5.39	-2.17	C	-8.82	-1.44	-6.29	C	-7.48	6.07	-0.02
C	-6.42	4.75	-3.40	C	-8.99	1.40	-5.63	C	-8.67	6.35	0.69
C	-6.76	3.04	-5.89	C	-7.37	-3.21	-5.45	H	-9.61	6.17	-1.77
C	-6.44	-1.17	-6.40	C	-8.65	-2.73	-5.78	H	-9.75	5.09	-3.93
C	-6.79	1.79	-6.51	C	-7.14	-5.57	-1.86	H	-9.80	2.93	-4.39
C	-6.27	-2.46	-5.92	C	-7.20	-4.25	-4.40	H	-9.83	-1.07	-6.43
C	-6.08	-4.15	-3.54	C	-8.21	-5.15	-4.02	H	-9.85	0.77	-5.45
C	-6.04	-6.01	0.36	C	-7.21	-5.88	-0.42	H	-9.54	-3.30	-5.51
C	-6.05	-4.79	-2.31	C	-8.43	-5.77	0.28	H	-9.07	-5.31	-4.67
C	-6.06	-5.80	1.74	C	-8.19	-5.79	-2.78	H	-9.36	-5.69	-0.28
C	-6.16	-3.84	3.92	C	-7.26	-5.45	2.40	H	-9.02	-6.43	-2.50
C	-6.47	-0.55	6.67	C	-8.45	-5.56	1.66	H	-9.40	-5.32	2.13
C	-6.23	-2.85	4.89	C	-7.37	-2.69	5.70	H	-9.15	-5.35	4.48
C	-6.64	0.83	6.75	C	-7.23	-4.72	3.68	H	-9.73	-1.44	6.38
C	-6.91	3.69	5.98	C	-8.32	-4.65	4.58	H	-9.26	-3.63	6.21
C	-6.44	5.54	2.14	C	-7.57	-1.40	6.39	H	-10.03	0.96	6.61
C	-6.84	4.71	5.03	C	-8.85	-0.82	6.51	H	-10.00	2.49	5.21
C	-6.34	5.77	0.77	C	-8.38	-3.67	5.57	H	-9.73	6.28	2.55
C	-7.48	5.83	-1.48	C	-7.91	1.43	6.59	H	-9.88	4.27	3.58
C	-8.70	5.79	-2.21	C	-9.02	0.56	6.62	H	-9.56	6.68	0.16
C	-7.66	4.52	-4.02	C	-7.88	4.90	4.09	C	-9.44	-2.78	-0.77
C	-8.78	5.15	-3.45	C	-8.01	2.80	6.03	C	-8.90	-2.35	-1.97
C	-7.86	0.90	-6.32	C	-9.12	3.13	5.22	C	-7.70	-1.54	-2.02
C	-7.81	3.46	-5.04	C	-7.69	5.61	2.80	C	-7.31	-0.61	-3.05
C	-8.96	2.65	-5.02	C	-8.77	6.12	2.06	C	-6.46	0.47	-2.78
C	-7.72	-0.57	-6.47	C	-9.05	4.15	4.27	C	-8.83	-2.45	0.50

C	-9.47	-2.36	1.80	H	-10.40	-3.30	-0.78	H	-5.74	1.45	6.80
C	-8.95	-1.57	2.82	H	-9.44	-2.55	-2.89	H	-5.47	-0.95	6.71
C	-5.50	2.18	0.49	H	-7.77	-0.68	-4.02	H	-5.43	-2.11	4.93
C	-5.49	1.95	-0.88	H	-6.30	1.20	-3.57	H	-5.31	-3.83	3.24
C	-5.93	0.70	-1.46	H	-10.43	-2.85	1.96	H	-5.13	-5.84	2.29
C	-6.15	-0.33	-0.54	H	-9.51	-1.46	3.74	H	-5.35	5.47	-1.70
C	-7.02	-1.43	-0.81	H	-5.27	3.17	0.86	H	-5.51	4.32	-3.83
C	-7.57	-1.88	0.42	H	-5.25	2.78	-1.54	H	-5.88	3.67	-6.01
C	-7.04	-1.05	1.46	H	-7.85	0.67	4.26	H	-5.92	1.49	-7.10
C	-7.75	-0.78	2.63	H	-6.37	2.31	3.26	H	-5.55	-0.57	-6.59
C	-7.37	0.43	3.32	H	-5.38	5.60	0.30	H	-5.26	-2.84	-5.80
C	-6.52	1.36	2.74	H	-5.57	5.19	2.68	H	-5.29	-3.45	-3.77
C	-5.96	1.17	1.42	H	-5.95	5.32	4.98	H	-5.23	-4.58	-1.64
C	-6.16	-0.10	0.87	H	-6.07	3.54	6.65	H	-5.09	-6.21	-0.13

SUMC[9]CPP

C	-9.13	-5.40	3.24	C	-8.20	-1.53	-6.03	H	-10.16	-4.80	-0.34
C	-9.14	-5.78	1.90	C	-6.98	-2.04	-5.54	H	-10.24	-4.02	-4.88
C	-9.29	-4.99	-0.97	C	-8.17	2.72	-5.89	H	-10.21	-4.06	-2.66
C	-9.32	-3.47	-5.05	C	-8.29	-0.09	-6.35	H	-10.29	-2.04	-6.31
C	-9.32	-4.57	-2.29	C	-7.18	0.67	-6.78	H	-10.30	0.08	-5.56
C	-9.35	-2.34	-5.86	C	-7.96	3.98	-5.14	H	-9.99	4.75	-5.28
C	-9.42	0.63	-5.89	C	-6.72	4.20	-4.52	H	-10.20	2.48	-5.18
C	-9.03	4.82	-4.76	C	-7.12	2.05	-6.56	H	-9.79	6.27	-3.37
C	-9.36	2.00	-5.67	C	-7.73	5.74	-2.91	H	-9.83	5.97	-1.19
C	-8.92	5.68	-3.67	C	-6.61	5.06	-3.42	H	-9.30	6.35	3.52
C	-8.87	6.15	-0.72	C	-7.55	6.16	1.33	H	-9.70	5.93	1.24
C	-8.46	5.67	3.66	C	-7.71	6.23	-1.51	H	-9.29	4.88	5.47
C	-8.80	6.13	0.67	C	-6.49	6.50	-0.84	H	-9.74	2.77	5.97
C	-8.46	4.83	4.78	C	-7.43	5.61	2.70	H	-10.15	-1.36	5.91
C	-8.85	2.19	6.18	C	-6.34	4.76	2.98	H	-10.02	0.49	6.72
C	-9.25	-1.97	5.91	C	-6.42	6.46	0.55	H	-10.17	-3.42	4.64
C	-9.01	0.87	6.59	C	-7.44	3.88	4.98	C	-9.13	2.54	0.47
C	-9.26	-3.16	5.19	C	-6.34	3.92	4.09	C	-8.91	1.69	-0.63
C	-8.00	-4.80	3.81	C	-7.90	-0.01	6.69	C	-8.63	0.34	-0.34
C	-6.81	-4.80	3.05	C	-7.58	2.72	5.88	C	-7.86	-0.24	-1.41
C	-8.01	-5.58	1.08	C	-6.47	1.93	6.25	C	-6.95	-1.27	-1.14
C	-6.82	-5.18	1.71	C	-8.05	-1.47	6.48	C	-5.75	-1.39	-1.87
C	-8.18	-4.64	-3.12	C	-6.95	-2.35	6.49	C	-8.95	2.08	1.81
C	-8.11	-5.51	-0.40	C	-6.63	0.60	6.63	C	-4.95	-2.15	1.71
C	-7.01	-5.71	-1.26	C	-8.09	-3.91	4.99	C	-6.78	-1.74	0.21
C	-8.14	-3.83	-4.35	C	-6.96	-3.54	5.76	C	-7.51	-1.17	1.25
C	-6.95	-3.16	-4.71	H	-10.05	-5.51	3.82	C	-8.45	-0.11	0.97
C	-7.05	-5.29	-2.58	H	-10.06	-6.18	1.47	C	-8.55	0.76	2.07

C	-7.79	0.10	3.24	H	-7.14	0.82	3.76	H	-5.73	-0.01	6.77
C	-5.71	-1.57	2.77	H	-5.23	-1.45	3.74	H	-6.03	-2.06	6.99
C	-6.98	-1.01	2.54	H	-7.93	2.88	-2.20	H	-6.05	-4.14	5.72
C	-8.50	1.95	-2.10	H	-9.36	2.04	-2.77	H	-5.91	-4.34	3.46
C	-7.63	0.71	-2.43	H	-6.25	1.23	-4.01	H	-5.92	-5.01	1.12
C	-6.50	0.52	-3.23	H	-4.64	-0.54	-3.52	H	-6.10	-6.16	-0.87
C	-5.56	-0.52	-2.95	H	-3.77	-1.80	-0.98	H	-5.67	5.08	-2.88
C	-4.78	-2.23	-1.00	H	-4.69	-3.26	-1.37	H	-5.86	3.60	-4.79
C	-5.46	-2.19	0.40	H	-5.59	6.68	-1.41	H	-6.22	2.59	-6.83
H	-9.29	3.60	0.32	H	-5.45	6.60	1.03	H	-6.32	0.17	-7.22
H	-8.98	2.82	2.61	H	-5.53	4.67	2.26	H	-6.07	-1.46	-5.65
H	-3.93	-2.44	1.91	H	-5.53	3.20	4.19	H	-6.02	-3.42	-4.22
H	-8.47	-0.31	4.00	H	-5.46	2.32	6.15	H	-6.16	-5.42	-3.20

[10]CPP

C	6.50	0.49	-1.20	C	-6.98	-0.15	-0.20	C	6.72	-1.66	0.04
C	6.88	-0.19	-0.03	C	-6.81	1.32	-0.27	C	6.16	-2.23	1.20
C	6.87	1.97	1.13	C	-6.59	-0.83	0.97	H	6.30	-0.07	-2.11
C	7.15	0.60	1.11	C	-6.96	-2.30	-1.36	H	7.03	2.53	2.05
C	6.22	1.86	-1.19	C	-7.24	-0.94	-1.35	H	7.52	0.13	2.02
C	5.57	3.89	0.10	C	-6.40	-2.94	-0.24	H	5.80	2.31	-2.08
C	6.31	2.61	0.00	C	-6.31	-2.19	0.96	H	4.98	3.55	2.15
C	4.83	4.17	1.27	C	-4.92	-4.50	-1.50	H	4.14	6.25	-1.92
C	4.32	5.66	-1.02	C	-5.66	-4.22	-0.33	H	5.96	4.60	-1.91
C	5.35	4.72	-1.02	C	-4.41	-6.00	0.79	H	3.17	5.19	2.14
C	3.46	5.81	0.09	C	-5.44	-5.06	0.78	H	1.88	5.87	-2.10
C	3.80	5.10	1.26	C	-3.89	-5.44	-1.49	H	-0.48	7.41	1.97
C	1.38	6.25	-1.22	C	-2.20	-6.75	-0.21	H	1.96	7.14	2.01
C	2.11	6.41	-0.02	C	-3.55	-6.14	-0.32	H	-0.54	6.14	-2.15
C	0.03	7.07	1.07	C	-1.47	-6.58	0.99	H	-2.09	5.78	2.05
C	1.42	6.92	1.10	C	-0.12	-7.41	-1.30	H	-4.79	5.77	-2.11
C	0.00	6.40	-1.24	C	-1.51	-7.25	-1.33	H	-2.66	6.99	-2.05
C	-2.17	6.43	-0.01	C	0.63	-7.06	-0.16	H	-4.21	4.57	1.99
C	-0.72	6.73	-0.07	C	-0.09	-6.74	1.01	H	-5.14	3.51	-2.28
C	-2.70	5.82	1.15	C	2.61	-6.16	-1.38	H	-7.44	1.78	1.75
C	-4.21	5.77	-1.19	C	2.08	-6.76	-0.22	H	-6.43	4.01	1.81
C	-3.00	6.46	-1.16	C	4.12	-6.11	0.96	H	-6.14	1.29	-2.33
C	-4.65	5.01	-0.08	C	2.91	-6.80	0.93	H	-6.39	-0.26	1.88
C	-3.91	5.13	1.11	C	3.82	-5.47	-1.34	H	-7.12	-2.87	-2.28
C	-5.68	3.16	-1.40	C	5.55	-4.26	-0.02	H	-7.62	-0.46	-2.25
C	-5.64	3.92	-0.21	C	4.55	-5.35	-0.15	H	-5.89	-2.65	1.85
C	-6.94	2.15	0.86	C	5.59	-3.50	1.17	H	-5.07	-3.89	-2.39
C	-6.36	3.42	0.89	C	6.85	-2.49	-1.10	H	-4.23	-6.58	1.69
C	-6.25	1.90	-1.43	C	6.27	-3.76	-1.12	H	-6.05	-4.93	1.68

H	-3.26	-5.53	-2.37	H	2.00	-6.11	-2.28	H	7.35	-2.11	-1.98
H	-1.98	-6.20	1.87	H	4.70	-6.11	1.88	H	6.34	-4.35	-2.04
H	0.39	-7.74	-2.20	H	2.57	-7.33	1.82	H	6.05	-1.63	2.10
H	-2.05	-7.47	-2.25	H	4.12	-4.90	-2.22				
H	0.45	-6.47	1.92	H	5.05	-3.85	2.04				

CORC[10]CPP-lying

C	6.59	0.75	-1.13	C	-5.53	-4.17	-0.36	H	-2.70	7.07	-2.21
C	6.94	0.09	0.07	C	-4.26	-5.88	0.82	H	-4.25	4.66	1.83
C	6.85	2.26	1.20	C	-5.30	-4.96	0.78	H	-5.14	3.57	-2.43
C	7.15	0.90	1.21	C	-3.74	-5.39	-1.48	H	-7.41	1.82	1.62
C	6.28	2.11	-1.14	C	-2.04	-6.62	-0.14	H	-6.44	4.08	1.65
C	5.55	4.14	0.11	C	-3.39	-6.05	-0.28	H	-6.11	1.33	-2.46
C	6.32	2.87	0.05	C	-1.33	-6.41	1.06	H	-6.32	-0.17	1.76
C	4.78	4.41	1.26	C	0.08	-7.26	-1.19	H	-6.98	-2.86	-2.34
C	4.29	5.87	-1.06	C	-1.31	-7.14	-1.24	H	-7.52	-0.47	-2.36
C	5.33	4.95	-1.02	C	0.80	-6.89	-0.04	H	-5.78	-2.55	1.78
C	3.41	6.02	0.03	C	0.06	-6.54	1.11	H	-4.93	-3.88	-2.42
C	3.73	5.33	1.22	C	2.80	-6.00	-1.25	H	-4.07	-6.44	1.74
C	1.35	6.44	-1.31	C	2.25	-6.57	-0.08	H	-5.91	-4.82	1.67
C	2.06	6.61	-0.11	C	4.25	-5.85	1.12	H	-3.10	-5.49	-2.35
C	-0.05	7.23	0.95	C	3.05	-6.56	1.08	H	-1.84	-6.01	1.93
C	1.33	7.10	1.00	C	3.99	-5.29	-1.21	H	0.61	-7.61	-2.07
C	-0.03	6.57	-1.36	C	5.66	-4.00	0.12	H	-1.83	-7.38	-2.16
C	-2.22	6.54	-0.17	C	4.70	-5.12	0.00	H	0.58	-6.24	2.01
C	-0.78	6.87	-0.21	C	5.65	-3.21	1.30	H	2.21	-5.99	-2.17
C	-2.75	5.94	0.99	C	6.95	-2.23	-0.96	H	4.81	-5.80	2.05
C	-4.23	5.84	-1.36	C	6.40	-3.51	-0.98	H	2.70	-7.06	1.98
C	-3.03	6.55	-1.32	C	6.79	-1.38	0.16	H	4.31	-4.75	-2.10
C	-4.67	5.09	-0.25	C	6.21	-1.94	1.31	H	5.09	-3.55	2.16
C	-3.95	5.23	0.95	H	6.42	0.17	-2.03	H	7.46	-1.86	-1.85
C	-5.68	3.21	-1.55	H	6.97	2.83	2.11	H	6.49	-4.11	-1.88
C	-5.65	3.98	-0.37	H	7.50	0.44	2.13	H	6.06	-1.32	2.19
C	-6.92	2.20	0.72	H	5.88	2.55	-2.05	C	1.02	-3.10	0.26
C	-6.36	3.48	0.74	H	4.91	3.81	2.15	C	2.22	-2.39	0.30
C	-6.23	1.94	-1.57	H	4.12	6.44	-1.97	C	2.27	-1.00	0.69
C	-6.91	-0.11	-0.32	H	5.96	4.83	-1.91	C	3.25	0.00	0.33
C	-6.78	1.36	-0.40	H	3.08	5.41	2.08	C	2.95	1.36	0.33
C	-6.52	-0.76	0.87	H	1.87	6.07	-2.19	C	-0.25	-2.48	0.60
C	-6.84	-2.28	-1.44	H	-0.59	7.55	1.84	C	-1.58	-2.85	0.17
C	-7.14	-0.92	-1.45	H	1.85	7.32	1.93	C	-2.62	-1.93	0.13
C	-6.28	-2.89	-0.29	H	-0.55	6.29	-2.28	C	-0.39	3.22	0.22
C	-6.21	-2.12	0.88	H	-2.15	5.90	1.90	C	0.99	3.08	0.26
C	-4.79	-4.47	-1.51	H	-4.81	5.82	-2.28	C	1.63	1.85	0.67

C	0.77	0.90	1.22	C	-1.28	2.13	0.58	H	-3.57	-2.24	-0.30
C	1.08	-0.49	1.23	C	-0.65	1.03	1.17	H	-0.82	4.13	-0.20
C	-0.15	-1.22	1.19	H	1.02	-4.11	-0.15	H	1.60	3.90	-0.12
C	-1.22	-0.28	1.15	H	3.12	-2.87	-0.07	H	-4.18	0.48	-0.31
C	-2.43	-0.55	0.53	H	4.22	-0.32	-0.03	H	-3.21	2.71	-0.28
C	-3.19	0.61	0.12	H	3.69	2.06	-0.05				
C	-2.64	1.89	0.14	H	-1.75	-3.85	-0.24				

CORC[10]CPP-stand

C	6.41	1.23	-1.30	C	-6.18	-1.78	1.09	H	1.77	7.84	1.86
C	6.81	0.59	-0.11	C	-4.72	-4.09	-1.33	H	-0.72	6.84	-2.30
C	6.69	2.76	1.01	C	-5.45	-3.81	-0.16	H	-2.16	6.29	1.93
C	7.03	1.41	1.02	C	-4.12	-5.49	1.00	H	-4.97	6.19	-2.15
C	6.07	2.58	-1.31	C	-5.19	-4.60	0.98	H	-2.90	7.51	-2.13
C	5.37	4.63	-0.07	C	-3.65	-4.99	-1.30	H	-4.22	4.98	1.92
C	6.12	3.36	-0.14	C	-1.89	-6.18	0.00	H	-5.21	3.88	-2.29
C	4.66	4.95	1.10	C	-3.26	-5.63	-0.11	H	-7.42	2.16	1.80
C	4.12	6.38	-1.22	C	-1.15	-5.92	1.17	H	-6.47	4.42	1.80
C	5.14	5.43	-1.21	C	0.19	-6.86	-1.08	H	-6.15	1.63	-2.29
C	3.29	6.57	-0.09	C	-1.20	-6.74	-1.10	H	-6.31	0.17	1.96
C	3.64	5.89	1.09	C	0.95	-6.44	0.03	H	-6.98	-2.56	-2.13
C	1.21	7.03	-1.39	C	0.24	-6.05	1.18	H	-7.56	-0.18	-2.15
C	1.94	7.17	-0.19	C	2.92	-5.62	-1.25	H	-5.73	-2.20	1.99
C	-0.15	7.71	0.94	C	2.39	-6.14	-0.06	H	-4.89	-3.51	-2.23
C	1.24	7.63	0.94	C	4.43	-5.41	1.07	H	-3.90	-6.04	1.92
C	-0.19	7.11	-1.39	C	3.23	-6.11	1.08	H	-5.79	-4.48	1.88
C	-2.33	6.96	-0.12	C	4.13	-4.92	-1.26	H	-3.02	-5.08	-2.19
C	-0.90	7.35	-0.20	C	5.79	-3.56	0.01	H	-1.65	-5.50	2.04
C	-2.79	6.31	1.05	C	4.86	-4.71	-0.07	H	0.69	-7.24	-1.97
C	-4.36	6.21	-1.25	C	5.80	-2.78	1.18	H	-1.75	-7.02	-1.99
C	-3.19	6.96	-1.24	C	6.91	-1.72	-1.14	H	0.78	-5.71	2.06
C	-4.74	5.43	-0.13	C	6.44	-3.03	-1.13	H	2.32	-5.64	-2.16
C	-3.97	5.57	1.04	C	6.75	-0.88	-0.02	H	5.01	-5.35	1.99
C	-5.73	3.53	-1.40	C	6.27	-1.47	1.17	H	2.89	-6.58	2.01
C	-5.70	4.31	-0.23	H	6.21	0.64	-2.19	H	4.43	-4.42	-2.17
C	-6.94	2.53	0.90	H	6.82	3.35	1.92	H	5.31	-3.15	2.08
C	-6.40	3.82	0.90	H	7.41	0.97	1.94	H	7.35	-1.32	-2.05
C	-6.27	2.25	-1.40	H	5.62	3.00	-2.21	H	6.52	-3.63	-2.03
C	-6.92	0.21	-0.12	H	4.80	4.35	2.00	H	6.12	-0.86	2.06
C	-6.80	1.68	-0.22	H	3.93	6.94	-2.13	C	2.14	-1.89	1.94
C	-6.51	-0.43	1.07	H	5.72	5.27	-2.11	C	2.62	-2.22	0.68
C	-6.83	-1.97	-1.22	H	3.02	6.00	1.98	C	3.08	-1.22	-0.25
C	-7.16	-0.61	-1.24	H	1.71	6.70	-2.29	C	3.15	-1.29	-1.69
C	-6.24	-2.56	-0.09	H	-0.67	7.99	1.85	C	3.10	-0.15	-2.49

C	2.07	-0.52	2.40	C	2.33	1.79	1.55	H	3.05	-0.27	-3.57
C	1.19	0.05	3.39	C	1.32	2.30	2.36	H	0.70	-0.61	4.11
C	0.83	1.40	3.38	C	0.70	3.52	1.87	H	0.08	1.75	4.08
C	1.89	3.40	-1.76	C	0.96	4.01	0.59	H	1.39	4.23	-2.27
C	2.42	2.37	-2.53	C	1.86	3.34	-0.32	H	2.32	2.42	-3.61
C	2.97	1.17	-1.92	C	2.60	2.30	0.24	H	-0.07	4.01	2.47
C	3.13	1.24	-0.54	H	1.71	-2.68	2.56	H	0.39	4.87	0.24
C	3.19	0.07	0.28	H	2.55	-3.26	0.35				
C	2.70	0.41	1.57	H	3.14	-2.27	-2.17				

SUMC[10]CPP-lying

C	6.46	0.67	-1.00	C	-7.06	-0.81	-1.13	H	5.93	4.69	-1.84
C	6.82	0.00	0.19	C	-6.26	-2.80	0.03	H	3.31	5.58	2.27
C	6.84	2.17	1.31	C	-6.18	-2.03	1.21	H	1.92	6.04	-2.02
C	7.08	0.80	1.32	C	-4.83	-4.44	-1.19	H	-0.44	7.65	2.02
C	6.21	2.04	-1.01	C	-5.56	-4.10	-0.03	H	1.99	7.38	2.07
C	5.61	4.12	0.22	C	-4.36	-5.88	1.14	H	-0.50	6.30	-2.07
C	6.31	2.81	0.16	C	-5.36	-4.91	1.11	H	-2.13	6.17	2.16
C	4.94	4.49	1.40	C	-3.83	-5.41	-1.17	H	-4.70	5.84	-2.06
C	4.33	5.82	-0.96	C	-2.18	-6.72	0.15	H	-2.58	7.07	-2.03
C	5.36	4.88	-0.93	C	-3.51	-6.09	0.03	H	-4.24	4.96	2.13
C	3.51	6.04	0.16	C	-1.45	-6.54	1.35	H	-5.03	3.65	-2.13
C	3.90	5.43	1.37	C	-0.09	-7.39	-0.93	H	-7.29	1.94	1.93
C	1.42	6.44	-1.14	C	-1.48	-7.24	-0.96	H	-6.34	4.20	1.94
C	2.15	6.63	0.05	C	0.66	-7.03	0.21	H	-5.98	1.41	-2.14
C	0.07	7.30	1.13	C	-0.07	-6.69	1.38	H	-6.24	-0.08	2.09
C	1.45	7.15	1.16	C	2.61	-6.11	-1.03	H	-6.94	-2.75	-2.03
C	0.04	6.59	-1.17	C	2.10	-6.70	0.14	H	-7.42	-0.35	-2.05
C	-2.13	6.65	0.05	C	4.11	-5.93	1.30	H	-5.78	-2.48	2.11
C	-0.68	6.94	-0.01	C	2.92	-6.67	1.29	H	-4.96	-3.85	-2.10
C	-2.70	6.15	1.24	C	3.79	-5.38	-1.02	H	-4.19	-6.45	2.05
C	-4.14	5.91	-1.13	C	5.48	-4.07	0.27	H	-5.95	-4.74	2.00
C	-2.94	6.61	-1.11	C	4.52	-5.19	0.18	H	-3.20	-5.53	-2.04
C	-4.60	5.22	0.01	C	5.52	-3.29	1.45	H	-1.95	-6.15	2.23
C	-3.91	5.45	1.22	C	6.75	-2.31	-0.85	H	0.42	-7.73	-1.83
C	-5.57	3.31	-1.25	C	6.19	-3.58	-0.85	H	-2.01	-7.47	-1.88
C	-5.56	4.09	-0.08	C	6.63	-1.46	0.28	H	0.47	-6.41	2.28
C	-6.80	2.31	1.03	C	6.08	-2.02	1.45	H	2.01	-6.11	-1.94
C	-6.26	3.60	1.04	H	6.24	0.09	-1.90	H	4.69	-5.89	2.22
C	-6.11	2.03	-1.26	H	7.00	2.75	2.22	H	2.60	-7.18	2.19
C	-6.81	0.00	0.00	H	7.44	0.34	2.24	H	4.08	-4.83	-1.91
C	-6.66	1.47	-0.09	H	5.81	2.48	-1.92	H	4.99	-3.63	2.33
C	-6.44	-0.66	1.19	H	5.12	3.95	2.32	H	7.24	-1.94	-1.75
C	-6.79	-2.18	-1.12	H	4.12	6.35	-1.89	H	6.25	-4.19	-1.75

H	5.97	-1.40	2.34	C	-2.66	0.17	-0.42	H	0.77	-4.28	0.05
C	-2.28	2.42	0.53	C	-3.02	-1.34	-0.41	H	-3.81	-1.58	-1.13
C	-0.97	2.47	0.02	C	-1.07	-3.22	-0.39	H	-3.39	-1.66	0.57
C	-0.58	1.41	-0.82	C	-1.67	-2.01	-0.76	H	-1.66	-4.03	0.03
C	0.85	1.26	-0.81	C	0.32	3.21	0.46	H	0.33	3.39	1.54
C	1.42	0.00	-1.01	C	1.44	2.22	0.04	H	0.42	4.18	-0.03
C	2.62	-0.38	-0.38	C	2.69	1.90	0.57	H	3.19	2.58	1.26
C	-3.12	1.28	0.31	C	3.28	0.61	0.36	H	4.20	0.38	0.90
C	0.36	-3.37	-0.38	C	2.66	-1.93	-0.36	H	2.94	-2.32	0.62
C	0.58	-1.15	-1.23	C	1.20	-2.31	-0.74	H	3.40	-2.33	-1.07
C	-0.81	-1.00	-1.24	H	-2.63	3.18	1.21				
C	-1.40	0.30	-1.03	H	-4.07	1.24	0.83				

SUMC[10]CPP-stand

C	6.43	0.47	-1.22	C	-6.82	1.30	-0.33	H	6.19	-0.10	-2.12
C	6.89	-0.20	-0.07	C	-6.80	-0.85	0.93	H	7.08	2.51	2.00
C	6.89	1.95	1.09	C	-6.96	-2.31	-1.43	H	7.62	0.12	1.94
C	7.19	0.59	1.06	C	-7.22	-0.94	-1.44	H	5.67	2.28	-2.07
C	6.14	1.83	-1.20	C	-6.51	-2.96	-0.26	H	4.97	3.51	2.16
C	5.55	3.87	0.11	C	-6.55	-2.22	0.94	H	4.12	6.26	-1.88
C	6.28	2.58	-0.01	C	-4.97	-4.50	-1.47	H	5.93	4.59	-1.90
C	4.82	4.14	1.28	C	-5.73	-4.22	-0.32	H	3.17	5.16	2.18
C	4.30	5.66	-0.99	C	-4.41	-5.90	0.86	H	1.88	5.90	-2.06
C	5.33	4.71	-1.00	C	-5.48	-5.01	0.82	H	-0.49	7.36	2.03
C	3.45	5.79	0.13	C	-3.90	-5.39	-1.44	H	1.94	7.09	2.08
C	3.80	5.08	1.30	C	-2.19	-6.64	-0.13	H	-0.54	6.17	-2.11
C	1.38	6.27	-1.17	C	-3.54	-6.05	-0.24	H	-2.12	5.74	2.08
C	2.11	6.41	0.03	C	-1.46	-6.48	1.07	H	-4.77	5.76	-2.10
C	0.02	7.04	1.13	C	-0.11	-7.28	-1.22	H	-2.65	7.00	-2.01
C	1.41	6.89	1.16	C	-1.49	-7.13	-1.25	H	-4.23	4.52	1.99
C	0.00	6.42	-1.19	C	0.64	-6.95	-0.08	H	-5.01	3.46	-2.27
C	-2.17	6.41	0.02	C	-0.08	-6.63	1.09	H	-7.54	1.79	1.65
C	-0.73	6.72	-0.02	C	2.63	-6.10	-1.31	H	-6.50	4.01	1.74
C	-2.71	5.80	1.17	C	2.09	-6.67	-0.14	H	-6.04	1.24	-2.35
C	-4.20	5.76	-1.18	C	4.16	-6.07	1.01	H	-6.67	-0.29	1.86
C	-2.99	6.46	-1.13	C	2.92	-6.71	1.00	H	-7.05	-2.86	-2.36
C	-4.64	4.99	-0.09	C	3.86	-5.46	-1.30	H	-7.51	-0.46	-2.37
C	-3.91	5.10	1.12	C	5.65	-4.30	-0.03	H	-6.24	-2.69	1.87
C	-5.60	3.12	-1.42	C	4.62	-5.36	-0.12	H	-5.12	-3.90	-2.37
C	-5.62	3.89	-0.24	C	5.81	-3.58	1.17	H	-4.21	-6.45	1.78
C	-6.99	2.14	0.79	C	6.83	-2.49	-1.17	H	-6.09	-4.88	1.72
C	-6.40	3.41	0.84	C	6.28	-3.77	-1.18	H	-3.26	-5.46	-2.31
C	-6.19	1.86	-1.46	C	6.78	-1.68	-0.01	H	-1.96	-6.09	1.95
C	-7.04	-0.16	-0.27	C	6.35	-2.30	1.18	H	0.40	-7.61	-2.13

H	-2.03	-7.34	-2.17	C	2.30	-2.90	0.52	C	1.05	-2.87	2.59
H	0.46	-6.36	2.00	C	-3.43	-1.67	-0.74	H	-3.03	-1.08	-2.78
H	2.01	-6.04	-2.20	C	0.36	-2.29	3.67	H	-4.29	-1.02	-0.68
H	4.75	-6.08	1.92	C	0.27	-3.39	1.55	H	0.91	-1.83	4.50
H	2.57	-7.20	1.91	C	-1.12	-3.24	1.52	H	-4.00	-2.72	2.31
H	4.17	-4.92	-2.19	C	-1.80	-3.12	0.26	H	-3.41	-1.06	2.16
H	5.37	-3.96	2.09	C	-2.96	-2.33	0.41	H	-1.53	-1.56	4.44
H	7.25	-2.08	-2.09	C	-3.17	-2.11	1.93	H	-0.09	-1.20	-3.29
H	6.28	-4.33	-2.11	C	-1.06	-2.14	3.64	H	-0.26	-2.87	-3.85
H	6.31	-1.72	2.10	C	-1.81	-2.55	2.53	H	2.77	-1.71	-2.66
C	-2.69	-1.71	-1.96	C	-0.21	-2.24	-2.95	H	3.94	-1.92	-0.51
C	-1.47	-2.41	-2.05	C	0.94	-2.67	-2.00	H	2.94	-1.76	2.30
C	-1.08	-3.16	-0.93	C	2.27	-2.26	-1.86	H	3.16	-3.51	2.46
C	0.35	-3.32	-0.90	C	2.95	-2.37	-0.60				
C	1.01	-3.43	0.32	C	2.50	-2.73	2.05				

[11]CPP

C	0.51	-4.36	-6.74	C	-0.59	-6.57	-3.86	C	-0.50	7.25	-2.95
C	0.42	-5.48	-5.91	C	-1.74	-6.89	-3.10	C	-0.66	7.16	0.05
C	0.65	-6.97	-3.32	C	-0.27	-7.72	0.28	C	0.50	5.77	-4.62
C	0.90	-7.24	0.92	C	-1.36	-8.06	1.11	C	-0.55	6.60	-4.19
C	0.75	-7.49	-2.03	C	-1.64	-7.38	-1.80	C	0.08	2.28	-7.08
C	0.92	-6.98	2.28	C	-0.23	-7.17	3.08	C	0.32	4.75	-5.68
C	0.85	-6.33	5.21	C	-1.34	-7.79	2.47	C	-0.92	4.10	-5.80
C	1.12	-2.51	7.07	C	-0.23	-4.51	6.44	C	0.02	0.84	-7.42
C	0.88	-5.36	6.22	C	-0.29	-6.50	4.40	C	-1.19	0.20	-7.78
C	1.19	-1.15	7.37	C	-1.45	-5.77	4.74	C	-1.04	2.89	-6.48
C	1.22	1.80	7.88	C	-0.09	-3.22	7.16	C	-0.27	-1.99	-7.25
C	1.59	5.04	5.11	C	-1.19	-2.55	7.73	C	-1.33	-1.18	-7.69
C	1.30	3.11	7.40	C	-1.42	-4.80	5.74	H	1.39	-4.23	-7.38
C	1.66	5.88	4.00	C	0.05	-0.44	7.78	H	1.23	-6.21	-5.93
C	1.68	7.55	1.51	C	-1.13	-1.19	8.03	H	1.57	-6.78	-3.87
C	1.73	6.40	-2.61	C	0.22	3.71	6.72	H	1.77	-6.96	0.32
C	1.70	7.67	0.12	C	0.05	1.04	7.69	H	1.73	-7.73	-1.64
C	1.68	5.76	-3.84	C	-1.08	1.70	7.17	H	1.80	-6.51	2.71
C	1.40	4.22	-6.42	C	0.39	4.89	5.84	H	1.73	-6.93	5.03
C	1.12	0.01	-7.15	C	-0.67	5.75	5.51	H	2.00	-2.99	6.63
C	1.28	3.01	-7.11	C	-1.00	3.00	6.69	H	1.79	-5.23	6.80
C	0.99	-1.38	-7.07	C	0.54	6.62	3.57	H	2.11	-0.62	7.17
C	-0.48	-3.36	-6.72	C	-0.60	6.60	4.40	H	2.08	1.36	8.35
C	-1.64	-3.61	-5.95	C	0.55	7.39	-0.65	H	2.44	4.39	5.33
C	-0.65	-5.64	-5.01	C	0.51	7.15	2.19	H	2.24	3.66	7.51
C	-1.72	-4.72	-5.12	C	-0.67	7.04	1.44	H	2.56	5.87	3.39
C	-0.39	-7.61	-1.20	C	0.61	7.09	-2.10	H	2.59	7.73	2.07

H	2.61	6.27	-1.98	H	-2.25	-8.51	0.67	H	-1.46	7.21	4.15
H	2.63	7.93	-0.38	H	-2.55	-7.50	-1.22	H	-1.60	6.74	1.92
H	2.51	5.13	-4.14	H	-2.22	-8.01	3.07	H	-1.35	7.84	-2.63
H	2.36	4.74	-6.41	H	-2.35	-5.88	4.14	H	-1.56	6.94	-0.51
H	2.08	0.46	-6.88	H	-2.13	-3.08	7.89	H	-1.45	6.70	-4.80
H	2.15	2.61	-7.62	H	-2.29	-4.17	5.89	H	-1.78	4.47	-5.25
H	1.83	-1.97	-6.73	H	-2.01	-0.69	8.42	H	-2.05	0.80	-8.08
H	-2.43	-2.87	-5.91	H	-2.01	1.14	7.01	H	-1.99	2.36	-6.45
H	-2.57	-4.80	-4.45	H	-1.59	5.73	6.10	H	-2.30	-1.63	-7.92
H	-2.73	-6.68	-3.50	H	-1.86	3.43	6.18				

CORC[11]CPP-lying

C	0.41	-3.71	-6.80	C	-0.32	-7.34	2.75	C	-0.39	-1.35	-7.25
C	0.33	-4.87	-6.03	C	-1.44	-7.89	2.10	C	-1.46	-0.56	-7.72
C	0.56	-6.56	-3.57	C	-0.32	-4.74	6.13	H	1.28	-3.55	-7.44
C	0.83	-7.29	0.60	C	-0.39	-6.72	4.09	H	1.14	-5.60	-6.09
C	0.66	-7.21	-2.35	C	-1.56	-6.01	4.46	H	1.48	-6.32	-4.10
C	0.84	-7.13	1.98	C	-0.17	-3.43	6.80	H	1.70	-6.98	0.04
C	0.75	-6.56	4.91	C	-1.27	-2.71	7.32	H	1.65	-7.50	-1.99
C	1.05	-2.74	6.68	C	-1.52	-5.04	5.46	H	1.73	-6.70	2.45
C	0.78	-5.59	5.91	C	-0.01	-0.62	7.27	H	1.64	-7.15	4.71
C	1.13	-1.37	6.91	C	-1.19	-1.34	7.55	H	1.92	-3.25	6.28
C	1.19	1.60	7.25	C	0.20	3.50	6.08	H	1.70	-5.45	6.48
C	1.54	4.85	4.48	C	0.01	0.85	7.11	H	2.06	-0.85	6.68
C	1.28	2.90	6.74	C	-1.12	1.51	6.58	H	2.06	1.15	7.72
C	1.62	5.77	3.44	C	0.36	4.70	5.24	H	2.36	4.15	4.63
C	1.68	7.76	1.19	C	-0.69	5.61	5.00	H	2.23	3.43	6.83
C	1.75	7.01	-2.99	C	-1.03	2.80	6.08	H	2.50	5.78	2.81
C	1.71	8.04	-0.17	C	0.52	6.60	3.12	H	2.60	7.85	1.78
C	1.68	6.42	-4.24	C	-0.61	6.54	3.96	H	2.63	6.82	-2.37
C	1.33	4.89	-6.80	C	0.57	7.87	-0.97	H	2.65	8.35	-0.63
C	1.00	0.66	-7.23	C	0.50	7.29	1.81	H	2.50	5.78	-4.57
C	1.18	3.65	-7.42	C	-0.68	7.29	1.04	H	2.29	5.39	-6.84
C	0.86	-0.72	-7.08	C	0.65	7.69	-2.44	H	1.95	1.12	-6.97
C	-0.59	-2.72	-6.73	C	-0.46	7.92	-3.29	H	2.03	3.21	-7.94
C	-1.72	-2.99	-5.94	C	-0.65	7.57	-0.32	H	1.71	-1.30	-6.71
C	-0.74	-5.08	-5.13	C	0.50	6.48	-5.01	H	-2.51	-2.25	-5.86
C	-1.79	-4.14	-5.16	C	-0.53	7.33	-4.55	H	-2.63	-4.25	-4.48
C	-0.47	-7.41	-1.53	C	-0.03	2.92	-7.32	H	-2.82	-6.20	-3.69
C	-0.68	-6.09	-4.05	C	0.27	5.46	-6.05	H	-2.35	-8.46	0.25
C	-1.83	-6.47	-3.33	C	-0.98	4.82	-6.11	H	-2.63	-7.26	-1.51
C	-0.35	-7.68	-0.08	C	-0.11	1.47	-7.56	H	-2.33	-8.14	2.67
C	-1.45	-8.07	0.72	C	-1.32	0.82	-7.87	H	-2.46	-6.12	3.86
C	-1.73	-7.10	-2.09	C	-1.13	3.58	-6.73	H	-2.21	-3.22	7.50

H	-2.40	-4.42	5.61	C	-0.08	-3.03	2.64	C	0.68	2.39	-0.28
H	-2.08	-0.81	7.90	C	0.29	-3.12	1.24	C	0.62	1.86	-1.57
H	-2.05	0.96	6.45	C	-0.20	-4.02	0.22	C	0.81	0.45	-1.83
H	-1.59	5.56	5.61	C	-0.14	-3.70	-1.14	C	1.26	-0.29	-0.74
H	-1.89	3.24	5.57	C	0.62	-0.65	2.78	H	-0.31	-1.82	4.39
H	-1.45	7.21	3.78	C	0.44	0.74	3.17	H	-0.57	-3.87	3.12
H	-1.61	6.94	1.49	C	0.59	1.79	2.27	H	-0.72	-4.93	0.52
H	-1.30	8.52	-2.93	C	0.35	-0.35	-2.95	H	-0.61	-4.37	-1.85
H	-1.55	7.43	-0.91	C	0.17	-1.73	-2.84	H	0.09	0.96	4.18
H	-1.42	7.47	-5.15	C	0.42	-2.44	-1.60	H	0.34	2.80	2.60
H	-1.82	5.23	-5.56	C	1.07	-1.70	-0.63	H	0.05	0.14	-3.87
H	-2.17	1.40	-8.20	C	1.01	-2.03	0.76	H	-0.27	-2.27	-3.68
H	-2.08	3.06	-6.64	C	1.17	-0.82	1.51	H	0.42	3.44	-0.14
H	-2.42	-1.03	-7.92	C	1.32	0.25	0.58	H	0.32	2.52	-2.39
C	0.08	-1.85	3.37	C	0.93	1.56	0.88				

CORC[11]CPP-stand

C	0.66	-4.22	-6.69	C	-0.53	-6.41	-3.84	C	-0.60	7.24	-2.92
C	0.58	-5.30	-5.82	C	-1.70	-6.72	-3.11	C	-0.70	7.18	0.08
C	0.69	-6.81	-3.26	C	-0.34	-7.73	0.27	C	0.40	5.78	-4.60
C	0.85	-7.45	0.97	C	-1.49	-7.96	1.05	C	-0.66	6.59	-4.15
C	0.75	-7.36	-1.98	C	-1.64	-7.25	-1.83	C	0.02	2.33	-7.13
C	0.85	-7.22	2.34	C	-0.34	-7.25	3.09	C	0.23	4.77	-5.67
C	0.71	-6.41	5.23	C	-1.50	-7.72	2.43	C	-1.00	4.07	-5.76
C	1.08	-2.53	7.00	C	-0.31	-4.50	6.38	C	-0.01	0.90	-7.52
C	0.76	-5.41	6.21	C	-0.41	-6.54	4.38	C	-1.21	0.24	-7.86
C	1.17	-1.17	7.31	C	-1.53	-5.73	4.66	C	-1.10	2.88	-6.47
C	1.25	1.79	7.82	C	-0.15	-3.21	7.09	C	-0.22	-1.94	-7.37
C	1.63	5.05	5.09	C	-1.24	-2.52	7.65	C	-1.31	-1.15	-7.78
C	1.35	3.10	7.36	C	-1.48	-4.74	5.64	H	1.58	-4.05	-7.24
C	1.69	5.90	3.99	C	0.04	-0.44	7.72	H	1.45	-5.95	-5.73
C	1.66	7.59	1.50	C	-1.14	-1.17	7.97	H	1.63	-6.61	-3.77
C	1.66	6.44	-2.62	C	0.27	3.72	6.71	H	1.78	-7.28	0.43
C	1.66	7.70	0.11	C	0.07	1.04	7.65	H	1.73	-7.61	-1.57
C	1.59	5.79	-3.85	C	-1.06	1.72	7.14	H	1.77	-6.88	2.82
C	1.30	4.29	-6.45	C	0.44	4.92	5.84	H	1.57	-7.06	5.10
C	1.12	0.09	-7.30	C	-0.62	5.79	5.54	H	1.95	-3.03	6.57
C	1.20	3.10	-7.17	C	-0.96	3.03	6.68	H	1.66	-5.31	6.81
C	1.02	-1.29	-7.23	C	0.56	6.65	3.59	H	2.11	-0.65	7.11
C	-0.40	-3.30	-6.82	C	-0.56	6.64	4.44	H	2.12	1.32	8.28
C	-1.60	-3.62	-6.15	C	0.49	7.41	-0.64	H	2.47	4.40	5.30
C	-0.56	-5.53	-5.02	C	0.51	7.19	2.21	H	2.29	3.63	7.47
C	-1.68	-4.70	-5.28	C	-0.69	7.07	1.47	H	2.57	5.89	3.36
C	-0.41	-7.52	-1.19	C	0.54	7.11	-2.08	H	2.59	7.77	2.04

H	2.55	6.32	-2.01	H	-1.42	7.27	4.20	C	-1.60	-2.86	-2.66
H	2.58	7.96	-0.40	H	-1.60	6.76	1.98	C	-1.62	-3.66	-1.48
H	2.44	5.18	-4.17	H	-1.45	7.81	-2.57	C	-0.28	-4.09	-1.21
H	2.24	4.84	-6.47	H	-1.61	6.96	-0.46	C	0.56	-3.56	-2.24
H	2.07	0.56	-7.04	H	-1.57	6.66	-4.74	C	1.91	-3.28	-2.03
H	2.06	2.74	-7.73	H	-1.85	4.40	-5.17	C	2.47	-2.32	-2.95
H	1.89	-1.86	-6.91	H	-2.09	0.82	-8.12	C	1.68	-1.57	-3.82
H	-2.45	-2.94	-6.21	H	-2.02	2.31	-6.42	C	0.24	-1.73	-3.86
H	-2.59	-4.83	-4.70	H	-2.27	-1.62	-7.99	C	-0.25	-2.80	-3.13
H	-2.68	-6.49	-3.53	C	-0.85	-4.37	1.10	H	-0.58	-4.63	2.11
H	-2.42	-8.27	0.58	C	-2.15	-3.96	0.84	H	-2.86	-3.91	1.67
H	-2.57	-7.36	-1.28	C	-2.56	-3.47	-0.47	H	-4.46	-2.43	-0.10
H	-2.42	-7.85	2.98	C	-3.65	-2.58	-0.81	H	-4.43	-1.08	-2.12
H	-2.41	-5.80	4.03	C	-3.63	-1.81	-1.97	H	2.06	-4.51	1.19
H	-2.18	-3.04	7.81	C	0.18	-4.34	0.07	H	3.50	-3.64	-0.56
H	-2.33	-4.06	5.74	C	1.61	-4.27	0.23	H	-0.47	0.05	-4.94
H	-2.02	-0.65	8.36	C	2.44	-3.77	-0.77	H	-2.77	-0.05	-4.14
H	-1.99	1.18	6.99	C	-0.77	-0.78	-4.30	H	3.54	-2.09	-2.89
H	-1.53	5.77	6.15	C	-2.08	-0.84	-3.85	H	2.14	-0.79	-4.41
H	-1.82	3.48	6.19	C	-2.52	-1.85	-2.90				

SUMC[11]CPP-lying

C	0.67	-3.59	-7.22	C	-0.27	-2.55	-7.19	C	-0.99	1.43	7.08
C	0.58	-4.67	-6.33	C	-1.38	-2.69	-6.33	C	0.49	4.55	5.60
C	0.81	-6.11	-3.70	C	-0.46	-4.74	-5.38	C	-0.57	5.39	5.22
C	1.01	-6.75	0.51	C	-1.47	-3.75	-5.44	C	-0.90	2.71	6.53
C	0.89	-6.71	-2.45	C	-0.25	-6.87	-1.64	C	0.68	6.20	3.29
C	1.03	-6.66	1.90	C	-0.42	-5.67	-4.23	C	-0.48	6.20	4.09
C	0.92	-6.35	4.89	C	-1.58	-5.98	-3.49	C	0.80	7.28	-0.88
C	1.23	-2.73	7.05	C	-0.15	-7.12	-0.19	C	0.69	6.78	1.92
C	0.95	-5.50	5.99	C	-1.26	-7.55	0.59	C	-0.47	6.71	1.13
C	1.30	-1.38	7.39	C	-1.50	-6.55	-2.22	C	0.89	7.19	-2.35
C	1.30	1.58	7.80	C	-0.13	-6.92	2.66	C	-0.19	7.50	-3.19
C	1.70	4.66	4.87	C	-1.25	-7.44	1.97	C	-0.41	6.95	-0.24
C	1.39	2.86	7.25	C	-0.15	-4.66	6.28	C	0.81	6.25	-5.03
C	1.79	5.47	3.74	C	-0.21	-6.41	4.04	C	-0.23	7.05	-4.51
C	1.88	7.23	1.31	C	-1.36	-5.71	4.45	C	0.34	3.02	-7.78
C	2.01	6.55	-2.93	C	0.00	-3.43	7.09	C	0.61	5.38	-6.21
C	1.93	7.48	-0.06	C	-1.10	-2.76	7.67	C	-0.65	4.77	-6.39
C	1.96	6.09	-4.24	C	-1.33	-4.85	5.54	C	0.27	1.58	-8.13
C	1.69	4.89	-6.99	C	0.14	-0.67	7.78	C	-0.95	0.94	-8.45
C	1.38	0.75	-7.85	C	-1.03	-1.41	8.00	C	-0.78	3.61	-7.16
C	1.55	3.74	-7.76	C	0.31	3.42	6.53	C	-0.04	-1.23	-7.82
C	1.22	-0.63	-7.70	C	0.14	0.80	7.65	C	-1.10	-0.43	-8.29

H	1.51	-3.54	-7.91	H	-2.41	-6.67	-1.65	C	-0.59	-0.79	-2.00
H	1.34	-5.44	-6.36	H	-2.14	-7.72	2.53	C	-1.23	-0.54	-0.78
H	1.73	-5.92	-4.25	H	-2.25	-5.73	3.82	C	-1.34	-1.53	0.21
H	1.89	-6.41	-0.03	H	-2.04	-3.29	7.79	C	-1.33	-1.16	1.60
H	1.87	-7.00	-2.07	H	-2.19	-4.22	5.73	C	-0.80	-2.20	2.38
H	1.91	-6.26	2.40	H	-1.92	-0.92	8.38	C	-0.26	-1.83	3.63
H	1.80	-6.94	4.65	H	-1.91	0.86	6.93	C	-0.31	-3.13	-1.24
H	2.10	-3.20	6.62	H	-1.50	5.38	5.79	C	-0.82	-2.82	0.03
H	1.85	-5.44	6.59	H	-1.76	3.11	5.99	C	-0.63	-3.43	1.45
H	2.22	-0.84	7.21	H	-1.34	6.81	3.80	C	-0.12	2.06	2.95
H	2.17	1.16	8.31	H	-1.40	6.35	1.56	C	-0.34	2.29	1.43
H	2.54	4.02	5.13	H	-1.04	8.06	-2.79	C	0.27	3.10	0.46
H	2.32	3.41	7.34	H	-1.30	6.78	-0.85	C	0.26	2.73	-0.93
H	2.70	5.44	3.15	H	-1.11	7.26	-5.12	H	0.40	-0.23	4.92
H	2.77	7.37	1.91	H	-1.50	5.12	-5.82	H	-0.78	0.89	-3.44
H	2.86	6.29	-2.31	H	-1.80	1.54	-8.76	H	0.88	0.59	-2.92
H	2.87	7.79	-0.51	H	-1.73	3.09	-7.16	H	0.32	-2.38	-3.17
H	2.79	5.48	-4.62	H	-2.08	-0.88	-8.47	H	0.19	-2.57	4.28
H	2.65	5.39	-6.94	C	-0.13	-0.45	4.00	H	0.12	-4.10	-1.45
H	2.34	1.20	-7.60	C	-0.54	0.58	3.14	H	0.35	-3.89	1.56
H	2.42	3.36	-8.30	C	-1.20	0.18	1.96	H	-1.36	-4.22	1.67
H	2.07	-1.22	-7.35	C	-1.08	1.20	0.95	H	-0.72	2.75	3.56
H	-2.12	-1.90	-6.28	C	-1.09	0.84	-0.40	H	0.92	2.23	3.23
H	-2.27	-3.76	-4.71	C	-0.36	1.55	-1.37	H	0.88	3.96	0.75
H	-2.56	-5.71	-3.88	C	-0.16	0.59	-2.58	H	0.87	3.33	-1.62
H	-2.15	-7.92	0.09	C	-0.20	-2.11	-2.25				

SUMC[11]CPP-stand

C	1.07	-3.77	-6.21	C	1.87	7.96	0.14	C	-0.42	-7.15	2.71
C	0.98	-4.92	-5.44	C	1.68	6.03	-3.80	C	-1.60	-7.61	2.09
C	0.66	-7.29	-3.65	C	1.25	4.47	-6.39	C	-0.21	-4.41	6.00
C	0.73	-7.42	0.58	C	1.18	0.28	-7.46	C	-0.42	-6.45	4.01
C	0.60	-7.81	-2.36	C	1.13	3.27	-7.08	C	-1.54	-5.66	4.38
C	0.76	-7.14	1.94	C	1.17	-1.11	-7.49	C	-0.01	-3.12	6.70
C	0.75	-6.30	4.79	C	-0.04	-3.26	-6.91	C	-1.06	-2.43	7.34
C	1.22	-2.45	6.57	C	-1.21	-4.05	-6.92	C	-1.43	-4.66	5.34
C	0.85	-5.30	5.76	C	-0.24	-5.62	-5.32	C	0.26	-0.37	7.42
C	1.35	-1.11	6.92	C	-1.31	-5.20	-6.14	C	-0.93	-1.09	7.69
C	1.53	1.81	7.61	C	-0.54	-7.62	-1.55	C	0.57	3.83	6.63
C	1.92	5.21	5.05	C	-0.42	-6.55	-4.19	C	0.32	1.11	7.42
C	1.65	3.15	7.22	C	-1.62	-6.54	-3.45	C	-0.80	1.84	6.99
C	1.97	6.10	3.98	C	-0.48	-7.73	-0.08	C	0.75	5.06	5.82
C	1.91	7.84	1.53	C	-1.63	-7.90	0.73	C	-0.30	5.98	5.59
C	1.79	6.71	-2.59	C	-1.68	-7.06	-2.16	C	-0.68	3.18	6.60

C	0.86	6.88	3.63	H	2.85	8.00	2.05	C	0.54	-3.43	-2.30
C	-0.25	6.87	4.52	H	2.71	6.62	-2.02	C	0.50	-4.02	-0.98
C	0.68	7.69	-0.57	H	2.78	8.21	-0.40	C	-0.72	-4.29	-0.38
C	0.77	7.45	2.27	H	2.52	5.43	-4.15	C	-0.91	-4.19	1.01
C	-0.45	7.35	1.56	H	2.15	5.06	-6.51	C	-2.44	-4.04	1.25
C	0.68	7.37	-2.02	H	2.13	0.79	-7.45	C	-4.05	-2.94	-0.65
C	-0.49	7.46	-2.81	H	1.94	2.95	-7.73	C	-2.98	-3.71	-0.17
C	-0.49	7.47	0.18	H	2.12	-1.64	-7.53	C	-1.95	-4.00	-1.08
C	0.46	5.97	-4.49	H	-2.07	-3.74	-7.51	C	-1.91	-3.44	-2.36
C	-0.60	6.77	-4.01	H	-2.25	-5.75	-6.13	C	-0.64	-3.14	-2.97
C	0.00	2.43	-6.91	H	-2.47	-5.98	-3.83	C	-0.76	-2.04	-3.83
C	0.24	4.91	-5.51	H	-2.57	-8.20	0.27	C	0.40	-1.30	-4.08
C	-0.94	4.15	-5.44	H	-2.57	-6.89	-1.57	C	-4.00	-2.36	-1.97
C	-0.02	1.01	-7.33	H	-2.52	-7.70	2.67	C	-2.90	-2.55	-2.81
C	-1.23	0.28	-7.41	H	-2.46	-5.75	3.82	C	-2.28	-1.73	-3.97
C	-1.06	2.94	-6.12	H	-2.00	-2.94	7.53	C	2.58	-2.87	-1.20
C	-0.03	-1.85	-7.36	H	-2.28	-4.00	5.51	C	1.62	-3.61	-0.23
C	-1.23	-1.11	-7.41	H	-1.77	-0.57	8.14	C	1.48	-3.62	1.16
H	1.99	-3.19	-6.15	H	-1.75	1.34	6.84	C	0.22	-3.91	1.78
H	1.82	-5.20	-4.81	H	-1.19	5.95	6.21	H	2.45	-0.91	-3.53
H	1.58	-7.39	-4.22	H	-1.54	3.67	6.16	H	-2.87	-4.97	1.64
H	1.63	-7.26	0.00	H	-1.10	7.52	4.33	H	-2.67	-3.25	1.97
H	1.47	-8.32	-1.95	H	-1.35	7.06	2.09	H	-4.86	-2.64	0.01
H	1.68	-6.78	2.38	H	-1.34	8.03	-2.44	H	0.37	-0.41	-4.71
H	1.60	-6.94	4.60	H	-1.43	7.26	-0.33	H	-4.79	-1.65	-2.23
H	2.06	-2.94	6.08	H	-1.54	6.81	-4.57	H	-2.49	-0.66	-3.88
H	1.79	-5.19	6.30	H	-1.74	4.45	-4.77	H	-2.66	-2.05	-4.95
H	2.29	-0.59	6.69	H	-2.18	0.81	-7.40	H	3.47	-3.48	-1.44
H	2.39	1.30	8.01	H	-1.94	2.33	-5.95	H	2.94	-1.93	-0.77
H	2.76	4.53	5.21	H	-2.19	-1.62	-7.36	H	2.29	-3.28	1.81
H	2.61	3.64	7.33	C	1.62	-1.59	-3.40	H	0.14	-3.78	2.86
H	2.85	6.09	3.33	C	1.69	-2.63	-2.45				

[12]CPP

C	7.67	-3.03	-3.78	C	-6.69	-3.66	-3.73	C	6.63	4.84	-3.76
C	5.56	-6.88	-3.90	C	-8.29	0.32	-3.83	C	8.92	1.08	-3.89
C	7.03	-4.26	-3.78	C	-6.98	3.03	-3.70	C	7.38	3.66	-3.76
C	4.39	-7.63	-3.90	C	-4.87	6.89	-3.82	C	8.98	-0.32	-3.90
C	1.39	-7.86	-3.77	C	-6.34	4.26	-3.70	C	8.58	-1.06	-5.02
C	-3.01	-7.96	-3.87	C	-3.69	7.63	-3.82	C	6.94	-5.04	-4.95
C	0.00	-7.92	-3.76	C	-0.69	7.86	-3.72	C	8.26	-2.51	-4.95
C	-4.25	-7.32	-3.87	C	3.70	7.96	-3.86	C	8.30	-3.35	-6.08
C	-5.94	-4.83	-3.73	C	0.70	7.92	-3.72	C	5.94	-6.13	-5.03
C	-8.22	-1.07	-3.83	C	4.94	7.32	-3.86	C	5.17	-6.28	-6.20

C	7.66	-4.59	-6.08	C	2.85	7.92	-4.98	H	8.50	3.76	-6.97
C	3.54	-7.66	-5.02	C	3.36	7.34	-6.16	H	7.18	5.83	-6.96
C	4.00	-7.03	-6.20	C	0.66	8.64	-6.02	H	4.91	6.15	-7.06
C	-0.72	-8.23	-4.93	C	5.38	6.60	-5.00	H	2.74	7.28	-7.05
C	2.13	-8.10	-4.94	C	4.60	6.69	-6.17	H	1.17	8.96	-6.93
C	1.41	-8.56	-6.07	C	8.01	3.20	-4.94	H	-1.28	8.85	-6.92
C	-2.17	-7.91	-5.01	C	6.47	5.60	-4.93	H	3.37	8.47	-2.95
C	-2.69	-7.32	-6.17	C	7.22	5.22	-6.06	H	1.24	7.61	-2.84
C	0.02	-8.63	-6.07	C	8.45	1.79	-5.02	H	-1.20	7.50	-2.82
C	-4.70	-6.59	-4.99	C	8.20	1.05	-6.19	H	-3.40	8.17	-2.92
C	-3.92	-6.68	-6.17	C	7.97	4.05	-6.06	H	-5.47	6.85	-2.92
C	-7.32	-3.19	-4.90	C	8.26	-0.34	-6.20	H	-5.79	4.57	-2.81
C	-5.79	-5.60	-4.91	H	1.95	-8.83	-6.97	H	-6.92	2.40	-2.82
C	-6.55	-5.21	-6.03	H	-0.50	-8.94	-6.97	H	-8.60	0.83	-2.92
C	-7.77	-1.78	-4.97	H	-2.07	-7.26	-7.07	H	4.10	-8.17	-2.99
C	-7.52	-1.03	-6.14	H	-4.24	-6.13	-7.06	H	-6.69	-3.04	-2.83
C	-7.29	-4.03	-6.03	H	-6.51	-5.81	-6.94	H	-5.37	-5.10	-2.84
C	-7.89	1.07	-4.96	H	-7.83	-3.74	-6.93	H	-4.85	-7.34	-2.96
C	-7.58	0.36	-6.13	H	-7.17	-1.54	-7.03	H	5.55	7.33	-2.96
C	-6.26	5.04	-4.87	H	-7.28	0.90	-7.02	H	6.07	5.10	-2.86
C	-7.57	2.51	-4.88	H	-8.13	3.03	-6.90	H	7.39	3.04	-2.87
C	-7.62	3.36	-6.00	H	-7.00	5.21	-6.90	H	9.19	1.62	-2.99
C	-5.26	6.13	-4.95	H	-4.76	5.73	-7.02	H	9.30	-0.83	-3.00
C	-4.50	6.29	-6.13	H	-2.70	7.05	-7.03	H	7.62	-2.41	-2.88
C	-6.98	4.60	-6.00	H	3.37	-7.03	-7.08	H	6.49	-4.57	-2.88
C	-2.85	7.67	-4.96	H	5.43	-5.71	-7.09	H	6.17	-6.85	-3.00
C	-3.32	7.04	-6.13	H	7.67	-5.19	-6.98	H	1.90	-7.50	-2.88
C	1.41	8.24	-4.90	H	8.80	-3.01	-6.98	H	-0.54	-7.61	-2.87
C	-1.44	8.11	-4.89	H	7.94	-0.88	-7.09	H	-2.67	-8.47	-2.97
C	-0.74	8.58	-6.02	H	7.84	1.56	-7.08	H	-8.49	-1.62	-2.93

CORC[12]CPP-lying

C	7.50	-3.76	0.96	C	-7.20	3.06	1.19	C	8.08	-1.66	-0.25
C	5.84	-7.81	0.75	C	-5.49	7.08	1.06	C	7.06	-5.82	-0.26
C	7.05	-5.07	0.94	C	-6.75	4.38	1.19	C	7.99	-3.13	-0.20
C	4.69	-8.59	0.75	C	-4.34	7.86	1.06	C	8.16	-3.94	-1.35
C	1.70	-8.70	0.95	C	-1.37	8.01	1.19	C	6.17	-7.00	-0.36
C	-2.66	-8.26	0.91	C	2.98	7.53	1.07	C	5.41	-7.18	-1.54
C	0.31	-8.62	0.98	C	0.02	7.95	1.20	C	7.70	-5.26	-1.37
C	-3.80	-7.46	0.93	C	4.12	6.72	1.04	C	3.82	-8.61	-0.36
C	-5.23	-4.81	1.04	C	5.55	4.09	1.05	C	4.26	-7.96	-1.53
C	-7.73	-1.18	1.05	C	8.10	0.49	0.91	C	-0.45	-8.84	-0.18
C	-5.96	-3.62	1.06	C	6.30	2.91	1.02	C	2.39	-8.99	-0.24
C	-7.99	0.18	1.07	C	8.36	-0.88	0.89	C	1.62	-9.38	-1.36

C	-1.84	-8.33	-0.24	H	6.56	-5.47	1.82	H	-1.84	9.02	-2.02
C	-2.30	-7.68	-1.40	H	4.43	-9.14	1.65	H	1.99	7.13	-2.16
C	0.23	-9.31	-1.33	H	2.26	-8.40	1.84	H	0.61	8.90	-2.01
C	-4.18	-6.70	-0.20	H	-2.38	-8.81	1.81	H	3.99	5.73	-2.21
C	-3.44	-6.89	-1.38	H	-0.17	-8.27	1.89	H	6.26	5.22	-2.08
C	-6.68	-3.19	-0.07	H	-4.39	-7.40	1.84	H	6.99	0.87	-2.28
C	-5.17	-5.61	-0.11	H	-4.62	-5.07	1.90	H	7.57	3.14	-2.12
C	-5.96	-5.22	-1.22	H	-7.89	-1.77	1.95	H	7.43	-1.54	-2.31
C	-7.23	-1.82	-0.11	H	-5.91	-2.98	1.94	C	2.18	0.41	0.60
C	-7.12	-1.04	-1.28	H	-8.35	0.64	1.98	C	2.36	1.79	0.52
C	-6.70	-4.04	-1.20	H	-7.05	2.46	2.08	C	1.27	2.71	0.79
C	-7.76	0.98	-0.07	H	-6.07	7.00	1.98	C	1.10	4.07	0.31
C	-7.38	0.33	-1.26	H	-6.26	4.76	2.08	C	-0.17	4.65	0.21
C	-6.76	5.16	0.01	H	-4.04	8.37	1.98	C	0.91	-0.18	0.97
C	-7.68	2.46	0.01	H	-1.90	7.70	2.08	C	0.39	-1.50	0.66
C	-7.84	3.29	-1.12	H	2.71	8.03	1.99	C	-0.98	-1.76	0.63
C	-5.87	6.34	-0.07	H	0.53	7.58	2.09	C	-3.68	3.14	0.18
C	-5.15	6.57	-1.26	H	4.71	6.61	1.95	C	-2.73	4.16	0.15
C	-7.40	4.61	-1.12	H	4.95	4.31	1.92	C	-1.37	3.94	0.60
C	-3.51	7.93	-0.07	H	8.30	1.06	1.82	C	-1.15	2.74	1.26
C	-4.00	7.35	-1.26	H	6.26	2.24	1.88	C	0.14	2.14	1.35
C	0.77	8.17	0.02	H	8.75	-1.36	1.78	C	-0.04	0.72	1.44
C	-2.08	8.31	0.02	H	8.61	-3.52	-2.24	C	-1.44	0.45	1.41
C	-1.33	8.71	-1.11	H	5.64	-6.59	-2.42	C	-1.97	-0.74	0.91
C	2.15	7.66	-0.07	H	7.80	-5.83	-2.29	C	-3.35	-0.66	0.49
C	2.60	7.06	-1.27	H	3.62	-7.96	-2.41	C	-4.02	0.55	0.37
C	0.06	8.64	-1.11	H	2.11	-9.69	-2.27	C	-3.37	1.81	0.67
C	4.48	6.02	-0.12	H	-1.69	-7.71	-2.30	C	-2.13	1.70	1.30
C	3.74	6.26	-1.29	H	-0.34	-9.56	-2.22	H	2.99	-0.24	0.29
C	7.00	2.51	-0.13	H	-3.70	-6.32	-2.27	H	3.30	2.17	0.15
C	5.48	4.92	-0.09	H	-5.99	-5.85	-2.11	H	1.95	4.61	-0.08
C	6.25	4.57	-1.21	H	-6.73	-1.49	-2.19	H	-0.25	5.63	-0.26
C	7.56	1.15	-0.22	H	-7.28	-3.76	-2.07	H	1.07	-2.28	0.34
C	7.41	0.39	-1.40	H	-7.18	0.91	-2.16	H	-1.32	-2.74	0.29
C	7.00	3.39	-1.23	H	-8.29	2.88	-2.03	H	-4.66	3.33	-0.26
C	7.66	-0.97	-1.42	H	-5.41	6.03	-2.17	H	-3.00	5.10	-0.32
H	7.36	-3.17	1.87	H	-7.49	5.20	-2.02	H	-3.86	-1.57	0.15
H	6.46	-7.76	1.65	H	-3.39	7.39	-2.17	H	-5.03	0.56	-0.04

CORC[12]CPP-stand

C	7.37	-2.92	1.25	C	0.84	-7.43	1.19	C	-6.60	-4.68	1.15
C	5.06	-6.65	1.12	C	-3.54	-7.63	1.09	C	-8.86	-0.93	0.99
C	6.66	-4.12	1.25	C	-0.55	-7.49	1.19	C	-7.36	-3.51	1.13
C	3.85	-7.34	1.11	C	-4.81	-7.05	1.08	C	-8.92	0.46	0.98

C	-7.65	3.16	1.11	C	-3.64	6.87	-1.24	H	1.44	-8.54	-1.97
C	-5.27	6.84	1.01	C	1.09	8.08	0.06	H	-2.69	-7.10	-2.15
C	-6.96	4.36	1.12	C	-1.76	7.92	0.02	H	-1.02	-8.66	-1.98
C	-4.05	7.52	1.04	C	-1.04	8.39	-1.09	H	-4.90	-6.08	-2.18
C	-1.03	7.67	1.20	C	2.54	7.80	0.01	H	-7.10	-5.67	-2.07
C	3.37	7.87	1.15	C	3.10	7.25	-1.16	H	-7.87	-1.44	-2.22
C	0.36	7.74	1.22	C	0.35	8.47	-1.07	H	-8.43	-3.62	-2.09
C	4.63	7.28	1.16	C	5.12	6.59	0.04	H	-7.95	0.99	-2.24
C	6.41	4.86	1.29	C	4.35	6.65	-1.15	H	-8.58	3.11	-2.17
C	8.73	1.13	1.15	C	7.83	3.26	0.12	H	-5.12	5.62	-2.16
C	7.19	3.70	1.29	C	6.24	5.63	0.12	H	-7.34	5.22	-2.15
C	8.77	-0.26	1.14	C	7.02	5.27	-1.00	H	-2.99	6.82	-2.12
C	8.35	-1.00	0.01	C	8.28	1.85	0.03	H	-1.58	8.66	-2.00
C	6.54	-4.89	0.07	C	8.03	1.12	-1.15	H	2.49	7.17	-2.06
C	7.98	-2.43	0.08	C	7.80	4.12	-1.01	H	0.88	8.80	-1.97
C	7.99	-3.27	-1.05	C	8.07	-0.27	-1.16	H	4.70	6.13	-2.04
C	5.49	-5.93	-0.01	H	7.34	-2.30	2.15	H	6.98	5.89	-1.90
C	4.73	-6.05	-1.19	H	5.66	-6.64	2.03	H	7.69	1.64	-2.04
C	7.29	-4.48	-1.05	H	6.11	-4.41	2.14	H	8.34	3.85	-1.91
C	3.01	-7.34	-0.03	H	3.52	-7.86	2.01	H	7.75	-0.80	-2.06
C	3.52	-6.74	-1.20	H	1.34	-7.04	2.07	C	-3.20	-1.18	3.31
C	-1.26	-7.87	0.03	H	-3.17	-8.07	2.02	C	-3.39	0.20	3.31
C	1.59	-7.74	0.04	H	-1.10	-7.14	2.06	C	-4.11	0.87	2.25
C	0.89	-8.23	-1.08	H	-5.39	-7.04	1.99	C	-3.99	2.25	1.81
C	-2.72	-7.61	-0.05	H	-6.04	-4.92	2.04	C	-4.33	2.64	0.52
C	-3.29	-7.13	-1.25	H	-9.11	-1.46	1.91	C	-3.70	-2.02	2.24
C	-0.51	-8.30	-1.09	H	-7.36	-2.88	2.01	C	-3.20	-3.31	1.79
C	-5.31	-6.42	-0.08	H	-9.21	0.98	1.89	C	-3.40	-3.76	0.49
C	-4.55	-6.55	-1.26	H	-7.67	2.56	2.01	C	-4.79	0.66	-2.71
C	-7.97	-3.06	-0.05	H	-5.90	6.86	1.90	C	-4.78	1.79	-1.90
C	-6.42	-5.44	-0.02	H	-6.46	4.66	2.03	C	-4.83	1.70	-0.46
C	-7.16	-5.07	-1.16	H	-3.76	8.05	1.94	C	-5.11	0.43	0.04
C	-8.43	-1.65	-0.14	H	-1.55	7.30	2.09	C	-4.77	0.03	1.36
C	-8.22	-0.92	-1.33	H	3.00	8.36	2.05	C	-4.56	-1.38	1.35
C	-7.92	-3.90	-1.18	H	0.89	7.44	2.12	C	-4.77	-1.85	0.02
C	-8.53	1.19	-0.16	H	5.22	7.32	2.07	C	-4.12	-2.97	-0.49
C	-8.27	0.47	-1.34	H	5.83	5.10	2.18	C	-4.03	-3.02	-1.94
C	-6.75	5.09	-0.07	H	9.00	1.66	2.06	C	-4.38	-1.92	-2.73
C	-8.18	2.63	-0.09	H	7.19	3.07	2.17	C	-4.84	-0.68	-2.15
C	-8.12	3.45	-1.24	H	9.07	-0.79	2.05	C	-5.11	-0.73	-0.79
C	-5.67	6.10	-0.12	H	8.52	-2.96	-1.95	H	-2.56	-1.62	4.07
C	-4.85	6.18	-1.27	H	5.02	-5.50	-2.08	H	-2.90	0.79	4.08
C	-7.41	4.65	-1.23	H	7.28	-5.08	-1.95	H	-3.53	2.98	2.48
C	-3.18	7.50	-0.07	H	2.90	-6.72	-2.10	H	-4.14	3.67	0.22

H -2.57 -3.89 2.45
H -2.92 -4.68 0.18

H -4.65 0.78 -3.78
H -4.64 2.77 -2.37

H -3.59 -3.89 -2.41
H -4.20 -1.98 -3.80

SUMC[12]CPP-lying

C 7.39 -3.72 1.03
C 5.61 -7.72 0.82
C 6.89 -5.01 1.00
C 4.44 -8.48 0.82
C 1.45 -8.57 1.00
C -2.92 -8.22 0.95
C 0.06 -8.51 1.02
C -4.09 -7.45 0.96
C -5.58 -4.84 1.06
C -8.12 -1.25 1.03
C -6.34 -3.67 1.07
C -8.36 0.12 1.04
C -7.48 2.98 1.15
C -5.62 6.93 1.00
C -6.96 4.27 1.14
C -4.46 7.69 1.01
C -1.48 7.84 1.17
C 2.88 7.46 1.09
C -0.09 7.80 1.18
C 4.04 6.69 1.08
C 5.54 4.09 1.11
C 8.11 0.51 0.98
C 6.31 2.93 1.09
C 8.34 -0.87 0.96
C 8.05 -1.64 -0.19
C 6.88 -5.77 -0.19
C 7.91 -3.11 -0.14
C 8.06 -3.93 -1.28
C 5.96 -6.92 -0.30
C 5.20 -7.08 -1.47
C 7.55 -5.23 -1.30
C 3.58 -8.48 -0.30
C 4.03 -7.84 -1.47
C -0.70 -8.74 -0.14
C 2.15 -8.86 -0.19
C 1.39 -9.26 -1.31
C -2.10 -8.27 -0.20
C -2.58 -7.65 -1.37
C -0.01 -9.20 -1.28
C -4.49 -6.72 -0.17

C -3.74 -6.89 -1.35
C -7.06 -3.26 -0.07
C -5.51 -5.65 -0.09
C -6.32 -5.30 -1.19
C -7.63 -1.89 -0.12
C -7.52 -1.13 -1.30
C -7.08 -4.13 -1.18
C -8.11 0.91 -0.11
C -7.76 0.24 -1.29
C -6.92 5.03 -0.05
C -7.98 2.39 -0.03
C -8.10 3.21 -1.17
C -5.99 6.18 -0.13
C -5.25 6.39 -1.31
C -7.58 4.50 -1.18
C -3.61 7.74 -0.12
C -4.09 7.15 -1.31
C 0.66 8.04 0.02
C -2.19 8.12 -0.02
C -1.43 8.53 -1.14
C 2.06 7.57 -0.05
C 2.54 6.98 -1.25
C -0.04 8.49 -1.12
C 4.44 5.99 -0.07
C 3.71 6.22 -1.26
C 7.02 2.54 -0.06
C 5.46 4.92 -0.03
C 6.26 4.59 -1.14
C 7.58 1.17 -0.15
C 7.43 0.43 -1.33
C 7.02 3.43 -1.16
C 7.66 -0.95 -1.35
H 7.27 -3.12 1.93
H 6.22 -7.68 1.72
H 6.39 -5.40 1.88
H 4.17 -9.03 1.71
H 2.01 -8.26 1.88
H -2.62 -8.75 1.85
H -0.43 -8.16 1.92
H -4.68 -7.40 1.88

H -4.96 -5.07 1.92
H -8.28 -1.82 1.94
H -6.29 -3.02 1.94
H -8.71 0.60 1.95
H -7.36 2.37 2.04
H -6.22 6.87 1.91
H -6.46 4.63 2.03
H -4.17 8.21 1.92
H -2.02 7.52 2.05
H 2.58 7.96 2.01
H 0.41 7.44 2.08
H 4.62 6.60 2.00
H 4.93 4.30 1.98
H 8.30 1.06 1.89
H 6.27 2.26 1.95
H 8.71 -1.36 1.86
H 8.52 -3.52 -2.17
H 5.44 -6.50 -2.35
H 7.64 -5.81 -2.22
H 3.40 -7.83 -2.35
H 1.89 -9.57 -2.22
H -1.97 -7.66 -2.27
H -0.56 -9.47 -2.18
H -4.02 -6.33 -2.25
H -6.33 -5.93 -2.08
H -7.15 -1.60 -2.21
H -7.67 -3.87 -2.06
H -7.55 0.81 -2.19
H -8.56 2.82 -2.07
H -5.51 5.83 -2.21
H -7.65 5.10 -2.09
H -3.47 7.17 -2.20
H -1.94 8.83 -2.05
H 1.94 7.03 -2.15
H 0.51 8.76 -2.02
H 3.99 5.69 -2.17
H 6.26 5.24 -2.01
H 7.03 0.91 -2.22
H 7.61 3.18 -2.04
H 7.42 -1.51 -2.25

C	1.25	-0.99	0.78	C	-1.14	0.08	1.71	H	-3.47	4.92	0.77
C	1.24	0.35	1.19	C	-1.18	-1.23	1.19	H	-3.08	4.33	-0.84
C	0.03	0.84	1.71	C	0.05	-1.78	0.78	H	-5.25	2.28	-0.55
C	-0.04	2.27	1.56	C	-4.41	0.45	0.26	H	0.09	-2.77	0.33
C	-1.28	2.89	1.41	C	-3.33	-0.15	0.93	H	-5.14	-0.15	-0.27
C	-1.45	4.04	0.62	C	-2.66	-1.54	0.85	H	-2.76	-1.98	-0.15
C	-2.95	4.12	0.23	C	2.13	1.58	0.85	H	-3.10	-2.26	1.56
C	-4.47	1.88	0.09	C	1.12	2.76	0.94	H	2.96	1.70	1.56
C	-3.48	2.72	0.61	C	1.00	3.99	0.26	H	2.57	1.50	-0.15
C	-2.49	2.10	1.41	C	-0.28	4.62	0.10	H	1.85	4.42	-0.27
C	-2.42	0.72	1.56	H	2.14	-1.43	0.33	H	-0.33	5.49	-0.55

SUMC[12]CPP-stand

C	7.65	-2.97	1.16	C	3.27	-7.39	0.01	C	0.37	8.32	-0.96
C	5.34	-6.71	1.10	C	3.75	-6.80	-1.18	C	5.19	6.47	-0.02
C	6.96	-4.18	1.18	C	-1.01	-7.87	0.16	C	4.39	6.53	-1.18
C	4.13	-7.39	1.13	C	1.84	-7.78	0.11	C	7.97	3.20	-0.02
C	1.12	-7.47	1.28	C	1.11	-8.26	-0.99	C	6.34	5.53	0.03
C	-3.28	-7.64	1.26	C	-2.46	-7.60	0.11	C	7.08	5.19	-1.12
C	-0.27	-7.51	1.30	C	-3.05	-7.10	-1.08	C	8.45	1.80	-0.12
C	-4.55	-7.08	1.26	C	-0.28	-8.31	-0.97	C	8.19	1.06	-1.29
C	-6.43	-4.76	1.35	C	-5.08	-6.45	0.11	C	7.88	4.05	-1.14
C	-8.79	-1.09	1.24	C	-4.32	-6.55	-1.07	C	8.25	-0.33	-1.29
C	-7.23	-3.63	1.35	C	-7.87	-3.19	0.17	H	7.64	-2.35	2.05
C	-8.86	0.30	1.24	C	-6.22	-5.52	0.18	H	5.96	-6.70	2.00
C	-7.53	2.96	1.36	C	-6.98	-5.17	-0.96	H	6.43	-4.46	2.08
C	-5.17	6.64	1.29	C	-8.37	-1.80	0.09	H	3.82	-7.90	2.04
C	-6.84	4.17	1.37	C	-8.19	-1.06	-1.09	H	1.65	-7.08	2.15
C	-3.94	7.31	1.29	C	-7.79	-4.03	-0.96	H	-2.89	-8.08	2.18
C	-0.94	7.45	1.33	C	-8.50	1.05	0.10	H	-0.79	-7.16	2.19
C	3.45	7.72	1.16	C	-8.25	0.33	-1.09	H	-5.13	-7.09	2.18
C	0.45	7.53	1.31	C	-6.70	4.94	0.20	H	-5.85	-4.99	2.24
C	4.72	7.15	1.13	C	-8.13	2.47	0.18	H	-9.02	-1.63	2.15
C	6.56	4.77	1.20	C	-8.12	3.32	-0.95	H	-7.25	-3.00	2.23
C	8.95	1.09	0.99	C	-5.64	5.97	0.14	H	-9.14	0.81	2.16
C	7.36	3.63	1.17	C	-4.89	6.14	-1.05	H	-7.50	2.33	2.24
C	9.01	-0.30	0.99	C	-7.42	4.53	-0.94	H	-5.74	6.59	2.21
C	8.58	-1.05	-0.13	C	-3.13	7.35	0.14	H	-6.28	4.44	2.27
C	6.81	-4.95	0.01	C	-3.67	6.81	-1.05	H	-3.60	7.78	2.21
C	8.23	-2.48	-0.03	C	1.14	7.90	0.14	H	-1.43	7.05	2.22
C	8.22	-3.34	-1.16	C	-1.71	7.74	0.19	H	3.10	8.19	2.07
C	5.75	-5.99	-0.04	C	-1.03	8.25	-0.94	H	1.01	7.19	2.18
C	4.96	-6.12	-1.20	C	2.59	7.64	0.04	H	5.34	7.19	2.02
C	7.52	-4.54	-1.14	C	3.12	7.10	-1.15	H	6.00	5.00	2.10

H	9.24	1.63	1.89	H	2.49	7.03	-2.03	C	-3.57	-3.38	0.62
H	7.40	3.00	2.06	H	0.86	8.68	-1.86	C	-3.85	-0.88	-3.71
H	9.36	-0.82	1.89	H	4.72	6.02	-2.08	C	-4.31	-1.63	-2.62
H	8.72	-3.03	-2.07	H	7.00	5.80	-2.01	C	-3.96	-3.03	-2.05
H	5.24	-5.58	-2.10	H	7.80	1.57	-2.17	C	-3.93	-0.18	2.90
H	7.49	-5.15	-2.04	H	8.41	3.79	-2.06	C	-4.29	1.02	1.98
H	3.11	-6.78	-2.06	H	7.91	-0.87	-2.18	C	-3.80	2.33	1.87
H	1.64	-8.57	-1.89	C	-3.56	-2.67	1.86	C	-3.87	3.04	0.63
H	-2.45	-7.06	-1.99	C	-4.17	-1.41	1.97	H	-2.96	-3.07	2.67
H	-0.82	-8.66	-1.85	C	-4.89	-0.95	0.85	H	-4.96	3.39	-2.43
H	-4.69	-6.08	-1.98	C	-4.96	0.49	0.86	H	-3.23	3.06	-2.27
H	-6.91	-5.76	-1.86	C	-5.02	1.19	-0.35	H	-3.42	1.08	-4.52
H	-7.85	-1.56	-1.99	C	-4.42	2.45	-0.51	H	-2.98	-4.30	0.55
H	-8.32	-3.76	-1.87	C	-4.23	2.67	-2.04	H	-3.30	-1.37	-4.52
H	-7.96	0.87	-1.99	C	-3.91	0.55	-3.71	H	-2.94	-3.33	-2.29
H	-8.62	3.01	-1.86	C	-4.45	1.25	-2.62	H	-4.63	-3.81	-2.45
H	-5.22	5.65	-1.96	C	-5.02	0.47	-1.59	H	-4.57	-0.22	3.80
H	-7.39	5.13	-1.84	C	-4.96	-0.92	-1.60	H	-2.89	-0.14	3.24
H	-3.08	6.82	-1.96	C	-4.89	-1.64	-0.35	H	-3.24	2.78	2.68
H	-1.59	8.55	-1.82	C	-4.18	-2.84	-0.52	H	-3.37	4.01	0.57

TS of CORC[10]CPP (Imaginary Frequency = $124i \text{ cm}^{-1}$)

C	3.94	5.38	1.23	C	2.14	-6.63	-0.04	C	-6.27	3.59	1.11
C	3.52	6.01	0.04	C	2.68	-6.11	-1.23	C	-6.83	2.31	1.11
C	5.34	4.84	-1.11	C	-0.02	-6.67	1.23	C	-5.63	4.11	-0.04
C	4.31	5.79	-1.11	C	0.69	-6.93	0.04	C	-5.75	3.36	-1.23
C	4.96	4.43	1.23	C	-1.47	-7.05	-1.11	C	-3.90	5.41	1.23
C	6.35	2.78	-0.03	C	-0.09	-7.22	-1.11	C	-4.63	5.21	0.04
C	5.62	4.07	0.04	C	-1.40	-6.50	1.23	C	-2.96	6.57	-1.11
C	6.33	2.03	-1.23	C	-3.51	-5.98	-0.03	C	-4.17	5.89	-1.11
C	7.18	0.78	1.11	C	-2.15	-6.59	0.04	C	-2.69	6.09	1.23
C	6.88	2.14	1.11	C	-3.94	-5.36	-1.23	C	-0.68	6.90	-0.04
C	6.97	-0.02	-0.04	C	-5.35	-4.85	1.11	C	-2.13	6.60	0.04
C	6.63	0.66	-1.23	C	-4.30	-5.77	1.11	C	0.03	6.65	-1.23
C	6.33	-2.08	1.23	C	-5.65	-4.08	-0.04	C	1.47	7.07	1.11
C	6.81	-1.49	0.04	C	-4.98	-4.44	-1.23	C	0.09	7.20	1.11
C	6.25	-3.58	-1.11	C	-6.35	-2.04	1.23	C	2.17	6.62	-0.04
C	6.84	-2.31	-1.11	C	-6.38	-2.80	0.04	C	1.42	6.52	-1.23
C	5.75	-3.34	1.23	C	-7.16	-0.78	-1.11	H	3.36	5.52	2.14
C	4.61	-5.18	-0.03	C	-6.89	-2.15	-1.11	H	5.88	4.66	-2.03
C	5.60	-4.09	0.04	C	-6.62	-0.67	1.23	H	4.09	6.32	-2.03
C	3.88	-5.40	-1.23	C	-6.77	1.48	-0.04	H	5.14	3.87	2.14
C	2.96	-6.58	1.11	C	-6.94	0.01	0.04	H	5.95	2.47	-2.14
C	4.16	-5.88	1.11	C	-6.31	2.08	-1.23	H	7.52	0.32	2.03

H	7.00	2.70	2.03	H	-6.25	1.50	-2.14	C	1.88	-1.74	-0.01
H	6.47	0.10	-2.14	H	-6.28	4.16	2.03	C	0.88	-0.81	-0.01
H	6.29	-1.49	2.14	H	-7.26	1.93	2.03	C	1.04	0.58	0.00
H	6.25	-4.15	-2.03	H	-5.28	3.72	-2.14	C	-0.23	1.17	0.00
H	7.28	-1.94	-2.03	H	-4.22	4.91	2.14	C	-1.18	0.14	0.00
H	5.27	-3.69	2.14	H	-2.62	7.03	-2.03	C	-2.55	0.30	0.00
H	4.19	-4.90	-2.14	H	-4.74	5.84	-2.03	C	-3.22	-1.00	-0.01
H	2.63	-7.05	2.03	H	-2.10	6.09	2.14	C	-2.53	-2.23	0.00
H	4.74	-5.82	2.03	H	-0.51	6.42	-2.14	C	-1.07	-2.33	-0.01
H	2.10	-6.12	-2.14	H	2.02	7.25	2.03	C	-0.50	-1.08	0.00
H	0.52	-6.44	2.14	H	-0.41	7.49	2.03	H	0.70	4.38	0.01
H	-2.02	-7.23	-2.03	H	1.90	6.18	-2.14	H	2.88	3.37	-0.01
H	0.40	-7.52	-2.03	C	0.74	3.29	0.00	H	4.38	0.69	0.00
H	-1.88	-6.16	2.14	C	2.02	2.70	-0.01	H	4.10	-1.69	-0.02
H	-3.36	-5.49	-2.14	C	2.24	1.25	-0.01	H	-2.32	3.78	0.00
H	-5.90	-4.68	2.03	C	3.36	0.31	0.00	H	-3.95	2.02	0.02
H	-4.07	-6.30	2.04	C	3.19	-1.09	-0.01	H	-0.34	-4.42	-0.02
H	-5.17	-3.88	-2.14	C	-0.50	2.51	0.00	H	2.01	-3.95	0.00
H	-5.97	-2.49	2.14	C	-1.94	2.76	0.00	H	-4.31	-1.04	-0.01
H	-7.50	-0.32	-2.03	C	-2.90	1.72	0.01	H	-3.14	-3.13	0.01
H	-7.03	-2.71	-2.03	C	-0.05	-3.37	-0.01				
H	-6.44	-0.11	2.14	C	1.34	-3.10	-0.01				

TS of SUMC[10]CPP (Imaginary Frequency = $127i \text{ cm}^{-1}$)

C	6.73	1.67	-1.22	C	-5.06	5.25	-0.92	C	-2.98	-5.64	-1.36
C	7.15	1.03	-0.03	C	-3.95	6.10	-0.90	C	-1.13	-6.76	-0.14
C	6.62	3.10	1.16	C	-5.35	4.40	0.17	C	-2.55	-6.34	-0.21
C	7.19	1.83	1.14	C	-4.58	4.57	1.33	C	-0.41	-6.64	1.07
C	6.17	2.95	-1.19	C	-6.22	2.48	-1.17	C	1.02	-6.94	-1.30
C	4.99	4.72	0.12	C	-6.20	3.20	0.05	C	-0.37	-7.02	-1.31
C	6.00	3.64	0.02	C	-7.19	1.24	1.13	C	1.72	-6.58	-0.12
C	4.19	4.79	1.28	C	-6.79	2.57	1.17	C	0.98	-6.54	1.08
C	3.44	6.29	-0.93	C	-6.61	1.14	-1.20	C	3.48	-5.28	-1.31
C	4.62	5.54	-0.96	C	-6.95	-1.02	0.01	C	3.09	-6.03	-0.18
C	2.57	6.25	0.18	C	-7.02	0.46	-0.03	C	5.07	-5.16	0.96
C	3.01	5.53	1.31	C	-6.51	-1.67	1.18	C	3.96	-6.00	0.94
C	0.43	6.60	-1.08	C	-6.53	-3.10	-1.20	C	4.59	-4.44	-1.29
C	1.16	6.70	0.12	C	-7.05	-1.81	-1.16	C	6.30	-3.15	-0.02
C	-0.96	6.97	1.31	C	-5.91	-3.68	-0.07	C	5.38	-4.31	-0.13
C	0.43	6.99	1.30	C	-6.01	-2.96	1.14	C	6.41	-2.44	1.19
C	-0.97	6.60	-1.07	C	-4.16	-4.89	-1.34	C	7.32	-1.24	-1.14
C	-3.08	6.14	0.21	C	-4.95	-4.80	-0.18	C	6.87	-2.55	-1.17
C	-1.69	6.66	0.14	C	-3.42	-6.38	0.89	C	7.21	-0.45	0.02
C	-3.47	5.41	1.35	C	-4.60	-5.63	0.91	C	6.85	-1.12	1.21

H	6.70	1.11	-2.15	H	-3.16	-6.96	1.77	C	1.12	-0.62	0.23
H	6.61	3.65	2.10	H	-5.22	-5.64	1.80	C	2.26	-1.35	0.49
H	7.60	1.42	2.06	H	-2.34	-5.57	-2.23	C	1.71	-2.77	0.99
H	5.73	3.34	-2.11	H	-0.95	-6.49	2.00	C	-1.13	-3.25	1.19
H	4.42	4.16	2.14	H	1.56	-7.08	-2.23	C	0.12	-2.60	0.95
H	3.17	6.88	-1.81	H	-0.88	-7.23	-2.24	C	1.51	2.85	-1.00
H	5.24	5.57	-1.85	H	1.48	-6.30	2.01	C	-0.06	2.59	-0.93
H	2.37	5.46	2.18	H	2.83	-5.26	-2.18	C	-1.35	3.16	-1.15
H	0.94	6.40	-2.01	H	5.70	-5.13	1.85	C	-2.59	2.43	-0.89
H	-1.48	7.14	2.24	H	3.74	-6.60	1.81	C	-3.55	-0.12	0.04
H	0.96	7.18	2.23	H	4.77	-3.80	-2.14	C	-2.53	-1.27	0.47
H	-1.49	6.40	-2.00	H	6.00	-2.87	2.11	H	4.35	1.27	-0.41
H	-2.83	5.40	2.23	H	7.69	-0.80	-2.06	H	4.43	-1.01	0.36
H	-5.67	5.21	-1.82	H	6.90	-3.11	-2.10	H	-3.29	-3.21	1.17
H	-3.73	6.69	-1.79	H	6.77	-0.57	2.14	H	2.07	-3.00	2.00
H	-4.76	3.93	2.19	C	3.39	0.79	-0.25	H	2.05	-3.58	0.34
H	-5.80	2.92	-2.06	C	2.16	1.47	-0.50	H	-1.17	-4.27	1.56
H	-7.58	0.78	2.03	C	1.07	0.67	-0.23	H	1.81	3.69	-0.35
H	-6.88	3.12	2.10	C	-0.16	1.29	-0.46	H	1.84	3.11	-2.01
H	-6.48	0.59	-2.13	C	-1.33	0.61	-0.22	H	-1.47	4.17	-1.51
H	-6.44	-1.11	2.11	C	-2.61	1.09	-0.41	H	-3.50	2.98	-1.09
H	-6.56	-3.66	-2.14	C	3.43	-0.59	0.22	H	-4.20	-0.45	-0.78
H	-7.46	-1.38	-2.07	C	-2.41	-2.60	0.96	H	-4.21	0.16	0.86
H	-5.57	-3.37	2.05	C	-1.28	-0.71	0.26				
H	-4.38	-4.26	-2.20	C	-0.07	-1.32	0.48				

TS of CORC[11]CPP (Imaginary Frequency = $113i$ cm⁻¹)

C	4.84	-6.39	0.82	C	6.23	3.83	1.33	C	-7.57	-1.56	-0.01
C	3.61	-7.04	0.81	C	8.14	1.52	1.16	C	-6.42	-4.16	0.10
C	0.63	-7.27	1.16	C	7.13	-2.61	1.18	C	-6.48	-3.45	-1.11
C	-3.42	-5.99	1.40	C	8.33	0.14	1.12	C	-7.72	-0.09	0.02
C	-0.75	-7.27	1.29	C	6.45	-3.82	1.13	C	-7.99	0.67	-1.13
C	-4.61	-5.27	1.39	C	5.21	-5.51	-0.21	C	-7.04	-2.18	-1.17
C	-7.10	-3.62	1.21	C	4.34	-5.40	-1.32	C	-7.17	2.70	-0.05
C	-7.33	0.61	1.18	C	2.68	-6.81	-0.23	C	-7.72	2.04	-1.17
C	-7.67	-2.35	1.16	C	3.10	-6.03	-1.32	C	-4.47	6.02	-0.16
C	-7.06	1.97	1.15	C	-1.59	-7.16	0.16	C	-6.48	4.00	-0.16
C	-6.31	4.86	0.95	C	1.25	-7.18	-0.11	C	-5.74	4.29	-1.33
C	-2.45	6.63	1.16	C	0.41	-7.25	-1.24	C	-3.18	6.72	-0.04
C	-5.33	5.85	0.95	C	-3.01	-6.74	0.28	C	-2.52	7.28	-1.16
C	-1.09	6.92	1.20	C	-3.92	-6.86	-0.79	C	-4.76	5.28	-1.32
C	1.87	7.45	1.16	C	-0.98	-7.22	-1.11	C	-0.40	7.32	0.04
C	5.28	4.85	1.34	C	-5.43	-5.25	0.25	C	-1.16	7.57	-1.12
C	3.20	7.03	1.19	C	-5.11	-6.13	-0.81	C	3.80	6.41	0.08

C	1.08	7.25	0.01	H	4.63	4.97	2.20	C	2.91	-0.97	-0.04
C	1.72	6.74	-1.15	H	3.77	7.16	2.11	C	2.21	0.32	-0.03
C	5.05	5.63	0.19	H	6.29	3.17	2.19	C	2.54	1.75	0.00
C	5.91	5.44	-0.91	H	8.35	2.06	2.09	C	1.56	2.78	0.01
C	3.05	6.34	-1.11	H	7.11	-2.02	2.09	C	0.77	-2.34	-0.07
C	6.98	3.54	0.18	H	8.68	-0.38	2.01	C	-0.24	-3.40	-0.10
C	6.86	4.42	-0.92	H	5.90	-4.15	2.01	C	-1.63	-3.15	-0.10
C	7.99	-0.61	-0.03	H	4.59	-4.72	-2.12	C	-2.41	2.65	-0.01
C	7.62	2.21	0.05	H	2.41	-5.82	-2.13	C	-1.14	3.26	0.00
C	7.46	1.50	-1.15	H	0.84	-7.26	-2.24	C	0.12	2.51	-0.01
C	7.71	-2.06	0.01	H	-3.68	-7.50	-1.64	C	-0.13	1.15	-0.03
C	7.73	-2.86	-1.15	H	-1.58	-7.16	-2.01	C	0.84	0.14	-0.04
C	7.64	0.12	-1.19	H	-5.76	-6.19	-1.68	C	0.18	-1.10	-0.06
C	6.30	-4.52	-0.08	H	-5.97	-3.84	-1.99	C	-1.20	-0.85	-0.06
C	7.03	-4.06	-1.20	H	-8.36	0.18	-2.03	C	-2.20	-1.80	-0.08
H	5.52	-6.54	1.66	H	-6.95	-1.60	-2.08	C	-3.52	-1.16	-0.07
H	3.35	-7.69	1.64	H	-7.88	2.59	-2.10	C	-3.71	0.24	-0.05
H	1.24	-7.25	2.06	H	-5.84	3.65	-2.20	C	-2.60	1.20	-0.04
H	-2.75	-5.87	2.25	H	-3.07	7.43	-2.09	C	-1.39	0.55	-0.04
H	-1.18	-7.29	2.29	H	-4.12	5.39	-2.19	H	2.85	-3.11	-0.07
H	-4.83	-4.60	2.22	H	-0.67	7.96	-2.01	H	3.99	-0.99	-0.03
H	-7.14	-4.18	2.15	H	1.13	6.56	-2.05	H	3.58	2.07	0.01
H	-7.11	0.06	2.09	H	5.81	6.08	-1.79	H	1.92	3.80	0.02
H	-8.14	-1.94	2.04	H	3.47	5.85	-1.98	H	0.07	-4.44	-0.11
H	-6.64	2.45	2.03	H	7.47	4.27	-1.80	H	-2.29	-4.01	-0.12
H	-6.92	4.71	1.83	H	7.06	2.00	-2.03	H	-3.28	3.31	-0.01
H	-2.92	6.20	2.04	H	8.24	-2.50	-2.04	H	-1.12	4.35	0.01
H	-5.19	6.46	1.84	H	7.38	-0.42	-2.10	H	-4.42	-1.78	-0.08
H	-0.53	6.71	2.11	H	7.00	-4.63	-2.13	H	-4.74	0.59	-0.05
H	1.43	7.89	2.04	C	2.24	-2.21	-0.06				

TS of SUMC[11]CPP (Imaginary Frequency = $121i$ cm⁻¹)

C	4.93	-6.37	0.81	C	-5.58	5.70	0.93	C	2.82	-6.96	-0.26
C	3.75	-7.11	0.79	C	-1.39	6.94	1.17	C	3.20	-6.17	-1.36
C	0.80	-7.48	1.13	C	1.53	7.64	1.13	C	-1.43	-7.39	0.14
C	-3.22	-6.16	1.36	C	5.00	5.15	1.34	C	1.41	-7.40	-0.14
C	-0.58	-7.50	1.26	C	2.87	7.27	1.17	C	0.57	-7.50	-1.27
C	-4.40	-5.43	1.35	C	5.93	4.12	1.34	C	-2.84	-6.96	0.26
C	-6.95	-3.86	1.20	C	7.80	1.76	1.18	C	-3.77	-7.10	-0.79
C	-7.32	0.37	1.17	C	6.91	-2.42	1.17	C	-0.82	-7.48	-1.13
C	-7.55	-2.60	1.14	C	8.00	0.38	1.14	C	-5.26	-5.46	0.23
C	-7.12	1.75	1.13	C	6.32	-3.68	1.12	C	-4.95	-6.36	-0.81
C	-6.52	4.67	0.93	C	5.24	-5.47	-0.23	C	-7.47	-1.81	-0.02
C	-2.73	6.58	1.13	C	4.39	-5.44	-1.35	C	-6.25	-4.38	0.09

C	-6.32	-3.66	-1.12	H	-6.98	-4.42	2.13	H	7.06	-0.19	-2.08
C	-7.68	-0.35	0.01	H	-7.06	-0.17	2.08	H	6.97	-4.44	-2.13
C	-7.99	0.40	-1.14	H	-8.05	-2.21	2.03	C	-0.74	-3.49	0.01
C	-6.91	-2.40	-1.17	H	-6.71	2.24	2.01	C	-1.50	-2.28	0.02
C	-7.27	2.47	-0.07	H	-7.12	4.49	1.82	C	-0.69	-1.16	0.01
C	-7.79	1.78	-1.18	H	-3.17	6.10	2.01	C	-1.39	0.05	0.02
C	-4.74	5.91	-0.17	H	-5.47	6.31	1.83	C	-0.70	1.24	0.01
C	-6.65	3.80	-0.18	H	-0.81	6.75	2.07	C	-1.26	2.50	0.02
C	-5.92	4.13	-1.34	H	1.07	8.07	2.02	C	0.72	-3.49	-0.01
C	-3.47	6.67	-0.06	H	4.37	5.29	2.21	C	2.69	2.43	-0.04
C	-2.86	7.28	-1.17	H	3.44	7.42	2.09	C	0.70	1.24	-0.01
C	-4.99	5.16	-1.34	H	6.00	3.47	2.21	C	1.39	0.05	-0.02
C	-0.73	7.41	0.02	H	8.00	2.30	2.10	C	0.69	-1.17	-0.01
C	-1.51	7.65	-1.13	H	6.83	-1.84	2.09	C	1.49	-2.29	-0.02
C	3.49	6.66	0.06	H	8.35	-0.13	2.03	C	2.98	-1.69	-0.04
C	0.75	7.41	-0.02	H	5.79	-4.05	1.99	C	3.42	1.17	-0.04
C	1.40	6.94	-1.17	H	4.59	-4.75	-2.17	C	2.76	-0.10	-0.04
C	4.75	5.90	0.17	H	2.51	-6.02	-2.19	C	-2.99	-1.68	0.04
C	5.60	5.68	-0.93	H	0.99	-7.51	-2.26	C	-2.76	-0.09	0.04
C	2.74	6.57	-1.13	H	-3.55	-7.76	-1.62	C	-3.42	1.18	0.04
C	6.66	3.79	0.18	H	-1.43	-7.44	-2.03	C	-2.68	2.44	0.03
C	6.53	4.65	-0.93	H	-5.62	-6.45	-1.66	C	0.01	3.49	0.00
C	7.68	-0.36	-0.01	H	-5.80	-4.04	-1.99	C	1.27	2.50	-0.02
C	7.28	2.45	0.07	H	-8.35	-0.11	-2.03	H	-1.21	-4.46	0.02
C	7.12	1.73	-1.13	H	-6.83	-1.82	-2.09	H	1.20	-4.47	-0.02
C	7.46	-1.83	0.02	H	-8.00	2.32	-2.10	H	3.31	3.33	-0.04
C	7.55	-2.62	-1.14	H	-6.00	3.48	-2.21	H	3.53	-2.01	-0.93
C	7.32	0.35	-1.17	H	-3.42	7.43	-2.09	H	3.56	-2.02	0.83
C	6.24	-4.39	-0.09	H	-4.36	5.30	-2.21	H	4.51	1.24	-0.05
C	6.94	-3.87	-1.20	H	-1.05	8.08	-2.02	H	-3.57	-2.01	-0.83
H	5.61	-6.46	1.66	H	0.83	6.74	-2.07	H	-3.54	-2.00	0.93
H	3.53	-7.77	1.62	H	5.48	6.30	-1.83	H	-4.50	1.26	0.05
H	1.41	-7.44	2.03	H	3.19	6.09	-2.01	H	-3.29	3.34	0.04
H	-2.53	-6.01	2.19	H	7.13	4.48	-1.82	H	0.02	4.14	0.88
H	-1.01	-7.51	2.26	H	6.72	2.23	-2.01	H	0.00	4.14	-0.88
H	-4.61	-4.74	2.17	H	8.04	-2.23	-2.03				

TS of COR (Imaginary Frequency = $122i \text{ cm}^{-1}$)

C	0.86	-3.27	0.00	C	-2.47	0.68	0.00	H	1.40	-4.21	0.00
C	-0.55	-3.33	0.00	C	-1.15	0.32	0.00	H	-1.00	-4.32	0.00
C	-1.41	-2.14	0.00	C	-0.66	-1.00	0.00	H	-3.57	-2.63	0.00
C	-2.84	-1.83	0.00	C	0.75	-0.93	0.00	H	-4.42	-0.38	0.00
C	-3.34	-0.50	0.00	C	1.12	0.42	0.00	H	3.80	-2.29	0.00
C	1.60	-2.00	0.00	C	2.40	0.91	0.00	H	4.44	0.03	0.00
C	3.00	-1.55	0.00	C	2.40	2.37	0.00	H	-1.73	4.09	0.00
C	3.37	-0.19	0.00	C	1.23	3.15	0.00	H	-3.61	2.59	0.00
C	-1.51	3.02	0.00	C	-0.12	2.56	0.00	H	3.35	2.91	0.00
C	-2.61	2.14	0.00	C	-0.06	1.19	0.00	H	1.34	4.23	0.00

TS of SUM (Imaginary Frequency = $130i \text{ cm}^{-1}$)

C	2.45	-2.64	0.00	C	-0.08	-2.76	0.00	H	1.30	-4.48	0.00
C	2.48	-1.21	0.00	C	-1.66	-3.02	0.00	H	-4.53	1.11	0.00
C	1.21	-0.68	0.00	C	-3.51	-0.80	0.00	H	-1.97	-3.59	0.88
C	1.18	0.73	0.00	C	-2.29	-1.54	0.00	H	-1.97	-3.59	-0.88
C	-0.02	1.39	0.00	C	3.44	0.07	0.00	H	-4.48	-1.30	0.00
C	-0.19	2.76	0.00	C	2.43	1.32	0.00	H	4.09	0.08	0.88
C	1.20	-3.39	0.00	C	2.34	2.73	0.00	H	4.09	0.08	-0.88
C	-3.54	0.66	0.00	C	1.06	3.44	0.00	H	3.23	3.36	0.00
C	-1.22	0.66	0.00	C	-1.78	2.94	0.00	H	1.11	4.53	0.00
C	-1.19	-0.71	0.00	C	-2.35	1.45	0.00	H	-2.12	3.50	-0.88
C	0.04	-1.39	0.00	H	3.36	-3.23	0.00	H	-2.12	3.50	0.88

Tetrazine

N	-1.68	-0.21	0.00	N	-2.36	0.93	0.00	N	-0.31	2.17	0.00
C	-0.34	-0.11	0.00	H	0.22	-1.04	0.00	N	0.38	1.03	0.00
C	-1.65	2.07	0.00	H	-2.21	3.00	0.00				

TS of Tetrazine + COR (Imaginary Frequency = $454i \text{ cm}^{-1}$)

C	-1.69	2.90	-0.13	C	-0.44	1.27	1.11	H	1.38	-3.90	0.18
C	-2.74	1.99	-0.28	C	0.75	0.54	1.35	H	-1.02	-4.10	-0.23
C	-2.63	0.62	0.17	C	2.00	1.01	0.98	H	3.93	0.26	0.29
C	-3.35	-0.55	-0.30	C	3.07	0.00	0.91	H	3.38	-2.06	0.28
C	-2.83	-1.83	-0.17	C	2.71	-1.43	0.87	N	3.13	-0.13	3.58
C	-0.44	2.52	0.48	C	1.31	-1.85	0.95	C	4.06	0.25	2.60
C	0.87	3.10	0.28	C	0.41	-0.87	1.34	C	3.54	-2.17	2.67
C	2.03	2.37	0.51	H	-1.79	3.88	-0.58	N	2.85	-1.38	3.60
C	0.73	-3.07	0.46	H	-3.62	2.29	-0.84	H	4.29	1.31	2.56
C	-0.64	-3.19	0.22	H	-4.27	-0.41	-0.86	H	3.27	-3.21	2.63
C	-1.54	-2.08	0.44	H	-3.36	-2.66	-0.64	N	4.88	-1.86	2.47
C	-0.98	-0.98	1.09	H	0.95	4.09	-0.17	N	5.17	-0.60	2.45
C	-1.51	0.34	0.95	H	2.99	2.82	0.25				

TS of Tetrazine + CORC[10]CPP (Imaginary Frequency = 486i cm⁻¹)

C	-6.56	-1.85	-1.36	C	0.07	6.52	0.98	H	4.89	5.68	1.50
C	-6.97	-1.24	-0.16	C	-1.45	7.25	-1.23	H	1.92	6.01	-2.45
C	-6.51	-3.35	0.98	C	-0.06	7.35	-1.28	H	0.65	6.17	1.83
C	-7.03	-2.06	0.99	C	-2.11	6.71	-0.11	H	-2.03	7.55	-2.10
C	-6.04	-3.14	-1.37	C	-1.32	6.43	1.03	H	0.42	7.72	-2.18
C	-4.94	-5.00	-0.12	C	-3.93	5.56	-1.37	H	-1.78	6.00	1.91
C	-5.91	-3.89	-0.18	C	-3.48	6.16	-0.17	H	-3.37	5.70	-2.29
C	-4.11	-5.11	1.01	C	-5.31	5.05	0.99	H	-5.85	4.87	1.92
C	-3.42	-6.50	-1.29	C	-4.26	5.96	0.98	H	-4.00	6.48	1.91
C	-4.61	-5.78	-1.25	C	-4.98	4.64	-1.36	H	-5.21	4.10	-2.27
C	-2.50	-6.47	-0.22	C	-6.36	3.01	-0.07	H	-5.66	2.62	1.94
C	-2.92	-5.84	0.97	C	-5.63	4.29	-0.16	H	-7.81	0.63	-2.05
C	-0.44	-6.51	-1.61	C	-6.18	2.21	1.08	H	-7.23	3.01	-2.05
C	-1.07	-6.81	-0.38	C	-7.34	1.06	-1.17	H	-6.23	0.26	1.94
C	1.14	-7.06	0.61	C	-7.02	2.42	-1.17	C	-1.71	2.92	-0.20
C	-0.24	-7.17	0.70	C	-7.03	0.23	-0.07	C	-2.75	2.01	-0.33
C	0.94	-6.40	-1.69	C	-6.51	0.86	1.08	C	-2.64	0.64	0.12
C	3.14	-6.05	-0.58	H	-6.51	-1.26	-2.28	C	-3.37	-0.53	-0.34
C	1.77	-6.59	-0.57	H	-6.52	-3.93	1.90	C	-2.85	-1.82	-0.22
C	3.68	-5.45	0.57	H	-7.42	-1.66	1.92	C	-0.44	2.53	0.40
C	4.91	-4.97	-1.87	H	-5.61	-3.53	-2.29	C	0.87	3.10	0.18
C	3.86	-5.87	-1.79	H	-4.33	-4.52	1.90	C	2.04	2.38	0.43
C	5.31	-4.21	-0.75	H	-3.16	-7.05	-2.20	C	0.72	-3.05	0.40
C	4.74	-4.55	0.49	H	-5.26	-5.78	-2.12	C	-0.65	-3.16	0.15
C	5.77	-2.12	-2.01	H	-2.25	-5.79	1.82	C	-1.55	-2.06	0.38
C	6.05	-2.93	-0.89	H	-1.04	-6.23	-2.47	C	-0.98	-0.96	1.02
C	7.13	-1.01	0.16	H	1.75	-7.30	1.49	C	-1.51	0.36	0.88
C	6.80	-2.37	0.16	H	-0.69	-7.48	1.64	C	-0.44	1.29	1.03
C	6.10	-0.76	-2.00	H	1.38	-6.04	-2.62	C	0.75	0.55	1.28
C	6.64	1.31	-0.74	H	3.18	-5.59	1.53	C	2.00	1.03	0.92
C	6.71	-0.16	-0.88	H	5.39	-4.80	-2.83	C	3.08	0.01	0.93
C	6.30	1.87	0.50	H	3.54	-6.40	-2.69	C	2.71	-1.42	0.87
C	6.11	3.45	-1.78	H	5.05	-4.01	1.39	C	1.31	-1.84	0.89
C	6.63	2.16	-1.86	H	5.19	-2.51	-2.83	C	0.41	-0.85	1.27
C	5.56	3.94	-0.57	H	7.65	-0.60	1.02	H	-1.81	3.90	-0.63
C	5.76	3.15	0.59	H	7.07	-2.98	1.02	H	-3.65	2.32	-0.86
C	3.76	5.25	-1.68	H	5.76	-0.14	-2.83	H	-4.31	-0.40	-0.87
C	4.58	5.05	-0.55	H	6.32	1.24	1.39	H	-3.39	-2.64	-0.67
C	3.06	6.48	0.72	H	6.07	4.07	-2.67	H	0.96	4.09	-0.27
C	4.25	5.75	0.63	H	6.98	1.80	-2.83	H	2.99	2.82	0.16
C	2.58	5.98	-1.59	H	5.38	3.50	1.54	H	1.37	-3.88	0.12
C	0.73	6.90	-0.20	H	3.98	4.73	-2.61	H	-1.02	-4.08	-0.31
C	2.16	6.54	-0.37	H	2.81	6.96	1.66	H	3.97	0.26	0.36

H	3.42	-2.07	0.36	C	3.39	-2.12	2.79	H	3.12	-3.17	2.75
N	2.88	-0.06	3.58	N	2.61	-1.31	3.62	N	4.74	-1.81	2.71
C	3.90	0.29	2.66	H	4.12	1.35	2.63	N	5.02	-0.55	2.67

Cycloadduct of Tetrazine + COR

C	-1.79	2.94	-0.29	C	-0.56	1.32	0.98	H	1.22	-3.89	0.25
C	-2.83	2.04	-0.47	C	0.61	0.59	1.29	H	-1.16	-4.07	-0.27
C	-2.73	0.67	-0.01	C	1.86	1.07	0.98	H	3.68	0.26	0.18
C	-3.46	-0.50	-0.47	C	3.00	0.06	1.02	H	3.13	-1.96	0.18
C	-2.96	-1.79	-0.30	C	2.62	-1.48	1.02	N	3.05	-0.12	3.47
C	-0.54	2.57	0.36	C	1.14	-1.83	0.98	C	3.88	0.29	2.31
C	0.76	3.14	0.20	C	0.26	-0.83	1.29	C	3.30	-2.08	2.31
C	1.92	2.41	0.49	H	-1.87	3.93	-0.75	N	2.75	-1.33	3.47
C	0.57	-3.05	0.48	H	-3.70	2.35	-1.05	N	4.74	-1.83	2.20
C	-0.80	-3.15	0.19	H	-4.37	-0.37	-1.05	N	5.05	-0.62	2.20
C	-1.68	-2.04	0.35	H	-3.49	-2.62	-0.75	H	4.21	1.32	2.42
C	-1.12	-0.92	0.98	H	0.87	4.13	-0.26	H	3.10	-3.15	2.42
C	-1.63	0.39	0.80	H	2.89	2.85	0.25				

Cycloadduct of Tetrazine + COR \subset [10]CPP

C	-6.58	-1.86	-1.39	C	5.74	-2.10	-2.05	C	-3.95	5.57	-1.40
C	-6.98	-1.25	-0.19	C	6.03	-2.92	-0.94	C	-3.50	6.17	-0.20
C	-6.53	-3.36	0.95	C	7.13	-1.01	0.10	C	-5.32	5.04	0.97
C	-7.04	-2.07	0.96	C	6.80	-2.36	0.10	C	-4.28	5.96	0.96
C	-6.07	-3.16	-1.40	C	6.07	-0.75	-2.05	C	-5.00	4.65	-1.39
C	-4.96	-5.01	-0.15	C	6.63	1.31	-0.80	C	-6.37	3.00	-0.10
C	-5.94	-3.90	-0.21	C	6.70	-0.16	-0.94	C	-5.64	4.29	-0.18
C	-4.14	-5.13	0.98	C	6.29	1.87	0.45	C	-6.18	2.20	1.05
C	-3.44	-6.51	-1.33	C	6.09	3.46	-1.83	C	-7.35	1.06	-1.20
C	-4.63	-5.79	-1.28	C	6.61	2.17	-1.92	C	-7.03	2.41	-1.20
C	-2.52	-6.48	-0.25	C	5.54	3.94	-0.62	C	-7.04	0.23	-0.10
C	-2.95	-5.85	0.94	C	5.75	3.16	0.54	C	-6.51	0.85	1.05
C	-0.46	-6.50	-1.64	C	3.73	5.25	-1.72	H	-6.53	-1.27	-2.31
C	-1.09	-6.81	-0.42	C	4.56	5.05	-0.59	H	-6.54	-3.94	1.87
C	1.13	-7.06	0.57	C	3.04	6.48	0.68	H	-7.43	-1.66	1.89
C	-0.26	-7.17	0.66	C	4.23	5.75	0.58	H	-5.63	-3.54	-2.33
C	0.92	-6.39	-1.73	C	2.55	5.98	-1.63	H	-4.35	-4.54	1.87
C	3.13	-6.04	-0.63	C	0.71	6.91	-0.23	H	-3.18	-7.05	-2.23
C	1.75	-6.58	-0.61	C	2.14	6.55	-0.40	H	-5.28	-5.79	-2.15
C	3.67	-5.45	0.53	C	0.05	6.54	0.95	H	-2.27	-5.80	1.79
C	4.89	-4.95	-1.92	C	-1.47	7.26	-1.27	H	-1.07	-6.22	-2.50
C	3.83	-5.86	-1.84	C	-0.08	7.35	-1.31	H	1.74	-7.29	1.44
C	5.29	-4.20	-0.80	C	-2.13	6.71	-0.14	H	-0.70	-7.48	1.61
C	4.73	-4.55	0.44	C	-1.34	6.44	1.00	H	1.35	-6.02	-2.66

H	3.18	-5.59	1.49	H	-4.02	6.48	1.88	C	3.08	0.08	1.17
H	5.36	-4.78	-2.89	H	-5.23	4.11	-2.30	C	2.71	-1.47	1.17
H	3.51	-6.38	-2.74	H	-5.66	2.61	1.91	C	1.24	-1.84	1.04
H	5.04	-4.01	1.34	H	-7.82	0.62	-2.08	C	0.34	-0.84	1.34
H	5.15	-2.50	-2.87	H	-7.24	3.01	-2.08	H	-1.84	3.90	-0.68
H	7.66	-0.60	0.95	H	-6.23	0.25	1.91	H	-3.66	2.31	-0.96
H	7.08	-2.98	0.95	C	-1.74	2.91	-0.24	H	-4.31	-0.42	-0.96
H	5.72	-0.13	-2.87	C	-2.78	2.00	-0.40	H	-3.40	-2.66	-0.69
H	6.32	1.25	1.34	C	-2.67	0.63	0.05	H	0.92	4.10	-0.25
H	6.04	4.07	-2.72	C	-3.38	-0.55	-0.41	H	2.94	2.85	0.28
H	6.96	1.81	-2.88	C	-2.87	-1.83	-0.25	H	1.34	-3.88	0.28
H	5.38	3.50	1.50	C	-0.49	2.55	0.39	H	-1.03	-4.08	-0.26
H	3.95	4.72	-2.64	C	0.82	3.12	0.22	H	3.82	0.27	0.39
H	2.79	6.96	1.62	C	1.98	2.40	0.53	H	3.29	-1.97	0.39
H	4.88	5.69	1.45	C	0.68	-3.05	0.52	N	2.88	-0.05	3.62
H	1.89	6.01	-2.48	C	-0.68	-3.17	0.21	C	3.83	0.33	2.54
H	0.63	6.19	1.80	C	-1.59	-2.07	0.39	C	3.26	-2.04	2.54
H	-2.05	7.56	-2.14	C	-1.04	-0.95	1.02	N	2.59	-1.26	3.62
H	0.39	7.72	-2.22	C	-1.56	0.36	0.85	N	4.70	-1.77	2.59
H	-1.80	6.02	1.88	C	-0.50	1.30	1.03	N	4.99	-0.55	2.59
H	-3.39	5.71	-2.32	C	0.68	0.58	1.34	H	4.12	1.37	2.66
H	-5.86	4.86	1.89	C	1.93	1.07	1.05	H	3.06	-3.10	2.66